A multi-pronged approach targeting SARS-CoV-2 proteins using ultra-large virtual screening

Christoph Gorgulla[1,2,3,*], Krishna M. Padmanabha Das[1,3], Kendra E. Leigh[11], Marco Cespugli[14], Patrick D. Fischer[1,3,9], Zi-Fu Wang[1], Guilhem Tesseyre[4], Shreya Pandita[4], Alec Shnapir[4], Anthony Calderaio[18], Minko Gechev [4], Alexander Rose[17], Noam Lewis[4], Colin Hutcheson[4], Erez Yaffe[4], Roni Luxenburg[4], Henry D. Herce[1,3], Vedat Durmaz[14], Thanos D. Halazonetis[13], Konstantin Fackeldey[8,10], Justin J. Patten[16], Alexander Chuprina[5], Igor Dziuba[5a], Alla Plekhova[6], Yurii Moroz[6,7], Dmytro Radchenko[5,7], Olga Tarkhanova[6], Irina Yavnyuk[5], Christian Gruber[14,15], Ryan Yust[4], Dave Payne[4], Anders M. Näär[19], Mark N. Namchuk[1], Robert A. Davey[16], Gerhard Wagner[1], Jamie Kinney[4], Haribabu Arthanari[1,3,*]

Severe acute respiratory syndrome coronavirus 2 (SARS-CoV-2), previously known as 2019 novel coronavirus (2019-nCoV), has spread rapidly across the globe, creating an unparalleled global health burden and spurring a deepening economic crisis. As of July 7th, 2020, almost seven months into the outbreak, there are no approved vaccines and few treatments available. Developing drugs that target multiple points in the viral life cycle could serve as a strategy to tackle the current as well as future coronavirus pandemics. Here we leverage the power of our recently developed *in silico* screening platform, VirtualFlow, to identify inhibitors that target SARS-CoV-2. VirtualFlow is able to efficiently harness the power of computing clusters and cloud-based computing platforms to carry out ultra-large scale virtual screens. In this unprecedented structure-based multi-target virtual screening campaign, we have used VirtualFlow to screen an average of ~1 billion molecules against each of 40 different target sites on 17 different potential viral and host targets in the cloud. In addition to targeting the active sites of viral enzymes, we also target critical auxiliary sites such as functionally important protein-protein interaction interfaces. This multi-target approach not only increases the likelihood of finding a potent inhibitor, but could also help identify a collection of anti-coronavirus drugs that would retain efficacy in the face of viral mutation. Drugs belonging to different regimen classes could be combined to develop possible combination therapies, and top hits that bind at highly conserved sites would be potential candidates for further development as coronavirus drugs. Here, we present the top 200 *in silico* hits for each target site. While in-house experimental validation of some of these compounds is currently underway, we want to make this array of potential inhibitor candidates available to researchers worldwide in consideration of the pressing need for fast-tracked drug development.

Small-molecule inhibitors | SARS-CoV-2 | COVID-19 | coronavirus | *in silico* screening | drug discovery | structure-based virtual screening

Introduction

At the end of 2019, cases of pneumonia with an initially unknown etiology were identified in Wuhan City, in the Hubei Province of China (1–3). The cause was determined to be a novel coronavirus (CoV) (4), and by early July, 2020, there were over 12 million confirmed cases worldwide (5, 6) of what is now designated SARS-CoV-2 (7). A lineage B *Betacoronavirus* related to severe acute respiratory syndrome CoV (SARS-CoV), SARS-CoV-2 commonly causes fever, cough, myalgia, and/or fatigue (8, 9). While even half a year later, our clinical knowledge is still developing, in addition to asymptomatic and mild cases, dyspnoea, lymphopenia, and anosmia, with or without dysgeusia, have also been reported as clinical features (8, 10–12), and complications can include acute respiratory distress syndrome (ARDS), acute cardiac injury, and secondary infections (8). As of July 8th, 2020, over half a million deaths have been attributed to coronavirus disease 2019 (COVID-19) (5, 6), and the rapid expansion in case number in combination with severe symptoms requiring hospitalization has resulted in unprecedented strain on the global healthcare system.

Coronaviridae is comprised of a family of large positive-sense, single-stranded RNA viruses that derive their name from the 'corona' that fringes the virions in electron micrographs (14, 15). Coronavirus virions are composed of a lipid envelope, decorated with spike (S) protein, which facilitates entry and causes their corona-like appearance (16). Envelope (E) protein, which contributes to virion assembly and viral pathogenesis, as well as membrane (M) protein, which also facilitates virion assembly, are also both embedded in this bilayer (16), and the viral genome, in close association with nucleoprotein (N), is encapsulated within.

To initiate entry, the receptor binding domain of S must engage with its receptor on the surface of its target cell, and several studies have already identified the SARS-CoV recep-

[1]Department of Biological Chemistry and Molecular Pharmacology, Harvard Medical School, Harvard University, Boston, USA. [2]Department of Physics, Faculty of Arts and Sciences, Harvard University, Cambridge, USA. [3]Department of Cancer Biology, Dana-Farber Cancer Institute, Boston, USA. [4]Google, Mountain View, CA, USA. [5]Enamine, Kyiv, Ukraine. [6]Chemspace, Kyiv, Ukraine. [7]Taras Shevchenko National University of Kyiv, Ukraine. [5a]UkrOrgSyntez Ltd., Kyiv, Ukraine. [8]Zuse Institute Berlin (ZIB), Berlin, Germany. [9]Department of Pharmacy, Pharmaceutical and Medicinal Chemistry, Saarland University, Saarbrücken, Germany. [10]Institute of Mathematics, Technical University Berlin, Berlin, Germany. [11]Max-Planck-Institut für Biophysik, Frankfurt, Germany. [12]1Department of Mathematics and Computer Science, Freie Universität Berlin, Berlin, Germany. [13]Department of Molecular Biology, University of Geneva, Geneva, Switzerland. [14]Innophore GmbH, Graz, Austria. [15]Institute of Molecular Biosciences, University of Graz, Austria. [16]Department of Microbiology, Boston University Medical School, Boston University, Boston, USA. [17]Mol* Consortium, https://molstar.org. [18]VirtualFlow Organization, https://virtual-flow.org/. [19]Department of Nutritional Sciences & Toxicology, University of California Berkeley, USA. *email: cgorgulla@g.harvard.edu, hari@hms.harvard.edu

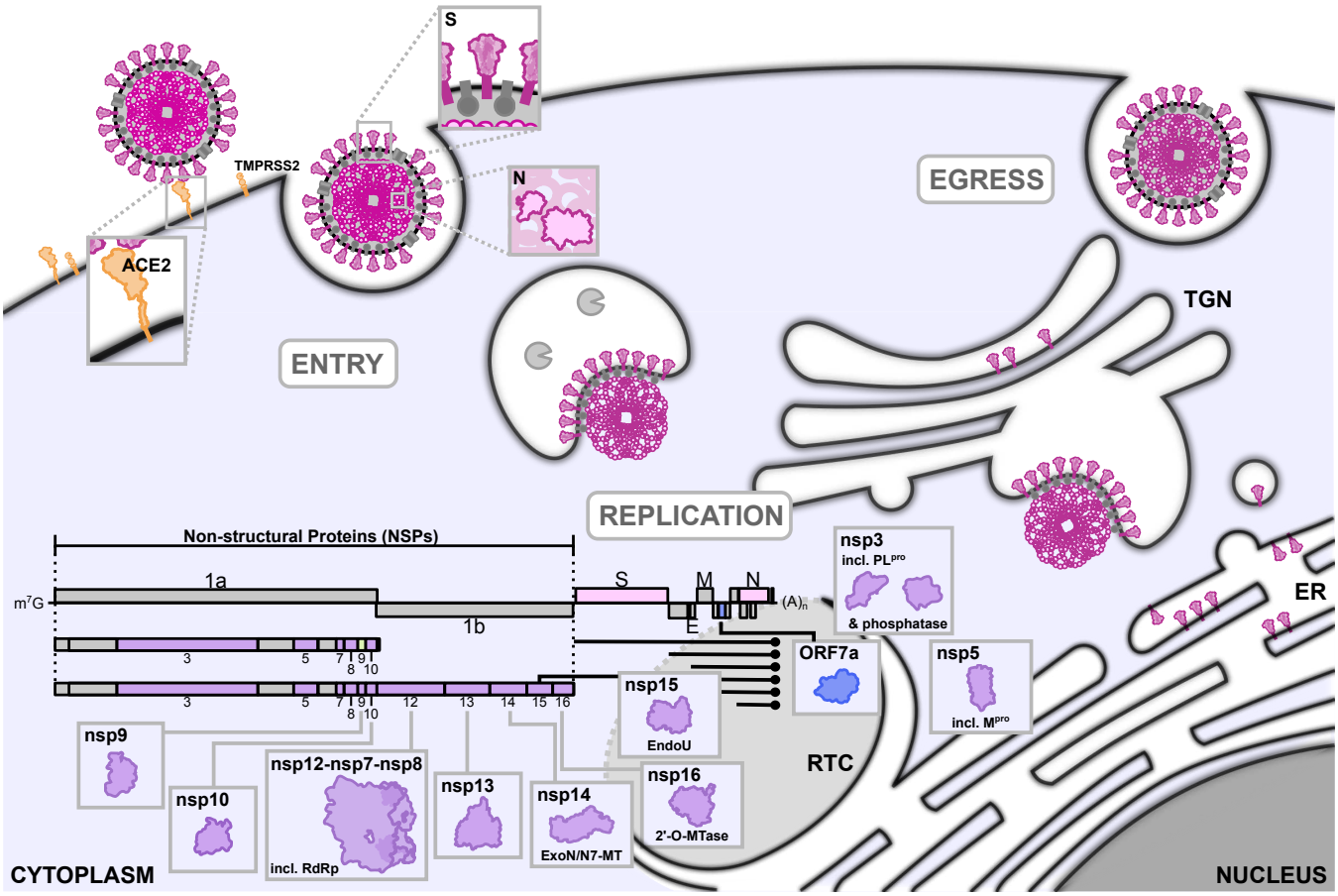

Fig. 1. A schematic of the viral lifecycle of SARS-CoV-2. The genome organization is based on other coronaviruses and published predictions (2, 13). ACE2: angiotensin-converting enzyme 2; TMPRSS2: transmembrane protease, serine 2; RdRp: RNA-dependent RNA polymerase; ExoN: exonuclease; N7-MT N7-methyl transferase; 2'O-MTase: 2'O-methyl transferase; EndoU: uridylate-specific endonuclease; RTC: replication and transcription complex; ER: endoplasmic reticulum; TGN: trans-Golgi network

tor, angiotensin-converting enzyme 2 (ACE2), as a possible receptor for SARS-CoV-2 (1, 17, 18). While engagement with the receptor initiates conformational rearrangements in S, the spike protein must also be cleaved at its S2' site as part of the entry process. Unlike the S1/S2 cleavage event, which can occur at any point from viral assembly to entry, S2' cleavage likely only occurs during entry, and involves host proteases at the cell surface, such as transmembrane protease, serine 2 (TMPRSS2), or in endosomes, such as cathepsins (19). Further conformational rearrangements in S result in membrane fusion, allowing release of the nucleocapsid into the cytoplasm.

As the genome is positive-sense, replication starts with the expression of ORF1a and ORF1ab. The resulting polyproteins (pp1a and pp1ab) are further processed into sixteen non-structural proteins (nsp1-16; see Fig. 1) that form, in conjunction with host proteins, membrane-associated replication and transcription complexes (RTCs) (13). The genome is replicated via an intermediate negative-sense copy of the genome and both structural and accessory proteins are expressed from 3'-co-terminal sub-genomic RNAs (20). Assembly occurs on membranes between the endoplasmic reticulum and the trans-Golgi Network, with the virions budding into vesicular compartments that then fuse with the plasma membrane, releasing their cargo (20) (see Fig. 1).

While low-pathogenicity human coronaviruses such as HCoV-229E, HCoV-OC43, HCov-NL63, and HCoV-HKU1 (21) continually circulate and generally cause mild disease, the emergence of SARS-CoV (22–25) in 2002 and Middle East respiratory syndrome CoV (MERS-CoV) (26–28) in 2012 as the result of zoonotic jumps into the human population (29) demonstrated that coronaviruses could cause serious morbidity and mortality. Their importance made them the subject of extensive research and attractive therapeutic targets. While research is only just beginning on SARS-CoV-2, comparison of the SARS-CoV-2 sequence early in the outbreak to previously identified coronavirus sequences revealed it to be most related to previously isolated bat SARS-like CoVs (1, 2, 30) and comparison to both a bat SARS-like virus (bat SL-CoVZC45) as well as a previous human SARS-CoV isolate (SARS-CoV Tor2) predicted that SARS-CoV-2 likely has a similar genomic organization and expresses similar proteins (2) (see Fig. 1). The assignment to the *Betacoronavirus* genus and in particular the similarity to SARS-CoV, allows us to also draw on a field of already published work to infer promising targets within the SARS-CoV-2 life cycle for small molecule intervention.

Therapeutics against viruses generally fall into two broad categories: i) vaccines, which prime the host immune system to mount a targeted defense against infection by the virus,

Protein index	Protein name	Alternative names	Screen ID	Target site	Structure used
1	ACE2	Angiotensin-converting enzyme 2	1	Spike RDB binding region – site 1	6m17
			2	Spike RDB binding region – site 1	6m18
			3	Spike RDB binding region – site 2	6m17
			4	Dynamic pocket 1 besides spike RDB binding region	DE Shaw MD simulation 10875754 frame 2715
			5	Dynamic pocket 2 besides spike RDB binding region	DE Shaw MD simulation 10875754 frame 5273
2	TMPRSS2	Transmembrane protease serine 2	6	Active site	Swissmodel of TMPRSS2 – Model 1
3	Spike	S-protein, S	7	Spike RDB – ACE2 interface	6w41
			8	Spike HR1 domain	6lxt
4	ORF7a	Protein 7a	9	Blind docking	6w37
5	nsp3-macrodomain	Phosphatase, (macro) X domain	10	Active site	6w6y chain A (closed active site)
			11	Active site	6w6y chain B (open active site)
6	nsp3-PL^{pro}	PL^{pro}, PLP, papain-like protease	12	Active site	6w9c
			13	Accessory pocket	6w9c
			14	DUB binding site	6w9c
			15	Active site and accessory pocket	6wx4*
7	nsp5	M^{pro}, main protease	16	Active site	6lu7
			17	Active site	M^{pro}-11*
			18	Dimerization site	6wqf
			19	α-helix 5 attachment site	hybrid in-house model
8	nsp7	Replicase polyprotein 1ab	20	Blind docking (nsp8 PPI, nsp12 PPI)	6wiq
9	nsp8	Primase complex	21	nsp7 PPI	6wiq
			22	nsp12 PPI	7bv1
10	nsp9	Replicase	23	Dimerization interface – site 1	6w4b
			24	Dimerization interface – site 2	6w4b
11	nsp10		25	nsp16 PPI	6w4h
			26	nsp16 PPI	Swissmodel of nsp10/14 - Model 3
			27	nsp14 PPI	Swissmodel of nsp10/14 - Model 3
12	nsp12	RNA dependent RNA-Polymerase (RdRP)	28	RNA binding interface – site 1	7bv1
			29	RNA binding interface – site 2	7bv1
			30	Nucleotide binding site	7bv1
			31	nsp8 PPI	6m71
			32	nsp7/8 PPI	7BV1
13	nsp13	Helicase	33	Active site	Swissmodel nsp13 – Model 1
			34	RNA binding interface – site 1	Swissmodel nsp13 – Model 1
			35	RNA binding interface – site 2	Swissmodel nsp13 – Model 1
14	nsp14	Exoribonuclease, N7 methyltransferase, N7-MTase	36	nsp10 PPI	Swissmodel of nsp10/14 - Model 3
			37	Active site (ExoN)	Swissmodel of nsp10/14 - Model 3
			38	Active site (N7-MT)	Swissmodel of nsp10/14 - Model 3
15	nsp15	Endoribonuclease, XendoU	39	Active site	6w01
16	nsp16	2'-O-MTase, 2'-O methyltransferase	40	nsp10 PPI	6w4b
			41	Active site (2'-O MT)	6w4b
17	nucleoprotein	N, NC, NP, RNP, ribonucleocapsid protein	42	NTD – RNA binding site	6yi3
			43	NTD – oligomerization site	6yi3
			44	CTD – dimerization interface	6wji
			45	CTD – oligomerization site	6wji

Table 1. Overview of the virtual screens that were carried out. A total of 45 virtual screens were performed, involving 17 different target proteins and 40 unique target sites. In each screen, approximately 1 billion molecules from the Enamine REAL library, and approximately 10 million compounds from the in-stock library ZINC 15 database were screened.

and ii) other agents with antiviral effects, which include, but are not limited to, small molecule inhibitors, peptides, and biologics. Although effective vaccines have been developed against several viruses, including polio and hepatitis B, there are many viruses for which there is still no vaccine, even after decades of research (31). HIV is the most prominent example of this, but there are also no approved vaccines for any of the human coronaviruses, including SARS-CoV and MERS-CoV.

Other therapeutics with antiviral properties can be broadly divided into two categories: i) drugs that target viral proteins, and ii) drugs that target host proteins, including the viral receptor, cellular proteins essential to the viral life cycle, and components of the immune system. Currently available viral therapeutics include protease inhibitors, reverse transcriptase and polymerase inhibitors (both nucleoside analogues and non-nucleoside inhibitors), integrase inhibitors, and viral entry blockers (Supplementary Fig. 23). Although there are no drugs specifically approved by the FDA for SARS-CoV, MERS-CoV or SARS-CoV-2, there have been a number of efforts to target proteins of the viral machinery, including the proteases, helicase and RNA-dependent RNA polymerase (RdRP). A partial list of these published small molecules is shown in Supplementary Table 2. For instance, Remdesivir, an RdRP inhibitor originally developed for hepatitis C, was previously tested against both SARS-CoV and MERS-CoV. Preliminary studies have suggested that Remdesivir may reduce the time to recovery in SARS-CoV-2 patients; however, this finding needs to be confirmed with larger studies (32).

For every virus, there are targets such as the entry pro-

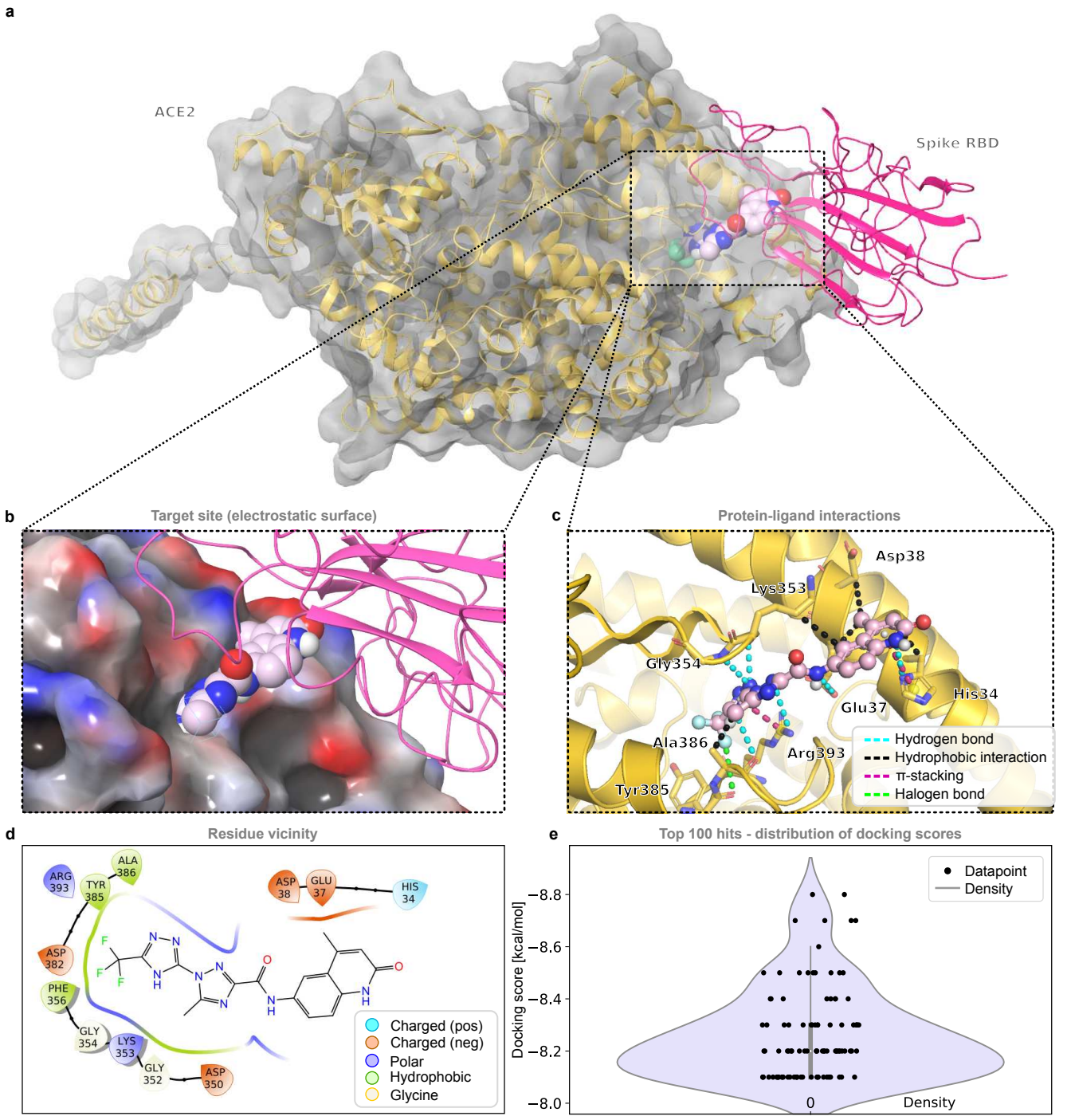

Fig. 2. The ACE2 receptor (open conformation) and an example compound from the top 0.0001% of screened compounds bound at the spike interaction interface (site1). **a**, The target protein ACE2 (gold) in an open conformation bound to the RBD of the spike protein (magenta) and an example compound (light pink) from the virtual screen bound to the spike interaction interface (site 1, around Glu37) (Screen ID: 1). **b**, The electrostatic surface of the target protein (ACE2) bound to the RBD domain of the spike protein (magenta) and an example compound (light pink). **c,** An overview of the interactions between the ligand and the receptor structure. **d,** Receptor residues within 4 Å of the ligand. **e,** Distribution of the docking scores of the top 100 virtual screening hits.

tein or the viral polymerase, which have direct effects on the ability of the virus to replicate, even under ideal conditions for the virus. There are also other targets that, if inhibited, would reduce the severity of the viral infection often referred to as the viral virulence. Some of these targets may only have an effect when inhibitors are evaluated in the context of a whole organism. For example, several viruses paralyze the host immune system by hijacking or sequestering, key signaling proteins, and targeting the viral proteins that mediate this effect would reduce the virulence of the virus. In this study we target an array of SARS-CoV-2 proteins in addition to two human proteins, and we posit that inhibitors, which target proteins that affect the viability and/or the virulence, could synergistically combine for more efficacious combination therapies.

In silico screening methods enable us to identify lead drug

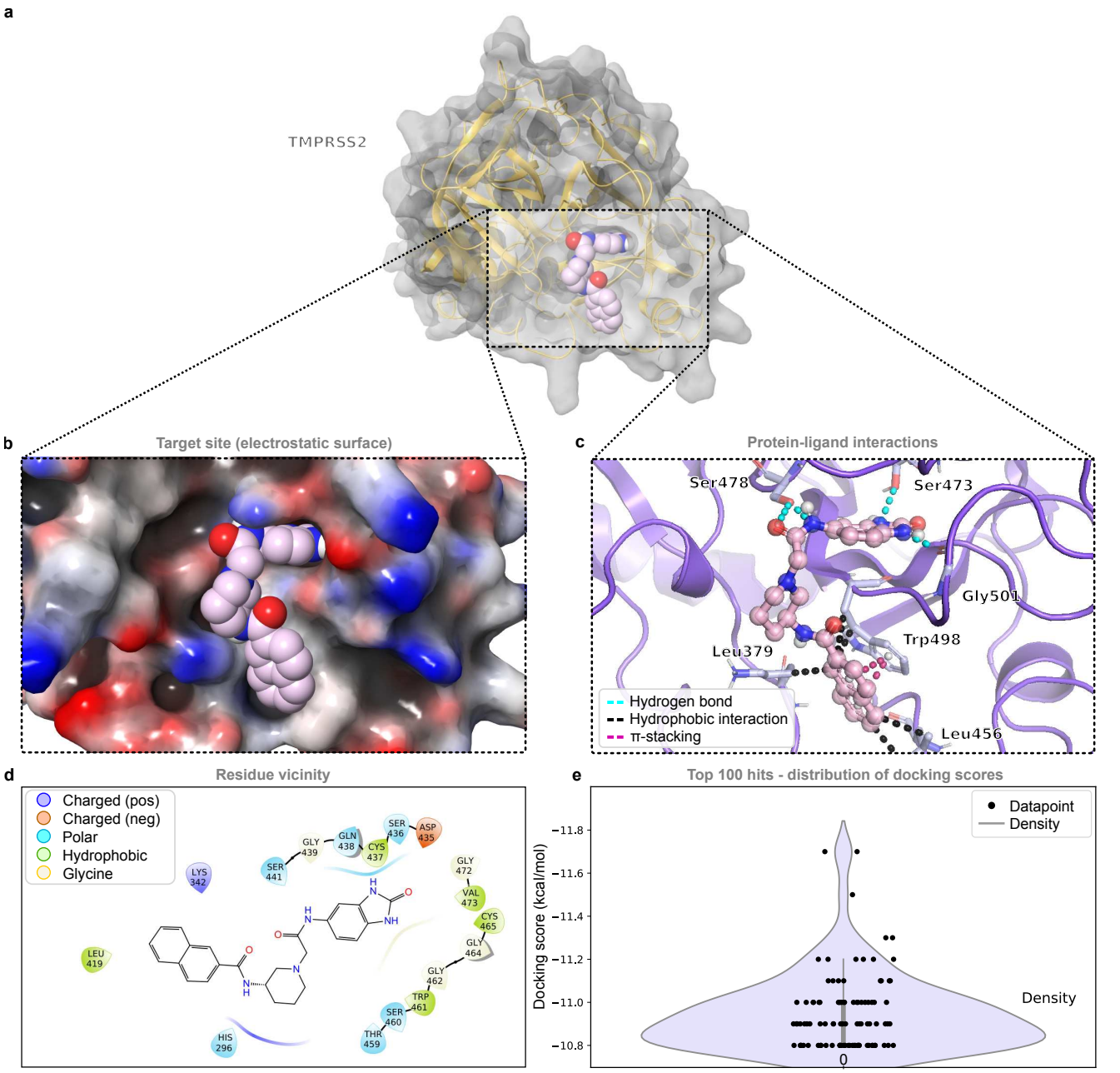

Fig. 3. TMPRSS2 and an example compound from the top 0.0001% of screened compounds bound at the active site of the serine protease domain. a, The target protein TMPRSS2 (gold) and an example compound (light pink) from the virtual screen bound at the active site of the serine protease domain (Screen ID: 6). **b**, Electrostatic surface of the target protein to which an example compound (light pink) is bound. **c,** An overview of the interactions between the inhibitor and protease structure. **d,** Residues within 4 Å of the inhibitor. **e,** Distribution of the docking scores of the top 100 virtual screening hits.

candidates for SARS-CoV-2 in an expedited manner, fueled by the availability of high-resolution structures of many of the SARS-CoV-2 proteins. Previous work has shown that the number of compounds screened in a structure-based *in silico* screen affects the quality of the resulting hits and the potency of the hits derived increases with the number of compounds screened (33). A flurry of recent papers have demonstrated that by using *in silico* screening to expand the chemical space (screening~100 million compounds), one can identify picomolar-affinity inhibitors (33–35). To become capable of screening billions of molecules in a relatively short period (weeks), we recently developed VirtualFlow, an open source computational drug discovery platform (36). VirtualFlow, with its linear scaling feature, leverages the power of computing clusters to perform ultra-large scale screens. Here we use the computational power of the Google Cloud Platform (GCP) to identify molecules that could inhibit SARS-CoV-2. We screened over one billion molecules against each of fifteen SARS-CoV-2 proteins and two human proteins, ACE2 and TMPRSS2. For some of the proteins we target multiple functional sites on the protein surface; an approach which provides two distinct advantages: i) the possibility of increasing efficacy using a cocktail approach, and ii) the identification of alternative ways to target the same protein, a ne-

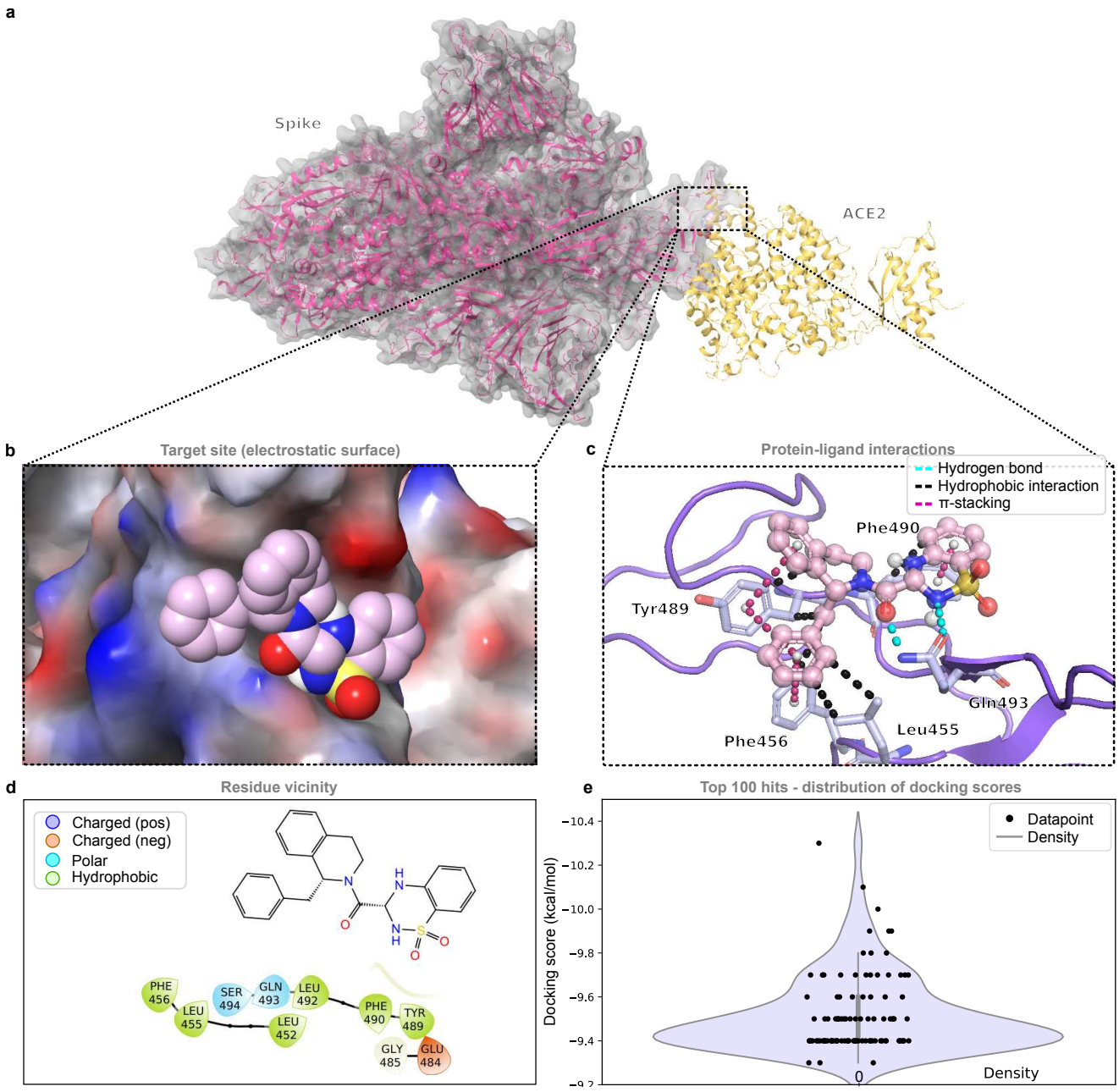

Fig. 4. The RBD of the spike protein and an example compound from the top 0.0001% of screened compounds bound at the ACE2 binding interface. a, The targeted spike protein (magenta) and an example compound (light pink) from the virtual screen bound to the ACE2 binding interface (Screen ID: 7). **b**, Electrostatic surface of the target protein to which an example compound (light pink) is bound. **c,** An overview of the interactions between the inhibitor and the receptor structure. **d,** Residues within 4 Å of the inhibitor. **e,** Distribution of the docking scores of the top 100 virtual screening hits.

cessity when faced with the possibility of resistance mutations. Whenever possible we used recently determined high-resolution structures of SARS-Cov-2 proteins in our screens. A complete list of the target proteins along with the models used can be found in 1.

In the realm of *in silico* screening, the probability of finding a true hit (a hit that is validated experimentally) increases with the number of molecules screened and the accuracy of the chosen structure relative to what exists in solution inside the cell. Small changes in structure or dynamics can be accommodated by flexible docking, but large conformational changes decrease the ability of *in silico* screening methods to identify potent binders. Large conformational changes can be tackled by ensemble docking methods (molecular dynamics simulations), but the trade-off for these approaches is additional computational time. Targeting protein-protein interactions (PPI) is also challenging for *in silico* screening. Typically in PPIs the off-rate between the two interacting proteins is slow and the interaction interface is large compared to a small molecule inhibitor. Thus targeting PPIs was approached with the rationale that a small molecule engaging the monomer at the hot spot of the PPI interface can prevent complex formation, driven by an excess concentration of the small molecule. In the absence of a solved

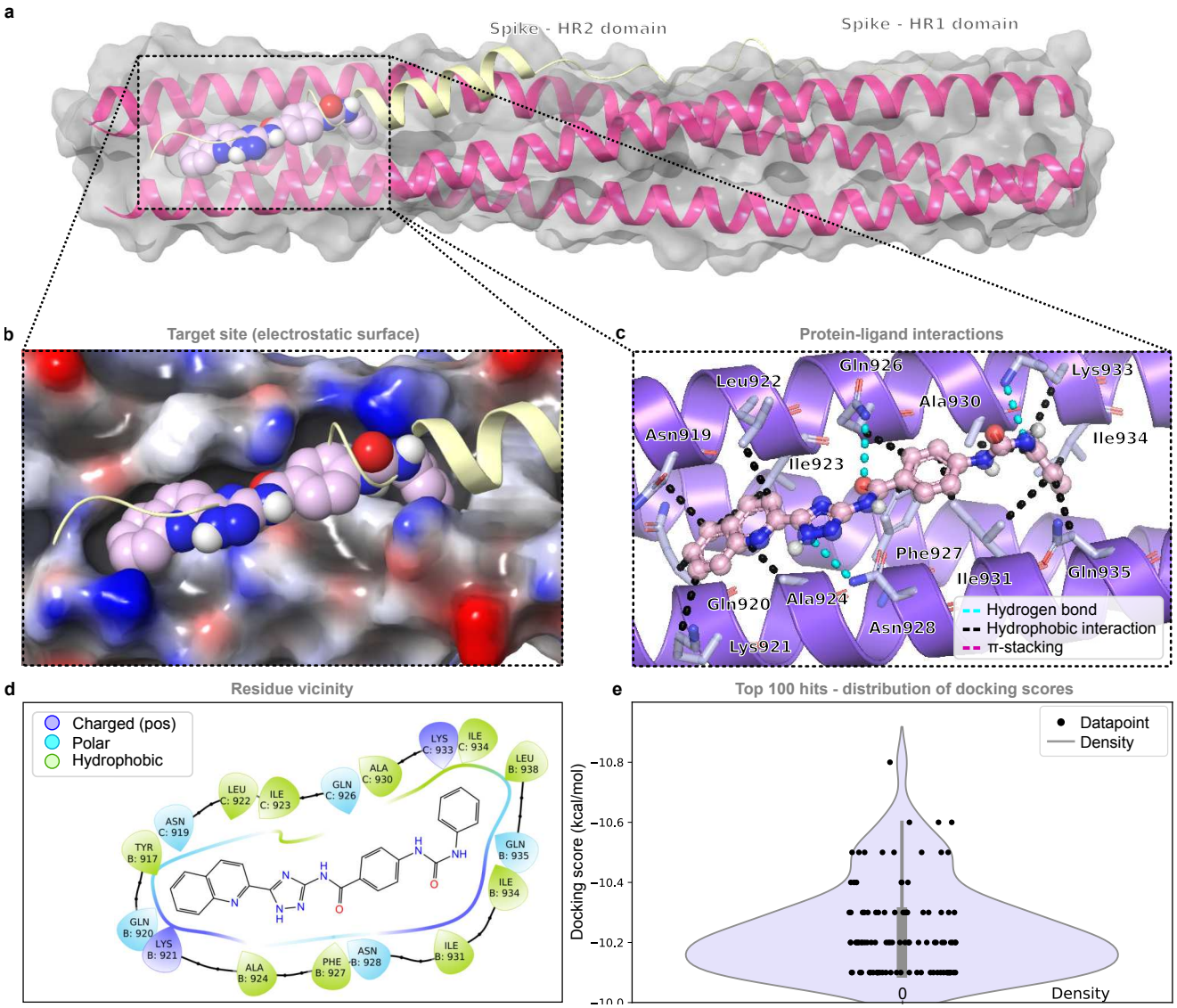

Fig. 5. The HR1 domain and an example compound from the top 0.0001% of screened compounds bound at the interaction interface to the HR2 domain of the spike protein. **a**, The HR1 domain of the targeted spike protein (magenta) and an example compound (light pink) from the virtual screen bound to the HR2 interaction interface. The H2 domain is shown in light gold (Screen ID: 8). **b**, Electrostatic surface of the target protein to which an example compound (light pink) is bound. **c,** An overview of the interactions between the inhibitor and the HR1 structure. **d,** Residues within 4 Å of the inhibitor. **e,** Distribution of the docking scores of the top 100 virtual screening hits.

dimeric/multimeric structure, we make the assumption that the structure of the monomer is similar to that of the protein in complex, which does not always hold true. For each of the targets that were screened we describe any potential limitations that we anticipate could affect the experimental outcome.

Methods

VirtualFlow was used to screen around 1 billion on-demand (synthesizable) compounds from the Enamine REAL library, and around 10 million in-stock compounds from the ZINC 15 library (37) for each targeted site. Both libraries were previously prepared with 'VirtualFlow for Ligand Preparation' (VFLP) (36). For each virtual screen a single receptor structure was used, and the protein was held rigid. QuickVina W was used to perform a blind docking procedure (38) for the HR1 domain of spike protein, the RNA binding interface of nucleoprotein, the RNA binding site of nsp12, as well as for nsp7 and ORF7a. For all the other docking routines, we used QuickVina 2 (39). Both docking programs are based on AutoDock Vina (40), and the exhaustiveness parameter was set to 1 during all virtual screens. This setting minimizes the search of the conformational space within the docking box and maximizes the computational efficiency.

To conduct VirtualFlow screens we needed to leverage a significant amount of high performance computing (HPC) time and infrastructure in order to complete multiple virtual screens in parallel. For this purpose we have taken advantage of Slurm (https://slurm.schedmd.com), a highly scalable and fault-tolerant workload manager capable of handling multiple jobs in parallel. In addition, the Elastifile Cloud File Storage (ECFS) was used, which is a POSIX-compliant and highly scalable NFS file service mounted to

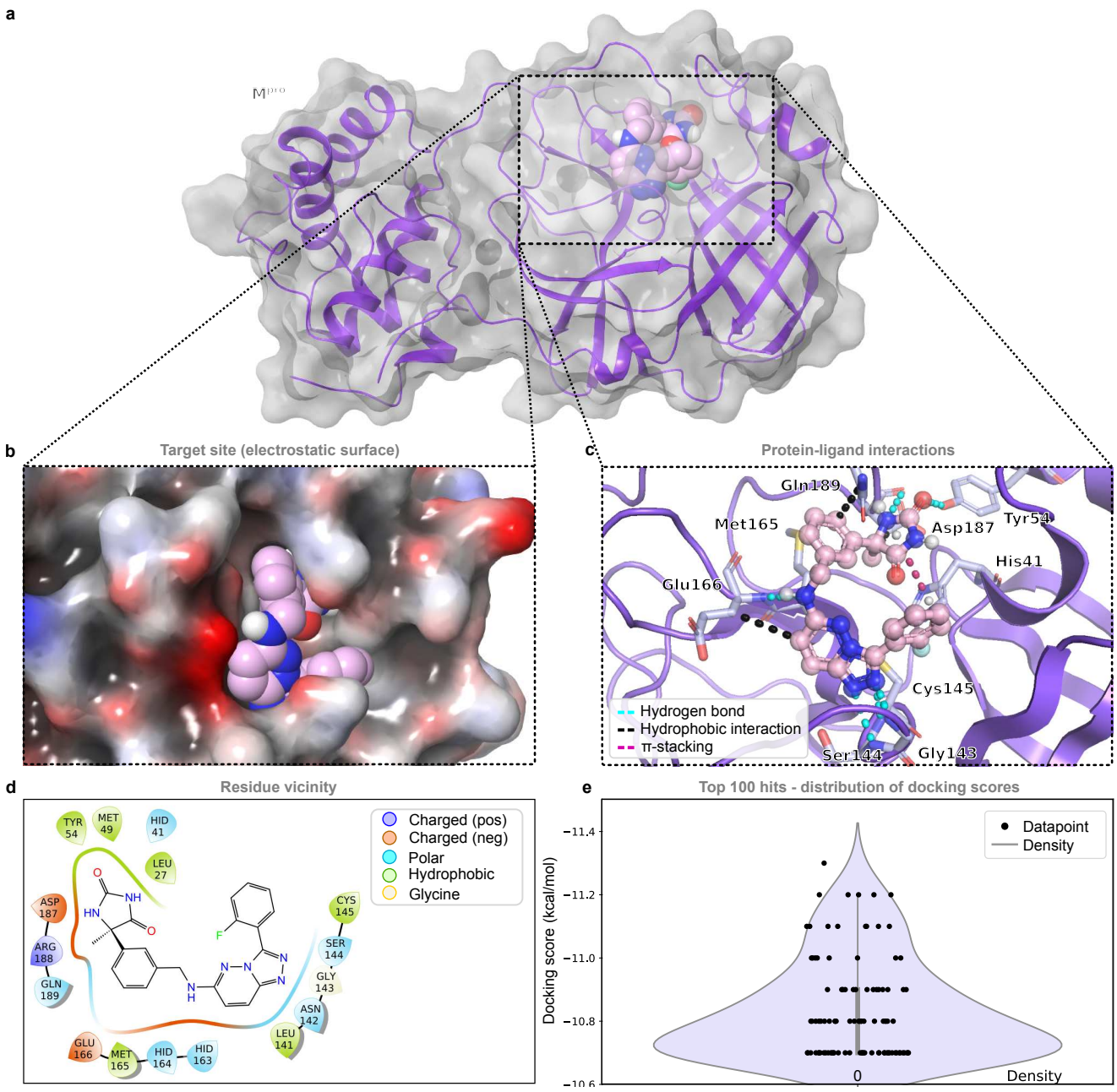

Fig. 6. M^{pro} and an example compound from the top 0.0001% of screened compounds bound at the enzymatic active site a, M^{pro} (violet) and an example compound (light pink) from the virtual screen bound to the active site. Here, the crystal structure with PBD ID 6lu7 was used (Screen ID: 16). **b**, Electrostatic surface of the target protein to which an example compound (light pink) is bound. **c,** An overview of the interactions between the inhibitor and the protease structure. **d,** Residues within 4 Å of the inhibitor. **e,** Distribution of the docking scores of the top 100 virtual screening hits.

the Slurm cluster compute nodes. ECFS provides a full suite of cloud-native NAS features (including snapshots and multi-zone accessibility). The Google Cloud Platform (GCP, https://cloud.google.com), which combines all of these components, including Google Compute Engine preemptible virtual machines, was used to provide the scale of computation required for the ultra-large virtual screens reported here. Google Cloud Storage was used to durably store the generated data.

We operated within a Google Cloud project that has a single Virtual Private Cloud to provide networking functionality to all the virtual instances. To set up this infrastructure we leveraged automated deployment tools like Terraform (https://www.terraform.io/) and the Google Cloud Deployment Manager to replicate this architecture across 3 different zones belonging to two different geographic regions. This resulted in three different clusters (Fig. 22) that were used for virtual screens against different targets in parallel. This globally distributed architecture allowed us to run hundreds of thousands of cores in parallel, consuming a total of approximately 100 million CPU hours in a total of about 3 weeks for all the virtual screens reported here. The types of nodes used are listed in Table 1.

The virtual hits resulting from these screens were filtered

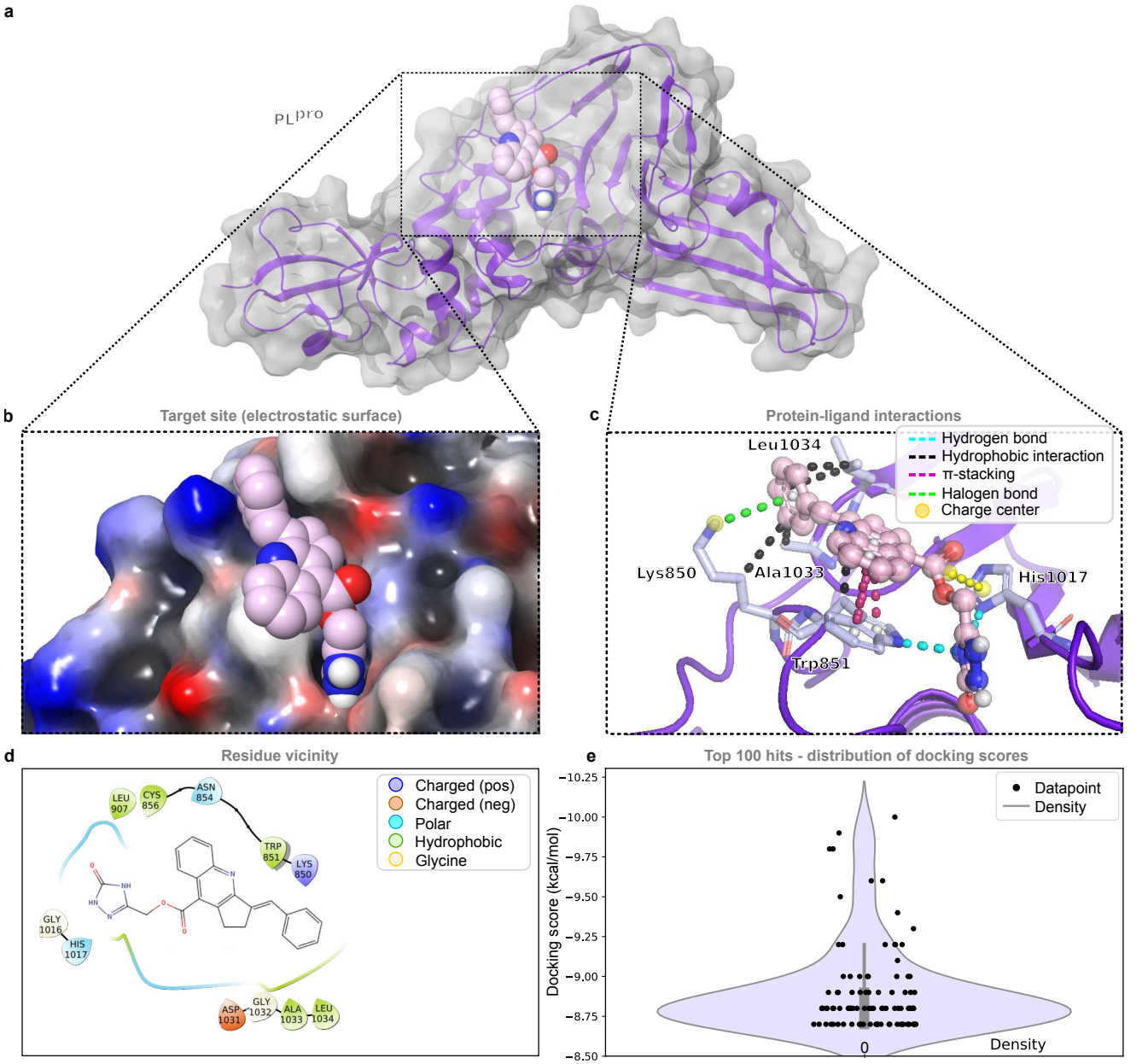

Fig. 7. PL^{pro} and an example compound from the top 0.0001% of screened compounds bound at the enzymatic active site. a, PL^{pro} (violet) and an example compound (light pink) from the virtual screen bound to the active site (Screen ID: 12). **b**, Electrostatic surface of the target protein to which an example compound (light pink) is bound. **c,** An overview of the interactions between the inhibitor and the protease structure. **d,** Residues within 4 Å of the inhibitor. **e,** Distribution of the docking scores of the top 100 virtual screening hits.

to remove compounds that have reactive functional groups, a molecular weight greater than 600 daltons, a cLogP greater than 6, or more than 10 hydrogen bond acceptors. A smaller number of non-druglike molecules from the ZINC library were also removed after visual inspection. The top 200 hits for each target site, after the filtering process, are included in the supplementary section. In addition, for each target site, we showcase one of the top hits in the manuscript. This hit was chosen based on consideration of a number of parameters including, but not limited to, docking score, 'drug-likeness' (which includes criteria such as Lipinski's rule of five, and the tendency to aggregate as estimated by a fraction of sp3-hybridized carbon atoms between 0.25 and 1), and the presence of PAINS (pan-assay interference compounds) or other potentially toxic moieties. The desire to highlight plausible small molecule-protein interactions that can be accommodated by the docking site was also taken into account when choosing the hit to be depicted. Due to these filtering criteria, it is therefore important to note that although the example hit molecule displayed in each figure is one of the top hits for the represented screen, it is often not the hit with the highest docking score.

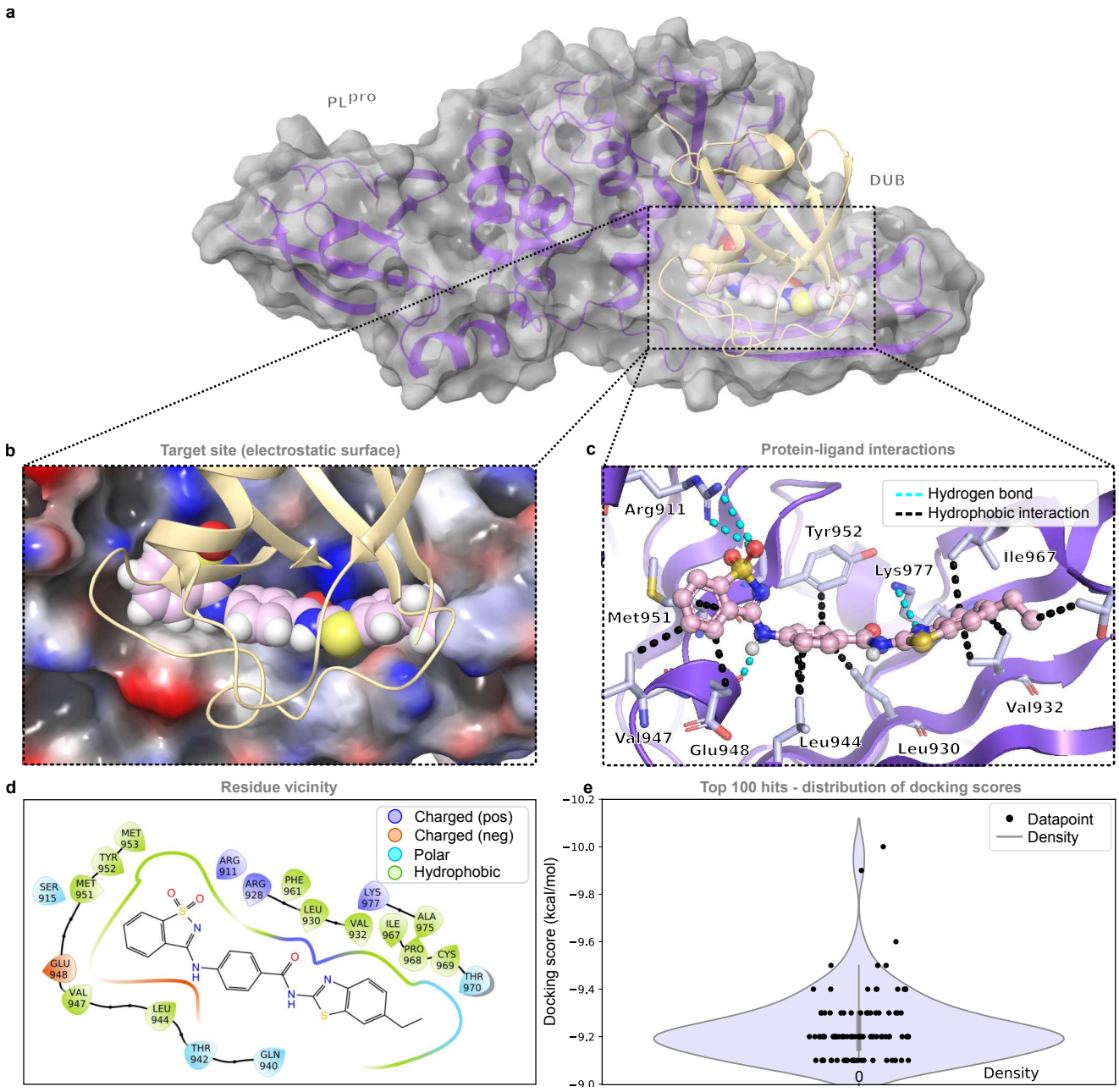

Fig. 8. PL^{pro} and an example compound from the top 0.0001% of screened compounds bound at the DUB binding site. a, PL^{pro} (violet) and an example compound (light pink) from the virtual screen bound at the DUB binding site (Screen ID: 14). **b**, Electrostatic surface of the target protein to which an example compound (light pink) is bound. **c,** An overview of the interactions between the inhibitor and the receptor structure. **d,** Receptor residues within 4 Å of the inhibitor. **e,** Distribution of the docking scores of the top 100 virtual screening hits.

Results

Preventing coronavirus entry

The spike protein forms the highly glycosylated trimeric receptor-binding protein that decorates the virion surface and facilitates entry into the host cell through interaction with its receptor ACE2 (41). Binding of the Receptor Binding Domain (RBD) of S to ACE2 induces large conformational changes in the S2 domain. These changes are followed by processing by host proteases such as TMPRSS2 and cathepsins and result in the formation of a stable six-helix bundle by heptad repeats 1 and 2 (HR1 and HR2) culminating in the fusion of the viral and cellular membranes (8). In order to develop compounds capable of preventing SARS-CoV-2 from entering cells, we focused on the following three targets: a) the interaction interface of the RBD and ACE2, b) the host protease TMPRSS2, and c) the HR2 hydrophobic binding groove of HR1.

ACE2-spike-RBD interaction. Recent studies have revealed molecular details of ACE2 binding with spike-RBD and multiple high-resolution structures of the RBD in complex with ACE2 have been released (PDB: 6M17, 6M0J, 6VW1) (17, 42, 43). As the primary mediator of host cell attachment, the spike trimer is a clear potential target for thera-

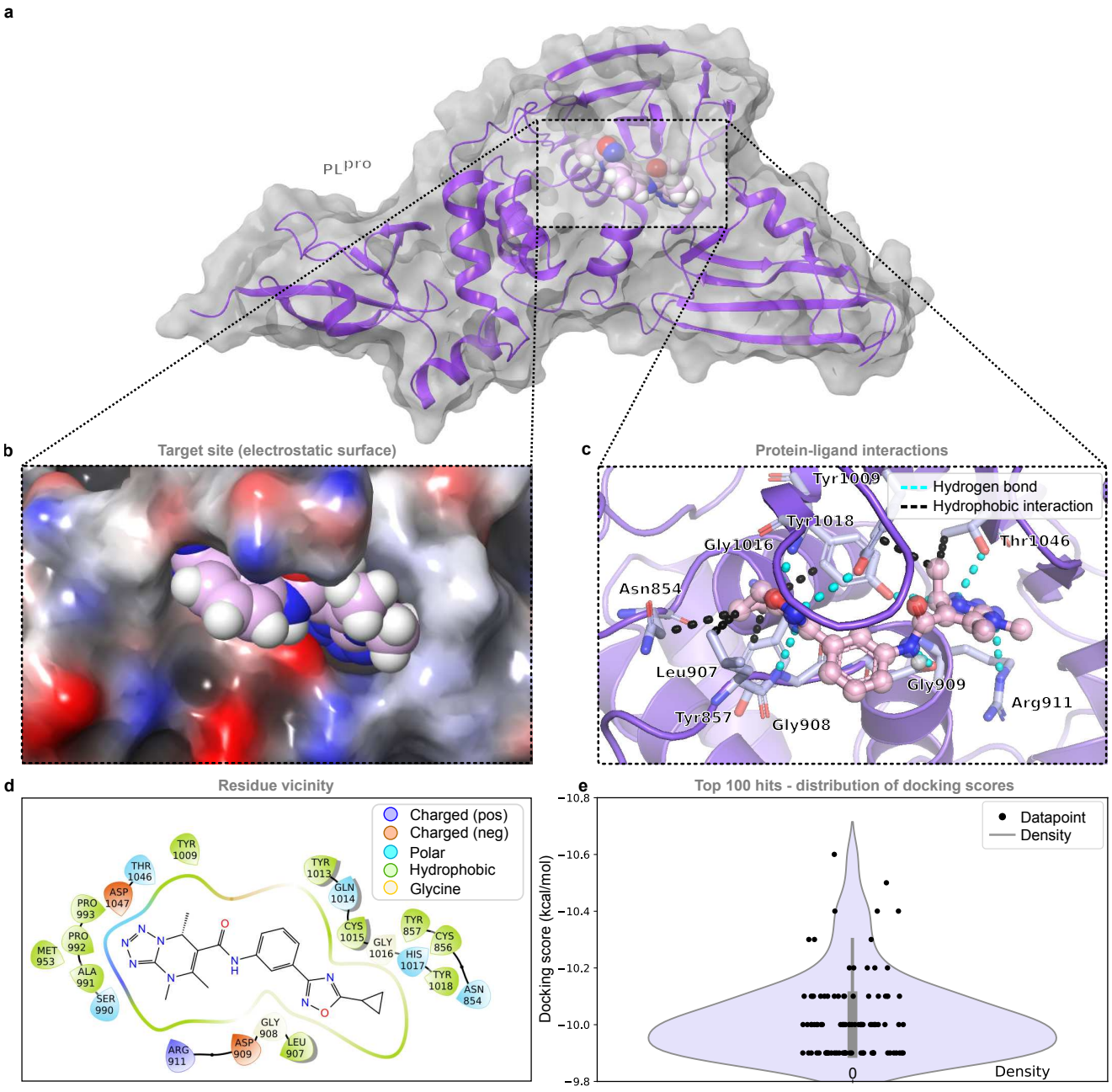

Fig. 9. PL^{pro} and an example compound from the top 0.0001% of screened compounds bound at the enzymatic active site (tunnel region). **a**, PL^{pro} (violet) and an example compound (light pink) from the virtual screen bound to the active site (tunnel region) (Screen ID: 15). **b**, Electrostatic surface of the target protein to which an example compound (light pink) is bound. **c,** An overview of the interactions between the inhibitor and the protease structure. **d,** Residues within 4 Å of the inhibitor. **e,** Distribution of the docking scores of the top 100 virtual screening hits.

peutic intervention, and in order to find an effective inhibitor of viral entry into host cells, we target both ACE2 and the RBD of spike in parallel.

Targeting the spike protein interaction interface on ACE2. The primary physiological function of the receptor, ACE2, is the maturation of angiotensin, a signalling peptide with cardiovascular regulatory effects (44), making any targeting of the catalytic site of ACE2 unfavourable. Fortunately, the structure of the complex shows that the peptidase (PD) domain of ACE2 has two distinct lobes that are essential for substrate engagement, and while the RBD-ACE2 binding interface includes one of these lobes, it does not obstruct the PD active site (17, 42) (Fig. 2, Supplementary Figs. 1, 2, 3, 4). This suggests that targeting the RBD interaction interface should not inhibit ACE2 functionality and therefore not affect angiotensin homeostasis. In fact, previous biochemical studies with SARS-CoV have shown that the ACE2 inhibitor MLN-4760, which favors the closed state, does not interfere with S protein binding and vice versa, also arguing for independence of ACE2 function and spike binding (45). We have targeted four different sites on the ACE2 surface. Two of them are located on the spike interaction interface, and would directly disrupt the ACE2-spike interaction (Fig. 2, Supplementary Figs. 1, 2). For the first of these two sites (cen-

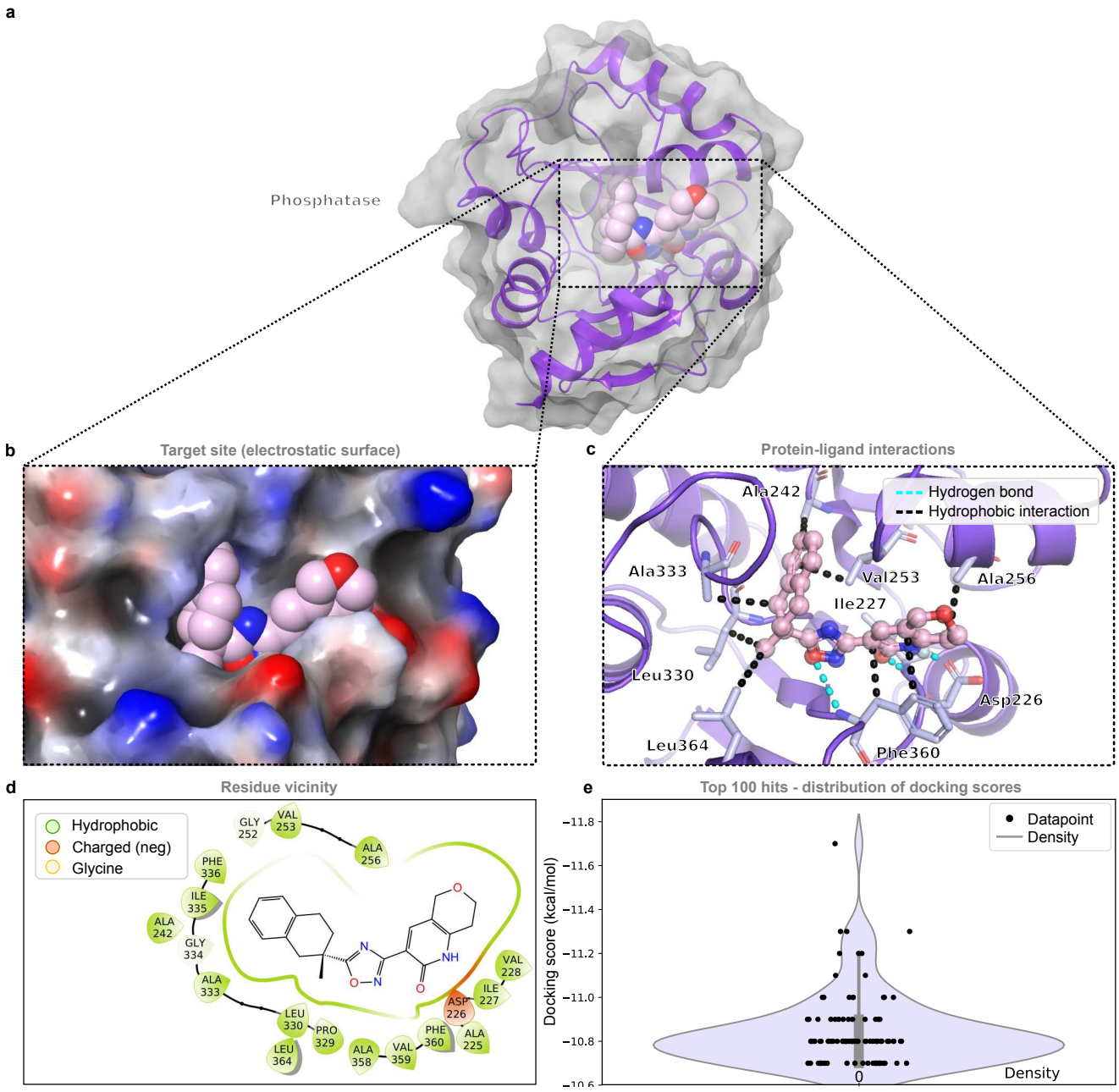

Fig. 10. The phosphatase (closed conformation) and an example compound from the top 0.0001% of screened compounds bound at the enzymatic active site. a, The phosphatase (violet), which is part of nsp3, and an example compound (light pink) from the virtual screen bound to the active site (closed conformation) (Screen ID :10). **b**, Electrostatic surface of the target protein to which an example compound (light pink) is bound. **c,** An overview of the interactions between the inhibitor and the phosphatase structure. **d,** Residues within 4 Å of the inhibitor. **e,** Distribution of the docking scores of the top 100 virtual screening hits.

tered around Glu37), two independent virtual screens were carried out (Screen IDs: 1 and 2): one using an ACE2 structure where no spike protein was bound (PDB: 6m17; Screen ID: 1), and one using an ACE2 structure to which the RBD domain of the spike protein was bound (PDB: 6m18; Screen ID: 2). The difference between these two conformations at the site of binding is relatively small (RMSD: 0.355 Å in the region of the first two N-terminal α-helices), yet significant for structure-based virtual screening. The second site that we targeted on the spike binding interface (Screen ID: 3) is centered around residue Gly354, and was chosen because there is a shallow hydrophobic pocket. The other two sites targeted were two dynamic pockets adjacent to the spike interface on ACE2 potentially capable of accommodating tighter binders (Screen IDs: 4 and 5) (Supplementary Figs. 1, 2). Compounds bound to the two dynamic pockets could be linked to each other, and the linker, which then would pass over the spike interaction interface, could potentially block the binding of spike protein.

Targeting the ACE2 interaction interface on the Spike RBD. *In vitro* measurements suggest that SARS-CoV-2 RBD binds to ACE2 with nanomolar affinity (18, 46). Each peptidase domain of ACE2 can accommodate one RBD and the interaction is mediated through polar interactions. It has previ-

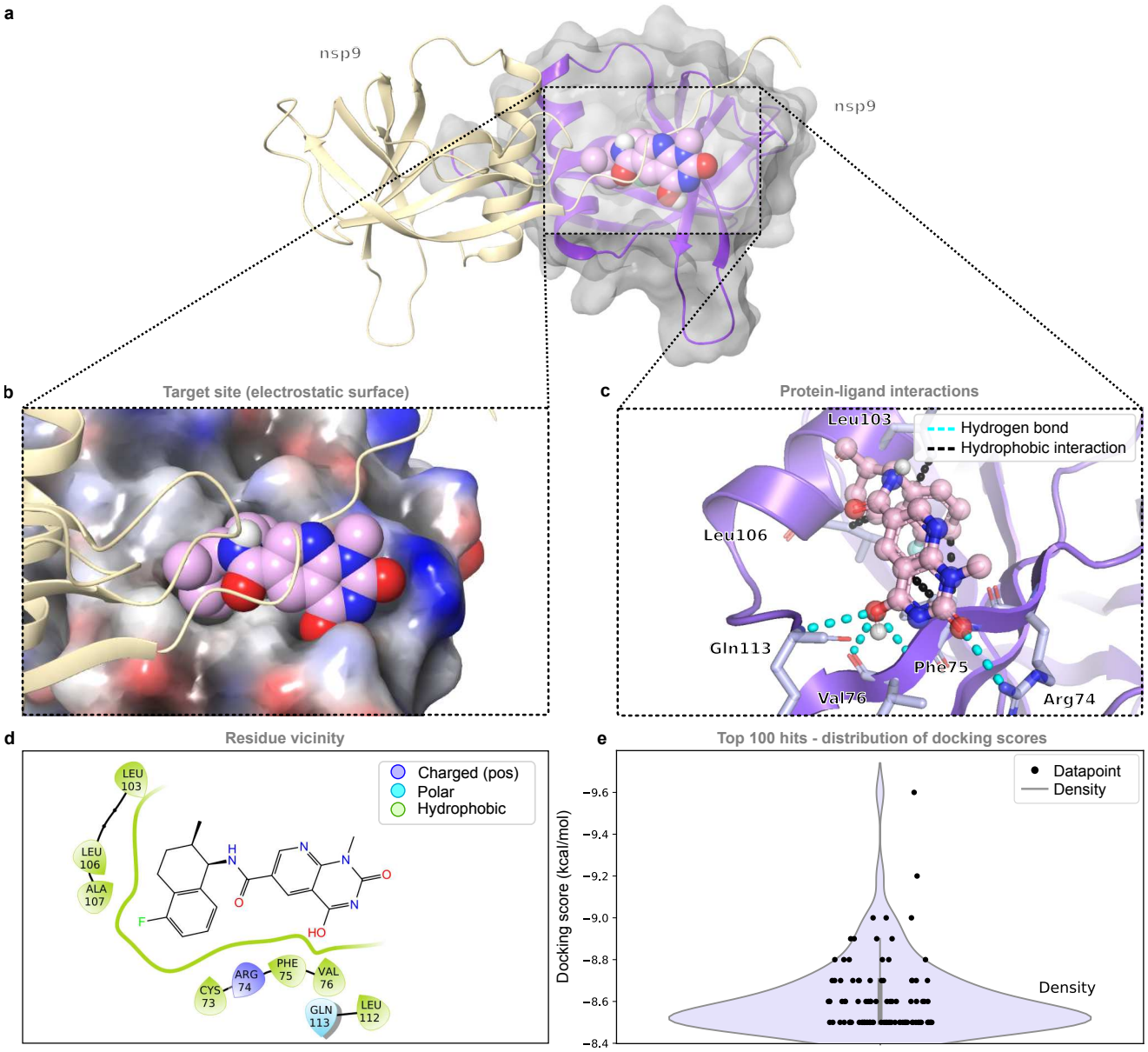

Fig. 11. nsp9 and an example compound from the top 0.0001% of screened compounds bound at the dimerization interface (site 2). **a**, The nsp9 dimer (one monomer in violet, one monomer in gold), where an example compound (light pink) from the virtual screen is bound to the dimerization interface (site 2) of the nsp9 monomer in violet (Screen ID: 24). **b**, Electrostatic surface of the target protein to which an example compound (light pink) and a second nsp9 monomer (light gold) is bound. **c,** An overview of the interactions between the inhibitor and the nsp9 structure. **d,** Residues within 4 Å of the inhibitor. **e,** Distribution of the docking scores of the top 100 virtual screening hits.

ously been shown that the "up" conformation of the RBD is required for receptor binding and that two spike protein trimers can bind to a single ACE2 dimer (17) (Fig. 4). The RBD itself consists of a core containing an anti-parallel β-sheet (β1 to β4 and β7), with three short α-helices and an extended loop. This extended loop engages the α1 helix of the ACE2-PD, and it is the center of this interface on the RBD that we have targeted by virtual screening (Screen ID: 7) (Fig. 4.

The spike interaction interface on ACE2 is relatively flat and polar, which makes it challenging to identify tight-binding molecules. This difficulty is reflected in the docking scores resulting from the virtual screen of this binding interface: the average docking score of the top 100 virtual hit compounds from this screen was approximately -8 kcal/mol, which is amongst the weakest docking score averages of all the target sites screened (see also Supplementary Fig. 21).

The SARS-CoV-2 RBD has significantly higher affinity for ACE2 as compared to that of the SARS-CoV RBD (43, 46); however, the full-length spike protein from SARS-CoV-2 shows either similar or weaker affinity for ACE2 (18, 47) when compared to that of the full-length SARS-CoV spike. This contrast in binding affinities between the RBD alone and the full-length spike protein could be a consequence of RBD dynamics where the protein switches between RBD "up" and "down" states as seen in case of SARS-CoV (48, 49). There is limited information available as to whether the SARS-CoV-2 spike favors a 'lying-

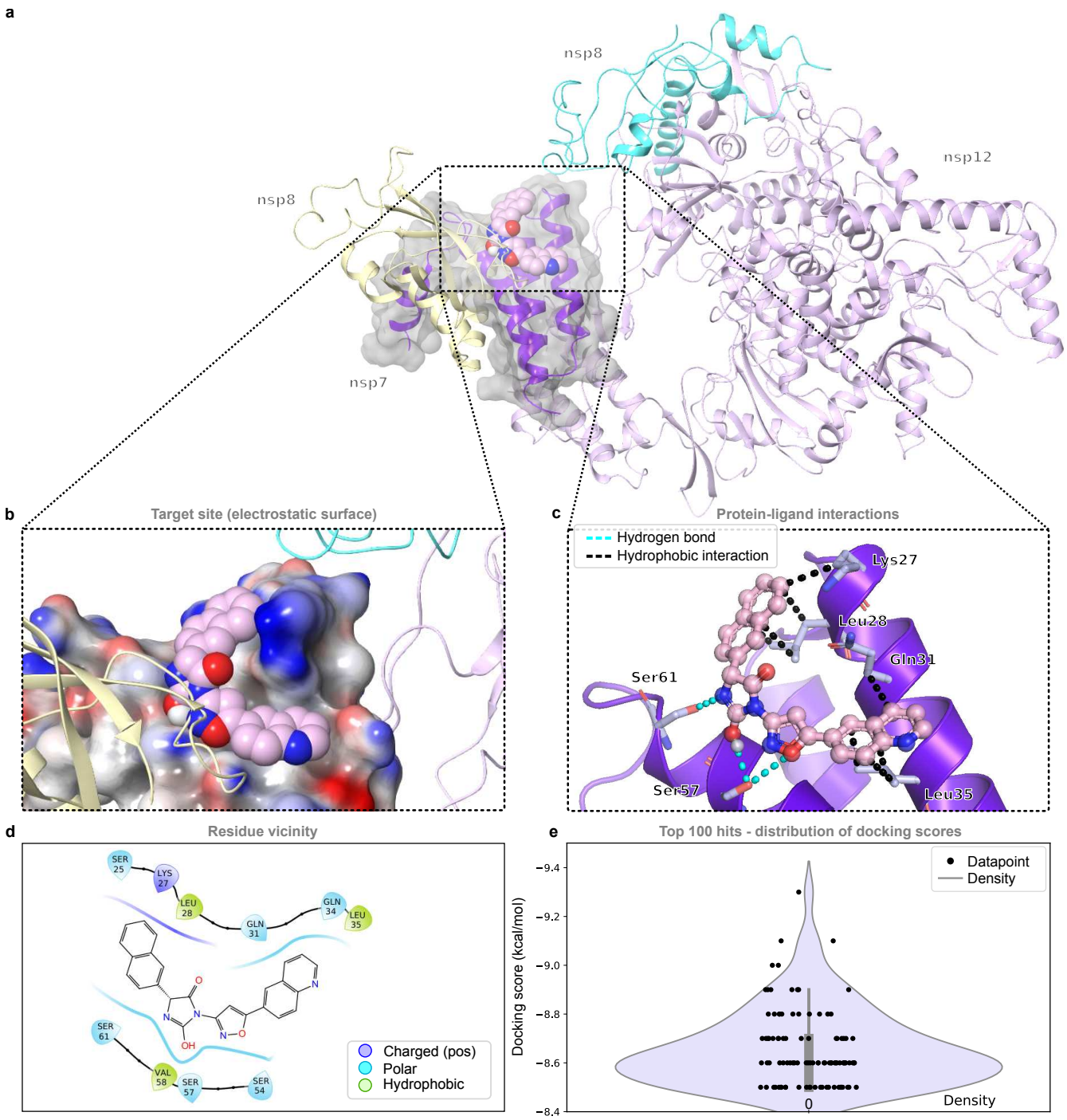

Fig. 12. nsp7 and an example compound from the top 0.0001% of screened compounds bound to the surface). a, nsp7 (violet), where an example compound (light pink) from the virtual screen is bound at the nsp8 (light gold) interface. In the virtual screen, a blind docking was carried out for each screened compound over the entire surrounding helical surface. This helical surface includes large parts of the nsp8 (light gold, cyan) and nsp12 (lavender) binding interfaces (Screen ID: 20). **b**, Electrostatic surface of nsp7 to which an example compound (light pink) is bound. Also shown are the protein-protein interaction partners nsp8 (light gold, cyan) and nsp12 (lavender). **c,** An overview of the interactions between the inhibitor and the nsp7 structure. **d,** Residues within 4 Å of the inhibitor. **e,** Distribution of the docking scores of the top 100 virtual screening hits.

down'binding-inactive state or a 'standing up' state capable of receptor binding (18, 46), and so far no SARS-CoV-2 spike trimer structure with two RBD domains in "up" position has been determined. Furthermore, there is no information on the inherent dynamics within the RBD domain itself, which is where the targeted molecules are expected to bind. This means that it is possible that local protein dynamics could adversely affect binding of some of the hits in ways that the screen is unable to predict.

It should be noted that while targeting the flat surface of the spike-binding interface with ACE2 (Screen IDs 1-3) resulted in compounds with an average binding energy of -8.275 kcal/mol, targeting the dynamic pockets resulted in hits with the potential for higher affinity binding. The binding

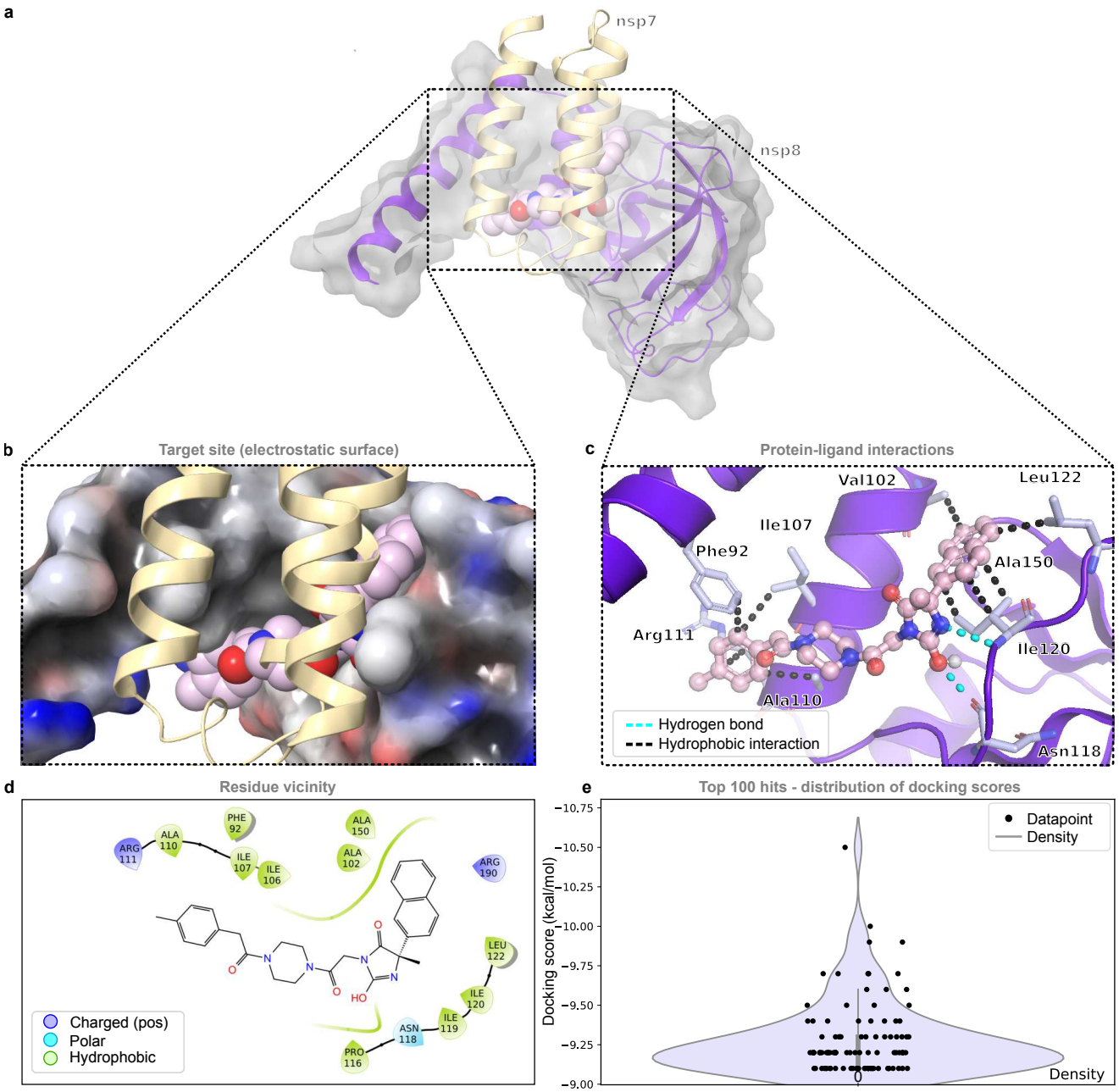

Fig. 13. nsp8 and an example compound from the top 0.0001% of screened compounds bound at the nsp7 binding interface. a, nsp8 (violet) bound to nsp7 (light gold) and an example compound (light pink) (Screen ID: 21). **b**, Electrostatic surface of the target protein to which an example compound (light pink) and nsp7 (light gold) bound. **c,** An overview of the interactions between the inhibitor and the nsp8 structure. **d,** Residues within 4 Å of the inhibitor. **e,** Distribution of the docking scores of the top 100 virtual screening hits.

energy of hits in the dynamic pockets was as high as -10.3 kcal/mol. Experimental validation of these hits would be required to confirm an affinity difference.

TMPRSS2. The essential priming of S during entry can be executed by the host serine protease TMPRSS2 in the case of SARS-CoV-2, making it a potential therapeutic target. In addition, recent research has shown that the TMPRSS2 inhibtor, camostat mesylate, can block viral entry in cell-based assays (41). Effective inhibition of TMPRSS2 could have multiple applications, since processing of ACE2 by TMPRSS2 has also been shown to be crucial for activation of S in SARS-CoV (50). Although TMPRSS2 has been shown to activate protease-activated receptor 2 (PAR-2) and hepatocyte growth factor (HGF), giving it possible roles in tumor metastasis and epithelial-mesenchymal transition (51), the exact physiological function of this protein is still unknown. TMPRSS2-deficient mice showed no significant phenotypic changes (52), and thus TMPRSS2 is considered to be dispensable for normal cellular function, making a TMPRSS2-specific inhibitor less likely to have side effects.

TMPRSS2 itself contains a cytoplasmic domain, a transmembrane domain, an extracellular low-density-lipoprotein-receptor (LDLR) domain, a scavenger-receptor cysteine-rich (SRCR) domain and a C-terminal serine protease domain.

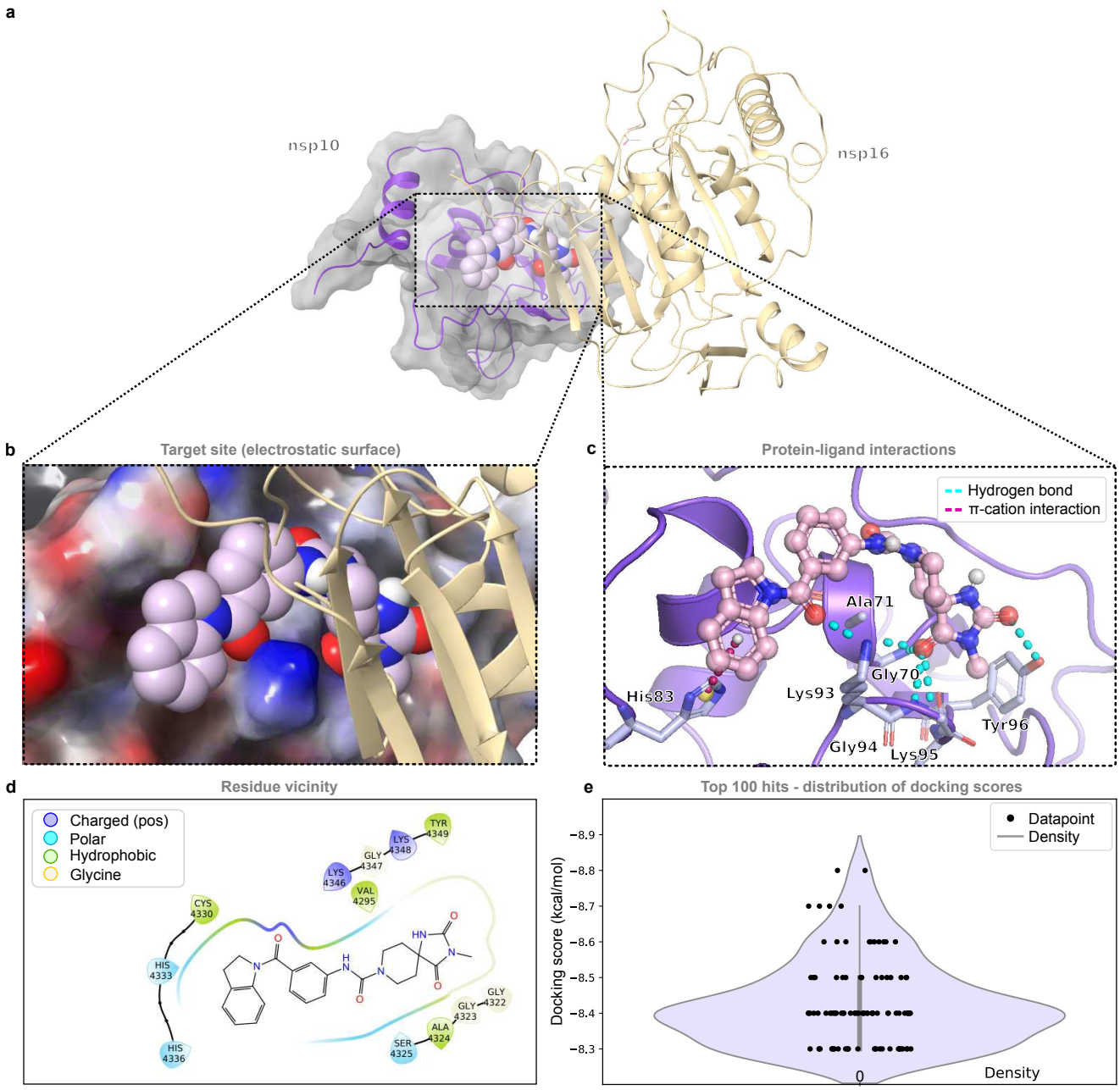

Fig. 14. nsp10 and an example compound from the top 0.0001% of screened compounds bound at the protein-protein interaction interface with nsp14 and nsp16. **a**, nsp10 (violet) bound to nsp14 (light gold) and an example compound (light pink), at the nsp14/nsp16 binding interface of nsp10 (Screen ID: 25). **b**, Electrostatic surface of nsp10 to which an example compound (light pink) as well nsp14 (light gold) are bound. **c,** An overview of the interactions between the inhibitor and the nsp10 structure. **d,** Residues within 4 Å of the inhibitor. **e,** Distribution of the docking scores of the top 100 virtual screening hits.

The TMPRSS2 precursor consists of 492 amino acids and auto-catalytic cleavage at Arg255 generates the active protease (53). As a chymotrypsinogen-like protease, TMPRSS2 contains a catalytic triad consisting of residues His296, Asp345 and Ser441. As there are currently no experimental structures available for TMPRSS2, we used a homology model from SWISS-MODEL that is based on the human serine protease hepsin (PDB: 5CE1.1A), which shares 33.82% sequence identity with TMPRSS2. Approximately 1 billion compounds were screened against the active site of this homology model (Fig. 3).

Since a homology model was used to screen for inhibitors, success would depend on the how closely the model represents the actual structure. The active site of TMPRSS2 is well conserved when compared to the template and other serine proteases, and contains Ser, His and Asp residues. The residues around the binding pocket are also well conserved, making it very likely that the predicted structure is sufficiently accurate in the region around the active site binding pocket, which is what we targeted (Screen ID: 6). Our top 10 hits had an average binding energy of -11.35 kcal/mol, which should ideally result in nanomolar inhibitors. It must be noted that experiments with the TMPRSS2 inhibitor camostst mesylate in cultured cells showed that complete inhibition of

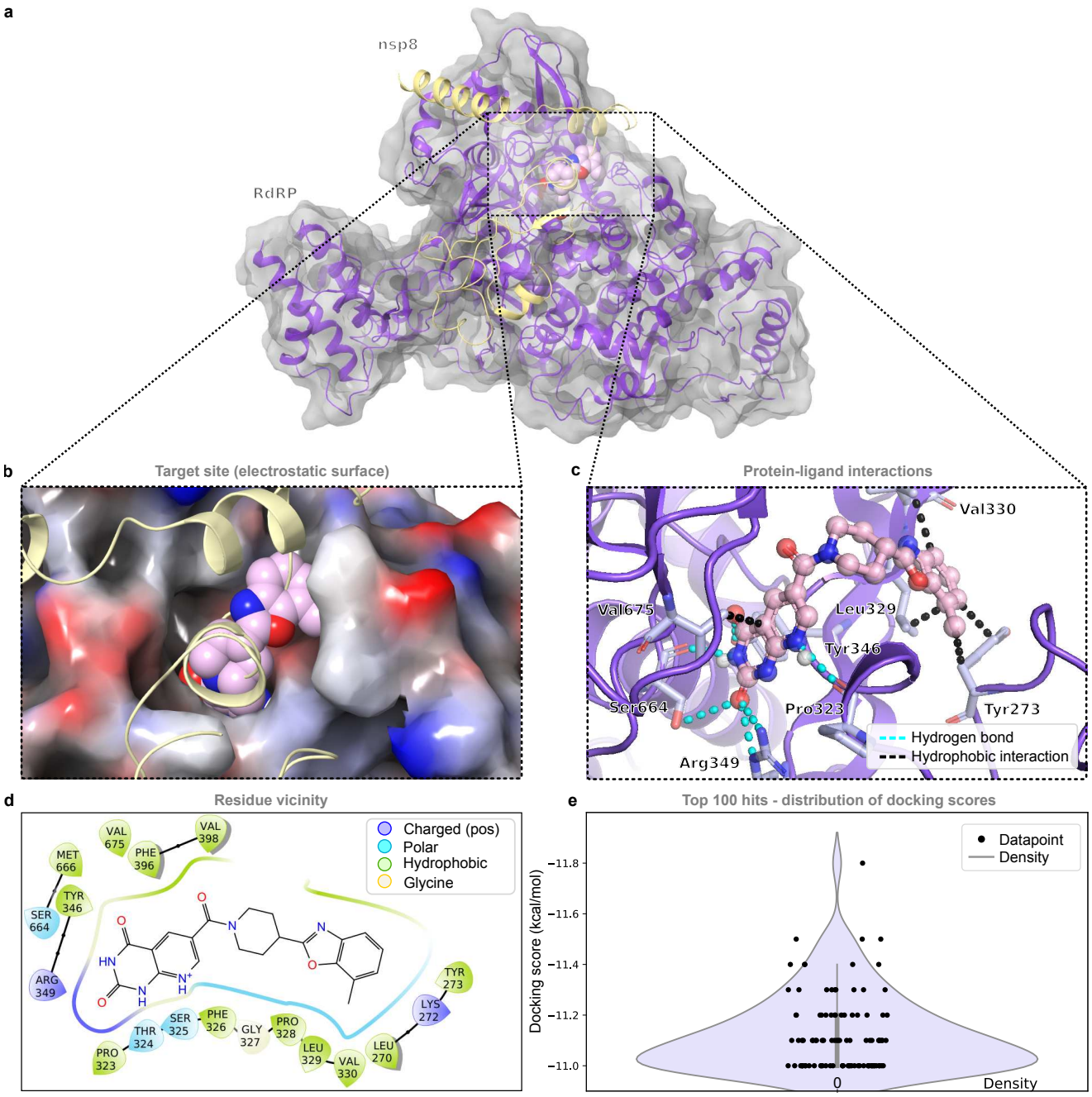

Fig. 15. nsp12 and an example compound from the top 0.0001% of screened compounds bound at the nsp8 binding interface. a, nsp12 (violet) bound to nsp8 (light gold) and an example compound (light pink) at the nsp8 binding interface of nsp12 . **b**, Electrostatic surface of nsp12 to which an example compound (light pink) as well as nsp8 (light gold) are bound. **c,** An overview of the interactions between the inhibitor and the nsp12 structure. **d,** Residues within 4 Å of the inhibitor. **e,** Distribution of the docking scores of the top 100 virtual screening hits.

viral entry is achieved only in conjunction with an inhibitor of CatB/L (E-64d) (41); however, the impact of this residual priming of S by CatB/L on viral pathogenesis *in vivo* has yet to be well studied.

HR1-HR2 interface. While the S1 subunit of the spike protein is crucial for host cell attachment, the S2 subunit plays an essential role in membrane fusion and subsequent entry into the host cell. Heptad repeats HR1 (residues 912-984) and HR2 (residues 1163-1213) in S2 interact to form the classic six-helix bundle (6-HB) of a class I entry protein (54, 55). The HR domains of the spike protein and their mode of interaction are known to be highly conserved across CoVs, making them an attractive target for the development of pan-coronavirus fusion inhibitors (56).

The central trimeric coiled-coil of HR1 has three hydrophobic grooves (Fig. 5) that are proposed to be potential drug binding sites for inhibition of viral fusion. The recent crystal structure of HR1-L6-HR2 (PDB: 6LXT) displays a 6-HB structure with the HR1 domains forming a parallel trimeric coiled-coil around the anti-parallel HR2 domain. The hydrophobic groove formed by the HR1 helices is

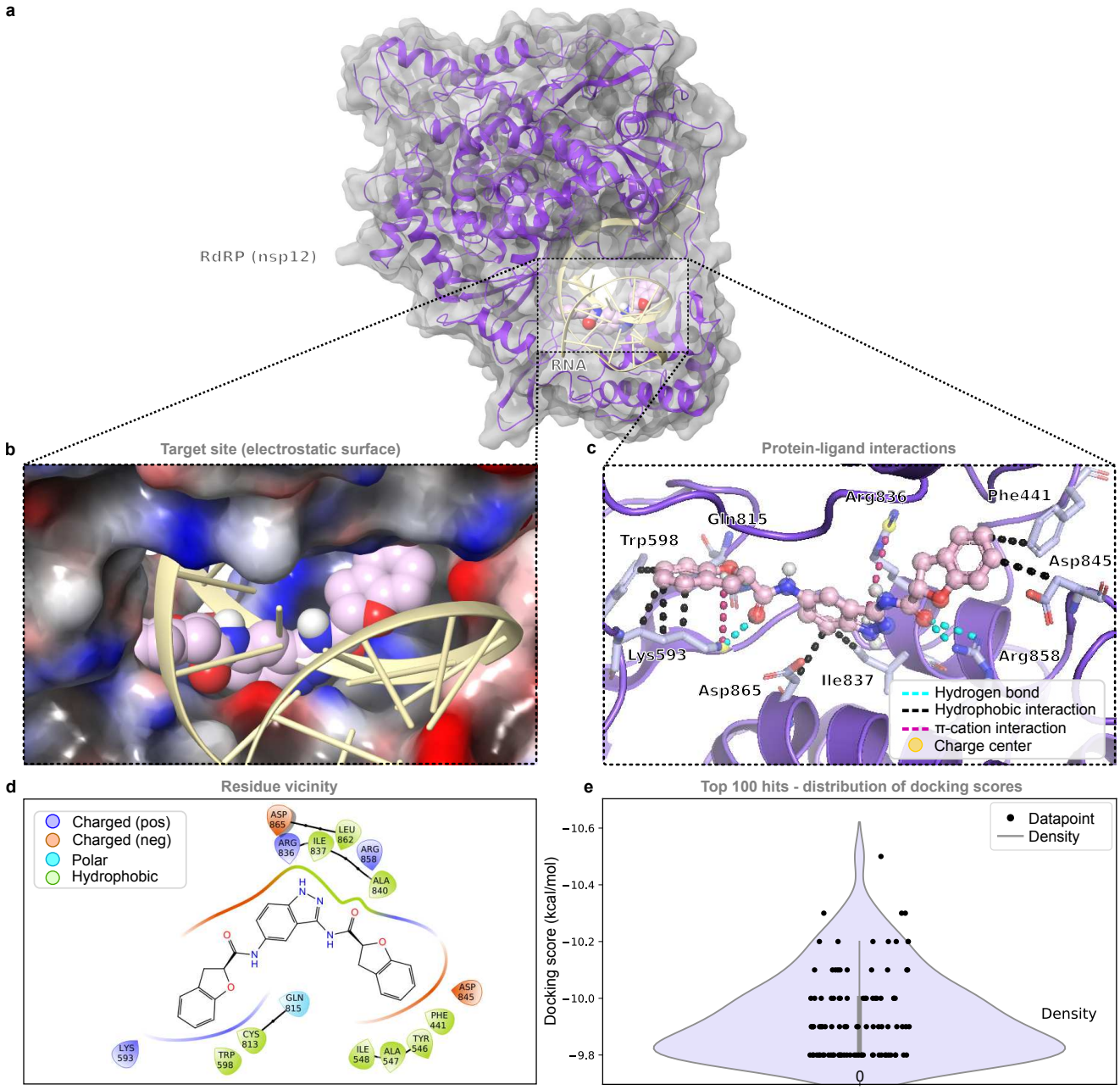

Fig. 16. nsp12 and an example compound from the top 0.0001% of screened compounds bound at site 1 of the the RNA binding interface. a, nsp12 (violet) bound to RNA (light gold) and an example compound (light pink) at site 1 of the RNA binding interface of nsp12 (Screen ID: 28). **b**, Electrostatic surface of nsp12 to which an example compound (light pink) is bound at site 1 of the RNA (light gold) binding interface. **c,** An overview of the interactions between the inhibitor and the nsp12 structure. **d,** Residues within 4 Å of the inhibitor. **e,** Distribution of the docking scores of the top 100 virtual screening hits.

also the binding interface for the HR2 domain (57). The hydrophobic interaction between HR1 and HR2 is in the area of the fusion core, and previous studies have shown that both HR1 and HR2 components of this fusion core interface could be effectively targeted using complementary peptides in SARS-CoV-2 and MERS-CoV (54, 58).

We performed a blind docking using QuickVina W against the entire surface of the trimeric alpha helix (Screen ID: 8) (Fig. 4). The resulting hits could not only potentially have high inhibitory activity against multiples CoVs, but could also have both prophylactic and therapeutic applications as was seen previously in the case of a peptide inhibitor (59). Ligands binding to each of the three different hydrophobic grooves could be identified and linked together in order to enhance the overall affinity and thereby increase the potency.

Preventing coronavirus replication and curtailing viral load

Once coronavirus enters the cell, translation of the replicase gene gives rise to two large polyproteins, PP1a and PP1ab, composed of nsp1-11 and nsp1-16, respectively. M^{pro} and PL^{pro} cleave these polyproteins into individual nsps, which facilitate genomic replication and transcription of subgenomic RNAs. In order to develop small molecules capa-

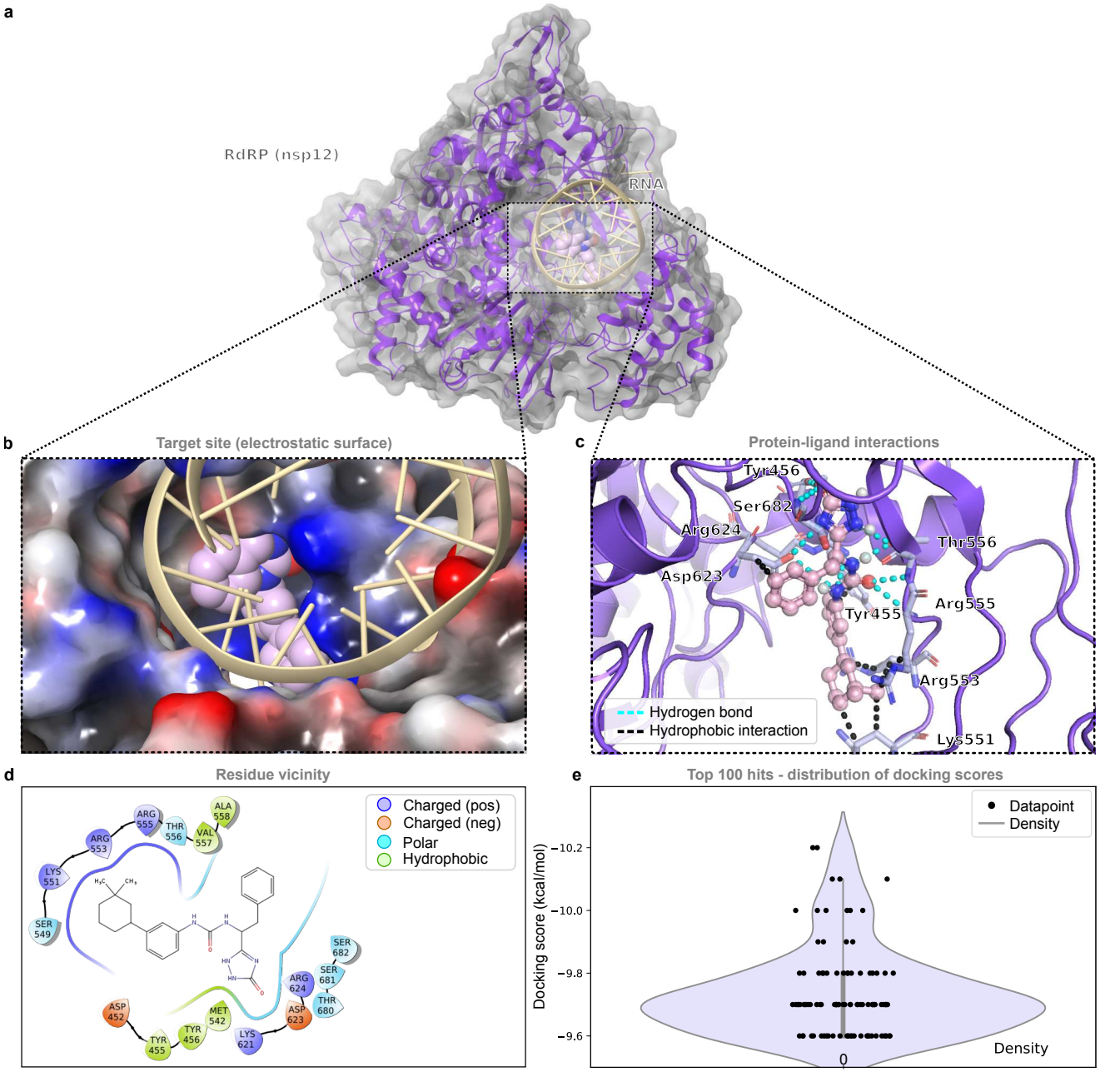

Fig. 17. nsp12 and an example compound from the top 0.0001% of screened compounds bound at the nucleotide binding site. a, nsp12 (violet) bound to RNA (light gold) and an example compound (light pink) at the nucleotide binding site (Screen ID: 30). **b**, Electrostatic surface of nsp12 to which an example compound (light pink) is bound at the nucleotide binding site. RNA is depicted in light gold. **c,** An overview of the interactions between the inhibitor and the nsp12 structure. **d,** Residues within 4 Å of the inhibitor. **e,** Distribution of the docking scores of the top 100 virtual screening hits.

ble of inhibiting replication we targeted the following five proteins and protein complexes, selected based on the availability of high-resolution structures and available information about their molecular mechanisms: a) the coronavirus primary protease (M^{pro}, nsp5), b) the papain-like protease (PL^{pro}, nsp3), c) the RNA-replication complex, composed of the RdRp (nsp12) and its co-factors nsp7 and nsp8, d) the helicase (nsp13), and e) the ssRNA-binding protein nsp9.

M^{pro} ($3CL^{pro}$). M^{pro} ($3CL^{pro}$), the main protease of coronavirus, cleaves PP1a and PP1ab into many of their constituent nsps (11 cleavage sites in PP1ab). The inhibition of M^{pro} would not only inhibit the protease itself, but also hinder downstream processes by preventing the production of key viral proteins through inhibition of their proteolytic processing. Proteolytic cleavage by M^{pro} via the catalytic dyad (Cys-His) occurs at the P1 glutamine residue in the cleavage motif (60). Dimerization is thought to create a substrate binding cleft (61), and simulations suggest that only one monomer is active at a time (62). M^{pro} is highly conserved not only in SARS-CoV and SARS-CoV-2, but also among other viruses of the *Nidovirales* order (enveloped positive-sense single-stranded RNA viruses that produce nested 3'-co-terminal genomic RNAs), making it a potential target for the development of antiviral drugs with broad efficacy (63).

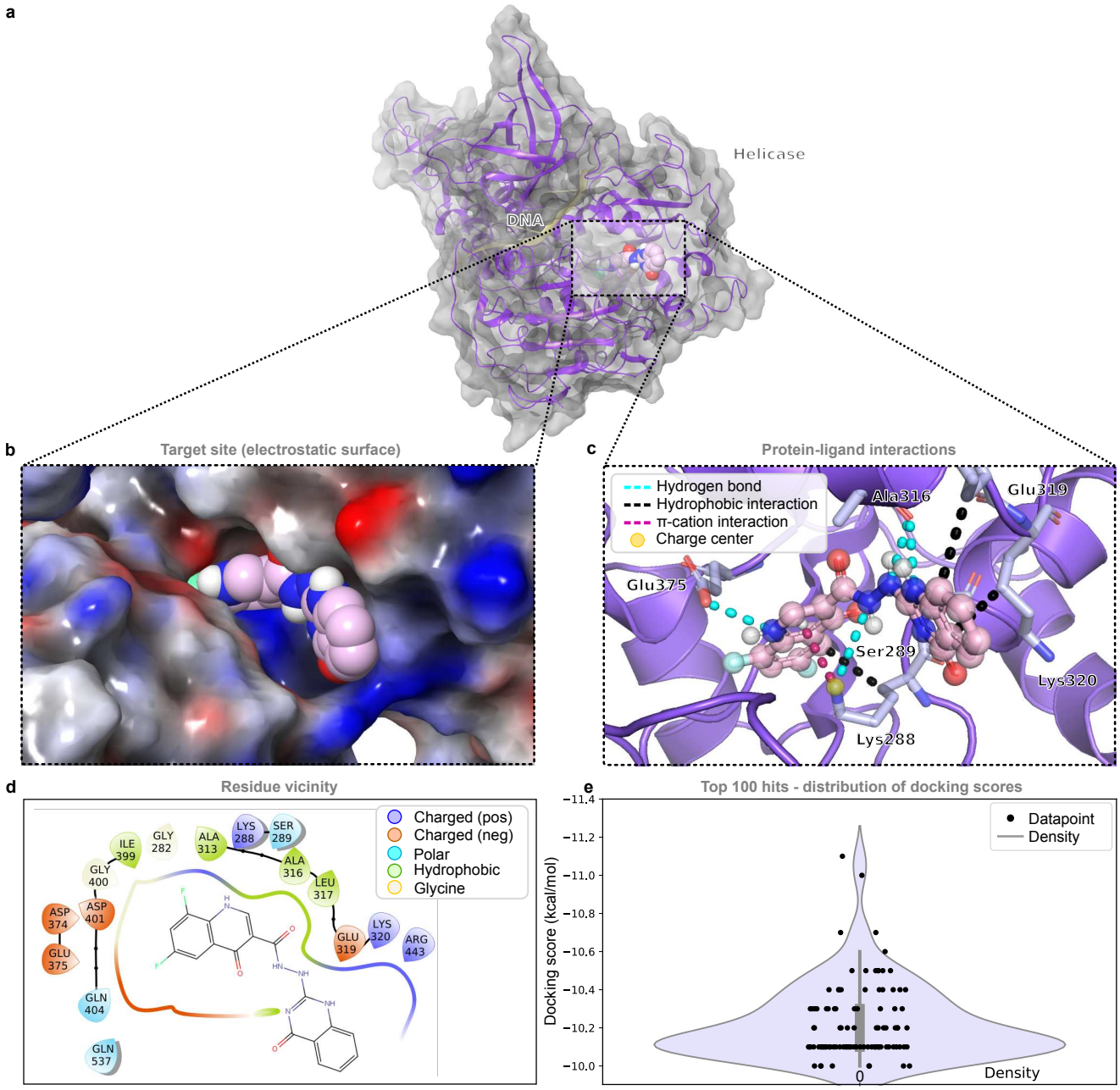

Fig. 18. The helicase (nsp13) and an example compound from the top 0.0001% of screened compounds bound at the enzymatic active site. a, The helicase (violet) bound to an example compound (light pink) at the enzymatic active site. A docked DNA strand is shown in light gold (Screen ID: 33). **b**, Electrostatic surface of the helicase to which an example compound (light pink) is bound. **c,** An overview of the interactions between the compound and the helicase structure. **d,** Residues within 4 Å of the inhibitor. **e,** Distribution of the docking scores of the top 100 virtual screening hits.

Using the same strategies that allowed crystallization of SARS-CoV M^{pro} (64), several groups determined the three-dimensional structure of SARS-CoV-2 M^{pro} in its apo form or bound to various inhibitors (65–71). These structures revealed that the N-terminus of SARS-CoV-2 M^{pro} contains two domains (domain I, residues 10-99; domain II, residues 100-184) that adopt a chymotrypsin-like fold, whereas the M^{pro} C-terminal Domain III (residues 201–303) is composed of five α-helices and is responsible for the intermolecular interactions critical for the dimerization. The protease active site of the picornavirus 3C-protease-like domain is located at the cleft formed between domains I and II and contains a Cys145-His41 catalytic dyad. A total of five protein segments comprised of residues 25-27 and 44-50 from domain I and residues 140-143, 165-168 and 188-190 from domain II form the walls of the active site (Supplementary Fig. 20a).

The M^{pro} active site seems to show significant conformational flexibility (72). Comparison of three apo structures and five structures in complex with inhibitors reveals changes in the conformation and position of the Gln189-containing loop and the short Ser46-containing α-helix (Supplementary Fig. 20b). Specifically, the cleft between domains I and II is narrower in the apo structures than in the structures of M^{pro} bound to inhibitors, consistent with an induced-fit or confor-

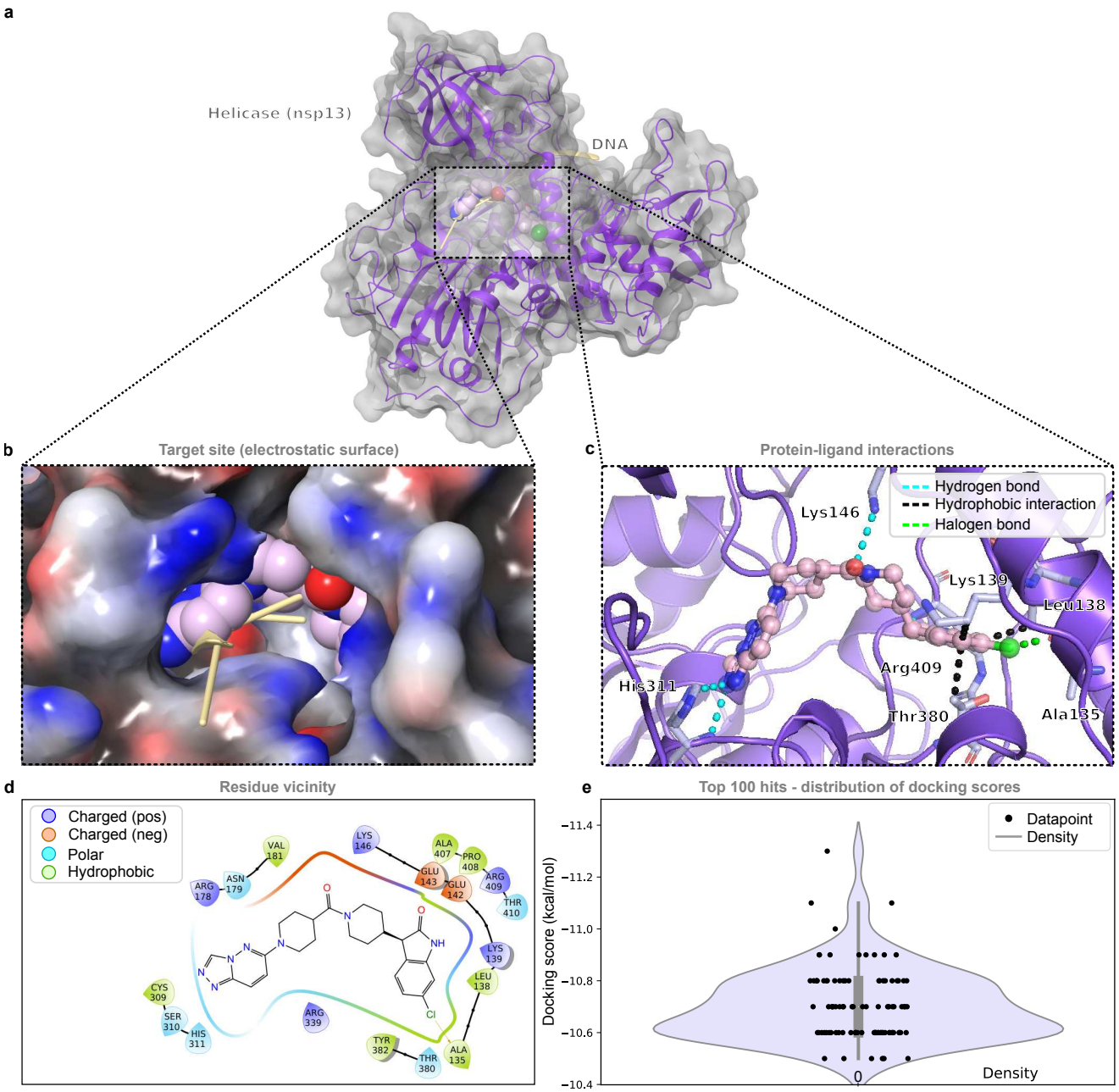

Fig. 19. The helicase (nsp13) and an example compound from the top 0.0001% of screened compounds bound at region 1 of the RNA-binding interface. **a**, The helicase (violet) bound to an example compound (light pink) at region 1 of the RNA-binding interface. A docked DNA strand is shown in light gold (Screen ID: 34). **b**, Electrostatic surface of the helicase to which an example compound (light pink) and a docked DNA strand (light gold) are bound. **c,** An overview of the interactions between the compound and the helicase structure. **d,** Residues within 4 Å of the inhibitor. **e,** Distribution of the docking scores of the top 100 virtual screening hits.

mational selection upon ligand binding.

Given the plasticity of the active site, we used two different conformations of M^{pro} for *in silico* screening (Screen IDs: 16 and 17) (Fig. 6, Supplementary Fig. 5). The first conformation corresponded to the structure of M^{pro} bound to the peptide-like inhibitor N3 (66). For this search, the protein model used was exactly the protein structure reported in the PDB file, after removal of all water molecules and bound ligands (Screen ID: 16) (Supplementary Fig. 20c). The second conformation corresponded to the structure of M^{pro} bound to inhibitor 11b, an inhibitor with peptide-like features (67). However, the model used for screening differed slightly from the conformation reported in the PDB file. In the crystal structure, the side chain of Met49 projects into the active site and thus would potentially interfere with compound docking. To avoid this, a different Met49 side chain rotamer was used that did not project as much into the active site. This change resulted in steric clashes with the side chain of Ser46, for which selection of a different side chain rotamer resolved these incompatibilities. Finally, a rotamer for Cys145 was selected that results in its side chain pointing towards the core of the protein. This rotamer was selected to allow the possible docking of compounds that could form covalent bonds with the Cys145 thiol group (Supplementary Fig. 20d).

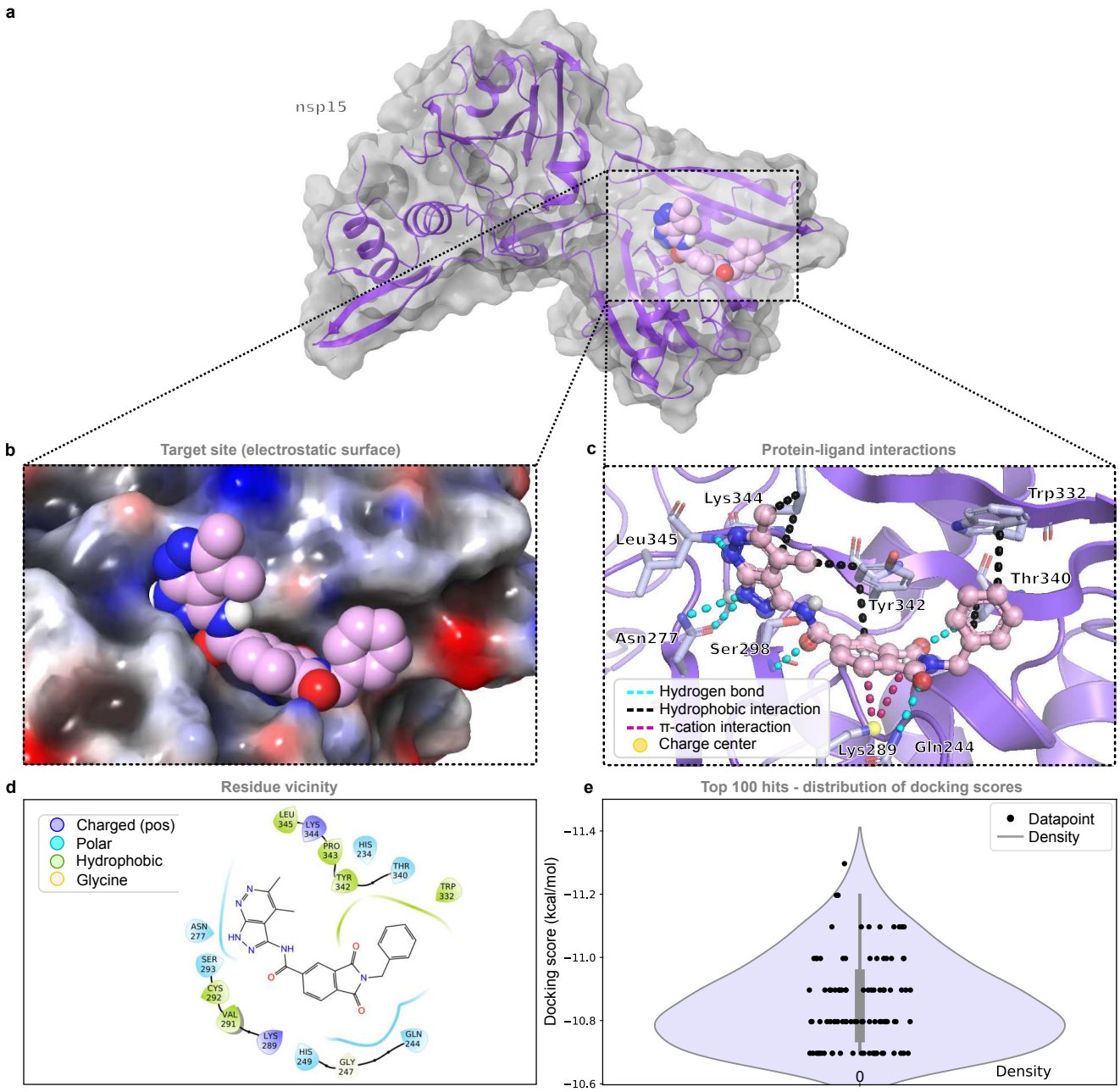

Fig. 20. nsp15 and an example compound from the top 0.0001% of screened compounds bound at the active site. a, nsp15 (violet) bound to an example compound (light pink) at the active site (Screen ID: 39. **b**, Electrostatic surface of nsp15 to which an example compound (light pink) is bound. **c,** An overview of the interactions between the compound and the nsp15 structure. **d,** Residues within 4 Å of the inhibitor. **e,** Distribution of the docking scores of the top 100 virtual screening hits.

The two conformations screened, hereafter referred to as M^{pro}-N3 (Screen ID: 16) and M^{pro}-11b* (Screen ID: 17), respectively, identified compounds that docked with high binding energies (Supplementary Fig. 20). Interestingly, the M^{pro}-11b* conformation resulted in predicted binding free energies that were approximately 0.5 kcal/mol lower than the binding free energies (docking scores) obtained from screening the M^{pro}-N3 conformation. Moreover, amongst the top 1000 hits identified by screening each of the two conformations (with the application of the standard filtering criteria of logP less than 6, molecular weight less than 600 daltons, and no reactive groups), only 12 hits overlapped. These results illustrate how screening closely related protein conformations can lead to the identification of a diverse set of docked compounds and this may be a generalizable strategy for *in silico* screening of proteins that exhibit conformational flexibility, such as SARS-CoV-2 M^{pro} (72).

Since the dimerization of M^{pro} is known to be essential for its catalytic activity (73–75), we also targeted the dimerization interface, which relies primarily on the α1 helix of the C-terminal domain (Screen ID: 18). Previous studies have shown that the inter-conversion of M^{pro} from monomer to dimer is mediated by an order-to-disorder transition of α5, and this aids domain swapping without exposure of the protein's hydrophobic core (76). Since the C-terminal region of M^{pro} is fully conserved between SARS-CoV and SARS-

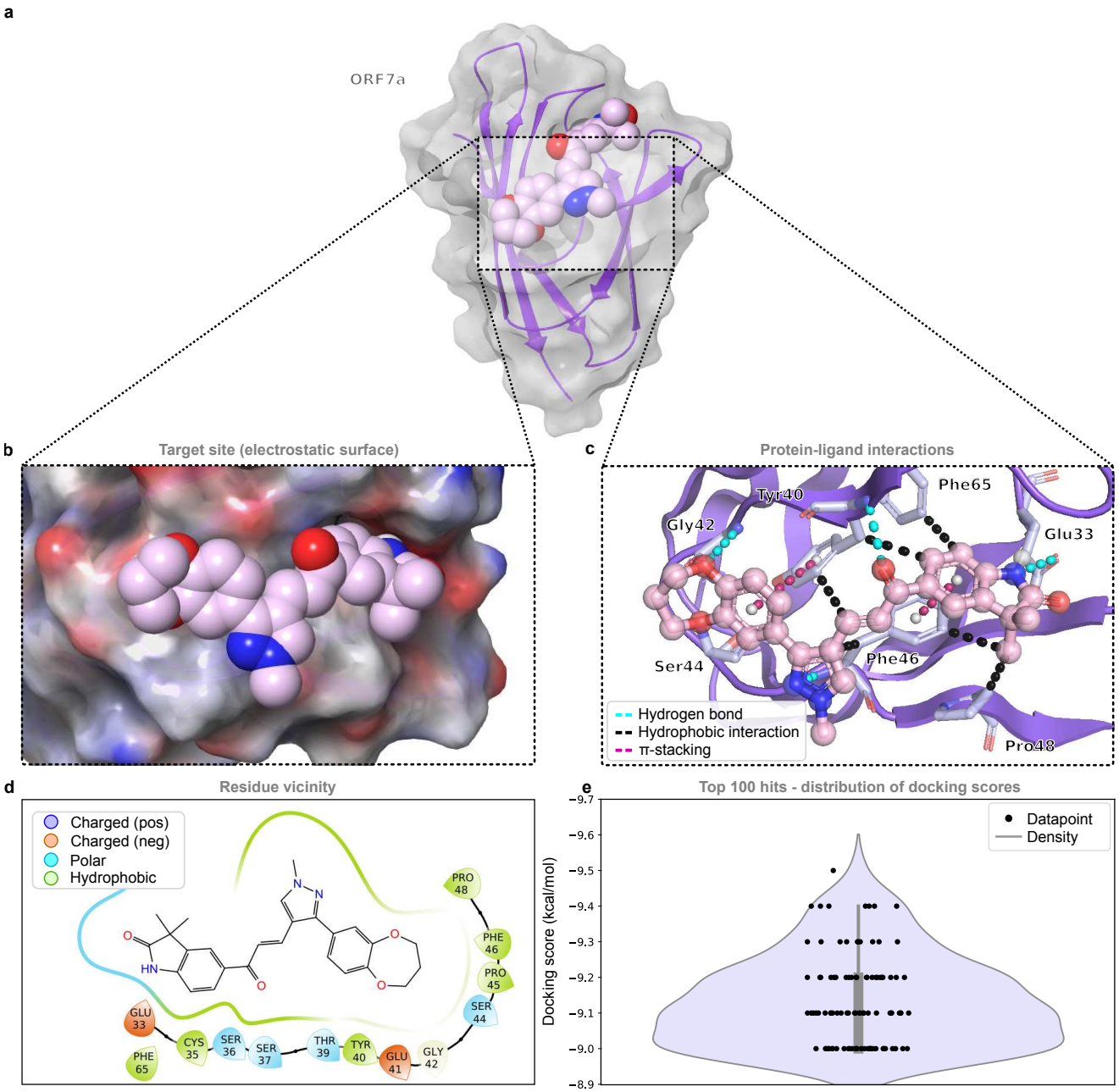

Fig. 21. ORF7a and an example compound from the top 0.0001% of screened compounds bound. a, ORF7a (violet) bound to an example compound (light pink) at the surface (Screen ID: 9). **b**, Electrostatic surface of ORF7a to which an example compound (light pink) is bound. **c,** An overview of the interactions between the compound and the ORF7a structure. **d,** Residues within 4 Å of the inhibitor. **e,** Distribution of the docking scores of the top 100 virtual screening hits.

CoV-2, we used an NMR ensemble of the SARS-CoV M^{pro} C-terminal domain (PDB: 2LIZ) to build a hybrid model of a disordered C-terminus. We subsequently used this model and screened against the attachment site of the α5 helix (Screen ID: 19). Potential binders at this position would be expected to trap the protein in its inactive monomeric form.

PL^{pro}. SARS-CoV-2 nsp3 is a multi-domain protein containing an N-terminal ubiquitin-like fold, a glutamic-acid-rich acidic domain, a phosphatase domain, a SARS unique domain (SUD), a catalytically active PL^{pro} domain, a marker domain (G2M), and two transmembrane domains (77). In addition to the protease activity, PL^{pro} also possesses deubiquitination and de-ISGylation activity that aids in the disruption of the interferon regulatory factor 3 (IRF3) pathway and host innate immune responses (78). The central α-helical "thumb" domain of PL^{pro} harbors the catalytic Cys112, while the C-terminal domain is mostly β-sheet and includes the "palm" domain, which harbors the other two residues of the catalytic triad, His275 and Asp287, and the "fingers", which coordinate a Zn^{2+} ion (PDB: 6W9C). PL^{pro} also has two blocking loops (BL1 and BL2) targeting which will prevent the substrate from entering the active site.

Comparison of the crystal structures of PL^{pro} in its unbound and peptide inhibitor-bound states (PDB: 6w9c and 6wx4, respectively) revealed conformational changes in both

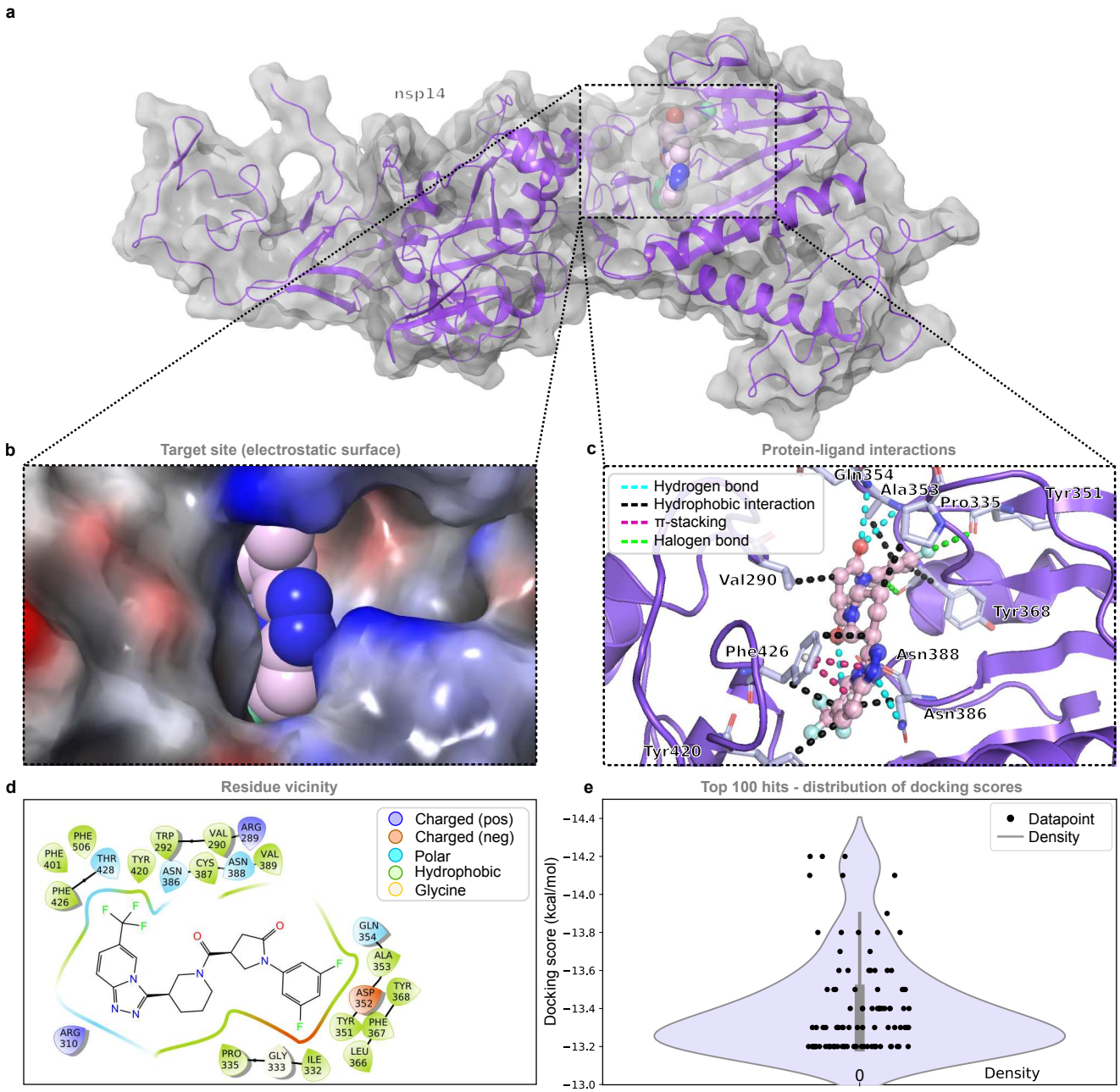

Fig. 22. nsp14 and an example compound from the top 0.0001% of screened compounds bound at the active site of the N7 methyltransferase domain. a, nsp14 (violet) bound to a example compound (light pink) at the active site of the N7 methyltransferase domain (Screen ID: 38). **b**, Electrostatic surface of nsp14 to which an example compound (light pink) is bound. **c,** An overview of the interactions between the compound and the nsp14 structure. **d,** Residues within 4 Å of the inhibitor. **e,** Distribution of the docking scores of the top 100 virtual screening hits.

the "finger" domain as well as the BL2 loop. We therefore targeted the active site in unliganded and the bound states, which correspond to the open and closed conformations the active site (Screen IDs: 12 and 15 respectively) Fig. 7(Fig. 9).In addition to this, we also targeted the accessory cleft leading to the active site which would prevent the substrate access to the active site (Screen ID: 13).(Supplementary Fig. 6). In addition to the three sites that are described here, the ubiquitin contact site in Pl^{pro} which is critical for the deubiquitination and deISGylation functions was also targeted, and is described in detail elsewhere in this manuscript.

Replication complex: nsp7, 8 and 12. nsp12, 7, and 8 form a minimal 160-kDa complex capable of nucleotide polymerization with additional nsps playing important roles in RNA modification (79, 80). nsp12 encodes for the RNA-dependent RNA polymerase (RdRp) while nsp7 and nsp8 are cofactors, which may form a hexadecameric supercomplex (81). When compared to the SARS-CoV replicase, key functional residues are found to be fully conserved in SARS-CoV-2; however, there are substitutions on the surface of the complex. The RNA polymerase domain of nsp12 has an N-terminal nidovirus-unique N-terminal extension (NiRAN) in addition to the "finger", "palm", and "thumb" domains com-

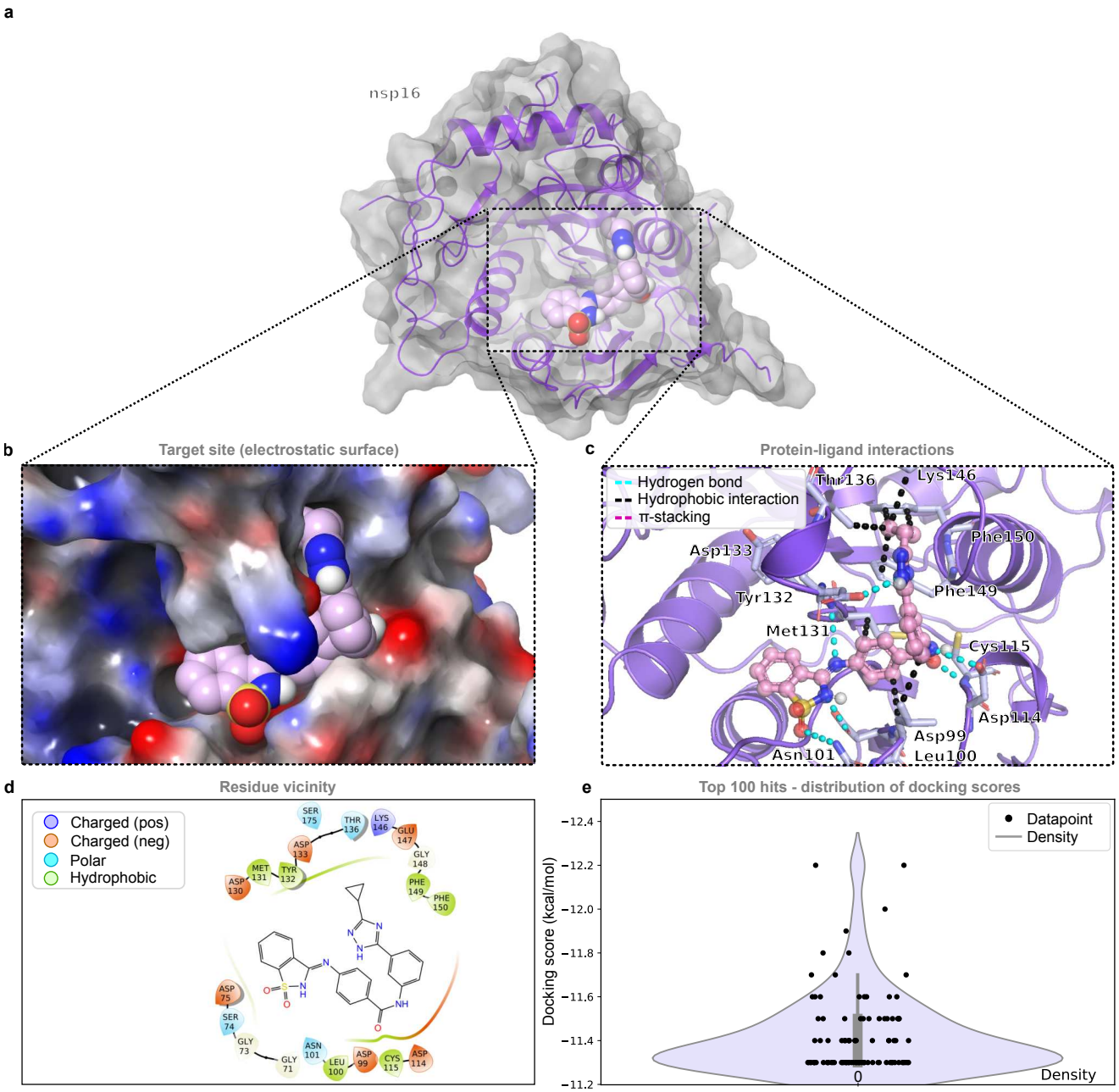

Fig. 23. nsp16 and an example compound from the top 0.0001% of screened compounds bound at the active site. a, nsp16 (violet) bound to an example compound (light pink) at the active site (Screen ID: 40). **b**, Electrostatic surface of nsp16 to which an example compound (light pink) is bound. **c,** An overview of the interactions between the compound and the nsp16 structure. **d,** Residues within 4 Å of the inhibitor. **e,** Distribution of the docking scores of the top 100 virtual screening hits.

mon to polymerases (82) (Figs. 15, 16, 17, Supplementary Figs. 12, 13). The seven catalytic motifs found in other known viral polymerases, and which are involved in template and nucleotide binding and catalysis, are also well conserved in the SARS-CoV-2 polymerase (82, 83).

The SARS-CoV-2 RNA synthesis machinery is governed largely by a number of protein-protein interactions, and this provides us with an opportunity to target these interfaces using small molecules. The C-terminal head domain of nsp8 wraps around the nsp7 helical bundle, forming a hexadecameric complex. nsp8 has been suggested to possess RdRp activity of its own, and produce the primers utilized by the primer-dependent nsp12 RdRp. This nsp12 activity requires the formation of a large oligomeric complex that brings active site residues into proximity with each other (84, 85). A previously determined crystal structure (PDB: 2AHM) shows nsp7 and nsp8 capable of interacting in at least two ways: i) residues on the C-terminal end of the nsp8 shaft form a hydrophobic core with residues in helix 1 of nsp7; and ii) helix 1 and the short helix of nsp7 interact with one of the helices of the nsp8 head domain (Fig. 12). The heterodimer formed by nsp7-nsp8 interaction binds to nsp12 on the polymerase "thumb" domain facing the NTP entry channel, thus placing the nsp12 polymerase "index finger" loop between nsp7-nsp8 and the polymerase "thumb" domain (Fig. 13). In addition to this interaction, a second nsp8 monomer binds to the nsp12

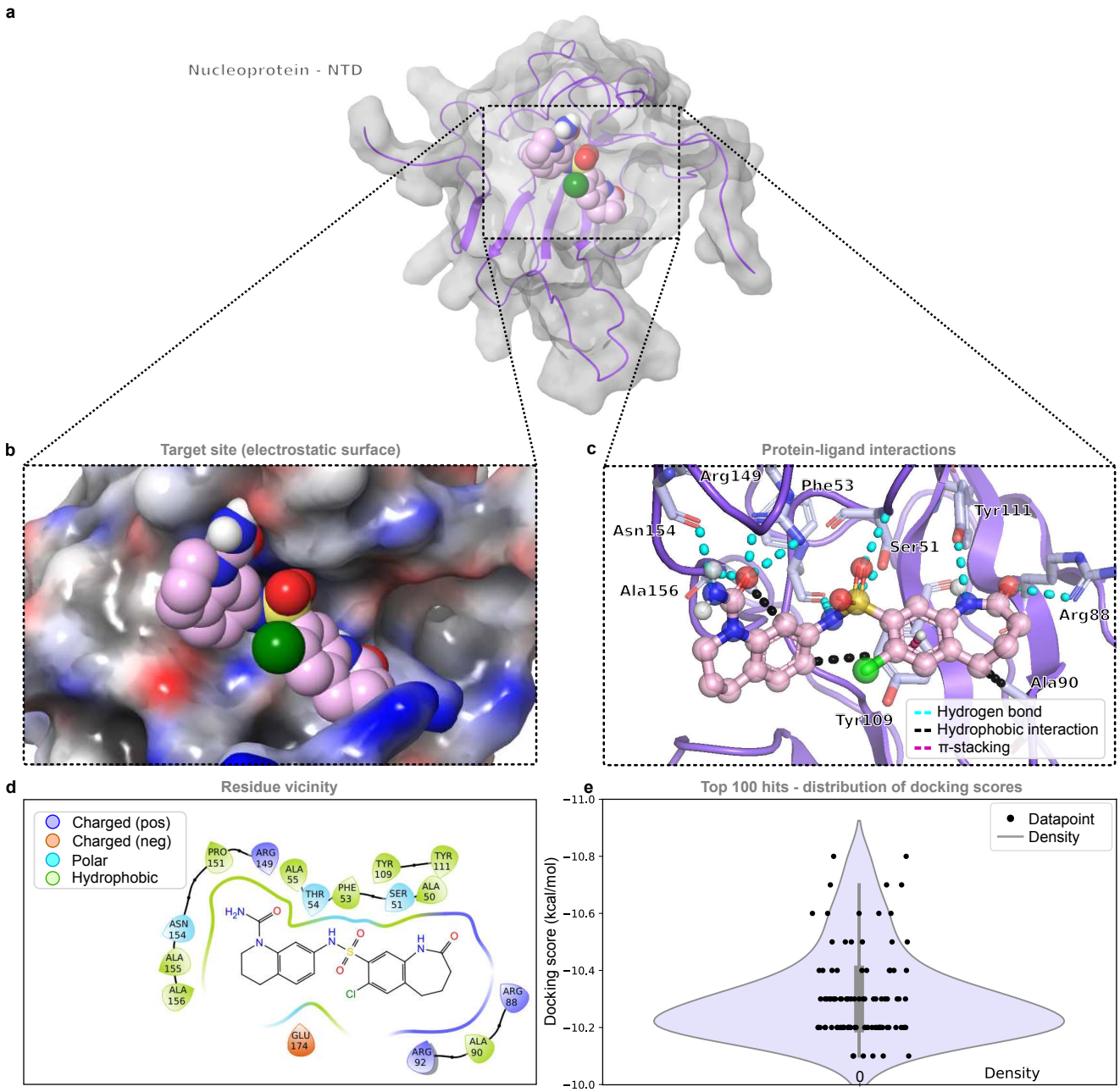

Fig. 24. N-terminal domain of the nucleoprotein and an example compound from the top 0.0001% of screened compounds bound at the RNA-binding interface. **a**, The N-terminal domain (NTD) of nucleoprotein (violet) bound to an example compound (light pink) at the RNA binding interface (Screen ID: 41). **b**, Electrostatic surface of nucleoprotein to which an example compound (light pink) is bound. **c,** An overview of the interactions between the compound and the NTD structure. **d,** Residues within 4 Å of the inhibitor. **e,** Distribution of the docking scores of the top 100 virtual screening hits.

interface domain in the vicinity of Leu117. We targeted the nsp12 binding interface on nsp8 (Screen ID: 22) (Fig. 9), the nsp7 binding interface on nsp8 (Screen ID: 21) (Fig. 13), the entire alpha-helical surface of nsp7 which includes the nsp8 and nsp12 binding interfaces (Screen ID: 20) (Fig. 12), the nsp8 binding interface on nsp12 (Screen ID: 31) (Fig. 15), two sites in the RNA binding region on nsp12 (Screen IDs: 28 and 29) (Fig. 16, Supplementary Fig. 12), and the nsp7 binding interface on nsp12 (Screen ID: 32) (Supplementary Fig. 13).

The nsp7 binding interface on nsp12 is relatively shallow, and the RNA binding sites are as well, but to a lesser degree. One of the principal challenges of targeting an RNA binding interface is the strong avidity effect, frequently in the nanomolar range, that restricts the ability of ligands from displacing RNA. Moreover, biological processes involving RNA-protein interactions are also known to often be dynamics-dependent. The average binding free energies of the top 100 hits from the screens of the RNA binding interfaces of nsp12 (Screen IDs: 28 and 29) were -11.8 and -10.2 kcal/mol, respectively.

nsp13: helicase. nsp13, which is one of the few proteins that is fully conserved in SARS-CoV and SARS-CoV-2, has known activity as an RNA helicase, NTPase, dNTPase, RT-

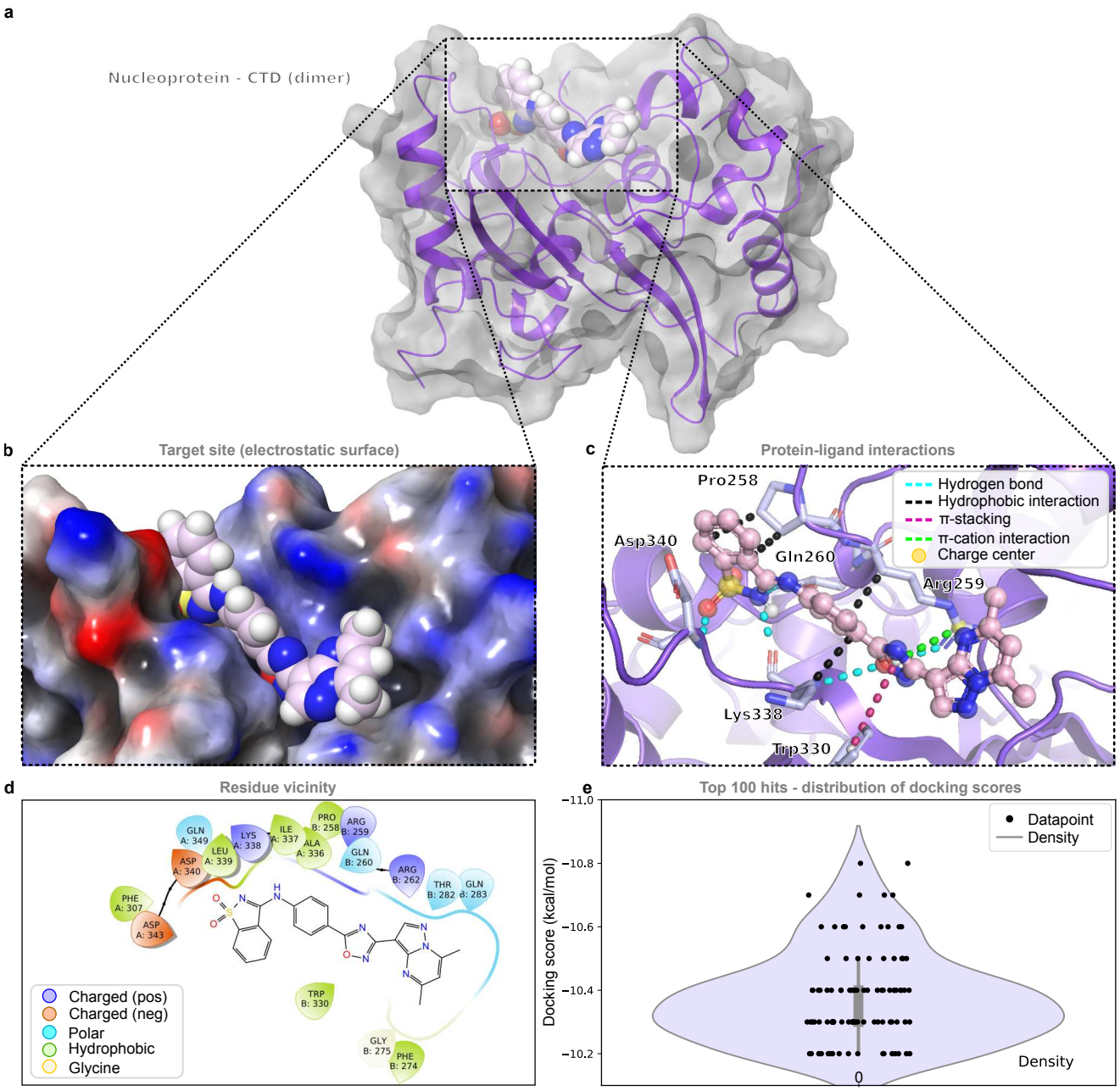

Fig. 25. C-terminal domain of the nucleoprotein and an example compound from the top 0.0001% of screened compounds bound at the oligomerization interface. **a**, The C-terminal domain (CTD) dimer of nucleoprotein (violet) bound to an example compound (light pink) at the oligomerization interface Screen ID: 45). **b**, Electrostatic surface of the CTD dimer of nucleoprotein to which an example compound (light pink) is bound. **c,** An overview of the interactions between the compound and the CTD structure. **d,** Residues within 4 Å of the inhibitor. **e,** Distribution of the docking scores of the top 100 virtual screening hits.

Pase, and DNA helicase (86). It is also known to interact with nsp12 (87). The helicase is 603 amino acids long, contains an N-terminal zinc binding domain, a stalk domain, RecA-like domains 1A, 1B and 2A, and forms a triangular shaped structure (Fig. 18) (88). There are multiple potential sites that could be targeted on this protein. We therefore chose to target the active (ATP binding) site (Screen ID: 33) (Fig. 18), and two sites on the RNA interaction interface (Screen IDs: 34 and 35) (Supplementary Figs. 19, 19).

Even though we used a homology model, this model is expected to be reliable because the helicase of SARS-CoV-2 shares 99.8% sequence identity with the template used (PDB:6JYT, structure of SARS-CoV nsp13). However there are currently no helicase structures available for CoVs with nucleic acid bound, and this uncertainty about the residues actually participating in RNA binding is a confounding factor while screening against this target. According to previously reported hydrogen-deuterium exchange experiments, the 1A and 2A domains undergo a series of conformational changes during nucleotide binding and ATP hydrolysis (88), and this inherent flexibility could impact the plasticity of the screened binding pockets and therefore the reliability of the model screened. Our two virtual screens for the RNA binding interface (Screen IDs: 34 and 35) resulted in top 100 hits

with an average binding free energy of -10.225 and -10.704 kcal/mol, respectively, and the screen for the active site inhibitors (Screen ID: 33) resulted in an average binding energy of -10.224 kcal/mol.

nsp9: ssRNA binding protein. nsp9 is known to co-localize with nsp7, nsp8 and nsp10 within the replication complex and is presumed to play a role in RNA replication (89). A study on SARS-CoV nsp9 has shown that nsp9 is an ssRNA-binding protein indispensable for viral RNA replication in mouse models (90). There are several high resolution crystal structures available for nsp9 (91, 92), including those of the protein from SARS-CoV-2 (PDB: 6W4B, 6W9Q). Since dimerization has been found to be essential for viral replication (93), we chose to target the dimerization interface as a method of inhibiting viral replication.

nsp9 contains seven antiparallel β-strands and an α-helix (Supplementary Fig. 8). The dimer interface is formed mainly by the parallel association of the C-terminal α-helices (Fig. 11), and this surface, in particular the GXXXG motif, was targeted using VirtualFlow (Screen ID: 23). We also targeted a shallow cavity around Phe75 that partially overlaps with the first targeted site centered on the α-helix (Screen ID: 24). This second site interacts with the NTD of the other nsp9 monomer, and is more concave in shape than the first site, making it more pocket-like. The average docking scores of the top 100 compounds of the second targeted site is -9.2 kcal/mol, making it slightly stronger than the first site with an average of -9.1 kcal/mol (see also Supplementary Fig. 21).

The C-terminal α-helix, which is responsible for dimerization has a high hydrophobic amino acid content, and the dimer is mainly facilitated by hydrophobic interactions. Targeting this region may lead to hits that are hydrophobic and interacting in a non-specific manner, something that would need to be addressed during follow-up experimental validation. Targeting the dimerization interface is made more difficult because it is not clear if the monomer alone adopts a different conformational state compared to the structure in dimeric form, which was targeted here. The interface is relatively hydrophobic and lacks deep pockets, making it challenging to find specific tight binding compounds.

Disrupting the ability of coronaviruses to evade or subvert host defenses

Initial studies on SARS-CoV-2 in *ex-vivo* systems and on clinical samples suggest that infection produces lower levels of interferon and differential cytokine/chemokine profiles, even when compared to the closely related SARS-CoV (94, 95). This suggests that SARS-CoV-2 is able to escape, at least initial, host immune surveillance, and when combined with robust early replication (95, 96), allows the virus to establish a strong foothold in the host, forcing the immune system play catch-up. In light of this, targeting SARS-CoV-2 immune evasion factors, particularly in combination with other inhibitors, could have clinical benefits.

Coronaviruses have an RNA genome and during its life cycle produce RNA species normally absent in the host cell's cytoplasm, such as dsRNA and RNA with a 5'-triphosphate. Sensing of RNA intermediates such as these is one way in which the host cell can detect viral infection and initiate an antiviral immune program (97). An effective way in which coronaviruses avoid recognition by these intrinsic immune sensors is by using methyl transferases to add a cap-structure to viral RNA in order to mimic the cell's own mRNA (98). Coronaviruses also encode an endoribonuclease, which prevents the accumulation of viral RNA that could activate dsRNA sensors in the cell (99). The deubiquitination and deISGylation activities of PL^{pro} further interfere with the host antiviral response by antagonizing the induction of type I interferon (IFN) pathways (100). With the goal of preventing coronavirus from being able to evade or subvert host defense mechanisms, we targeted the following four proteins: a) the guanine-N7 methyltransferase/ExoN (nsp10-14) complex, b) the 2'-O-ribose methyltransferase (nsp16), c) the uridylate-specific endoribonuclease (NendoU/nsp15), and d) the deubiquitination and deISGylation activities of PL^{pro}.

Guanine-N7 methyltransferase/ExoN (nsp10-14 complex). nsp14 is critical for viral replication and transcription, as it plays dual roles in proofreading and mRNA capping (101–103). Disruption of nsp14 exonuclease activity (104) has been shown to result in increased sensitivity of the virus to Ribavirin (RBV) and 5-fluorouracil (5-FU) (81), demonstrating the importance of this 3'-mismatched dsRNA excision activity (105). The ExoN activity relies on heterodimer formation of nsp14 with nsp10, and disruption of this interaction has been demonstrated to result in lowered replication fidelity (106). Unlike many other RNA viruses, coronaviruses have a low mutation rate by virtue of this ExoN activity, which supported the expansion of coronavirus genomes (107) and is directly linked to its virulence (108). Previous work with SARS-CoV has suggested that the limited efficacy of RBV *in vivo* may be due to excision by this ExoN activity (109), and work in MHV has shown that a mutant strain lacking ExoN activity was more sensitive to Remdesivir (110). These data suggest that use of a nucleoside analogue might be more effective if combined with an ExoN inhibitor (107). nsp14 also functions as a SAM-dependent guanine-N7 methyltrasferase (N7-MTase) (103). Mutation studies in a replicon system have shown that this N7-MTase activity is critical for viral replication and transcription (103). This activity is used to add a cap 0 structure at the 5' end of viral mRNA, thus mimicking a defining structural feature of host mRNAs and assisting translation (111) as well as in in evading host defenses (112). For nsp14 we targeted three sites, i) targeted the active site of the ExoN domain (Screen ID: 37) (Fig. 22) ii) the active site on the methyltransferase domain (Screen ID: 38)16 and iii) the PPI interface with nsp10 (Screen ID: 36)15.

In the bimodular nsp14, the N-terminal domain of nsp14 up to Lys288 interacts solely with nsp10 and forms the ExoN domain, whereas the C-terminal domain possess the N7-MTase activity. The ExoN domain is comprised of a twisted parallel β-sheet made up of five β-strands and are bordered by α-helices on both the sides (Fig. 22, Supplementary Figs.

15, 16) (113). The N7-MTase domain of nsp14 is made up of five β-strands, and the ligand binding pocket is situated between the β1 and β2 sheets (113). We screened against three distinct sites on nsp14: the nsp10 binding interface (Screen ID: 36)(Supplementary Fig. 15), the active site of the ExoN domain (Screen ID: 37) (Supplementary Fig. 16), and the active site of the N7-MTase domain (Screen ID: 38) (Fig. 10). As there are not yet any experimental structures available for the SARS-CoV-2 nsp10-14 complex, we used a high confidence homology model constructed from the SARS-CoV ExoN/N7-MTase structure (PDB:5C8U) for our docking experiments. It should be noted that while nsp10 is 97% conserved between the two viruses, nsp14 is only 73% identical.

The nsp10 interaction site on nsp14 has a shallow pocket that is fairly hydrophobic, resulting in relatively high docking scores for the top scoring compounds. However, due to the sparsity of polar atoms at this site, it is challenging to find compounds that form sufficient electrostatic interactions to provide the compounds with specificity. By comparison, the ExoN active site is more polar in nature, and forms a wide shallow pocket. This should lead to a larger proportion of the hits that bind with high specificity, but the absence of a deep pocket would affect the binding affinity. The third target site, the active site of the N7-MTase domain of nsp14, also harbors a relatively large hydrophobic cavity, but with with polar elements. The suitability of each of these nsp14 pockets to accommodate ligands is reflected in their mean docking scores (for the top 100 hits for each target site): -10.4 kcal/mol for the PPI site, -13.4 kcal/mol for the N7-MTase active site, and -9.8 kcal/mol for the ExoN active site.

2'-O-ribose methyltransferase (nsp16). RNA cap modifications are known to play a role in the host cell's identification of self-RNA. For example, foreign RNA which lacks 2'-O methylation is inhibited by IFIT1 (114). Pathogenic viruses such as coronaviruses that replicate in the cytoplasm have developed tactics to escape recognition by the host innate immune system. One such coronaviral mechanism is 2'-O-methyl capping of viral RNA by the nsp10-nsp16 complex. nsp16 is an m^7GpppA-specific, SAM-dependent, 2'-O-MTase that must form a complex with nsp10 for its function (115, 116). We therefore targeted the nsp10 binding interface on nsp16 (Supplementary Fig. 17).

nsp16 has a catalytic core comprised of a β-sheet flanked by eleven α-helices (Fig. 23, Supplementary Fig. 17). nsp10 has a small antiparallel β-sheet sandwiched between several α-helices and a large loop. The interaction surface of nsp10 with nsp16 is a mixture of hydrophobic, polar, and positively charged, and helps in the stabilization of the SAM binding site (PDB:6W75). However, since the interface is relatively flat and polar, it is rather challenging to find small molecules that bind with sufficient strength.

Earlier structural studies showed that stabilization of the SAM-binding pocket by the nsp10-16 interaction also expands the RNA-binding pocket of nsp16 (117), and short peptides derived from the interaction interface have been shown to inhibit 2'-O-methyltransferase activity of the nsp10-16 complex (118). Therefore, in addition to targeting the interaction interface of nsp10 and nsp16 (Screen ID: 40), we also targeted the putative SAM binding site (Screen ID: 41, Supplementary Fig. 17). SAM binding has been shown to be essential for both nsp10-16 complex formation as well its catalytic function in another highly pathogenic coronavirus, MERS-CoV (119).

Uridylate-specific endoribonuclease. nsp15 is a uridylate-specific endoribonuclease (NendoU) carrying a C-terminal catalytic EndoU domain that has been described as having various roles in immune evasion in different coronviruses. A recent study in mouse hepatitis virus (MHV), a murine coronavirus, showed that nsp15 was critical for evasion from host dsRNA sensors in macrophages (120), and in porcine deltacoronavirus, nsp15 was found to inhibit IFN-β production (121). The SARS-CoV-2 nsp15 monomer is composed of three distinct domains: a) an N-terminal domain containing an antiparallel β-sheet and two α-helices, b) a central domain composed of 10 β-strands and three short helices , and c) a C-terminal NendoU domain composed of two antiparallel β-sheets and five α-helices (PDB:6VWW) (122). The SARS-CoV-2 nsp15 monomer is capable of forming dimeric, trimeric, and double-ring hexameric assemblies. It has been shown that the hexameric form is essential for enzymatic activity and that the hexamer is stabilized by interactions of the N-terminal oligomerization domain (123). The NendoU active site itself is located in a groove between the two β-sheets, and conserved, crucial residues have been previously identified: His235, His250, Lys290, Thr341, Tyr343, and Ser294. With the aim of disrupting the endoribonuclease activity of nsp15, the active site was targeted in an *in silico* screen (Screen ID: 39, Fig. 20).

Deubiquitination and deISGylation activities of PL^{pro}. PL^{pro} (nsp3) cleaves at a consensus cleavage motif, LXGG, which is also the consensus sequence recognized by cellular deubiquitinating enzymes (DUBs). Coronaviruses attenuate the host anti-viral response by deubiquinating key components of the interferon-mediated immune response. While PL^{pro} uses its catalytic site for its deubiquitination function, ubiquitin itself makes contacts with the "palm" and "fingers" regions of PL^{pro} (124). This protein-protein interface is well conserved in SARS-CoV-2 and could be targeted in order to inhibit the deubiquitination function of nsp3. SARS-CoV has also been shown to possess deISGylation activity, in which ISG-15, a protein modifier consisting of two tandem ubiquitin-like domains involved in modulating the innate immune response, is cleaved (125). We therefore targeted the proximal 'S1' Ub contact site (S1Ub) of the "palm" of nsp3 (Fig. 8), inhibition of which could effectively block both the deubiquitination as well as deISGylation activities of PL^{pro} (Screen ID: 14). The binding interface is moderately hydrophobic and concave, making it an attractive drug target.

nsp3 macrodomain. The macrodomain, sometimes also called the X domain, is a highly conserved region of ~180 amino acids that binds to ADP ribose (126) and which has

been shown to be dispensable in RNA replication, at least in the context of an RNA replicon (127). However, it has been shown to have possible roles in evading host innate immune response (128, 129). Viral macrodomains are known to have two major enzymatic activities: i) ADP-ribose-1" phosphatase activity where the phosphate is removed from ADP-ribose-1" phosophate, and ii) ADP-ribose hydrolase activity where ADP ribose is removed from mono- or poly-ADP-ribosylated proteins (130).

Previous biochemical studies showed that the nsp3 macrodomain is responsible for processing of ADP-ribose-1"-phosphate, which is a byproduct of pre-tRNA splicing (131, 132). This phosphatase activity has been found to be specific for ADP-ribose-1"-phosphate, however the turnover was found to be very low (133, 134) with a kcat of 1.7 to 20 min^{-1}), making it unlikely that this activity has a strong direct effect on viral virulence.

ADP-ribosylation is a critical post-translational modification catalyzed mainly by poly (ADP-ribose) polymerases (PARPs) in which ADP-ribose is added to a protein (135). Several PARPs are known to be interferon-stimulated genes (ISGs), and some PARPS have been shown to have antiviral activities. Studies in SARS-CoV and MERS-CoV have shown that these viruses were less virulent in the absence of the macrodomain and that this directly associated with changes in pro-inflammatory cytokine expression (136, 137). Additional studies in HCoV-299E and SARS-CoV suggested that the nsp3 macrodomain may mediate the resistance to antiviral interferon responses (128). Mutation of the macrodomain in SARS-CoV also induced a strong interferon and inflammatory cytokine response in the lungs of infected mice (136). However, the exact mechanism linking the hydrolase/phosphatase activity of nsp3 and the observed cytokine production is unknown. The fact that a) the macrodomain participates in reversing antiviral ADP ribosylation (130, 138), and b) mutation of a highly conserved asparagine residue abolishes phosphatase and hydrolase activites and mitigates viral virulence (136, 139), suggests that targeting the ADP-ribose binding pocket could be an effective therapeutic strategy, particularly in combination with other targets. We observed two different conformations for the active site in the same X-ray structure, which indicated protein dynamics that could affect the ability of the docking to accurately recapitulate the solution-state structure. We therefore targeted both conformations of the active site of the macrodomain: one in which the active site is more closed (Screen ID: 11; Fig. 10), and a second conformation in which the active site is more open (Screen ID: 12; Supplementary Fig. 7). It is also important to note that the active site itself is very hydrophobic, which increases the risk that the resulting hits could bind non-specifically to membranes and hydrophobic pockets in other proteins, and this should be accounted for in any follow-up screening.

ORF7a. ORF7a is a non-essential accessory protein with a transmembrane helix at the C-terminus that is known to localize to the ER, Golgi, and cell surface (140, 141). The assembly of ORF7a into viral particles suggests that the protein is important in the viral replication cycle, and that it might have a function early on in the infection (142). In SARS-CoV, ORF7a is known to interact with a 'host restriction factor', bone marrow stromal antigen 2 (BST-2) (141), which inhibits viral replication by preventing virus budding from the plasma membrane (143). ORF7a, which otherwise localizes to the Golgi, has also been shown to localize to the ER when co-expressed with BST-2. Moreover, ORF7a interferes with the glycosylation of BST-2, which is essential for its tethering/restriction function (141). There are also indications that ORF7a may play a role in virus-induced apoptosis (144); however, further studies are needed to understand the mechanism of this role.

Structurally, ORF7a has an N-terminal signal peptide, an 80 amino-acid long luminal domain, a transmembrane domain, and a short C-terminal cytoplasmic tail (140). In the recent experimental structure of the SARS-COV-2 ORF7a (PDB:6W37, (145)), the luminal domain displays structural characteristics similar to that of previously published ORF7a structures, and is composed of a seven-stranded β-sandwich (Fig. 21) with topological similarities to the Ig super family. Interestingly, a very recent genomic analysis of a sample picked up during sentinel surveillance in the state of Arizona in the USA revealed a 27 amino-acid in-frame deletion in ORF7a, in a region pertaining to the N-terminal signal peptide (146). The functional consequences of this deletion, however, are not known. Since the molecular mechanism of the ORF7a interaction is largely unknown, we pursued a blind docking strategy for this protein that covers the complete protein structure (Screen ID: 9) (Fig. 21). Interestingly, almost all top scoring compounds bound at a shallow cavity around Phe46, while a few bound to the opposite side near Leu31.

During an experimental validation phase, it will need to be verified whether these hits can inhibit the interaction of ORF7a with small glutamine-rich tetratricopeptide repeat-containing protein (SGT)(147) or lymphocyte associated antigen 1 (LFA-1) (148), both of which are thought to play a role in virus-host interactions and host cell-cycle modulation. The presence of ORF7a on the viral surface means that LFA-1 could possibly be a viral attachment factor in leucocytes (142, 148); however there is currently insufficient data available about the possible residues and the structural dynamics that would be involved in this interaction. Moreover, the rather flat surface of ORF7a devoid of pockets or clefts make it challenging for finding small molecules with selective and potent binding.

Disrupting the viral assembly and packaging

As the viral lifecycle progresses, the structural proteins (S, E, M) are also expressed. These structural proteins are initially inserted into the endoplasmic reticulum (ER), but transition to the ER-Golgi intermediate compartment (ERGIC) where they aid the formation of mature virions (149). Nucleocapsid protein (N) forms large oligomeric complexes with the replicated viral genome. The resulting ribonucleoprotein (RNP) complexes associate with M, facilitating packaging of

the genome into a complete virion assembly. Since there is very little structural information available about M and E, our efforts to find compounds that can disrupt the viral assembly and packaging are centered on the nucleocapsid protein.

Nucleocapsid protein. The nucleocapsidprotein (N) packages the viral RNA into a helically ordered RNP (150) and plays a critical role in virion assembly by interacting with M. N is also known to play key roles in the regulation of viral RNA synthesis and modification of the host cell metabolism (151). The structure of N consists of an N-terminal RNA-binding domain (NTD, Fig. 24, Supplementary Fig. 18), an intrinsically disordered SR-rich linker, and a C-terminal dimerization domain (CTD, Fig. 25, Supplementary Fig. 19). The published crystal structure of the RNA-binding domain reveals a β-sheet core sandwiched between two loops. The β-sheet core has five antiparallel β-strands plus a short helix, and a longer β-hairpin between strands β2 and β5 (PDB:6M3M (152). The central β-strands of the β-sheet core contain a purine/pyramidine monophosphate binding site, and this ribonucleotide binding mechanism is essential for virulence, making it an attractive drug docking site (153). The NTD is also expected to interact with the CTD during RNA packaging. We have therefore targeted two minimally overlapping regions of the NTD, which together cover the entire surface of the NTD (screen IDs: 42 and 43) (Fig. 24, Supplementary Fig. 18). The first site includes the ribonucleotide-binding site reported in (153).

The CTD of N aids dimerization of the protein as well as RNA binding. The monomer consists of eight α-helices and a β-hairpin. The dimerization interface itself is composed of three helices (α5, α6 and α7) and one β-hairpin from each monomer, and involves a combination of hydrogen bonds and hydrophobic interactions, which result in a very stable dimer (PDB:6WJI). That the C-terminal domain has also been found to bind RNA (154) points to the critical role of this domain in the overall helical packaging of the viral genome (155). We targeted the dimerization interface of the CTD by removing one monomer from the crystallized dimer structure (Screen ID: 44) (Supplementary Fig. 19), and also screened the dimerization interface via a blind docking procedure against the entire dimer surface (screen ID: 45) (Fig. 25). The goal of these screens was to identify a small molecule that will bind to the monomer at the dimer interface and disrupt the formation of the nucleocapsid. However, the structure of the monomer alone has not been solved and given the extent of the interaction at the dimer interface, we anticipate considerable dynamics in the monomer. Therefore the structure extracted from the dimer may not adequately describe the monomer structure yielding imperfect hits. The other challenge of this target is that each virion has ~65 spike trimers and with a ratio of S trimer to N of 1:4 (156, 157), this amounts to ~260 monomers or ~130 dimer interfaces. The abundance of contacts that would need to be disrupted means that a higher concentration of the inhibitor would be required for efficacy.

Discussion

We screened against 17 proteins, 15 proteins of SARS-CoV-2 and two human proteins, targeting a total of 40 sites across these proteins with approximately 1.1 billion molecules per site. Due to the unprecedented global situation, we wanted to make the screening results available to researchers as soon as possible. The top 100 filtered hits as ranked by the docking score for each target site can be seen in Fig. 21. The top 1000 hits per virtual screen, along with additional information such as the docking scores, molecular properties, and docking poses, can be found online at https://vf4covid19.hms.harvard.edu/. In addition, the top million hits for each target site are available for download from the same website in DataWarrior format.

As discussed earlier, not all the functional surfaces that were targeted had similar potential to accommodate a small molecule. The targeted site that yielded the weakest virtual hit compounds is the first (site 1) of the two targeted sites located on the spike interaction interface of ACE2. The reason for the relatively weak predicted binding affinities of the top scoring compounds is the flat and polar nature of this target site, which makes it very challenging for small molecules to bind sufficiently well to disrupt the interaction with the spike protein. The target yielding the virtual hits with the highest predicted binding affinities is the active site of the ExoN domain of nsp14. The high affinities are a product of the remarkably deep, buried pocket of this active site and the relatively high number of hydrophobic sites within that pocket. If we consider the top 1000 filtered hits, the weakest screen (ACE2, Screen ID: 2) had a mean docking score of -7.6 kcal/mol (2.3 μM) while nsp14 (Screen ID: 37) had the best mean docking score of -12.9 kcal/mol (0.3 nM). Although the trend was the same, the mean docking scores were better for the top 100 hits: -8.2 kcal/mol (1.1 μM) for ACE2 (Screen ID: 2) and -13.4 kcal/mol (0.14 nM) for nsp14 (Screen ID: 37). Finally, as expected, the mean docking scores were even better for the top 10 hits: -8.52 kcal/mol (0.5 μM) for ACE2 (Screen ID: 2) and -14 kcal/mol (0.03 nM) for nsp14 (Screen ID: 37). The mean docking scores of the top 1000, 100, and 10 hits for each screen are shown in Fig. 21. Out of the 45 virtual screens, 41 had a mean docking score for the top 1000 compounds higher than -8.2 kcal/mol. These scores indicate that sub-micromolar binders should be identifiable from the hits for each target site. The hits derived from the rigid-docking procedures described here could be further improved for potency by a second-stage screen, in which the target proteins can be allowed to be flexible. This can be achieved either by ensemble docking or allowing flexible side chains. Another way of improving the docking results in second stage screenings consists of using alternative docking programs, such as AutoDock Vina, Smina or Gnina (40, 158, 159). For special types of ligands such as compounds containing carbohydrates or halogens, specialized docking programs such as VinaXB or Vina-Carb can be utilized to further increase the accuracy of the results (160, 161).

Small-molecule drug candidates that have been previously

pre-approved by the FDA or other regulatory bodies for other indications, and those molecules that have been vetted for use in humans, including preclinical candidates, neutraceuticals, metabolites, and select natural products are particularly desirable hits in any inhibitor screen (162). This is because these compounds can be fast-tracked to clinical trials on the basis of previous data. Here we mined for such compounds in the top 1% of our hits from the "in stock" compounds of the ZINC library. We found 161 drugs (with 491 occurrences across all the screens) that are "world approved" in our top 1%. We further filtered these drug candidates to only those with a docking score better than -8 kcal/mol and show these 80 approved drugs along with their screening target and docking score in Supplementary Table 3. Of these 80 drugs, 16 of them are currently being considered in clinical trials for COVID-19. The complete list of "world approved" hits along with their binding targets and docking score is available at https://vf4covid19.hms.harvard.edu/world-approved-drugs.

Several hits from the "world approved" drugs are from the steroid family. Corticosteroids such as betamethasone, ciclesonid, flumetasone and meprednisone acetate are already being investigated as COVID-19 treatments (163–165). For example, we identified betamethasone as binding to nsp14, the bifunctional enzyme that acts as a methyltransferase and an exoribonuclease. Betamethasone binds to the active site of the exoribonuclease of nsp 14 (Supplementary Fig. 24). While the usefulness of corticosteroids is largely attributed to their anti-inflammatory effects in the host, these screening results suggest the possibility of additional mechanisms of action that involve viral proteins. Other steroid hormones in clinical trial such as estradiol or dutasteride also came up as hits in our screens.

Of the non-steroid approved drug hits, tyrosine kinase inhibitors occupy a significant fraction. Drugs such as imatinib (Glivec®) are being tested in clinical trials due to their *in vitro* efficacy against SARS-CoV and MERS-CoV (166, 167); however, their mode of action is not yet fully understood. In our screens, imatinib binds to two targets: i) nsp14, but this time at the active site of the methyltransferase, and ii) the RNA-binding interface of the helicase, nsp13.

Of the 3897 "investigational" drugs in the ZINC15 database, 137 were hits (500 occurrences) and of the 101378 "in-man" compounds, 401 were hits (1061 occurrences). A full list of these molecules, along with their respective target sites and docking scores is available at (https://vf4covid19.hms.harvard.edu/investigational-drugs). Multiple occurrences of a hit molecule partly stem from the different docking scenarios that we used for the same target site. In addition, some of the compounds may be represented more than once in the list because of a different tautomeric, isomeric, or protonation state, any of which earns the molecule a unique ID in the ZINC database. Despite the abundance of approved hits, some of which are already involved in or related to drugs in clinical trials, experimental confirmation of the specificity of hits from our screen against SARS-CoV-2 proteins is still needed to determine an antiviral mechanism of action. As noted earlier, when testing these compounds in viral assays, one should bear in mind the nature of the targets and be cognizant of differential effects on viral viability versus viral virulence. Furthermore, correlating "pre-approved" hits from the virtual screens with patient data, particularly severity of infection and recovery time, through examination of patients' regular medication and supplement regimens could reveal if any hit positively correlates with either a milder disease course or a faster time to recovery

When performing *in silico* screening, we generally choose a 3D surface on the target protein, referred to as the "docking box", and evaluate the energetics of a molecule bound to that chosen surface. The docking box is judiciously chosen to target a known functional domain, either an active site, an allosteric site, or a protein-protein interaction interface. In practice, the docking box is typically extended to accommodate secondary interactions with the small molecule, especially when competing with a substrate. However, occasionally this results in identifying a tight binder that does not harbour any inhibitory function. It is important to take into account this possibility during follow-up experiments and test for binding using a direct binding assay such as ITC, SPR, MST or NMR. In particular, NMR and X-Ray structures can provide detailed information on the binding site and how the small molecule engages the target. It is possible to functionalize these non-inhibitory binders with warheads to degrade the targeted protein by established methods, referred to as proteolysis-targeting chimeras (PROTACS) (168, 169). However the effectiveness of these PROTACs will depend on the concentration, rate of turnover, and accessibility of the target viral proteins.

SARS-CoV-2 is not the first coronavirus to cause serious disease in the human population, and these other coronaviruses (SARS-CoV and MERS-CoV) have also been the subject of research into small molecule inhibitors. There have been several efforts in the past, both experimental and computational, to target specific viral proteins from these viruses. The proteins that were most often targeted in these efforts were the proteases, M^{Pro} (66, 170–172) and PL^{Pro} (170, 173–175), the polymerase (176, 177), the spike protein (59, 178, 179), the endoribonuclease (180), and the helicase (181–183) 2. Although direct binding affinities were not available for most of the molecules, the inhibitory potential, IC50, or the effective potential, EC50, were reported.

When the the exact binding site of a previously published inhibitor was reported, in order to determine if these SARS-CoV and MERS-CoV hits were also top hits against SARS-CoV-2, we calculated docking scores using the same computational methods used in the screens described here, allowing direct comparison with our hits. One of the best inhibitors for SARS-CoV M^{Pro} is an asymmetric aromatic disulfide molecule with an IC50 of 0.52 ± 0.06 µM (171). When we docked this molecule against SARS-CoV-2 M^{pro}, we got a docking score of -7.7 kcal/mol 2, whereas the top 100 hits from two of our recent screens described here, which targeted the active site of M^{pro} (Screen IDs: 16 and 17), resulted in

a mean docking scores of -10.83 and -11.41 kcal/mol. Similarly, in the case of PL^{pro}, the best previously described active site inhibitor (173) has a binding free energy of -7.2 kcal/mol, while the top 100 compounds from two of our VirtualFlow screens (Screen IDs: 12 and 15) have a mean binding scores of -8.90 and -10.02 kcal/mol respectively. 21. These energies, in principle, should result in inhibitors with affinities two orders of magnitude higher than that of the original inhibitor from Ghosh, *et al.*. Lee, *et al.* described a novel helicase inhibitor that can block both the dSDNA unwinding and ATP hydrolysis activities of the SARS-CoV helicase (181). Docking of this molecule to the SARS CoV-2 helicase gave a score of -7.9 kcal/mol. We also targeted the active site of the SARS-CoV-2 helicase (Screen ID: 33), in addition to its RNA binding interface, and that screen resulted in a top 100 hits with a mean docking sore of -10.22 kcal/mol. In addition, there have been multiple attempts to develop small molecule inhibitors that target the active site of the RdRp, considered a promising target, from both SARS-CoV and MERS-CoV (176, 177). Docking of the best molecules from these previously published studies against the SARS-CoV-2 RdRp resulted in docking scores of -6.1 and -6.8 kcal/mol, while our screens (Screen IDs 28 and 29) resulted in compounds with mean docking scores of -11.12 and -9.72 kcal/mol, respectively, for the top 100 hits. In general, our multi-target screening strategy resulted in hits with significantly higher docking scores than previously described hits re-tested against SARS-CoV-2 targets. However, the improvements in binding still needs to be experimentally validated.

In addition, there have already been multiple attempts to employ virtual screening of varying library sizes to identify approved drugs as well as discover new molecules that can effectively inhibit SARS-CoV-2 viral infection(66, 184–192), and more than one screen is focused solely on M^{pro} (184, 187, 190, 191). It is important to note that in the case of M^{pro}, the conformational plasticity of the active site means that screening against a single conformation,as is done in these studies, may be less effective at identifying functional hits. One work of note is that by Ton, *et al*. 1.3 billion compounds from the ZINC 15 library were screened against M^{pro} using a Deep Docking algorithm (188). While Deep Docking significantly accelerates the screening of ultra-large compound libraries, it relies heavily on the docking scores of a small random subset of compounds to eliminate a large chunk of the compounds early in the docking workflow, and this can be detrimental to finding an absolute docking score for individual compounds.

A recent mass-spectrometry-based study has identified several host proteins that interact with SARS-CoV-2 viral proteins, leading to the identification of multiple druggable host targets and a series of known modulating compounds for these targets that were then shown to have antiviral activity in cell-culture-based assays (193). The efficacy of these already approved host-directed compounds lends support to the development of these drugs as therapeutic interventions for SARS-CoV-2 infection. Coincidentally, some of the compounds from this mass spectrometry study were also identified as hits in our screens against diverse viral proteins. For example, 'Nafamostat', an approved anticoagulant identified in Gordon, *et al.* as having a possible impact on cell entry, was also identified in our screens as a hit with good scores against three viral proteins: ORF7a, PL^{pro}, and nucleoprotein. This compound is already undergoing clinical trials for COVID-19 (Ref:NCT04352400, NCT04418128). Similarly, 'progesterone', a common birth control drug that is also known to have anti-inflammatory properties was identified in the proteomics study as a ligand with antiviral activity that targets sigma-1 or sigma-2 receptors. In our screens, this compound was identified as an inhibitor for nsp16, nsp7 and spike. Progesterone is also in clinical trials for treatment of COVID-19 (NCT04365127). Silmitasertib (CX-4945), an inhibitor of casein kinase II (CK2), was identified both in the proteomics study as well as in another recent study that mapped the host phosphorylation landscape in the context of SARS-CoV-2 infection (193, 194). Silmitasertib was originally developed to be used in combination with chemotherapy. Here, we identify that Silmitasertib could potentially bind to nsp16. If some of these host-protein-targeted compounds can also directly inhibit some viral proteins, as suggested by the docking scores derived from our screens, this could form the basis for a unique regimen of multi-target drugs to treat COVID-19 that acts on both viral as well as host proteins simultaneously. A list of compounds that are common to both the interactome study and our virtual screens, along with their potential targets are provided in Supplementary Table 4.

Our ultra-large library size and the multi-pronged screening approach is not only unprecedented in terms of scale, significantly enhancing the chances of finding an effective antiviral, but also provides a pool of potential antiviral compounds that could be developed further as pan-coronavirus drugs as well as combination therapies. Combination regimens of reverse transcriptase inhibitors and protease inhibitors have been found to be effective as anti-retroviral therapy for human immunodeficiency virus (HIV) and has lead to dramatic improvement in HIV infected patient health and survival worldwide (195–197). Clinical studies have also shown that in case of severe influenza, a combination of multiple antiviral drugs is much more effective than a single one (198, 199). Therefore, it could also be beneficial to develop a combination therapy to treat severely affected COVID-19 patients. Considering that the success or efficacy of any future SARS-CoV-2 vaccines is still unknown, combination therapeutic strategies for the control and treatment of coronavirus infections should be developed in parallel. The mutating nature of coronaviruses and the potential for the emergence of novel coronaviruses in the future make the development of broad spectrum antivirals desirable. For a protein to qualify as a candidate target for pan-coronavirus drug development, it should be i) critical for the viral replication or virulence, and ii) highly conserved across all known CoVs and likely to be conserved in emerging CoVs. While the structural proteins (S, N, M and E) are not as well conserved, the accessory proteins are conserved to an even lesser ex-

tent across different CoV species (ProViz, (200)). Highly conserved nonstructural proteins and conserved host proteins would therefore be ideal targets for the development of broad spectrum CoV drugs (201). While studies (202) have suggested that the S and N genes of SARS-CoV-2 are undergoing episodic selection during human transmission, recent analyses of genome samples from across the world suggest that the greatest genetic diversity is occurring in S, ORF3a and ORF8 (203). Structural genomic analysis across multiple virus classes, including SARS-CoV-2, have shown that intra-viral interactions are more conserved than viral host-interactions (204–207). The protein-protein interaction interfaces involved in the heteromeric RNA polymerase complex (composed of nsp7,nsp8 and nsp12) are evolutionarily conserved (204) and our top hits against these crucial PPIs represent promising candidates for the development of pan-coronavirus inhibitors. Similarly, structural genomic analysis of the methyl transferase complexes (nsp10-nsp14 and nsp10-nsp16) also reveals PPIs that are fully conserved and with mutations limited to the the surface (204). Moreover, the substrate binding regions we used for PL^{pro}, M^{pro}, nsp14, nsp16 and the RNA binding site of the nucleocapsid protein have all been shown to be highly conserved (207), and the derived small molecules could also potentially be developed as pan-coronavirus therapeutics. Since most human coronaviruses differ in their use of host cell receptors and priming proteases (19), identifying a cell-based assay or functional animal model for developing pan-coronavirus therapeutics could be challenging. The use of normal human bronchial epithelia (NHBE) cells as a potential universal screening platform for multiple classes of coronaviruses is promising (208–210), and the general need for high-throughput *ex vivo* testing models will hopefully drive development in this area.

The work described here is only the first step in the drug discovery process. Virtual screening seeks to use structure and modelling-guided approaches to identify higher quality starting hits. Hits from these screens still need to be experimentally validated for binding, inhibition, and activity in the context of viral infection. Some of these targets, which affect viral immune evasion rather than replication, may need more complex evaluation in cell culture or in animal models to determine efficacy. While our own experimental validation of hits from these screens has begun, we believe that making these results available to a broader audience for experimentation is important in light of the current pandemic.

Conclusions

The alarming global spread of SARS-CoV-2 and the dearth of effective prophylaxis or treatment methods has resulted in a pressing need for accelerated drug discovery. Here we make use of the recent chemical space revolution that resulted in ultra-large make-on-demand libraries, to prioritize lead molecules and minimize the transition time from discovery to clinic. We have used the available-to-date SARS-CoV-2 structome to carry out detailed structure-based virtual screening against 17 different target proteins, frequently at multiple target sites, by leveraging the versatility of our recently developed *in silico* screening platform, VirtualFlow. The set of small molecule hits that we present here can aid drug development happening at multiple institutions worldwide, and the set of prospective drug molecules derived from this ultra-large multi-target screening campaign will potentially contribute to the building of a future arsenal of anti-coronaviral drugs, ready to tackle future outbreaks.

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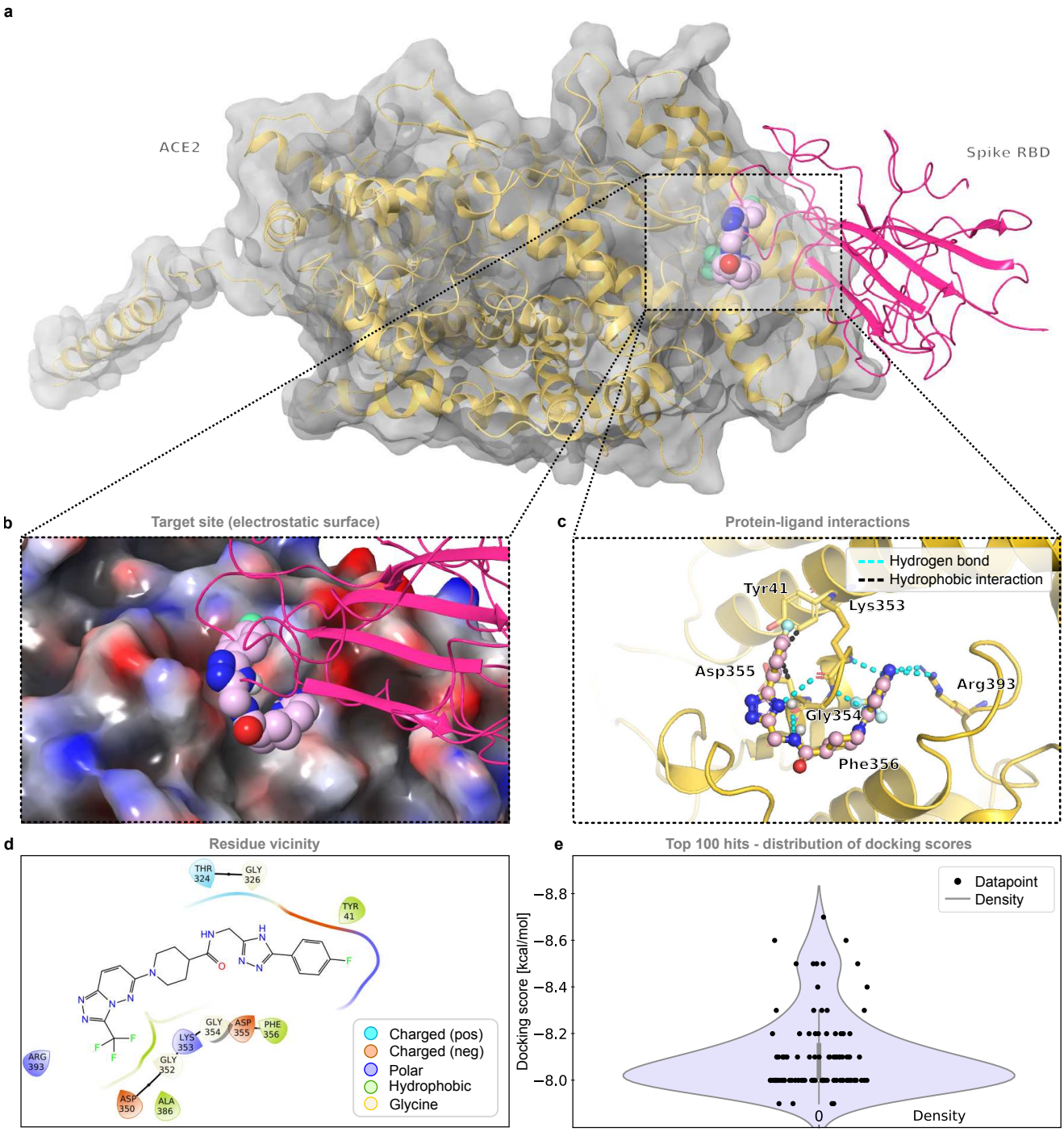
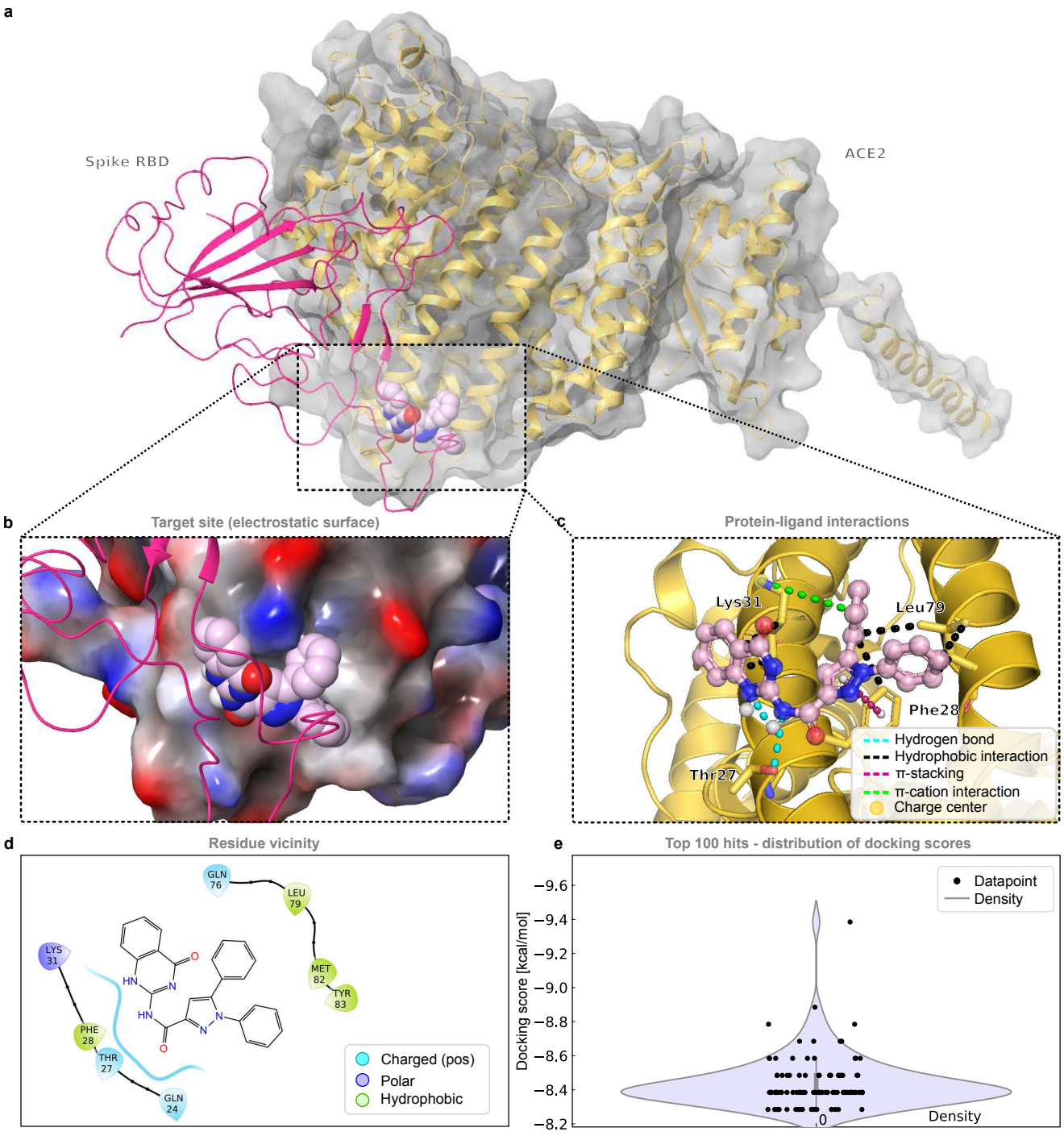
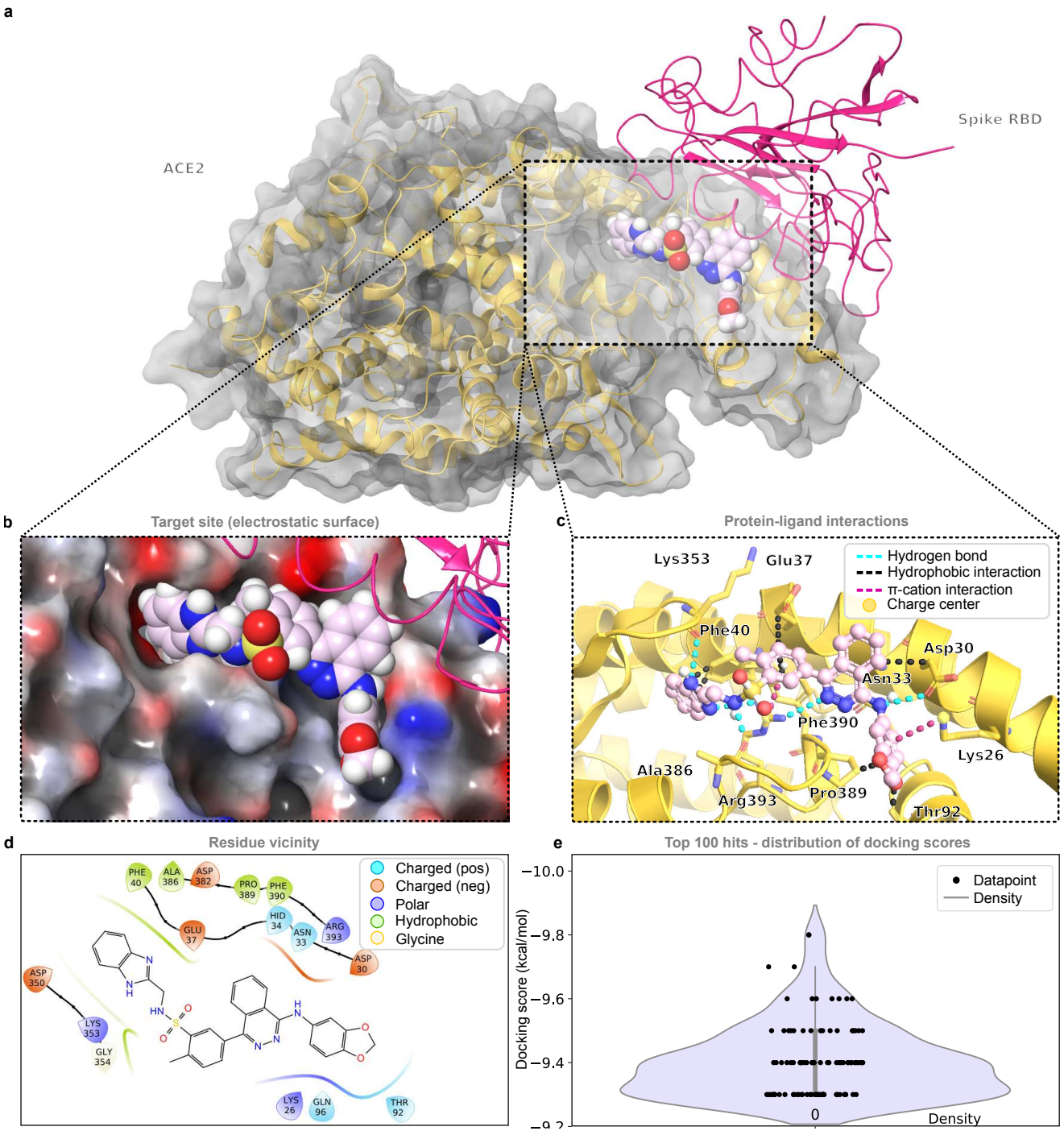
Supplementary Information



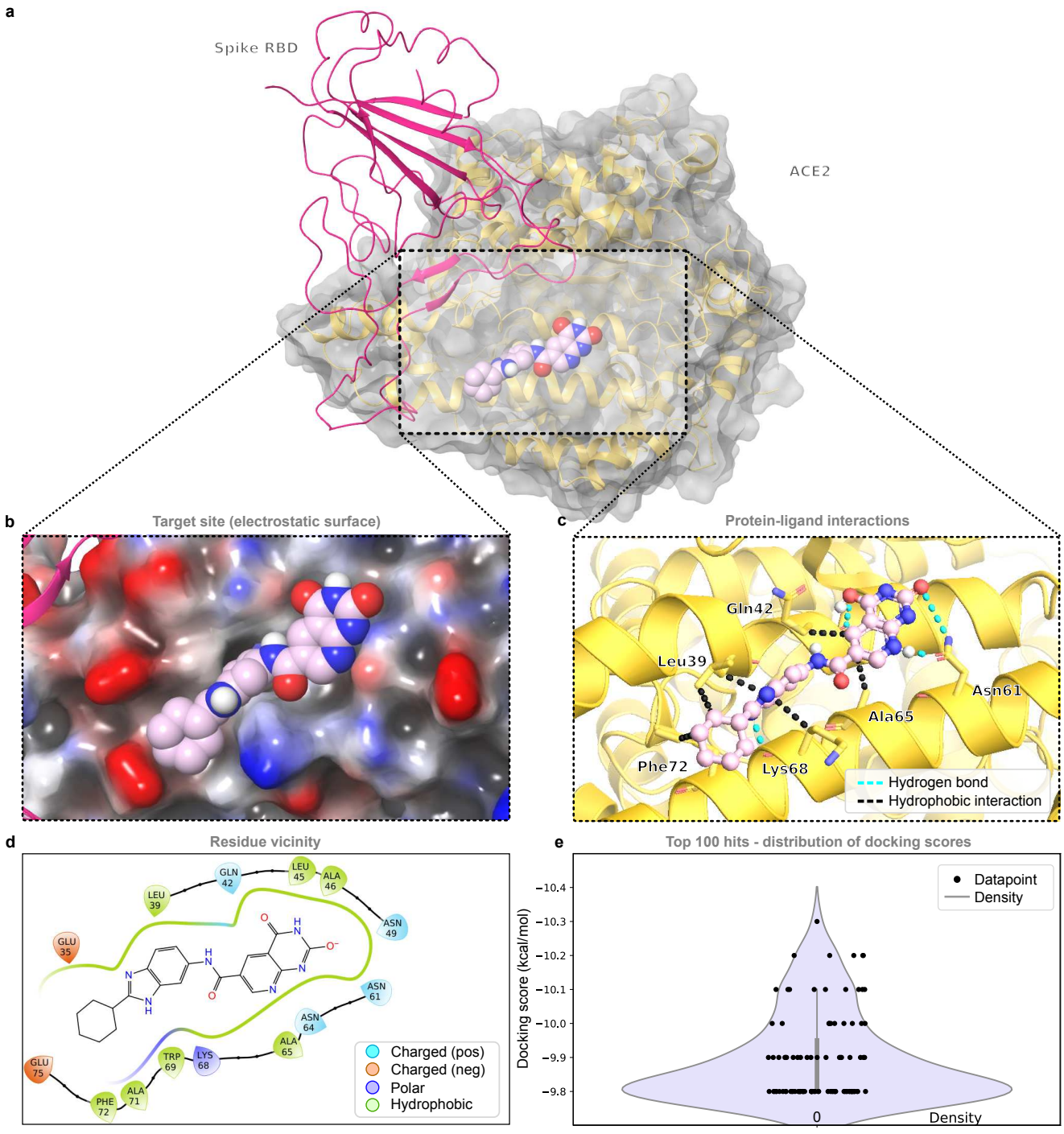
Supplementary Fig. 1. The ACE2 receptor (closed conformation) and an example compound from the top 0.0001% of screened compounds bound at the spike protein interaction interface (site 1). a, The target protein ACE2 (gold) in a closed conformation bound to the RBD of the spike protein (magenta) and an example compound (light pink) from the virtual screen bound to the spike protein interaction interface (Screen ID: 2)(site 1, around Glu37). **b**, Electrostatic surface of the target protein (ACE2) bound to the RBD domain of the spike protein and an example compound (light pink). **c,** An overview of the interactions between the ligand and the receptor structure. **d,** Residues within 4 Å of the ligand. **e,** Distribution of the docking scores of the top 100 virtual screening hits.



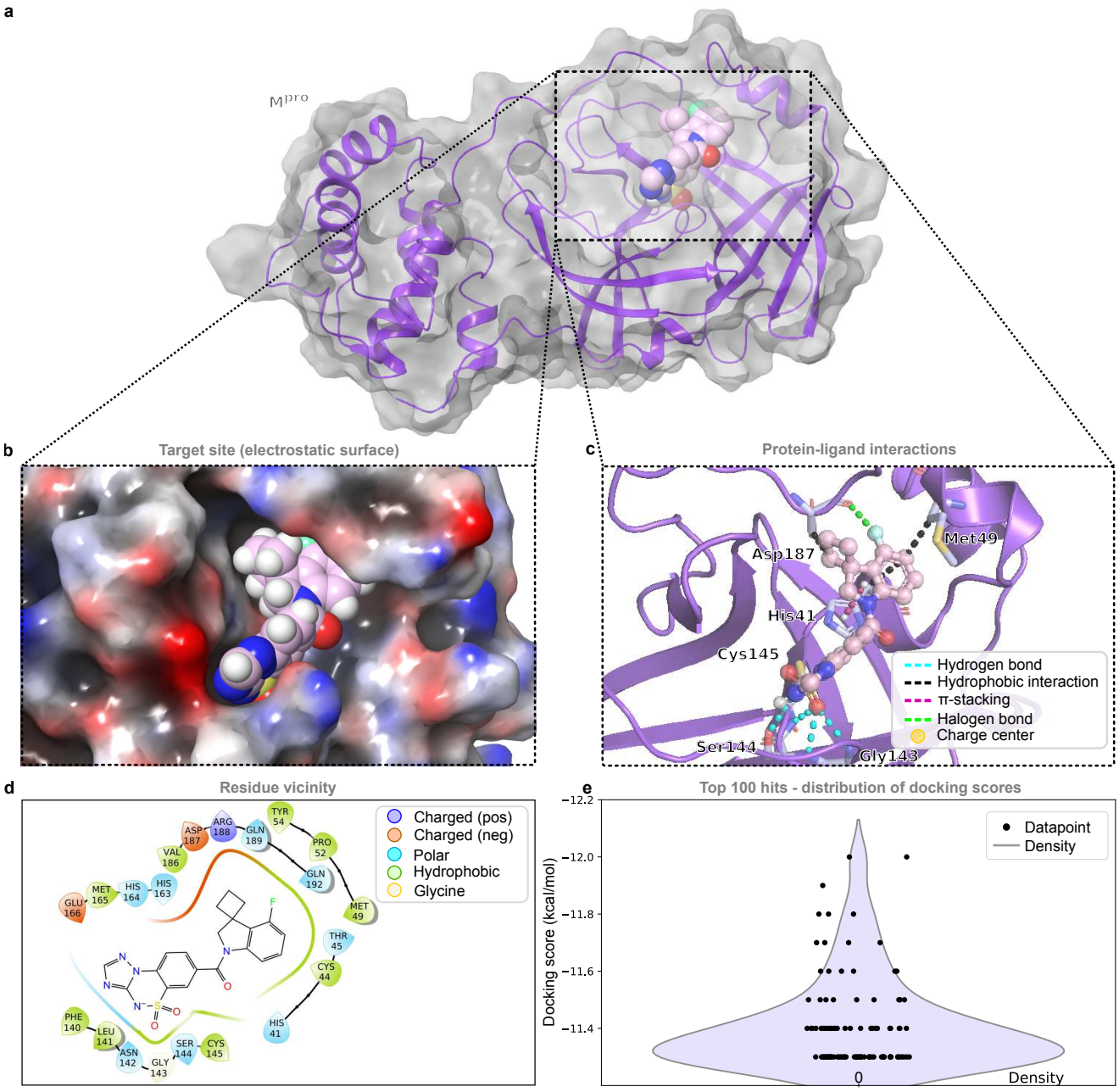
Supplementary Fig. 2. The ACE2 receptor (open conformation) and an example compound from the top 0.0001% of screened compounds bound at the spike interaction interface (site 2). a, The target protein ACE2 (gold) in a closed conformation bound to the RBD of the spike protein (magenta) and an example compound (light pink) from the virtual screen bound to the spike protein interaction interface (Screen ID: 3)(site 2, around Phe28). **b**, Electrostatic surface of the target protein (ACE2) bound to the RBD domain of the spike protein and an example compound (light pink). **c,** An overview of the interactions between the ligand and the receptor structure. **d,** Residues within 4 Å of the ligand. **e,** Distribution of the docking scores of the top 100 virtual screening hits.



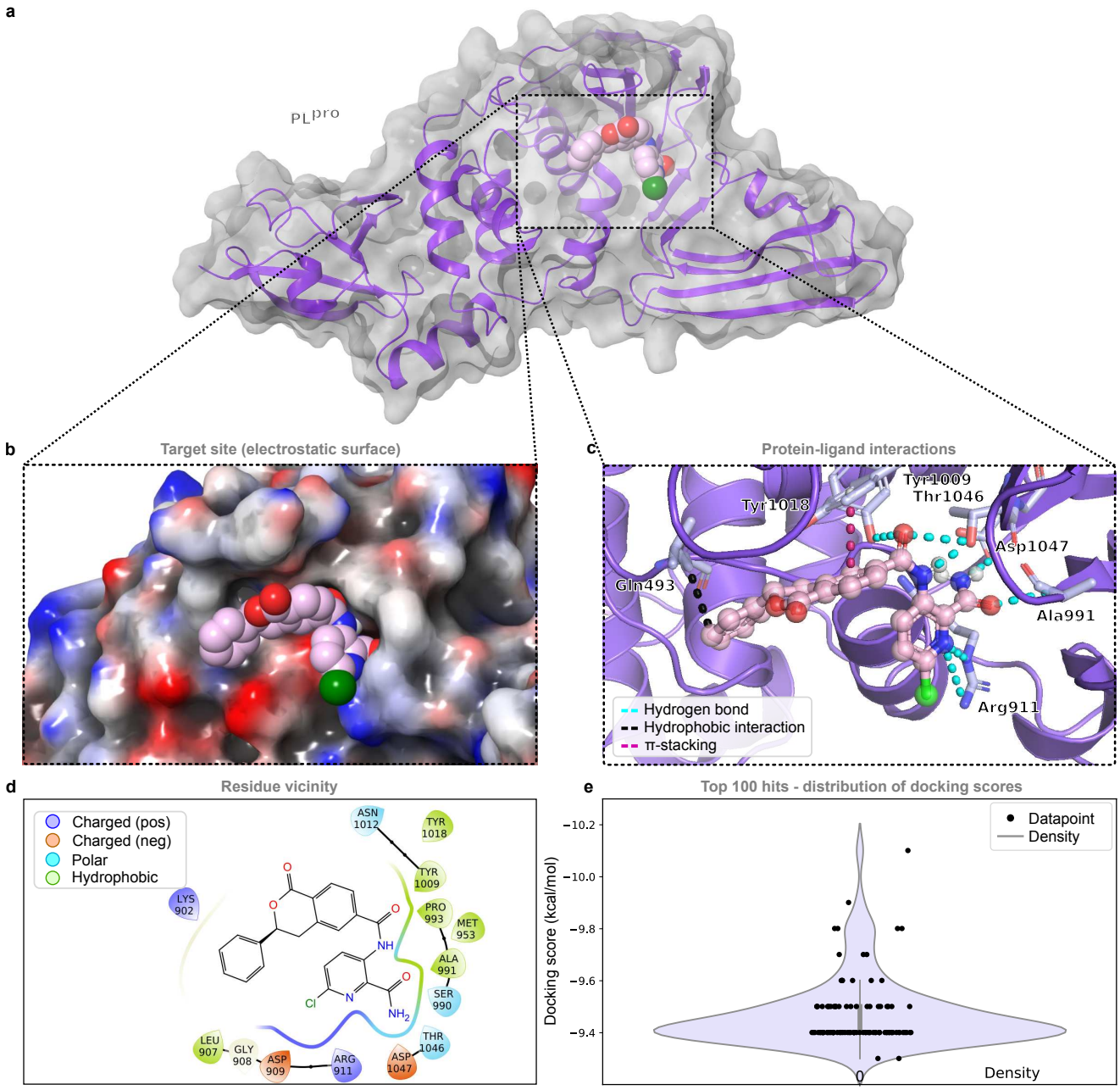
Supplementary Fig. 3. The ACE2 receptor (open conformation) and an example compound from the top 0.0001% of screened compounds bound near the spike interaction interface (site 3). a, The target protein ACE2 (gold) in a closed conformation bound to the RBD of the spike protein (magenta) and an example compound (light pink) from the virtual screen bound to target site 3 (around Phe40), which contains a dynamic pocket located adjacent to the RBD interface (Screen ID: 4). **b**, Electrostatic surface of the target protein (ACE2) bound to the RBD domain of the spike protein (magenta) and an example compound (light pink). **c,** An overview of the interactions between the ligand and the receptor structure. **d,** Residues within 4 Å of the ligand. **e,** Distribution of the docking scores of the top 100 virtual screening hits.



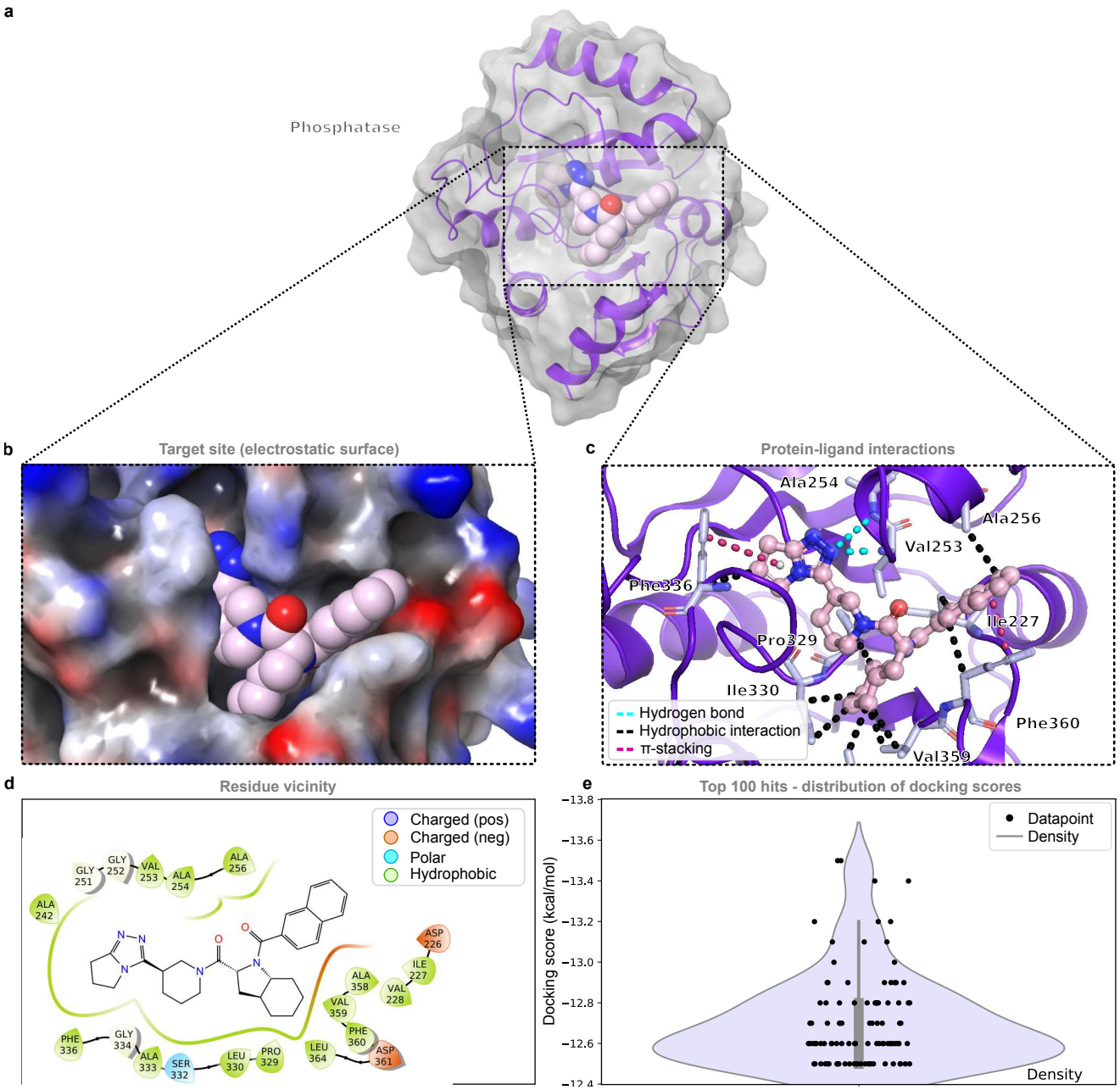
Supplementary Fig. 4. The ACE2 receptor (open conformation) and an example compound from the top 0.0001% of screened compounds bound near the spike interaction interface. a, The target protein ACE2 (gold) in a closed conformation bound to the RBD of the spike protein (magenta) and an example compound (light pink) from the virtual screen bound to target site 4 (around Leu39), which represents a dynamic pocket adjacent to the RBD binding interface (Screen ID:5). **b**, Electrostatic surface of the target protein (ACE2) bound to the RBD domain of the spike protein (magenta) and an example compound (light pink). **c,** An overview of the interactions between the ligand and the receptor structure. **d,** Residues within 4 Å of the ligand. **e,** Distribution of the docking scores of the top 100 virtual screening hits.



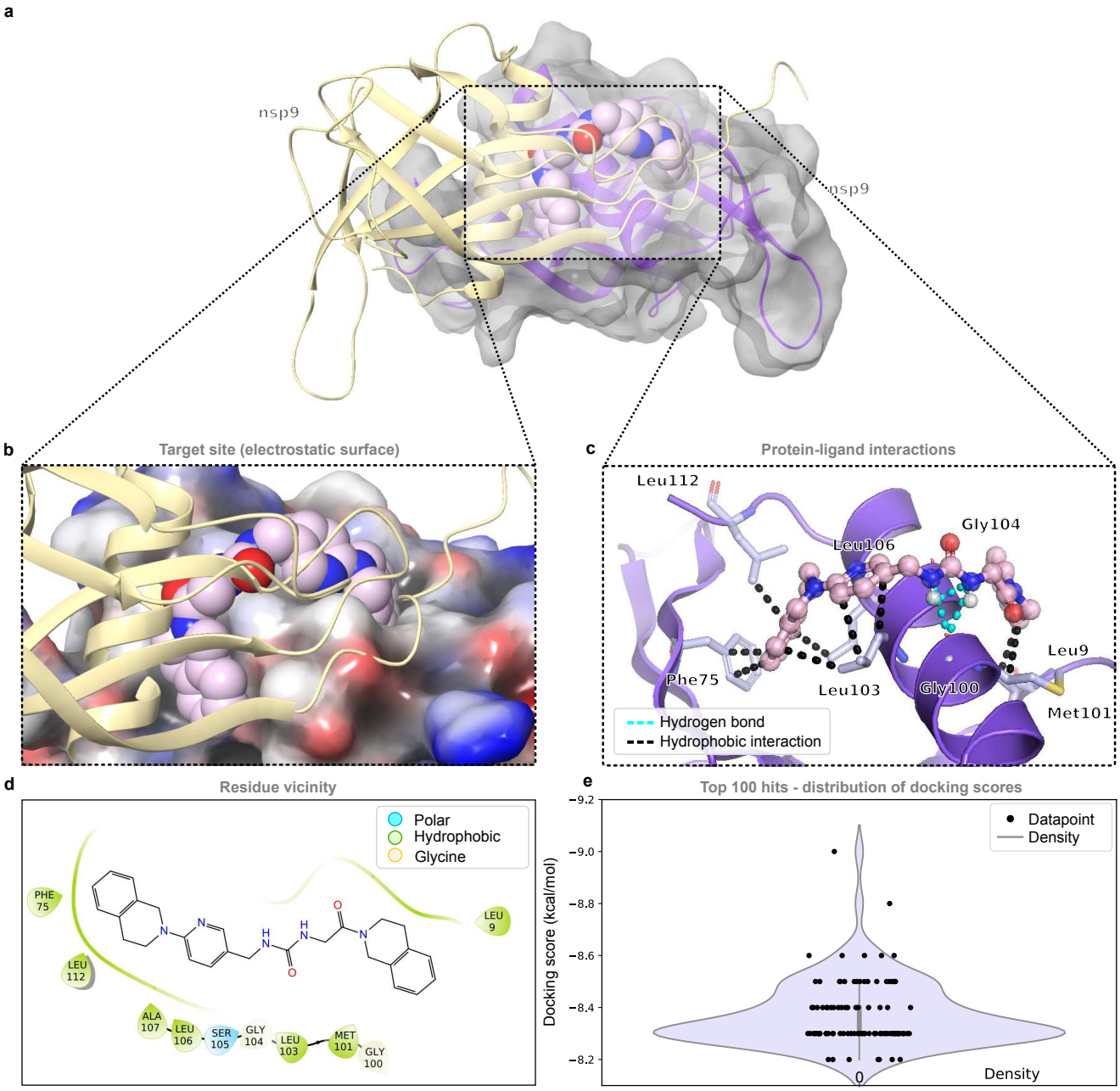
Supplementary Fig. 5. M^{pro} and an example compound from the top 0.0001% of screened compounds bound at the enzymatic active site a, M^{pro} (violet) and an example compound (light pink) from the virtual screen bound to the active site. Here, a modified version of the structure wth PDB ID 6m0k was used (details are described in the main text)(Screen ID: 17). **b**, Electrostatic surface of the target protein to which an example compound (light pink) is bound. **c,** An overview of the interactions between the inhibitor and the protease structure. **d,** Residues within 4 Å of the inhibitor. **e,** Distribution of the docking scores of the top 100 virtual screening hits.



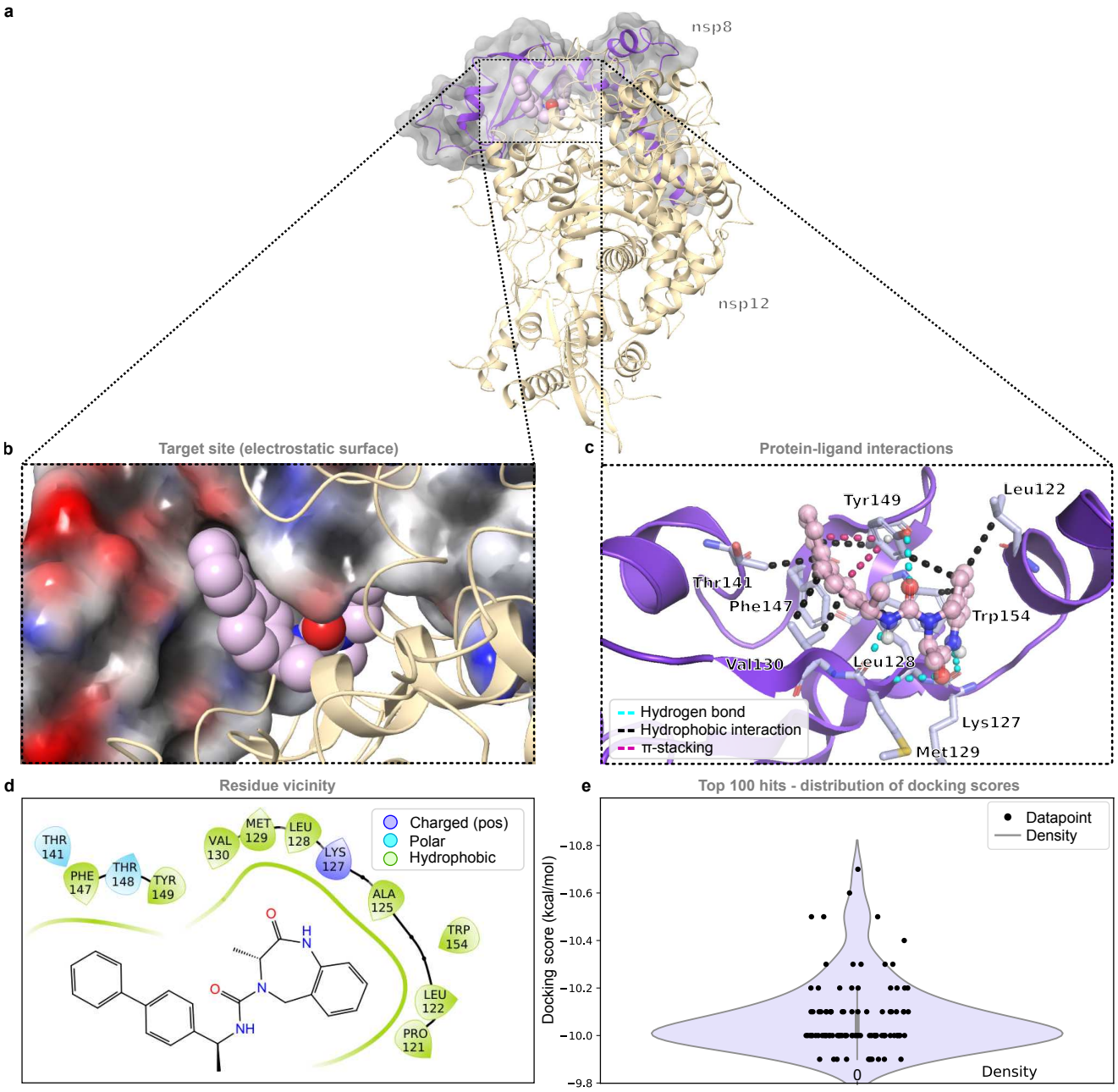
Supplementary Fig. 6. PL^{pro} and an example compound from the top 0.0001% of screened compounds bound at the accessory pocket near the active site. a, PL^{pro} (violet) and an example compound (light pink) from the virtual screen bound at the accessory pocket near the active site (screen ID:13). **b**, Electrostatic surface of the target protein to which an example compound (light pink) is bound. **c,** An overview of the interactions between the inhibitor and the protease structure. **d,** Residues within 4 Å of the inhibitor. **e,** Distribution of the docking scores of the top 100 virtual screening hits.



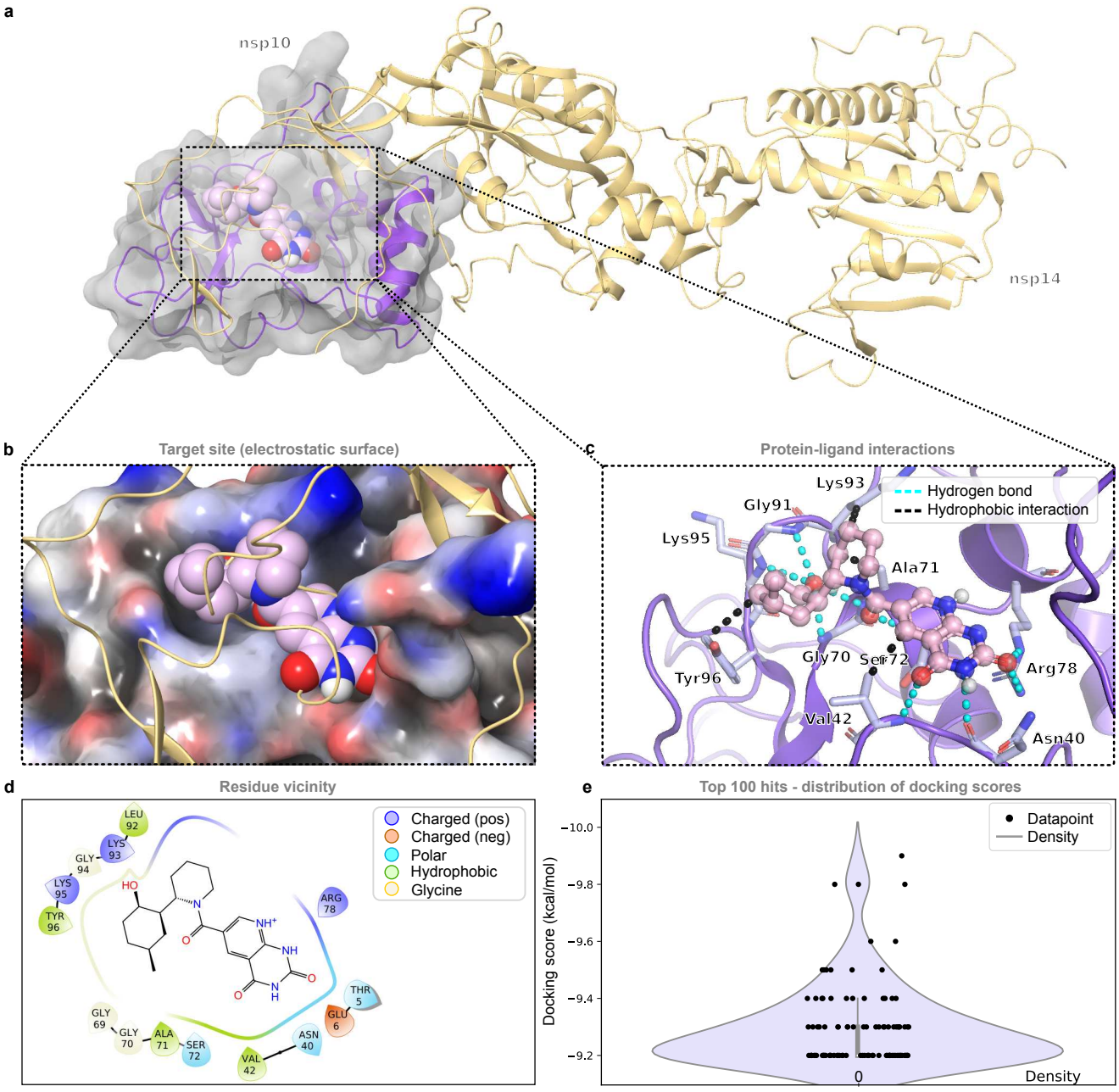
Supplementary Fig. 7. The phosphatase (open conformation) and an example compound from the top 0.0001% of screened compounds bound at the enzymatic active site. **a**, The phosphatase (violet) which is part of nsp3 and an example compound (light pink) from the virtual screen bound to the active site (closed conformation)(Screen ID: 11). **b**, Electrostatic surface of the target protein to which an example compound (light pink) is bound. **c,** An overview of the interactions between the inhibitor and the phosphatase structure. **d,** Residues within 4 Å of the inhibitor. **e,** Distribution of the docking scores of the top 100 virtual screening hits.



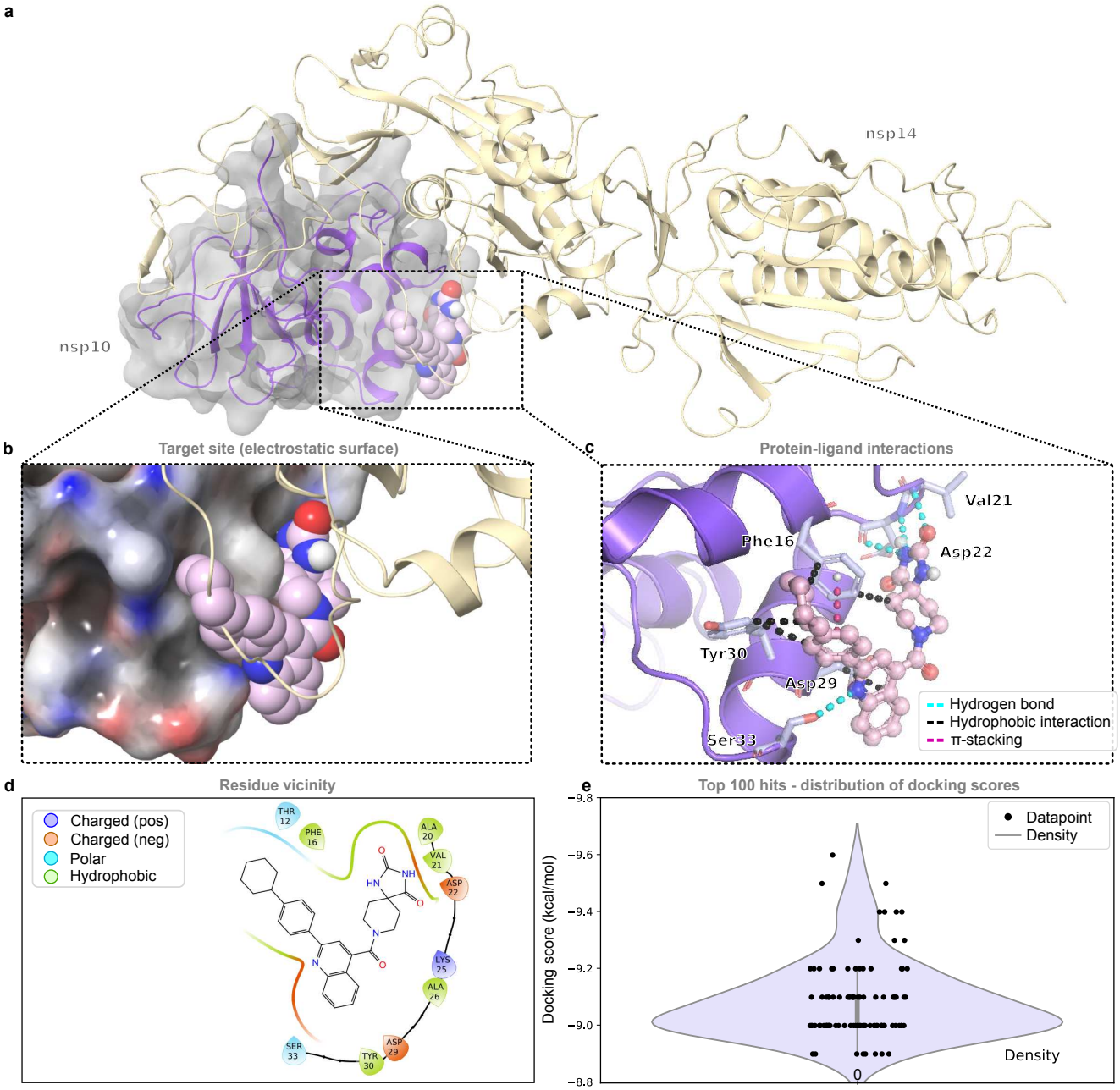
Supplementary Fig. 8. nsp9 and an example compound from the top 0.0001% of screened compounds bound at the dimerization interface (site 1). a, nsp9 dimer (one monomer in violet, one monomer in gold), where an example compound (light pink) from the virtual screen is bound to the dimerization interface (site 1) of the nsp9 monomer in violet(Screen ID:23). **b**, Electrostatic surface of the target protein to which an example compound (light pink) is bound. **c,** An overview of the interactions between the inhibitor and the nsp9 structure. **d,** Residues within 4 Å of the inhibitor. **e,** Distribution of the docking scores of the top 100 virtual screening hits.



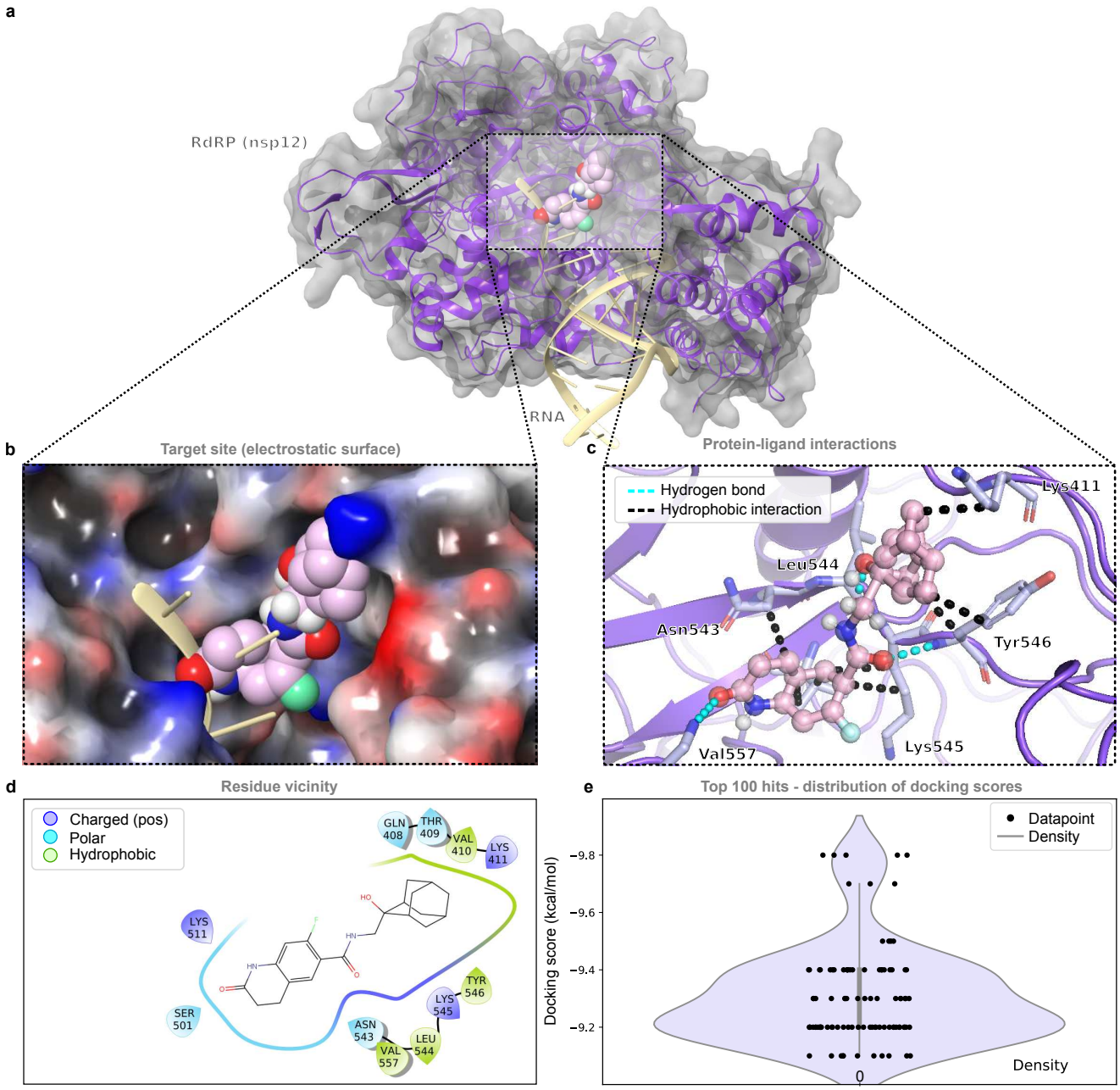
Supplementary Fig. 9. nsp8 and an example compound from the top 0.0001% of screened compounds bound at the nsp12 binding interface. **a**, nsp8 (violet) bound to nsp12 (in light gold) and an example compound (light pink) at the nsp12 binding interface (Screen ID: 22). **b**, Electrostatic surface of nsp8 to which an example compound (light pink) and nsp12 (light gold) is bound. **c,** An overview of the interactions between the inhibitor and the nsp8 structure. **d,** Residues within 4 Å of the inhibitor. **e,** Distribution of the docking scores of the top 100 virtual screening hits.



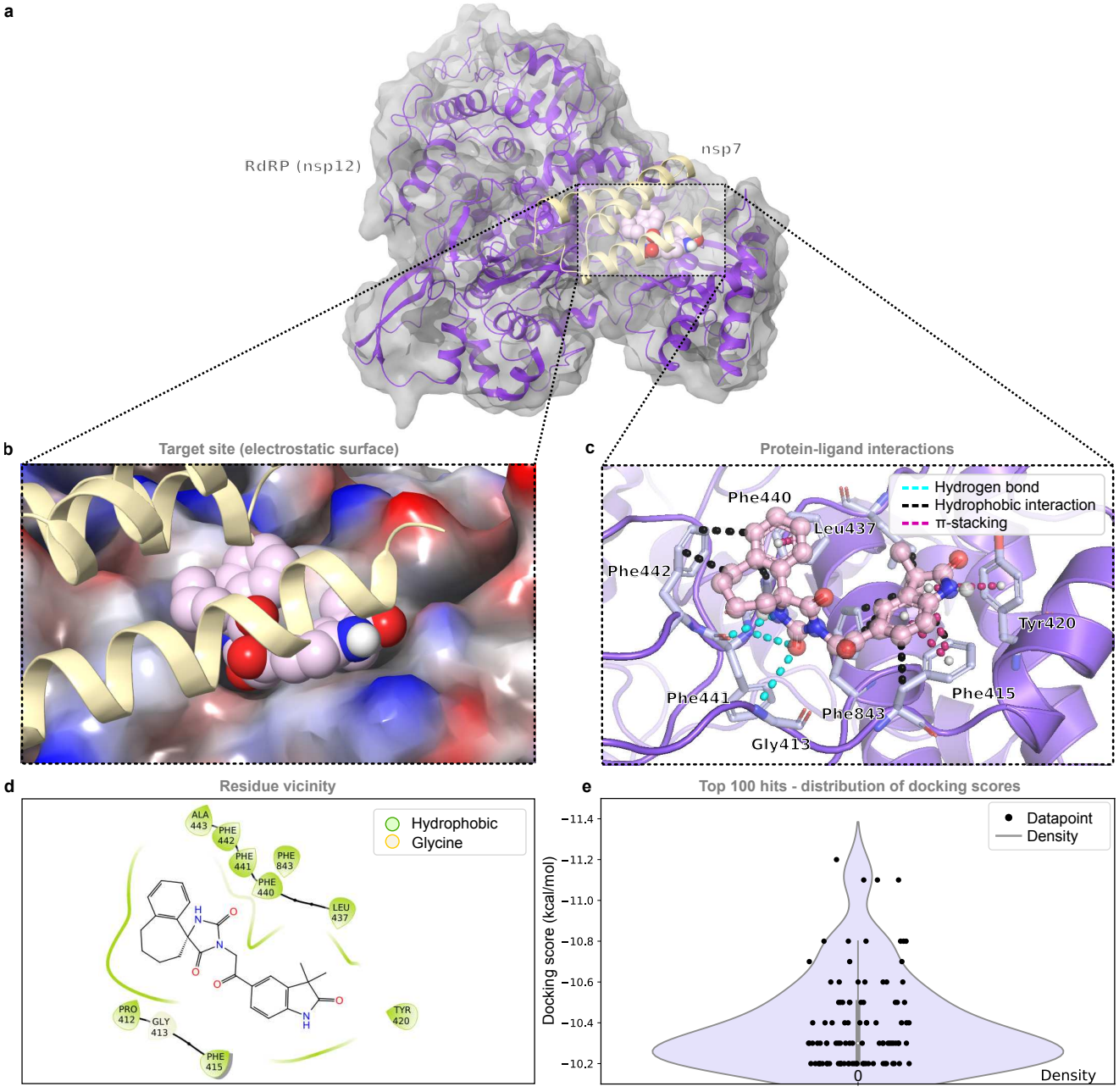
Supplementary Fig. 10. nsp10 and an example compound from the top 0.0001% of screened compounds bound at the binding interface to nsp14 and nsp16. a, nsp10 (violet) bound to nsp14 (light gold) and and example compound (light pink) at the binding interface of nsp10 to nsp14 and nsp16 (Screen ID: 26). **b**, Electrostatic surface of nsp10 to which an example compound (light pink) and nsp14 (light gold cartoon) are bound. **c,** An overview of the interactions between the inhibitor and the nsp10 structure. **d,** Residues within 4 Å of the inhibitor. **e,** Distribution of the docking scores of the top 100 virtual screening hits.



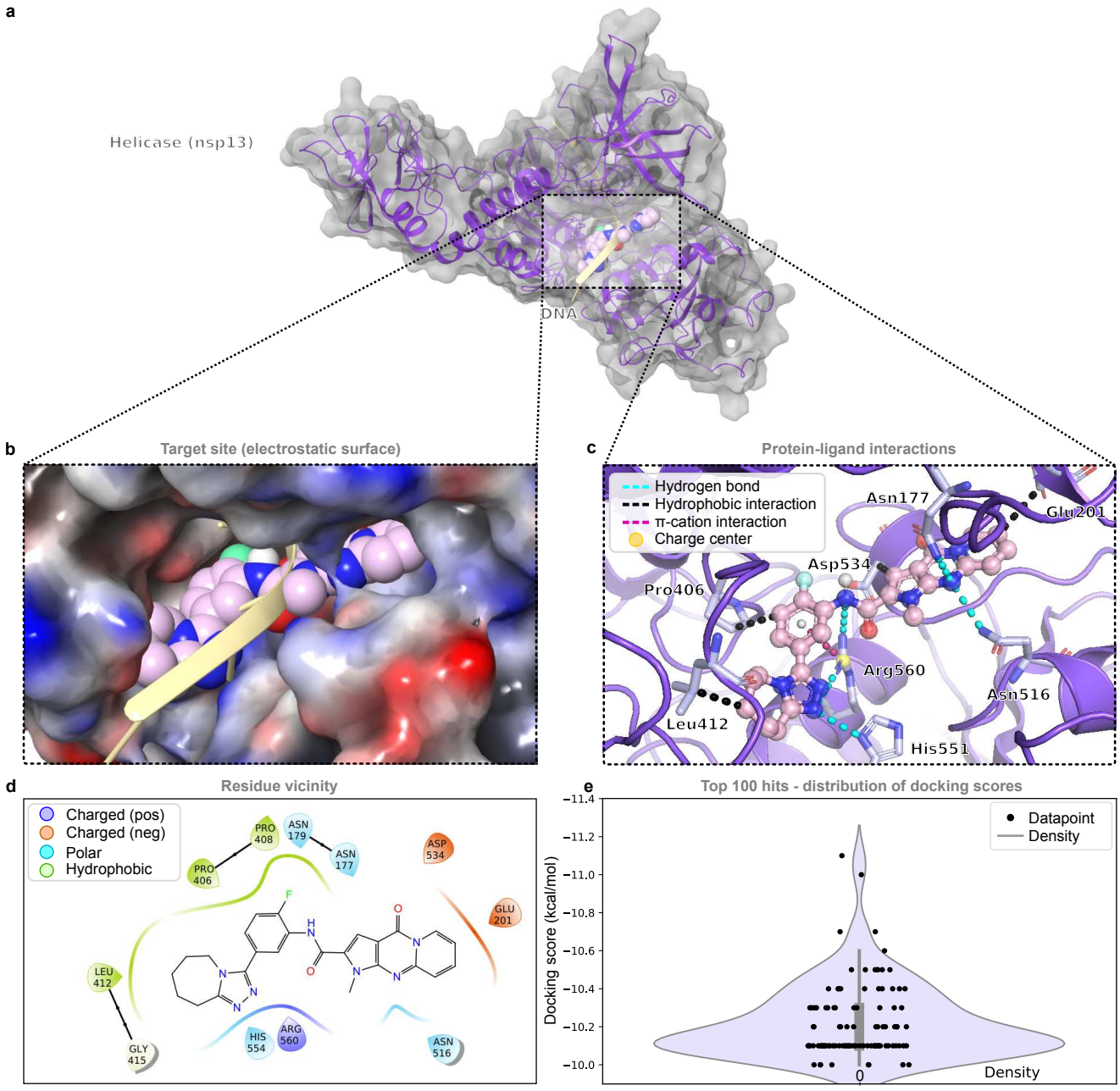
Supplementary Fig. 11. nsp10 and an example compound from the top 0.0001% of screened compounds bound at the nsp14 binding interface. a, nsp10 (violet) bound to nsp14 (light gold) and an example compound (light pink) at the nsp14 binding interface of nsp10 (Screen ID: 27). **b**, Electrostatic surface of nsp10 to which an example compound (light pink) and nsp14 (light gold) are bound. **c,** An overview of the interactions between the inhibitor and the nsp10 structure. **d,** Residues within 4 Å of the inhibitor. **e,** Distribution of the docking scores of the top 100 virtual screening hits.



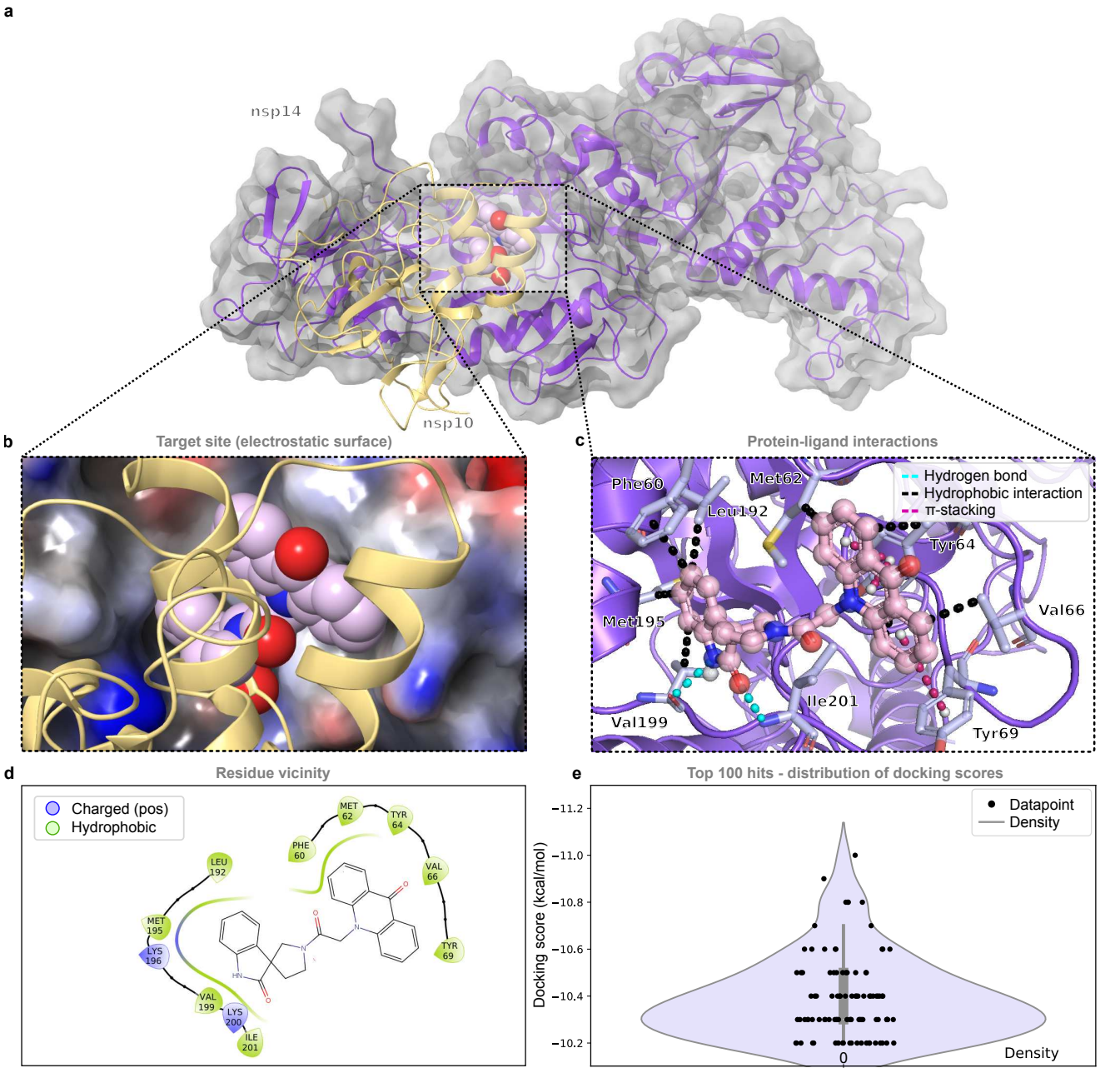
Supplementary Fig. 12. nsp12 and an example compound from the top 0.0001% of screened compounds bound at site 2 of the RNA binding interface. a, nsp12 (violet) bound to RNA (light gold) and an example compound (light pink) at site 2 of the RNA binding region (Screen ID:30). **b**, Electrostatic surface of nsp12 to which an example compound (light pink) at site 2 of the RNA binding region. RNA is shown in light gold. **c,** An overview of the interactions between the inhibitor and the nsp12 structure. **d,** Residues within 4 Å of the inhibitor. **e,** Distribution of the docking scores of the top 100 virtual screening hits.



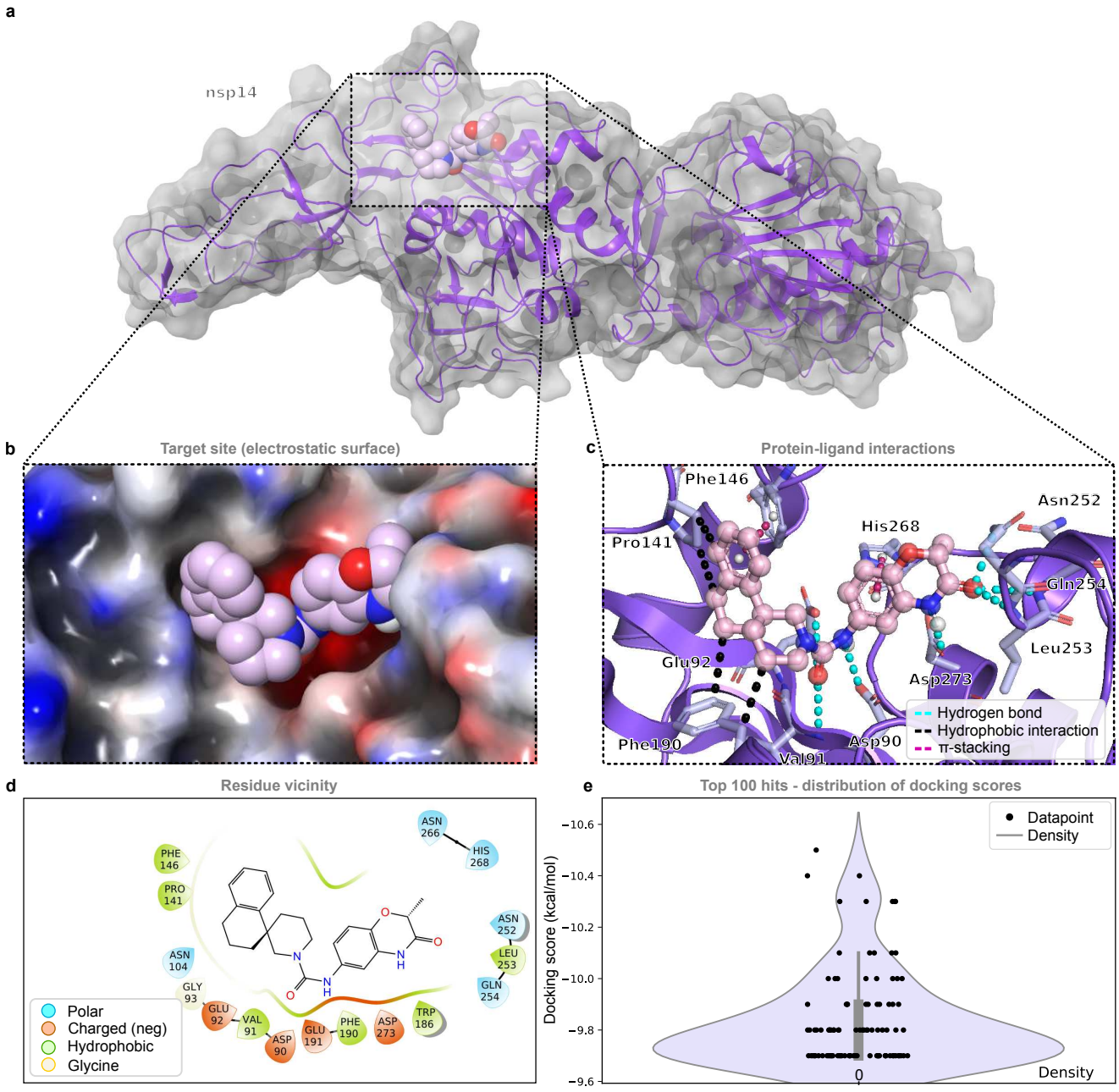
Supplementary Fig. 13. nsp12 and an example compound from the top 0.0001% of screened compounds bound at the nsp7 binding interface. a, nsp12 (violet) bound to nsp7 (light gold) and an example compound (light pink) at the nsp7 binding interface (Screen ID: 31). **b**, Electrostatic surface of nsp12 to which an example compound (light pink) is bound to the nsp7 binding site. nsp7 is shown in light gold. **c,** An overview of the interactions between the inhibitor and the nsp12 structure. **d,** Residues within 4 Å of the inhibitor. **e,** Distribution of the docking scores of the top 100 virtual screening hits.



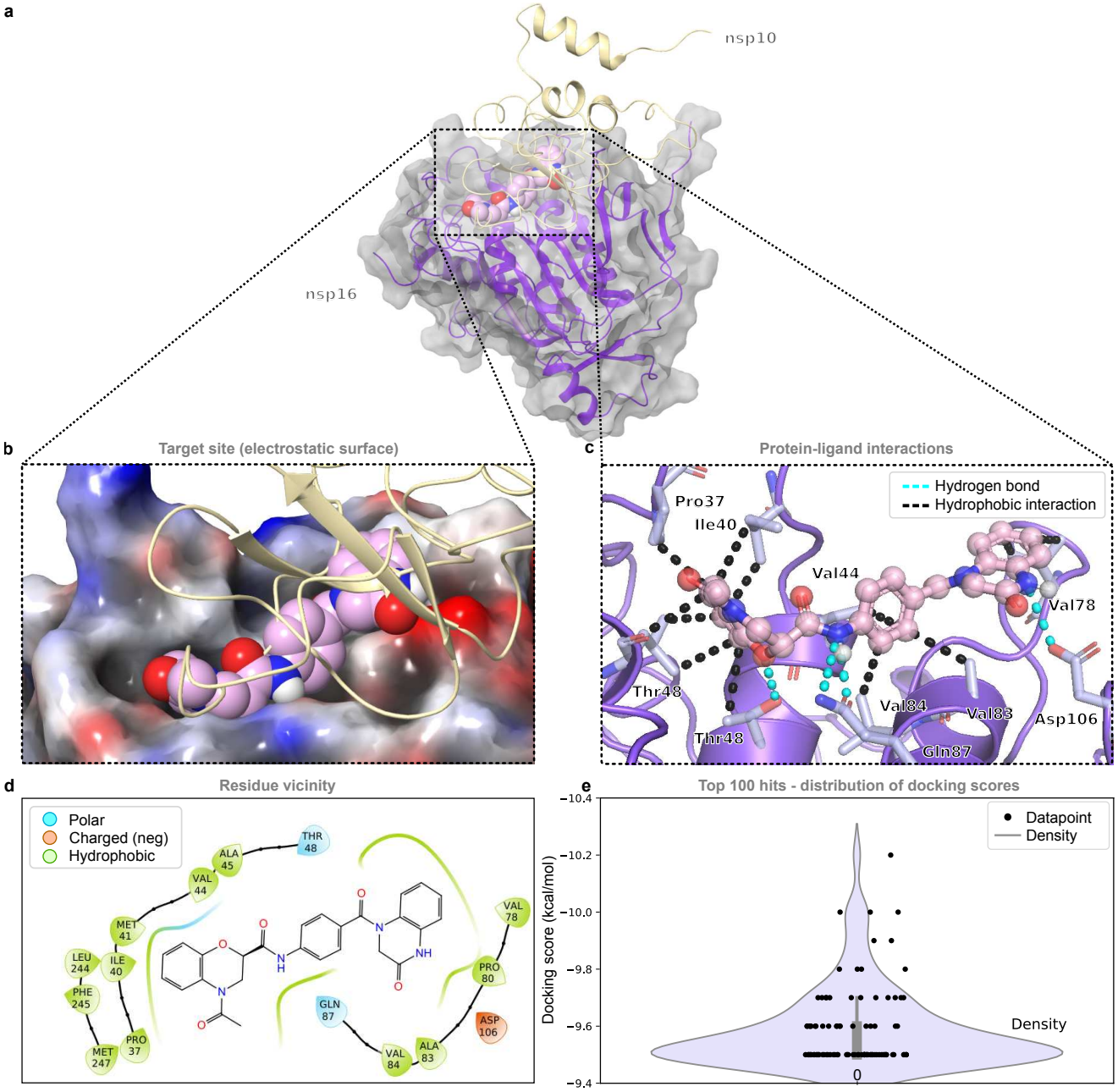
Supplementary Fig. 14. The helicase (nsp13) and an example compound from the top 0.0001% of screened compounds bound at region 2 of the RNA binding interface. a, The helicase (violet) bound to an example compound (light pink) at region 2 of the RNA binding interface. A docked DNA strand is shown in light gold (Screen ID:35). **b**, Electrostatic surface of the helicase to which an example compound (light pink) and a docked DNA strand (light gold) are bound. **c,** An overview of the interactions between the compound and the helicase structure. **d,** Reesidues within 4 Å of the inhibitor. **e,** Distribution of the docking scores of the top 100 virtual screening hits.



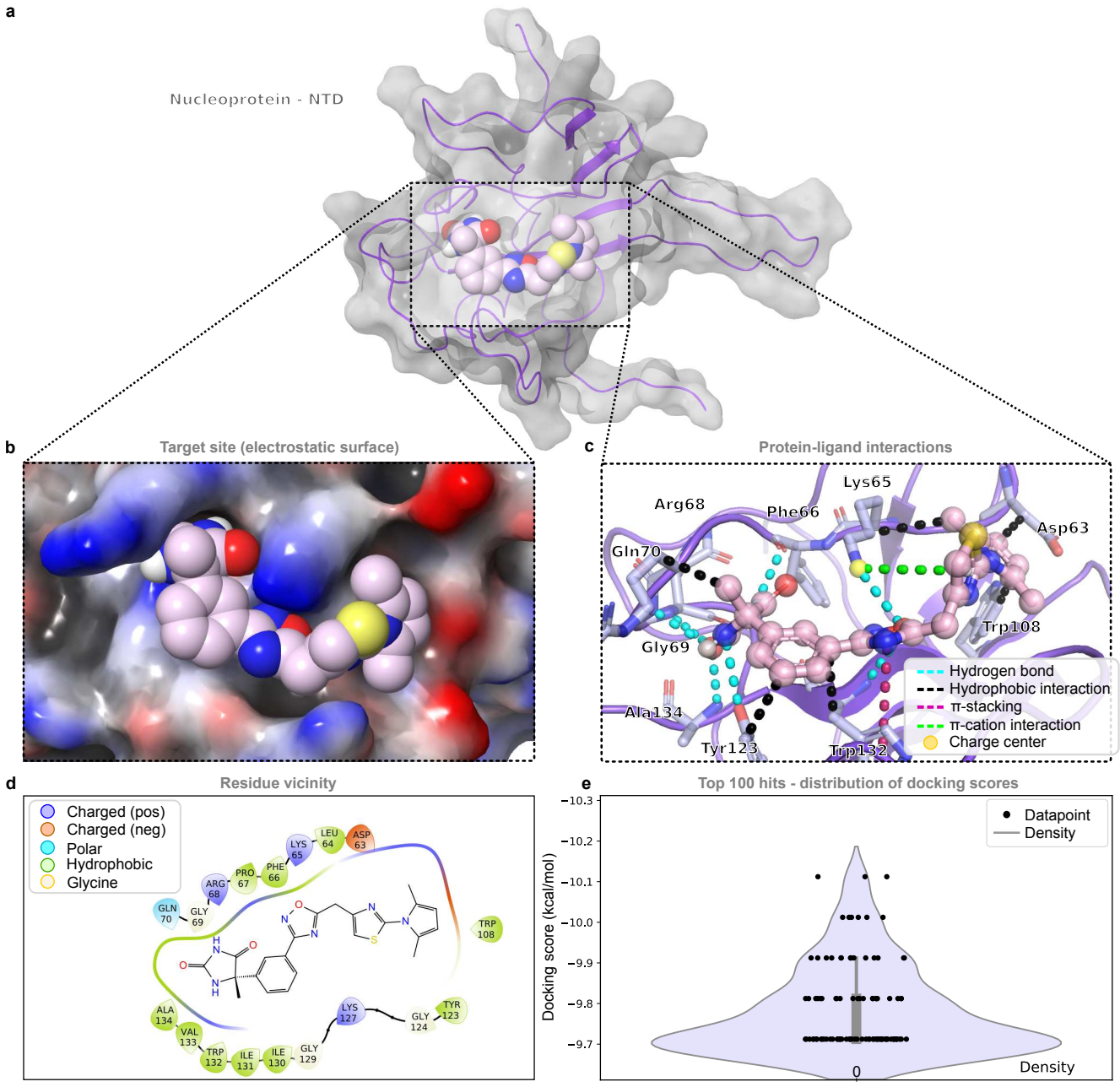
Supplementary Fig. 15. nsp14 and an example compound from the top 0.0001% of screened compounds bound at the nsp10 protein-protein interface. a, nsp14 (violet) bound to an example compound (light pink) at the nsp10 (light gold) binding interface (Screen ID: 36). **b**, Electrostatic surface of nsp14 to which an example compound (light pink) and nsp10 (light gold) are bound. **c,** An overview of the interactions between the compound and the nsp14 structure. **d,** Residues within 4 Å of the inhibitor. **e,** Distribution of the docking scores of the top 100 virtual screening hits.



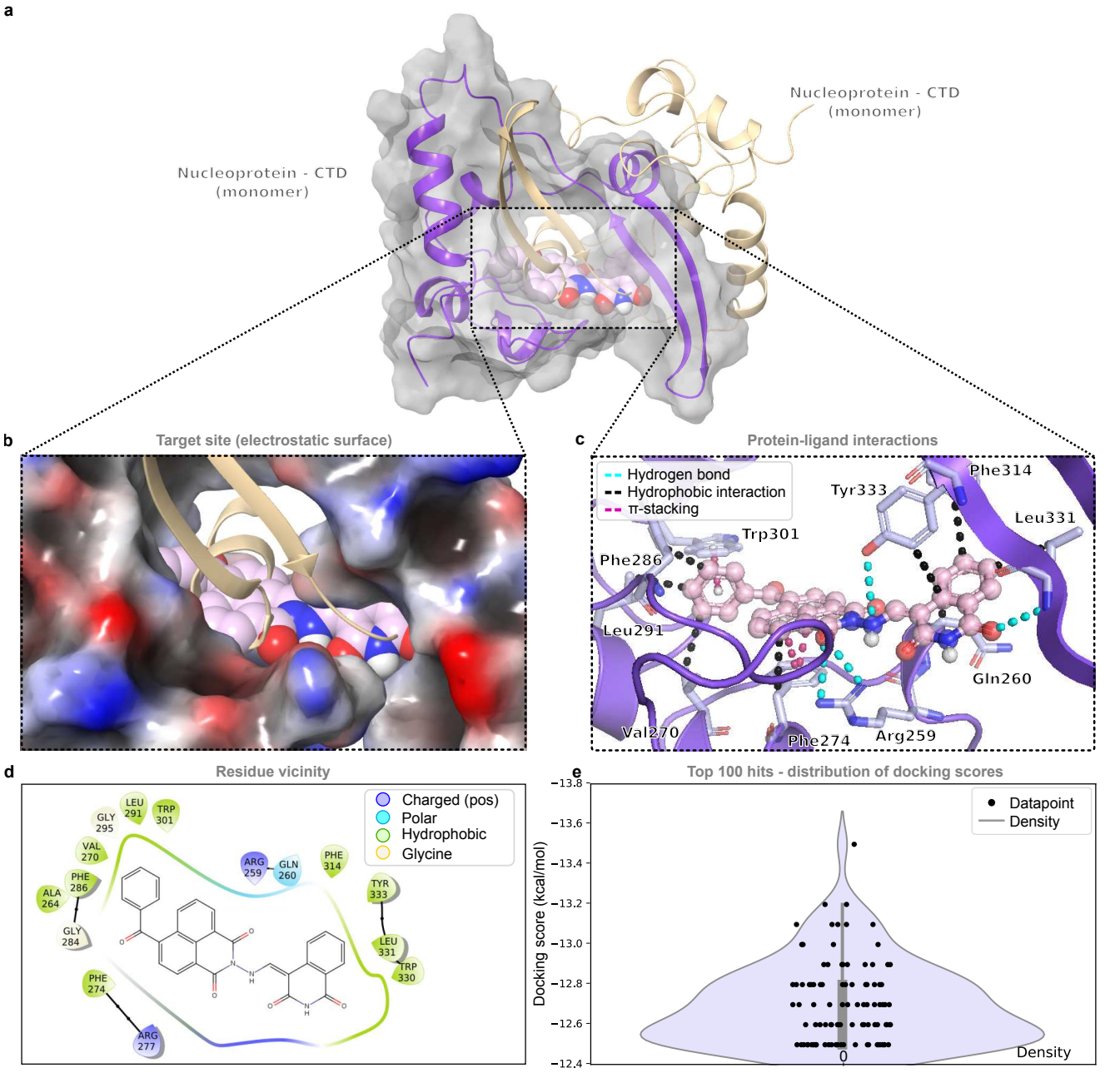
Supplementary Fig. 16. nsp14 and an example compound from the top 0.0001% of screened compounds bound at the active site of the exoribonuclease domain. **a**, nsp14 (violet) bound to an example compound (light pink) at the active site of the exoribonuclease domain (Screen ID:38). **b**, Electrostatic surface of nsp14 to which an example compound (light pink) is bound. **c,** An overview of the interactions between the compound and the nsp14 structure. **d,** Residues within 4 Å of the inhibitor. **e,** Distribution of the docking scores of the top 100 virtual screening hits.



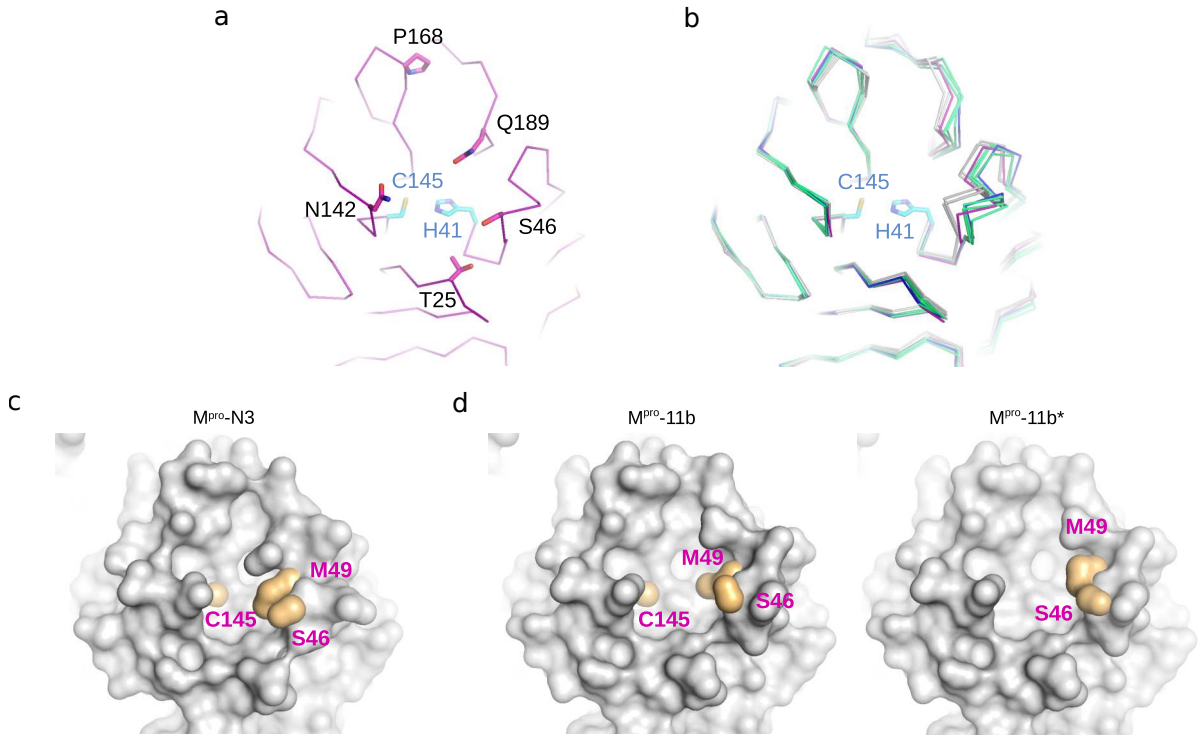
Supplementary Fig. 17. nsp16 and an example compound from the top 0.0001% of screened compounds bound at the nsp10 protein-protein interaction interface. **a**, nsp16 (violet) bound to an example compound (light pink) at the nsp10 (light gold) protein-protein interface (Screen ID:41). **b**, Electrostatic surface of nsp16 to which an example compound (light pink) and nsp10 (light gold) are bound. **c,** An overview of the interactions between the compound and the nsp16 structure. **d,** Residues within 4 Å of the inhibitor. **e,** Distribution of the docking scores of the top 100 virtual screening hits.



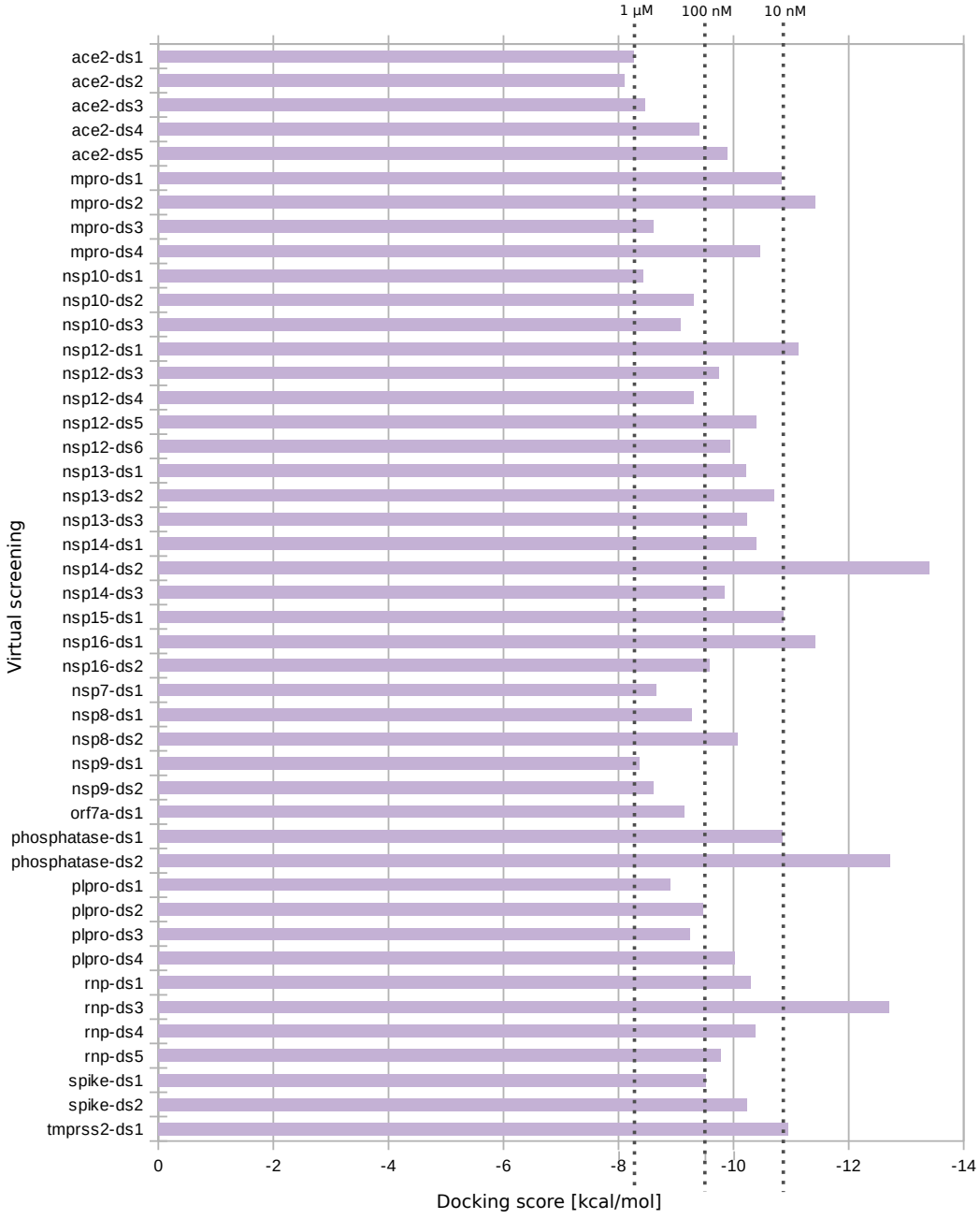
Supplementary Fig. 18. N-terminal domain of the nucleoprotein and an example compound from the top 0.0001% of screened compounds bound at the oligomerization interface. a, N-terminal domain (NTD) of the nucleoprotein (violet) bound to an example compound (light pink) at the oligomerization interface (Screen ID: 44). **b**, Electrostatic surface of the NTD of the nucleoprotein to which an example compound (light pink) is bound. **c,** An overview of the interactions between the compound and the NTD structure. **d,** Residues within 4 Å of the inhibitor. **e,** Distribution of the docking scores of the top 100 virtual screening hits.



Supplementary Fig. 19. C-terminal domain of the nucleoprotein and an example compound from the top 0.0001% of screened compounds bound at the dimerization interface. **a**, C-terminal domain (CTD) of the nucleoprotein (violet) bound to an example compound (light pink) at the dimerization interface. A second CTD of the nucleoprotein is shown in light gold (Screen ID:42). **b**, Electrostatic surface of the CTD of the nucleoprotein to which an example compound (light pink) and a second CTD of the nucldeoprotein (light gold) are bound. **c,** An overview of the interactions between the compound and the receptor structure. **d,** Residues within 4 Å of the inhibitor. **e,** Distribution of the docking scores of the top 100 virtual screening hits.



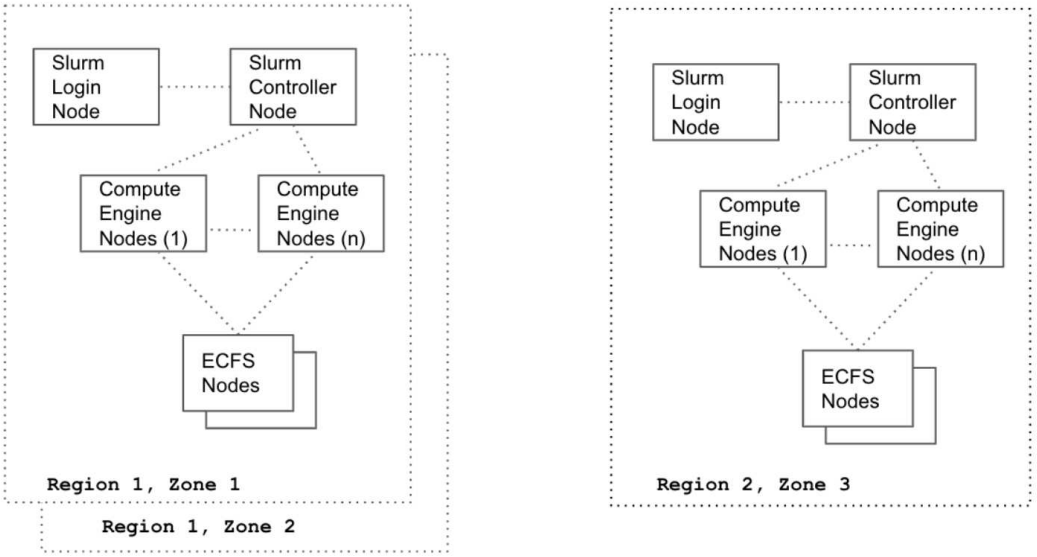
Supplementary Fig. 20. Conformation of the active site of M^{pro} and models for *in silico* screening. a, Secondary structural elements that form the active site of M^{pro}. The catalytic dyad Cys145 (C145)-His41 (H41) at the base of the active site is surrounded by secondary structural elements contributed by domains I and II of the protease. The side chains of selected residues are shown: Thr25 (T25), Ser46 (S46), Asn142 (N142), Pro168 (P168) and Gln189 (Q189). The structure of M^{pro} bound to the inhibitor N3 is shown (PDB ID 6lu7). **b**, Overlay of M^{pro} active site structures showing that binding of inhibitors induces conformational changes in two secondary structural elements, which form the walls of the active site: the loop harboring Gln189 and the short α-helix harboring Ser46 (see panel **a**). The main chain is colored gray for the three apo structures of M^{pro} (PDB IDs 6y2e, 6yb7, 6m2q), purple for the structure of M^{pro} bound to the inhibitor N3 (PDB ID 6lu7), blue for the structure of M^{pro} bound to the inhibitor 11b (PDB ID 6m0k) and green for three other structures of M^{pro} bound to inhibitors (PDB IDs 6m2n, 6y2g, 7buy). **c**, Van der Waals surface of the active site of M^{pro} bound to the inhibitor N3 (PDB ID 6lu7), after removing all water and ligand molecules. The side chains of Met49 (M49), Ser46 (S46) and Cys145 (C145) are colored. **d**, Van der Waals surface of the active site of M^{pro} bound to the inhibitor 11b (PDB ID 6m0k), after removing all water and ligand molecules (left) and the same structure after selecting different rotamers for the side chains of Met49, Ser46 and Cys145 (right). The images in panels **a-d** show M^{pro} from the same orientation and were generated using PyMOL.



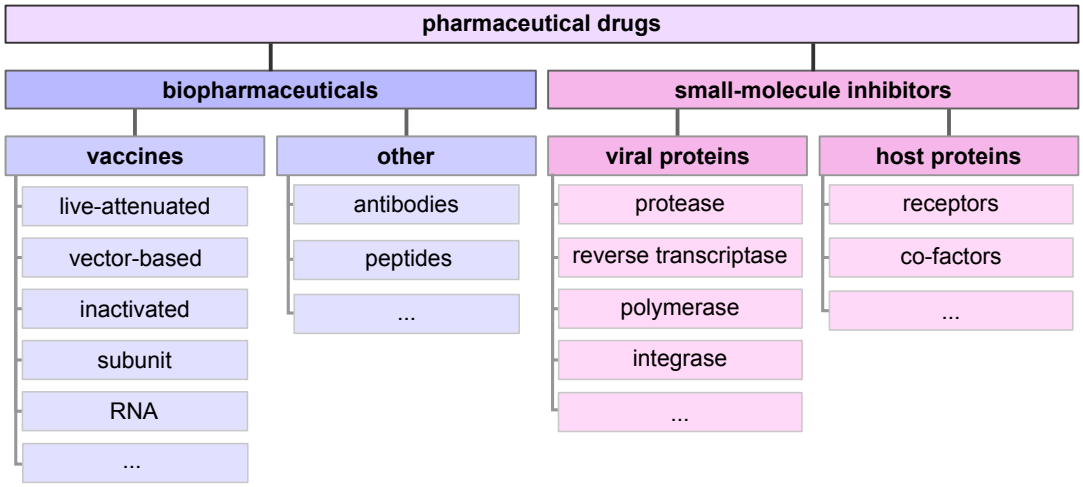
Supplementary Fig. 21. Average docking scores of the top hits. Average docking scores of the top 100 compounds of each virtual screen that was carried out. Only compounds with cLogP less than 6, molecular weight less than 600 dalton, no reactive groups, and at most ten hydrogen bond acceptors were considered (a smaller number of non-druglike molecules from the ZINC library were also removed by visual inspection). The docking scores estimate free energy of binding in kcal/mol. These are computational values that can diverge significantly from the experimental binding free energies. The dashed lines indicate the corresponding K_d values of 1 µM, 100 nM, and 10 nM under standard conditions..

Nodes	GCE instance type
Slurm controller node	n1-standard-16
Slurm login node	n1-standard-8
Slurm compute nodes	n2d-highcpu-64 (cluster 1 and 2), n1-highcpu-32 (cluster 3)
Elastifile management node	n1-standard-8
ECFS storage node	custom (16 vCPUs, 96 GB memory)

Supplementary Table 1. Vitual manchine types employed in the Google Cloud Platform.



Supplementary Fig. 22. Google Cloud Platform (VPC-1)



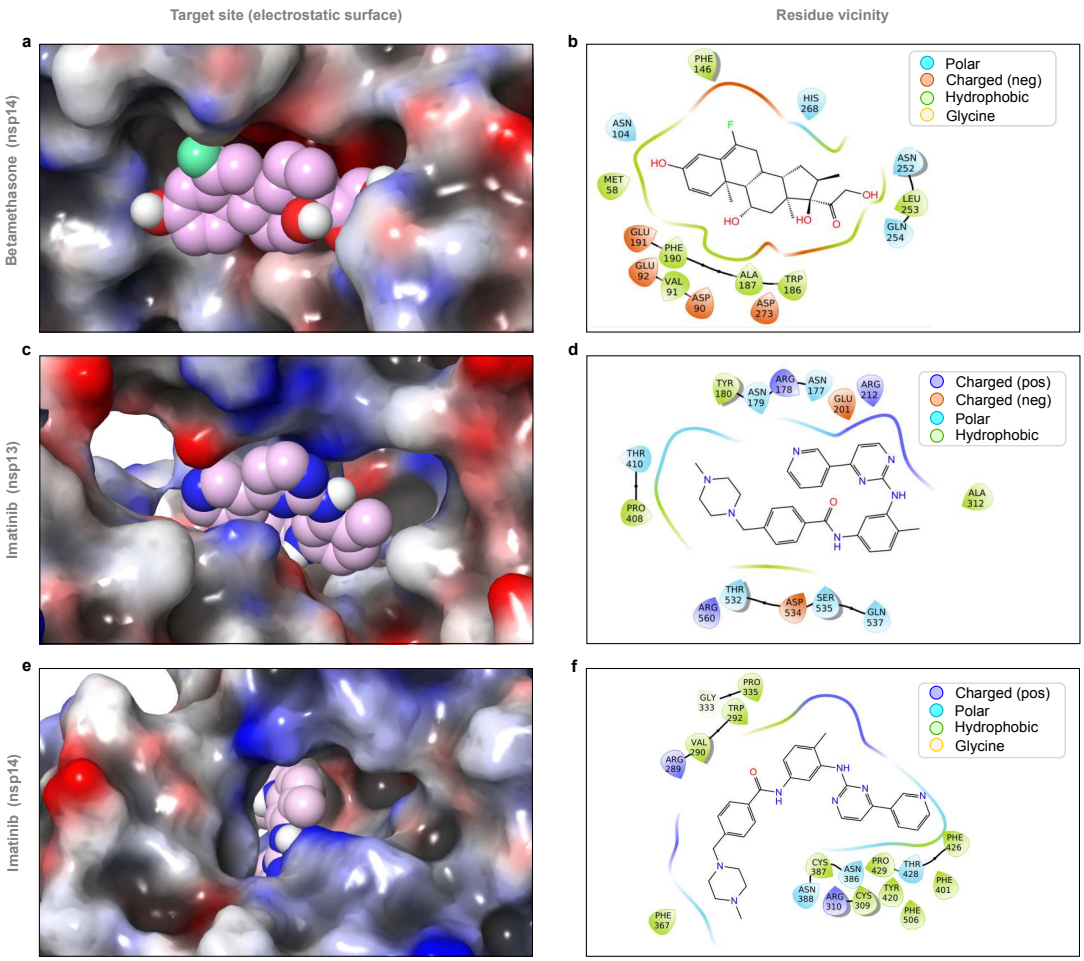
Supplementary Fig. 23. Classes of pharmaceutical drug: A non-exhaustive classification of pharmaceutical drugs that could potentially be leveraged against SARS-CoV-2, including possible small-molecule inhibitor targets

Index	Site	Target protein	Virus	Structure/Sequence	IC50 [uM]	Docking score	Reference	Similar hit compounds
1	Active site	PLPro	SARS	C[C@@H](N1CCC(C(NCC2=CC(OCO3)=C3C=C2)=O)CC1)C4=CC=CC5=C4C=CC=C5	0.32	-7.2	(173)	52
2	Near active site	PLPro	SARS MERS	S=C1C2=C(N=CN2)N=CN1	21.6 ± 1.8 26.9 ± 7.5	-4.3	(174, 175)	9
3	Near active site	PLPro	SARS MERS	S=C1C2=C(N=CN2)N=C(N)N1	5.0 ± 1.7 24.4 ± 4.3	-5	(174, 175)	97
4	Not specified non-competitive site	PLPro Mpro	SARS SARS	CC1=CC=CC2=C3C(C(OCC4C)=C4C(C3=O)=O)=CC=C12	4.9 ± 1.2 14.4 ± 0.7	-6.9	(170)	0
5	AS	Mpro	SARS	ClC1=CC=C(SSC2=NN=CO2)C=C1	0.52 ± 0.06	-7.7	(171)	0
6	Active site	MPro	SARS	CC1=NOC(C(N[C@@H](C)C(N[C@H](C(C)C)C(N[C@@H](CC(C)C)-C(N[C@@H](C[C@@H]2CCNC2=O)/C=C/C(OCC3=CC=CC=C3)=O)=O)=O)=O)=O)=C1	Ki = 9.0 ± 0.8	-5.9	(172)	≈ 1000
7	Not specified	Helicase	SARS	O=C(NC1=CC=C(S(=O)(N)=O)C=C1)/C=C/C2=CC=CO2	2.09 ± 0.3 (ATP-hydrolysis) 13.2 ± 0.9 (DNA unwinding)	-7.9	(181)	N/A
8	Not specified	Helicase	SARS	O=C1C2=C(N=C(S)N2CC)N(C)C(N1)=O	8.66 ± 0.26 (ATP-hydrolysis) 41.6 ± 2.3 (DNA unwinding)	N/A	(182)	N/A
9	Not specified	Helicase	MERS	CCC1=NC(C)=C(CN2CC(C3=CC=NC(C4=CC=CC(O)=C4)=C3)CC2)N1	KD = 47.6	N/A	(183)	N/A
10	Fusion peptide	Spike	SARS	KYEQYIKWPWYVWLGF (MPER peptide)	26	N/A	(178)	N/A
11	HR1 domain	Spike	SARS MERS	LKVLLYEEFKLLESLIMEILE YQKDSDIKENAEDTK (EK1 peptide)	0.27 ± 0.01 0.18 ± 0.01	N/A	(59)	N/A
12	Not specified	Spike/ACE2	SARS	OC(COC1=CC=CC(OCC(O)CN2CCCCC2)=C1)CN3CCCCC3	EC50 = 3	N/A	(179)	N/A
13	Active site	Nsp15	SARS	CC1=CC(C2=CC=C(/N=N/C3=C(N)C=CC4=C3C=CC(S(=O)(O)=O)=C4)C(C)=C2)=CC=C1/N=N/C5=C(N)C=CC6=C5C=CC(S(=O)(O)=O)=C6	0.2 ± 0.02	-8.6	(180)	4
14	Active site	RdRP	MERS	O=C1N=C(NO)C=CN1[C@H]2[C@H](O)[C@H](O)[C@@H](CO)O2	EC50 = 0.56	-6.1	(176)	≈ 200
15	Active site	RdRP	SARS MERS	NC1=NC=NN2C([C@@]3(C#N)[C@H](O)[C@H](O)[C@@H](CO[P@@]-(N[C@@H](C)C(OCC(CC)CC)=O)(OC4=CC=CC=C4)=O)O3)=CC=C12	0.07 0.03	-6.8	(177)	≈ 1600

Supplementary Table 2. Known inhibitors of SARS-CoV-2. The inhibitors that were previously reported for SARS-CoV-2 proteins were docked against respective targets and the docking scores were calculated using the same computational methods we used in the screens described in this manuscript.

ZINCID	Generic name	COVID clinical trial	Targets (Screen IDs)
ZINC000040165249	11-beta-Hydroxyandrosterone-3-glucuronide	No	nsp16 (41), TMPRSS2 (6)
ZINC000013540864	3'-Azido-3'-deoxy-5'- O-beta-D-glucopyranuronosylthymidine	No	nsp13 (33)
ZINC000040164488	5-alpha-Dihydrotestosterone glucuronide	No	ORF7a (9), nucleoprotein (44)
ZINC000208774715	Acalabrutinib	Yes	nucleoprotein (45)
ZINC000003861599	Aldactone	Yes	nsp14 (37)
ZINC000066166864	Alectinib	No	nsp12 (32)
ZINC000014261579	Alvesco	Yes	nsp13 (34)
ZINC000014768568	Aprepitant	No	nsp14 (38)
ZINC000003973334	Aromasin	No	nucleoprotein (44)
ZINC000012504271 *	Atavaquone	No	nsp15 (39), nsp16 (40, 41), nucleoprotein (44, 45)
ZINC000116473771 *	Atovaquone	Yes	nsp12 (31), nsp13 (33), macrodomain (10,11), nucleoprotein (45)
ZINC000003872931	Avapro	No	macrodomain (11)
ZINC000003932831 *	Avodart	Yes	nsp13 (34)
ZINC000009232411	Benperidol	No	macrodomain (10)
ZINC000004097384	Betamethasone	Yes	nsp14 (38)
ZINC000019203128	Biosone	No	mpro (19), nsp10 (26), nsp13 (34)
ZINC000003977868	Biosone	No	nsp10 (17)
ZINC000019203134	Biosone	No	nsp10 (26), nsp12 (29), nsp13 (34)
ZINC000019203131	Biosone	No	nsp13 (34)
ZINC000011677911	Bisoctrizole	No	nsp12 (32), nsp13 (34), nsp8 (21), nucleoprotein (43)
ZINC000148723177	Brigatinib	No	nsp12 (29), nsp13 (35)
ZINC000019364228	Buclizine	No	nsp12 (31)
ZINC000003977981	Capex	No	mpro (17)
ZINC000043195321 *	Capmatinib	No	mpro (16), nsp12 (28), nsp15 (39), macrodomain (11)
ZINC000004215257	Cipiramide	No	nsp13 (34,35)
ZINC000021981222	cgp74588	No	nsp12 (32), nsp14 (37)
ZINC000003993855	Cilais	No	mpro (16), TMPRSS2 (6)
ZINC000004098610	Daidzin	No	nucleoprotein(44)
ZINC000043710727	Dehydroepiandrosterone	No	macrodomain (10)
ZINC000003784182	Differin	No	nsp8 (21, 22), nsp12 (28), nucleoprotein (45)
ZINC000011677837	Eliquis	No	TMPRSS2 (6)
ZINC000011679756 *	Eltombopag	No	nsp14 (37), nucleoprotein (43), nsp16 (40), mpro (19)
ZINC000222731806	Enasidenib	No	ACE2 (4), mpro (16, 17)
ZINC000245204943	Eplerenone	No	nucleoprotein (41)
ZINC000238850852	Eptifibatide	No	nsp13 (34)
ZINC000238850855	Eptifibatide	No	mpro (17), nsp12 (29), nucleoprotein (42)
ZINC000238850853	Eptifibatide	No	nsp12 (28, 29, 32), nucleoprotein (43)
ZINC000238850854	Eptifibatide	No	nsp12 (29, 31), nsp14 (38)
ZINC000052955754*	Ergotamine	No	mpro (16, 17), nsp13 (34,35), nsp8 (22)
ZINC000003876078	Estradiol	Yes	nsp14 (38), spike (8)
ZINC000004099035	Estradiol 17b glucorinide	No	nsp10 (26), nsp13 (33), nucleoprotein (45)
ZINC000003881345	Estradiol benzoate	Yes	spike (8)
ZINC000004096817	Estradiol glucuronide	No	nsp13 (33)
ZINC000102136963	Estriol-3-glucuronide	No	plpro(12)
ZINC000102136971	Estriol-3-glucuronide	No	nucleoprotein (44)
ZINC000008234405	Estriol-3-glucuronide*	No	nsp10 (26), nsp12 (31), nsp13 (33), orf7a (9), nucleoprotein (44)
ZINC000004099004	Estrone glucoronide	No	nsp12 (31),nsp13 (33,35), nucleoprotein (44)
ZINC000001481815	Exjade	No	mpro(16), nsp12 (32), rnp (44), tmprss2 (6)
ZINC000008215434	FAD	No	mpro (17), nsp13 (35), rnp (42)
ZINC000003977985	Flumetasone	No	nsp15 (39)
ZINC000004097305	Flumisolide	No	nsp14 (38)
ZINC000001543181	Ibutamoren	No	nsp14 (41)
ZINC000013986658	Idelalisib	No	mpro (17), nsp13 (33)
ZINC000019632618	Imatinib	Yes	nsp13 (35), nsp14 (37)
ZINC000100005073	Indigo carmine	No	nucleoprotein (44)
ZINC000261527149	Ivermectin	Yes	nsp12 (29), nucleoprotein (45)
ZINC000000537877	Ketanserin	No	TMPRSS2 (6)
ZINC000031417974	Ketoprofen glucoronide	No	nsp13 (33)
ZINC000003781738*	Lestaurtinib	No	mpro (16)
ZINC000031290884	Lorazepam glucoronide	No	nsp13 (33)
ZINC000064033452 *	Lumacaftor	No	mpro (17), nsp12 (28), nsp13 (33), nsp14 (37), tmprss2 (6)
ZINC000118912516	Meprednisone acetate	No	mpro (19)
ZINC000100017856*	Mepron	Yes	nsp15 (39), nsp16 (40), rnp (43,44,45)
ZINC000013831810	Mizolastine	No	mpro (16), nsp12 (30)
ZINC000003874467	Nafamostat	Yes	ORF7a (9), plpro (13), nucleoprotein (44)
ZINC000003881613	Nandrolone phenpropionate	No	nsp12 (31), spike (8)
ZINC000011681563	Netupitant	No	nsp12 (31), nsp14 (36), rnp (42, 43)
ZINC000006716957 *	Nilotinib	No	mpro (16,17), nsp14 (37), rnp (43), tmprss2 (6)
ZINC000031460590	Oxazepam glucuronide	No	nsp13 (33)
ZINC000031460595	Oxazepam glucuronide	No	mpro (19), TMPSS2 (6)
ZINC000095626782	Oxytetracycline	Yes	nucleoprotein (44)
ZINC000001481956	Paliperidone	No	macrodomain (11), rnp (44), tmprss2 (6)
ZINC000004214700	Paliperidone	No	nucleoprotein (43)
ZINC000000538152	Pamoic acid	No	macrodomain (10)
ZINC000011617039	Pazopanib	No	nucleoprotein (44)
ZINC000004217252	Penfluridol	No	ace2 (5), nsp8 (22), rnp (43)
ZINC000334138264	Rifabutin	No	mpro (17), nsp12 (29,32)
ZINC000253848650	Rifabutin	No	nsp12 (29,32)
ZINC000003816514	Rolapitant	No	nsp14 (37), nsp16 (41)
ZINC000000598829	Rupatadine	No	nucleoprotein (43)
ZINC000000898237	Rutaecarpine	No	macrodomain (11)
ZINC000004096846	Rutaecarpine	No	mpro (17), nsp12 (29)
ZINC000072206342	Rutin	No	nsp12 (28)
ZINC000100074252	Sofosbuvir	Yes	plpro (15)
ZINC000000601275 *	Talniflumate	No	ace2 (5), mpro (16,19), nsp15 (39), nsp8 (22)
ZINC000001844627	Talniflumate	No	ace2 (5), mpro (16), nsp13 (33), nsp15 (39)
ZINC000000538415	Tamibarotene	No	nsp12 (28)
ZINC000011525121	Tetracycline hydrochloride	Yes	nsp14 (38), nsp16 (40), nucleoprotein (45)
ZINC000003812889	Tibolone	No	nsp12 (31)
ZINC000003938684	Toposar	Yes	nsp16 (40)
ZINC000003925861	Vorapaxar	No	ACE2 (4)
ZINC000218037687	Voxilaprevir	No	nsp12 (29, 30, 32), nucleoprotein (43)
ZINC000000577115 *	Xaliproden	No	nsp12 (28), nsp14 (36), macrodomain (11). tmprss2 (6)
ZINC000003927200	Yaz, Drospirenone	No	nsp12 (31), nsp15 (39), macrodomain (10), rnp (43)
ZINC000052509366	Zelboraf	No	mpro (17)
ZINC000003797541	Zytiga	No	nsp12 (31)

Supplementary Table 3. Approved drugs among the virtual screening hits. A table of "world approved" drugs that bind to SARS-CoV-2 proteins as identified by VirtualFlow. These drugs are mined from the top 1 % of the hits from "in stock" compounds of the ZINC library. The drugs presented here are the top 1 % of hits that were further filtered for a docking score of better than -8 kcal/mol. Some of the drugs are predicted to bind to multiple protein targets, and for some of the drugs (denoted by *) only the targets of the top five virtual screens as judged by the docking score are shown. Some of the drugs shown here are currently in clinical trials for the treatment of COVID-19 (highlighted in light green).



Supplementary Fig. 24. Docking poses of two exemplar approved drug hits that came up in the top 1% of the hits from "in stock" compounds of the ZINC library , against their respective targets. **a**, electrostatic surface of nsp14 N7 Methyl transferase's active site (N7-MTase) (Screen ID: 38) to which betamethasone is bound **b**, An overview of the interactions between betamethasone and the N7-MTase active site pocket of nsp14 **c**, electrostatic surface of the RNA binding pocket of nsp 13 helicase (Screen ID: 35) to which imatinib is bound **d**, overview of interactions between imatinib and the RNA binding pocket of the helicase nsp13 **e**, electrostatic surface representation of nsp14 methyl transferase ExoN Active site (Screen ID: 37) where imatinib is bound **f**,interaction interface diagram of imatinib with nsp14 Exon active site.

Compound name	ZINC_ID	Human gene	Viral bait	Indication	Clinical Trial identifier	Target 1 (Screen ID)	Docking score	Target 2 (Screen ID)	Docking score	Target 3 (Screen ID)	Docking score
Nafamostat	ZINC3874467	Cell Entry	-	Anticoagulant	NCT04352400, NCT04418128	orf7a (9)	-8	plpro(13)	-8.5	rnp(43)	-8.5
Pazopanib	ZINC11617039	MARK2	orf9b	Cancer	-	rnp (43)	-8.3				
progesterone	ZINC4428529	SIGMAR1/SIGMAR2	Nsp6/Orf9c	birth control	NCT04365127	plpro (12)	-7.1				
Pimoazide	ZINC4175630	SIGMAR1/SIGMAR2	Nsp6/Orf9c	Tourette syndrome	-	nsp16 (41)	-7.8	nsp7(20)	-7	spike(7)	-7.9
Silmitasertib	ZINC58638454	CSNK2A2	-	Cancer	under consideration	nsp16(40)	-9.6				

Supplementary Table 4. A list of drug hits that found to be in common between a previously published SARS-COV-2 interactome study (193) and our virtual screens. These drugs, upon experimental validation, could be potentially developed into multi-target drugs capable of modulating both host and viral targets simultaneously. Three of the drugs listed here are currently undergoing clinical trials for the treatment of COVID-19 (highlighted in light green).

Name	Catalog ID	Score	LE	MW	Library	SMILES
vMpro-as1-1	Z1002304178	-11.3	0.353	431.43	REAL	C[C@]1(c2cccc(CNc3ccc4nnc(-c5ccccc5F)n4n3)c2)NC(=O)NC1=O
vMpro-as1-2	Z1000940198	-11.2	0.32	473.488	REAL	Cc1cc(-c2cc(C(=O)NCc3cccc([C@@]4(C)NC(=O)NC4=O)c3)c3c(C)noc3n2)c(C)o1
vMpro-as1-3	Z1927967127	-11.2	0.373	407.379	REAL	Nc1ncc2c(n1)CCN(C(=O)c1cc(F)cc3c(=O)c4cc(F)ccc4[nH]c13)C2
vMpro-as1-4	Z993683084	-11.2	0.329	456.501	REAL	C[C@@]1(c2cccc(CNC(=O)[C@H]3CC(=O)N(c4cccc5ccccc45)C3)c2)NC(=O)NC1=O
vMpro-as1-5	ZINC000017189271	-11.2	0.361	433.403	ZINC15	O=C1NC(=O)/C(=N/c2cccc3c(O)nnc(O)c23)[C@@H](c2nc3ccccc3s2)C1=O
vMpro-as1-6	Z1000940282	-11.1	0.317	473.463	REAL	Cc1noc2nc(-c3ccc(F)cc3)ccc(C(=O)NCc3cccc([C@@]4(C)NC(=O)NC4=O)c3)c12
vMpro-as1-7	Z1014391890	-11.1	0.308	490.552	REAL	O=C([C@@H]1C[C@@H]2CCCC[C@H]2N1C(=O)c1ccc(F)cc1F)N1CC=C(c2c[nH]c3ncccc23)CC1
vMpro-as1-8	Z1614250722	-11.1	0.336	444.494	REAL	C[C@@]1(c2cccc(C(=O)N3CCC[C@H](c4n[nH]c(-c5cccc5)n4)C3)c2)NC(=O)NC1=O
vMpro-as1-9	Z68547169	-11.1	0.3	498.581	REAL	C[C@@H](OC(=O)c1cc(-c2ccncc2)nc2ccccc12)C(=O)NC(=O)NC12CC3CC(CC(C3)C1)C2
vMpro-as1-10	Z68550114	-11.1	0.3	498.581	REAL	C[C@@H](OC(=O)c1cc(-c2cccnc2)nc2ccccc12)C(=O)NC(=O)NC12CC3CC(CC(C3)C1)C2
vMpro-as1-11	Z1000939356	-11	0.314	469.5	REAL	Cc1ccc(-c2cc(C(=O)NCc3cccc([C@@]4(C)NC(=O)NC4=O)c3)c3c(C)noc3n2)cc1
vMpro-as1-12	Z1002304370	-11	0.355	413.44	REAL	C[C@]1(c2cccc(CNc3ccc4nnc(-c5ccccc5)n4n3)c2)NC(=O)NC1=O
vMpro-as1-13	Z1162536284	-11	0.333	449.493	REAL	O=C(Nc1nc2ccccc2c(=O)[nH]1)c1cc(-c2nc3ccccc3s2)nc2ccccc12
vMpro-as1-14	Z806293372	-11	0.306	480.523	REAL	C[C@@]1(c2cccc(NC(=O)[C@@H]3CC(=O)N(c4ccc5c(c4)Cc4ccccc4-5)C3)c2)NC(=O)NC1=O
vMpro-as1-15	Z1039095378	-10.9	0.33	482.33	REAL	C[C@]1(c2cccc(CNc3ccc4nnc(-c5cc(Cl)cc(Cl)c5)n4n3)c2)NC(=O)NC1=O
vMpro-as1-16	Z1451529036	-10.9	0.363	406.416	REAL	C[C@]1(c2cccc(C(=O)N3CCc4[nH]c5ccc(F)cc5c4C3)c2)NC(=O)NC1=O
vMpro-as1-17	Z1541650451	-10.9	0.352	422.471	REAL	O=C(Nc1nc2ccccn2n1)c1cc(-c2nc3ccccc3s2)nc2ccccc12
vMpro-as1-18	Z281532788	-10.9	0.295	493.522	REAL	CCn1c(NNC(=O)c2cc(-c3ccc4c(c3)OCCO4)nc3ccccc23)nc2ccccc2c1=O
vMpro-as1-19	ZINC000020572816	-10.9	0.295	496.497	ZINC15	O=C1Nc2cccc(F)cc2[C@]12N[C@@H](Cc1c[nH]c3ccc(O)cc13)[C@@H]1C(=O)N(c3ccccc3)C(=O)[C@@H]12
vMpro-as1-20	ZINC000020758902	-10.9	0.303	478.507	ZINC15	O=C1Nc2ccccc2[C@]12N[C@@H](Cc1c[nH]c3ccc(O)cc13)[C@@H]1C(=O)N(c3ccccc3)C(=O)[C@@H]12
vMpro-as1-21	ZINC000102513812	-10.9	0.311	490.554	ZINC15	Cc1ccc(/C(O)=C2\C(=O)C(=O)N(c3nc4ccc(F)cc4s3)[C@H]2c2ccc(C(C)(C)C)cc2)o1
vMpro-as1-22	ZINC000408975126	-10.9	0.363	388.429	ZINC15	O=C(Nc1ccc2ccccc2c1)c1ccc2[nH]c3nc4ccccc4nc3c2c1
vMpro-as1-23	PV-001955706104	-10.8	0.348	423.472	REAL	C[C@@]1(c2cccc(CNC(=O)NCc3cc4c(nc3O)CCCC4)c2)NC(=O)NC1=O
vMpro-as1-24	Z1007204568	-10.8	0.327	447.45	REAL	C[C@@]1(c2cccc(CNC(=O)c3c[nH]nc3-c3ccc4c(c3)OCCO4)c2)NC(=O)NC1=O
vMpro-as1-25	Z1643054649	-10.8	0.348	406.444	REAL	Cc1cc(NC(=O)c2cc(-c3cccc4ccccc34)nc3ccccc23)nc(=O)[nH]1
vMpro-as1-26	Z2002795192	-10.8	0.4	387.862	REAL	CCOCCOc1c(Cl)cccc1NC(=O)[C@@]12[C@@H]3C(=O)[C@H]4[C@@H]5[C@H]([C@H]41)[C@H]2[C@H]53
vMpro-as1-27	Z2142999535	-10.8	0.338	431.49	REAL	Cn1c(C(=O)N2C[C@@H](C(=O)N3CCCCC3)Oc3ccccc32)cc2ccccc2c1=O
vMpro-as1-28	Z296632530	-10.8	0.348	425.415	REAL	O=C1C[C@@H](C(=O)N2CCN(C(=O)c3cc4c(c3)OCO4)CC2)c2ccc(F)cc2N1
vMpro-as1-29	Z993686968	-10.8	0.36	406.441	REAL	C[C@@]1(c2cccc(CNC(=O)[C@H]3CC(=O)N(c4ccccc4)C3)c2)NC(=O)NC1=O
vMpro-as1-30	ZINC000003307955	-10.8	0.309	464.463	ZINC15	Cc1nn(-c2ccccc2)c2c1[C@]1(c3cc(F)ccc3NC1=O)N1N=NN(c3ccccc3)C1=N2
vMpro-as1-31	ZINC000020588479	-10.8	0.292	496.497	ZINC15	O=C1Nc2ccccc2[C@]12N[C@@H](Cc1c[nH]c3ccc(O)cc13)[C@@H]1C(=O)N(c3ccc(F)cc3)C(=O)[C@@H]12
vMpro-as1-32	ZINC000102877232	-10.8	0.309	486.566	ZINC15	CC(C)(C)c1ccc([C@H]2/C(=C(\O)c3ccccc3)C(=O)C(=O)N2c2nc3ccc(F)cc3s2)cc1
vMpro-as1-33	ZINC000245247236	-10.8	0.3	480.498	ZINC15	O=C1Nc2ccccc2[C@]12N[C@@H](Cc1c[nH]c3ccccc13)[C@H]1C(=O)N(c3ccccc3F)C(=O)[C@@H]12
vMpro-as1-34	PV-001955706148	-10.7	0.357	411.392	REAL	C[C@@]1(c2cccc(CNC(=O)NCc3noc4cc(F)ccc34)c2)NC(=O)NC1=O
vMpro-as1-35	Z1128746843	-10.7	0.306	489.555	REAL	Cc1cc(-c2cc(C(=O)NCc3cccc([C@@]4(C)NC(=O)NC4=O)c3)c3c(C)noc3n2)c(C)s1
vMpro-as1-36	Z137249204	-10.7	0.334	421.459	REAL	Cn1c(NNC(=O)c2cc(-c3ccccc3)nc3ccccc23)nc2ccccc2c1=O
vMpro-as1-37	Z1402639526	-10.7	0.334	445.913	REAL	Cn1cc(-c2nc3ccccn3c2NC(=O)N2CCc3[nH]c4ccc(Cl)cc4c3C2)cn1
vMpro-as1-38	Z1402639786	-10.7	0.334	429.458	REAL	Cn1cc(-c2nc3ccccn3c2NC(=O)N2CCc3[nH]c4ccc(F)cc4c3C2)cn1
vMpro-as1-39	Z1942531317	-10.7	0.357	404.512	REAL	O=C(c1cc(O)c2ccccc2c1)N1CCC[C@H](c2n[nH]c(C3CCCCC3)n2)C1
vMpro-as1-40	Z2157916861	-10.7	0.334	427.463	REAL	C[C@@]1(c2cccc(-c3noc(-c4cccc5c6c([nH]c45)CCCC6)n3)c2)NC(=O)NC1=O
vMpro-as1-41	Z993687126	-10.7	0.315	462.548	REAL	Cc1cc(C)cc(C(=O)N2CCC[C@H](C(=O)NCc3cccc([C@]4(C)NC(=O)NC4=O)c3)C2)c1
vMpro-as1-42	Z998726482	-10.7	0.297	482.518	REAL	O=C(Nc1ccc2[nH]c(-c3ccc(F)cc3)nc2c1)[C@H]1CCCN(C(=O)c2ccc3[nH]ncc3c2)C1
vMpro-as1-43	ZINC000000828265	-10.7	0.306	463.531	ZINC15	CC1(C)CC(=O)C2=C(C1)c1c(ccc3ccccc31)N[C@H]2c1ccc(-c2cccc(C(=O)O)c2)o1
vMpro-as1-44	ZINC000004785154	-10.7	0.334	421.499	ZINC15	Cc1cccc(-n2c(/C=C3/c4ccccc4N(C(C)C)C3=O)nc3ccccc3c2=O)c1
vMpro-as1-45	ZINC000006300868	-10.7	0.289	496.657	ZINC15	Cc1cc(C)c2[nH]c(=O)c([C@@H](c3nnnn3Cc3ccccc3)N3CCCC4(CCCCC4)C3)cc2c1
vMpro-as1-46	ZINC000008790287	-10.7	0.315	451.481	ZINC15	O=C(NCc1ccc2c(c1)OCO2)[C@@H]1Cc2c3ccccc3[nH]c2[C@H]2c3ccccc3C(=O)N21
vMpro-as1-47	ZINC000009668947	-10.7	0.324	431.458	ZINC15	Cc1ccc(NC2=N[C@]3(c4ccccc4NC3=O)n3c(nc4c3=Nc3ccccc3-4)=N2)cc1
vMpro-as1-48	ZINC000013593515	-10.7	0.297	488.518	ZINC15	O=C1Nc2ccc(F)cc2[C@]12N[C@@H](Cc1c[nH]c3ccc(O)cc13)[C@@H]1C(=O)N(C3CCC3)C(=O)[C@@H]12
vMpro-as1-49	ZINC000014246080	-10.7	0.315	446.473	ZINC15	Cc1nn(-c2ccccc2)c2c1[C@]1(c3ccccc3NC1=O)N1N=NN(c3ccccc3)C1=N2
vMpro-as1-50	ZINC000017988176	-10.7	0.268	521.571	ZINC15	O=C(Oc1ccc2ccccc2c1)c1cccc(N2C(=O)[C@H]3[C@@H](C2=O)C2c4ccccc4C3c3ccccc32)c1
vMpro-as1-51	ZINC000034795034	-10.7	0.334	421.499	ZINC15	Cc1cccc(-n2c(/C=C3\c4ccccc4N(C(C)C)C3=O)nc3ccccc3c2=O)c1
vMpro-as1-52	ZINC000085392618	-10.7	0.289	493.569	ZINC15	O=C([C@@H]1CC(=O)N(c2nc[nH]n2)C1)N1CCC(c2c[nH]c3ccccc32)(c2c[nH]c3ccccc32)CC1
vMpro-as1-53	ZINC000101833415	-10.7	0.306	489.885	ZINC15	Cc1ccc(N2C(=O)[C@@H]3[C@@H](c4cccc(F)c4)OC4(C(=O)c5ccccc5C4=O)[C@H]3C2=O)cc1Cl
vMpro-as1-54	ZINC000102879694	-10.7	0.315	476.527	ZINC15	CC(C)(C)c1ccc([C@H]2/C(=C(\O)c3ccco3)C(=O)C(=O)N2c2nc3ccc(F)cc3s2)cc1
vMpro-as1-55	ZINC000195529574	-10.7	0.297	473.483	ZINC15	O=C1c2ccccc2C(=O)C12O[C@H](c1ccccc1)[C@H]1C(=O)N(c3cccc4ccccc43)C(=O)[C@@H]12
vMpro-as1-56	ZINC000217751255	-10.7	0.306	474.42	ZINC15	COc1cc([C@H]2CC(=O)Oc3cc(O)c4c(=O)cc(-c5ccc(O)cc5)oc43)c2c1OCO2
vMpro-as1-57	ZINC000229870983	-10.7	0.274	575.461	ZINC15	O=C(c1ccccc1)[C@H]1[C@@H](C(=O)c2ccc(Br)cc2)N2c3ccccc3C=C[C@H]2[C@]12C(=O)Nc1ccccc12
vMpro-as1-58	ZINC000229980317	-10.7	0.268	529.57	ZINC15	O=C(Nc1ccccc1)[C@@H]1[C@H](C(=O)c2ccc(F)cc2)[C@]2(C(=O)Nc3ccccc32)[C@@H]2C=Cc3ccccc3N21
vMpro-as1-59	ZINC000253486913	-10.7	0.289	498.488	ZINC15	O=C1Nc2ccc(F)cc2[C@]12N[C@@H](Cc1c[nH]c3ccccc13)[C@H]1C(=O)N(c3ccc(F)cc3)C(=O)[C@@H]12
vMpro-as1-60	PV-001848284510	-10.6	0.353	411.465	REAL	CN(C)c1n[nH]c(C2CCN(C(=O)c3ccccc[C@]4(C)NC(=O)NC4=O)c3)CC2)n1
vMpro-as1-61	PV-001955708011	-10.6	0.342	421.456	REAL	C[C@H]1C(=O)Nc2ccccc2CN1C(=O)NCc1ccccc[C@]2(C)NC(=O)NC2=O)c1
vMpro-as1-62	Z1000935708	-10.6	0.312	459.461	REAL	C[C@@]1(c2cccc(CNC(=O)CN3C(=O)Cn4c(cc5ccccc54)C3=O)c2)NC(=O)NC1=O
vMpro-as1-63	Z1000941160	-10.6	0.303	493.586	REAL	C[C@H]1CCc2c(sc3nc(CCC(=O)NCc4cccc([C@]5(C)NC(=O)NC5=O)c4)[nH]c(=O)c23)C1
vMpro-as1-64	Z1005792310	-10.6	0.294	482.518	REAL	O=C(Nc1ccc2[nH]c(-c3cccc(F)c3)nc2c1)[C@H]1CCCN(C(=O)c2ccc3[nH]ncc3c2)C1
vMpro-as1-65	Z1018131998	-10.6	0.303	478.551	REAL	C[C@H](NC(=O)NCc1cccc([C@]2(C)NC(=O)NC2=O)c1)C(=O)Nc1cccc(N2CCCC2)c1
vMpro-as1-66	Z1028479320	-10.6	0.294	492.51	REAL	C[C@@]1(c2cccc(CNC(=O)N3CCC[C@H](c4nc(-c5cccc(F)c5)no4)C3)c2)NC(=O)NC1=O
vMpro-as1-67	Z1192942247	-10.6	0.321	444.45	REAL	Cc1ccc(-c2cc(C(=O)NNc3nc4ccccc4c(=O)n3C)c3c(C)noc3n2)c(C)o1
vMpro-as1-68	Z1281862994	-10.6	0.321	431.458	REAL	O=C(NNc1ncnc2nc[nH]c12)c1cc(-c2cccc3ccccc23)nc2ccccc12
vMpro-as1-69	Z1314080218	-10.6	0.331	440.455	REAL	C[C@H](C(=O)NCc1cccc([C@]2(C)NC(=O)NC2=O)c1)N1C(=O)[C@H]2[C@@H]3CC[C@@H](O3)[C@H]2C1=O
vMpro-as1-70	Z136505810	-10.6	0.312	453.476	REAL	CCn1c(NNC(=O)c2cc(-c3ccc(F)cc3)nc3ccccc23)nc2ccccc2c1=O
vMpro-as1-71	Z1452314983	-10.6	0.342	418.456	REAL	C[C@@]1(c2cccc(C(=O)N3CCC[C@H](c4nnc5cccn45)C3)c2)NC(=O)NC1=O
vMpro-as1-72	Z1470503086	-10.6	0.331	424.459	REAL	O=C1C[C@H](c2cccc(N/C=C3\C(=O)N(c4ccccn4)C(=O)c4ccccc43)c2)CN1
vMpro-as1-73	Z1503339335	-10.6	0.342	429.455	REAL	CC(C)[C@@H](NC(=O)N[C@@H]1CC(C)(C)Oc2cc(F)ccc21)c1nc(-c2nnc[nH]2)no1
vMpro-as1-74	Z1684582482	-10.6	0.342	421.387	REAL	C[C@]1(c2cccc(-c3noc([C@H]4CC(=O)Nc5cc(F)ccc54)n3)c2)NC(=O)NC1=O
vMpro-as1-75	Z1688940046	-10.6	0.342	427.435	REAL	O=C1C[C@@H](c2nc(CCN3C(=O)NC4(CCCCC4)C3=O)no2)c2ccc(F)cc2N1
vMpro-as1-76	Z1703923781	-10.6	0.321	444.49	REAL	O=C1CC[C@@H]2CN(C(=O)[C@@H]3CN(Cc4nc5ccccc5c(=O)[nH]4)CCO3)c3ccc1c32
vMpro-as1-77	Z1748664410	-10.6	0.342	420.551	REAL	C[C@@H]1CN(C(=O)[C@@H]2C[C@@H]3CCCC[C@H]3N2C(=O)c2ccc3ccccc3c2)CC[C@@H]1O
vMpro-as1-78	Z1769353608	-10.6	0.331	432.479	REAL	Cc1ccc2nc(C3CCN(C(=O)c4cccc([C@]5(C)NC(=O)NC5=O)c4)CC3)oc12
vMpro-as1-79	Z1819912470	-10.6	0.331	425.422	REAL	O=C(c1ccc2noc(-c3ccc(F)cc3)c2c1)N1Cc2cnnn2Cc2ccccc21
vMpro-as1-80	Z1890552009	-10.6	0.331	432.414	REAL	O=C1C[C@@H](c2nc(CC(=O)N3CCn4c3nc3ccccc34)no2)c2ccc(F)cc2N1
vMpro-as1-81	Z2002641727	-10.6	0.342	417.414	REAL	O=C1[C@@H]2[C@@H]3C[C@H]4[C@@H]2[C@@]2(C(=O)Nc5ccc6[nH]c(-c7cc(F)ccc7F)nc6c5)[C@H]1[C@@H]3[C@@H]42
vMpro-as1-82	Z203500650	-10.6	0.312	452.513	REAL	Cc1nc(NC(=O)c2cc(-c3ccc4c(c3)OCCO4)nc3ccccc23)nc2c1CCCC2
vMpro-as1-83	Z358736862	-10.6	0.321	478.608	REAL	CCc1ccc(C(=O)OCC(=O)N[C@H](C)[C@H]2C[C@@H]3CC[C@@H]2C3)cc1S(=O)(=O)N1CCOCC1
vMpro-as1-84	Z413039866	-10.6	0.321	447.533	REAL	C[C@@H]1c2cc3c(cc2C2(CCCC2)CN1C(=O)Nc1ccc2c(c1)CCC(=O)N2)OCCO3
vMpro-as1-85	Z423747092	-10.6	0.312	474.907	REAL	C[C@@]1(c2cccc3cccc3c2)NC(=O)N(CC(=O)Nc2nnc(-c3cccc3Cl)[nH]2)C1=O
vMpro-as1-86	Z452576762	-10.6	0.303	476.575	REAL	Cc1ccc(C(=O)Nc2ccccc2)cc1NC(=O)CN1C(=O)N[C@]2(C[C@H](C)CC(C)(C)C2)C1=O
vMpro-as1-87	Z651196130	-10.6	0.331	449.534	REAL	C[C@@]1(c2cccc(NC(=O)[C@@H]3CCCN(c4nc5ccccc5s4)C3)c2)NC(=O)NC1=O
vMpro-as1-88	Z738900228	-10.6	0.303	480.538	REAL	C[C@@H]1CC(C)(C)C[C@]2(C1)NC(=O)N(CC(=O)Nc1cccc(C(=O)Nc3cccc(F)c3)c1)C2=O
vMpro-as1-89	Z993685642	-10.6	0.312	469.54	REAL	C[C@@H]1CC(C)(C)C[C@]2(C1)NC(=O)N(CC(=O)NCc1cccc([C@]3(C)NC(=O)NC3=O)c1)C2=O
vMpro-as1-90	Z993687716	-10.6	0.303	473.488	REAL	CCCc1noc2nc(-c3ccco3)cc(C(=O)NCc3cccc([C@@]4(C)NC(=O)NC4=O)c3)c12
vMpro-as1-91	ZINC000000909918	-10.6	0.294	480.546	ZINC15	Cc1cc(C)c2[nH]c(=O)c([C@@H](c3nnnn3Cc3ccc(F)cc3)N3CCc4ccccc43)cc2c1
vMpro-as1-92	ZINC000000910138	-10.6	0.294	480.546	ZINC15	Cc1ccc(C)c2[nH]c(=O)c([C@@H](c3nnnn3Cc3ccc(F)cc3)N3CCc4ccccc43)cc12
vMpro-as1-93	ZINC000002251851	-10.6	0.303	461.48	ZINC15	Cc1ccc(Cn2cnc3c(c4nc5ccccc5nc4n3-c3ccc4c(c3)OCO4)c2=O)cc1
vMpro-as1-94	ZINC000002786787	-10.6	0.294	495.439	ZINC15	Cc1ccccc1Cn1cnc(NC(=O)c2cc3nc(-c4ccc(F)cc4)cc(C(F)(F)F)n3n2)n1
vMpro-as1-95	ZINC000008791455	-10.6	0.303	470.571	ZINC15	C[C@H](NC(=O)[C@@H]1Cc2c3ccccc3[nH]c2[C@H]2c3ccccc3C(=O)N21)C(=O)NC1CCCCC1
vMpro-as1-96	ZINC000008837336	-10.6	0.331	434.376	ZINC15	O=C1c2ccccc2C(O)=C(n2nnc3ccccc32)/C1=N/c1cccc(C(F)(F)F)c1
vMpro-as1-97	ZINC000008871106	-10.6	0.303	481.898	ZINC15	O=c1c2c3nc4ccccc4nc3n(-c3ccc4c(c3)OCO4)c2ncn1Cc1ccc(Cl)cc1
vMpro-as1-98	ZINC000009157962	-10.6	0.312	440.505	ZINC15	Cc1cccc(-c2nc3c4c(ncn3n2)Oc2c3ccccc3ccc2[C@@H]4c2ccccc2)c1
vMpro-as1-99	ZINC000009356565	-10.6	0.312	442.477	ZINC15	Oc1ccccc1-c1nc2c3c(ncn2n1)Oc1c2ccccc2ccc1[C@@H]3c1ccccc1
vMpro-as1-100	ZINC000009542118	-10.6	0.294	475.507	ZINC15	Cc1ccc(Cn2cnc3c(c4nc5ccccc5nc4n3-c3ccc4c(c3)OCCO4)c2=O)cc1

Supplementary Table 5. Top 100 virtual hits of the screen against the active site of M^{pro} in which the structure with PDB ID 6lu7 was used (Screen ID: 16). Compounds were filtered so that hits had MW < 600 dalton, cLogP < 6, number of hydrogen bond acceptors < 11, and no reactive functional groups. The name of each compound consists of the initial letter 'v' for virtual hit, followed by the target protein name and the target site ('as' for active site, 1 for docking scenario 1). The score is the docking score given by QuickVina 2 in kcal/mol. The ligand efficiency (LE) is computed as LE = -score/#NonH, where #NonH is the number of heavy (i.e. non hydrogen) atoms.

Name	Catalog ID	Score	LE	MW	Library	SMILES
vMpro-as1-101	ZINC000012771113	-10.6	0.312	456.48	ZINC15	Cc1cccc(-c2nn(-c3ccc(F)cc3)cc2C(=O)N2C[C@@H](C(N)=O)Oc3ccccc32)c1
vMpro-as1-102	ZINC000013509896	-10.6	0.331	421.50	ZINC15	CCCN1c2ccccc2/C(=C/c2nc3ccccc3c(=O)n2-c2cccc(C)c2)C1=O
vMpro-as1-103	ZINC000015858930	-10.6	0.286	493.52	ZINC15	Cc1ccc(-c2c3c(c4n2-c2ccccc2O[C@H]4c2ccc4c(c2)OCO4)n(C)c(=O)n(C)c3=O)cc1
vMpro-as1-104	ZINC000016577965	-10.6	0.331	445.95	ZINC15	CC1(C)CC(=O)C2=C(C1)c1c(ccc3ccccc31)N[C@H]2c1ccc(Cl)cc2c1OCOC2
vMpro-as1-105	ZINC000021524902	-10.6	0.286	492.53	ZINC15	Cc1cccc(-c2c3c(c4n2-c2ccccc2N[C@@H]4c2ccc4c(c2)OCO4)n(C)c(=O)n(C)c3=O)c1
vMpro-as1-106	ZINC000032609526	-10.6	0.331	421.50	ZINC15	CCCN1c2ccccc2/C(=C\c2nc3ccccc3c(=O)n2-c2cccc(C)c2)C1=O
vMpro-as1-107	ZINC000034921978	-10.6	0.272	525.58	ZINC15	Cc1ccc(CN2CCN(C(=O)c3cnc(-c4ccc5c(c4)OCO5)nc3Nc3cccc(F)c3)CC2)cc1
vMpro-as1-108	ZINC000096113733	-10.6	0.303	467.48	ZINC15	COc1ccc(NC(=O)[C@H]2Oc3c(c(=O)oc4ccccc34)[C@@H]2C2=Cc3ccccc3OC2)cc1
vMpro-as1-109	ZINC000096114039	-10.6	0.303	474.42	ZINC15	COc1cc([C@H]2CC(=O)Oc3c(O)c(O)c4c(=O)cc(-c5ccccc5)oc4c32)cc2c1OCO2
vMpro-as1-110	ZINC000100415678	-10.6	0.286	487.51	ZINC15	Cc1cccc([C@H]2OC3(C(=O)c4ccccc4C3=O)[C@@H]3C(=O)N(c4ccccc5ccccc54)C(=O)[C@@H]32)c1
vMpro-as1-111	ZINC000100505727	-10.6	0.286	488.54	ZINC15	O=C1[C@@H]2[C@H]3C=C[C@@H](C3)[C@@H]2C(=O)N1c1ccc2c(c1)-c1ccc(N3C(=O)[C@H]4[C@H]5C=C[C@H](C5)[C@@H]4C3=O)ccc1C2
vMpro-as1-112	ZINC000102521214	-10.6	0.312	492.59	ZINC15	CC(C)(C)c1ccc([C@H]2/C(=C(\O)c3cccs3)C(=O)C(=O)N2c2nc3ccc(F)cc3s2)cc1
vMpro-as1-113	ZINC000102655249	-10.6	0.312	498.36	ZINC15	O=C1c2ccccc2C(=O)C12O[C@H](c1ccc(Cl)cc1Cl)[C@H]1C(=O)N(C3CCCC3)C(=O)[C@@H]12
vMpro-as1-114	ZINC000102713153	-10.6	0.312	456.50	ZINC15	Cc1cc(N2C(=O)C(=O)/C(=C(/O)c3cc4ccccc4o3)[C@H]2c2ccc(C(C)(C)C)cc2)no1
vMpro-as1-115	ZINC000102719741	-10.6	0.303	466.54	ZINC15	Cc1cc(N2C(=O)C(=O)/C(=C(/O)c3ccc4ccccc4c3)[C@@H]2c2ccc(C(C)(C)C)cc2)no1
vMpro-as1-116	ZINC000102862874	-10.6	0.321	460.60	ZINC15	Cc1nc(N2C(=O)C(=O)/C(=C(/O)c3ccc(C)cc3)[C@@H]2c2ccc(C(C)(C)C)cc2)sc1C
vMpro-as1-117	ZINC000239305870	-10.6	0.312	471.90	ZINC15	Cc1ccc(N2C(=O)[C@@H]3[C@@H](c4ccccc4)OC4(C(=O)c5ccccc5C4=O)[C@H]3C2=O)cc1Cl
vMpro-as1-118	PV-001802203537	-10.5	0.318	451.57	REAL	Cc1cc(C)cc(-n2nc(NC(=O)CN3C(=O)N[C@]4(C[C@H](C)CC(C)(C)C4)C3=O)cc2C)c1
vMpro-as1-119	PV-001817570577	-10.5	0.328	451.35	REAL	O=C(N1CCc2c(NC(=O)C(F)(F)n3ccc(-c4ccccc4)nn3)cccc21)C(F)(F)F
vMpro-as1-120	PV-001844203081	-10.5	0.404	354.33	REAL	O=C(c1ccc(-n2[nH]c(=O)[nH]c2=O)cc1)N1CCc2n[nH]c(=O)cc2C1
vMpro-as1-121	PV-001855182446	-10.5	0.318	458.56	REAL	C[C@@H]1C[C@H](C)N(C(=O)c2cccc([C@]3(C)NC(=O)NC3=O)c2)C[C@H]1CNC(=O)OC(C)(C)C
vMpro-as1-122	PV-001950833703	-10.5	0.328	439.45	REAL	Cc1ccc(-c2noc([C@@H](C)NC(=O)Nc3cccc([C@@]4(C)COC(=O)N4)c3)n2)cc1F
vMpro-as1-123	PV-001955704740	-10.5	0.318	452.45	REAL	C[C@@H](NC(=O)NCc1cccc([C@]2(C)NC(=O)NC2=O)c1)c1nc(-c2ccccc(F)c2)no1
vMpro-as1-124	Z1000939726	-10.5	0.309	456.50	REAL	C[C@]1(c2cccc(CNC(=O)c3cc4ccccc4cc3NC(=O)C3CC3)c2)NC(=O)NC1=O
vMpro-as1-125	Z1000942566	-10.5	0.318	449.47	REAL	C[C@]1(c2cccc(CNC(=O)CCC(=O)N3CC(=O)Nc4ccccc43)c2)NC(=O)NC1=O
vMpro-as1-126	Z1018311930	-10.5	0.339	421.46	REAL	C[C@@]1(c2cccc(CNC(=O)NCC(=O)N3CCc4ccccc43)c2)NC(=O)NC1=O
vMpro-as1-127	Z104048044	-10.5	0.328	418.42	REAL	c1cc(-c2nnc(-c3cc(-c4ccncc4)nc4ccccc34)o2)cc(-n2cnnn2)c1
vMpro-as1-128	Z1094878064	-10.5	0.309	474.91	REAL	C[C@@]1(c2ccc3ccccc3c2)NC(=O)N(CC(=O)NC2nnc(-c3cccc(Cl)c3)[nH]2)C1=O
vMpro-as1-129	Z1129401799	-10.5	0.300	465.51	REAL	CN1C(=O)CCc2cc(NC(=O)c3cc(-c4ccc5c(c4)OCCO5)nc4ccccc34)ccc21
vMpro-as1-130	Z1144659239	-10.5	0.339	424.43	REAL	C[C@@]1(c2cccc(CNC(=O)[C@H]3CC(=O)N(c4ccc(F)cc4)C3)c2)NC(=O)NC1=O
vMpro-as1-131	Z1155700167	-10.5	0.309	467.51	REAL	O=C(Nc1cccc(-c2ccc3c(c2)OCCO3)n1)c1ncncn1-c1nc2ccccc2s1
vMpro-as1-132	Z1192944140	-10.5	0.375	377.38	REAL	Cc1cc(C(=O)NNc2nc3ccccc3c(=O)n2C)c2ccc(F)cc2n1
vMpro-as1-133	Z1250518867	-10.5	0.350	397.43	REAL	C[C@@H]1CN(C(=O)c2cc(-c3ccco3)nc3ccccc23)c2ccccc2NC1=O
vMpro-as1-134	Z1276147995	-10.5	0.350	406.40	REAL	CC(=O)N1C[C@H](C(=O)Nc2[nH]ncc2-c2ccc3c(c2)OCO3)Oc2ccccc21
vMpro-as1-135	Z1416053019	-10.5	0.318	436.47	REAL	O=C1NC(=O)N2CCN(C(=O)c3cc(-c4cccc5ccccc45)nc4ccccc34)C[C@H]12
vMpro-as1-136	Z1451354170	-10.5	0.318	449.51	REAL	C[C@@]1(c2cccc(C(=O)NCC3(c4ccc5c(c4)OCCO5)CCCC3)c2)NC(=O)NC1=O
vMpro-as1-137	Z1482232337	-10.5	0.339	420.41	REAL	O=C(c1ccc2noc(-c3ccc(F)cc3)c2c1)N1CCO[C@@H](c2ccc(F)cc2)C1
vMpro-as1-138	Z1531890994	-10.5	0.328	431.53	REAL	NC(=O)[C@H]1CCN(C(=O)[C@H]2C[C@@H]3CCCC[C@H]3N2C(=O)c2ccccc2)c2ccccc21
vMpro-as1-139	Z1614245151	-10.5	0.339	419.53	REAL	COc1ccc2nc(C(=O)N3CCC[C@H](c4n[nH]c(C5CCCCC5)n4)C3)ccc2c1
vMpro-as1-140	Z1620399497	-10.5	0.339	416.48	REAL	Cc1ccc2[nH]c3c(c2c1)C[C@@H](NC(=O)c1cccc([C@@]2(C)NC(=O)NC2=O)c1)CC3
vMpro-as1-141	Z1655759539	-10.5	0.328	433.42	REAL	C[C@]1(c2cccc(CNC(=O)c3cn[nH]c3-c3ccc4c(c3)OCO4)c2)NC(=O)NC1=O
vMpro-as1-142	Z1684580765	-10.5	0.328	432.44	REAL	C[C@@]1(c2cccc(-c3nocc([C@H]4C[C@H]4c4ccc5c(c4)OCCO5)n3)c2)NC(=O)NC1=O
vMpro-as1-143	Z1766394717	-10.5	0.339	426.37	REAL	O=C(c1cc(F)cc2c(=O)c3cc(F)ccc3[nH]c12)N1Cc2ccccc2C(F)(F)C1
vMpro-as1-144	Z1830769356	-10.5	0.318	447.51	REAL	O=C1C[C@@H](c2cccc(NC(=O)N3CCCC[C@H]3c3nc(-c4cccc(F)c4)c[nH]3)c2)CN1
vMpro-as1-145	Z1861943195	-10.5	0.339	439.94	REAL	O=C([C@@H]1C[C@@H]2CCCC[C@H]2N1C(=O)c1cccc(Cl)c1)N1CCc2cnc(O)c2C1
vMpro-as1-146	Z1896771126	-10.5	0.339	409.42	REAL	O=C(NNc1cnc2ccccc2n1)c1cc(-c2ccccc2)nc2cc(F)ccc12
vMpro-as1-147	Z1983291804	-10.5	0.328	431.53	REAL	C[C@@H](NC(=O)CN1C(=O)N[C@@]2(C[C@@H]3C[C@@H]2[C@H]2CCC[C@@H]32)C1=O)c1ccc2ccccc2c1
vMpro-as1-148	Z2177644532	-10.5	0.318	449.55	REAL	CC(=O)N1C[C@H]2CCC[C@H](NC(=O)[C@@H]3CCCN3C(=O)c3ccc4ccccc4c3O)[C@H]2C1
vMpro-as1-149	Z219443316	-10.5	0.292	494.43	REAL	Cc1noc2nc(-c3ccccc3C(F)(F)F)cc(C(=O)OCc3cc(=O)n4cccc(C)c4n3)c12
vMpro-as1-150	Z220407410	-10.5	0.300	484.54	REAL	O=C(Nc1nc2ccccc2nc1N1CCCC1)c1ccc2c(c1)S(=O)(=O)c1ccccc1C2=O
vMpro-as1-151	Z2231942151	-10.5	0.328	438.61	REAL	C[C@H]1CC(=O)C[C@@H](C(=O)N2C[C@@H]3[C@H]4CC[C@@H](C4)[C@H]3C2)[C@H]1C(=O)N1C[C@H]2[C@@H]3CC[C@@H](C3)[C@@H]2C1
vMpro-as1-152	Z2233156474	-10.5	0.339	418.43	REAL	O=C(c1cc(-c2ccccc2)nc2cc(F)ccc12)N1CCC(O)(c2nnn[nH]2)CC1
vMpro-as1-153	Z225729362	-10.5	0.284	498.52	REAL	O=C1NC(=O)C2(CCN(C(=O)c3cc(-c4ccccc4)nc4c3cnn4Cc3cccc(F)c3)CC2)N1
vMpro-as1-154	Z2524819091	-10.5	0.309	477.67	REAL	CC(C)NC(=O)CSc1ccccc1C(=O)N1C[C@H]2CC[C@H]1[C@H]1CN(Cc3ccccc3)C[C@H]21
vMpro-as1-155	Z2830959285	-10.5	0.292	488.49	REAL	O=C1N[C@@H](c2cn(Cc3ccccc3)nc2-c2ccc3c(c2)OCCO3)Nc2cc(F)c(F)cc21
vMpro-as1-156	Z284412618	-10.5	0.292	496.59	REAL	C[C@@H]1CC(C)(C)C[C@]2(C1)NC(=O)N(CC(=O)Nc1cc(-c3nnc4n3CCCCC4)ccc1F)C2=O
vMpro-as1-157	Z284424348	-10.5	0.318	463.54	REAL	O=C1CC[C@@]2(C(=O)Nc3cc(-c4nnc5n4CCCCC5)ccc3F)Sc3ccccc3N12
vMpro-as1-158	Z31287518	-10.5	0.309	469.39	REAL	O=C(NN/C=C1\C(=O)N(c2cccc(C(F)(F)F)c2)C(=O)c2ccccc21)c1ccccc1F
vMpro-as1-159	Z383608736	-10.5	0.292	485.50	REAL	C[C@]1(c2ccc(NC(=O)CN3C(=O)N[C@](C)(c4ccc5ccccc5c4)C3=O)cc2)NC(=O)NC1=O
vMpro-as1-160	Z392464174	-10.5	0.328	424.51	REAL	Cc1nc(NC(=O)c2cnc3c(c2)c(C2CC2)nn3-c2ccccc2)nc2c1CCCC2
vMpro-as1-161	Z424328336	-10.5	0.318	483.57	REAL	C[C@@]1(c2cccc(NC(=O)CSCc3nc4sc5c(c4c(=O)[nH]3)CCC5)c2)NC(=O)NC1=O
vMpro-as1-162	Z424329296	-10.5	0.328	451.51	REAL	C[C@@]1(c2cccc(NC(=O)CCc3nc4sc5c(c4c(=O)[nH]3)CCC5)c2)NC(=O)NC1=O
vMpro-as1-163	Z424333500	-10.5	0.309	497.60	REAL	C[C@@]1(c2cccc(NC(=O)CSCc3nc4sc5c(c4c(=O)[nH]3)CCCC5)c2)NC(=O)NC1=O
vMpro-as1-164	Z52367703	-10.5	0.309	449.51	REAL	O=C(Nc1cccc(-c2nc3ccccc3[nH]2)c1)c1ccc2c(=O)n3c(nc2c1)CCCCC3
vMpro-as1-165	Z595787930	-10.5	0.292	490.56	REAL	C[C@@H]1c2cc3c(cc2C2(CCCC2)CN1C(=O)Nc1cccc(N2C(=O)CN(C)C2=O)c1)OCCO3
vMpro-as1-166	Z729907406	-10.5	0.300	468.47	REAL	O=C1c2ccccc2N[C@@H](c2c[nH]nc2-c2ccc3c(c2)OCO3)N1c1ccc2c(c1)OCCO2
vMpro-as1-167	Z737501626	-10.5	0.300	470.48	REAL	CN(C(=O)[C@@H]1Cc2ccccc2C(=O)O1)c1cccc(NC(=O)[C@H]2Cc3ccccc3C(=O)O2)c1
vMpro-as1-168	Z963478490	-10.5	0.350	433.84	REAL	O=C1C[C@@H](C(=O)N2CCN(C(=O)c3ccc(F)cc3Cl)CC2)c2ccc(F)cc2N1
vMpro-as1-169	Z993685386	-10.5	0.309	461.48	REAL	C[C@@]1(c2cccc(CNC(=O)CN3C(=O)N[C@@]4(CCc5ccccc54)C3=O)c2)NC(=O)NC1=O
vMpro-as1-170	Z993686872	-10.5	0.318	449.51	REAL	C[C@@]1(c2cccc(CNC(=O)C3(c4ccc5c(c4)OCCO5)CCCC3)c2)NC(=O)NC1=O
vMpro-as1-171	Z998371692	-10.5	0.328	431.47	REAL	Cc1ccc(-c2cc(C(=O)N3CCO[C@@H](c4ccc(F)cc4)C3)c3c(C)noc3n2)cc1
vMpro-as1-172	Z998712162	-10.5	0.309	460.49	REAL	C[C@]1(c2cccc(NC(=O)[C@@H]3CCCN(C(=O)c4ccc5[nH]ncc5c4)C3)c2)NC(=O)NC1=O
vMpro-as1-173	ZINC000000894324	-10.5	0.300	462.56	ZINC15	Cc1ccc(C)c2[nH]c(=O)c([C@@H](c3nnnn3Cc3ccccc3)N3CCc4ccccc43)cc12
vMpro-as1-174	ZINC000001714458	-10.5	0.300	462.46	ZINC15	O=C1c2ccccc2C(=O)C(C(/C=C/c2ccccc2)C2=C(O)C(=O)c3ccccc3C2=O)=C1O
vMpro-as1-175	ZINC000002332302	-10.5	0.318	431.50	ZINC15	Cc1cccc(-n2c3nc4ccccc4nc3c3c2ncn([C@H](C)c2ccccc2)c3=O)c1
vMpro-as1-176	ZINC000002336524	-10.5	0.318	439.45	ZINC15	O=C(c1ccccc1)[C@H]1[C@H]2C(=O)N(c3cccc(F)c3)C(=O)[C@@H]2[C@H]2c3ccccc3CCN1C2=O
vMpro-as1-177	ZINC000002366044	-10.5	0.292	471.52	ZINC15	O=C(c1ccccc1)[C@H]1[C@H]2C(=O)N(c3ccc4ccccc4c3)C(=O)[C@@H]2[C@H]2c3ccccc3C=NN12
vMpro-as1-178	ZINC000003873988	-10.5	0.318	429.43	ZINC15	O=C1c2ccccc2C(=O)c2c(Nc3ccccc3)C(=O)c3ccccc3C4=Occcc21
vMpro-as1-179	ZINC000004698292	-10.5	0.339	408.46	ZINC15	Cn1c2ccccc2c2cc([C@H]3CC(=O)Oc4c5ccccc5n(C)c(=O)c43)ccc21
vMpro-as1-180	ZINC000008834551	-10.5	0.300	461.48	ZINC15	O=c1c2c3nc4ccccc4nc3n(-c3ccc4c(c3)OCCO4)c2ncn1Cc1ccccc1
vMpro-as1-181	ZINC000008870443	-10.5	0.300	482.56	ZINC15	CN1c2ccc(S(=O)(=O)Nc3cc4c5c(oc4c4ccccc34)CCCC5)c3cccc(c23)C1=O
vMpro-as1-182	ZINC000008871108	-10.5	0.292	495.93	ZINC15	O=c1c2c3nc4ccccc4nc3n(-c3ccc4c(c3)OCCO4)c2ncn1Cc1ccc(Cl)cc1
vMpro-as1-183	ZINC000009776804	-10.5	0.284	497.59	ZINC15	COc1ce2c(cc1OC)[C@@H](C(=O)N1CCN(c3cccc3)CC1)[C@@H]1c3cccc3CCN1C2=O
vMpro-as1-184	ZINC000012244659	-10.5	0.284	509.53	ZINC15	O=C(c1cc(-c2ccccc2)n[nH]1)N1CCC(n2c3ccc(C(F)(F)F)cc3nc2[C@@H]2CCCO2)CC1
vMpro-as1-185	ZINC000012559603	-10.5	0.269	508.58	ZINC15	O=C1NC(c2ccccc2)=C(c2nc3ccccc3[nH]2)[C@@H](c2cn(-c3ccccc3)nc2-c2ccccc2)N1
vMpro-as1-186	ZINC000012887862	-10.5	0.309	456.54	ZINC15	C[C@H](NC(=O)[C@@H]1Cc2c3ccccc3[nH]c2[C@H]2c3ccccc3C(=O)N21)C(=O)NC1CCCC1
vMpro-as1-187	ZINC000013590248	-10.5	0.339	407.47	ZINC15	Cc1ccc2c(c1)/C(=C/c1nc3ccccc3c(=O)n1-c1cccc(C)c1)C(=O)N2C
vMpro-as1-188	ZINC000013756054	-10.5	0.318	500.40	ZINC15	CCCN1C(=O)/C(=C\c2nc3ccccc3c(=O)n2-c2cccc(C)c2)c2cc(Br)ccc21
vMpro-as1-189	ZINC000018179959	-10.5	0.300	489.89	ZINC15	Cc1ccc(N2C(=O)[C@H]3[C@H](c4cccc(F)c4)OC4(C(=O)c5ccccc5C4=O)[C@@H]3C2=O)cc1Cl
vMpro-as1-190	ZINC000031687842	-10.5	0.300	462.46	ZINC15	O=C1c2ccccc2C(=O)C(C(/C=C\c2ccccc2)C2=C(O)C(=O)c3ccccc3C2=O)=C1O
vMpro-as1-191	ZINC000031829103	-10.5	0.339	407.47	ZINC15	Cc1ccc2c(c1)/C(=C\c1nc3ccccc3c(=O)n1-c1cccc(C)c1)C(=O)N2C
vMpro-as1-192	ZINC000034921958	-10.5	0.269	525.58	ZINC15	Cc1ccc(CN2CCN(C(=O)c3cnc(-c4ccc5c(c4)OCO5)nc3Nc3cccc3F)CC2)cc1
vMpro-as1-193	ZINC000035147335	-10.5	0.300	465.55	ZINC15	Cc1ccc(-c2n[nH]c3c2[C@@H](c2ccc(C(C)(C)C)cc2)N(c2ccc(C(=O)O)cc2)C3=O)cc1
vMpro-as1-194	ZINC000048523762	-10.5	0.292	464.48	ZINC15	O=C1c2ccccc2C(=O)C2=C3C=CC4=CC5=C(C(=O)c6ccccc6C5=O)C5=CC=C(C=C12)[C@H]3[C@H]45
vMpro-as1-195	ZINC000049006633	-10.5	0.309	451.45	ZINC15	Cc1cccc(-c2noc(-c3ccen4c3nn(Cc3cc(=O)n5ccccc5n3)c4=O)n2)c1
vMpro-as1-196	ZINC000095944224	-10.5	0.292	481.49	ZINC15	O=C(NCc1cccc(F)c1)[C@@]12CCC(=O)N1c1ccccc1-c1nc(=O)c(-c3ccccc3)nn12
vMpro-as1-197	ZINC000096115616	-10.5	0.309	453.45	ZINC15	CC(C)n1ncc2c1nc1c3ccc(O)cc3oc1c2-c1ccc(-c2cccc(C(=O)O)c2)o1
vMpro-as1-198	ZINC000101099901	-10.5	0.309	475.86	ZINC15	O=C1c2ccccc2C(=O)C12O[C@H](c1ccc(Cl)cc1)[C@H]1C(=O)N(c3cccc(F)c3)C(=O)[C@@H]12
vMpro-as1-199	ZINC000101169303	-10.5	0.328	443.37	ZINC15	O=C(CN1N=N[C@H]2C(=O)N(c3ccc(F)c(F)c3)C(=O)[C@@H]21)Nc1ccc2c(c1)OCCO2
vMpro-as1-200	ZINC000101262755	-10.5	0.300	482.42	ZINC15	O=C1[C@H]2[C@H](N=NN2Cc2nc(-c3cccc(C(F)(F)F)c3)no2)C(=O)N1c1ccc2c(c1)CCC2

Supplementary Table 6. Virtual screening hits 101 to 200 of the screen against the active site of M^{pro} in which the structure with PDB ID 6lu7 was used (Screen ID: 16). Compounds were filtered so that hits had MW < 600 dalton, cLogP < 6, number of hydrogen bond acceptors < 11, and no reactive functional groups. The name of each compound consists of the initial letter 'v' for virtual hit, followed by the target protein name and the target site ('as' for active site, 1 for docking scenario 1). The score is the docking score given by QuickVina 2 in kcal/mol. The ligand efficiency (LE) is computed as LE = -score/#NonH, where #NonH is the number of heavy (i.e. non hydrogen) atoms.

Name	Catalog ID	Score	LE	MW	Library	SMILES
vMpro-as2-1	ZINC000104480048	-11.8	0.328	490.945	ZINC	O=C(NC1=CC=C[C@H]2C(=O)c3ccccc3C(=O)[C@H]12)c1cc(-c2ccccc2Cl)nc2ccccc21
vMpro-as2-2	Z301905520	-11.7	0.344	460.58	REAL	O=C(c1ccc2c(=O)n3c(nc2c1)CCCCC3)N1CCC[C@@H](c2nnc3n2CCCCC3)C1
vMpro-as2-3	ZINC000056952873	-11.7	0.355	447.498	ZINC	Cn1c2nc(N3CCN(CC(N)=O)CC3)n(Cc3cccc4ccccc43)c2c(=O)[nH]c1=O
vMpro-as2-4	Z2698659161	-11.6	0.387	397.485	REAL	c1ccc2c(c1)CN(c1ccnc(N3CCC[C@@H](c4nnc5ccccn45)C3)n1)C2
vMpro-as2-5	Z2931718585	-11.6	0.414	377.403	REAL	O=C1NCC2(CCN(C(=O)c3ccc4nncn4c3)CC2)Oc2ccccc21
vMpro-as2-6	Z301914184	-11.6	0.331	470.571	REAL	O=C1O[C@H](c2ccccc2)Cc2cc(C(=O)N3CCC[C@@H](c4nnc5n4CCCCC5)C3)ccc21
vMpro-as2-7	PV-001859059041	-11.5	0.359	452.432	REAL	C[C@H](C(=O)N[C@@H]1Cc2ccccc2N(C(=O)C(F)(F)F)C1)N1C(=O)NC2(CCCC2)C1=O
vMpro-as2-8	PV-001859061038	-11.5	0.383	423.434	REAL	O=C1C[C@H](C(=O)N[C@H]2Cc3ccccc3N(C(=O)C(F)(F)F)C2)[C@@H]2CCCC[C@@H]2N1
vMpro-as2-9	Z1023503068	-11.5	0.319	487.533	REAL	O=C(c1ccc2c(=O)n3c(nc2c1)CCCCC3)N1CCC[C@@H](c2nc(-c3cccc(F)c3)no2)C1
vMpro-as2-10	Z1037871898	-11.5	0.319	482.546	REAL	O=C(Nc1ccccc1)[C@H]1CCc2ccccc2N1C(=O)C1CCN(c2ccc3nnnn3n2)CC1
vMpro-as2-11	Z1161084532	-11.5	0.311	491.55	REAL	O=C(Nc1ccc(-c2nnc3n2CCCC3)cc1)c1ccc2c(c1)C(=O)N(CCc1ccccc1)C2=O
vMpro-as2-12	Z2090596200	-11.5	0.371	432.914	REAL	Cc1nnc2c3ccccc3c(N3CCC([C@@H]4C(=O)Nc5cc(Cl)ccc54)CC3)nn12
vMpro-as2-13	Z2141651627	-11.5	0.371	416.488	REAL	O=C(C1CCN(c2ccc3nnnn3n2)CC1)N1CCCn2c(cc3ccccc32)C1
vMpro-as2-14	Z332863718	-11.5	0.371	413.523	REAL	O=C(c1cc2c(ccc3ccccc32)[nH]1)N1CCC[C@@H](c2nnc3n2CCCCC3)C1
vMpro-as2-15	PV-001824399245	-11.4	0.345	458.395	REAL	Cc1onc(-c2ccc(C(F)(F)F)cc2)c1C(=O)Nc1ccc([C@]2(C)NC(=O)NC2=O)cc1
vMpro-as2-16	PV-001855722215	-11.4	0.345	457.415	REAL	Cc1nc(-c2cc(NC(=O)C3=NN(c4ccccc4)C(=O)[C@@H](C)N3)cc(C(F)(F)F)c2)n[nH]1
vMpro-as2-17	Z1170374434	-11.4	0.38	425.443	REAL	O=C(c1ccc2c(c1)S(=O)(=O)Nc1ncnn1-2)N1CC2(CCC2)c2c(F)cccc21
vMpro-as2-18	Z119684146	-11.4	0.308	498.533	REAL	O=C1O[C@H](c2ccccc2)Cc2cc(C(=O)N3C[C@@H](C(=O)N4CCOCC4)Oc4ccccc43)ccc21
vMpro-as2-19	Z1637286208	-11.4	0.345	447.473	REAL	O=C(Nc1n[nH]c(Cc2cccc(F)c2)n1)[C@@H]1CCCN(C(=O)c2ccc3[nH]ncc3c2)C1
vMpro-as2-20	Z1685323021	-11.4	0.356	443.534	REAL	Cc1nnc(-c2cccc(-c3noc([C@H]4CCCN(c5nc6ccccc6s5)C4)n3)c2)[nH]1
vMpro-as2-21	Z1723440467	-11.4	0.326	487.539	REAL	Cn1c(=O)[nH]c2ncc(-c3cccc(C(=O)N4CCN(C(=O)c5cc6occc6s5)CC4)c3)cc21
vMpro-as2-22	Z2140567272	-11.4	0.38	405.409	REAL	O=C1COC[C@H](C[C@@H]2CN(C(=O)c3ccc4c(c3)C(=O)NC4=O)c3ccccc32)N1
vMpro-as2-23	Z2140571313	-11.4	0.356	425.487	REAL	O=C1COC[C@@H](C[C@@H]2CN(C(=O)c3cc4c(ccc5ccccc54)[nH]3)c3ccccc32)N1
vMpro-as2-24	Z2177648417	-11.4	0.356	439.461	REAL	CC(=O)N1C[C@@H]2CCC[C@@H](NC(=O)c3cc(F)cc4c(=O)c5cc(F)ccc5[nH]c34)[C@@H]2C1
vMpro-as2-25	Z237105250	-11.4	0.317	483.57	REAL	O=C(c1cccc(CN2C(=O)c3ccccc3C2=O)c1)N1CCC[C@@H](c2nnc3n2CCCCC3)C1
vMpro-as2-26	Z2931716788	-11.4	0.407	381.435	REAL	O=C1NCC2(CCN(C(=O)[C@H]3CCc4nncn4C3)CC2)Oc2ccccc21
vMpro-as2-27	ZINC000020086598	-11.4	0.335	456.461	ZINC	Cc1n[nH]c2c1[C@@H](c1ccc([C@@H]3c4c(C)n[nH]c4NC4=C3C(=O)OC4)cc1)C1=C(COC1=O)N2
vMpro-as2-28	ZINC000026780145	-11.4	0.317	490.945	ZINC	O=C(NC1=CC=C[C@H]2C(=O)c3ccccc3C(=O)[C@H]12)c1cc(-c2ccccc2Cl)nc2ccccc21
vMpro-as2-29	ZINC000101343710	-11.4	0.326	460.488	ZINC	O=C(c1cccc1)[C@@H]1[C@@H]2C(=O)N(c3ccc4ccccc4c3)C(=O)[C@H]2[C@@H]2c3ccccc3C=CN21
vMpro-as2-30	PV-001847889949	-11.3	0.365	422.487	REAL	Cc1nnc2[nH]nc(NC(=O)[C@@H]3CN(C(=O)OC(C)(C)C)Cc4ccccc43)c2c1C
vMpro-as2-31	PV-001875531219	-11.3	0.39	446.321	REAL	O=C(c1ccc2nnc(S)n2c1)N1C[C@@H]2[C@@H](C1)C(F)(F)C(F)(F)C(F)(F)C2(F)F
vMpro-as2-32	Z1037998952	-11.3	0.323	499.424	REAL	O=C(Nc1ccc(-c2noc(C(F)(F)F)n2)cc1)c1ccc2c(c1)S(=O)(=O)c1ccccc1C2=O
vMpro-as2-33	Z1067808706	-11.3	0.365	406.444	REAL	Cc1ccc2cccc(N/C=C3/C(=O)N(c4cccn4)C(=O)c4ccccc43)c2n1
vMpro-as2-34	Z109823584	-11.3	0.305	496.561	REAL	O=C1O[C@H](c2ccccc2)Cc2cc(C(=O)N3C[C@@H](C(=O)N4CCCCC4)Oc4ccccc43)ccc21
vMpro-as2-35	Z1231685987	-11.3	0.353	436.461	REAL	Cc1ccc(Nc2cccc(C(=O)N3CCC(C(=O)c4cc(F)ccc4F)CC3)c2)nn1
vMpro-as2-36	Z1401587733	-11.3	0.365	421.479	REAL	O=C(C1CCN(c2ccc3nnnn3n2)CC1)N1CCC(=Cc2ccccc2F)CC1
vMpro-as2-37	Z1548458207	-11.3	0.377	431.515	REAL	O=C1NC(=O)N2CCN(C(=O)[C@H]3CCCN(C(=O)N4CCc5sccc5C4)C3)C[C@H]12
vMpro-as2-38	Z1594871022	-11.3	0.353	448.913	REAL	Cc1nc(-c2ccc(NC(=O)c3ccc4c(=O)n5c(nc4c3)CCCCC5)cc2Cl)n[nH]1
vMpro-as2-39	Z1723432082	-11.3	0.305	491.55	REAL	Cn1c(=O)[nH]c2ncc(-c3cccc(C(=O)N4CCN(C(=O)c5cccc6ccccc56)CC4)c3)cc21
vMpro-as2-40	Z1870844731	-11.3	0.404	380.378	REAL	O=C(c1cnc2[nH]c(=O)[nH]c(=O)c2c1)N1CC2(CCCC2)c2cccc(F)c21
vMpro-as2-41	Z2002480587	-11.3	0.353	431.53	REAL	C[C@H]1c2cc3c(cc2C2(CCCC2)CN1C(=O)[C@@]12[C@H]4C(=O)[C@H]5[C@H]6C[C@@H]([C@@H]51)[C@@H]2[C@H]64)OCCO3
vMpro-as2-42	Z2003834871	-11.3	0.365	429.906	REAL	O=C1[C@@H]2[C@H]3C[C@H]4[C@@H]2[C@@]2(C(=O)Nc5nc6ccccc6n5Cc5ccc(Cl)cc5)[C@@H]1[C@@H]3[C@@H]42
vMpro-as2-43	Z2033632139	-11.3	0.365	416.44	REAL	Cc1nnc2c3ccccc3c(N3CCN(C(=O)c4ccc5c(c4)OCO5)CC3)nn12
vMpro-as2-44	Z2067513613	-11.3	0.353	438.545	REAL	CN(C)C(=O)CN1[C@H]2CC[C@H]1CC(N[C@@H](C(=O)Nc1ccc(F)cc1)c1ccccc1)C2
vMpro-as2-45	Z2141487675	-11.3	0.342	448.505	REAL	O=C(C1CCN(c2ccc3nnnn3n2)CC1)N1CCC(c2c[nH]c3ccc(F)cc23)CC1
vMpro-as2-46	Z2143208950	-11.3	0.377	396.453	REAL	Cc1nnc2[nH]nc(NC(=O)c3cn(Cc4ccccc4)c4ccccc34)c2c1C
vMpro-as2-47	Z219422428	-11.3	0.342	445.434	REAL	NC1=Nc2nc3cc4c(cc3n2[C@@H](c2ccc(-c3ccc(C(=O)O)cc3)o2)N1)OCCCO4
vMpro-as2-48	Z288393008	-11.3	0.323	487.942	REAL	O=C(c1ccccc(Cl)c1)N1CCN(C(=O)c2cccc(CN3C(=O)c4ccccc4C3=O)c2)CC1
vMpro-as2-49	Z2931718970	-11.3	0.404	376.415	REAL	O=C1NCC2(CCN(C(=O)c3ccc4[nH]ncc4c3)CC2)Oc2ccccc21
vMpro-as2-50	Z301920758	-11.3	0.342	448.525	REAL	O=C(c1c[nH]nc1-c1ccc2c(c1)OCCO2)N1CCC[C@H](c2nnc3n2CCCCC3)C1
vMpro-as2-51	Z301923952	-11.3	0.323	486.642	REAL	O=C(c1ccc(SCc2cn3ccccc3n2)cc1)N1CCC[C@@H](c2nnc3n2CCCCC3)C1
vMpro-as2-52	Z3137732023	-11.3	0.404	383.49	REAL	O=C1C[C@H](C(=O)N[C@@H]2C[C@@]3(CCNC3)Oc3ccccc32)[C@@H]2CCCC[C@@H]2N1
vMpro-as2-53	Z653575014	-11.3	0.332	489.498	REAL	Cc1cc(NS(=O)(=O)c2cccc(C(=O)N3CCC(C(=O)c4cc(F)ccc4F)CC3)c2)no1
vMpro-as2-54	Z728499368	-11.3	0.365	421.479	REAL	O=C(C1CCN(c2ccc3nnnn3n2)CC1)N1CCC(=Cc2cccc(F)c2)CC1
vMpro-as2-55	Z748894022	-11.3	0.323	475.462	REAL	O=C(Nc1ccc2[nH]c(-c3cc(F)ccc3F)nc2c1)C1CCN(c2ccc3nnnn3n2)CC1
vMpro-as2-56	Z748894468	-11.3	0.323	474.474	REAL	O=C(Nc1ccc2[nH]c(-c3cc(F)ccc3F)nc2c1)C1CCN(c2ccc3nncn3n2)CC1
vMpro-as2-57	Z961061888	-11.3	0.353	444.47	REAL	Cc1n[nH]c(-c2ccc(NC(=O)c3ccc4c(c3)S(=O)(=O)c3ccccc3C4=O)cc2)n1
vMpro-as2-58	Z977441774	-11.3	0.404	380.378	REAL	O=C(c1cnc2[nH]c(=O)[nH]c(=O)c2c1)N1CC2(CCCC2)c2c(F)cccc21
vMpro-as2-59	ZINC000009332188	-11.3	0.323	460.488	ZINC	O=C(c1cccc1)[C@@H]1[C@@H]2C(=O)N(c3cccc4ccccc43)C(=O)[C@H]2[C@@H]2c3ccccc3C=CN21
vMpro-as2-60	ZINC000020086593	-11.3	0.332	456.461	ZINC	Cc1n[nH]c2c1[C@H](c1ccc([C@H]3c4c(C)n[nH]c4NC4=C3C(=O)OC4)cc1)C1=C(COC1=O)N2
vMpro-as2-61	ZINC000020393147	-11.3	0.323	460.488	ZINC	O=C(c1cccc1)[C@@H]1[C@@H]2C(=O)N(c3cccc4ccccc43)C(=O)[C@@H]2[C@@H]2c3ccccc3C=CN21
vMpro-as2-62	ZINC000033292519	-11.3	0.305	498.585	ZINC	Cc1cccc(N2CCN(C(=O)c3nc(Cn4nc(-c5ccc(C)c(C)c5)ccc4=O)no3)C[C@H]2C)c1
vMpro-as2-63	ZINC000071759495	-11.3	0.39	391.438	ZINC	Nc1nc2[nH]ncc2c(N2CCC(c3n[nH]c(=O)n3Cc3ccccc3)CC2)n1
vMpro-as2-64	ZINC000096345456	-11.3	0.342	447.469	ZINC	O=C([C@@H]1CC(=O)N(c2n[nH]c3ccccc32)C1)N1CCC(c2noc3cc(F)ccc32)CC1
vMpro-as2-65	ZINC000104480052	-11.3	0.314	490.945	ZINC	O=C(NC1=CC=C[C@@H]2C(=O)c3ccccc3C(=O)[C@H]12)c1cc(-c2ccccc2Cl)nc2ccccc21
vMpro-as2-66	ZINC000104480060	-11.3	0.314	490.945	ZINC	O=C(NC1=CC=C[C@@H]2C(=O)c3ccccc3C(=O)[C@@H]12)c1cc(-c2ccccc2Cl)nc2ccccc21
vMpro-as2-67	ZINC000239426033	-11.3	0.297	504.541	ZINC	O=C(c1cccc(N2C(=O)[C@@H]3[C@H]4C=C[C@@H](C4)[C@H]3C2=O)c1)c1cccc(N2C(=O)[C@@H]3[C@H]4C=C[C@@H](C4)[C@H]3C2=O)c1
vMpro-as2-68	PV-001810155719	-11.2	0.339	458.374	REAL	Cc1nc(-c2cc(NC(=O)c3ccc(=O)n(-c4ccc(F)cc4)n3)cc(C(F)(F)F)c2)n[nH]1
vMpro-as2-69	PV-001810157304	-11.2	0.339	458.374	REAL	Cc1nc(-c2cc(NC(=O)c3ccc(=O)n(-c4ccccc4F)n3)cc(C(F)(F)F)c2)n[nH]1
vMpro-as2-70	PV-001860197053	-11.2	0.415	371.396	REAL	Cc1cc(C(=O)N2NC(=O)C[C@@]23CCCC[C@@H]3C)nc2nc(O)[nH]c(=O)c12
vMpro-as2-71	PV-001863061710	-11.2	0.373	445.261	REAL	Cc1onc(-c2ccc(Cl)c(Cl)c2)c1C(=O)Nc1ccc([C@@H]2NC(=O)NC2=O)cc1
vMpro-as2-72	PV-001944141884	-11.2	0.4	398.296	REAL	O=C1COc2c(cc(C(F)(F)F)cc2NC(=O)N2CC[C@H]3C(=O)NC(=O)[C@H]3C2)N1
vMpro-as2-73	PV-001944143911	-11.2	0.361	442.393	REAL	O=C1COc2c(cc(C(F)(F)F)cc2NC(=O)N2CCC3(CC2)C[C@H](O)CNC3=O)N1
vMpro-as2-74	PV-001948674531	-11.2	0.386	410.399	REAL	Cc1nc(-c2cc(NC(=O)N3[C@@H](C)C(=O)N[C@@H](C)[C@H]3C)cc(C(F)(F)F)c2)n[nH]1
vMpro-as2-75	PV-001962078606	-11.2	0.373	420.502	REAL	O=C(N[C@@H]1CCCN(C(=O)N2CCCC2)C1)N1CCC[C@@H](c2ccc(F)c(F)c2)C1
vMpro-as2-76	Z1024049144	-11.2	0.32	465.508	REAL	O=C1Nc2ccccc2[C@@H]1C1CCN(C(=O)c2cccc(N3C(=O)c4ccccc4C3=O)c2)CC1
vMpro-as2-77	Z1072128894	-11.2	0.32	471.559	REAL	Cc1ccc2[nH]c([C@@H]3CCCN(C(=O)CN4C(=O)c5ccccc5N5C(=O)CC[C@]45)C3)nc2c1
vMpro-as2-78	Z1091306320	-11.2	0.35	426.479	REAL	COc1cccc(Cn2c(NC(=O)c3cc(C)nc4[nH]nc(C)c34)nc3ccccc32)c1
vMpro-as2-79	Z1102796065	-11.2	0.303	493.522	REAL	O=C(Nc1cccc(N2C(=O)c3ccccc3C2=O)c1)[C@H]1CCCN(C(=O)c2ccc3[nH]ncc3c2)C1
vMpro-as2-80	Z1171598481	-11.2	0.361	412.427	REAL	Cc1nnc2[nH]nc(NC(=O)c3cc(-c4ccc(F)cc4)nc4ccccc34)c2c1C
vMpro-as2-81	Z1251065307	-11.2	0.361	423.476	REAL	Cc1cc(C(=O)N2CCC[C@H](c3nnc4n3CCCCC4)C2)nc2nc(O)[nH]c(=O)c12
vMpro-as2-82	Z1265801277	-11.2	0.339	449.509	REAL	O=C(c1ncoc1-c1ccc2c(c1)OCCO2)N1CCC[C@H](c2nnc3n2CCCCC3)C1
vMpro-as2-83	Z1360866759	-11.2	0.361	419.44	REAL	O=C1CCCN1CC[C@@H]1CN(C(=O)c2cnc3[nH]c(=O)[nH]c(=O)c3c2)c2ccccc21
vMpro-as2-84	Z1620593776	-11.2	0.361	414.511	REAL	Cc1ccc2[nH]c3c(c2c1)C[C@H](NC(=O)Nc1cc(-c2n[nH]c(C)n2)ccc1C)CC3
vMpro-as2-85	Z1723433635	-11.2	0.329	456.461	REAL	CN1CC(=O)N(c2cccc(NC(=O)c3cccc(-c4cnc5[nH]c(=O)n(C)c5c4)c3)c2)C1=O
vMpro-as2-86	Z1723437098	-11.2	0.303	498.517	REAL	Cn1c(=O)[nH]c2ncc(-c3cccc(C(=O)N4CCC[C@H](c5nc(-c6ccc(F)cc6)no5)C4)c3)cc21
vMpro-as2-87	Z1723438783	-11.2	0.329	476.963	REAL	Cn1c(=O)[nH]c2ncc(-c3cccc(C(=O)N4CCC([C@H](O)c5ccc(Cl)cc5)CC4)c3)cc21
vMpro-as2-88	Z1766655795	-11.2	0.329	449.513	REAL	O=C(c1ccc2[nH]c3ccccc3c(=O)c2c1)N1CCC[C@@H](c2n[nH]c(-c3ccccc3)n2)C1
vMpro-as2-89	Z1827693751	-11.2	0.361	417.428	REAL	O=C(Nc1ccc(-n2nn[nH]c2=O)cc1)c1ccc2c(=O)n3c(nc2c1)CCCCC3
vMpro-as2-90	Z2159830273	-11.2	0.339	441.45	REAL	Cc1nnc2ccc(-c3noc(-c4cccc(NN5C(=O)[C@@H]6CC=CC[C@@H]6C5=O)c4)n3)cn12
vMpro-as2-91	Z2199970353	-11.2	0.35	435.439	REAL	Cn1c(=O)[nH]c(=O)c2cc(C(=O)N3C[C@@H](C[C@@H]4COCC(=O)N4)c4ccccc43)cnc21
vMpro-as2-92	Z223087504	-11.2	0.32	490.582	REAL	O=C1c2ccccc2S(=O)(=O)c2cc(C(=O)N3CCC[C@@H](c4nnc5n4CCCCC5)C3)ccc21
vMpro-as2-93	Z237105240	-11.2	0.35	428.534	REAL	O=C(Cc1coc2ccc3ccccc3c12)N1CCC[C@@H](c2nnc3n2CCCCC3)C1
vMpro-as2-94	Z237105536	-11.2	0.361	412.535	REAL	O=C(c1ccc2c(c1)-c1ccccc1C2)N1CCC[C@@H](c2nnc3n2CCCCC3)C1
vMpro-as2-95	Z424739836	-11.2	0.32	480.546	REAL	Cc1ccc(CNC(=O)C2CCN(C(=O)C3CCN(c4ccc5nnnn5n4)CC3)CC2)cc1F
vMpro-as2-96	Z460472820	-11.2	0.311	489.593	REAL	Cc1cc(C)cc(C(=O)N2CCC[C@H](C(=O)Nc3ccc(F)c(-c4nnc5n4CCCCC5)c3)C2)c1
vMpro-as2-97	Z512936300	-11.2	0.311	481.598	REAL	Cc1ccc(CNC(=O)c2cccc(CNC(=O)N3CCC[C@H](c4nc5ccccc5[nH]4)C3)c2)cc1
vMpro-as2-98	Z738431044	-11.2	0.329	456.484	REAL	O=C(Nc1ccc2[nH]c(-c3cccc(F)c3)nc2c1)C1CCN(c2ccc3nncn3n2)CC1
vMpro-as2-99	Z795993874	-11.2	0.329	455.469	REAL	Cc1cccn2c(=O)cc(COC(=O)c3cccc(NC(=O)[C@@H]4Cc5ccccc5O4)c3)nc12
vMpro-as2-100	Z992191116	-11.2	0.339	454.411	REAL	Cc1cc(C(=O)Nc2nc3cc(C(F)(F)F)ccc3n2Cc2ccco2)c2c(C)n[nH]c2n1

Supplementary Table 7. Top 100 virtual hits of the screen against the active site of M^{pro} in which a modified receptor structure based on the structure with PDB ID 6m0k was used (Screen ID: 17). The modifications are described in the main text. The name of each compound consists of the initial letter 'v' for virtual hit, followed by the target protein name and the target site ('as' for active site, 2 for docking scenario 2 of this target site). The score is the docking score given by QuickVina 2 in kcal/mol. The ligand efficiency (LE) is computed as LE = -score/#NonH, where #NonH is the number of heavy (i.e. non hydrogen) atoms.

Name	Catalog ID	Score	LE	MW	Library	SMILES
vMpro-as2-101	ZINC000001352198	-11.2	0.320	478.50	ZINC	Cc1ccc(C)c(Cn2nnc3c2nc(C2CCN(C(=O)c4cc(F)cc(F)c4)CC2)[nH]c3=O)c1
vMpro-as2-102	ZINC000003879166	-11.2	0.311	473.44	ZINC	O=C(O)c1ccc2c(c1Nc1ccnc3c1C(=O)c1ccccc1C3=O)C(=O)c1ccccc1C2=O
vMpro-as2-103	ZINC000009353751	-11.2	0.329	454.49	ZINC	C/C(=N\Nc1nc2c(c(=O)[nH]c(=O)n2C)n1Cc1ccccc2ccccc21)c1ccc(O)cc1
vMpro-as2-104	ZINC000012133624	-11.2	0.350	433.47	ZINC	Cc1cc(=O)n(CC(=O)N2CCC(n3nnc4c3nc(C)nc4O)CC2)c2ccccc12
vMpro-as2-105	ZINC000020086595	-11.2	0.329	456.46	ZINC	Cc1n[nH]c2c1[C@@H](c1ccc([C@H]3c4c(C)n[nH]c4NC4=C3C(=O)OC4)cc1)C1=C(COC1=O)N2
vMpro-as2-106	ZINC000024832512	-11.2	0.303	492.49	ZINC	C[C@@H](OC(=O)c1cccc(Nc2ncccn2)c1)C(=O)Nc1cccc2c1C(=O)c1ccccc1C2=O
vMpro-as2-107	ZINC000102643339	-11.2	0.339	438.50	ZINC	c1n[nH]c2ncn3nc(C45C[C@@H]6C[C@@H](C4)CC(n4nnc(-c7ccccc7)n4)(C6)C5)nc3c12
vMpro-as2-108	ZINC000408679806	-11.2	0.295	498.58	ZINC	Cc1cc(C)cc(NC(=O)c2cccc(N3C(=O)[C@@H]4[C@@H](C3=O)C3c5ccccc5C4c4ccccc43)c2)c1
vMpro-as2-109	PV-001825573645	-11.1	0.358	421.50	REAL	Cc1cn2nc(C(=O)Nc3cc(C(=O)N4C[C@@H](C)C[C@H](C)C4)ccc3C)cc2c(=O)[nH]1
vMpro-as2-110	PV-001847889872	-11.1	0.383	395.35	REAL	Cc1nnc2[nH]nc(NC(=O)C3=NN(c4ccc(F)cc4)C=O)CC3=O)c2c1C
vMpro-as2-111	PV-001855726145	-11.1	0.383	406.37	REAL	Cc1nc(-c2cc(NC(=O)[C@@H]3CCc4nnnn4CC3)cc(C(F)(F)F)c2)n[nH]1
vMpro-as2-112	PV-001867457597	-11.1	0.396	376.39	REAL	Cc1cc(C(=O)NCC(=O)c2ccc(F)c3ccccc23)c2c(C)n[nH]c2n1
vMpro-as2-113	PV-001947183848	-11.1	0.358	455.30	REAL	O=C(Nc1cccc2c(=O)[nH]ccc12)N1C[C@@H]2[C@H](C1)C(F)(F)C(F)(F)C(F)(F)C2(F)F
vMpro-as2-114	PV-001948675364	-11.1	0.383	408.38	REAL	Cc1nc(-c2cc(NC(=O)N3[C@@H]4CC[C@H]3CC(=O)NC4)cc(C(F)(F)F)c2)n[nH]1
vMpro-as2-115	Z1006856166	-11.1	0.317	493.54	REAL	Cc1cc(NS(=O)(=O)c2cccc(C(=O)N3CCN(C(=O)c4cc5ccccc5[nH]4)CC3)c2)no1
vMpro-as2-116	Z1088490864	-11.1	0.347	435.46	REAL	Cc1nnnn1-c1cc(NC(=O)N2CCC([C@H]3C(=O)Nc4ccccc43)CC2)ccc1F
vMpro-as2-117	Z1090637620	-11.1	0.347	427.46	REAL	COc1cccc(Cn2c(NC(=O)c3cc(C)nc4onc(C)c34)nc3ccccc32)c1
vMpro-as2-118	Z1117087294	-11.1	0.358	416.48	REAL	Cc1nc(-c2cccc(NC(=O)N3CCC([C@H]4C(=O)Nc5ccccc54)CC3)c2)n[nH]1
vMpro-as2-119	Z1127930141	-11.1	0.336	447.51	REAL	CC(=O)N1Cc2ccccc2C[C@H]1C(=O)Nc1ccc(F)c(-c2nnc3n2CCCCC3)c1
vMpro-as2-120	Z115522690	-11.1	0.317	497.45	REAL	O=C1/C(=C/NC2=NS(=O)(=O)c3ccccc32)c2ccccc2C(=O)N1c1cccc(C(F)(F)F)c1
vMpro-as2-121	Z1158453094	-11.1	0.336	447.51	REAL	CC(=O)N1Cc2ccccc2C[C@H]1C(=O)Nc1cc(-c2nnc3n2CCCCC3)ccc1F
vMpro-as2-122	Z1277644619	-11.1	0.347	437.43	REAL	Cc1nnnn1-c1cc(NC(=O)N2CCc3c(cccc3N3CCOC3=O)C2)ccc1F
vMpro-as2-123	Z1286733709	-11.1	0.336	443.55	REAL	Cc1cc(C)cc(C(=O)N2CCC[C@H](C(=O)N3CCn4c(nnc4-c4ccccc4)C3)C2)c1
vMpro-as2-124	Z1421880231	-11.1	0.347	429.48	REAL	Cc1nc([C@@H]2CCCN(CC(=O)Nc3ccc4c(c3)C(=O)c3ccccc3C4=O)C2)n[nH]1
vMpro-as2-125	Z1542344028	-11.1	0.347	428.45	REAL	O=C(Nc1ccccc1)Nc1cccc2c1CCN(C(=O)c1ccc3n[nH]c(=O)n3c1)C2
vMpro-as2-126	Z1552595589	-11.1	0.347	435.50	REAL	CC(=O)N1CCN(C(=O)c2ccc3noc(-c4ccc(F)cc4)c3c2)CC12CCCCC2
vMpro-as2-127	Z1576976549	-11.1	0.347	444.42	REAL	Cc1c(N2CCN(C(=O)c3ccc4[nH]cnc4c3)CC2)nn2c(C(F)(F)F)nnc2c1C
vMpro-as2-128	Z1585243691	-11.1	0.358	422.53	REAL	O=C1CCCc2cc(NC(=O)N3CCC[C@H](c4nnc5n4CCCCC5)C3)ccc2N1
vMpro-as2-129	Z1587197720	-11.1	0.358	444.93	REAL	Cc1noc([C@@H]2CCCN(c3ncc(Cl)c(N4CCC[C@H](c5nc(C)no5)C4)n3)C2)n1
vMpro-as2-130	Z1620486757	-11.1	0.396	386.36	REAL	O=C1NC(=O)N2CCN(C(=O)Nc3ccc(F)cc3-c3ccc(F)cc3)C[C@H]12
vMpro-as2-131	Z1653582205	-11.1	0.336	448.52	REAL	C[C@H](C(=O)Nc1cccc2c1C(=O)c1ccccc1C2=O)N1CCC[C@H](C2(C)OCCO2)C1
vMpro-as2-132	Z1684082603	-11.1	0.336	438.42	REAL	Nc1nc(Cc2noc(-c3ccc4noc(-c5ccc(F)cc5)c4c3)n2)nc2ccccc12
vMpro-as2-133	Z1684581770	-11.1	0.336	441.45	REAL	Cc1ccc(Nc2cccc(-c3nc(-c4cccc([C@]5(C)NC(=O)NC5=O)c4)no3)c2)nn1
vMpro-as2-134	Z1723429876	-11.1	0.317	484.58	REAL	Cn1c(=O)[nH]c2ncc(-c3cccc(C(=O)N4CCN(C5nc6ccccc6s5)CC4)c3)cc21
vMpro-as2-135	Z1723430355	-11.1	0.317	471.52	REAL	Cn1c(=O)[nH]c2ncc(-c3cccc(C(=O)N4CCC(C(=O)Nc5ccccc5O)CC4)c3)cc21
vMpro-as2-136	Z1723437031	-11.1	0.317	473.51	REAL	Cn1c(=O)[nH]c2ncc(-c3cccc(C(=O)N4CCC(C(=O)Nc5cccc(F)c5)CC4)c3)cc21
vMpro-as2-137	Z1723437103	-11.1	0.308	479.54	REAL	Cn1c(=O)[nH]c2ncc(-c3cccc(C(=O)N4CCC(c5nc(-c6ccccc6)n[nH]5)CC4)c3)cc21
vMpro-as2-138	Z1723438662	-11.1	0.326	460.51	REAL	Cn1c(=O)[nH]c2ncc(-c3cccc(C(=O)N4CCC([C@H](O)c5ccc(F)cc5)CC4)c3)cc21
vMpro-as2-139	Z1723442803	-11.1	0.317	472.48	REAL	Cc1cc(-c2noc([C@@H](C)NC(=O)c3cccc(-c4cnc5[nH]c(=O)n(C)c5c4)c3)n2)cc1F
vMpro-as2-140	Z1765886231	-11.1	0.347	431.40	REAL	O=C(NCc1cc(=O)[nH]c2ccccc12)c1cc(F)cc2c(=O)c3cc(F)ccc3[nH]c12
vMpro-as2-141	Z1766320930	-11.1	0.358	426.46	REAL	O=C(c1cc(F)cc2c(=O)c3cc(F)ccc3[nH]c12)N1CCOC2(CCCCC2)C1
vMpro-as2-142	Z19083170	-11.1	0.317	488.54	REAL	CC1(C)C(=O)Nc2ccccc2N1C(=O)CSc1nc2ccccc2c(=O)n1-c1ccccc1F
vMpro-as2-143	Z1937461390	-11.1	0.358	418.43	REAL	O=C(Nc1ccc(-c2nc[nH]n2)cc1F)c1ccc2c(=O)n3c(nc2c1)CCCCC3
vMpro-as2-144	Z2113902315	-11.1	0.370	412.54	REAL	C[C@H]1c2nnc(C3CCCC3)n2CCN1C(=O)N[C@H](C)c1nnc2n1CCCCC2
vMpro-as2-145	Z2179585869	-11.1	0.370	394.48	REAL	Cc1[nH]c2ccccc2c1C1=CCN(c2nn3c(C)nnc3ccccc23)CC1
vMpro-as2-146	Z2188335341	-11.1	0.336	446.51	REAL	O=C([C@@H]1CN(Cc2nc3ccccc3c(=O)[nH]2)CCO1)N1Cc2ccc(O)cc2C2(CC2)C1
vMpro-as2-147	Z2227338125	-11.1	0.383	434.28	REAL	O=C(Nc1[nH]nc2nc(O)ccc12)[C@@H]1CCCN(C(=O)c2ccc(Cl)c(Cl)c2)C1
vMpro-as2-148	Z2227338471	-11.1	0.383	401.37	REAL	O=C(Nc1[nH]nc2nc(O)ccc12)C1CCN(C(=O)c2ccc(F)cc2F)CC1
vMpro-as2-149	Z2407090427	-11.1	0.383	397.41	REAL	Cc1cc(F)cc(-n2nc(C(=O)N3CCN4C(=O)NC(=O)[C@H]4C3)c3c2CCC3)c1
vMpro-as2-150	Z2903064710	-11.1	0.358	434.48	REAL	O=C1N=CC=C[C@@H]1c1noc(-c2cccc(S(=O)(=O)N3CCc4ccccc4C3)c2)n1
vMpro-as2-151	Z2903469901	-11.1	0.300	498.54	REAL	Cn1cc(-c2noc(CCC(=O)N3CCN(C4c5ccccc5-c5ccccc54)CC3)n2)c(=O)[nH]c1=O
vMpro-as2-152	Z2974805043	-11.1	0.411	365.39	REAL	Cc1noc2ncnc(N3CCC4(CC3)CNC(=O)c3ccccc3O4)c12
vMpro-as2-153	Z365636896	-11.1	0.347	435.53	REAL	Cc1cc(NC(=O)CN2CCN(C(=O)c3ccc4[nH]c5c(c4c3)CCCCC5)CC2)no1
vMpro-as2-154	Z381129036	-11.1	0.358	414.47	REAL	Cn1cnnc1-c1ccc(NC(=O)c2ccc3c(=O)n4c(nc3c2)CCCC4)cc1
vMpro-as2-155	Z395357220	-11.1	0.347	435.57	REAL	O=C1CCCCN1Cc1ccc(C(=O)N2CCC[C@@H](c3nnc4n3CCCCC4)C2)cc1
vMpro-as2-156	Z454430608	-11.1	0.317	471.60	REAL	Cc1cc(C)cc(C(=O)N2CCC[C@H](C(=O)Nc3cccc(-c4nnc5n4CCCCC5)c3)C2)c1
vMpro-as2-157	Z644350534	-11.1	0.326	475.58	REAL	O=C(c1cc(F)ccc1F)C1CCN(CC(=O)N2CCC(C(=O)N3CCCCC3)CC2)CC1
vMpro-as2-158	Z651757526	-11.1	0.326	456.48	REAL	O=C(Nc1ccc2[nH]c(-c3ccc(F)cc3)nc2c1)C1CCN(c2ccc3nncn3n2)CC1
vMpro-as2-159	Z738431014	-11.1	0.326	457.47	REAL	O=C(Nc1ccc2[nH]c(-c3cccc(F)c3)nc2c1)C1CCN(c2ccc3nnnn3n2)CC1
vMpro-as2-160	Z767245730	-11.1	0.370	408.39	REAL	Cc1onc(-c2ccc(F)cc2)c1C(=O)Nc1ccc([C@]2(C)NC(=O)NC2=O)cc1
vMpro-as2-161	Z786227244	-11.1	0.317	469.50	REAL	O=C(Nc1ccc(NC(=O)[C@H]2CCCO2)cc1)c1cccc(NC(=O)c2ccc3[nH]cnc3c2)c1
vMpro-as2-162	Z795993688	-11.1	0.317	470.48	REAL	O=CN1CCc2cc(C(=O)COC(=O)c3cccc(NC(=O)[C@@H]4Cc5ccccc5O4)c3)ccc21
vMpro-as2-163	Z806433434	-11.1	0.300	496.61	REAL	COc1ccc(C(=O)N2CCC[C@H](C(=O)N3CCC(c4c[nH]c5ncccc45)CC3)C2)c2ccccc12
vMpro-as2-164	Z808686756	-11.1	0.326	455.51	REAL	O=C(Nc1ccc(CC(=O)N2CCN(c3ccc(O)cc3)CC2)cc1)c1cc2ccccc2o1
vMpro-as2-165	Z899254338	-11.1	0.370	405.50	REAL	O=C(Cn1ccc(=O)c2ccccc21)N1CCC[C@@H](c2nnc3n2CCCCC3)C1
vMpro-as2-166	Z95870366	-11.1	0.300	491.55	REAL	O=C(c1cc(-c2ccc3c(c2)OCCO3)nc2ccccc12)N1CCC(c2nnc3ccccn23)CC1
vMpro-as2-167	Z98336198	-11.1	0.336	458.50	REAL	NC1=Nc2nc3cc4c(cc3n2[C@@H](c2ccc(-c3nc5ccccc5s3)o2)N1)OCCCO4
vMpro-as2-168	Z999696386	-11.1	0.308	478.55	REAL	O=C(Nc1ccc(Cn2cnc3ccccc32)cc1)[C@H]1CCCN(C(=O)c2ccc3[nH]ncc3c2)C1
vMpro-as2-169	ZINC000001238226	-11.1	0.300	497.53	ZINC	O=C(Nc1cccc2ccccc21)N1CCC(c2nc(=O)c3nnn(Cc4ccc(F)cc4)c3[nH]2)CC1
vMpro-as2-170	ZINC000001352206	-11.1	0.317	478.50	ZINC	Cc1ccc(C)c(Cn2nnc3c2nc(C2CCN(C(=O)c4ccc(F)c(F)c4)CC2)[nH]c3=O)c1
vMpro-as2-171	ZINC000003861401	-11.1	0.317	459.46	ZINC	Nc1ccc(Nc2ccc(N)c3c2C(=O)c2ccccc2C3=O)c2c1C(=O)c1ccccc1C2=O
vMpro-as2-172	ZINC000009192689	-11.1	0.326	454.49	ZINC	C/C(=N\Nc1nc2c(c(=O)[nH]c(=O)n2C)n1Cc1ccccc2ccccc21)c1ccccc1O
vMpro-as2-173	ZINC000014329813	-11.1	0.326	449.51	ZINC	CN1CCCN(C(=O)Cn2c3ccccc3c(=O)c3ccccc32)c2nc3ccccc3nc21
vMpro-as2-174	ZINC000098023312	-11.1	0.252	584.54	ZINC	O=C1c2ccc(Oc3cccc(Oc4ccc5c(c4)C(=O)N(c4ccccc4O)C5=O)c3)cc2C(=O)N1c1ccccc1O
vMpro-as2-175	ZINC000101064563	-11.1	0.278	597.42	ZINC	O=C(c1ccccc1)C1=C[C@H]2[C@H]3C(=O)N(c4ccc5c(c4)OCO5)C(=O)[C@@H]3[C@H](C(=O)c3ccc(Br)cc3)N2C=C1
vMpro-as2-176	ZINC000101064566	-11.1	0.278	597.42	ZINC	O=C(c1ccccc1)C1=C[C@H]2[C@@H]3C(=O)N(c4ccc5c(c4)OCO5)C(=O)[C@@H]3[C@H](C(=O)c3ccc(Br)cc3)N2C=C1
vMpro-as2-177	ZINC000102666371	-11.1	0.370	420.90	ZINC	CC1(C)CC(O)=C2C(=NC(Nc3nc4ccccc4o3)=N[C@@H]2c2ccccc2Cl)C1
vMpro-as2-178	ZINC000103518122	-11.1	0.300	494.53	ZINC	Cc1ccc2c(c1)[C@H](N[C@@H](Cc3c[nH]c4ccccc34)[C@H]3C(=O)N(c4ccc(F)cc4)C(=O)[C@@H]31)C(=O)N2
vMpro-as2-179	ZINC000229699794	-11.1	0.300	488.55	ZINC	Cc1ccccc1N1C(=O)[C@@H]2[C@H](C1=O)[C@@H]1CCCN1[C@@]21c2ccccc2-n2c1nc1ccccc1c2=O
vMpro-as2-180	ZINC000247703670	-11.1	0.308	479.47	ZINC	O=C([C@@H]1[C@H]2C(=O)N(c3ccc(F)cc3)C(=O)[C@H]2[C@H]2C=Cc3ccccc3N21)n1nnc2ccccc21
vMpro-as2-181	ZINC000253414836	-11.1	0.308	476.58	ZINC	CN1c2ccccc2C(=O)N2CCc3c4ccccc4n(CC(=O)N4CCc5ccccc5C4)c3[C@@H]12
vMpro-as2-182	ZINC000408978119	-11.1	0.292	495.49	ZINC	O=C(Oc1ccc2nc3c4ccccc4c4ccccc4c3nc2c1)c1ccc(N2C(=O)C=CC2=O)cc1
vMpro-as2-183	PV-000287469996	-11.0	0.355	417.51	REAL	Cc1cc(C(=O)N2C[C@@H]3CCN(C(=O)[C@@H]4C[C@@H]5O[C@H]4[C@@H]4C[C@@H]54)[C@@H]3C2)nc2ccccc12
vMpro-as2-184	PV-000378122571	-11.0	0.407	366.38	REAL	Cc1cc(C(=O)N2[C@H]3CC[C@@H]2C[C@H]3NC(=O)c2cccn3nnnc23)[nH]n1
vMpro-as2-185	PV-001810155786	-11.0	0.344	440.38	REAL	Cc1nc(-c2cc(NC(=O)c3ccc(=O)n(-c4ccccc4)n3)cc(C(F)(F)F)c2)n[nH]1
vMpro-as2-186	PV-001818619514	-11.0	0.355	457.32	REAL	CC(C)c1noc2ncc(C(=O)N3C[C@@H]4[C@@H](C3)C(F)(F)C(F)(F)C(F)(F)C4(F)F)cc12
vMpro-as2-187	PV-001840750949	-11.0	0.355	417.42	REAL	COC(=O)c1cc(-c2ccccc2CNC(=O)c2ccc3c(=O)[nH]c(C)nc3c2)[nH]n1
vMpro-as2-188	PV-001875529051	-11.0	0.367	440.29	REAL	O=C(c1cc2ccccc2c(=O)[nH]1)N1C[C@H]2[C@H](C1)C(F)(F)C(F)(F)C(F)(F)C2(F)F
vMpro-as2-189	PV-001875530016	-11.0	0.379	428.28	REAL	Cc1nnc2ccc(C(=O)N3C[C@@H]4[C@@H](C3)C(F)(F)C(F)(F)C(F)(F)C4(F)F)cn12
vMpro-as2-190	PV-001958523432	-11.0	0.367	444.32	REAL	Cc1ccc2c(c1)[C@H](NC(=O)N1C[C@H]3[C@H](C1)C(F)(F)C(F)(F)C(F)(F)C3(F)F)CO2
vMpro-as2-191	PV-002008078398	-11.0	0.379	421.56	REAL	C[C@H](CC#N)N(C)c1nnc([C@@H]2CCS(=O)(=O)C2)n1CC[C@@]1(O)C[C@H]2CC[C@H]1C2
vMpro-as2-192	Z1025056226	-11.0	0.344	433.47	REAL	O=C1NC2ccccc2[C@H]1C1CCN(C(=O)Nc2cccc(N3C(=O)CNC3=O)c2)CC1
vMpro-as2-193	Z1042997160	-11.0	0.355	417.42	REAL	O=C(Nc1ccc(-c2noc(=O)[nH]2)cc1)c1ccc2c(=O)n3c(nc2c1)CCCCC3
vMpro-as2-194	Z1104835886	-11.0	0.355	418.50	REAL	O=C1CCCc2cc(NC(=O)N3CCC([C@@H]4C(=O)Nc5ccccc54)CC3)ccc2N1
vMpro-as2-195	Z1130902954	-11.0	0.355	421.48	REAL	Cc1nc2[nH]n(C)c(=O)c2c(C)c1CCC(=O)N1CCc2[nH]c3ccc(F)cc3c2C1
vMpro-as2-196	Z1171597597	-11.0	0.367	394.44	REAL	Cc1nnc2[nH]nc(NC(=O)c3cc(-c4ccccc4)nc4ccccc34)c2c1C
vMpro-as2-197	Z1174755033	-11.0	0.344	446.46	REAL	O=C([C@@H]1C[C@@H]2CCCC[C@H]2N1C(=O)c1ccc(F)cc1F)N1CCO[C@H](c2nnn[nH]2)C1
vMpro-as2-198	Z1187918644	-11.0	0.344	430.55	REAL	Cc1ccc(NC(=O)c2ccc(N3CCC[C@@H](c4nnc5n4CCCCC5)C3)nc2)cc1
vMpro-as2-199	Z1204855483	-11.0	0.379	389.42	REAL	O=C(Nc1cccc(-c2nnc[nH]2)c1)C1CCN(c2ccc3nncn3n2)CC1
vMpro-as2-200	Z1231782892	-11.0	0.355	418.46	REAL	Cc1ccc(Nc2ccccc(C(=O)N3CCN(C(=O)c4ccc(=O)[nH]c4)CC3)c2)nn1

Supplementary Table 8. Virtual screening hits 101 to 200 of the screen against the active site of M^{pro} in which a modified structure based on the structure with PDB ID 6m0k was used (Screen ID: 17). The modifications are described in the main text. Compounds were filtered so that hits had MW < 600 dalton, cLogP < 6, number of hydrogen bond acceptors < 11, and no reactive functional groups. The name of each compound consists of the initial letter 'v' for virtual hit, followed by the target protein name and the target site ('as' for active site, 2 for docking scenario 2 of this target site). The score is the docking score given by QuickVina 2 in kcal/mol. The ligand efficiency (LE) is computed as LE = -score/#NonH, where #NonH is the number of heavy (i.e. non hydrogen) atoms.

Name	Catalog ID	Score	LE	MW	Library	SMILES
vAce2-spike1-1	PV-001861465482	-8.8	0.293	418.338	REAL	Cc1cc(O)nc2ccc(NC(=O)c3nc(C)n(-c4nnc(C(F)(F)F)[nH]4)n3)cc12
vAce2-spike1-2	Z1323896259	-8.8	0.275	449.392	REAL	Cc1nc(C(=O)Nc2ccc3c(c2)OC2(CCCCC2)O3)nn1-c1nnc(C(F)(F)F)[nH]1
vAce2-spike1-3	Z1323884037	-8.7	0.281	425.373	REAL	Cc1nc(C(=O)Nc2ccc3c(c2)Cc2ccccc2-3)nn1-c1nnc(C(F)(F)F)[nH]1
vAce2-spike1-4	Z1613949112	-8.7	0.281	420.422	REAL	O=C(Nc1n[nH]c(Cc2cccc(F)c2)n1)c1nn(-c2ccccc2F)c2c1CCC2
vAce2-spike1-5	Z1664931328	-8.7	0.29	397.433	REAL	Cc1ccc(-c2nnc([C@H]3CC(=O)N(c4ccc5c(c4)Cc4ccccc4-5)C3)o2)o1
vAce2-spike1-6	Z2160483899	-8.7	0.29	398.421	REAL	Cc1nc(-c2noc([C@H]3CC(=O)N(c4ccc5c(c4)Cc4ccccc4-5)C3)n2)co1
vAce2-spike1-7	Z810425300	-8.6	0.246	493.63	REAL	Cc1cccc(NC(=O)[C@H]2CCCN(C(=O)CCc3nc4sc5c(c4c(=O)[nH]3)CC[C@@H](C)C5)C2)n1
vAce2-spike1-8	PV-001818840757	-8.5	0.283	408.392	REAL	O=C(C[C@@H]1NC(=O)c2ccccc2NC1=O)Nc1n[nH]c(Cc2cccc(F)c2)n1
vAce2-spike1-9	PV-001868042535	-8.5	0.274	438.388	REAL	Cc1nc(C(=O)Nc2ccc(N3CCCC3)c(F)c2)nn1-c1nnc(C(F)(F)F)[nH]1
vAce2-spike1-10	Z1235131928	-8.5	0.274	413.48	REAL	Cc1cc(NNC(=O)[C@@H]2CC(=O)N(c3ccc4c(c3)Cc3ccccc3-4)C2)nc(C)n1
vAce2-spike1-11	Z1272302699	-8.5	0.258	446.485	REAL	Cc1nc(-c2ccc(N3CCC[C@H](c4nc(-c5cccc(F)c5)no4)C3)nc2)[nH]c(=O)c1C
vAce2-spike1-12	Z1324897279	-8.5	0.266	445.408	REAL	Cc1nc(C(=O)Nc2ccc3c(c2)nc2n3CCCCC2)nn1-c1nnc(C(F)(F)F)[nH]1
vAce2-spike1-13	Z1325147839	-8.5	0.304	393.328	REAL	Cc1nc(C(=O)Nc2ccc3c(c2)CCCO3)nn1-c1nnc(C(F)(F)F)[nH]1
vAce2-spike1-14	Z3167706395	-8.5	0.293	395.47	REAL	Cc1cccc(NC(=O)[C@H]2CCCN(c3nnc(Cc4n[nH]c(C)n4)n3C)C2)n1
vAce2-spike1-15	PV-001842100988	-8.4	0.29	459.307	REAL	Cc1cc(N2CCC[C@H](NC(=O)c3nc(C)n(-c4nnc[nH]4)n3)C2=O)ccc1Br
vAce2-spike1-16	PV-001957904638	-8.4	0.29	404.44	REAL	C[C@@H](NC(=O)N1CCC2(CC1)C[C@@H](O)CCO2)c1nc(-c2cccc(F)c2)no1
vAce2-spike1-17	Z1323893567	-8.4	0.29	417.254	REAL	Cc1nc(C(=O)Nc2ccc3c(c2)OC(F)(F)O3)nn1-c1nnc(C(F)(F)F)[nH]1
vAce2-spike1-18	Z1546238198	-8.4	0.255	444.537	REAL	Cc1cc(C)nc(-n2nc(C(=O)N3CCC(C(=O)N4CCc5ccccc54)CC3)cc2C)n1
vAce2-spike1-19	Z2087173589	-8.4	0.271	435.365	REAL	Cc1nc(C(=O)Nc2ccc3c(c2)C(=O)CC(C)(C)O3)nn1-c1nnc(C(F)(F)F)[nH]1
vAce2-spike1-20	Z2232287256	-8.4	0.255	437.502	REAL	Cc1c(C(=O)Nc2ccc3c(c2)N(C(=O)Cc2ccccc2)CC3)nnn1-c1ccccc1
vAce2-spike1-21	PV-001826352288	-8.3	0.268	454.843	REAL	Cc1nc(C(=O)Nc2ccc(N3CCCC3)c(Cl)c2)nn1-c1nnc(C(F)(F)F)[nH]1
vAce2-spike1-22	PV-001840548514	-8.3	0.259	456.378	REAL	Cc1nc(C(=O)Nc2cc(F)c(N3CCCC3)c(F)c2)nn1-c1nnc(C(F)(F)F)[nH]1
vAce2-spike1-23	PV-001871319755	-8.3	0.259	434.498	REAL	CNC(=O)Nc1ccc(C(=O)N2CCC(Cc3nc(-c4cccc(C)n4)no3)CC2)cc1
vAce2-spike1-24	PV-001874465013	-8.3	0.307	374.281	REAL	O=C(Nc1cnc2[nH]ncc2c1)c1cccc(-c2noc(C(F)(F)F)n2)c1
vAce2-spike1-25	Z1027770464	-8.3	0.252	449.485	REAL	O=C(Nc1ccc(N2CCCC2=O)cc1)N1CCC[C@@H](c2nc(-c3cccc(F)c3)no2)C1
vAce2-spike1-26	Z1325370435	-8.3	0.296	421.403	REAL	Cc1nc(C(=O)N[C@@H]2CCC[C@@H](S(C)(=O)=O)C2)nn1-c1nnc(C(F)(F)F)[nH]1
vAce2-spike1-27	Z1430648589	-8.3	0.277	419.37	REAL	Cc1cccc2nc(CNC(=O)c3nc(C)n(-c4nnc(C(F)(F)F)[nH]4)n3)n(C)c12
vAce2-spike1-28	Z1530493105	-8.3	0.268	433.437	REAL	Cc1nc(C(=O)Nc2ccc3c(c2)C(C)(C)CC3(C)C)nn1-c1nnc(C(F)(F)F)[nH]1
vAce2-spike1-29	Z1637282921	-8.3	0.307	368.342	REAL	O=C(Nc1n[nH]c(Cc2cccc(F)c2)n1)C1=Cc2cc(F)ccc2OC1
vAce2-spike1-30	Z1683565629	-8.3	0.259	449.359	REAL	O=C1C[C@H](c2nc(-c3ccF)ccc3C(F)(F)F)no2)CN1c1cccc2c(c1)OCCO2
vAce2-spike1-31	Z1750746709	-8.3	0.307	365.327	REAL	O=C(Nc1n[nH]c(Cc2cccc(F)c2)n1)c1cc2c(=O)[nH]cnc2cn1
vAce2-spike1-32	Z1823377971	-8.3	0.277	433.311	REAL	O=C(Nc1ccc(C(F)(F)F)nn1)N[C@H]1CC(=O)N(c2cccc(C(F)(F)F)c2)C1
vAce2-spike1-33	Z1891575450	-8.3	0.259	425.447	REAL	NC(=O)c1c[nH]c(-c2noc([C@H]3CC(=O)N(c4ccc5c(c4)Cc4ccccc4-5)C3)n2)c1
vAce2-spike1-34	Z2206298590	-8.3	0.277	425.312	REAL	O=C(N[C@@H]1COc2c(F)cc(F)cc2C1)c1cccc(-c2noc(C(F)(F)F)n2)c1
vAce2-spike1-35	Z2413550394	-8.3	0.332	368.382	REAL	C[C@@H]1CCN[C@H](c2nc(-c3ccc4sc(C(F)(F)F)nc34)no2)C1
vAce2-spike1-36	Z983988696	-8.3	0.231	489.574	REAL	Cc1cc(NC(=O)CN2CCN(C(=O)NCc3ccc(-c4ccc5c(c4)CCCO5)cc3)CC2)no1
vAce2-spike1-37	PV-001810541003	-8.2	0.293	385.304	REAL	O=C(Nc1cc2ccccc2nn1)c1cccc(-c2noc(C(F)(F)F)n2)c1
vAce2-spike1-38	PV-001837033462	-8.2	0.315	379.322	REAL	O=C(Nc1ccc2nc(S)oc2c1)c1cncc2nc(C(F)(F)F)[nH]c12
vAce2-spike1-39	PV-001846781053	-8.2	0.273	417.346	REAL	O=C(Nc1cccc(N2C(=O)CCCC2=O)c1)c1cncc2nc(C(F)(F)F)[nH]c12
vAce2-spike1-40	PV-001957902804	-8.2	0.256	438.437	REAL	C[C@@H](NC(=O)N[C@@H](C)c1ccc(-n2cccn2)c(F)c1)c1nc(-c2cccc(F)c2)no1
vAce2-spike1-41	Z1323948822	-8.2	0.283	427.773	REAL	Cc1nc(C(=O)N[C@@H]2CCOc3c(Cl)cccc32)nn1-c1nnc(C(F)(F)F)[nH]1
vAce2-spike1-42	Z1324950851	-8.2	0.273	442.744	REAL	Cc1nc(C(=O)Nc2cc3c(cc2Cl)NC(=O)CO3)nn1-c1nnc(C(F)(F)F)[nH]1
vAce2-spike1-43	Z1404562288	-8.2	0.273	417.354	REAL	Cc1nc(C(=O)N2CC(c3nc4ccccc4[nH]3)C2)nn1-c1nnc(C(F)(F)F)[nH]1
vAce2-spike1-44	Z1416543572	-8.2	0.283	388.426	REAL	CNC(=O)Cc1noc([C@H]2CC(=O)N(c3ccc4c(c3)Cc3ccccc3-4)C2)n1
vAce2-spike1-45	Z1683768061	-8.2	0.248	436.47	REAL	NC(=O)c1cccc(-c2noc([C@H]3CC(=O)N(c4ccc5c(c4)Cc4ccccc4-5)C3)n2)c1
vAce2-spike1-46	Z1684179630	-8.2	0.304	378.411	REAL	Cc1cccc(-c2noc(-c3csc(-c4ccc5c(c4)OCCO5)n3)n2)n1
vAce2-spike1-47	Z1685323420	-8.2	0.265	413.444	REAL	Cc1cc(C)nc(-n2nc(-c3nc(-c4cccc(-c5nnc(C)[nH]5)c4)no3)cc2C)n1
vAce2-spike1-48	Z1741672460	-8.2	0.256	445.448	REAL	Cc1nc(C(=O)N2C[C@H](c3ccccc3)[C@H]3CCCC[C@H]32)nn1-c1nnc(C(F)(F)F)[nH]1
vAce2-spike1-49	Z1873469736	-8.2	0.273	416.358	REAL	CN1C(=O)CCc2cc(NC(=O)c3cccc(-c4noc(C(F)(F)F)n4)c3)cccc21
vAce2-spike1-50	Z1981822081	-8.2	0.265	441.456	REAL	Cc1nc(C(=O)N2CCCC[C@@H]2[C@H]2C[C@@H](C)CC[C@@H]2O)nn1-c1nnc(C(F)(F)F)[nH]1
vAce2-spike1-51	Z2089425314	-8.2	0.293	378.387	REAL	Cc1cccc(-c2nnc([C@H]3CC(=O)N(c4ccc5c(c4)OCCO5)C3)o2)n1
vAce2-spike1-52	Z2091204875	-8.2	0.293	407.738	REAL	O=C(Nc1nc2c(Cl)cccc2[nH]1)c1cccc(-c2noc(C(F)(F)F)n2)c1
vAce2-spike1-53	Z2118684250	-8.2	0.273	416.318	REAL	O=C(NNc1nc2ccccc2c(=O)[nH]1)c1cccc(-c2noc(C(F)(F)F)n2)c1
vAce2-spike1-54	Z2159675548	-8.2	0.273	436.745	REAL	Cc1nc(-c2nc(-c3c(Cl)nc4ccccn34)no2)nn1-c1nnc(C(F)(F)F)[nH]1
vAce2-spike1-55	Z2229810567	-8.2	0.265	428.369	REAL	Cc1cc2cc(NC(=O)c3cccc(-c4noc(C(F)(F)F)n4)c3)ccc2n(C)c1=O
vAce2-spike1-56	Z2234572537	-8.2	0.304	390.348	REAL	Nc1cc(-c2noc(-c3csc(-c4cccc(C(F)(F)F)c4)n3)n2)ncn1
vAce2-spike1-57	Z2284942574	-8.2	0.273	399.449	REAL	Cc1cccc(-c2nnc(-c3ccc(C(=O)N4C[C@H]5[C@@H]6C=C[C@@H](O6)[C@@H]5C4)cc3)o2)c1
vAce2-spike1-58	Z2477230542	-8.2	0.283	398.397	REAL	C[C@@H](NC(=O)NCc1ncc2c(n1)CCOC2)c1nc(-c2cccc(F)c2)no1
vAce2-spike1-59	Z499291430	-8.2	0.228	483.535	REAL	Cc1ncc2c(n1)CC[C@H](NC(=O)NNC(=O)c1ccc(Cn3nnc(-c4ccccc4)n3)cc1)C2
vAce2-spike1-60	Z509797392	-8.2	0.248	443.506	REAL	CCc1cc(=O)[nH]c(-c2cccc(NC(=O)C3CCN(c4nc5ccccc5o4)CC3)c2)n1
vAce2-spike1-61	Z647619990	-8.2	0.248	444.494	REAL	Cc1ccc2c(O)c(C(=O)N3CCN([C@@H](C)c4nc(-c5ccccc5)no4)CC3)cnc2n1
vAce2-spike1-62	PV-001829221598	-8.1	0.261	452.464	REAL	Cc1cc(NC(=O)c2nc(C)n(-c3nnc(C(F)(F)F)[nH]3)n2)ccc1N1CCSCC1
vAce2-spike1-63	PV-001841154561	-8.1	0.27	411.382	REAL	O=C(Nc1cc(Cc2ccccc2)ccc1O)c1cccn2cc(C(F)(F)F)nc12
vAce2-spike1-64	PV-001846557694	-8.1	0.3	380.329	REAL	O=C(Nc1cc([C@H]2CCCOC2)[nH]n1)c1cncc2nc(C(F)(F)F)[nH]c12
vAce2-spike1-65	PV-001850123693	-8.1	0.289	375.383	REAL	O=C1CC(c2cccc(NC(=O)c3cccc4ccc(O)nc34)c2)CC(=O)N1
vAce2-spike1-66	PV-001855678163	-8.1	0.27	423.834	REAL	O=C(Nc1n[nH]c(Cc2cccc(F)c2)n1)c1cccc(Oc2ccc(Cl)cn2)c1
vAce2-spike1-67	PV-001856308878	-8.1	0.261	446.271	REAL	Cc1nc(C(=O)Nc2ccc3nc(C(F)(F)F)oc3c2)nn1-c1nnc(C(F)(F)F)[nH]1
vAce2-spike1-68	PV-001864277680	-8.1	0.261	434.381	REAL	Cc1nc(C(=O)Nc2ccc3c(c2)[C@@H](C)CC(=O)N3C)nn1-c1nnc(C(F)(F)F)[nH]1
vAce2-spike1-69	PV-001866524845	-8.1	0.27	421.338	REAL	Cc1nc(C(=O)NC[C@@H]2CC(=O)c3ccccc3O2)nn1-c1nnc(C(F)(F)F)[nH]1
vAce2-spike1-70	PV-001872451883	-8.1	0.279	415.375	REAL	Cc1nc(C(=O)NC[C@H]2CC[C@@]3(CO[C@H](C)C3)O2)nn1-c1nnc(C(F)(F)F)[nH]1
vAce2-spike1-71	PV-001874645292	-8.1	0.261	429.357	REAL	C[C@H](NC(=O)c1cccc(N2C(=O)c3ccccc3C2=O)c1)c1nnc(C(F)(F)F)[nH]1
vAce2-spike1-72	PV-001877476707	-8.1	0.3	378.309	REAL	O=C(Nc1nc2c(o1)CCCC2)c1cccc(-c2noc(C(F)(F)F)n2)c1
vAce2-spike1-73	PV-001944811377	-8.1	0.245	450.541	REAL	COc1cccc(-c2noc([C@@H](C)NC(=O)Nc3cnc(N4CCCC[C@H]4C)c(C)c3)n2)c1
vAce2-spike1-74	PV-001946418667	-8.1	0.312	372.35	REAL	C[C@@H](NC(=O)Nc1cc(C2(C)CCCC2)on1)c1nnc(C(F)(F)F)[nH]1
vAce2-spike1-75	PV-001957890232	-8.1	0.279	412.876	REAL	COc1cccc(-c2noc([C@H](C)NC(=O)N[C@@H]3CCc4cc(Cl)ccc43)n2)c1
vAce2-spike1-76	PV-001961056425	-8.1	0.289	396.336	REAL	O=C(NCc1nc(C(F)(F)F)n[nH]1)N[C@H]1CCN(c2ccc3nncn3n2)C1
vAce2-spike1-77	Z1004161658	-8.1	0.245	444.469	REAL	O=C(Nc1cnc(-c2ccccc2)nc1)N1CCC[C@H](c2nc(-c3cccc(F)c3)no2)C1
vAce2-spike1-78	Z1200974302	-8.1	0.253	424.459	REAL	COc1cc(-c2noc([C@H]3CC(=O)N(c4ccc5c(c4)Cc4ccccc4-5)C3)n2)ccn1
vAce2-spike1-79	Z1231830924	-8.1	0.279	387.402	REAL	Cc1ccc(Nc2cccc(C(=O)NNc3nc(-c4ccccc4)no3)c2)nn1
vAce2-spike1-80	Z1255854579	-8.1	0.27	406.441	REAL	O=C(Nc1nc2ccccc2c(=O)[nH]1)[C@H]1CCCN(C(=O)COc2ccccc2)C1
vAce2-spike1-81	Z1282835000	-8.1	0.289	384.385	REAL	C[C@@H](NC(=O)N[C@@H]1CCc2cc(F)ccc21)c1nc(-c2cccc(F)c2)no1
vAce2-spike1-82	Z1323989330	-8.1	0.27	420.354	REAL	Cc1nc(C(=O)Nc2ccc3c(c2)CCC(=O)N3C)nn1-c1nnc(C(F)(F)F)[nH]1
vAce2-spike1-83	Z1324964303	-8.1	0.261	427.345	REAL	Cc1nc(C(=O)Nc2ccc3c(c2)oc2ccccc23)nn1-c1nnc(C(F)(F)F)[nH]1
vAce2-spike1-84	Z1325454487	-8.1	0.279	405.343	REAL	Cc1nc(C(=O)Nc2ccc3c(c2)nc(C)n3C)nn1-c1nnc(C(F)(F)F)[nH]1
vAce2-spike1-85	Z1365980511	-8.1	0.279	392.422	REAL	Cc1cc(C)n2nc(NC(=O)N[C@H](C)c3nc(Cc4ccccc4)no3)nc2n1
vAce2-spike1-86	Z1393742145	-8.1	0.279	390.446	REAL	Cc1nc(-c2ccc(C)c(NC(=O)N[C@H](C)c3ccc4c(c3)CC(=O)N4)c2)n[nH]1
vAce2-spike1-87	Z1550812699	-8.1	0.279	418.786	REAL	O=C(N[C@H]1CCN(c2ccc(Cl)c(F)c2)C1=O)c1noc(-c2cccc(F)c2)n1
vAce2-spike1-88	Z1605008992	-8.1	0.253	445.448	REAL	Cc1nc(C(=O)N[C@@H]2C[C@H]3CCC(C)(C)c4cccc2c43)nn1-c1nnc(C(F)(F)F)[nH]1
vAce2-spike1-89	Z1613949484	-8.1	0.279	397.384	REAL	O=C(Nc1n[nH]c(Cc2cccc(F)c2)n1)c1cc(N2CCCC2=O)ccc1F
vAce2-spike1-90	Z1637284819	-8.1	0.245	442.453	REAL	O=C(Nc1n[nH]c(Cc2cccc(F)c2)n1)c1cccc(OCc2cn3ccccc3n2)c1
vAce2-spike1-91	Z1649059253	-8.1	0.261	436.397	REAL	Cc1cc(NC(=O)c2nc(C)n(-c3nnc(C(F)(F)F)[nH]3)n2)ccc1N1CCOCC1
vAce2-spike1-92	Z1842760471	-8.1	0.289	393.833	REAL	O=C(NNc1nc2ccccn2n1)c1cccc(OCc2cccc(Cl)c2)c1
vAce2-spike1-93	Z1907428393	-8.1	0.27	418.338	REAL	Cc1nc(C(=O)Nc2ccc3ccc(=O)n(C)c3c2)nn1-c1nnc(C(F)(F)F)[nH]1
vAce2-spike1-94	Z1926547692	-8.1	0.261	413.415	REAL	Cc1cc(F)cc(-n2cc(C(=O)Nc3cccc(-c4cn5ccncc5n4)c3)nn2)c1
vAce2-spike1-95	Z2159549788	-8.1	0.3	388.403	REAL	Cc1ccc(-c2noc([C@H]3CC(=O)N(c4cccc(S(N)(=O)=O)c4)C3)n2)o1
vAce2-spike1-96	Z2160489151	-8.1	0.312	350.377	REAL	Cc1nc(-c2noc([C@H]3CC(=O)N(c4ccc5c(c4)CCC5)C3)n2)co1
vAce2-spike1-97	Z230724288	-8.1	0.253	463.92	REAL	Cc1cc(NC(=O)CN2CCN(C(=O)NCc3cc(Cl)c4c(c3)OCCCO4)CC2)no1
vAce2-spike1-98	Z2902883057	-8.1	0.3	453.272	REAL	NS(=O)(=O)c1cccc(N2C[C@@H](c3nc(-c4ccc(Br)o4)no3)CC2=O)c1
vAce2-spike1-99	Z2903061099	-8.1	0.261	410.432	REAL	O=C1N=CC=C[C@H]1c1noc([C@H]2CC(=O)N(c3ccc4c(c3)Cc3ccccc3-4)C2)n1
vAce2-spike1-100	Z2903497765	-8.1	0.279	397.34	REAL	Cn1ccc(-c2noc(-c3ccc(NC(=O)c4cc(F)cc(F)c4)cc3O)n2)n1

Supplementary Table 9. Top 100 virtual hits of the screen against ACE2 at the Spike interaction site in which the structure with PDB ID 6M17 was used (Screen ID: 1). The name of each compound consists of the initial letter 'v' for virtual hit, followed by the target protein name and the target site ('spike' for spike interaction site, 1 for docking scenario 1). The score is the docking score given by QuickVina 2 in kcal/mol. The ligand efficiency (LE) is computed as LE = -score/#NonH, where #NonH is the number of heavy (i.e. non hydrogen) atoms.

Name	Catalog ID	Score	LE	MW	Library	SMILES
vAce2-spike1-101	Z29404494	-8.1	0.253	450.52	REAL	Cc1cc(C)n2nc(C(=O)N3CCN(S(=O)(=O)c4ccc5ccccc5c4)CC3)nc2n1
vAce2-spike1-102	Z748748616	-8.1	0.219	493.53	REAL	O=C(NCc1ccc(-c2ccccc2)o1)NNC(=O)c1ccc(Cn2nnc(-c3ccccc3)n2)cc1
vAce2-spike1-103	Z991832880	-8.1	0.261	415.47	REAL	O=C(Cc1ccc2ccccc2c1)N1CCC[C@H](c2nc(-c3cccc(F)c3)no2)C1
vAce2-spike1-104	ZINC000002990413	-8.1	0.231	461.52	ZINC	Cn1c2ccccc2c2cc(/C=C(\NC(=O)c3ccccc3)C(=O)Nc3cccc(O)c3)ccc21
vAce2-spike1-105	PV-001799987693	-8.0	0.276	403.36	REAL	Cc1ccc2c(c1)N(C(=O)c1cccc(-c3noc(C(F)(F)F)n3)c1)C[C@@H](C)O2
vAce2-spike1-106	PV-001802154262	-8.0	0.286	390.32	REAL	O=C(Nc1cnc2c(c1)COCC2)c1cccc(-c2noc(C(F)(F)F)n2)c1
vAce2-spike1-107	PV-001812042826	-8.0	0.250	444.34	REAL	O=C(Nc1ccc(-n2ccccc2=O)cc1F)c1cccc(-c2noc(C(F)(F)F)n2)c1
vAce2-spike1-108	PV-001818839233	-8.0	0.286	380.35	REAL	O=C(Nc1n[nH]c(Cc2cccc(F)c2)n1)c1ccc(-c2ccccc2F)o1
vAce2-spike1-109	PV-001818839658	-8.0	0.296	425.26	REAL	O=C(Nc1n[nH]c(Cc2cccc(F)c2)n1)c1ccc2cc(Br)ccc2c1
vAce2-spike1-110	PV-001818840190	-8.0	0.286	459.20	REAL	O=C(Nc1n[nH]c(Cc2cccc(F)c2)n1)c1ccc(Br)c(OC(F)(F)F)c1
vAce2-spike1-111	PV-001818840306	-8.0	0.308	431.29	REAL	O=C(Nc1n[nH]c(Cc2cccc(F)c2)n1)c1ccc2scc(Br)c2c1
vAce2-spike1-112	PV-001824311775	-8.0	0.250	454.46	REAL	Cc1nc(C(=O)N2CCC(C(=O)N3CCC[C@H](C)C3)CC2)nn1-c1nnc(C(F)(F)F)[nH]1
vAce2-spike1-113	PV-001826511942	-8.0	0.276	410.82	REAL	Cc1nc(C(=O)Nc2ccc(=O)n(Cc3ccccc3Cl)c2)nn1-c1nnc[nH]1
vAce2-spike1-114	PV-001827368914	-8.0	0.267	422.41	REAL	Cc1ccc(C(=O)Nc2cccc(C(F)(F)F)c2)cc1NC(=O)C[C@@H](C)NC(N)=O
vAce2-spike1-115	PV-001828681739	-8.0	0.250	454.46	REAL	Cc1nc(C(=O)N2CCC(C(=O)NC3CCCCC3)CC2)nn1-c1nnc(C(F)(F)F)[nH]1
vAce2-spike1-116	PV-001836295889	-8.0	0.250	446.43	REAL	CN1CCN(C(=O)Cc2cccc(NC(=O)c3cncc4nc(C(F)(F)F)[nH]c34)c2)CC1
vAce2-spike1-117	PV-001839417734	-8.0	0.308	379.73	REAL	O=C(Nc1n[nH]c2c(Cl)cccc12)c1cccn2cc(C(F)(F)F)nc12
vAce2-spike1-118	PV-001843835041	-8.0	0.250	450.38	REAL	COCN1C(=O)CCc2cc(NC(=O)c3nc(C)n(-c4nnc(C(F)(F)F)[nH]4)n3)ccc21
vAce2-spike1-119	PV-001847552810	-8.0	0.276	459.35	REAL	Cc1cc(Br)cc(C)c1N1CCC[C@H](NC(=O)c2nc(C)n(-c3nnc[nH]3)n2)C1
vAce2-spike1-120	PV-001851565105	-8.0	0.308	363.26	REAL	O=C(Nc1[nH]nc2nc(O)ccc12)c1cncc2nc(C(F)(F)F)[nH]c12
vAce2-spike1-121	PV-001854461363	-8.0	0.258	448.33	REAL	Cc1nc(C(=O)Nc2ccc(N(C)C)c(C(F)(F)F)c2)nn1-c1nnc(C(F)(F)F)[nH]1
vAce2-spike1-122	PV-001855674479	-8.0	0.250	455.47	REAL	O=C(Nc1n[nH]c(Cc2cccc(F)c2)n1)c1cccc(S(=O)(=O)NCc2ccco2)c1
vAce2-spike1-123	PV-001855681852	-8.0	0.286	396.81	REAL	O=C(Nc1n[nH]c(Cc2cccc(F)c2)n1)c1cc(-c2ccc(Cl)cc2)n[nH]1
vAce2-spike1-124	PV-001858912921	-8.0	0.267	420.35	REAL	Cc1nc(C(=O)Nc2ccc3c(c2)CCN(C)C3=O)nn1-c1nnc(C(F)(F)F)[nH]1
vAce2-spike1-125	PV-001867408624	-8.0	0.276	402.34	REAL	Cc1nc(C(=O)N[C@@H]2Cc3ccc(C#N)cc3C2)nn1-c1nnc(C(F)(F)F)[nH]1
vAce2-spike1-126	PV-001871318674	-8.0	0.250	447.42	REAL	Cc1cccc(-c2noc(CC3CCN(C(=O)c4ccc(C(F)(F)F)c(=O)[nH]4)CC3)n2)n1
vAce2-spike1-127	PV-001871635515	-8.0	0.267	414.42	REAL	Cc1cc(=O)[nH]c(N2CCC[C@@H](NC(=O)c3ccn(-c4cc(F)cc(F)c4)n3)C2)n1
vAce2-spike1-128	PV-001872294817	-8.0	0.276	402.38	REAL	O=C1CCC[C@H](c2cccc(NC(=O)c3cccn4cc(C(F)(F)F)nc34)c2)N1
vAce2-spike1-129	PV-001874881335	-8.0	0.258	433.44	REAL	Cc1nc(C(=O)N[C@@H]2CCC[C@@H](c3ccccc3)CC2)nn1-c1nnc(C(F)(F)F)[nH]1
vAce2-spike1-130	PV-001875446345	-8.0	0.250	450.38	REAL	Cc1cc(NC(=O)c2nc(C)n(-c3nnc(C(F)(F)F)[nH]3)n2)ccc1N1CCOCC1=O
vAce2-spike1-131	PV-001901300710	-8.0	0.286	406.34	REAL	O=C(Nc1cc(-c2ccs2)on1)c1cccc(-c2noc(C(F)(F)F)n2)c1
vAce2-spike1-132	PV-001941894789	-8.0	0.267	418.38	REAL	C[C@H](NC(=O)Nc1cccc(NC(=O)c2ccccc2)c1)c1nnc(C(F)(F)F)[nH]1
vAce2-spike1-133	PV-001943072271	-8.0	0.296	414.78	REAL	Cc1nc(Cl)cc(NNC(=O)Nc2nc3cc4c(cc3s2)OC(F)(F)O4)n1
vAce2-spike1-134	PV-001945405654	-8.0	0.267	401.47	REAL	CC(C)c1ccc(Cn2ncc2NC(=O)NNc2cnc3ccenc23)cc1
vAce2-spike1-135	PV-001945833550	-8.0	0.308	367.33	REAL	Cc1oc2ccc(NC(=O)N[C@H](C)c3nnc(C(F)(F)F)[nH]3)cc2c1C
vAce2-spike1-136	PV-001948471911	-8.0	0.276	410.86	REAL	O=C(NCc1nc(-c2cccc(Cl)c2)no1)Nc1ccc2c(c1)C(=O)CCCC2
vAce2-spike1-137	PV-001957903211	-8.0	0.267	421.33	REAL	C[C@H](NC(=O)NNc1cccc2c1OC(F)(F)O2)c1nc(-c2cccc(F)c2)no1
vAce2-spike1-138	PV-001957903615	-8.0	0.267	428.89	REAL	C[C@@H]1CN(C(=O)N[C@H](C)c2nc(-c3cccc(F)c3)no2)CCc2ccc(Cl)cc21
vAce2-spike1-139	PV-001965160239	-8.0	0.250	457.59	REAL	C[C@@H]1CC[C@H](NC(=O)N2CCN(c3cccc(OCc4ccccc4)c3)CC2)CS1(=O)=O
vAce2-spike1-140	PV-001970528943	-8.0	0.286	397.32	REAL	Cn1ncc2c(=O)[nH]c(NNC(=O)NCc3cccc(OC(F)(F)F)c3)nc21
vAce2-spike1-141	PV-002013387594	-8.0	0.267	410.54	REAL	Cc1cc(C)n(Cc2nnc(N3CCCCCCC3)n2CCc2ccc(F)cc2)n1
vAce2-spike1-142	Z1006501812	-8.0	0.276	389.42	REAL	CC(C)c1nnc(NC(=O)c2cccc(NC(=O)c3ccc4[nH]cnc4c3)c2)[nH]1
vAce2-spike1-143	Z1023503370	-8.0	0.242	455.49	REAL	O=C(CN1C(=O)NC2(CCCCC2)C1=O)N1CCC[C@H](c2nc(-c3cccc(F)c3)no2)C1
vAce2-spike1-144	Z1027845972	-8.0	0.229	479.51	REAL	O=C(Nc1cccc(C(=O)N2CCOCC2)c1)N1CCC[C@@H](c2nc(-c3cccc(F)c3)no2)C1
vAce2-spike1-145	Z1028150836	-8.0	0.222	495.53	REAL	O=C(NC1CCN(C(=O)c2ccccc2F)CC1)N1CCC[C@@H](c2nc(-c3cccc(F)c3)no2)C1
vAce2-spike1-146	Z1029996306	-8.0	0.250	438.41	REAL	O=C(Nc1cccc(-c2nc(C3CC3)n[nH]2)c1)c1cccc(-n2nccc2C(F)(F)F)c1
vAce2-spike1-147	Z1067308502	-8.0	0.242	440.50	REAL	COc1cccc(CC(=O)N2CCc3ccc(NC(=O)c4cn5c(C)cccc5n4)cc32)c1
vAce2-spike1-148	Z1094946062	-8.0	0.222	481.51	REAL	CC(=O)Nc1cccc(C(=O)Nc2ccc3nc(NC(=O)c4cccc(NC(C)=O)c4)ccc3c2)c1
vAce2-spike1-149	Z1127879692	-8.0	0.242	450.50	REAL	C[C@@H]1c2cc3c(cc2C2(CCCC2)CN1C(=O)CCc1nc(-c2nnc[nH]2)no1)OCCO3
vAce2-spike1-150	Z1133076467	-8.0	0.229	472.59	REAL	Cc1cccC(=O)N2CCC(NC(=O)N3CCC(c4nc(-c5ccccc5)n[nH]4)CC3)CC2)cc1
vAce2-spike1-151	Z1134147875	-8.0	0.258	416.46	REAL	Cc1cc(N2CCC[C@@H](c3nc(-c4cccc(F)c4)no3)C2)nc(-c2ccccn2)n1
vAce2-spike1-152	Z1232656614	-8.0	0.267	411.39	REAL	Fc1cccc(-c2noc([C@@H]3CCCN(c4cnc5cc(F)c(F)cc5n4)C3)n2)c1
vAce2-spike1-153	Z1263759940	-8.0	0.267	398.47	REAL	C/C(=N\Nc1nc(-c2ccccn2)nc2c1CCC2)c1ccc2c(c1)CCC(=O)N2
vAce2-spike1-154	Z1318935695	-8.0	0.250	425.45	REAL	Cc1ccc(-c2cc(C(=O)NNC(=O)Cc3cn4ccccc4n3)c3ccccc3n2)o1
vAce2-spike1-155	Z1323919328	-8.0	0.258	431.38	REAL	Cc1cc(C)n(-c2cccc(NC(=O)c3nc(C)n(-c4nnc(C(F)(F)F)[nH]4)n3)c2)n1
vAce2-spike1-156	Z1323963726	-8.0	0.267	421.34	REAL	Cc1nc(C(=O)Nc2ccc3c(c2)n(C)c(=O)n3C)nn1-c1nnc(C(F)(F)F)[nH]1
vAce2-spike1-157	Z1324998090	-8.0	0.296	378.28	REAL	Cc1nc(C(=O)Nc2nnc3ccccn23)nn1-c1nnc(C(F)(F)F)[nH]1
vAce2-spike1-158	Z1373137869	-8.0	0.242	445.52	REAL	C[C@@H](NC(=O)N1CCC([C@@H]2C(=O)Nc3ccccc32)CC1)c1nc(Cc2ccccc2)no1
vAce2-spike1-159	Z1389739471	-8.0	0.258	424.46	REAL	Cc1cc(NC(=O)CN2CCN(C(=O)NCc3cn(-c4ccccc4)nn3)CC2)no1
vAce2-spike1-160	Z1392733282	-8.0	0.267	403.44	REAL	Cc1[nH]nc2ncc(C(=O)N3CCC[C@H](NC(=O)c4cc5ccccc5o4)C3)cc12
vAce2-spike1-161	Z1435411180	-8.0	0.267	401.43	REAL	Cc1ccc(-c2nnc(NC(=O)c3cccc(C(=O)N(C)c4ccccc4)c3)[nH]2)o1
vAce2-spike1-162	Z1463888467	-8.0	0.286	373.38	REAL	Cn1ncc2c(=O)[nH]c(NNC(=O)c3cc4c(ccc5ccccc54)[nH]3)nc21
vAce2-spike1-163	Z1466173248	-8.0	0.258	418.46	REAL	Cc1nc(-c2cccc(NC(=O)N3CCN(c4nccn5cnnc45)[C@H](C)C3)c2)n[nH]1
vAce2-spike1-164	Z1466829197	-8.0	0.286	447.20	REAL	O=C(Nc1nc(-c2ccc(Br)cc2F)n[nH]1)c1noc(-c2cccc(F)c2)n1
vAce2-spike1-165	Z1613948689	-8.0	0.267	423.43	REAL	O=C(Nc1n[nH]c(Cc2cccc(F)c2)n1)c1csc(-c2ccc3c(c2)OCO3)n1
vAce2-spike1-166	Z1637286342	-8.0	0.286	397.80	REAL	O=C(Nc1n[nH]c(Cc2cccc(F)c2)n1)c1cn(-c2ccc(Cl)cc2)nn1
vAce2-spike1-167	Z1656857031	-8.0	0.258	413.44	REAL	Cc1cccc(-c2nnc(-c3ccc(C(=O)N4CCc5c(nc[nH]c5=O)C4)cc3)o2)c1
vAce2-spike1-168	Z1677216700	-8.0	0.348	324.37	REAL	Cc1nc(NC(=O)c2cccc3[nH]c(-c4cccs4)nc23)n[nH]1
vAce2-spike1-169	Z1684172639	-8.0	0.258	435.91	REAL	Cc1ccc(-n2nc(C)c(Cc3nc(Cc4cccc(C(N)=O)c4)no3)c2C)cc1Cl
vAce2-spike1-170	Z1684868533	-8.0	0.276	411.84	REAL	Cc1ccc(Cl)cc1-c1noc([C@@H]2CCN(c3ccc4c(c3)OCCO4)C2=O)n1
vAce2-spike1-171	Z1685319633	-8.0	0.242	435.45	REAL	Cc1nnc(-c2cccc(-c3noc(-c4nnn(-c5cccc6cnccc56)c4C)n3)c2)[nH]1
vAce2-spike1-172	Z1685323835	-8.0	0.250	443.53	REAL	Cc1nnc(-c2cccc(-c3noc(C4CCN(c5nc6ccccc6s5)CC4)n3)c2)[nH]1
vAce2-spike1-173	Z1732737917	-8.0	0.267	406.44	REAL	COc1cccc(-c2noc([C@@H](C)NC(=O)Nc3ccc4oc(C)c(C)c4c3)n2)c1
vAce2-spike1-174	Z1743436488	-8.0	0.276	393.37	REAL	O=C(Nc1cccc(-c2noc(C[C@@H](O)c3cccc(F)c3)n2)c1)c1ccco1
vAce2-spike1-175	Z1767690035	-8.0	0.308	353.31	REAL	O=C1CCc2ccc(OC(=O)c3noc(-c4cccc(F)c4)n3)cc2N1
vAce2-spike1-176	Z1846548259	-8.0	0.258	416.40	REAL	Cc1nc(COc2cccc(C(=O)Nc3nnc(-c4cc5ccccc5o4)[nH]3)c2)no1
vAce2-spike1-177	Z1846557233	-8.0	0.267	401.43	REAL	C[C@H]1C[C@@H]1C(=O)Nc1cccc(C(=O)Nc2nnc(-c3cc4ccccc4o3)[nH]2)c1
vAce2-spike1-178	Z1870107070	-8.0	0.276	392.39	REAL	C[C@@H](c1nc(-c2cccc(F)c2)no1)N1C(=O)[C@H]2Cc3ccccc3CN2C1=O
vAce2-spike1-179	Z1873361625	-8.0	0.276	401.30	REAL	O=C(Nc1ccc2oc(=O)ccc2c1)c1cccc(-c2noc(C(F)(F)F)n2)c1
vAce2-spike1-180	Z1873528282	-8.0	0.276	401.31	REAL	O=C(Nc1cnn(-c2nccn2)c1)c1cccc(-c2noc(C(F)(F)F)n2)c1
vAce2-spike1-181	Z1903349704	-8.0	0.276	413.80	REAL	O=C(NCc1nc(-c2cccc(F)c2)no1)Nc1cc(-c2cccc(Cl)c2)on1
vAce2-spike1-182	Z1905696049	-8.0	0.276	390.49	REAL	Cc1ccnc(-c2n[nH]c([C@@H](C)NC(=O)N[C@@H]3CC(C)(C)c4ccccc43)n2)c1
vAce2-spike1-183	Z1918078017	-8.0	0.296	361.40	REAL	Cc1ccnc(-c2noc([C@H]3CC(=O)N(c4ccc5c(c4)CCC5)C3)n2)n1
vAce2-spike1-184	Z1995846816	-8.0	0.250	446.34	REAL	O=C(OCc1nnn(CC(F)(F)F)n1)c1ccc2c(=O)n(-c3ccccc3)c(=O)[nH]c2c1
vAce2-spike1-185	Z2089226546	-8.0	0.267	398.51	REAL	Cc1ccc(Nc2cccc(C(=O)N3C[C@@H](c4ccccc4)[C@H]4CCC[C@@H]43)c2)nn1
vAce2-spike1-186	Z2110662642	-8.0	0.276	399.33	REAL	O=C(Nc1cc(-c2ccccc2)n[nH]1)c1cccc(-c2noc(C(F)(F)F)n2)c1
vAce2-spike1-187	Z2111544837	-8.0	0.267	426.86	REAL	CC1(C)CC(=O)c2cc(NC(=O)NCc3nc(-c4cccc(Cl)c4)no3)ccc2O1
vAce2-spike1-188	Z2119259111	-8.0	0.276	418.36	REAL	O=C(Nc1nnc(-c2ccncc2)s1)c1cccc(-c2noc(C(F)(F)F)n2)c1
vAce2-spike1-189	Z2126518026	-8.0	0.276	407.35	REAL	O=C(Nc1cc([C@@H]2CCCOC2)[nH]n1)c1cccc(-c2noc(C(F)(F)F)n2)c1
vAce2-spike1-190	Z2157252686	-8.0	0.250	442.36	REAL	Cc1nc(-c2nc(COc3ccc4ccccc4c3)no2)nn1-c1nnc(C(F)(F)F)[nH]1
vAce2-spike1-191	Z2160349465	-8.0	0.267	396.45	REAL	Cn1ccc(-c2noc([C@H]3CC(=O)N(c4ccc5c(c4)Cc4ccccc4-5)C3)n2)c1
vAce2-spike1-192	Z2160482443	-8.0	0.308	378.33	REAL	Cc1nc(-c2noc(-c3csc(-c4cccc(C(F)(F)F)c4)n3)n2)co1
vAce2-spike1-193	Z2183206551	-8.0	0.267	404.47	REAL	C[C@@H](NC(=O)N1CC[C@]2(CCc3ccccc3O2)C1)c1cnoc(-c2ccccc2)n1
vAce2-spike1-194	Z2224596539	-8.0	0.276	433.85	REAL	Cc1cc(Cn2nnc(C(=O)Nc3nnc(-c4c(F)cccc4Cl)s3)c2C)on1
vAce2-spike1-195	Z2231650779	-8.0	0.250	448.41	REAL	Cc1nc(C(=O)N2CCCNC(=O)[C@@H]2Cc2ccccc2)nn1-c1nnc(C(F)(F)F)[nH]1
vAce2-spike1-196	Z2307425796	-8.0	0.296	361.45	REAL	CCc1nc(CNC(=O)N[C@H]2CCc3ccc(-c4ccccc4)cc32)n[nH]1
vAce2-spike1-197	Z2335172622	-8.0	0.276	389.41	REAL	Cc1nnc(-c2cccc(C(=O)N3CC[C@]4(CC(=O)c5ccccc5O4)C3)c2)o1
vAce2-spike1-198	Z2438906663	-8.0	0.296	383.84	REAL	Cc1nc(-c2cccc(NC(=O)N3CCc4cc(Cl)nnc4C3)c2)oc1C
vAce2-spike1-199	Z2444515687	-8.0	0.296	366.38	REAL	O=C(Nc1ccccc1)N1CCC(c2nc(-c3cc(O)ncn3)no2)CC1
vAce2-spike1-200	Z2445229313	-8.0	0.276	388.47	REAL	CC(C)[C@H](N)c1noc([C@@H]2CC(=O)N(c3ccc4c(c3)Cc3ccccc3-4)C2)n1

Supplementary Table 10. Top 100 virtual hits of the screen against ACE2 at the Spike interaction site in which the structure with PDB ID 6M17 was used (Screen ID: 1). The name of each compound consists of the initial letter 'v' for virtual hit, followed by the target protein name and the target site ('spike' for spike interaction site, 1 for docking scenario 1). The score is the docking score given by QuickVina 2 in kcal/mol. The ligand efficiency (LE) is computed as LE = -score/#NonH, where #NonH is the number of heavy (i.e. non hydrogen) atoms.

Name	Catalog ID	Score	LE	MW	Library	SMILES
vAce2-spike2-1	Z226992964	-8.7	0.256	477.45	REAL	O=C(NNC(=O)C1CCN(c2ccc3nnc(C(F)(F)F)n3n2)CC1)c1n[nH]c2c1CCCC2
vAce2-spike2-2	Z1021139114	-8.6	0.261	462.395	REAL	Cc1cc(=O)n2nc(NC(=O)C3CCN(c4ccc5nnc(C(F)(F)F)n5n4)CC3)[nH]c2n1
vAce2-spike2-3	Z1137565832	-8.6	0.246	489.436	REAL	O=C(NCc1nc(-c2ccc(F)cc2)n[nH]1)C1CCN(c2ccc3nnc(C(F)(F)F)n3n2)CC1
vAce2-spike2-4	Z1024050858	-8.5	0.258	446.513	REAL	O=C1Nc2ccccc2[C@@H]1C1CCN(C(=O)C2CCN(c3ccc4nnnn4n3)CC2)CC1
vAce2-spike2-5	Z226773826	-8.5	0.243	492.461	REAL	COc1ccc(NCC(=O)NNC(=O)C2CCN(c3ccc4nnc(C(F)(F)F)n4n3)CC2)cc1
vAce2-spike2-6	Z226804070	-8.5	0.25	476.462	REAL	Cc1ccc(NCC(=O)NNC(=O)C2CCN(c3ccc4nnc(C(F)(F)F)n4n3)CC2)cc1
vAce2-spike2-7	Z212284580	-8.4	0.24	486.457	REAL	CN(Cc1nc2ccccc2c(=O)[nH]1)C(=O)C1CCN(c2ccc3nnc(C(F)(F)F)n3n2)CC1
vAce2-spike2-8	Z826159176	-8.4	0.24	488.448	REAL	O=C(NCc1ccc(-n2ccnc2)c(F)c1)C1CCN(c2ccc3nnc(C(F)(F)F)n3n2)CC1
vAce2-spike2-9	Z212382148	-8.3	0.237	495.436	REAL	C[C@H](Oc1ccc(F)cc1)C(=O)NNC(=O)C1CCN(c2ccc3nnc(C(F)(F)F)n3n2)CC1
vAce2-spike2-10	ZINC000008656000	-8.3	0.231	486.324	ZINC	Oc1nnc(O)c2nc3c(nc12)c1nc2c(O)nnc(O)c2nc1c1nc2c(O)nnc(O)c2nc31
vAce2-spike2-11	ZINC000010816319	-8.3	0.259	465.434	ZINC	O=C(Nc1nc2ccc(F)cc2s1)C1CCN(c2ccc3nnc(C(F)(F)F)n3n2)CC1
vAce2-spike2-12	PV-001828987124	-8.2	0.265	440.429	REAL	NC(=O)N1CCCN(C(=O)C2CCN(c3ccc4nnc(C(F)(F)F)n4n3)CC2)CC1
vAce2-spike2-13	PV-001864748066	-8.2	0.265	457.818	REAL	O=C(NNc1ccc(F)c(Cl)c1)C1CCN(c2ccc3nnc(C(F)(F)F)n3n2)CC1
vAce2-spike2-14	Z212133020	-8.2	0.234	493.532	REAL	O=C(C1CCN(C(=O)C2CCN(c3ccc4nnc(C(F)(F)F)n4n3)CC2)CC1)N1CCCCC1
vAce2-spike2-15	Z212363428	-8.2	0.248	466.423	REAL	Cc1cc(NC(=O)CN(C)C(=O)C2CCN(c3ccc4nnc(C(F)(F)F)n4n3)CC2)no1
vAce2-spike2-16	Z215609940	-8.2	0.234	494.448	REAL	Cc1ccc(CNC(=O)COC(=O)C2CCN(c3ccc4nnc(C(F)(F)F)n4n3)CC2)cc1F
vAce2-spike2-17	Z226817806	-8.2	0.234	492.461	REAL	COc1ccccc1NCC(=O)NNC(=O)C1CCN(c2ccc3nnc(C(F)(F)F)n3n2)CC1
vAce2-spike2-18	Z758013340	-8.2	0.248	483.837	REAL	O=C(NNC(=O)C1CCN(c2ccc3nnc(C(F)(F)F)n3n2)CC1)c1ccc(Cl)cc1O
vAce2-spike2-19	PV-001850522725	-8.1	0.261	437.429	REAL	CC(C)c1nnc(CNC(=O)C2CCN(c3ccc4nnc(C(F)(F)F)n4n3)CC2)[nH]1
vAce2-spike2-20	PV-001869515859	-8.1	0.27	422.414	REAL	Cc1n[nH]c(CNC(=O)C2CCN(c3ccc4nnc(C(F)(F)F)n4n3)CC2)c1C
vAce2-spike2-21	PV-001869938968	-8.1	0.27	424.361	REAL	O=C(NNc1ccc(F)cn1)C1CCN(c2ccc3nnc(C(F)(F)F)n3n2)CC1
vAce2-spike2-22	PV-001875896075	-8.1	0.261	457.818	REAL	O=C(NNc1ccc(Cl)cc1F)C1CCN(c2ccc3nnc(C(F)(F)F)n3n2)CC1
vAce2-spike2-23	Z1037873644	-8.1	0.219	492.577	REAL	O=C(Nc1ccccc1)[C@H]1CCc2ccccc2N1C(=O)c1ccc2c(=O)n3c(nc2c1)CCCCC3
vAce2-spike2-24	Z1129810280	-8.1	0.231	486.457	REAL	O=C(Cn1ccc2ccccc21)NNC(=O)C1CCN(c2ccc3nnc(C(F)(F)F)n3n2)CC1
vAce2-spike2-25	Z1487169776	-8.1	0.27	423.373	REAL	O=C(NNc1cccc(F)c1)C1CCN(c2ccc3nnc(C(F)(F)F)n3n2)CC1
vAce2-spike2-26	Z1684206556	-8.1	0.261	435.453	REAL	C[C@@H]1CCC[C@H](c2noc(C3CCN(c4ccc5nnc(C(F)(F)F)n5n4)CC3)n2)C1
vAce2-spike2-27	Z2094121710	-8.1	0.27	424.361	REAL	O=C(NNc1cccc(F)n1)C1CCN(c2ccc3nnc(C(F)(F)F)n3n2)CC1
vAce2-spike2-28	Z212178528	-8.1	0.238	481.409	REAL	O=C(COc1ccccc1F)NNC(=O)C1CCN(c2ccc3nnc(C(F)(F)F)n3n2)CC1
vAce2-spike2-29	Z215604958	-8.1	0.238	483.45	REAL	CC(=O)N1CCN(C(=O)COC(=O)C2CCN(c3ccc4nnc(C(F)(F)F)n4n3)CC2)CC1
vAce2-spike2-30	Z216411668	-8.1	0.27	419.41	REAL	Cc1ccc(NNC(=O)C2CCN(c3ccc4nnc(C(F)(F)F)n4n3)CC2)cc1
vAce2-spike2-31	Z216418378	-8.1	0.27	423.373	REAL	O=C(NNc1ccc(F)cc1)C1CCN(c2ccc3nnc(C(F)(F)F)n3n2)CC1
vAce2-spike2-32	Z2179910169	-8.1	0.3	374.369	REAL	FC(F)(F)c1nc(N2CCCN3c4ccccc4C[C@@H]3C2)c2nc[nH]c2n1
vAce2-spike2-33	Z295543308	-8.1	0.238	471.446	REAL	O=C(NCc1ccc(-n2ccnc2)nc1)C1CCN(c2ccc3nnc(C(F)(F)F)n3n2)CC1
vAce2-spike2-34	Z295744302	-8.1	0.261	433.437	REAL	C[C@@H]1c2cccn2CCN1C(=O)C1CCN(c2ccc3nnc(C(F)(F)F)n3n2)CC1
vAce2-spike2-35	Z344230510	-8.1	0.231	487.528	REAL	C[C@@H](CNC(=O)C1CCN(c2ccc3nnc(C(F)(F)F)n3n2)CC1)N1CCc2ccccc2C1
vAce2-spike2-36	Z453257488	-8.1	0.231	493.532	REAL	O=C(CC1CCN(C(=O)C2CCN(c3ccc4nnc(C(F)(F)F)n4n3)CC2)CC1)N1CCCC1
vAce2-spike2-37	Z512234510	-8.1	0.238	472.47	REAL	Cc1c([C@@H](C)NC(=O)C2CCN(c3ccc4nnc(C(F)(F)F)n4n3)CC2)oc2ccccc12
vAce2-spike2-38	Z758988114	-8.1	0.245	458.447	REAL	Cc1ccn2cc(CNC(=O)C3CCN(c4ccc5nnc(C(F)(F)F)n5n4)CC3)nc2c1
vAce2-spike2-39	Z808254112	-8.1	0.279	411.431	REAL	O=C(NC1CCCCC1)NC1CCN(c2ccc3nnc(C(F)(F)F)n3n2)CC1
vAce2-spike2-40	PV-001810444094	-8	0.258	441.413	REAL	C[C@H]1OCC[C@@H]1C(=O)NNC(=O)C1CCN(c2ccc3nnc(C(F)(F)F)n3n2)CC1
vAce2-spike2-41	PV-001820016009	-8	0.258	441.388	REAL	CC(C)(F)c1cc(NC(=O)C2CCN(c3ccc4nnc(C(F)(F)F)n4n3)CC2)no1
vAce2-spike2-42	PV-001853294706	-8	0.25	451.456	REAL	CC(C)(C)c1nc(CNC(=O)C2CCN(c3ccc4nnc(C(F)(F)F)n4n3)CC2)n[nH]1
vAce2-spike2-43	PV-001866942754	-8	0.258	457.818	REAL	O=C(NNc1cc(Cl)ccc1F)C1CCN(c2ccc3nnc(C(F)(F)F)n3n2)CC1
vAce2-spike2-44	PV-001877277346	-8	0.258	454.839	REAL	O=C(NCc1cccc(Cl)c1O)C1CCN(c2ccc3nnc(C(F)(F)F)n3n2)CC1
vAce2-spike2-45	PV-001967929628	-8	0.267	409.449	REAL	CC(C)c1nc([C@H]2COCCN2C(=O)NCc2ccnc(-c3cccn3)n2)no1
vAce2-spike2-46	Z1024228616	-8	0.242	461.447	REAL	NC(=O)c1cccc(CCNC(=O)C2CCN(c3ccc4nnc(C(F)(F)F)n4n3)CC2)c1
vAce2-spike2-47	Z1082946418	-8	0.25	450.42	REAL	COc1cccc(CNC(=O)C2CCN(c3ccc4nnc(C(F)(F)F)n4n3)CC2)c1O
vAce2-spike2-48	Z1137565350	-8	0.258	422.427	REAL	O=C(NCc1nc(-c2ccc(F)cc2)n[nH]1)C1CCN(c2ccc3nnnn3n2)CC1
vAce2-spike2-49	Z1173764006	-8	0.276	404.37	REAL	Fc1ccc2c(C3CCN(c4ccc5nnc(C(F)(F)F)n5n4)CC3)c[nH]c2c1
vAce2-spike2-50	Z1345915131	-8	0.258	422.531	REAL	Cc1ccc(N2CC[C@H](NC(=O)NC3CCN(c4cc(C)nc(C)n4)CC3)C2=O)cc1
vAce2-spike2-51	Z1683430120	-8	0.25	447.395	REAL	Cc1cc(F)cc(-c2noc(C3CCN(c4ccc5nnc(C(F)(F)F)n5n4)CC3)n2)c1
vAce2-spike2-52	Z1685040243	-8	0.258	434.381	REAL	Cc1cc(Cc2noc(C3CCN(c4ccc5nnc(C(F)(F)F)n5n4)CC3)n2)no1
vAce2-spike2-53	Z1768354113	-8	0.258	436.397	REAL	COc1ccc(NNC(=O)C2CCN(c3ccc4nnc(C(F)(F)F)n4n3)CC2)nc1
vAce2-spike2-54	Z1842699865	-8	0.267	420.398	REAL	Cc1ccccnc1NNC(=O)C1CCN(c2ccc3nnc(C(F)(F)F)n3n2)CC1
vAce2-spike2-55	Z212189084	-8	0.235	483.4	REAL	O=C(CNC(=O)C1CCN(c2ccc3nnc(C(F)(F)F)n3n2)CC1)Nc1ccc(F)c(F)c1
vAce2-spike2-56	Z2150418015	-8	0.267	423.394	REAL	O=C1CCc2cc(NC(=O)N3CCCC[C@@H]3c3nnc(CC(F)(F)F)o3)ccc2N1
vAce2-spike2-57	Z215604224	-8	0.235	482.505	REAL	C[C@@H]1CCC[C@H](NC(=O)COC(=O)C2CCN(c3ccc4nnc(C(F)(F)F)n4n3)CC2)[C@H]1C
vAce2-spike2-58	Z215607016	-8	0.229	481.477	REAL	O=C(OCc1ccc(-c2ccccc2)cc1)C1CCN(c2ccc3nnc(C(F)(F)F)n3n2)CC1
vAce2-spike2-59	Z216413728	-8	0.267	419.41	REAL	Cc1cccc(NNC(=O)C2CCN(c3ccc4nnc(C(F)(F)F)n4n3)CC2)c1
vAce2-spike2-60	Z217378022	-8	0.242	467.494	REAL	O=C(C1CCN(c2ccc3nnc(C(F)(F)F)n3n2)CC1)N1CCN(C[C@H]2CCCO2)CC1
vAce2-spike2-61	Z2179889851	-8	0.276	406.342	REAL	Fc1ccc2c(C3CCN(c4ccc5nnc(C(F)(F)F)n5n4)CC3)noc2c1
vAce2-spike2-62	Z226262034	-8	0.229	484.481	REAL	COc1ccc2cc(CNC(=O)C3CCN(c4ccc5nnc(C(F)(F)F)n5n4)CC3)ccc2c1
vAce2-spike2-63	Z236324916	-8	0.229	487.528	REAL	Cc1ccn(C(=O)C2CCN(c3ccc4nnc(C(F)(F)F)n4n3)CC2)c(=NC2CCCCC2)c1
vAce2-spike2-64	Z3095057191	-8	0.296	366.471	REAL	Cc1nc(Cc2nnc(N(C)[C@H]3CCCN(c4ccccc4)C3)n2C)n[nH]1
vAce2-spike2-65	Z332660660	-8	0.235	459.509	REAL	C[C@H](Oc1ccc2ccccc2c1)C(=O)NNC(=O)C1CCN(c2ccc3nncn3n2)CC1
vAce2-spike2-66	Z338034064	-8	0.242	460.502	REAL	CC(C)(C)c1ccc(CNC(=O)C2CCN(c3ccc4nnc(C(F)(F)F)n4n3)CC2)cc1
vAce2-spike2-67	Z354295622	-8	0.222	493.492	REAL	Cc1cc2nc(N3CCN(Cc4nc(-c5cccc(C(F)(F)F)c5)no4)CC3)c3ccccc3n2n1
vAce2-spike2-68	Z729564886	-8	0.229	487.485	REAL	CC(=O)Nc1cccc2c1CCCN2C(=O)C1CCN(c2ccc3nnc(C(F)(F)F)n3n2)CC1
vAce2-spike2-69	Z758992822	-8	0.222	498.512	REAL	Cc1cc(C)c(-c2cc(NC(=O)C3CCN(c4ccc5nnc(C(F)(F)F)n5n4)CC3)[nH]n2)cc1C
vAce2-spike2-70	Z827247468	-8	0.25	448.448	REAL	C[C@@H](O)c1ccc(CNC(=O)C2CCN(c3ccc4nnc(C(F)(F)F)n4n3)CC2)cc1
vAce2-spike2-71	Z909365366	-8	0.235	473.501	REAL	C[C@@H]1Cc2ccccc2N1CCNC(=O)C1CCN(c2ccc3nnc(C(F)(F)F)n3n2)CC1
vAce2-spike2-72	Z941476112	-8	0.229	490.485	REAL	CC(C)(CNC(=O)C1CCN(c2ccc3nnc(C(F)(F)F)n3n2)CC1)c1ccc2c(c1)OCO2
vAce2-spike2-73	Z942115388	-8	0.25	443.432	REAL	O=C(NCc1cc2ccccc2[nH]1)C1CCN(c2ccc3nnc(C(F)(F)F)n3n2)CC1
vAce2-spike2-74	PV-001813574306	-7.9	0.282	395.348	REAL	Cc1nn[nH]c1NC(=O)C1CCN(c2ccc3nnc(C(F)(F)F)n3n2)CC1
vAce2-spike2-75	PV-001813819918	-7.9	0.247	451.412	REAL	CNC(=O)c1c(C)n[nH]c1NC(=O)C1CCN(c2ccc3nnc(C(F)(F)F)n3n2)CC1
vAce2-spike2-76	PV-001836495854	-7.9	0.263	422.414	REAL	Cc1nc(CNC(=O)C2CCN(c3ccc4nnc(C(F)(F)F)n4n3)CC2)[nH]c1C
vAce2-spike2-77	PV-001839207957	-7.9	0.247	453.399	REAL	COc1cc(F)cc(NNC(=O)C2CCN(c3ccc4nnc(C(F)(F)F)n4n3)CC2)c1
vAce2-spike2-78	PV-001859311846	-7.9	0.255	457.818	REAL	O=C(NNc1cc(F)cc(Cl)c1)C1CCN(c2ccc3nnc(C(F)(F)F)n3n2)CC1
vAce2-spike2-79	PV-001876373820	-7.9	0.272	409.375	REAL	Cc1n[nH]c(CNC(=O)C2CCN(c3ccc4nnc(C(F)(F)F)n4n3)CC2)n1
vAce2-spike2-80	PV-001914618042	-7.9	0.263	426.348	REAL	O=C(NCC[C@@H]1CN(c2ccc3nnc(C(F)(F)F)n3n2)c2ccccc21)C(F)(F)F
vAce2-spike2-81	PV-001957969271	-7.9	0.239	451.5	REAL	CCOC(=O)c1nc(-c2cccc(CNC(=O)N[C@H]3c4cccc(F)c4CC[C@@H]3C)c2)n[nH]1
vAce2-spike2-82	Z100348012	-7.9	0.293	371.321	REAL	Cc1cccc2c1N=C(O)/C2=N/Nc1nc(C(F)(F)F)nc2ccccc12
vAce2-spike2-83	Z1127241276	-7.9	0.232	475.405	REAL	O=C(Nc1cc(-c2ccccc2F)no1)C1CCN(c2ccc3nnc(C(F)(F)F)n3n2)CC1
vAce2-spike2-84	Z1317683514	-7.9	0.282	395.344	REAL	Cc1cnc(NC(=O)C2CCN(c3ccc4nnc(C(F)(F)F)n4n3)CC2)o1
vAce2-spike2-85	Z1433642705	-7.9	0.255	416.488	REAL	CN(Cc1nc(-c2ccccc2)c[nH]1)C(=O)C1CCN(c2ccc3nncn3n2)CC1
vAce2-spike2-86	Z1492669540	-7.9	0.239	446.517	REAL	Cc1ccc(-c2nnc(C)[nH]2)c(NC(=O)CN2CCN(c3ncn4cnnc34)[C@H](C)C2)c1
vAce2-spike2-87	Z1544028682	-7.9	0.255	437.429	REAL	CCc1nc([C@H](C)NC(=O)C2CCN(c3ccc4nnc(C(F)(F)F)n4n3)CC2)n[nH]1
vAce2-spike2-88	Z1631630247	-7.9	0.255	436.397	REAL	COc1cccc(NNC(=O)C2CCN(c3ccc4nnc(C(F)(F)F)n4n3)CC2)n1
vAce2-spike2-89	Z1636458668	-7.9	0.255	420.403	REAL	Cc1cc(C(=O)N2CCc3c(ncn3-c3ccc(F)cc3)C2)nc2nc(O)[nH]c(=O)c12
vAce2-spike2-90	Z1684209528	-7.9	0.255	435.453	REAL	CC1CCC(c2noc(C3CCN(c4ccc5nnc(C(F)(F)F)n5n4)CC3)n2)CC1
vAce2-spike2-91	Z1684721158	-7.9	0.247	447.395	REAL	Cc1cc(F)ccc1-c1noc(C2CCN(c3ccc4nnc(C(F)(F)F)n4n3)CC2)n1
vAce2-spike2-92	Z1731652930	-7.9	0.247	422.487	REAL	O=C(Nc1ccccc1-c1ccc(-c2ccccc2)cc1)N1CCc2n[nH]c(=O)cc2C1
vAce2-spike2-93	Z1827668256	-7.9	0.247	445.408	REAL	O=C(NCc1nc2ccenc2[nH]1)C1CCN(c2ccc3nnc(C(F)(F)F)n3n2)CC1
vAce2-spike2-94	Z1842474056	-7.9	0.255	435.413	REAL	C[C@H]1c2nncn2CCN1C(=O)C1CCN(c2ccc3nnc(C(F)(F)F)n3n2)CC1
vAce2-spike2-95	Z1933265157	-7.9	0.272	428.805	REAL	Cc1n[nH]c(NC(=O)C2CCN(c3ccc4nnc(C(F)(F)F)n4n3)CC2)c1Cl
vAce2-spike2-96	Z2094456664	-7.9	0.263	423.402	REAL	Cc1nnc([C@@H](C)NC(=O)C2CCN(c3ccc4nnc(C(F)(F)F)n4n3)CC2)[nH]1
vAce2-spike2-97	Z212148704	-7.9	0.232	496.876	REAL	Cc1ccc(Cl)cc1NC(=O)COC(=O)C1CCN(c2ccc3nnc(C(F)(F)F)n3n2)CC1
vAce2-spike2-98	Z212315474	-7.9	0.219	498.512	REAL	Cc1nn(-c2ccccc2)c(C)c1CNC(=O)C1CCN(c2ccc3nnc(C(F)(F)F)n3n2)CC1
vAce2-spike2-99	Z212337178	-7.9	0.255	436.397	REAL	Cn1cccc1C(=O)NNC(=O)C1CCN(c2ccc3nnc(C(F)(F)F)n3n2)CC1
vAce2-spike2-100	Z215605474	-7.9	0.226	487.441	REAL	Cc1ccc2nc(COC(=O)C3CCN(c4ccc5nnc(C(F)(F)F)n5n4)CC3)cc(=O)n2c1

Supplementary Table 11. Virtual hits 101 to 200 of the screen against ACE2 at the Spike interaction site in which the structure with PDB ID 6M18 was used (Screen ID: 2). Compounds were filtered so that hits had MW < 600 dalton, cLogP < 6, number of hydrogen bond acceptors < 11, and no reactive functional groups. The name of each compound consists of the initial letter 'v' for virtual hit, followed by the target protein name and the target site ('spike' for spike interaction site, 2 for docking scenario 2). The score is the docking score given by QuickVina 2 in kcal/mol. The ligand efficiency (LE) is computed as LE = -score/#NonH, where #NonH is the number of heavy (i.e. non hydrogen) atoms.

Name	Catalog ID	Score	LE	MW	Library	SMILES
vAce2-spike2-101	Z215608452	-7.9	0.232	483.45	REAL	NC(=O)[C@@H]1CCCCN1C(=O)COC(=O)C1CCN(c2ccc3nnc(C(F)(F)F)n3n2)CC1
vAce2-spike2-102	Z215609324	-7.9	0.226	494.45	REAL	C[C@H](OC(=O)C1CCN(c2ccc3nnc(C(F)(F)F)n3n2)CC1)C(=O)NCc1ccc(F)cc1
vAce2-spike2-103	Z223759864	-7.9	0.226	490.49	REAL	O=C(NCc1ccc(N2CCOCC2)nc1)C1CCN(c2ccc3nnc(C(F)(F)F)n3n2)CC1
vAce2-spike2-104	Z2271388199	-7.9	0.272	397.53	REAL	C[C@H]1C[C@@H]1c1nnc2ccc(N3CCC(NC(=O)NC4CCCCC4)CC3)nn12
vAce2-spike2-105	Z243109748	-7.9	0.247	445.40	REAL	CN(C(=O)C1CCN(c2ccc3nnc(C(F)(F)F)n3n2)CC1)c1nc2ccccc2o1
vAce2-spike2-106	Z272465156	-7.9	0.247	444.46	REAL	CN(C(=O)C1CCN(c2ccc3nnc(C(F)(F)F)n3n2)CC1)[C@H]1CCc2ccccc21
vAce2-spike2-107	Z2802159234	-7.9	0.293	381.46	REAL	Cn1c2ccccc2c2cc(C(=O)N3CCC[C@H](c4nnc(N)o4)C3)sc21
vAce2-spike2-108	Z288227882	-7.9	0.226	477.53	REAL	C[C@@H]1CC(=O)Nc2ccccc2N1C(=O)CN(C)C(=O)C1CCN(c2ccc3nnnn3n2)CC1
vAce2-spike2-109	Z2902402979	-7.9	0.226	486.46	REAL	Cc1ccc(NC(=O)Cc2noc(C3CCN(c4ccc5nnc(C(F)(F)F)n5n4)CC3)n2)cc1
vAce2-spike2-110	Z332645614	-7.9	0.255	423.43	REAL	O=C(NNC(=O)[C@H]1COc2ccccc2O1)C1CCN(c2ccc3nncn3n2)CC1
vAce2-spike2-111	Z332770094	-7.9	0.255	419.45	REAL	Cc1nc2ccccn2c1C(=O)NNC(=O)C1CCN(c2ccc3nncn3n2)CC1
vAce2-spike2-112	Z335389708	-7.9	0.255	466.37	REAL	O=C(Nc1nnc(C(F)(F)F)s1)C1CCN(c2ccc3nnc(C(F)(F)F)n3n2)CC1
vAce2-spike2-113	Z343593188	-7.9	0.247	447.42	REAL	NC(=O)c1cccc(CNC(=O)C2CCN(c3ccc4nnc(C(F)(F)F)n4n3)CC2)c1
vAce2-spike2-114	Z354275670	-7.9	0.239	478.50	REAL	Cc1cc(N2CCN(Cc3nc4sc(C)c(C)c4c(=O)[nH]3)CC2)n2nc(C(F)(F)F)nc2n1
vAce2-spike2-115	Z364476496	-7.9	0.232	493.56	REAL	C[C@H](CNC(=O)C1CCN(c2ccc3nnc(C(F)(F)F)n3n2)CC1)N1CCc2scc2C1
vAce2-spike2-116	Z417488960	-7.9	0.226	486.45	REAL	Cc1ccc(-c2cc(COC(=O)C3CCN(c4ccc5nnc(C(F)(F)F)n5n4)CC3)on2)cc1
vAce2-spike2-117	Z666176542	-7.9	0.247	468.83	REAL	O=C(NNC(=O)C1CCN(c2ccc3nnc(C(F)(F)F)n3n2)CC1)c1ccc(Cl)nc1
vAce2-spike2-118	Z737630648	-7.9	0.232	467.55	REAL	C[C@H]1CN(c2ccc(CNC(=O)C3CCN(c4ccc5nncn5n4)CC3)cc2F)C[C@@H](C)O1
vAce2-spike2-119	Z905989898	-7.9	0.226	486.50	REAL	CCn1c([C@H](C)NC(=O)C2CCN(c3ccc4nnc(C(F)(F)F)n4n3)CC2)nc2ccccc21
vAce2-spike2-120	ZINC000025538970	-7.9	0.247	430.51	ZINC	O=C(C1CCN(c2ccc3nnnn3n2)CC1)N1CCC(c2c[nH]c3ccccc32)CC1
vAce2-spike2-121	ZINC000033284077	-7.9	0.219	479.54	ZINC	Cc1ccc2c(=O)c(-c3nc(-c4ccccc4C)no3)cn(CC(=O)Nc3ccc(C)c(C)c3)c2n1
vAce2-spike2-122	PV-001799272195	-7.8	0.252	456.83	REAL	O=C(NCc1cccc(Cl)c1F)C1CCN(c2ccc3nnc(C(F)(F)F)n3n2)CC1
vAce2-spike2-123	PV-001803582159	-7.8	0.252	454.43	REAL	O=C(COc1ccc2ccc(=O)oc2c1)N1CCCN(c2nnc(C(F)(F)F)s2)CC1
vAce2-spike2-124	PV-001808613223	-7.8	0.260	425.41	REAL	C[C@@]1(CNC(=O)C2CCN(c3ccc4nnc(C(F)(F)F)n4n3)CC2)CCC(=O)N1
vAce2-spike2-125	PV-001809498175	-7.8	0.252	438.50	REAL	CC1(C)CCC[C@@H](CNC(=O)C2CCN(c3ccc4nnc(C(F)(F)F)n4n3)CC2)C1
vAce2-spike2-126	PV-001809813662	-7.8	0.244	453.47	REAL	NC(=O)[C@H]1CC[C@H](CNC(=O)C2CCN(c3ccc4nnc(C(F)(F)F)n4n3)CC2)CC1
vAce2-spike2-127	PV-001818929020	-7.8	0.252	440.47	REAL	CC1(C)CCC[C@H](CNC(=O)C2CCN(c3ccc4nnc(C(F)(F)F)n4n3)CC2)O1
vAce2-spike2-128	PV-001849107277	-7.8	0.260	426.44	REAL	O=C(NC[C@@H]1CCCC[C@H]1O)C1CCN(c2ccc3nnc(C(F)(F)F)n3n2)CC1
vAce2-spike2-129	PV-001871635270	-7.8	0.260	421.38	REAL	Cc1cc(=O)[nH]c(N2CCC[C@@H](NC(=O)c3cncc4nc(C(F)(F)F)[nH]c34)C2)n1
vAce2-spike2-130	PV-001916834661	-7.8	0.269	401.30	REAL	O=C(Cn1nnc(C(F)(F)F)n1)Nc1cccc2c1C(=O)c1ccccc1C2=O
vAce2-spike2-131	PV-001945917134	-7.8	0.269	397.44	REAL	CN(C)c1ncn(-c2cccc(NC(=O)N3CCC[C@H](c4nc(=O)[nH][nH]4)C3)c2)n1
vAce2-spike2-132	PV-001948672876	-7.8	0.260	419.37	REAL	Cc1nc(-c2cc(NC(=O)N3CCc4n[nH]c(=O)cc4C3)cc(C(F)(F)F)c2)n[nH]1
vAce2-spike2-133	PV-001964840766	-7.8	0.260	428.51	REAL	CS(=O)(=O)Nc1cccc2c1CCN(C(=O)N[C@H]1CCc3ccccc3NC1=O)C2
vAce2-spike2-134	Z100348054	-7.8	0.279	406.39	REAL	O=S1(=O)CC/C(=N\Nc2nc(C(F)(F)F)nc3ccccc23)c2ccccc21
vAce2-spike2-135	Z1014272304	-7.8	0.229	473.46	REAL	O=C(NCC(=O)N1CCc2ccccc21)C1CCN(c2ccc3nnc(C(F)(F)F)n3n2)CC1
vAce2-spike2-136	Z1030605578	-7.8	0.252	482.35	REAL	O=C(NCc1nc(-c2ccc(Br)cc2)n[nH]1)C1CCN(c2ccc3nncn3n2)CC1
vAce2-spike2-137	Z1093604380	-7.8	0.223	490.44	REAL	O=C(COC(=O)C1CCN(c2ccc3nnc(C(F)(F)F)n3n2)CC1)NCC(=O)c1ccccc1
vAce2-spike2-138	Z1175821707	-7.8	0.269	411.86	REAL	O=C(NCc1nc2cc(Cl)ccc2[nH]1)C1CCN(c2ccc3nnnn3n2)CC1
vAce2-spike2-139	Z1209600481	-7.8	0.260	440.82	REAL	O=C(NNc1ncccc1Cl)C1CCN(c2ccc3nnc(C(F)(F)F)n3n2)CC1
vAce2-spike2-140	Z1230919530	-7.8	0.244	448.45	REAL	Cc1cccc(NCCNC(=O)C2CCN(c3ccc4nnc(C(F)(F)F)n4n3)CC2)n1
vAce2-spike2-141	Z1276117521	-7.8	0.236	448.49	REAL	COc1cccc(-c2noc([C@H](C)NC(=O)C3CCN(c4ccc5nncn5n4)CC3)n2)c1
vAce2-spike2-142	Z1303409061	-7.8	0.269	391.44	REAL	Cc1ccc2[nH]c(CNC(=O)C3CCN(c4ccc5nnnn5n4)CC3)nc2c1
vAce2-spike2-143	Z1324790246	-7.8	0.244	448.41	REAL	O=C(Cc1ccncc1)NNC(=O)C1CCN(c2ccc3nnc(C(F)(F)F)n3n2)CC1
vAce2-spike2-144	Z132927986	-7.8	0.223	478.43	REAL	Cc1ccc(N2C(=O)/C(=C\Nc3cc(C)n4nc(C(F)(F)F)nc4n3)c3ccccc3C2=O)cc1
vAce2-spike2-145	Z1334095596	-7.8	0.269	395.40	REAL	O=C(NCc1nc2cc(F)ccc2[nH]1)C1CCN(c2ccc3nnnn3n2)CC1
vAce2-spike2-146	Z1335551796	-7.8	0.252	440.47	REAL	C[C@]1(CNC(=O)C2CCN(c3ccc4nnc(C(F)(F)F)n4n3)CC2)CCCC[C@@H]1O
vAce2-spike2-147	Z13970692	-7.8	0.211	494.51	REAL	O=C(COC(=O)c1c2c(nc3ccccc13)/C(=C/c1ccco1)CCC2)Nc1ccc2[nH]c(=O)[nH]c2c1
vAce2-spike2-148	Z1535281063	-7.8	0.260	425.35	REAL	O=C(NNc1ncc(F)cn1)C1CCN(c2ccc3nnc(C(F)(F)F)n3n2)CC1
vAce2-spike2-149	Z1558764253	-7.8	0.269	399.37	REAL	O=C(c1cccc(Oc2ccc(C(F)(F)F)nn2)c1)N1CCc2ccccc2C1
vAce2-spike2-150	Z1608663192	-7.8	0.300	364.44	REAL	C[C@H](OC(=O)Cn1cc([C@H](C)O)nn1)C(=O)N[C@H](C)[C@H]1C[C@@H]2CC[C@@H]1C2
vAce2-spike2-151	Z1613948795	-7.8	0.252	422.43	REAL	O=C(Nc1n[nH]c(Cc2cccc(F)c2)n1)C1CCN(c2ccc3nnnn3n2)CC1
vAce2-spike2-152	Z1613948798	-7.8	0.252	421.44	REAL	O=C(Nc1n[nH]c(Cc2cccc(F)c2)n1)C1CCN(c2ccc3nncn3n2)CC1
vAce2-spike2-153	Z1636268754	-7.8	0.260	424.36	REAL	O=C(NNc1ccnc(F)c1)C1CCN(c2ccc3nnc(C(F)(F)F)n3n2)CC1
vAce2-spike2-154	Z1890804295	-7.8	0.244	449.37	REAL	Oc1ccc(-c2noc(C3CCN(c4ccc5nnc(C(F)(F)F)n5n4)CC3)n2)c(F)c1
vAce2-spike2-155	Z1899413276	-7.8	0.252	418.46	REAL	Cc1nc(Cn2nnc(C(=O)NCc3nn(-c4ccccc4)c4c3CCC4)c2C)no1
vAce2-spike2-156	Z1997039396	-7.8	0.252	437.43	REAL	C[C@@H]1COCC[C@H]1c1noc(C2CCN(c3ccc4nnc(C(F)(F)F)n4n3)CC2)n1
vAce2-spike2-157	Z2041539816	-7.8	0.260	402.42	REAL	Cc1nc2c(-c3noc(C4CCN(c5ccc6nnnn6n5)CC4)n3)cccc2[nH]1
vAce2-spike2-158	Z2086862814	-7.8	0.260	424.36	REAL	O=C(NNc1ncccc1F)C1CCN(c2ccc3nnc(C(F)(F)F)n3n2)CC1
vAce2-spike2-159	Z212148694	-7.8	0.229	476.46	REAL	Cc1ccc(NC(=O)COC(=O)C2CCN(c3ccc4nnc(C(F)(F)F)n4n3)CC2)cc1C
vAce2-spike2-160	Z212434048	-7.8	0.229	497.86	REAL	COc1cc(Cl)ccc1C(=O)NNC(=O)C1CCN(c2ccc3nnc(C(F)(F)F)n3n2)CC1
vAce2-spike2-161	Z2143329031	-7.8	0.269	400.39	REAL	O=C1COC[C@@H](C[C@H]2CN(c3ccc4nnc(C(F)(F)F)n4n3)c3ccccc32)N1
vAce2-spike2-162	Z215605824	-7.8	0.223	489.41	REAL	O=C(OCc1cc(=O)oc2cc(O)ccc12)C1CCN(c2ccc3nnc(C(F)(F)F)n3n2)CC1
vAce2-spike2-163	Z216675370	-7.8	0.260	440.45	REAL	CC(C)c1nnc(NC(=O)C2CCN(c3ccc4nnc(C(F)(F)F)n4n3)CC2)s1
vAce2-spike2-164	Z2193899714	-7.8	0.279	437.26	REAL	CCc1onc(-c2ccc(Br)cc2)c1-c1nc(-c2ccc3[nH]nnc3c2)no1
vAce2-spike2-165	Z2193902139	-7.8	0.289	358.36	REAL	CCc1onc(-c2ccccc2)c1-c1nc(-c2ccc3[nH]nnc3c2)no1
vAce2-spike2-166	Z246075346	-7.8	0.223	486.50	REAL	CC(C)[C@@H](NC(=O)C1CCN(c2ccc3nnc(C(F)(F)F)n3n2)CC1)c1nc2ccccc2[nH]1
vAce2-spike2-167	Z2617836095	-7.8	0.312	336.36	REAL	Cc1nnc2ccc(-c3noc(-c4cn[nH]c4[C@@H]4CCNC4)n3)cn12
vAce2-spike2-168	Z269249736	-7.8	0.223	494.45	REAL	Cc1ccc(F)cc1NC(=O)[C@H](C)OC(=O)C1CCN(c2ccc3nnc(C(F)(F)F)n3n2)CC1
vAce2-spike2-169	Z2790009816	-7.8	0.339	306.37	REAL	Cc1ccc(N2N=C(c3ccc4c(c3)CCC4)CCC2=O)nn1
vAce2-spike2-170	Z2861631236	-7.8	0.279	384.43	REAL	FC(F)c1nnc2ccc(N3C[C@@H]4CCN(Cc5eccc5)C[C@@H]4C3)nn12
vAce2-spike2-171	Z289806774	-7.8	0.223	486.45	REAL	Cc1ccc(-c2nc(COC(=O)C3CCN(c4ccc5nnc(C(F)(F)F)n5n4)CC3)co2)cc1
vAce2-spike2-172	Z290274156	-7.8	0.252	420.43	REAL	Cc1cccc2c(=O)[nH]c(COC(=O)C3CCN(c4ccc5nnnn5n4)CC3)nc12
vAce2-spike2-173	Z2923628161	-7.8	0.289	377.37	REAL	FC(F)(F)[C@H]1CCC[C@@H](Cc2nc(Cc3ccc4ccccc4n3)no2)O1
vAce2-spike2-174	Z317205804	-7.8	0.252	418.46	REAL	CN(Cc1nc2ccccc2c(=O)[nH]1)C(=O)C1CCN(c2ccc3nncn3n2)CC1
vAce2-spike2-175	Z332660820	-7.8	0.252	427.44	REAL	C[C@H](Oc1ccccc1F)C(=O)NNC(=O)C1CCN(c2ccc3nncn3n2)CC1
vAce2-spike2-176	Z332750910	-7.8	0.252	416.44	REAL	O=C(NNC(=O)C1CCN(c2ccc3nncn3n2)CC1)c1ccc2ccccc2n1
vAce2-spike2-177	Z381708480	-7.8	0.223	487.45	REAL	COc1ccccc1-c1nnc(NC(=O)C2CCN(c3ccc4nnc(C(F)(F)F)n4n3)CC2)[nH]1
vAce2-spike2-178	Z383796282	-7.8	0.229	495.89	REAL	CN(CC(=O)Nc1cccc(Cl)c1)C(=O)C1CCN(c2ccc3nnc(C(F)(F)F)n3n2)CC1
vAce2-spike2-179	Z728957546	-7.8	0.236	447.46	REAL	Cn1nc(C(=O)NNC(=O)C2CCN(c3ccc4nncn4n3)CC2)c2ccccc2c1=O
vAce2-spike2-180	Z740502884	-7.8	0.229	476.48	REAL	O=C(C1CCN(c2ccc3nnc(C(F)(F)F)n3n2)CC1)N1CCC[C@H]1Cc1ccc(F)cc1
vAce2-spike2-181	Z773724760	-7.8	0.223	466.51	REAL	O=C(Nc1ccccc1-c1nc(-c2ccccc2)n[nH]1)C1CCN(c2ccc3nnnn3n2)CC1
vAce2-spike2-182	Z793013988	-7.8	0.223	498.46	REAL	O=C(OCC(=O)N1CCC2(CC1)OCCO2)C1CCN(c2ccc3nnc(C(F)(F)F)n3n2)CC1
vAce2-spike2-183	Z804765886	-7.8	0.229	483.60	REAL	Cc1ccc(S(=O)(=O)N2CCC[C@@H](C(=O)N3CCN(c4cc(C)nc5ncnn45)CC3)C2)cc1
vAce2-spike2-184	Z814254088	-7.8	0.223	487.95	REAL	O=C(NNC(=O)c1ccc(Cn2nnc(-c3cccc3)n2)cc1)N[C@@H]1CCc2c(Cl)cccc21
vAce2-spike2-185	Z872959800	-7.8	0.229	471.50	REAL	O=C(CNC(=O)c1cc(-c2ccs2)nc2ccccc12)Nc1ccccc2c(=O)[nH][nH]c(=O)c12
vAce2-spike2-186	Z899979886	-7.8	0.236	463.42	REAL	O=C(NCc1cccc(C(F)(F)F)c1)NNC(=O)C1CCN(c2ccc3nnnn3n2)CC1
vAce2-spike2-187	Z941503214	-7.8	0.229	473.50	REAL	CN1CCCc2cc(CNC(=O)C3CCN(c4ccc5nnc(C(F)(F)F)n5n4)CC3)ccc21
vAce2-spike2-188	Z961737308	-7.8	0.217	497.43	REAL	O=C(CNC(=O)c1ccccc1Nc1cccc(C(F)(F)F)c1)Nc1cccc2c(=O)[nH][nH]c(=O)c12
vAce2-spike2-189	Z966257664	-7.8	0.229	475.47	REAL	CCc1cccc(NC(=O)CNC(=O)C2CCN(c3ccc4nnc(C(F)(F)F)n4n3)CC2)c1
vAce2-spike2-190	Z981218732	-7.8	0.229	476.48	REAL	O=C(NCC1(c2ccc(F)cc2)CCC1)C1CCN(c2ccc3nnc(C(F)(F)F)n3n2)CC1
vAce2-spike2-191	Z994401724	-7.8	0.244	454.45	REAL	O=C(C1CCN(c2ccc3nnc(C(F)(F)F)n3n2)CC1)N1CCC(C2OCCO2)CC1
vAce2-spike2-192	Z996743762	-7.8	0.229	459.51	REAL	O=C(c1cc2ccccc2[nH]1)N1CCN(C(=O)C2CCN(c3ccc4nnnn4n3)CC2)CC1
vAce2-spike2-193	Z997928598	-7.8	0.252	423.48	REAL	Cc1ccc(OCC(=O)NNC(=O)C2CCN(c3ccc4nncn4n3)CC2)cc1C
vAce2-spike2-194	ZINC000008393088	-7.8	0.325	329.28	ZINC	FC(F)(F)c1nc2ccccc2c(Nc2ccc3[nH]ncc3c2)n1
vAce2-spike2-195	ZINC000033284100	-7.8	0.217	483.50	ZINC	Cc1ccc(NC(=O)Cn2cc(-c3nc(-c4ccccc4C)no3)c(=O)c3ccc(C)nc32)c(F)c1
vAce2-spike2-196	PV-000011265908	-7.7	0.285	382.35	REAL	Cc1[nH]c(=O)[nH]c1C(=O)N[C@@H]1C[C@H]2CC[C@@H]1N2c1ccc(C(F)(F)F)nn1
vAce2-spike2-197	PV-000383415738	-7.7	0.285	369.43	REAL	O=C(N[C@]12CCC[C@H]1CN(C(=O)[C@H]1CCc3[nH]ncc3C1)C2)c1nc[nH]n1
vAce2-spike2-198	PV-001825398303	-7.7	0.285	372.43	REAL	C[C@@H]1CC[C@@H](C(N)=O)CN1C(=O)C1CCN(c2ccc3nnnn3n2)CC1
vAce2-spike2-199	PV-001840701220	-7.7	0.296	360.29	REAL	O=C1C[C@H](NC(=O)c2cncc3nc(C(F)(F)F)[nH]c23)c2ccccc21
vAce2-spike2-200	PV-001863137649	-7.7	0.296	356.38	REAL	COc1cccc2c1OCC(C(=O)N1CCC[C@H](c3nnc(N)o3)C1)=C2

Supplementary Table 12. Virtual hits 101 to 200 of the screen against ACE2 at the Spike interaction site in which the structure with PDB ID 6M18 was used (Screen ID: 2). Compounds were filtered so that hits had MW < 600 dalton, cLogP < 6, number of hydrogen bond acceptors < 11, and no reactive functional groups. The name of each compound consists of the initial letter 'v' for virtual hit, followed by the target protein name and the target site ('spike' for spike interaction site, 2 for docking scenario 2). The score is the docking score given by QuickVina 2 in kcal/mol. The ligand efficiency (LE) is computed as LE = -score/#NonH, where #NonH is the number of heavy (i.e. non hydrogen) atoms.

Name	Catalog ID	Score	LE	MW	Library	SMILES
vAce2-spike3-1	Z1452691933	-9.4	0.285	445.493	REAL	O=C(NC[C@H]1[C@@H]2Cc3ccccc3[C@H]12)NNC(=O)c1ccccc1OCc1ccc(F)cc1
vAce2-spike3-2	Z1487641111	-8.7	0.281	417.511	REAL	O=C(NNc1ccnc2c1CCCC2)[C@H]1CCCN(C(=O)c2ccc3[nH]ncc3c2)C1
vAce2-spike3-3	Z1610522351	-8.7	0.29	411.488	REAL	O=C(NNc1ccc2ccccc2n1)c1cc(-c2cccs2)n(-c2ccccc2)n1
vAce2-spike3-4	PV-001921200564	-8.6	0.253	476.473	REAL	Cc1cc(-c2noc([C@@H](C)N3CC[C@H](c4ccccc4)[C@H](NC(=O)C(F)(F)F)C3)n2)ccc1F
vAce2-spike3-5	PV-001921201010	-8.6	0.253	472.509	REAL	Cc1ccc(-c2nnc([C@@H](C)N3CC[C@H](c4ccccc4)[C@H](NC(=O)C(F)(F)F)C3)o2)cc1C
vAce2-spike3-6	Z1032694568	-8.6	0.261	442.517	REAL	Cc1cccc(-c2cccc(CNC(=O)NCc3cccc([C@]4(C)NC(=O)NC4=O)c3)c2)c1
vAce2-spike3-7	Z1162536265	-8.6	0.277	407.432	REAL	O=C(Nc1nc2ccccc2c(=O)[nH]1)c1cc(-c2ccccc2)n(-c2ccccc2)n1
vAce2-spike3-8	Z1458999179	-8.6	0.253	448.564	REAL	O=C(NC[C@H]1[C@H]2Cc3ccccc3[C@H]12)c1cccc(C(=O)NC[C@H]2[C@@H]3Cc4ccccc4[C@H]23)c1
vAce2-spike3-9	Z1610505267	-8.6	0.277	408.416	REAL	O=C(NNc1ccc2ccccc2n1)c1cccc(N2C(=O)c3ccccc3C2=O)c1
vAce2-spike3-10	Z1610513255	-8.6	0.277	406.448	REAL	O=C(NNc1ccc2ccccc2n1)c1nc(-c2ccccc2)n(-c2ccccc2)n1
vAce2-spike3-11	Z1752546889	-8.6	0.277	411.504	REAL	O=C(NCCc1cccc(-c2ccccc2)c1)N1CC[C@@]2(C1)C(=O)Nc1ccccc12
vAce2-spike3-12	PV-001921200548	-8.5	0.25	476.473	REAL	Cc1ccc(-c2noc([C@@H](C)N3CC[C@H](c4ccccc4)[C@H](NC(=O)C(F)(F)F)C3)n2)cc1F
vAce2-spike3-13	PV-001944224354	-8.5	0.283	399.493	REAL	Cc1cccc(-c2cccc(CNC(=O)Nc3ccc4c(c3)C(=O)N(C)CC4)c2)c1
vAce2-spike3-14	PV-001949168003	-8.5	0.283	399.493	REAL	Cc1cccc(-c2cccc(CNC(=O)Nc3ccc4c(c3)CCN(C)C4=O)c2)c1
vAce2-spike3-15	Z1082330718	-8.5	0.274	408.42	REAL	O=C(Nc1nc2ccccc2c(=O)[nH]1)c1nc(-c2ccccc2)n(-c2ccccc2)n1
vAce2-spike3-16	Z1182419955	-8.5	0.266	444.877	REAL	C[C@@H](NC(=O)c1cccc(N2C(=O)c3ccccc3C2=O)c1)c1nc2cc(Cl)ccc2[nH]1
vAce2-spike3-17	Z1472745038	-8.5	0.258	442.478	REAL	Cc1n[nH]c(NC(=O)c2nc(C3CC3)n(-c3ccccc3)n2)c1-c1ccc2c(c1)OCCO2
vAce2-spike3-18	Z1521946606	-8.5	0.258	443.412	REAL	O=C(Nc1ccccc1-n1ncc2c(=O)[nH]cnc21)c1cccc(-c2c(F)cccc2F)c1
vAce2-spike3-19	Z1610522224	-8.5	0.283	412.476	REAL	O=C(NNc1ccc2ccccc2n1)c1nc(-c2cccs2)n(-c2ccccc2)n1
vAce2-spike3-20	Z1896770477	-8.5	0.283	412.476	REAL	O=C(NNc1cnc2ccccc2n1)c1cc(-c2cccs2)n(-c2ccccc2)n1
vAce2-spike3-21	Z2161652971	-8.5	0.283	397.473	REAL	O=C1O[C@@H](c2ccccc2)C[C@H]1C(=O)N1Cc2ccccc2[C@H](c2ccccc2)C1
vAce2-spike3-22	Z2166788903	-8.5	0.258	434.502	REAL	Cn1c(-c2n[nH]c(=O)c3ccccc23)nnc1N1Cc2ccccc2[C@H](c2ccccc2)C1
vAce2-spike3-23	Z406928108	-8.5	0.23	498.513	REAL	O=C(Nc1ccc2c(c1)OCCO2)c1ccccc1NC(=O)c1nn(-c2ccccc2F)c2c1CCC2
vAce2-spike3-24	Z448673852	-8.5	0.236	479.539	REAL	Cn1nc(C(=O)NNC(=O)NC[C@H]2CC3c4ccccc4C2c2ccccc23)c2ccccc2c1=O
vAce2-spike3-25	ZINC000008449797	-8.5	0.224	493.561	ZINC	O=C1[C@H]2[C@H](C(=O)N1c1ccc(Oc3ccc4ccccc4c3)cc1)C1c3ccccc3C2c2ccccc21
vAce2-spike3-26	PV-001921200029	-8.4	0.262	444.456	REAL	C[C@H](c1noc(-c2ccccc2)n1)N1CC[C@H](c2ccccc2)[C@H](NC(=O)C(F)(F)F)C1
vAce2-spike3-27	PV-001944224487	-8.4	0.28	399.493	REAL	Cc1ccc(-c2cccc(CNC(=O)Nc3ccc4c(c3)C(=O)N(C)CC4)c2)cc1
vAce2-spike3-28	PV-001947857635	-8.4	0.262	429.479	REAL	Cc1cc(NC(=O)NCc2cccc([C@]3(C)NC(=O)NC3=O)c2)ccc1-c1ccncc1
vAce2-spike3-29	PV-001948062037	-8.4	0.255	454.48	REAL	Cc1cc(NC(=O)N[C@@H](C)c2ccc(N3CCCNC3=O)cc2)nn1-c1ccc(F)cc1F
vAce2-spike3-30	Z1024049144	-8.4	0.24	465.508	REAL	O=C1Nc2ccccc2[C@H]1C1CCN(C(=O)c2ccc(N3C(=O)c4ccccc4C3=O)c2)CC1
vAce2-spike3-31	Z1032433622	-8.4	0.28	399.493	REAL	CC(=O)N1CCc2cc(NC(=O)NCc3cccc(-c4cccc(C)c4)c3)ccc21
vAce2-spike3-32	Z106765072	-8.4	0.233	478.515	REAL	Cc1ccc(-c2cc(NC(=O)Cn3nnc(-c4ccc(C(N)=O)cc4)n3)n(-c3ccccc3)n2)cc1
vAce2-spike3-33	Z1095050546	-8.4	0.247	464.512	REAL	O=C(Nc1nc(-c2ccc3ccccc3n2)n[nH]1)c1nc(-c2cccs2)n(-c2ccccc2)n1
vAce2-spike3-34	Z1129351503	-8.4	0.24	496.576	REAL	O=C(c1cccc(S(=O)(=O)N2CCc3ccccc3C2)c1)N1CCC(c2ccc(F)c(F)c2)CC1
vAce2-spike3-35	Z1272406433	-8.4	0.262	422.491	REAL	Cc1ccc(C[C@H](Nc2nc3c(cnn3-c3ccccc3)c(=O)[nH]2)c2cccn2)cc1
vAce2-spike3-36	Z1304269314	-8.4	0.262	425.447	REAL	O=C1c2ccccc2C(=O)N1[C@@H]1CCC/C(=N\Nc2ncnc3c2oc2ccccc23)C1
vAce2-spike3-37	Z1429436295	-8.4	0.271	420.472	REAL	O=C1c2ccccc2C(=O)N1[C@@H]1CCC/C(=N\Nc2nccc(N3CCOCC3)n2)C1
vAce2-spike3-38	Z1462331439	-8.4	0.255	443.458	REAL	C[C@@]1(c2ccccc(C(=O)OCC(=O)Nc3ccccc3-c3ccccc3)c2)NC(=O)NC1=O
vAce2-spike3-39	Z1472740852	-8.4	0.262	437.405	REAL	Cc1n[nH]c(NC(=O)c2ccn(-c3c(F)cccc3F)n2)c1-c1ccc2c(c1)OCCO2
vAce2-spike3-40	Z1522176995	-8.4	0.29	389.404	REAL	O=C(c1cccc(-c2c(F)cccc2F)c1)N1CC(c2nc3ccccc3[nH]2)C1
vAce2-spike3-41	Z1545558790	-8.4	0.255	445.497	REAL	Cc1ccc(-n2nc(C(=O)N[C@H](C)Cn3ncc4ccccc4c3=O)c3c2CCC3)c(F)c1
vAce2-spike3-42	Z1564045157	-8.4	0.271	434.886	REAL	CN1C(=O)C[C@@H](Nc2nc3c(cnn3-c3ccccc3)c(=O)[nH]2)[C@@H]1c1ccc(Cl)cc1
vAce2-spike3-43	Z1695804414	-8.4	0.28	413.464	REAL	O=C(NNc1cnc2ccccc2n1)c1nc(-c2cccs2)n(-c2ccccc2)n1
vAce2-spike3-44	Z2011962315	-8.4	0.255	448.515	REAL	O=C(c1nn(-c2ccccc2F)c2c1CCC2)N1CCC(N2CCc3cc(F)ccc32)CC1
vAce2-spike3-45	Z2118428859	-8.4	0.28	403.524	REAL	CC(=O)N1CC[C@H](NC(=O)N2C[C@@H](c3ccccc3)[C@@H]3CCC[C@H]32)c2ccccc21
vAce2-spike3-46	Z2178243919	-8.4	0.255	448.472	REAL	O=C(c1nn(-c2ccccc2F)c2c1CCC2)N1CCC(c2noc3cc(F)ccc23)CC1
vAce2-spike3-47	Z2182692015	-8.4	0.247	448.529	REAL	CCn1c(-c2n[nH]c(=O)c3ccccc23)nnc1N1Cc2ccccc2[C@H](c2ccccc2)C1
vAce2-spike3-48	Z2212550647	-8.4	0.255	437.498	REAL	O=C1CNC(=O)c2ccc(C(=O)NC[C@H]3CC4c5ccccc5C3c3ccccc34)cc2N1
vAce2-spike3-49	Z493332470	-8.4	0.255	460.967	REAL	C[C@H]1c2[nH]c3ccccc3c2[C@H](c2ccccc2Cl)CN1C(=O)NCc1nnc2n1CCC2
vAce2-spike3-50	Z499057712	-8.4	0.255	448.565	REAL	Cc1ncc2c(n1)CC[C@H](NC(=O)N1CC3(CCCC3)c3cc4c(cc3[C@@H]1C)OCCO4)C2
vAce2-spike3-51	Z73312516	-8.4	0.24	489.594	REAL	CC(=O)N1CCc2cc(NC(=O)[C@@H]3Cc4ccccc4CN3S(=O)(=O)c3ccc(C)cc3)ccc21
vAce2-spike3-52	Z738255640	-8.4	0.24	459.464	REAL	O=C(Nc1cccc(-c2cn3ccccn3n2)c1)c1ccc(N2C(=O)c3ccccc3C2=O)c1
vAce2-spike3-53	Z848648470	-8.4	0.233	483.523	REAL	O=C1CCC(=O)N(c2ccc(C(=O)OCC(=O)N3Cc4ccccc4[C@H](c4ccccc4)C3)cc2)N1
vAce2-spike3-54	ZINC000003146073	-8.4	0.247	441.529	ZINC	Cc1ccc(N2C(=O)[C@H]3C4c5ccccc5C(c5ccccc54)[C@@]3(c3ccccc3)C2=O)cc1
vAce2-spike3-55	ZINC000016919178	-8.4	0.247	448.517	ZINC	O=C1c2ccccc2C(=O)[C@H]2CC3=C(CC4=C(C3)C[C@@H]3C(=O)c5ccccc5C(=O)[C@@H]3C4)C[C@@H]12
vAce2-spike3-56	ZINC000036370631	-8.4	0.233	464.563	ZINC	O=C1[C@@H]2C3c4ccccc4C(c4ccccc43)[C@H]2C(=O)[C@H]2C3c4ccccc4C(c4ccccc43)[C@@H]12
vAce2-spike3-57	ZINC000230043899	-8.4	0.24	464.495	ZINC	O=C1[C@@H]2ON(c3ccccc3)[C@@H](c3ccccc3F)[C@H]2C(=O)N1c1ccccc1-c2ccccc2)c1
vAce2-spike3-58	ZINC000408679806	-8.4	0.221	498.58	ZINC	Cc1cc(C)cc(NC(=O)c2cccc(N3C(=O)[C@@H]4[C@@H](C3=O)C3c5ccccc5C4c4ccccc43)c2)c1
vAce2-spike3-59	PV-001921200006	-8.3	0.252	466.409	REAL	O=C(N[C@@H]1CN(Cc2noc(-c3ccc(F)cc3F)n2)CC[C@@H]1c1ccccc1)C(F)(F)F
vAce2-spike3-60	PV-001921200472	-8.3	0.259	444.456	REAL	Cc1ccccc1-c1nc(CN2CC[C@H](c3ccccc3)[C@H](NC(=O)C(F)(F)F)C2)no1
vAce2-spike3-61	PV-001921201118	-8.3	0.252	478.901	REAL	C[C@H](c1nc(-c2ccc(Cl)cc2)no1)N1CC[C@H](c2ccccc2)[C@H](NC(=O)C(F)(F)F)C1
vAce2-spike3-62	PV-001921201131	-8.3	0.259	448.419	REAL	O=C(N[C@@H]1CN(Cc2nnc(-c3cccc(F)c3)o2)CC[C@@H]1c1ccccc1)C(F)(F)F
vAce2-spike3-63	PV-001921202114	-8.3	0.259	446.428	REAL	O=C(N[C@@H]1CN(Cc2nnc(-c3cccc(O)c3)o2)CC[C@@H]1c1ccccc1)C(F)(F)F
vAce2-spike3-64	PV-001941456346	-8.3	0.286	385.466	REAL	Cc1cc(-c2ccccc2)ccc1NC(=O)N[C@@H]1C(=O)N(C)Cc2ccccc21
vAce2-spike3-65	PV-001944975953	-8.3	0.259	452.945	REAL	Cc1cc(NC(=O)N[C@@H](C)c2ccc(N3CCCNC3=O)cc2)nn1-c1ccc(Cl)c1
vAce2-spike3-66	PV-001947996802	-8.3	0.277	410.52	REAL	Cc1cc(NC(=O)N[C@@H](C)c2ccc(N3CCNC3=O)cc2)nn1C1CCCCC1
vAce2-spike3-67	PV-001947997857	-8.3	0.268	425.531	REAL	Cc1cc(NC(=O)N[C@@H](C)c2ccc(N3CCCOC3=O)cc2)nn1C1CCCCC1
vAce2-spike3-68	PV-001949168167	-8.3	0.277	399.493	REAL	Cc1ccc(-c2cccc(CNC(=O)Nc3ccc4c(c3)CCN(C)C4=O)c2)cc1
vAce2-spike3-69	Z1003199094	-8.3	0.252	468.576	REAL	Cc1nn(C)c2ncc(S(=O)(=O)N3CC4(CCCC4)c4cc5c(cc4[C@@H]3C)OCCO5)cc12
vAce2-spike3-70	Z1032434760	-8.3	0.277	401.465	REAL	Cc1cccc(-c2cccc(CNC(=O)Nc3ccc4c(c3)NC(=O)[C@H](C)O4)c2)c1
vAce2-spike3-71	Z1070219674	-8.3	0.231	499.953	REAL	O=C1Nc2cc(Cl)ccc2[C@@H]1C1CCN(C(=O)c2cccc(N3C(=O)c4ccccc4C3=O)c2)CC1
vAce2-spike3-72	Z1101910521	-8.3	0.231	496.542	REAL	O=C(Nc1cccc(N2C(=O)c3ccccc3C2=O)c1)c1cccc(CS(=O)(=O)c2ccccc2)c1
vAce2-spike3-73	Z1103258393	-8.3	0.237	498.558	REAL	C[C@@H]1c2cc3c(cc2C2(CCCC2)CN1S(=O)(=O)c1cnc2c(c1)c(=O)[nH]c(=O)n2C)OCCO3
vAce2-spike3-74	Z1192446367	-8.3	0.286	386.45	REAL	O=C(c1cccc2ccccc12)N1CCN(C(=O)[C@H]2COc3ccccc32)CC1
vAce2-spike3-75	Z1212740717	-8.3	0.268	406.492	REAL	Cc1ccc(C[C@H](Nc2ccc3nnc(-c4ccccc4)n3n2)c2ccccn2)cc1
vAce2-spike3-76	Z1337297021	-8.3	0.252	437.458	REAL	Cc1nc(-c2ccc(C)c(NC(=O)c3cccc(N4C(=O)c5ccccc5C4=O)c3)c2)n[nH]1
vAce2-spike3-77	Z1389963584	-8.3	0.252	441.529	REAL	O=C(NCCN1C(=O)[C@H]2[C@@H]3C=C[C@@H](C3)[C@@H]2C1=O)N1CCc2ccccc2[C@H](c2ccccc2)C1
vAce2-spike3-78	Z1411312008	-8.3	0.277	399.493	REAL	CC(=O)N1CCc2cc(NC(=O)NCc3cccc(-c4ccc(C)cc4)c3)ccc21
vAce2-spike3-79	Z1446868147	-8.3	0.268	416.48	REAL	Cc1ccc(-c2nnc(C)[nH]2)c(NC(=O)COc2ccc3oc4c(c3c2)CCCC4)c1
vAce2-spike3-80	Z1453108616	-8.3	0.259	431.451	REAL	Cc1nnc([C@@H]2Cc3ccccc3CN2C(=O)c2cccc([C@@]3(C)NC(=O)NC3=O)c2)o1
vAce2-spike3-81	Z1472742620	-8.3	0.268	415.452	REAL	Cc1n[nH]c(NC(=O)c2cc(C)n(-c3ccccc3)n2)c1-c1ccc2c(c1)OCCO2
vAce2-spike3-82	Z1531746394	-8.3	0.259	448.433	REAL	O=C(Nc1ccn(-c2ncccc2F)n1)c1ccc2c(c1)S(=O)(=O)c1ccccc1C2=O
vAce2-spike3-83	Z1548269969	-8.3	0.244	449.513	REAL	C[C@H](Cn1ncc2ccccc2c1=O)NC(=O)c1cc(-c2ccccc2)n(-c2ccccc2)n1
vAce2-spike3-84	Z1559005930	-8.3	0.259	442.909	REAL	O=c1[nH]c(N[C@@H](Cc2ccc(Cl)cc2)c2ccccn2)nc2c1nn2-c1ccccc1
vAce2-spike3-85	Z1632228538	-8.3	0.259	434.494	REAL	Cc1nc([C@H]2COCCN2C(=O)N[C@@H](c2ccccc2)c2ccc3c(c2)CCCO3)no1
vAce2-spike3-86	Z1687911235	-8.3	0.259	428.491	REAL	Cc1cc(NC(=O)NCc2cccc([C@]3(C)NC(=O)NC3=O)c2)ccc1-c1ccccc1
vAce2-spike3-87	Z1695804767	-8.3	0.268	408.464	REAL	O=C(NNc1cnc2ccccc2n1)C1=NN(c2ccccc2)[C@@H](c2ccccc2)C1
vAce2-spike3-88	Z1896759932	-8.3	0.268	406.448	REAL	O=C(NNc1cnc2ccccc2n1)c1cc(-c2ccccc2)n(-c2ccccc2)n1
vAce2-spike3-89	Z1919288439	-8.3	0.286	385.466	REAL	Cc1cccc(-c2cccc(CNC(=O)Nc3ccc4c(c3)CC(=O)N4C)c2)c1
vAce2-spike3-90	Z2032886619	-8.3	0.252	446.501	REAL	C[C@H]1Oc2ccc(C(=O)C3CCN(C(=O)[C@H]4CCC(=O)c5ccccc54)CC3)cc2NC1=O
vAce2-spike3-91	Z2171875536	-8.3	0.259	429.479	REAL	Cc1nc(NC(=O)NCc2cccc([C@]3(C)NC(=O)NC3=O)c2)ccc1-c1ccccc1
vAce2-spike3-92	Z2172023837	-8.3	0.277	411.504	REAL	Cc1cc(NC(=O)N[C@@H](C)c2ccc(N3CCOC3=O)cc2)nn1C1CCCCC1
vAce2-spike3-93	Z2174898637	-8.3	0.259	429.518	REAL	O=C(c1ccc2c(=O)n3c(nc2c1)CCCCC3)N1CC[C@]2(CCc3ccccc3O2)C1
vAce2-spike3-94	Z2182755069	-8.3	0.252	434.502	REAL	CCn1c(-c2n[nH]c(=O)c3ccccc23)nnc1N1C[C@@H](c2ccccc2)c2ccccc21
vAce2-spike3-95	Z2185412311	-8.3	0.252	446.553	REAL	Cc1cc(C)c2c(c1)CN(c1nnc(C(=O)Nc3cccn3)n1C[C@@H]1CCCCO1)CC2
vAce2-spike3-96	Z2190144208	-8.3	0.259	432.526	REAL	Cc1ccc(-n2nc(NC(=O)N[C@@H](C)c3ccc(N4CCCNC4=O)cc3)cc2C)cc1
vAce2-spike3-97	Z2190145665	-8.3	0.259	436.49	REAL	Cc1cc(NC(=O)N[C@@H](C)c2ccc(N3CCCNC3=O)cc2)nn1-c1cccc(F)c1
vAce2-spike3-98	Z284317138	-8.3	0.231	499.957	REAL	C[C@H]1c2[nH]c3ccccc3c2[C@H](c2ccccc2Cl)CN1C(=O)c1cnc2c(c1)c(=O)[nH]c(=O)n2C
vAce2-spike3-99	Z316831526	-8.3	0.224	489.53	REAL	O=C(c1cccc(N2C(=O)c3ccccc3C2=O)c1)N1CCN(C(=O)c2ccc3ccccc23)CC1
vAce2-spike3-100	Z325118426	-8.3	0.286	395.497	REAL	Cc1ccc(C23C[C@H]4C[C@@H](CC(C(=O)OCCN5C(=O)CCC5=O)(C4)C2)C3)cc1

Supplementary Table 13. Top 100 virtual hits of the screen against ACE2 at the Spike interaction interface in which the structure with PDB ID 6M17 was used (Screen ID: 3). Compounds were filtered so that hits had MW < 600 dalton, cLogP < 6, number of hydrogen bond acceptors < 11, and no reactive functional groups. The name of each compound consists of the initial letter 'v' for virtual hit, followed by the target protein name and the target site ('spike' for spike interaction site, 3 for docking scenario 3). The score is the docking score given by QuickVina 2 in kcal/mol. The ligand efficiency (LE) is computed as LE = -score/#NonH, where #NonH is the number of heavy (i.e. non hydrogen) atoms.

Name	Catalog ID	Score	LE	MW	Library	SMILES
vAce2-spike3-101	Z343948116	-8.3	0.268	409.44	REAL	O=C(O)c1ccc2[nH]c3c(c2c1)CN(C(=O)c1cc2c(ccc4ccccc42)[nH]1)CC3
vAce2-spike3-102	Z412184662	-8.3	0.231	488.59	REAL	Cc1cc(C)nc(-n2nc(C)cc2NC(=O)N2CC3(CCCC3)c3cc4c(cc3[C@@H]2C)OCCO4)n1
vAce2-spike3-103	Z448914410	-8.3	0.277	396.49	REAL	C[C@@H](NC(=O)N1Cc2ccccc2[C@H](c2ccccc2)C1)c1nc2ccccc2[nH]1
vAce2-spike3-104	Z666678018	-8.3	0.224	488.59	REAL	O=C(Cc1nc2cc3ccccc3cc2c(=O)[nH]1)N1CCN(C(c2ccccc2)c2ccccc2)CC1
vAce2-spike3-105	Z73312466	-8.3	0.237	493.56	REAL	CC(=O)N1CCc2cc(NC(=O)[C@@H]3Cc4ccccc4CN3S(=O)(=O)c3ccc(F)cc3)ccc21
vAce2-spike3-106	Z740561090	-8.3	0.259	455.53	REAL	C[C@H]1c2cc3c(cc2C2(CCCC2)CN1S(=O)(=O)c1ccc2c(c1)C(=O)OC2)OCCO3
vAce2-spike3-107	Z774371686	-8.3	0.259	423.43	REAL	Cc1nc(-c2cccc(NC(=O)c3cccc(N4C(=O)c5ccccc5C4=O)c3)c2)n[nH]1
vAce2-spike3-108	Z88505027	-8.3	0.268	410.43	REAL	C[C@@H](NC(=O)c1cccc(N2C(=O)c3ccccc3C2=O)c1)c1nc2ccccc2[nH]1
vAce2-spike3-109	Z993684752	-8.3	0.252	446.51	REAL	C[C@]1(c2cccc(CNC(=O)[C@H]3CC(=O)N(c4ccc5c(c4)CCC5)C3)c2)NC(=O)NC1=O
vAce2-spike3-110	ZINC000000894512	-8.3	0.224	484.55	ZINC	CC(=O)Nc1ccc(-c2ccc(N3C(=O)[C@@H]4[C@@H](C3=O)C3c5ccccc5C4c4ccccc43)cc2)cc1
vAce2-spike3-111	ZINC000001570225	-8.3	0.296	358.44	ZINC	O=C1c2ccccc2C(=C(c2ccccc2)c2ccccc2)c2ccccc21
vAce2-spike3-112	ZINC000002291141	-8.3	0.244	452.52	ZINC	Cc1cc2nc(NC(=N)NC(=O)c3ccccc3NC(=O)c3ccccc3)nc(C)c2cc1C
vAce2-spike3-113	ZINC000013807019	-8.3	0.237	464.50	ZINC	O=C1[C@@H]2[C@H](c3ccccc3F)N(c3ccccc3)O[C@@H]2C(=O)N1c1ccccc1)C(F)(F)F
vAce2-spike3-114	ZINC000100081501	-8.3	0.237	454.53	ZINC	O=C1[C@@H]2[C@H]3C=C[C@@H](C3=C(c3ccccc3)c3ccccc3)[C@H]2C(=O)N1c1ccccc2ccnc21
vAce2-spike3-115	ZINC000135602460	-8.3	0.237	464.50	ZINC	O=C1[C@@H]2ON(c3ccccc3)[C@@H](c3ccccc3F)[C@@H]2C(=O)N1c1ccccc(-c2ccccc2)c1
vAce2-spike3-116	ZINC000211010329	-8.3	0.296	372.39	ZINC	O=C1N=C(NNC2=NC(=O)/C(=C/c3ccccc3)N2)N/C1=C\c1ccccc1
vAce2-spike3-117	PV-001843315235	-8.2	0.273	407.55	REAL	COc1cccc(C[C@]2(C(=O)N[C@@H](CO)Cc3ccc(C)cc3)C[C@H]3CC[C@H]2C3)c1
vAce2-spike3-118	PV-001921200373	-8.2	0.248	466.41	REAL	O=C(N[C@@H]2[C@H](c3ccccc3F)N(c3ccccc3)O[C@@H]2C(=O)N1c1ccccc1)C(F)(F)F
vAce2-spike3-119	PV-001921200483	-8.2	0.248	462.45	REAL	Cc1cc(-c2noc(CN3CC[C@H](c4ccccc4)[C@H](NC(=O)C(F)(F)F)C3)n2)cc1F
vAce2-spike3-120	PV-001921200560	-8.2	0.256	445.44	REAL	C[C@H](c1nc(-c2cccnc2)no1)N1CC[C@H](c2ccccc2)[C@H](NC(=O)C(F)(F)F)C1
vAce2-spike3-121	PV-001921200969	-8.2	0.248	476.52	REAL	Cc1ccc2nc(NC(=O)CN3CC[C@H](c4ccccc4)[C@H](NC(=O)C(F)(F)F)C3)sc2c1
vAce2-spike3-122	PV-001921200994	-8.2	0.248	480.49	REAL	O=C(CN1CC[C@H](c2ccccc2)[C@H](NC(=O)C(F)(F)F)C1)Nc1nc2ccc(F)cc2s1
vAce2-spike3-123	PV-001921201041	-8.2	0.241	476.50	REAL	C[C@H](C(=O)NC(=O)NCc1ccccc1)N1CC[C@H](c2ccccc2)[C@H](NC(=O)C(F)(F)F)C1
vAce2-spike3-124	PV-001921201117	-8.2	0.248	458.48	REAL	Cc1ccccc1-c1noc([C@@H](C)N2CC[C@H](c3ccccc3)[C@H](NC(=O)C(F)(F)F)C2)n1
vAce2-spike3-125	PV-001921201119	-8.2	0.248	460.46	REAL	COc1cccc(-c2nnc(CN3CC[C@H](c4ccccc4)[C@H](NC(=O)C(F)(F)F)C3)o2)c1
vAce2-spike3-126	PV-001921202221	-8.2	0.256	445.44	REAL	Cc1cncc(-c2nc(CN3CC[C@H](c4ccccc4)[C@H](NC(=O)C(F)(F)F)C3)no2)c1
vAce2-spike3-127	PV-001940697547	-8.2	0.248	442.52	REAL	CC(=O)N1CCc2cc(NC(=O)N[C@H](C)c3cccc(NC(=O)c4ccccc4)c3)ccc21
vAce2-spike3-128	PV-001944065836	-8.2	0.273	399.49	REAL	CC(=O)N1Cc2ccc(NC(=O)NCc3cccc(-c4ccc(C)cc4)c3)cc2C1
vAce2-spike3-129	PV-001944651211	-8.2	0.273	409.42	REAL	C[C@H](NC(=O)Nc1ccn(-c2nccnc2F)n1)c1ccc(N2CCNC2=O)cc1
vAce2-spike3-130	PV-001944907645	-8.2	0.265	418.50	REAL	Cc1ccc(-n2nc(NC(=O)N[C@@H](C)c3ccc(N4CCNC4=O)cc3)cc2C)cc1
vAce2-spike3-131	PV-001944952232	-8.2	0.256	437.47	REAL	Cc1cc(NC(=O)N[C@@H](C)c2ccc(N3CCCOC3=O)cc2)nn1-c1cccc(F)c1
vAce2-spike3-132	PV-001944952919	-8.2	0.265	422.46	REAL	Cc1cc(NC(=O)N[C@@H](C)c2ccc(N3CCNC3=O)cc2)nn1-c1ccc(F)c1
vAce2-spike3-133	PV-001944976049	-8.2	0.265	438.92	REAL	Cc1cc(NC(=O)N[C@@H](C)c2ccc(N3CCNC3=O)cc2)nn1-c1cccc(Cl)c1
vAce2-spike3-134	PV-001945052947	-8.2	0.265	419.48	REAL	Cc1cc(NC(=O)N[C@@H](C)c2ccc(N3CCCOC3=O)cc2)nn1-c1ccccc1
vAce2-spike3-135	PV-001945053615	-8.2	0.273	404.47	REAL	Cc1cc(NC(=O)N[C@@H](C)c2ccc(N3CCNC3=O)cc2)nn1-c1ccccc1
vAce2-spike3-136	PV-001945885952	-8.2	0.265	435.45	REAL	O=C(N[C@H](c1cccc2ccccc12)C(F)(F)F)N1CCC2(CC1)C[C@H](O)CNC2=O
vAce2-spike3-137	PV-001948063025	-8.2	0.248	455.46	REAL	Cc1cc(NC(=O)N[C@@H](C)c2ccc(N3CCCOC3=O)cc2)nn1-c1ccc(F)cc1F
vAce2-spike3-138	PV-001948063170	-8.2	0.256	440.45	REAL	Cc1cc(NC(=O)N[C@@H](C)c2ccc(N3CCNC3=O)cc2)nn1-c1ccc(F)cc1F
vAce2-spike3-139	PV-001950613958	-8.2	0.248	444.49	REAL	Cc1cccc(Oc2cccc(NC(=O)NCc3cccc([C@]4(C)NC(=O)NC4=O)c3)c2)c1
vAce2-spike3-140	PV-001951312107	-8.2	0.256	435.48	REAL	C[C@@H](NC(=O)Nc1ccc2c(=O)n(C)c(=O)n(C)c2c1)c1cccc(N2CCCC2=O)c1
vAce2-spike3-141	PV-001952042441	-8.2	0.283	392.43	REAL	O=C(NCc1c(O)ccc2c1CCCC2)Nc1ccc(-c2ccccc2F)nn1
vAce2-spike3-142	PV-001964844732	-8.2	0.256	445.48	REAL	CC1(C)[C@@H](c2cccc(C(F)(F)F)c2)CCN1C(=O)N[C@H]1CCc2ccccc2NC1=O
vAce2-spike3-143	PV-001964845097	-8.2	0.273	399.49	REAL	O=C(NCCc1cccc(-c2ccccc2)c1)N[C@H]1CCc2ccccc2NC1=O
vAce2-spike3-144	Z1021061774	-8.2	0.241	450.54	REAL	C[C@H](NC(=O)c1[nH]nc2ccccc12)C(=O)NC[C@H]1CC2c3ccccc3C1c1ccccc12
vAce2-spike3-145	Z1066385418	-8.2	0.228	482.51	REAL	COc1ccc([C@H]2CC(c3ccccc3)=NN2C(=O)Cn2nc(-c3ccccc3F)ccc2=O)cc1
vAce2-spike3-146	Z1092437218	-8.2	0.256	422.45	REAL	O=C(NNc1nc(-c2ccccc2)no1)c1cc(-c2ccccc2)n(-c2ccccc2)n1
vAce2-spike3-147	Z1095050614	-8.2	0.256	421.46	REAL	O=C(Nc1nc(-c2ccc3ccccc3n2)n[nH]1)c1nn(-c2ccccc2)c2c1CCC2
vAce2-spike3-148	Z1132548632	-8.2	0.273	399.49	REAL	Cc1cccc(-c2cccc(CNC(=O)Nc3ccc4c(c3)CCC(=O)N4C)c2)c1
vAce2-spike3-149	Z1136005230	-8.2	0.241	455.51	REAL	O=C1CCNc2cccc(C(=O)OCC(=O)N3Cc4ccccc4[C@H](c4ccccc4)C3)cc2N1
vAce2-spike3-150	Z1147982922	-8.2	0.248	439.52	REAL	Cc1ccc(-c2nnn(CC(=O)N[C@H](c3ccccc3)c3ccc4c(c3)CCCO4)n2)cc1
vAce2-spike3-151	Z1148473113	-8.2	0.234	473.58	REAL	Cc1cc(-c2cc(C(=O)N3CCC[C@H](c4nnc5n4CCC5)C3)c3cnn(C(C)C)c3n2)c(C)o1
vAce2-spike3-152	Z1150337726	-8.2	0.256	432.45	REAL	Cc1ccc(-n2nc(C(=O)O[C@@H](C)c3nc4ccccc4c(=O)[nH]3)c3c2CCC3)c(F)c1
vAce2-spike3-153	Z1150338652	-8.2	0.241	468.46	REAL	Cc1ccc(-n2nc(C(=O)O[C@H](C)C(=O)NC(=O)Nc3ccccc3F)c3c2CCC3)c(F)c1
vAce2-spike3-154	Z1150338722	-8.2	0.234	479.51	REAL	Cc1ccc(-n2nc(C(=O)O[C@H](C)C(=O)Nc3ccc4c(c3)OCCCO4)c3c2CCC3)c(F)c1
vAce2-spike3-155	Z1150338890	-8.2	0.234	476.46	REAL	Cc1ccc(-n2nc(C(=O)OCC(=O)Nc3ccc4c(c3)C(=O)N(C)C4=O)c3c2CCC3)c(F)c1
vAce2-spike3-156	Z1150338952	-8.2	0.228	494.48	REAL	Cc1ccc(-n2nc(C(=O)OCC(=O)NNC(=O)[C@H]3COc4ccccc4O3)c3c2CCC3)c(F)c1
vAce2-spike3-157	Z1175699434	-8.2	0.256	419.44	REAL	O=C(Nc1ccnc(-c2ccccc2)c1)c1cccc(N2C(=O)c3ccccc3C2=O)c1
vAce2-spike3-158	Z1177534330	-8.2	0.248	439.56	REAL	O=C(CCNC(=O)N1CCc2ccccc2C1)N1Cc2ccccc2[C@H](c2ccccc2)C1
vAce2-spike3-159	Z1212624188	-8.2	0.273	400.40	REAL	CN1C(=O)c2ccc(C(=O)Nc3n[nH]c4c3c(-c3ccccc3)nn4C)cc2C1=O
vAce2-spike3-160	Z1264171309	-8.2	0.265	411.50	REAL	O=C([C@H]1C[C@H]1c1ccc2c(c1)OCCO2)N1Cc2ccccc2[C@H](c2ccccc2)C1
vAce2-spike3-161	Z1272249238	-8.2	0.265	414.47	REAL	C[C@H](Nc1nc2c(cnn2-c2ccccc2)c(=O)[nH]1)c1cccc(N2CCCC2=O)c1
vAce2-spike3-162	Z1272282454	-8.2	0.248	443.46	REAL	O=c1[nH]c(N[C@@H](Cc2cccc(F)c2)c2cccc(F)c2)nc2c1cnn2-c1ccccc1
vAce2-spike3-163	Z1303272370	-8.2	0.248	438.49	REAL	Cc1ccc(-n2c(NC(=O)c3cccc(N4C(=O)CCC4=O)c3)nc3cc(C)ccc32)cc1
vAce2-spike3-164	Z1324849333	-8.2	0.241	445.48	REAL	O=C(C#Cc1ccccc1)NNC(=O)c1ccc(CN2C(=O)c3cccc4cccc2c34)cc1
vAce2-spike3-165	Z1355701961	-8.2	0.273	399.49	REAL	CC(=O)N1Cc2ccc(NC(=O)NCc3cccc(-c4cccc(C)c4)c3)cc2C1
vAce2-spike3-166	Z1382201413	-8.2	0.248	448.57	REAL	O=C(NCc1cc(=O)[nH]c2ccccc12)N1CCN(C(=O)C23CC4CC(CC(C4)C2)C3)CC1
vAce2-spike3-167	Z1409360871	-8.2	0.256	442.91	REAL	C[C@H]1c2[nH]c3ccccc3c2[C@H](c2ccccc2Cl)CN1C(=O)c1ccc2nnnn2c1
vAce2-spike3-168	Z1412310977	-8.2	0.265	422.53	REAL	C[C@H]1c2cc3c(cc2C2(CCCC2)CN1C(=O)N[C@H]1CCc2cn[nH]c2C1)OCCO3
vAce2-spike3-169	Z1421207109	-8.2	0.248	438.44	REAL	C[C@@H](NC(=O)c1cccc(N2C(=O)c3ccccc3C2=O)c1)c1noc(-c2ccccc2)n1
vAce2-spike3-170	Z1423390904	-8.2	0.265	415.47	REAL	Cc1ccc(-n2nc(C(=O)N3CC(c4nc5ccccc5[nH]4)C3)c3c2CCC3)c(F)c1
vAce2-spike3-171	Z1437253500	-8.2	0.273	395.46	REAL	Cc1onc(-c2ccnc2)c1C(=O)N1Cc2ccccc2[C@H](c2ccccc2)C1
vAce2-spike3-172	Z1451727055	-8.2	0.256	430.51	REAL	Cc1[nH]c2ccccc2c1C1CCN(C(=O)c2cccc([C@]3(C)NC(=O)NC3=O)c2)CC1
vAce2-spike3-173	Z1452297979	-8.2	0.273	404.47	REAL	C[C@@]1(c2cccc(CNC(=O)NC[C@@H]3[C@H]4Cc5ccccc5[C@@H]34)c2)NC(=O)NC1=O
vAce2-spike3-174	Z1453173921	-8.2	0.265	413.48	REAL	C[C@]1(c2cccc(C(=O)NCCc3cccc(-c4cccc4)c3)c2)NC(=O)NC1=O
vAce2-spike3-175	Z1460804037	-8.2	0.256	430.44	REAL	C[C@@H](NC(=O)c1cncc(-c2ccc3c(c2)CCO3)c1)c1nc(-c2cccc(F)c2)no1
vAce2-spike3-176	Z1493127209	-8.2	0.273	400.48	REAL	O=C(c1cccc2ccccc12)N1CCN(C(=O)[C@H]2OCCc3ccccc32)CC1
vAce2-spike3-177	Z1506345444	-8.2	0.265	420.51	REAL	O=C(Nc1ccc2c(c1)OC1(CCCCC1)O2)N1CCO[C@@]2(CCc3ccccc32)C1
vAce2-spike3-178	Z1506531298	-8.2	0.265	415.49	REAL	O=C(Nc1cccn(Cc2ccccc2)c1=O)N1CCO[C@]2(CCc3ccccc32)C1
vAce2-spike3-179	Z1523926013	-8.2	0.248	443.46	REAL	O=C(NNc1nc(-c2cccn2)nc2c1CCC2)c1cccc(-c2c(F)cccc2F)c1
vAce2-spike3-180	Z1538688134	-8.2	0.293	399.55	REAL	COc1cccc(C[C@@]2(C(=O)N[C@H](CCO)c3cccs3)C[C@H]3CC[C@H]2C3)c1
vAce2-spike3-181	Z1557996037	-8.2	0.265	419.48	REAL	Cc1n[nH]c(NC(=O)c2cccc([C@H]3CCCOC3)c2)c1-c1ccc2c(c1)OCCO2
vAce2-spike3-182	Z1590843453	-8.2	0.248	445.57	REAL	Cc1cc(NC(=O)c2nnn(-c3cccc4c3CCN(C)C4)c2C)n([C@@H]2C[C@@H]3CC[C@H]2C3)n1
vAce2-spike3-183	Z1602460109	-8.2	0.265	418.48	REAL	Cc1nccn1-c1ccc([C@H](C)NC(=O)Nc2ccc(C)n(-c3cccc(F)c3)n2)cc1
vAce2-spike3-184	Z1608175908	-8.2	0.248	440.50	REAL	CC(=O)c1cccc(C(=O)N2C[C@@H](C)N(C(=O)c3cccc(C(C)=O)c3)c3ccccc32)c1
vAce2-spike3-185	Z1618349191	-8.2	0.265	416.52	REAL	Cc1ccc2[nH]c3c(c2c1)C[C@H](NC(=O)NCc1ccccc(N2CCCC2=O)c1)CC3
vAce2-spike3-186	Z1632201994	-8.2	0.265	415.54	REAL	Cc1cccc(-c2cccc(CNC(=O)N3CCC[C@H](c4n[nH]c(C5CC5)n4)C3)c2)c1
vAce2-spike3-187	Z1651046671	-8.2	0.283	382.46	REAL	O=C1Cc2ccc(CC(=O)N3Cc4ccccc4[C@H](c4ccccc4)C3)cc2N1
vAce2-spike3-188	Z1682559164	-8.2	0.256	425.41	REAL	Cc1ccc(-c2noc(Cc3noc(-c4c[nH]n5c4nc(=O)c4ccccc45)n3)n2)cc1
vAce2-spike3-189	Z1682561676	-8.2	0.265	420.44	REAL	Cc1ccc(-c2noc(Cc3noc(C4(c5cccc(F)c5)CCOCC4)n3)n2)cc1
vAce2-spike3-190	Z1684080397	-8.2	0.273	403.49	REAL	CC(C)c1cc(-c2nc(Cc3nc(N)c4ccccc4n3)no2)c(O)c(C(C)C)c1
vAce2-spike3-191	Z1695803522	-8.2	0.265	407.44	REAL	O=C(NNc1cnc2ccccc2n1)c1nc(-c2ccccc2)n(-c2ccccc2)n1
vAce2-spike3-192	Z1705104924	-8.2	0.256	437.41	REAL	Cc1n[nH]c(NC(=O)c2ccn(-c3ccc(F)cc3F)n2)c1-c1ccc2c(c1)OCCO2
vAce2-spike3-193	Z1709226393	-8.2	0.273	399.49	REAL	CC(=O)N1CCc2c(NC(=O)NCc3cccc(-c4cccc(C)c4)c3)ccc21
vAce2-spike3-194	Z1719583462	-8.2	0.273	398.50	REAL	O=C(NCCc1cccc(-c2ccccc2)c1)N1CC[C@@]2(C1)OCc1ccccc12
vAce2-spike3-195	Z1829491286	-8.2	0.256	432.52	REAL	Cc1cc(C)c(N2CC[C@@H](NC(=O)N3CC[C@@]4(C3)C(=O)Nc3ccccc34)C2=O)c(C)c1
vAce2-spike3-196	Z1850533638	-8.2	0.256	429.52	REAL	Cc1ccc(-n2cnc3c2CCN(C(=O)NCC(=O)N2CCc4ccccc4C2)C3)cc1
vAce2-spike3-197	Z1903278885	-8.2	0.248	440.50	REAL	Cn1c(=O)ccc2ccc(NC(=O)N3CCN(C(=O)c4cccc5ccccc45)CC3)cc21
vAce2-spike3-198	Z1907869846	-8.2	0.248	437.50	REAL	NC(=O)N1CCCc2ccc(NC(=O)c3cc(-c4ccccc4)n(-c4ccccc4)n3)cc21
vAce2-spike3-199	Z1908692485	-8.2	0.248	445.50	REAL	Cc1ccnc(-c2n[nH]c([C@@H](C)NC(=O)c3nn(-c4ccc(C)cc4F)c4c3CCC4)n2)c1
vAce2-spike3-200	Z1919227875	-8.2	0.265	424.48	REAL	CC1(c2ccc(NC(=O)N[C@H]3CCc4nnc(-c5ccc(F)cc5)n4C3)no2)CCCC1

Supplementary Table 14. Virtual screening hits 101-200 of the screen against ACE2 at the Spike interaction interface in which the structure with PDB ID 6M17 was used (Screen ID: 3). The name of each compound consists of the initial letter 'v' for virtual hit, followed by the target protein name and the target site ('spike' for spike interaction site, 3 for docking scenario 3). The score is the docking score given by QuickVina 2 in kcal/mol. The ligand efficiency (LE) is computed as LE = -score/#NonH, where #NonH is the number of heavy (i.e. non hydrogen) atoms.

Name	Catalog ID	Score	LE	MW	Library	SMILES
vAce2-spike4-1	Z358867962	-9.8	0.327	415.532	REAL	Cc1cccc([C@@H](CC(=O)O[C@@H](C)C(=O)N[C@@H](C)[C@H]2C[C@H]3CC[C@H]2C3)NC(N)=O)c1
vAce2-spike4-2	ZINC000001080232	-9.8	0.288	446.505	ZINC	O=C1C[C@H](c2ccccc2)CC2=C1[C@@H](c1ccc3c(c1)OCO3)c1ccc3ncccc3c1N2
vAce2-spike4-3	ZINC000006161704	-9.7	0.237	564.625	ZINC	Cc1ccc(-c2nnc(Nc3ccc4c(c3)OCO4)c3ccccc32)cc1S(=O)(=O)NCc1nc2ccccc2[nH]1
vAce2-spike4-4	PV-000377205688	-9.6	0.343	382.423	REAL	O=C(N[C@@H]1C[C@H]2CC[C@@H]1N2C(=O)[C@H]1CCCc2[nH]ncc21)c1ccc(=O)[nH]n1
vAce2-spike4-5	PV-001877208919	-9.6	0.331	392.458	REAL	CC1(C)CCC[C@H](c2cccc(NC(=O)c3cnc4[nH]c(=O)[nH]c(=O)c4c3)c2)C1
vAce2-spike4-6	ZINC000006079679	-9.6	0.24	548.669	ZINC	Cc1ccc(Nc2nnc(-c3ccc(C)c(S(=O)(=O)NCc4nc5ccccc5[nH]4)c3)c3ccccc32)c(C)c1
vAce2-spike4-7	ZINC000006161729	-9.6	0.229	588.613	ZINC	Cc1ccc(-c2nnc(Nc3cccc(C(F)(F)F)c3)c3ccccc32)cc1S(=O)(=O)NCc1nc2ccccc2[nH]1
vAce2-spike4-8	ZINC000007423120	-9.6	0.32	403.397	ZINC	Cc1cc(NC(=O)c2cc(=O)c3ccccc3o2)n(-c2nc3c(c(=O)[nH]2)CCC3)n1
vAce2-spike4-9	ZINC000021780241	-9.6	0.274	489.598	ZINC	CC(=O)N1c2ccc(S(=O)(=O)N3CCN(c4nc5ccccc5n5eccc45)CC3)cc2C[C@H]1C
vAce2-spike4-10	Z1494997312	-9.5	0.328	429.524	REAL	CN1CC[C@H](C(=O)Nc2nnc(NS(=O)(=O)c3ccccc3)s2)c2ccccc21
vAce2-spike4-11	Z1610101091	-9.5	0.306	412.496	REAL	Cc1ccc(-n2nc(C(=O)N3CCC[C@H]3c3nc(-c4ccccc4)n[nH]3)cc2C)cc1
vAce2-spike4-12	Z1610101093	-9.5	0.306	416.459	REAL	Cc1cc(C(=O)N2CCC[C@H]2c2nc(-c3ccccc3)n[nH]2)nn1-c1ccc(F)cc1
vAce2-spike4-13	Z1684581689	-9.5	0.297	439.377	REAL	C[C@@]1(c2ccccc(-c3nnoc([C@H]4CC(c5cc(F)ccc5F)=NO4)n3)c2)NC(=O)NC1=O
vAce2-spike4-14	Z1748295971	-9.5	0.306	421.456	REAL	O=C([C@H]1CCCCN1C(=O)c1ccc(=O)[nH]n1)N1CC[C@@]2(C1)C(=O)Nc1ccccc12
vAce2-spike4-15	Z2226999403	-9.5	0.306	431.413	REAL	O=C1CNC(=O)c2ccc(C(=O)N3CCC[C@H](c4cccc(C(F)(F)F)c4)C3)cc2N1
vAce2-spike4-16	ZINC000002229890	-9.5	0.279	477.5	ZINC	CC(=O)Nc1ccc(S(=O)(=O)Nc2nc3ccccc3nc2Nc2ccccc(C(=O)O)c2)cc1
vAce2-spike4-17	ZINC000003283106	-9.5	0.271	484.535	ZINC	O=S(=O)(Nc1nc2ccccc2nc1Nc1cccc2ccccc21)c1ccc2c(c1)OCCO2
vAce2-spike4-18	ZINC000010215018	-9.5	0.264	477.519	ZINC	C[C@@]1(c2ccc3ccccc3c2)NC(=O)N(CC(=O)c2ccc(NC(=O)c3ccccc3)cc2)C1=O
vAce2-spike4-19	ZINC000013730160	-9.5	0.288	479.584	ZINC	O=C(c1ccc2nc(NS(=O)(=O)c3ccccc3)sc2c1)N1CCN(c2ccccn2)CC1
vAce2-spike4-20	ZINC000017159713	-9.5	0.25	520.616	ZINC	Cc1ccc(-c2nnc(Nc3ccccc3)c3ccccc32)cc1S(=O)(=O)NCc1nc2ccccc2[nH]1
vAce2-spike4-21	ZINC000095474117	-9.5	0.271	468.52	ZINC	Cc1nn(-c2ncnc3[nH]cnc32)c2c1[C@@]1(CC(O)=N2)c2cccc3c2N(C1=O)C(C)(C)C[C@H]3C
vAce2-spike4-22	ZINC000263618603	-9.5	0.271	474.538	ZINC	O=C(NC1CCN(Cc2nnn3c2CO[C@H](c2ccc(F)cc2)C3)CC1)c1cccc2[nH]ccc21
vAce2-spike4-23	ZINC000952862595	-9.5	0.237	542.638	ZINC	O=C([C@H]1Cc2ccccc2C(=O)N1)N1CCC2(Cc3cn(nn3)CCCOc3ccc(cc3)CCNC2=O)CC1
vAce2-spike4-24	PV-001882414886	-9.4	0.313	447.47	REAL	O=C1C[C@H](C(=O)Nc2nnc(NS(=O)(=O)c3ccccc3)s2)c2ccc(F)cc2N1
vAce2-spike4-25	PV-001946364913	-9.4	0.303	422.459	REAL	Cc1c(NC(=O)N[C@H](C)C(=O)N2c3ccccc3[C@H]2C)noc1-c1ccccc1F
vAce2-spike4-26	PV-001948009740	-9.4	0.324	405.375	REAL	O=C(Nc1cccc2[nH]c(=O)oc12)N1CCC[C@@H](c2ccc(C(F)(F)F)c2)C1
vAce2-spike4-27	PV-001965891477	-9.4	0.336	390.404	REAL	O=C(N[C@H]1CCc2ccc(O)cc21)NC1(c2ccc(C(F)(F)F)c2)CCC1
vAce2-spike4-28	Z1010550230	-9.4	0.261	494.542	REAL	C[C@H](OC(=O)[C@H]1C[C@H](O)CN1C(=O)c1ccc2c(c1)CCC2)C(=O)N[C@H]1COc2ccccc2O1
vAce2-spike4-29	Z1095049158	-9.4	0.303	413.392	REAL	O=C(COc1ccc2ccc(=O)oc2c1)Nc1nc(-c2ccc3ccccc3n2)n[nH]1
vAce2-spike4-30	Z1281111006	-9.4	0.285	443.589	REAL	O=C([C@@H]1C[C@@]2(CCOC1)CCCc1ccccc12)N1CCN(CC(=O)N2CCCc3ccccc32)CC1
vAce2-spike4-31	Z1303089142	-9.4	0.294	433.467	REAL	Cc1ccc(-c2cc(C(=O)NC[C@H]3CCC[C@@]34NC(=O)NC4=O)c3c(C)noc3n2)cc1
vAce2-spike4-32	Z1337005506	-9.4	0.285	446.509	REAL	O=C([C@@H]1CCCCN1C(=O)c1ccc(=O)[nH]n1)N1CCN(c2ccc3ccccc3n2)CC1
vAce2-spike4-33	Z1523178777	-9.4	0.303	423.472	REAL	CC(=O)N1CC[C@@H](NC(=O)[C@@H]2CCCCN2C(=O)c2ccc(=O)[nH]n2)c2ccccc21
vAce2-spike4-34	Z1608788445	-9.4	0.294	430.514	REAL	Cc1cc(C)cc(-n2nc(NC(=O)C3CCN(c4ccc5nncn5n4)CC3)cc2C)c1
vAce2-spike4-35	Z1610637700	-9.4	0.294	445.408	REAL	Cc1cc(C)cc(-n2nc(NC(=O)c3nc(C)n(-c4nnc(C(F)(F)F)[nH]4)n3)cc2C)c1
vAce2-spike4-36	Z1967731006	-9.4	0.294	435.518	REAL	C[C@@H]1C[C@@]2(CCO1)CN(C(=O)c1ccc3c(c1)C[C@@H](c1ccccc1)OC3=O)C[C@@H](C)O2
vAce2-spike4-37	Z2077157563	-9.4	0.303	412.408	REAL	Cc1noc2nc(-c3ccccc3)cc(C(=O)Nc3cccc(-c4n[nH]c(=O)[nH]4)c3)c12
vAce2-spike4-38	Z2151031713	-9.4	0.313	414.426	REAL	Cc1cc(=O)[nH]c2cc(C(=O)N3CCC[C@H](c4cccc(C(F)(F)F)c4)C3)ccc12
vAce2-spike4-39	Z2201098239	-9.4	0.336	385.506	REAL	C[C@H]1[C@H](NC(=O)NCC[C@@]2(O)C[C@H]3CC[C@H]2C3)CC(=O)N1Cc1ccccc1
vAce2-spike4-40	Z2311242839	-9.4	0.324	398.461	REAL	CCOC(=O)c1ccn(-c2cccc(NC(=O)NCC[C@H]3C[C@H]4CC[C@H]3O4)c2)n1
vAce2-spike4-41	Z2790043058	-9.4	0.348	363.42	REAL	O=C1[C@@H]2CCCc3ccccc3C2=NN1c1nccc(N2CCOCC2)n1
vAce2-spike4-42	ZINC000002933884	-9.4	0.254	494.452	ZINC	O=c1oc(-c2cccc(F)c2)nc2cc(Cc3ccc4c(=O)oc(-c5cccc(F)c5)nc4c3)ccc12
vAce2-spike4-43	ZINC000006161742	-9.4	0.241	536.615	ZINC	Cc1ccc(-c2nnc(Nc3cccc(O)c3)c3ccccc32)cc1S(=O)(=O)NCc1nc2ccccc2[nH]1
vAce2-spike4-44	ZINC000008424887	-9.4	0.294	433.384	ZINC	O=C1OC(c2ccc3ccccc3c2)=N/C1=C\c1ccc(-c2cccc(C(F)(F)F)c2)o1
vAce2-spike4-45	ZINC000009377815	-9.4	0.254	499.522	ZINC	C[C@]1(c2ccc3c(c2)OCCCO3)NC(=O)N(CC(=O)c2ccc(NC(=O)c3ccccc3)cc2)C1=O
vAce2-spike4-46	ZINC000012363521	-9.4	0.247	524.576	ZINC	Cc1cc(N2C(=O)C[C@@H](N3CCC(C4CCN([C@H]5CC(=O)N(c6cc(C)on6)C5=O)CC4)CC3)C2=O)no1
vAce2-spike4-47	ZINC000014746024	-9.4	0.261	478.55	ZINC	O=C(N[C@H]1C[C@H]2C(=O)N[C@@H](Cc3c[nH]c4ccccc34)C(=O)N2C1)c1ccc(-c2ccccc2)cc1
vAce2-spike4-48	ZINC000071853331	-9.4	0.269	477.538	ZINC	O=C(Nc1ccccc1)N1CCC[C@H](C(=O)N2CCC[C@@H](c3nc(-c4ccc(F)cc4)no3)C2)C1
vAce2-spike4-49	PV-001806344665	-9.3	0.31	415.414	REAL	Cc1nc2cc(C(=O)N3CCC[C@H](c4cccc(C(F)(F)F)c4)C3)ccc2c(=O)[nH]1
vAce2-spike4-50	PV-001921651657	-9.3	0.3	420.555	REAL	COc1ccc(-n2c(C)c(C)c(C#N)c2NC(=O)CN[C@H](C)[C@@]23CCCC[C@H]2C3)cc1
vAce2-spike4-51	PV-001962864474	-9.3	0.321	410.395	REAL	CC1(C)CN(C(=O)NCc2ccc(=O)[nH]n2)C[C@H](c2cccc(C(F)(F)F)c2)O1
vAce2-spike4-52	Z1095050540	-9.3	0.3	434.479	REAL	O=C(Nc1nc(-c2ccc3ccccc3n2)n[nH]1)c1cccc(N2CCCS2(=O)=O)c1
vAce2-spike4-53	Z1303091958	-9.3	0.3	418.452	REAL	Cc1ccc(-c2cc(C(=O)NC[C@H]3CCC[C@@]34NC(=O)NC4=O)c3ccccc3n2)o1
vAce2-spike4-54	Z1341820887	-9.3	0.332	385.379	REAL	C[C@@]1(C2CCN(C(=O)Nc3ccc4c(c3)C(=O)NC4=O)CC2)NC(=O)NC1=O
vAce2-spike4-55	Z1591928563	-9.3	0.3	439.495	REAL	Cc1ccc2[nH]c([C@H]3CCCN(S(=O)(=O)c4ccc5[nH]c(=O)[nH]c(=O)c5c4)C3)nc2c1
vAce2-spike4-56	Z1613247547	-9.3	0.3	411.424	REAL	O=C(NCc1nc(-c2ccccc2)n[nH]1)Nc1ccc2nc(-c3ccccn3)oc2c1
vAce2-spike4-57	Z1623274417	-9.3	0.291	448.869	REAL	Nc1nc(Cl)cc(NNC(=O)c2cc(-c3ccc4c(c3)OCCO4)nc3ccccc23)n1
vAce2-spike4-58	Z1634212503	-9.3	0.291	435.418	REAL	Cn1c(=O)[nH]c(=O)c2cc(C(=O)N[C@@H]3CCc4nnc(-c5ccc(F)cc5)n4C3)cnc21
vAce2-spike4-59	Z1663681893	-9.3	0.282	443.51	REAL	Cc1cc(C)cc(C(=O)N2CCC[C@H](c3nnc(Cn4nnc(-c5ccccc5)n4o3)C2)c1
vAce2-spike4-60	Z1684582120	-9.3	0.3	421.387	REAL	C[C@@]1(c2ccccc(-c3noc([C@H]4CC(c5cccc(F)c5)=NO4)n3)c2)NC(=O)NC1=O
vAce2-spike4-61	Z1684605096	-9.3	0.282	449.513	REAL	C[C@@H]1CC(C)(C)C[C@@]2(C1)NC(=O)N(Cc1nc(Cc3nc(-c4ccccc4)n[nH]3)no1)C2=O
vAce2-spike4-62	Z1862836773	-9.3	0.282	439.482	REAL	O=C(Nc1ccc2[nH]c(-c3ccccc3)nc2c1)C1CCN(c2ccc3nnnn3n2)CC1
vAce2-spike4-63	Z1917838623	-9.3	0.31	411.411	REAL	C[C@H](NC(=O)Nc1cc(-c2ccc(F)cc2F)nn1C)c1ccc2c(c1)CC(=O)N2
vAce2-spike4-64	Z1929431734	-9.3	0.3	421.539	REAL	Cc1ccc(C23C[C@@H]4C[C@H](CC(C(=O)N5CCC[C@]6(C5)NC(=O)NC6=O)C4)C2)C3)cc1
vAce2-spike4-65	Z1948615421	-9.3	0.344	361.444	REAL	O=C(Cc1c[nH]c2ccccc12)NNC(=O)[C@@H]1[C@@H]2[C@H]3C[C@@H]4[C@@H]5[C@H]3C[C@H]2[C@@H]5[C@H]41
vAce2-spike4-66	Z2144773071	-9.3	0.321	390.398	REAL	Cc1cc(=O)[nH]c2cc(C(=O)Nc3cccc([C@@]4(C)NC(=O)NC4=O)c3)ccc12
vAce2-spike4-67	Z2192934806	-9.3	0.291	449.868	REAL	Cn1c(=O)cc(C(=O)Nc2ncc(Cl)cc2C(=O)Cc2cccc(F)c2)c2ccccc21
vAce2-spike4-68	Z2308828546	-9.3	0.344	380.369	REAL	O=C(NCc1ccc(=O)[nH]n1)N1CCC[C@@H](c2cccc(C(F)(F)F)c2)C1
vAce2-spike4-69	Z292933652	-9.3	0.332	403.553	REAL	Cc1cc(C)n(-c2nnc(S[C@H](C)C(=O)N[C@H](C)[C@H]3C[C@H]4CC[C@H]3C4)n2N)n1
vAce2-spike4-70	Z729290334	-9.3	0.291	420.431	REAL	O=c1cc(/C=C/c2cn(-c3ccccc3)nc2-c2cc3ccccc3o2)nc2nc[nH]n12
vAce2-spike4-71	ZINC000001306298	-9.3	0.245	542.581	ZINC	Cc1ccc(-c2nnc(Nc3cccc(C(F)(F)F)c3)c3ccccc32)cc1S(=O)(=O)NC[C@H]1CCCO1
vAce2-spike4-72	ZINC000001588362	-9.3	0.274	440.509	ZINC	Nc1nc(-c2ccc3ccccc3c2)cc(-c2cc(-c3ccc4ccccc4c3)nc(N)n2)n1
vAce2-spike4-73	ZINC000002272171	-9.3	0.282	461.545	ZINC	CC(=O)Nc1ccc(S(=O)(=O)Nc2nc3ccccc3nc2Nc2ccc(C)c(C)c2)cc1
vAce2-spike4-74	ZINC000002859412	-9.3	0.258	472.499	ZINC	Cc1ccc(-c2nc3ccccc3o2)cc1NC(=O)c1ccc(-c2cc3ccccc3oc2=O)c1
vAce2-spike4-75	ZINC000002908937	-9.3	0.251	494.452	ZINC	O=c1oc(-c2cccc(F)c2)nc2cc(Cc3ccc4nc(-c5cccc(F)c5)oc(=O)c4c3)ccc12
vAce2-spike4-76	ZINC000006161730	-9.3	0.238	555.061	ZINC	Cc1ccc(-c2nnc(Nc3ccc(Cl)c3)c3ccccc32)cc1S(=O)(=O)NCc1nc2ccccc2[nH]1
vAce2-spike4-77	ZINC000006166473	-9.3	0.282	513.326	ZINC	O=S(=O)(Nc1nc2ccccc2nc1Nc1ccc(Cl)c(C(F)(F)F)c1)c1ccc(Cl)cc1
vAce2-spike4-78	ZINC000008870444	-9.3	0.258	496.586	ZINC	C[C@@H]1CCc2oc3c(cc(NS(=O)(=O)c4ccc5c6c(cccc64)C(=O)N5C)c4ccccc34)c2C1
vAce2-spike4-79	ZINC000009369230	-9.3	0.274	455.438	ZINC	FC(F)(F)c1ccnc(/N=c2\oc3ccc4ccccc4c3cc2-c2nc3ccccc3[nH]2)c1
vAce2-spike4-80	ZINC000009561375	-9.3	0.291	421.463	ZINC	O=C(c1ccc(Nc2nc3ccccc3n3nnnc23)cc1)N1CCc2ccccc2C1
vAce2-spike4-81	ZINC000012514899	-9.3	0.274	494.958	ZINC	O=C(Nc1nnc(-c2cccc(Cl)c2)o1)c1ccc(S(=O)(=O)N2CCc3ccccc3C2)cc1
vAce2-spike4-82	ZINC000012525007	-9.3	0.3	410.48	ZINC	c1ccc2c(c1)ccnc2[C@H]1C=C(c2ccc(N3CCOCC3)cc2)N=C2N=NNN21
vAce2-spike4-83	ZINC000013639629	-9.3	0.31	396.405	ZINC	O=c1c2c(nce3c2C[C@@H](c2ccccc2)CC3=O)[nH]n1-c1nc2ccccc2o1
vAce2-spike4-84	ZINC000016491517	-9.3	0.3	432.463	ZINC	O=c1[nH]c2ccc(Nc3nc4ccccc4nc3NS(=O)(=O)c3ccccc3)cc2[nH]1
vAce2-spike4-85	ZINC000040069859	-9.3	0.274	452.488	ZINC	Cc1noc2nc(-c3ccccc3F)cc(C(=O)N3CCn4cccc4[C@@H]3c3ccccc3)c12
vAce2-spike4-86	ZINC000040484406	-9.3	0.274	452.513	ZINC	COc1ccc(-c2cc(=O)n3c4ccccc4n(CC(=O)Nc4ccc(C)cc4C)c3n2)cc1
vAce2-spike4-87	ZINC000048523764	-9.3	0.258	464.475	ZINC	O=C1c2ccccc2C(=O)C2=C3C=CC4=CC5=C(C(=O)c6ccccc6C5=O)C5=CC=C(C=C12)[C@@H]3[C@@H]45
vAce2-spike4-88	ZINC000057494737	-9.3	0.266	466.5	ZINC	Cc1cccc(-c2noc(-c3ccn4c(=O)n(CC(=O)N5CCCc6ccccc65)nc34)n2)c1
vAce2-spike4-89	ZINC000067261396	-9.3	0.31	405.382	ZINC	Fc1ccc(-c2nnn3c2nc(NCc2ccc(F)cc2F)c2ccccc23)cc1
vAce2-spike4-90	ZINC000095474115	-9.3	0.266	468.52	ZINC	Cc1nn(-c2ncnc3[nH]cnc32)c2c1[C@@]1(CC(O)=N2)c2cccc3c2N(C1=O)C(C)(C)C[C@@H]3C
vAce2-spike4-91	ZINC000095549603	-9.3	0.266	462.551	ZINC	Cc1cccc(C(=O)N2CCc3cc(CNC(=O)c4n[nH]c5c4CCc4ccccc4-5)ccc32)c1
vAce2-spike4-92	ZINC000257357009	-9.3	0.274	452.548	ZINC	O=C1[C@@H]2C[C@@H]3C(=O)[C@H]4Cc5ccccc5C[C@H]4C(=O)[C@H]3C[C@H]2C(=O)[C@H]2Cc3ccccc3C[C@@H]12
vAce2-spike4-93	ZINC000604404113	-9.3	0.274	451.441	ZINC	O=C(CN1C(=O)c2ccccc2N2C(=O)c3ccccc3[C@@H]21)Nc1ccc2ncnc(O)c2c1
vAce2-spike4-94	PV-001807541512	-9.2	0.341	369.547	REAL	COc1cccc(C[C@]2(C(=O)NC[C@H]3CCCC3(C)C)C[C@H]3CC[C@H]2C3)c1
vAce2-spike4-95	PV-001825234235	-9.2	0.307	419.362	REAL	O=C(c1cccc(C(F)(F)F)c1)N1CCN(C(=O)c2ccnc3[nH]c(O)nc23)CC1
vAce2-spike4-96	PV-001825235385	-9.2	0.287	443.424	REAL	Cc1c(C(=O)N2CCN(C(=O)c3cccc(C(F)(F)F)c3)CC2)c2ccccc2[nH]c1=O
vAce2-spike4-97	PV-001874090146	-9.2	0.297	429.426	REAL	C[C@H]1CCN(c2ccc(F)cc2F)CCN1C(=O)c1cnc2c(c1)c(=O)[nH]c(=O)n2C
vAce2-spike4-98	PV-001882415667	-9.2	0.329	418.472	REAL	O=C(Nc1nnc(NS(=O)(=O)c2ccccc2)s1)[C@H]1CCc2cc(F)ccc21
vAce2-spike4-99	PV-001946130439	-9.2	0.329	390.364	REAL	O=C(Nc1ccc2nonc12)N1CCC[C@@H](c2cccc(C(F)(F)F)c2)C1
vAce2-spike4-100	PV-001957990487	-9.2	0.317	411.339	REAL	O=C1NC(=O)C2(CN(C(=O)N[C@H]3CC(=O)N(c4cccc(C(F)(F)F)c4)C3)C2)N1

Supplementary Table 15. Top 100 virtual hits of the screen against ACE2 at a site adjacent to the Spike interaction interface (Screen ID: 4). Compounds were filtered so that hits had MW < 600 dalton, cLogP < 6, number of hydrogen bond acceptors < 11, and no reactive functional groups. The name of each compound consists of the initial letter 'v' for virtual hit, followed by the target protein name and the target site ('spike' for spike interaction site, 4 for docking scenario 4). The score is the docking score given by QuickVina 2 in kcal/mol. The ligand efficiency (LE) is computed as LE = -score/#NonH, where #NonH is the number of heavy (i.e. non hydrogen) atoms.

Name	Catalog ID	Score	LE	MW	Library	SMILES
vAce2-spike4-101	PV-001965892100	-9.2	0.341	378.39	REAL	CC(C)(NC(=O)N[C@H]1CCc2ccc(O)cc21)c1cccc(C(F)(F)F)c1
vAce2-spike4-102	Z1069340454	-9.2	0.279	442.48	REAL	O=C(Nc1ccnn1[C@H]1CCCc2ccccc21)c1cnc2c(c1)c(=O)[nH]c(=O)n2C1CC1
vAce2-spike4-103	Z1127362355	-9.2	0.329	378.34	REAL	C[C@]1(c2cccc(NC(=O)c3ccc4c(c3)C(=O)NC4=O)c2)NC(=O)NC1=O
vAce2-spike4-104	Z1245911612	-9.2	0.287	429.45	REAL	O=C(c1cccc2ccccc12)N1CCN(C(=O)c2cc(=O)[nH]c3cc(F)ccc23)CC1
vAce2-spike4-105	Z1314145283	-9.2	0.279	449.51	REAL	O=C1Nc2ccccc2[C@@H]1C1CCN(C(=O)[C@H]2CCCCN2C(=O)c2ccc(=O)[nH]n2)CC1
vAce2-spike4-106	Z1334452954	-9.2	0.307	401.47	REAL	C[C@]1(C2CCN(c3nc(-c4ccccc4)nc4ccccc34)CC2)NC(=O)NC1=O
vAce2-spike4-107	Z1348480998	-9.2	0.307	410.48	REAL	O=C(Nc1cc([C@H]2C[C@@H]3CC[C@H]2C3)[nH]n1)[C@@H]1CCCCN1C(=O)c1ccc(=O)[nH]n1
vAce2-spike4-108	Z1550501417	-9.2	0.297	417.45	REAL	Cc1nc(C(=O)N2CCC[C@H]2c2nc(-c3ccccc3)n[nH]2)nn1-c1ccc(F)cc1
vAce2-spike4-109	Z1559358547	-9.2	0.287	447.56	REAL	CS(=O)(=O)Nc1ccc(N2CCN(C(=O)c3ccc4c(c3)-c3ccccc3C4)CC2)cc1
vAce2-spike4-110	Z1612154384	-9.2	0.307	400.44	REAL	O=C(Nc1cc(-c2ccccc2)on1)N1CCC[C@@H]1c1nc(-c2ccccc2)n[nH]1
vAce2-spike4-111	Z1613078336	-9.2	0.307	410.48	REAL	Cc1cc(C)cc(-n2nc(NC(=O)N3CCC4(CC3)NC(=O)N(C)C4=O)cc2C)c1
vAce2-spike4-112	Z1684581929	-9.2	0.279	444.45	REAL	Cc1cccc(N2N=C(c3nc(-c4cccc([C@]5(C)NC(=O)NC5=O)c4)no3)CCC2=O)c1
vAce2-spike4-113	Z1684605062	-9.2	0.287	426.48	REAL	O=C1C[C@H](c2nc(Cc3nc(-c4ccccc4)n[nH]3)no2)CN1c1ccc2c(c1)CCC2
vAce2-spike4-114	Z1693558636	-9.2	0.279	448.57	REAL	O=C(N[C@H]1CCO[C@@H](c2ccccc2)C1)N1CCN([C@H]2CCN(c3ccccc3)C2=O)CC1
vAce2-spike4-115	Z1693559789	-9.2	0.279	447.54	REAL	O=C(N[C@H]1CCO[C@@H](c2ccccc2)C1)N1CCN(Cc2nc3ccccc3c(=O)[nH]2)CC1
vAce2-spike4-116	Z1730117979	-9.2	0.297	417.40	REAL	O=C(c1ccc(-c2noc(-c3ccc(F)cc3)n2)cc1)N1CCc2n[nH]c(=O)cc2C1
vAce2-spike4-117	Z1731749860	-9.2	0.287	432.46	REAL	Cc1cc(-c2nc3cc(F)ccc3n2C)ccc1NC(=O)N1CCc2n[nH]c(=O)cc2C1
vAce2-spike4-118	Z1743879838	-9.2	0.317	403.36	REAL	O=C(N[C@H]1CCN(c2ccccc2C(F)(F)F)C1)c1ccc2c(=O)[nH]cnc2cn1
vAce2-spike4-119	Z17749227	-9.2	0.279	441.42	REAL	C[C@@H](C(=O)Nc1ccc2c(c1)C(=O)c1ccccc1C2=O)n1nnc(-c2ccc(F)cc2)n1
vAce2-spike4-120	Z1846556951	-9.2	0.307	402.37	REAL	O=C(COc1ccc2ccc(=O)oc2c1)Nc1nnc(-c2cc3ccccc3o2)[nH]1
vAce2-spike4-121	Z1846569519	-9.2	0.297	417.42	REAL	O=C(COc1cccc(N2CCCC2=O)c1)Nc1nnc(-c2cc3ccccc3o2)[nH]1
vAce2-spike4-122	Z1896776640	-9.2	0.329	389.51	REAL	COCCN(C(=O)NC[C@@H]1CCN(c2ccc(F)cc2)C1)[C@@H]1C[C@@H]2CC[C@@H]1C2
vAce2-spike4-123	Z1918849374	-9.2	0.279	448.52	REAL	COc1cccc(CC(=O)N2CCc3ccc(NC(=O)N4CC[C@]5(CNC(=O)C5)C4)cc32)c1
vAce2-spike4-124	Z1953218972	-9.2	0.279	446.51	REAL	O=C([C@@H]1CCCCN1C(=O)c1ccc(=O)[nH]n1)N1CCN(c2cncc3ccccc23)CC1
vAce2-spike4-125	Z2008042887	-9.2	0.279	441.49	REAL	Cn1c(-c2nn(C)c(=O)c3ccccc23)nnc1N1CCC[C@@H](c2nc3ccccc3o2)C1
vAce2-spike4-126	Z2011462392	-9.2	0.297	444.49	REAL	O=c1[nH]c(=O)c2cc(S(=O)(=O)N3CCC(N4CCc5cc(F)ccc54)CC3)ccc2[nH]1
vAce2-spike4-127	Z2077302320	-9.2	0.307	420.41	REAL	O=C1CCc2cc(C(=O)N3CCC[C@H](c4cccc(C(F)(F)F)c4)C3)c(F)cc2N1
vAce2-spike4-128	Z2091788341	-9.2	0.279	443.51	REAL	Cc1ccc2nc(-c3ccnc3)cc(C(=O)N3CCC[C@H]3C[C@]3(C)NC(=O)NC3=O)c2c1
vAce2-spike4-129	Z2091800037	-9.2	0.279	446.51	REAL	Cc1nn(C)c2nc(-c3ccccc3)cc(C(=O)N3CCC[C@H]3C[C@]3(C)NC(=O)NC3=O)c12
vAce2-spike4-130	Z2142733947	-9.2	0.317	385.43	REAL	Cc1cccc(-c2cncc(C(=O)Nc3cc(-c4n[nH]c(=O)[nH]4)ccc3C)c2)c1
vAce2-spike4-131	Z2160281118	-9.2	0.297	415.42	REAL	O=c1cc(-c2noc(C3CCN(c4ccc5nnnn5n4)CC3)n2)c2ccccc2[nH]1
vAce2-spike4-132	Z2228335002	-9.2	0.317	407.39	REAL	C[C@H]1CO[C@@H](c2cccc(C(F)(F)F)c2)CN1C(=O)/C=C\c1ccc(O)c(O)c1
vAce2-spike4-133	Z225721626	-9.2	0.279	446.46	REAL	Cc1ccc(C)c(N2C(=O)c3ccc(C(=O)N4CCC5(CC4)NC(=O)NC5=O)cc3C2=O)c1
vAce2-spike4-134	Z2308829654	-9.2	0.354	366.34	REAL	O=C(NCc1ccc(=O)[nH]n1)NC1(c2ccccc(C(F)(F)F)c2)CCC1
vAce2-spike4-135	Z2484316466	-9.2	0.317	398.46	REAL	CC(C)(C)Cc1nc(-c2cccc(C(=O)NNC(=O)[C@H]3C[C@@H]4CC[C@@H]3O4)c2)no1
vAce2-spike4-136	Z2625123242	-9.2	0.317	389.50	REAL	O=C1NCCc2cc(NC(=O)N3CCC[C@]4(CCCc5ccccc54)C3)ccc21
vAce2-spike4-137	Z2634736442	-9.2	0.329	392.48	REAL	Cc1ccc2[nH]c([C@@H]3CCCN(C(=O)c4ccc5oc(S)nc5c4)C3)nc2c1
vAce2-spike4-138	Z2802528018	-9.2	0.317	386.45	REAL	Cn1c(C(=O)N2CCC[C@H](c3c[nH]c4ncccc34)C2)cc(=O)c2ccccc21
vAce2-spike4-139	Z282725144	-9.2	0.297	414.47	REAL	CNC(=O)Nc1cccc(NC(=O)c2cc(-c3ccccc3)nc3c2c(C)nn3C)c1
vAce2-spike4-140	Z316833126	-9.2	0.256	482.54	REAL	O=C(CN1C(=O)N[C@@]2(CCc3ccccc32)C1=O)N1CCN(C(=O)c2cccc3ccccc23)CC1
vAce2-spike4-141	Z770167530	-9.2	0.317	387.48	REAL	O=C1CCCc2cc(C(=O)N3CCC[C@@H](c4cc5ccccc5[nH]4)C3)ccc2N1
vAce2-spike4-142	Z786229024	-9.2	0.297	417.40	REAL	NC(=O)c1cc(NC(=O)c2cccc(NC(=O)c3ccc4[nH]cnc4c3)c2)ccc1F
vAce2-spike4-143	Z803605870	-9.2	0.271	476.60	REAL	Cc1c(C(=O)N2CCN(Cc3nc4sc5c(c4c(=O)[nH]3)CCCC5)CC2)oc2c(C)cccc12
vAce2-spike4-144	Z804390806	-9.2	0.249	495.63	REAL	O=C([C@@H]1CC(=O)N(c2ccc3c(c2)Cc2ccccc2-3)C1)N1CCC[C@@H](c2nnc3n2CCCCC3)C1
vAce2-spike4-145	Z812597010	-9.2	0.263	490.63	REAL	Cc1ccc(C)c2c(C)c(C(=O)N3CCN(Cc4nc5sc6c(c5c(=O)[nH]4)CCCC6)CC3)oc12
vAce2-spike4-146	Z853698182	-9.2	0.287	433.47	REAL	Cn1c(=O)[nH]c(=O)c2cc(C(=O)N3CCC(C(=O)N4CCc5ccccc54)CC3)cnc21
vAce2-spike4-147	Z908882368	-9.2	0.297	419.48	REAL	Cn1c(=O)[nH]c(=O)c2cc(C(=O)N3CCC(N4CCc5ccccc5C4)CC3)cnc21
vAce2-spike4-148	Z920795562	-9.2	0.297	412.49	REAL	CC(=O)N1C[C@@H](C(=O)N2CC=C(c3cccc4ccccc34)CC2)Oc2ccccc21
vAce2-spike4-149	Z998973034	-9.2	0.279	446.47	REAL	Cc1oncc1C(=O)Nc1ccc(NC(=O)C2CCN(c3ccc4nncn4n3)CC2)cc1
vAce2-spike4-150	ZINC000002272003	-9.2	0.263	491.53	ZINC	CC(=O)Nc1ccc(S(=O)(=O)Nc2nc3ccccc3nc2Nc2ccc3c(c2)OCCO3)cc1
vAce2-spike4-151	ZINC000002275183	-9.2	0.271	477.50	ZINC	CC(=O)Nc1ccc(S(=O)(=O)Nc2nc3ccccc3nc2Nc2ccc(C(=O)O)cc2)cc1
vAce2-spike4-152	ZINC000002326512	-9.2	0.287	462.56	ZINC	Cc1ccc(Nc2nc3ccccc3nc2NS(=O)(=O)c2cccc3nsnc32)cc1C
vAce2-spike4-153	ZINC000002639248	-9.2	0.249	498.49	ZINC	Cc1cc(=O)oc2cc(OCc3ccc(C(=O)OCC(=O)N4CC(=O)Nc5ccccc54)cc3)ccc12
vAce2-spike4-154	ZINC000002861543	-9.2	0.263	464.48	ZINC	Cc1cc(NC(=O)c2ccc(-c3cc4ccccc4oc3=O)cc2)ccc1NC(=O)c1ccco1
vAce2-spike4-155	ZINC000002956095	-9.2	0.287	473.86	ZINC	O=c1oc2ccc3ccccc3c2cc1-c1nnc(Nc2cc(C(F)(F)F)ccc2Cl)s1
vAce2-spike4-156	ZINC000003137151	-9.2	0.287	447.52	ZINC	CC(=O)Nc1ccc(S(=O)(=O)Nc2nc3ccccc3nc2Nc2cccc(C)c2)cc1
vAce2-spike4-157	ZINC000003271774	-9.2	0.287	478.88	ZINC	O=S(=O)(Nc1nc2ccccc2nc1Nc1cccc(C(F)(F)F)c1)c1ccc(Cl)cc1
vAce2-spike4-158	ZINC000003283259	-9.2	0.279	486.91	ZINC	O=S(=O)(Nc1nc2ccccc2nc1Nc1ccc(F)c(Cl)c1)c1ccc2c(c1)OCCO2
vAce2-spike4-159	ZINC000003289817	-9.2	0.287	458.46	ZINC	Cc1ccc(S(=O)(=O)Nc2nc3ccccc3nc2Nc2ccc(C(F)(F)F)cc2)cc1
vAce2-spike4-160	ZINC000003328289	-9.2	0.297	484.91	ZINC	O=S(=O)(Nc1nc2ccccc2nc1Nc1cccc(C(F)(F)F)c1)c1ccc(Cl)s1
vAce2-spike4-161	ZINC000004911112	-9.2	0.317	387.53	ZINC	Cc1ccc(Nc2cc(C(=O)N[C@@H]3CCCC[C@H]3C)c3ccccc3n2)c(C)c1
vAce2-spike4-162	ZINC000006074254	-9.2	0.279	459.91	ZINC	CC(=O)n1cc([C@H]2Oc3ccc(Cl)cc3[C@@H]3CC(c4ccc(F)cc4)=NN32)c2ccccc21
vAce2-spike4-163	ZINC000009066553	-9.2	0.287	433.38	ZINC	O=C1OC(c2cccc3ccccc32)=N/C1=C\c1ccc(-c2cccc(C(F)(F)F)c2)o1
vAce2-spike4-164	ZINC000009192115	-9.2	0.249	489.51	ZINC	O=C(c1ccc(F)cc1)[C@H]1[C@H]2C(=O)N(c3ccc4ccccc4c3)C(=O)[C@H]2[C@@H]2c3ccccc3C=NN12
vAce2-spike4-165	ZINC000009274534	-9.2	0.263	481.58	ZINC	Cc1ccc(C)c(Nc2nn3c(nc4cc(C(=O)N5CCc6ccccc6C5)ccc4c3=O)s2)c1
vAce2-spike4-166	ZINC000009865194	-9.2	0.263	467.48	ZINC	C[C@@]1(c2cc3ccccc3o2)NC(=O)N(CC(=O)c2ccc(NC(=O)c3ccccc3)cc2)C1=O
vAce2-spike4-167	ZINC000013163846	-9.2	0.249	498.53	ZINC	O=C(Nc1ccc2c(c1)OCO2)C1CCN(C(=O)c2ccc3c(c2)C[C@@H](c2ccccc2)OC3=O)CC1
vAce2-spike4-168	ZINC000013370522	-9.2	0.271	451.46	ZINC	O=C(Nc1cccc(-c2nc3ccccc3o2)c1)c1ccc(NC(=O)c2ccccc2F)cc1
vAce2-spike4-169	ZINC000013564757	-9.2	0.279	459.57	ZINC	O=C(N1CCC(Nc2nc3c(c(=O)[nH]2)CCC3)CC1)N1c2ccccc2Sc2ccccc21
vAce2-spike4-170	ZINC000013653657	-9.2	0.297	415.45	ZINC	Cc1ccc2c(=O)cc(C(=O)Nc3nonc3-c3ccc4c(c3)CCCC4)oc2c1C
vAce2-spike4-171	ZINC000014728806	-9.2	0.297	433.51	ZINC	O=C(Cc1csc(-c2cccc(F)c2)n1)Nc1nc2ccccc2nc1N1CCCC1
vAce2-spike4-172	ZINC000016525737	-9.2	0.279	453.48	ZINC	O=C(Nc1nc2ccc(NC(=O)c3cc4ccccc4o3)cc2s1)c1cc2ccccc2o1
vAce2-spike4-173	ZINC000017988176	-9.2	0.230	521.57	ZINC	O=C(Oc1ccc2ccccc2c1)c1cccc(N2C(=O)[C@H]3[C@@H](C2=O)C2c4ccccc4C3c3ccccc32)c1
vAce2-spike4-174	ZINC000021663879	-9.2	0.271	478.62	ZINC	O=C([C@H]1CCCN(c2nn3c(nc4c(c3=O)CCCC4)s2)C1)N1CCN(c2ccccc2)CC1
vAce2-spike4-175	ZINC000021867469	-9.2	0.256	486.48	ZINC	O=C(c1ccc2c(O)nc3c(-c4cccc(F)c4)nnn3c2c1)N1CCN(c2ccc(F)cc2)CC1
vAce2-spike4-176	ZINC000027794956	-9.2	0.297	435.87	ZINC	Cc1cc2oc(C(=O)Nc3nonc3-c3ccc4c(c3)CCCC4)cc(=O)c2cc1Cl
vAce2-spike4-177	ZINC000033254412	-9.2	0.263	493.99	ZINC	Cc1nc(-c2ccc(C(=O)N3CCC(C(=O)N4CCN(c5cccc(Cl)c5)CC4)CC3)cc2)no1
vAce2-spike4-178	ZINC000033266725	-9.2	0.287	429.50	ZINC	Cc1cccc(NC(=O)C2CCN(c3ncn4nc(-c5ccc(F)cc5)cc34)CC2)c1
vAce2-spike4-179	ZINC000033324788	-9.2	0.279	439.52	ZINC	Cc1ccc(-c2nc3n(n2)c(=O)c2c(n3CC(=O)N3CCc4ccccc4C3)CCC2)cc1
vAce2-spike4-180	ZINC000034837496	-9.2	0.256	485.52	ZINC	O=C(NCc1ccc2c(c1)OCO2)c1nnc(N2CCN(c3ccccc3F)CC2)c2ccccc21
vAce2-spike4-181	ZINC000037246226	-9.2	0.263	465.59	ZINC	O=C1c2ccccc2C(=O)c2cc3c(cc21)N[C@@H]1CC[C@@H]2[C@@H]4CCCC[C@@H]4C(=O)[C@H]4CC[C@H]3[C@H]1[C@H]24
vAce2-spike4-182	ZINC000040155218	-9.2	0.279	440.48	ZINC	Cc1noc2nc(-c3ccccc3F)cc(C(=O)N3CCc4c5ccccc5[nH]c4[C@H]3C)c12
vAce2-spike4-183	ZINC000047892326	-9.2	0.271	472.53	ZINC	O=C(CN1C(=O)N[C@]2(CCCc3ccccc32)C1=O)Nc1nn2cc(-c3ccccc3)nc2s1
vAce2-spike4-184	ZINC000048985193	-9.2	0.279	437.51	ZINC	Cc1nn(-c2ccc(Nc3ccc(NC(=O)c4c[nH]c5ccccc45)cc3)nn2)c(C)c1C
vAce2-spike4-185	ZINC000049967677	-9.2	0.256	484.47	ZINC	Cc1cc(=O)oc2cc(NC(=O)c3cc(C(=O)Nc4ccc5c(C)cc(=O)oc5c4)n(C)n3)ccc12
vAce2-spike4-186	ZINC000067261402	-9.2	0.307	421.84	ZINC	Fc1ccc(-c2nnn3c2nc(NCc2ccc(F)cc2Cl)c2ccccc23)cc1
vAce2-spike4-187	ZINC000067261404	-9.2	0.287	437.40	ZINC	Fc1ccc(-c2nnn3c2nc(NCc2cccc(C(F)(F)F)c2)c2ccccc23)cc1
vAce2-spike4-188	ZINC000067262664	-9.2	0.317	390.42	ZINC	NC(=O)C1CCN(c2nc3c(-c4ccc(F)cc4)nnn3c3ccccc32)CC1
vAce2-spike4-189	ZINC000072312266	-9.2	0.307	401.47	ZINC	C[C@]1(C2CCN(c3nc(-c4cccc4)nc4ccccc43)CC2)NC(=O)NC1=O
vAce2-spike4-190	ZINC000096344127	-9.2	0.279	447.49	ZINC	O=C([C@@H]1CC(=O)N(c2n[nH]c3ccccc32)C1)N1CCN(Cc2ccc3c(e2)OCO3)CC1
vAce2-spike4-191	ZINC000169684223	-9.2	0.249	487.51	ZINC	Cc1cccc([C@@H]2OC3(C(=O)c4ccccc4C3=O)[C@H]3C(=O)N(c4cccc5ccccc54)C(=O)[C@@H]23)c1
vAce2-spike4-192	ZINC000225481762	-9.2	0.271	491.60	ZINC	CCn1c2ccccc2c2cc(NS(=O)(=O)c3nnc(NC(=O)c4cccc(C)c4)s3)ccc21
vAce2-spike4-193	ZINC000225801637	-9.2	0.271	498.63	ZINC	Cc1ccccc1C(=O)Nc1nnc(S(=O)(=O)N[C@@H]2CC3(CCCCC3)Oc3ccccc32)s1
vAce2-spike4-194	ZINC000239439294	-9.2	0.249	487.51	ZINC	Cc1ccc(N2C(=O)[C@@H]3[C@H](c4cccc5ccccc54)OC4(C(=O)c5ccccc5C4=O)[C@H]3C2=O)cc1
vAce2-spike4-195	ZINC000247710661	-9.2	0.249	486.53	ZINC	O=C(Nc1ccccc1)[C@@H]1[C@@H]2C(=O)N(c3cccc4ccccc43)C(=O)[C@H]2[C@@H]2c3ccccc3C=NN21
vAce2-spike4-196	ZINC000253399265	-9.2	0.249	496.45	ZINC	O=C(O)c1ccccc1-c1ccc([C@@H]2CC(=O)Oc3cce4c(=O)c(-c5ccc(F)cc5)coc4c32)o1
vAce2-spike4-197	ZINC000257197297	-9.2	0.307	396.49	ZINC	O=C(c1ccc2ncccc2c1)N1CCC2(CC1)NCCc1c3ccccc3[nH]c12
vAce2-spike4-198	ZINC000257356626	-9.2	0.307	402.58	ZINC	O=C1C[C@@H]([C@@H]2C(=O)C[C@@H]3C[C@]45C=CC[C@@H]4CC[C@@H]5[C@@H]32)[C@H]2C[C@]34C=CC[C@@H]3CC[C@H]4[C@H]12
vAce2-spike4-199	ZINC000408679806	-9.2	0.242	498.58	ZINC	Cc1cc(C)cc(NC(=O)c2cccc(N3C(=O)[C@@H]4[C@@H](C3=O)C3c5ccccc5C4c4ccccc43)c2)c1
vAce2-spike4-200	ZINC000408733453	-9.2	0.249	485.54	ZINC	Cc1ccc2c(c1)OC(=O)[C@@H]1C2=C[C@H](c2ccccc2)[C@H]2C(=O)N(c3cccc4ccccc43)C(=O)[C@@H]21

Supplementary Table 16. Virtual hits 101-200 of the screen against ACE2 at a site adjacent to the Spike interaction interface (Screen ID: 4). The name of each compound consists of the initial letter 'v' for virtual hit, followed by the target protein name and the target site ('spike' for spike interaction site, 4 for docking scenario 4). The score is the docking score given by QuickVina 2 in kcal/mol. The ligand efficiency (LE) is computed as LE = -score/#NonH, where #NonH is the number of heavy (i.e. non hydrogen) atoms.

Name	Catalog ID	Score	LE	MW	Library	SMILES
vAce2-spike5-1	ZINC000001588361	-10.2	0.3	440.509	ZINC	Nc1nc(-c2cc(-c3cccc4ccccc43)nc(N)n2)cc(-c2cccc3ccccc32)n1
vAce2-spike5-2	ZINC000002896234	-10.2	0.283	472.499	ZINC	Cc1ccccc1-c1nc2ccc(-c3ccc4nc(-c5ccccc5C)oc(=O)c4c3)cc2c(=O)o1
vAce2-spike5-3	ZINC000013661067	-10.2	0.309	434.494	ZINC	Cc1ccc([C@H]2[C@H]3C(=O)N(c4ccc5ccccc54)C(=O)[C@H]3ON2c2ccccc2)cc1
vAce2-spike5-4	ZINC000033433929	-10.2	0.283	476.554	ZINC	Cc1ccc(C2=N/C(=C\c3cn(C)c4ccccc34)C(=O)N2CCc2c[nH]c3cc(F)ccc23)cc1
vAce2-spike5-5	ZINC000100961974	-10.2	0.309	434.494	ZINC	Cc1ccc([C@H]2[C@@H]3C(=O)N(c4ccc5ccccc54)C(=O)[C@H]3ON2c2ccccc2)cc1
vAce2-spike5-6	PV-001872272336	-10.1	0.316	437.542	REAL	Cc1cc(C)cc(C(=O)N2CCC[C@H](C(=O)N3CCN(c4nc(C)cc(=O)[nH]4)CC3)C2)c1
vAce2-spike5-7	Z1420416669	-10.1	0.326	433.487	REAL	O=c1[nH]c(=O)c2cc(S(=O)(=O)N3CCCc4cc(-c5ccccc5)ccc43)ccc2[nH]1
vAce2-spike5-8	Z2072789500	-10.1	0.337	394.473	REAL	Cn1c(C(=O)N2CCCc3cc(-c4ccccc4)ccc32)cc2ccccc2c1=O
vAce2-spike5-9	ZINC000021867174	-10.1	0.273	492.581	ZINC	Cc1cccc(-c2nnn3c2nc(O)c2ccc(C(=O)N4CCN(c5cc(C)ccc5C)CC4)cc23)c1
vAce2-spike5-10	ZINC000039742926	-10.1	0.306	434.454	ZINC	O=C(Nc1nnc(-c2ccccc2)o1)c1cccc(NC(=O)c2cccc3ccccc32)c1
vAce2-spike5-11	Z1334275055	-10	0.333	404.429	REAL	O=C(Nc1ccc2[nH]c(C3CCCCC3)nc2c1)c1cnc2[nH]c(=O)[nH]c(=O)c2c1
vAce2-spike5-12	Z1557588975	-10	0.345	385.47	REAL	Cc1[nH]c2ccccc2c1C1=CCN(C(=O)Nc2cc(C)c3cn[nH]c3c2)CC1
vAce2-spike5-13	Z1744195451	-10	0.313	419.483	REAL	O=C(c1cc(-c2ccccc2)nc2ccccc12)N1CC[C@]2(C1)C(=O)Nc1ccccc12
vAce2-spike5-14	Z1887042759	-10	0.333	411.426	REAL	O=C([C@H]1CCc2[nH]nc(C(F)(F)F)c2C1)N1C[C@@H](c2ccccc2)c2ccccc21
vAce2-spike5-15	ZINC000002933672	-10	0.278	513.335	ZINC	O=c1oc(-c2ccccc2Cl)nc2ccc(-c3ccc4nc(-c5ccccc5Cl)oc(=O)c4c3)cc21
vAce2-spike5-16	ZINC000003671068	-10	0.286	459.5	ZINC	O=C(O)[C@H]1C2c3ccccc3C(c3ccccc32)[C@@H]1C(=O)Nc1ccc2c(c1)oc1ccccc12
vAce2-spike5-17	ZINC000006610219	-10	0.323	401.468	ZINC	O=c1[nH]c(-c2cn(Cc3cccc4ccccc43)c3ccccc23)nc2ccccc12
vAce2-spike5-18	ZINC000009062176	-10	0.303	450.521	ZINC	O=C(Nc1nnc(-c2ccccc2)s1)c1cccc(NC(=O)c2cccc3ccccc32)c1
vAce2-spike5-19	PV-001801324572	-9.9	0.319	422.542	REAL	Cc1cc(C)cc(C(=O)N2CCC[C@H](C(=O)N3[C@H](C)Cc4cc(F)ccc4[C@@H]3C)C2)c1
vAce2-spike5-20	PV-001876884527	-9.9	0.309	436.554	REAL	Cc1cc(C)cc(C(=O)N2CCC[C@@H](C(=O)N[C@H]3CC[C@H](c4nccc(O)n4)CC3)C2)c1
vAce2-spike5-21	Z1276023341	-9.9	0.33	402.399	REAL	O=C(c1cc(=O)[nH]c2ccc(F)cc12)N1CCc2cc(-c3cccc(F)c3)ccc21
vAce2-spike5-22	Z1419338114	-9.9	0.33	416.5	REAL	O=c1ccc2cc(S(=O)(=O)N3CCCc4cc(-c5ccccc5)ccc43)ccc2[nH]1
vAce2-spike5-23	Z1420928818	-9.9	0.33	396.489	REAL	CC(=O)N1CCc2cc(C(=O)N3CCCc4cc(-c5ccccc5)ccc43)ccc21
vAce2-spike5-24	Z1626784209	-9.9	0.309	424.507	REAL	O=C(C1CCN(c2ccc3nncn3n2)CC1)N1CC=C(c2cccc3ccccc23)C1
vAce2-spike5-25	Z2008630353	-9.9	0.309	426.526	REAL	Cn1c(-c2ccc(-n3cnnn3)cc2)nnc1N1CCC[C@@]2(CCCc3ccccc32)C1
vAce2-spike5-26	Z770368506	-9.9	0.3	454.613	REAL	Cc1cccc(NC(=O)N2CCC[C@H](C(=O)N3CCC(C(=O)N4CCC[C@H](C)C4)CC3)C2)c1
vAce2-spike5-27	Z773166186	-9.9	0.3	454.613	REAL	Cc1cccc(NC(=O)N2CCC[C@H](C(=O)N3CCC(C(=O)N4CCC(C)CC4)CC3)C2)c1
vAce2-spike5-28	Z998654188	-9.9	0.291	465.596	REAL	C[C@H]1CCCN(C(=O)C2CCN(C(=O)[C@H]3CCCN(C(=O)c4ccc5[nH]ncc5c4)C3)CC2)C1
vAce2-spike5-29	ZINC000001588362	-9.9	0.291	440.509	ZINC	Nc1nc(-c2ccc3ccccc3c2)cc(-c2cc(-c3ccc4ccccc4c3)nc(N)n2)n1
vAce2-spike5-30	ZINC000001588368	-9.9	0.291	446.517	ZINC	Cc1[nH]c2ccccc2c1-c1cc(-c2cc(-c3c(C)[nH]c4ccccc43)nc(N)n2)nc(N)n1
vAce2-spike5-31	ZINC000004728718	-9.9	0.319	399.448	ZINC	O=C1c2ccccc2C(=O)N1c1ccc2c(c1)C1c3ccccc3C2c2ccccc21
vAce2-spike5-32	ZINC000008771513	-9.9	0.283	458.563	ZINC	Cc1ccc(C2=N/C(=C\c3cn(C)c4ccccc34)C(=O)N2CCc2c[nH]c3ccccc23)cc1
vAce2-spike5-33	ZINC000013629718	-9.9	0.3	441.413	ZINC	O=C1OC(c2ccccc2F)=N/C1=C1/C=C(c2ccc3c(c2)OCCO3)Oc2ccccc21
vAce2-spike5-34	ZINC000257325672	-9.9	0.3	442.493	ZINC	Cc1cc(-c2ccc(F)cc2)cc([C@H]2CCCN(C(=O)c3n[nH]c(=O)c4ccccc43)C2)n1
vAce2-spike5-35	Z1069479288	-9.8	0.316	418.491	REAL	C[C@H]1Oc2ccc(C(=O)C3CCN(C(=O)c4cccc5c4CCC5)CC3)ccc2NC1=O
vAce2-spike5-36	Z1069479908	-9.8	0.306	432.479	REAL	Cc1cc(C(=O)N2CCC(C(=O)c3ccc4c(c3)NC(=O)[C@@H](C)O4)CC2)c2n[nH]cc2c1
vAce2-spike5-37	Z1245954502	-9.8	0.306	429.41	REAL	O=C(Nc1cccc(Cn2nc3ccccn3c2=O)c1)c1cc(=O)[nH]c2cc(F)ccc12
vAce2-spike5-38	Z1248573568	-9.8	0.338	379.422	REAL	Cc1nnc(-c2cccc(-c3nc4ccc(-c5ccccc5)cc4c(=O)[nH]3)c2)[nH]1
vAce2-spike5-39	Z1276025054	-9.8	0.363	357.387	REAL	O=C(c1cccc2[nH]ncc12)N1CCc2cc(-c3cccc(F)c3)ccc21
vAce2-spike5-40	Z1348016768	-9.8	0.316	411.504	REAL	C[C@@H]1C(=O)Nc2cc(C(=O)N3CC=C(c4cccc5ccccc45)CC3)ccc2N1C
vAce2-spike5-41	Z1443313670	-9.8	0.35	368.439	REAL	Cc1cc(C(=O)N2CCc3cc(-c4ccccc4)ccc32)c2c(C)n[nH]c2n1
vAce2-spike5-42	Z1546665942	-9.8	0.316	424.471	REAL	Cc1cc(C(=O)N2CCC(C(=O)c3ccc4c(c3)NC(=O)[C@@H](C)O4)CC2)cc(C)c1F
vAce2-spike5-43	Z1720528731	-9.8	0.327	401.436	REAL	O=C(c1ccc(F)cc1)c1cccc1C(=O)N1CC[C@@]2(C1)OCc1ccccc12
vAce2-spike5-44	Z1724785157	-9.8	0.306	428.455	REAL	O=c1cc2c(n[nH]1)CCN(c1nc(N3CCc4n[nH]c(=O)cc4C3)c3ccccc3n1)C2
vAce2-spike5-45	Z1739733200	-9.8	0.306	420.431	REAL	Cn1c(=O)[nH]c2ncc(-c3cccc(-c4nc(-c5cccc6ncccc56)no4)c3)cc21
vAce2-spike5-46	Z1744514456	-9.8	0.306	420.471	REAL	O=C(c1cc(-c2cccnc2)nc2ccccc12)N1CC[C@]2(C1)C(=O)Nc1ccccc12
vAce2-spike5-47	Z1784008149	-9.8	0.363	358.375	REAL	O=C(c1cccc2nn[nH]c12)N1CCc2cc(-c3cccc(F)c3)ccc21
vAce2-spike5-48	Z1941081203	-9.8	0.338	390.481	REAL	Cc1ccc2c(c1)[C@H]1CN(C)CC[C@@H]1N2C(=O)[C@]1(C)Cc2ccccc2C(=O)O1
vAce2-spike5-49	Z2160288780	-9.8	0.316	409.448	REAL	Cc1ccccc1-n1nc(-c2nc(-c3cc(=O)[nH]c4ccccc34)no2)c2c1CCC2
vAce2-spike5-50	Z226359370	-9.8	0.338	390.481	REAL	Cc1ccc2c(c1)[C@@H]1CN(C)CC[C@@H]1N2C(=O)[C@]1(C)Cc2ccccc2C(=O)O1
vAce2-spike5-51	Z263069322	-9.8	0.265	497.593	REAL	C[C@H](OC(=O)c1c2c(nc3ccccc13)/C(=C/c1ccccc1)CCC2)C(=O)N1CCC[C@@H](C(N)=O)C1
vAce2-spike5-52	Z822271430	-9.8	0.306	422.487	REAL	O=C(c1ccc2c(c1)-c1ccccc1C2)N1CCN(C(=O)c2ccc3[nH]cnc3c2)CC1
vAce2-spike5-53	Z999014250	-9.8	0.297	449.513	REAL	COc1ccnc(N2CCN(C(=O)[C@H]3CCCN(C(=O)c4ccc5[nH]ncc5c4)C3)CC2)n1
vAce2-spike5-54	ZINC000000653912	-9.8	0.306	485.434	ZINC	Cc1cccc([C@@H]2Nc3ccc(S(=O)(=O)Nc4cc(Cl)ccc4Cl)cc3[C@@H]3C=CC[C@H]32)c1
vAce2-spike5-55	ZINC000002755716	-9.8	0.297	456.51	ZINC	C[C@@H]1CC[C@@H]2[C@@H]([CC[C@H](C)N2C(=O)c2cc3nc(-c4ccccc4)cc(C(F)(F)F)n3n2)C1
vAce2-spike5-56	ZINC000002859412	-9.8	0.272	472.499	ZINC	Cc1ccc(-c2nc3ccccc3o2)cc1NC(=O)c1cccc(-c2cc3ccccc3oc2=O)c1
vAce2-spike5-57	ZINC000002865873	-9.8	0.251	515.52	ZINC	COc1ccc(-c2cc3ccccc3oc2=O)cc1NC(=O)c1cccc(-c2cc3ccccc3oc2=O)c1
vAce2-spike5-58	ZINC000002935991	-9.8	0.272	480.425	ZINC	O=c1oc(-c2cccc(F)c2)nc2ccc(-c3ccc4nc(-c5cccc(F)c5)oc(=O)c4c3)cc21
vAce2-spike5-59	ZINC000004175991	-9.8	0.316	398.464	ZINC	O=C1[C@@H]2[C@@H](c3nc4cccc5cccc(c54)n31)C1c3ccccc3C2c2ccccc21
vAce2-spike5-60	ZINC000004503052	-9.8	0.338	375.426	ZINC	O=C(Nc1ccc2c(c1)oc1ccccc12)C1c2ccccc2-c2ccccc21
vAce2-spike5-61	ZINC000005955032	-9.8	0.272	495.929	ZINC	O=C1NC2=NN3C(=O)C(/C=C\c4ccc(Cl)cc4)=NN[C@@H]3N2NC12c1ccccc1-c1ccccc12
vAce2-spike5-62	ZINC000008912515	-9.8	0.306	430.55	ZINC	Cc1ccc(C)c(N2CCN(C(=O)c3ccc4c(c3)nc3n(c4=O)CCCCC3)CC2)c1
vAce2-spike5-63	ZINC000013477069	-9.8	0.265	484.554	ZINC	CC(=O)Nc1ccc(-c2ccc(N3C(=O)[C@H]4[C@@H](C3=O)C3c5ccccc5C4c4ccccc43)cc2)cc1
vAce2-spike5-64	ZINC000019878192	-9.8	0.288	454.387	ZINC	O=c1c2cc3cc4e(cc3cc2c(=O)n1-c1cccc(F)c1)c(=O)n(-c1cccc(F)c1)c4=O
vAce2-spike5-65	ZINC000020634876	-9.8	0.316	409.492	ZINC	Cc1cccc([C@H]2CC(=O)c3c(C)nc(Nc4nc(C)c5ccccc5n4)nc3C2)c1
vAce2-spike5-66	ZINC000043769601	-9.8	0.306	444.597	ZINC	Cc1cccc([C@@H]2Nc3ccc(S(=O)(=O)Nc4cc(C)ccc4C)cc3[C@@H]3C=CC[C@H]32)c1
vAce2-spike5-67	ZINC000046056854	-9.8	0.297	441.573	ZINC	Cc1nn(-c2ccc(C)c(C)c2)c2c1[C@@H](C(=O)c1ccc(C3CCCC3)cc1)CC(=O)N2
vAce2-spike5-68	ZINC000065074788	-9.8	0.288	488.601	ZINC	O=S(=O)(c1ccc2c(c1)CCCC2)N1CCC2(CC1)NCCN=C2NCc1cc(F)cc(F)c1
vAce2-spike5-69	ZINC000072340943	-9.8	0.306	445.419	ZINC	Cc1cc2nc([C@H]3CCCN(C(=O)c4cc5ccc(F)c5[nH]4)C3)cc(C(F)(F)F)n2n1
vAce2-spike5-70	ZINC000072353608	-9.8	0.306	431.495	ZINC	Cc1cc(-c2cnc(N)nc2)cc([C@H]2CCCN(C(=O)c3ccc4c(c3)OCCO4)C2)n1
vAce2-spike5-71	ZINC000103904800	-9.8	0.327	392.457	ZINC	Cc1cc2c(cc1C)NC1=C(O)[C@@H](c3c4ccccc4cc4ccccc43)OC1=N2
vAce2-spike5-72	ZINC000198754475	-9.8	0.272	464.475	ZINC	O=C1c2ccccc2C(=O)C2=C3C=CC4=CC5=C(C(=O)c6ccccc6C5=O)C5=CC=C(C=C12)[C@@H]3[C@H]45
vAce2-spike5-73	ZINC000229966438	-9.8	0.28	470.567	ZINC	Cc1ccc(N2C(=O)C[C@@H]([C@H]3C=C(C)[C@H]4C(=O)N(c5ccc(C)c(C)c5)C(=O)[C@H]4C3)C2=O)cc1C
vAce2-spike5-74	ZINC000245380417	-9.8	0.28	470.567	ZINC	Cc1ccc(N2C(=O)C[C@@H]([C@H]3C=C(C)[C@@H]4C(=O)N(c5ccc(C)c(C)c5)C(=O)[C@H]4C3)C2=O)cc1C
vAce2-spike5-75	ZINC000257286381	-9.8	0.306	424.503	ZINC	Cc1cc(-c2ccccc2)cc([C@H]2CCCN(C(=O)c3n[nH]c(=O)c4ccccc43)C2)n1
vAce2-spike5-76	ZINC000409160388	-9.8	0.338	383.49	ZINC	COc1ccccc1[C@@H]2Nc3ccc(-c4ccccc4)cc3[C@@H]3C=CC[C@H]32)c1OC
vAce2-spike5-77	ZINC000409332220	-9.8	0.272	471.515	ZINC	N#C/C(=C\c1cn(CC(=O)Nc2ccc3c(c2)OCO3)c2ccccc12)c1ccccc2ccccc21
vAce2-spike5-78	PV-001802204803	-9.7	0.359	359.472	REAL	Cc1cc(C)cc(-n2nc(NC(=O)c3ccc(C)c4c3CCC4)cc2C)c1
vAce2-spike5-79	PV-001808974499	-9.7	0.334	395.343	REAL	O=C(Nc1cc(-c2nnn[nH]2)ccc1F)c1cccc(-c2c(F)cccc2F)c1
vAce2-spike5-80	PV-001822608693	-9.7	0.359	358.44	REAL	Cc1ccccc(-c2cccc(C(=O)N[C@@H]3CCCc4[nH]c(=O)ccc43)c2)c1
vAce2-spike5-81	PV-001847827967	-9.7	0.359	358.4	REAL	Cc1ccc2c(C(=O)Nc3cccc(-c4n[nH]c(=O)[nH]4)c3)c(C)ccc2c1
vAce2-spike5-82	PV-001850120660	-9.7	0.334	391.401	REAL	Cc1cc(C(=O)Nc2cccc(C3CC(=O)NC(=O)C3)c2)c2ccc(F)cc2n1
vAce2-spike5-83	PV-001852209655	-9.7	0.334	394.449	REAL	CNC(=O)Nc1cccc(C(=O)N2CCC(c3c[nH]c4ccc(F)cc34)CC2)c1
vAce2-spike5-84	PV-001868158927	-9.7	0.346	375.442	REAL	O=C(N[C@H]1c2ccccc2CC[C@@H]1F)c1cc(Cc2ccccc2)cc1O
vAce2-spike5-85	PV-001869165148	-9.7	0.346	372.387	REAL	Cc1nc(-c2ccccc2)ncc1C(=O)NNc1cc(O)nc2ncccc12
vAce2-spike5-86	PV-001952047195	-9.7	0.323	416.377	REAL	O=C(Nc1ccc(-c2cccc2F)nn1)N1CCc2c(cccc2C(F)(F)F)C1
vAce2-spike5-87	Z1224578717	-9.7	0.346	376.498	REAL	Cc1ccc2c(c1)[C@@H]1CN(C)CC[C@@H]1N2C(=O)C[C@@H]1CCOc2ccccc21
vAce2-spike5-88	Z1239173478	-9.7	0.303	429.41	REAL	O=C(Nc1cccc(Cn2nc3ccccn3c2=O)c1)c1cc(=O)[nH]c2ccc(F)cc12
vAce2-spike5-89	Z1313836952	-9.7	0.313	412.448	REAL	Cc1cc(C(=O)N2CC=C(c3cccc4ccccc34)CC2)nc2nc(O)[nH]c(=O)c12
vAce2-spike5-90	Z1439725110	-9.7	0.303	430.55	REAL	Cc1ccc(C)c(N2CCN(C(=O)c3ccc4c(=O)n5c(nc4c3)CCCCC5)CC2)c1
vAce2-spike5-91	Z1449831502	-9.7	0.313	411.508	REAL	O=C1Nc2ccccc2[C@@H]1C1CCN(c2nc(-c3cccnc3)nc3c2CCC3)CC1
vAce2-spike5-92	Z1466305736	-9.7	0.303	433.457	REAL	O=C(c1cncc(C(=O)N2CCc3ccc(F)cc3C2)c1)N1CCc2ccc(F)cc2C1
vAce2-spike5-93	Z1472869473	-9.7	0.303	422.487	REAL	O=C(Nc1cccc(C(=O)N[C@H]2[C@H]3CCc4ccccc4[C@@H]32)c1)c1ccc2[nH]cnc2c1
vAce2-spike5-94	Z1494941980	-9.7	0.303	429.518	REAL	COc1ccc(C(=O)N2CCC[C@@H](C(=O)N3CCc4nccc4C3)C2)c2ccccc12
vAce2-spike5-95	Z1529176911	-9.7	0.323	396.489	REAL	CN1C(=O)CCc2cc(C(=O)N3CCCc4cc(-c5ccccc5)ccc43)ccc21
vAce2-spike5-96	Z1656881171	-9.7	0.323	399.453	REAL	O=C(Nc1ccc(-n2ncc3ccccc32)cc1)N[C@@H]1CCCc2[nH]c(=O)ccc21
vAce2-spike5-97	Z1684735758	-9.7	0.323	397.412	REAL	Fc1ccc(-n2nc(-c3nc(-c4ccc5cncc45)no3)c3c2CCC3)cc1
vAce2-spike5-98	Z1684738963	-9.7	0.323	397.412	REAL	Fc1ccccc1-n1nc(-c2nc(-c3ccc4cnccc34)no2)c2c1CCC2
vAce2-spike5-99	Z1688216974	-9.7	0.313	417.507	REAL	C[C@@H]1CCCCN1c1ccc2c(c1)CCCN2C(=O)c1ccc2c(c1)C(=O)N(C)C2=O
vAce2-spike5-100	Z169619690	-9.7	0.313	414.479	REAL	O=C(Nc1ccc2c(c1)Cc1ccccc1-2)[C@@H]1CCCN(C(=O)c2ccc(F)cc2)C1

Supplementary Table 17. Top 100 virtual hits of the screen against ACE2 at a site adjacent to the Spike interaction interface (Screen ID: 5). Compounds were filtered so that hits had MW < 600 dalton, cLogP < 6, number of hydrogen bond acceptors < 11, and no reactive functional groups. The name of each compound consists of the initial letter 'v' for virtual hit, followed by the target protein name and the target site ('spike' for spike interaction site, 5 for docking scenario 5). The score is the docking score given by QuickVina 2 in kcal/mol. The ligand efficiency (LE) is computed as LE = -score/#NonH, where #NonH is the number of heavy (i.e. non hydrogen) atoms.

Name	Catalog ID	Score	LE	MW	Library	SMILES
vAce2-spike5-101	Z1744511504	-9.7	0.303	420.47	REAL	O=C(c1cc(-c2ccncc2)nc2ccccc12)N1CC[C@]2(C1)C(=O)Nc1ccccc12
vAce2-spike5-102	Z1748297916	-9.7	0.303	420.47	REAL	O=C(c1cc(-c2ccccn2)nc2ccccc12)N1CC[C@]2(C1)C(=O)Nc1ccccc12
vAce2-spike5-103	Z1833691044	-9.7	0.303	430.50	REAL	C[C@H]1CN(C(=O)[C@@H]2CC(=O)c3ccccc32)[C@H](C)CN1C(=O)[C@H]1CC(=O)c2ccccc21
vAce2-spike5-104	Z1834345526	-9.7	0.313	414.40	REAL	O=C(Nc1cccc(C(=O)Nc2n[nH]c3cc(F)ccc23)c1)c1ccc2[nH]cnc2c1
vAce2-spike5-105	Z1864436399	-9.7	0.323	398.44	REAL	Cn1cc(C(=O)N2CCc3cc(-c4cccc(F)c4)ccc32)c2ccccc2c1=O
vAce2-spike5-106	Z1927950648	-9.7	0.294	445.52	REAL	COc1ccc(C(=O)N2CCC[C@@H](C(=O)N3CCc4nc(N)ncc4C3)C2)c2ccccc12
vAce2-spike5-107	Z1941074391	-9.7	0.346	376.50	REAL	Cc1ccc2c(c1)[C@@H]1CN(C)CC[C@@H]1N2C(=O)C[C@@H]1CCOc2ccccc21
vAce2-spike5-108	Z1941079505	-9.7	0.346	376.46	REAL	Cc1ccc2c(c1)[C@@H]1CN(C)CC[C@@H]1N2C(=O)C[C@@H]1OC(=O)c2ccccc21
vAce2-spike5-109	Z1972443566	-9.7	0.334	385.39	REAL	O=C(c1cc2ccccc2c(=O)o1)N1CCc2cc(-c3cccc(F)c3)ccc21
vAce2-spike5-110	Z1988035038	-9.7	0.303	438.57	REAL	C[C@H]1CC[C@H](O)[C@H]([C@H]2CCCN2C(=O)[C@H]2CCCN(C(=O)c3ccc4[nH]ncc4c3)C2)C1
vAce2-spike5-111	Z2003353290	-9.7	0.359	358.38	REAL	O=C(c1cc(F)ccc2[nH]nnc12)N1CCc2cc(-c3ccccc3)ccc21
vAce2-spike5-112	Z2041558328	-9.7	0.303	420.43	REAL	Cn1c(=O)[nH]c2ncc(-c3cccc(-c4nc(-c5cccc6ncccc56)no4)c3)cc21
vAce2-spike5-113	Z2071945217	-9.7	0.323	398.44	REAL	Cn1c(C(=O)N2CCc3cc(-c4cccc(F)c4)ccc32)cc2ccccc2c1=O
vAce2-spike5-114	Z2089212994	-9.7	0.313	416.53	REAL	O=C(C1CCN(c2ccc3nncn3n2)CC1)N1C[C@@H](c2ccccc2)[C@@H]2CCC[C@H]21
vAce2-spike5-115	Z2089239784	-9.7	0.359	361.44	REAL	O=C1O[C@@H](CC(=O)N2C[C@@H](c3ccccc3)[C@@H]3CCC[C@H]32)c2ccccc21
vAce2-spike5-116	Z2128561236	-9.7	0.313	418.50	REAL	O=C1NC(=O)C2(CCC(NC(=O)N3CC=C(c4cccc5ccccc45)CC3)CC2)N1
vAce2-spike5-117	Z2160279449	-9.7	0.313	409.45	REAL	Cc1ccc(-n2nc(-c3nc(-c4cc(=O)[nH]c5ccccc45)no3)c3c2CCC3)cc1
vAce2-spike5-118	Z2160283676	-9.7	0.313	413.41	REAL	O=c1cc(-c2noc(-c3nn(-c4ccc(F)cc4)c4c3CCC4)n2)c2ccccc2[nH]1
vAce2-spike5-119	Z2160285388	-9.7	0.313	413.41	REAL	O=c1cc(-c2noc(-c3nn(-c4ccccc4F)c4c3CCC4)n2)c2ccccc2[nH]1
vAce2-spike5-120	Z2178346573	-9.7	0.334	391.45	REAL	Cc1cc(F)c2nc(O)cc(C(=O)N3CCCN4c5ccccc5C[C@@H]4C3)c2c1
vAce2-spike5-121	Z2193902273	-9.7	0.313	409.40	REAL	O=C1O[C@H](c2ccccc2)Cc2cc(-c3nc(-c4ccc5[nH]nnc5c4)no3)ccc21
vAce2-spike5-122	Z2299756832	-9.7	0.359	380.84	REAL	O=C(c1ccc2[nH]nnc2c1)N1CCCC[C@@H]1c1nc2cc(Cl)ccc2[nH]1
vAce2-spike5-123	Z273919126	-9.7	0.269	478.51	REAL	Cc1ccc(C)c(N2C(=O)c3ccc(C(=O)Nc4ccc5nc6n(c(=O)c5c4)CCC6)cc3C2=O)c1
vAce2-spike5-124	Z2789939496	-9.7	0.346	382.37	REAL	O=C1C[C@]2(CCCc3ccccc32)C(=O)NN1c1nc2cc(F)c(F)cc2[nH]1
vAce2-spike5-125	Z2913275989	-9.7	0.346	375.47	REAL	O=C(c1ccc2[nH]c(CO)nc2c1)N1CCC2(CCc3ccccc3C2)CC1
vAce2-spike5-126	Z829081616	-9.7	0.313	416.37	REAL	O=C(Nc1ccc2[nH]c(-c3cccc(F)c3)nc2c1)c1cnc2[nH]c(=O)[nH]c(=O)c2c1
vAce2-spike5-127	Z998902016	-9.7	0.285	465.60	REAL	CC1CCN(C(=O)C2CCN(C(=O)[C@H]3CCCN(C(=O)c4ccc5[nH]ncc5c4)C3)CC2)CC1
vAce2-spike5-128	ZINC000002260525	-9.7	0.346	370.49	ZINC	CC1(C)C[C@@](C)(c2ccccc2)c2ccccc2N1C(=O)Nc1ccccc1
vAce2-spike5-129	ZINC000002915254	-9.7	0.303	426.45	ZINC	COc1cccc([C@H]2C3=C(N=C4N=CNN42)c2ccccc2O[C@H]3c2cccc(F)c2)c1
vAce2-spike5-130	ZINC000005607051	-9.7	0.269	470.44	ZINC	Nc1c(-c2nc3cc4c(cc3o2)C(=O)c2ccccc2C4=O)ccc2c1C(=O)c1ccccc1C2=O
vAce2-spike5-131	ZINC000007096974	-9.7	0.346	367.45	ZINC	O=C(O)c1ccccc1[C@@H]1Nc2ccc(-c3ccccc3)cc2[C@@H]2C=CC[C@H]21
vAce2-spike5-132	ZINC000008826511	-9.7	0.285	441.49	ZINC	O=C1[C@@H]2[C@@H](C(=O)N1c1ccc3c(c1)oc1ccccc13)C1c3ccccc3C2c2ccccc21
vAce2-spike5-133	ZINC000008995230	-9.7	0.303	443.84	ZINC	O=C1OC(c2ccc(Cl)cc2)=N/C1=C1/C=C(c2ccc3c(c2)OCO3)Oc2ccccc21
vAce2-spike5-134	ZINC000009340277	-9.7	0.294	441.41	ZINC	O=C1OC(c2ccc(F)cc2)=N/C1=C1/C=C(c2ccc3c(c2)OCCO3)Oc2ccccc21
vAce2-spike5-135	ZINC000009619640	-9.7	0.262	494.55	ZINC	O=C(Nc1ccc2c(c1)OCO2)C1CCN(C(=O)c2cc(-c3ccccc3)nn2-c2ccccc2)CC1
vAce2-spike5-136	ZINC000009647851	-9.7	0.285	478.57	ZINC	O=C(N[C@@H]1CCCc2ccccc21)c1ccnc(NS(=O)(=O)c2ccc3c(c2)OCCO3)c1
vAce2-spike5-137	ZINC000011852849	-9.7	0.294	445.55	ZINC	Cn1c2ccc3ccccc3c2s/c1=N/C(=O)c1cc(-c2ccccc2)nc2ccccc21
vAce2-spike5-138	ZINC000012528008	-9.7	0.269	479.54	ZINC	O=C(c1ccc2c(c1)OCCO2)C1CCN(C(=O)c2cc(-c3ccnc3)nc3ccccc32)CC1
vAce2-spike5-139	ZINC000014114786	-9.7	0.277	467.52	ZINC	O=C(c1ccc2c(c1)C[C@@H](c1ccccc1)OC2=O)N1CCC(n2c(=O)[nH]c3ccccc32)CC1
vAce2-spike5-140	ZINC000015931255	-9.7	0.294	456.51	ZINC	C[C@@H]1CC[C@@H]2[C@@H](CC[C@@H](C)N2C(=O)c2cc3nc(-c4ccccc4)cc(C(F)(F)F)n3n2)C1
vAce2-spike5-141	ZINC000015990071	-9.7	0.243	527.63	ZINC	Cc1cccc(Nc2nnc(-c3ccc(C(=O)N4C[C@H]5C[C@@H](C4)c4ccccc4)n4C5)cc3)c3ccccc32)c1
vAce2-spike5-142	ZINC000016526081	-9.7	0.323	390.39	ZINC	O=c1oc2ccc3ccccc3c2cc1-c1cc2c(ccc3ccccc32)oc1=O
vAce2-spike5-143	ZINC000019585662	-9.7	0.294	445.48	ZINC	CN(C)c1ncc2c(cc([C@H]3CCCN(C(=O)c4n[nH]c(=O)c5ccccc54)C3)[nH]c2=O)n1
vAce2-spike5-144	ZINC000020440415	-9.7	0.262	490.57	ZINC	O=C(c1cccc1)N1CCC[C@H](c2nc(=O)c3nnn(Cc4ccc(-c5ccccc5)cc4)c3[nH]2)C1
vAce2-spike5-145	ZINC000033010640	-9.7	0.303	420.52	ZINC	O=C(N[C@@H]1CCCc2ccccc21)c1cccc(Nc2cc(-c3ccccc3)ncn2)c1
vAce2-spike5-146	ZINC000033876541	-9.7	0.303	485.43	ZINC	Cc1cc(Cl)ccc1NS(=O)(=O)c1ccc2c(c1)[C@@H]1C=CC[C@H]1[C@H](c1cccc(Cl)c1)N2
vAce2-spike5-147	ZINC000035110890	-9.7	0.303	448.56	ZINC	Cc1ccc(NS(=O)(=O)c2ccc3c(c2)[C@@H]2C=CC[C@H]2[C@H](c2ccccc2F)N3)c(C)c1
vAce2-spike5-148	ZINC000046057326	-9.7	0.294	441.57	ZINC	Cc1nn(-c2cccc(C)c2C)c2c1[C@@H](C(=O)c1ccc(C3CCCC3)cc1)CC(=O)N2
vAce2-spike5-149	ZINC000048272370	-9.7	0.285	458.51	ZINC	O=C(N1CC=C(c2c[nH]c3cc(F)ccc32)CC1)N1CC=C(c2c[nH]c3cc(F)ccc32)CC1
vAce2-spike5-150	ZINC000064605434	-9.7	0.277	465.55	ZINC	Cc1ccc(CNC(=O)Cn2c(=O)cc(C(=O)N3CCc4ccccc4C3)c3ccccc32)cc1
vAce2-spike5-151	ZINC000065096478	-9.7	0.313	417.37	ZINC	O=C(Nc1cccc(Oc2nc3ccccc3n3nnnc23)c1)c1c(F)cccc1F
vAce2-spike5-152	ZINC000065235425	-9.7	0.323	412.42	ZINC	CN1c2cc(F)ccc2C(=O)NC12CCN(C(=O)Nc1ccc3c(c1)OCO3)CC2
vAce2-spike5-153	ZINC000100688988	-9.7	0.313	416.44	ZINC	Cc1nn(-c2nc3ccccc3o2)c(O)c1[C@H]1CC(=O)N(c2ccc(C)cc2C)C1=O
vAce2-spike5-154	ZINC000100344967	-9.7	0.334	382.55	ZINC	C1=C[C@H]2c3ccc(C45CC6CC(CC(C6)C4)C5)ccc3N[C@@H](c3ccccn3)[C@@H]2C1
vAce2-spike5-155	ZINC000100737710	-9.7	0.294	431.45	ZINC	O=C(Nc1cccc2c1C(=O)[C@H]1C=CC=C[C@H]1C2=O)c1cccc2c1C(=O)c1ccccc1-2
vAce2-spike5-156	ZINC000100962359	-9.7	0.277	466.54	ZINC	Cc1cc([C@H]2CC(=O)N(c3ccc(C)c(C)c3)C2=O)cc2c1C(=O)N(c1ccc(C)c(C)c1)C2=O
vAce2-spike5-157	ZINC000104268210	-9.7	0.249	511.58	ZINC	Cc1ccc(N2C(=O)[C@@H]3[C@H](C2=O)[C@@H]2c4ccccc4C=NN2[C@@H]3C(=O)c2ccc(-c3ccccc3)cc2)cc1
vAce2-spike5-158	ZINC000208949977	-9.7	0.277	467.51	ZINC	Cc1cnn(C)c1C(=O)Nc1cc(Nc2ccc3c(/C=C/c4ccccn4)n[nH]c3c2)ccc1F
vAce2-spike5-159	ZINC000408812889	-9.7	0.277	477.56	ZINC	O=C1NC(=Nc2cccc3ccccc32)S/C1=C\c1cn(Cc2ccc(F)cc2)c2ccccc12
vAce2-spike5-160	ZINC000604404772	-9.7	0.262	490.56	ZINC	O=C(CCCN1C(=O)c2ccccc2N2C(=O)c3ccccc3[C@@H]21)N1CCc2c3ccccc3[nH]c2C1
vAce2-spike5-161	PV-001793579003	-9.6	0.343	366.42	REAL	O=C1C[C@@H](C(=O)Nc2cccc(C#Cc3ccccc3)c2)c2ccccc2N1
vAce2-spike5-162	PV-001806014991	-9.6	0.300	435.43	REAL	Cc1cc(N2C[C@@H](C(=O)Nc3nccc3C(=O)c3ccc(F)cc3)CC2=O)ccc1F
vAce2-spike5-163	PV-001810912572	-9.6	0.320	423.83	REAL	O=C1C[C@H](C(=O)Nc2nccc2C(=O)c2cccc(Cl)c2)c2ccc(F)cc2N1
vAce2-spike5-164	PV-001810957861	-9.6	0.310	422.54	REAL	Cc1cc(C)cc(C(=O)N2CCC[C@H](C(=O)N3CCc4ccc(F)cc4[C@@H](C)C3)C2)c1
vAce2-spike5-165	PV-001825441477	-9.6	0.331	396.37	REAL	Cc1cc(F)cc(C(=O)Nc2ccc3[nH]c(-c4cc(F)ccc4F)nc3c2)c1N
vAce2-spike5-166	PV-001839935705	-9.6	0.343	372.47	REAL	Cc1ccnc(Nc2cccc(C(=O)N[C@]3(C)CCCc4ccccc43)c2)n1
vAce2-spike5-167	PV-001857682220	-9.6	0.310	423.53	REAL	Cc1cccc(NC(=O)N2CCC[C@H](C(=O)N3CCc4ccc(F)cc4[C@@H](C)C3)C2)c1
vAce2-spike5-168	PV-001860077366	-9.6	0.331	403.33	REAL	O=C(c1cc(F)cc2ccccc12)N1Cc2ccc(NC(=O)C(F)(F)F)cc2C1
vAce2-spike5-169	PV-001866975555	-9.6	0.320	404.36	REAL	O=C(Nc1ccc(F)c(C(=O)c2ccccc2)c1)c1cnc2[nH]c(=O)[nH]c(=O)c2c1
vAce2-spike5-170	PV-001868161286	-9.6	0.343	376.43	REAL	Cc1ccnc(Nc2cccc(C(=O)N[C@H]3c4ccccc4CC[C@@H]3F)c2)n1
vAce2-spike5-171	PV-001872270966	-9.6	0.310	443.93	REAL	Cc1cc(=O)[nH]c(N2CCN(C(=O)[C@H]3CCCN(C(=O)c4ccc(Cl)cc4)C3)CC2)n1
vAce2-spike5-172	PV-001942298927	-9.6	0.320	417.36	REAL	O=C(Nc1cc(C(F)(F)F)c[nH]c1=O)N1CCc2cc(-c3cccc(F)c3)ccc21
vAce2-spike5-173	Z1020977516	-9.6	0.310	423.38	REAL	O=C(NNc1nc(-c2ccncc2)no1)c1nn(-c2ccc(F)c(F)c2)c2c1CCC2
vAce2-spike5-174	Z1069484694	-9.6	0.320	406.48	REAL	Cc1ccc(C)c(C(=O)N2CCC(C(=O)c3ccc4c(c3)NC(=O)[C@@H](C)O4)CC2)c1
vAce2-spike5-175	Z1069484696	-9.6	0.320	406.48	REAL	Cc1cc(C)cc(C(=O)N2CCC(C(=O)c3ccc4c(c3)NC(=O)[C@@H](C)O4)CC2)c1
vAce2-spike5-176	Z1082328850	-9.6	0.320	407.38	REAL	O=C(Nc1nc2ccccc2c(=O)[nH]1)c1nn(-c2ccc(F)c(F)c2)c2c1CCC2
vAce2-spike5-177	Z1131297999	-9.6	0.320	401.43	REAL	O=C1NC(=O)c2cc(C(=O)N3CCC(c4nc(-c5ccccc5)n[nH]4)CC3)ccc21
vAce2-spike5-178	Z1165694785	-9.6	0.320	403.48	REAL	O=C1NC(=O)C2(CCC(C(=O)N3CC=C(c4cccc5ccccc45)CC3)CC2)N1
vAce2-spike5-179	Z1171698418	-9.6	0.310	417.37	REAL	O=C(Nc1ccc2[nH]c(-c3cc(F)ccc3F)nc2c1)c1n[nH]c2ccccc2c1=O
vAce2-spike5-180	Z1172231620	-9.6	0.331	379.46	REAL	O=c1[nH]c(NC[C@@H]2CC3c4ccccc4C2c2ccccc23)nc2ccccc12
vAce2-spike5-181	Z1192869169	-9.6	0.310	418.45	REAL	C[C@H]1Oc2ccc(C(=O)C3CCN(C(=O)c4coc5ccccc45)CC3)cc2NC1=O
vAce2-spike5-182	Z1210042740	-9.6	0.343	376.50	REAL	Cc1ccc2c(c1)[C@@H]1CN(C)CC[C@@H]1N2C(=O)C[C@@H]1OCCc2ccccc21
vAce2-spike5-183	Z1220621607	-9.6	0.310	411.51	REAL	O=C1Nc2ccccc2[C@@H]1C1CCN(c2nc(-c3ccccn3)nc3c2CCC3)CC1
vAce2-spike5-184	Z1223959326	-9.6	0.331	383.45	REAL	O=C1NCCc2ccc(NC(=O)N3Cc4ccccc4-c4ccccc4C3)cc21
vAce2-spike5-185	Z1267441036	-9.6	0.331	391.45	REAL	C[C@H]1C[C@H](c2ccccc(F)c2)N(C(=O)c2ccc3c(=O)n4c(nc3c2)CCC4)C1
vAce2-spike5-186	Z1276023412	-9.6	0.320	402.42	REAL	O=C1Nc2ccccc2O[C@H]1CC(=O)N1CCc2cc(-c3cccc(F)c3)ccc21
vAce2-spike5-187	Z1276023884	-9.6	0.320	402.40	REAL	O=C(c1cc(=O)[nH]c2cc(F)ccc12)N1CCc2cc(-c3cccc(F)c3)ccc21
vAce2-spike5-188	Z1276024508	-9.6	0.310	416.41	REAL	Cn1c(=O)[nH]c(=O)c2cc(C(=O)N3CCc4cc(-c5cccc(F)c5)ccc43)cnc21
vAce2-spike5-189	Z1312817852	-9.6	0.310	412.45	REAL	Cc1cc(C(=O)N2Cc3ccccc3[C@@H](c3ccccc3)C2)nc2nc(O)[nH]c(=O)c12
vAce2-spike5-190	Z1313872032	-9.6	0.310	413.52	REAL	CN1CCC(=O)Nc2cc(C(=O)N3CCC(c4cccc5ccccc45)CC3)ccc21
vAce2-spike5-191	Z1330295780	-9.6	0.300	422.49	REAL	Cc1nc(-c2ccccn2)[nH]c(=O)c1CC(=O)N(C)C1c2ccccc2-c2ccccc21
vAce2-spike5-192	Z1335192124	-9.6	0.300	434.47	REAL	C[C@@]1(c2ccc(C(=O)N3CCC(c4c[nH]c5ccc(F)ccc45)CC3)cc2)NC(=O)NC1=O
vAce2-spike5-193	Z1417812245	-9.6	0.356	362.38	REAL	O=C1NC(=O)c2cc(C(=O)N3CCC4(CC3)OCc3ccccc34)ccc21
vAce2-spike5-194	Z1419338558	-9.6	0.320	424.50	REAL	CC(=O)Nc1cc(S(=O)(=O)N2CCCc3cc(-c4ccccc4)ccc32)ccc1F
vAce2-spike5-195	Z1420919075	-9.6	0.310	418.40	REAL	O=C(c1ccc(N2C(=O)c3ccccc3C2=O)cc1)N1CCCc2c(F)ccc(F)c21
vAce2-spike5-196	Z1420929299	-9.6	0.300	424.50	REAL	O=C1C[C@@H](Cc2ccc(C(=O)N3CCCc4cc(-c5ccccc5)ccc43)cc2)C(=O)N1
vAce2-spike5-197	Z1443316589	-9.6	0.331	384.41	REAL	O=C(c1cc(=O)[nH]c2ccc(F)cc12)N1CCc2cc(-c3ccccc3)ccc21
vAce2-spike5-198	Z1449006270	-9.6	0.331	399.47	REAL	O=C(c1ccc2c(=O)[nH]c(S)nc2c1)N1CCc2cc(-c3ccccc3)ccc21
vAce2-spike5-199	Z1451813869	-9.6	0.300	423.52	REAL	O=C(NC[C@@H]1[C@H]2Cc3ccccc3[C@H]12)Nc1cccc(C(=O)N2CCc3ccccc32)c1
vAce2-spike5-200	Z1470610225	-9.6	0.343	376.42	REAL	O=C(Nc1cccc(N2C(=O)CNC2=O)c1)N[C@@H]1[C@H]2CCc3ccccc3[C@H]21

Supplementary Table 18. Virtual hits 101-200 of the screen against ACE2 at a site adjacent to the Spike interaction interface (Screen ID: 5). Compounds were filtered so that hits had MW < 600 dalton, cLogP < 6, number of hydrogen bond acceptors < 11, and no reactive functional groups. The name of each compound consists of the initial letter 'v' for virtual hit, followed by the target protein name and the target site ('spike' for spike interaction site, 5 for docking scenario 5). The score is the docking score given by QuickVina 2 in kcal/mol. The ligand efficiency (LE) is computed as LE = -score/#NonH, where #NonH is the number of heavy (i.e. non hydrogen) atoms.

Name	Catalog ID	Score	LE	MW	Library	SMILES
vPhos-as1-1	ZINC000100504092	-11.7	0.377	404.512	ZINC	O=c1cccc2n1C[C@H]1C[C@H]2CN(Cc2ccc3ccc4ccccc5ccc2c3c45)C1
vPhos-as1-2	Z1428257796	-11.3	0.404	373.411	REAL	O=C(c1cc(O)nc2ccccc12)N1CCCC[C@@H]1c1nc2ccccc2o1
vPhos-as1-3	ZINC000100219587	-11.3	0.365	411.508	ZINC	Cc1cc2nc3c(cc(O)n2n1)C[C@H]1CC[C@H](C3)N1Cc1ccc(-c2cccn2)cc1
vPhos-as1-4	Z1983287764	-11.2	0.386	395.433	REAL	O=C1N[C@@]2(C[C@H]3C[C@H]2[C@H]2CCC[C@H]32)C(=O)N1Cc1ncc(-c2ccc(F)cc2)o1
vPhos-as1-5	Z362739648	-11.2	0.311	475.551	REAL	O=C(c1cccc(C(=O)N2CCc3[nH]c4ccccc4c3C2)n1)N1CCc2[nH]c3ccccc3c2C1
vPhos-as1-6	ZINC000004090796	-11.2	0.4	371.435	ZINC	O=C1CCCC2=C1[C@H](c1ccccc1)C=C1c3cc4c(cc3CCN12)OCO4
vPhos-as1-7	ZINC000004660212	-11.1	0.347	419.527	ZINC	Cc1[nH]c2ccccc2c1C1(c2c(C)[nH]c3ccccc32)c2cc(C)cc(C)c2NC1=O
vPhos-as1-8	ZINC000005451173	-11.1	0.383	389.425	ZINC	O=C1CCCC2=C1[C@H](c1ccc(F)cc1)C=C1c3cc4c(cc3CCN12)OCO4
vPhos-as1-9	PV-001815193777	-11	0.393	382.409	REAL	C[C@]1(Cc2ccc(F)c(F)c2)CCCN1C(=O)c1cc(O)nc2ccccc12
vPhos-as1-10	Z1616250975	-11	0.379	399.44	REAL	O=C1CCc2cc(F)c(NC(=O)N3CCC[C@@H](c4ccc(F)cc4)CC3)cc2N1
vPhos-as1-11	Z1663738465	-11	0.344	424.546	REAL	O=C([C@@H]1C[C@@H]2CCCC[C@@H]2N1c1nccn1)N1Cc2ccccc2-c2ccccc2C1
vPhos-as1-12	Z1897866162	-11	0.367	419.46	REAL	O=S(=O)(Nc1nnc(-c2ccc3ccccc3c2)o1)C1=Cc2ccccc2OCC1
vPhos-as1-13	Z2668909623	-11	0.407	368.382	REAL	O=C(c1cc(O)nc2ccccc12)N1CCCC[C@@H]1c1ccc(F)cc1F
vPhos-as1-14	Z2719795306	-11	0.393	381.406	REAL	O=C(N[C@@H]1Cc2ccccc2NC1=O)[C@H]1CCC(=O)N(c2cccc(F)c2)C1
vPhos-as1-15	ZINC000409044452	-11	0.324	465.979	ZINC	Cc1ccc(C(=C2[C@H]3C=C[C@H]2[C@@H]2C(=O)N(c4cccc(Cl)c4)C(=O)[C@@H]32)c2ccc(C)cc2)cc1
vPhos-as1-16	ZINC000409372284	-11	0.306	475.551	ZINC	Cc1ccc(-c2n[nH]c(O)c2C(c2c[nH]c3ccccc32)c2c(O)[nH]nc2-c2ccc(C)cc2)cc1
vPhos-as1-17	PV-001806635110	-10.9	0.419	366.847	REAL	O=C(c1cc(O)nc2ccccc12)N1CCCC[C@@H]1c1ccc(Cl)cc1
vPhos-as1-18	PV-001814964519	-10.9	0.389	398.864	REAL	C[C@]1(Cc2ccc(Cl)c(F)c2)CCCN1C(=O)c1cc(O)nc2ccccc12
vPhos-as1-19	PV-001859058609	-10.9	0.352	433.36	REAL	O=C(N[C@H]1Cc2ccccc2N(C(=O)C(F)(F)F)C1)c1cc(=O)[nH]c2cc(F)ccc12
vPhos-as1-20	Z1724349206	-10.9	0.404	353.424	REAL	Cn1nc2ccccc2c1C(=O)N1Cc2ccccc2-c2ccccc2C1
vPhos-as1-21	Z1887045622	-10.9	0.376	384.394	REAL	O=C(c1cnc2[nH]c(=O)[nH]c(=O)c2c1)N1C[C@@H](c2ccccc2)c2ccccc21
vPhos-as1-22	Z1897888291	-10.9	0.389	391.45	REAL	O=S(=O)(Nc1nnc(-c2ccc3c(c2)CCC3)o1)c1ccc2ccccc2c1
vPhos-as1-23	Z2011293929	-10.9	0.376	402.433	REAL	O=S(=O)(Nc1nnc(-c2ccc3ccccc3c2)o1)c1cnc2ccccc2c1
vPhos-as1-24	Z226401112	-10.9	0.389	368.435	REAL	NC(=O)[C@@H]1Cc2ccccc2CN1C(=O)c1ccc2c(c1)-c1ccccc1C2
vPhos-as1-25	Z2869806474	-10.9	0.389	387.385	REAL	O=C(Nc1cc2oc(=O)[nH]c2cc1F)N1CCCC[C@@H](c2ccc(F)cc2)CC1
vPhos-as1-26	Z978768214	-10.9	0.376	386.454	REAL	C[C@H](NC(=O)Nc1ccc2c(c1)Cc1ccccc1-2)c1ccc(NC(N)=O)cc1
vPhos-as1-27	ZINC000100572803	-10.9	0.389	368.479	ZINC	O=c1cccc2n1C[C@H]1C[C@H]2CN(Cc2ccc3c(c2)Cc2ccccc2-3)C1
vPhos-as1-28	PV-001804564206	-10.8	0.338	449.937	REAL	CC(=O)Nc1ccc(N2C[C@@H](C(=O)N[C@@H](C)c3ccc(Cl)c4ccccc34)CC2=O)cc1
vPhos-as1-29	PV-001816161915	-10.8	0.386	376.498	REAL	Cc1ccc([C@@H]2CCN(C(=O)c3ccc4c(c3)CCCC(=O)N4)C2(C)C)cc1
vPhos-as1-30	PV-001844794610	-10.8	0.348	434.432	REAL	O=C([C@@H]1CCCN(c2ccccc2)C1=O)N1CC[C@@](F)(c2ccccc(C(F)(F)F)c2)C1
vPhos-as1-31	PV-001859060412	-10.8	0.36	414.382	REAL	O=C(N[C@H]1Cc2ccccc2N(C(=O)C(F)(F)F)C1)c1ccccc2cc(O)ccc12
vPhos-as1-32	PV-001859060877	-10.8	0.36	415.37	REAL	O=C(N[C@H]1Cc2ccccc2N(C(=O)C(F)(F)F)C1)c1ccccc2cc(O)ncc12
vPhos-as1-33	PV-001859061465	-10.8	0.348	426.437	REAL	Cc1ccc2c(C(=O)N[C@H]3Cc4ccccc4N(C(=O)C(F)(F)F)C3)c(C)ccc2c1
vPhos-as1-34	PV-001885014963	-10.8	0.36	407.444	REAL	Cc1ccc(N2C[C@@H](C(=O)Nc3cc(-c4ccccc4F)no3)CCC2=O)cc1C
vPhos-as1-35	PV-001950625177	-10.8	0.36	413.448	REAL	CC1(C)COc2cc(NC(=O)N[C@@H]3CCCOc4ccc(F)cc43)ccc2NC1=O
vPhos-as1-36	PV-001950627027	-10.8	0.36	413.448	REAL	CC1(C)COc2cc(NC(=O)N[C@@H]3CCCOc4cc(F)ccc43)ccc2NC1=O
vPhos-as1-37	Z1014477988	-10.8	0.3	482.582	REAL	C[C@@H](NC(=O)[C@H]1C[C@H]2CCCC[C@@H]2N1C(=O)c1ccc2ccccc2c1)c1ccc2[nH]c(=O)[nH]c2c1
vPhos-as1-38	Z1014568628	-10.8	0.338	428.534	REAL	O=C([C@@H]1C[C@@H]2CCCC[C@@H]2N1C(=O)c1ccc2ccccc2c1)N1CCc2[nH]ncc2C1
vPhos-as1-39	Z1134728050	-10.8	0.4	364.419	REAL	O=C(c1cc(O)nc2ccccc12)N1CCCC[C@@H]1Cc1ccc(F)cc1
vPhos-as1-40	Z1173004777	-10.8	0.45	319.407	REAL	Cc1ccc([C@H]2CCCN2c2nc3ccccc3c(=O)[nH]2)cc1C
vPhos-as1-41	Z1269832101	-10.8	0.348	414.464	REAL	O=C(Nc1ccc2c(c1)Cc1ccccc1-2)[C@H]1CCCCN1C(=O)c1ccc(=O)[nH]n1
vPhos-as1-42	Z1312794175	-10.8	0.327	442.474	REAL	O=C(Nc1ccc(-c2cc3ccccc3o2)cc1)[C@H]1CCCCN1C(=O)c1ccc(=O)[nH]n1
vPhos-as1-43	Z1535729802	-10.8	0.327	441.421	REAL	NC(=O)c1n[nH]c2ccc(NC(=O)c3ccccc3-c3ncc(-c4ccc(F)cc4)o3)cc12
vPhos-as1-44	Z1616968098	-10.8	0.338	431.466	REAL	O=C(CN1C(=O)Cn2c(cc3ccccc32)C1=O)N[C@@H]1CC=C(c2ccc(F)cc2)CC1
vPhos-as1-45	Z1693249791	-10.8	0.386	377.486	REAL	C[C@H]1CCCc2ccccc2[C@H]1NC(=O)Nc1ccc2c(c1)CCCC(=O)N2
vPhos-as1-46	Z1765810445	-10.8	0.372	386.425	REAL	C[C@@H]1c2ccc(F)cc2CCN1C(=O)c1ccc2[nH]c3ccccc3c(=O)c2c1
vPhos-as1-47	Z1766236220	-10.8	0.36	404.415	REAL	C[C@@H]1c2cc(F)cc(F)c2CCN1C(=O)c1ccc2[nH]c3ccccc3c(=O)c2c1
vPhos-as1-48	Z1766525781	-10.8	0.338	433.373	REAL	NC(=O)c1n[nH]c2ccc(NC(=O)c3cc(F)cc4c(=O)c5cc(F)ccc5[nH]c34)cc12
vPhos-as1-49	Z1885378240	-10.8	0.386	368.435	REAL	O=C1CCc2cc(C(=O)N3C[C@@H](c4ccccc4)c4ccccc43)ccc2N1
vPhos-as1-50	Z2141012606	-10.8	0.36	397.433	REAL	O=C(c1nn(Cc2ccccc2)c(=O)c2ccccc12)N1Cc2ccccc2CO1
vPhos-as1-51	Z2497462462	-10.8	0.415	347.417	REAL	O=C(c1cccc2[nH]c(=O)[nH]c12)N1CC[C@@H]2CCCC[C@@]21c1ccccc1
vPhos-as1-52	Z2830784081	-10.8	0.292	495.534	REAL	O=C1c2ccccc2C(=O)N1[C@H]1CCC[C@@]2(C1)Nc1ccccc1C(=O)N2c1ccc2c(c1)OCCO2
vPhos-as1-53	Z2843561962	-10.8	0.386	384.478	REAL	COc1cccc(C[C@]2(C(=O)N[C@@H](C)c3n[nH]c(=O)n3C)C[C@H]3CC[C@H]2C3)c1
vPhos-as1-54	Z383337534	-10.8	0.348	413.519	REAL	CC(C)C(=O)N[C@H](Cc1c[nH]c2ccccc12)C(=O)NCc1cccc2ccccc12
vPhos-as1-55	Z615602838	-10.8	0.309	491.498	REAL	O=C1CCc2cc(S(=O)(=O)NC(=O)c3ccccc3-c3ncc(-c4ccccc4F)o3)ccc2N1
vPhos-as1-56	Z810429462	-10.8	0.348	416.523	REAL	Cc1cccc(NC(=O)[C@@H]2CCCN(C(=O)c3ccc4c5c([nH]c34)CCCC5)C2)n1
vPhos-as1-57	ZINC000001445915	-10.8	0.4	355.392	ZINC	O=C1CCC2=C1[C@H](c1ccc3c(c1)OCO3)c1c(ccc3ccccc31)N2
vPhos-as1-58	ZINC000003357442	-10.8	0.36	395.461	ZINC	O=C(c1nn(Cc2ccccc2)c(=O)c2ccccc21)N1CCc2ccccc2C1
vPhos-as1-59	ZINC000040486311	-10.8	0.386	368.479	ZINC	c1ccc2c(c1)cccc2C1=NN2[C@@H](C1)c1ccccc1OC21CCCCC1
vPhos-as1-60	ZINC000253623741	-10.8	0.292	493.47	ZINC	O=C1c2ccc3c(c2O/C1=C\c1ccc2c(c1)OCCO2)[C@@H](c1cc2ccccc2nc1O)CC(=O)O3
vPhos-as1-61	ZINC000263585291	-10.8	0.348	413.428	ZINC	Cc1cc2oc(=O)c3c(c2c2c1[C@@H](c1cc4ccccc4nc1O)CC(=O)O2)CCC3
vPhos-as1-62	PV-000381535369	-10.7	0.382	378.446	REAL	O=C(N[C@@H]1C[C@H]2CC[C@@H]1N2C(=O)c1ccc(F)c1)C1Cc2ccccc2C1
vPhos-as1-63	PV-001808249024	-10.7	0.334	433.482	REAL	CC(=O)Nc1ccc(N2C[C@@H](C(=O)N[C@@H](C)c3ccc(F)c4ccccc34)CC2=O)cc1
vPhos-as1-64	PV-001815530815	-10.7	0.382	382.546	REAL	CC1(C)CC[C@@H](NC(=O)[C@H]2CC(=O)N[C@@H]3CCCC[C@@H]32)[C@@H](c2ccccc2)C1
vPhos-as1-65	PV-001817751674	-10.7	0.357	401.465	REAL	Cn1c(=O)c2ccc(NC(=O)C(C)(C)c3ccc4ccccc4c3)cc2n(C)c1=O
vPhos-as1-66	PV-001859058574	-10.7	0.345	433.36	REAL	O=C(N[C@H]1Cc2ccccc2N(C(=O)C(F)(F)F)C1)c1cc(=O)[nH]c2ccc(F)cc12
vPhos-as1-67	PV-001859059057	-10.7	0.369	402.375	REAL	Cc1cc(C(=O)N[C@H]2Cc3ccccc3N(C(=O)C(F)(F)F)C2)c2n[nH]cc2c1
vPhos-as1-68	PV-001948775444	-10.7	0.412	346.433	REAL	C[C@H]1CCCc2ccccc2[C@H]1NC(=O)Nc1cc2ccccc2nn1
vPhos-as1-69	PV-001948776476	-10.7	0.396	364.423	REAL	O=C(Nc1cc2ccccc2nn1)N1CCC[C@@H](c2ccc(F)cc2)CC1
vPhos-as1-70	Z1022405620	-10.7	0.334	429.406	REAL	Cn1c(=O)oc2ccc(NC(=O)c3ccccc3-c3ncc(-c4ccccc4F)o3)cc21
vPhos-as1-71	Z1157948085	-10.7	0.396	356.424	REAL	O=C1CCc2cc(NC(=O)[C@H]3C[C@H]3c3ccc4ccccc4c3)ccc2N1
vPhos-as1-72	Z1318763034	-10.7	0.382	366.419	REAL	O=C1NCCc2ccc(NC(=O)c3c4ccccc4cc4ccccc34)cc21
vPhos-as1-73	Z1410038912	-10.7	0.369	391.47	REAL	O=C1CCCc2cc(NC(=O)N[C@H]3CC4(CCC4)Oc4ccccc43)ccc2N1
vPhos-as1-74	Z1558880056	-10.7	0.369	382.418	REAL	O=C(CCc1cc2ccccc2[nH]c1=O)Nc1ccc2c(c1)oc1ccccc12
vPhos-as1-75	Z1560190040	-10.7	0.382	377.443	REAL	O=C1COc2cc(NC(=O)N3C[C@H]4CCCC[C@@]43c3ccccc3)ccc2N1
vPhos-as1-76	Z1599581175	-10.7	0.324	439.518	REAL	O=C(Nc1nc2ccccn2n1)[C@@H]1C[C@H]2CCCC[C@H]2N1C(=O)c1ccc2ccccc2c1
vPhos-as1-77	Z1614410881	-10.7	0.382	370.451	REAL	C[C@H]1CN(C(=O)[C@H]2C[C@H]2c2ccc3ccccc3c2)c2ccccc2C(=O)N1
vPhos-as1-78	Z1764103969	-10.7	0.369	390.373	REAL	O=C1CCc2cc(F)c(NC(=O)c3c[nH]nc3-c3c4ccccc4o3)cc2N1
vPhos-as1-79	Z1883096696	-10.7	0.345	407.472	REAL	O=C(c1ccc2c(=O)n3c(nc2c1)CCC3)N1C[C@@H](c2ccccc2)c2ccccc21
vPhos-as1-80	Z1890092232	-10.7	0.357	401.396	REAL	O=C1CCc2cc(F)c(NC(=O)c3ccc4c(=O)c5ccccc5[nH]c34)cc2N1
vPhos-as1-81	Z1897887786	-10.7	0.382	393.466	REAL	O=S(=O)(Nc1nnc(-c2ccc3c(c2)CCC3)o1)C1=Cc2ccccc2CC1
vPhos-as1-82	Z1902476072	-10.7	0.382	370.451	REAL	Cn1c(=O)ccc2ccc(NC(=O)C(C)(C)c3ccc4ccccc4c3)cc21
vPhos-as1-83	Z1907861800	-10.7	0.324	448.428	REAL	NC(=O)N1CCCc2ccc(NC(=O)c3cc(F)cc4c(=O)c5cc(F)ccc5[nH]c34)cc21
vPhos-as1-84	Z2001428616	-10.7	0.334	425.53	REAL	O=C(c1ccc2c(=O)n3c(nc2c1)CCCCC3)N1[C@@H]2C=C(c3ccccc3)C[C@H]1CC2
vPhos-as1-85	Z2002795192	-10.7	0.396	387.862	REAL	CCOCCOc1c(Cl)cccc1NC(=O)[C@@]12[C@@H]3C(=O)[C@H]4[C@@H]5C[C@H]([C@H]41)[C@H]2[C@H]53
vPhos-as1-86	Z2008687310	-10.7	0.357	399.497	REAL	Cn1c([C@@H]2Cc3ccccc3O2)nnc1N1CCC[C@@H](c2cc3ccccc3[nH]2)C1
vPhos-as1-87	Z2011294091	-10.7	0.382	392.438	REAL	O=S(=O)(Nc1nnc(-c2ccc3c(c2)CCC3)o1)c1cnc2ccccc2c1
vPhos-as1-88	Z2090580623	-10.7	0.382	376.455	REAL	O=C1Nc2ccccc2[C@@H]1CC(=O)N1C[C@@H](c2ccccc2)[C@@H]2COCC[C@@H]21
vPhos-as1-89	Z2222967991	-10.7	0.369	389.454	REAL	O=C1CNC(=O)c2ccc(C(=O)N3C[C@@H]4CCCC[C@@]43c3ccccc3)cc2N1
vPhos-as1-90	Z2304871385	-10.7	0.369	392.414	REAL	O=C(Nc1nc2cc3c(cc2[nH]1)OCO3)[C@H]1CCCCN1C(=O)c1ccccc1
vPhos-as1-91	Z2408749245	-10.7	0.396	354.452	REAL	O=C([C@@H]1CCc2ccccc21)N1Cc2ccccc2[C@H](c2ccccc2)C1
vPhos-as1-92	Z2879686466	-10.7	0.396	363.416	REAL	C[C@]1(c2nc(-c3cc4c([nH]c3=O)CCOC4)no2)CCc2ccccc2C1
vPhos-as1-93	Z2959698572	-10.7	0.369	390.481	REAL	O=C1C[C@@H](CC(=O)N2C[C@@H](c3ccccc3)[C@@H]3COCC[C@@H]32)c2ccccc2N1
vPhos-as1-94	Z300528004	-10.7	0.369	382.462	REAL	O=C(Nc1ccc2c(c1)Cc1ccccc1-2)[C@H]1CCCN1C(=O)c1ccccc1
vPhos-as1-95	Z364622518	-10.7	0.369	384.434	REAL	O=C(CC1c2ccccc2Oc2ccccc21)Nc1ccc2c(c1)CCC(=O)N2
vPhos-as1-96	Z510547088	-10.7	0.324	438.482	REAL	Cc1c(-c2ccccc2)oc2c(C(=O)N[C@H](C)c3ccc4c(c3)CC(=O)N4)cccc2c1=O
vPhos-as1-97	ZINC000005603194	-10.7	0.382	376.455	ZINC	c1ccc2c(c1)OC1(CCCCC1)N1N=C(c3ccc4c(c3)OCCO4)C[C@@H]21
vPhos-as1-98	ZINC000006383000	-10.7	0.357	396.449	ZINC	O=C(Nc1nc2ccccc2[nH]1)[C@@H]1Cc2ccccc2CN1C(=O)c1ccccc1
vPhos-as1-99	ZINC000006624286	-10.7	0.357	401.421	ZINC	Cc1coc2c1c(C)cc1oc(=O)c(CC(=O)N=c3[nH]c4ccccc4[nH]3)c(C)c21
vPhos-as1-100	ZINC000009090034	-10.7	0.396	361.448	ZINC	Cc1ccc(NC(=N)Nc2nc(C)c(Cc3ccccc3)c(O)n2)cc1C

Supplementary Table 19. Top 100 virtual hits of the screen against the active site of the macrodomain in closed conformation (Screen ID: 10). Compounds were filtered so that hits had MW < 600 dalton, cLogP < 6, number of hydrogen bond acceptors < 11, and no reactive functional groups. The name of each compound consists of the initial letter 'v' for virtual hit, followed by the target protein name and the target site ('as' for active site, 1 for docking scenario 1). The score is the docking score given by QuickVina 2 in kcal/mol. The ligand efficiency (LE) is computed as LE = -score/#NonH, where #NonH is the number of heavy (i.e. non hydrogen) atoms.

Name	Catalog ID	Score	LE	MW	Library	SMILES
vPhos-as1-101	ZINC000015016813	-10.7	0.345	425.92	ZINC	Cc1[nH]c2ccccc2c1C1(c2c(C)[nH]c3ccccc32)c2cc(Cl)ccc2NC1=O
vPhos-as1-102	ZINC000032759491	-10.7	0.369	382.46	ZINC	O=C(Nc1ccc2c(c1)Cc1ccccc1-2)[C@H]1CCCN1C(=O)c1ccccc1
vPhos-as1-103	ZINC000409362960	-10.7	0.357	416.44	ZINC	O=C(c1ccc(-c2ccccc2)cc1)N1N=C(C2CCCCC2)C[C@]1(O)C(F)(F)F
vPhos-as1-104	PV-001806634444	-10.6	0.393	384.84	REAL	O=C(c1cc(=O)[nH]c2cc(F)ccc12)N1CCCC[C@@H]1c1ccc(Cl)cc1
vPhos-as1-105	PV-001807255310	-10.6	0.342	430.47	REAL	O=C1C[C@@H](C(=O)N2CCC[C@H](c3ccccc3)C2)CN1Cc1ccnc(C(F)(F)F)c1
vPhos-as1-106	PV-001807376560	-10.6	0.393	357.46	REAL	Cc1nn(C)c2cc(NC(=O)C(C)(C)c3ccc4ccccc4c3)ccc12
vPhos-as1-107	PV-001809535912	-10.6	0.379	376.50	REAL	Cc1ccc(N2C[C@H](C(=O)N3CCCc4ccc(C)c(C)c43)CC2=O)cc1C
vPhos-as1-108	PV-001810029930	-10.6	0.342	443.91	REAL	CC(=O)Nc1ccc(N2C[C@H](C(=O)N3CCCc4c(C)c(F)cc(Cl)c43)CC2=O)cc1
vPhos-as1-109	PV-001810540264	-10.6	0.379	374.44	REAL	Cc1ccc(N2C[C@@H](C(=O)Nc3ccc4ccccc4nn3)CCC2=O)cc1C
vPhos-as1-110	PV-001811634811	-10.6	0.353	400.48	REAL	CC(=O)c1ccc2ccccc2c1NC(=O)[C@]1(C)CCCN1C(=O)c1ccccc1
vPhos-as1-111	PV-001814320429	-10.6	0.353	412.57	REAL	Cc1cc(C)c(/C=C\C(=O)N[C@@H]2C[C@H]3CC[C@H]([C@H]2C)N3C(=O)OC(C)(C)C)cc1C
vPhos-as1-112	PV-001816322703	-10.6	0.366	419.50	REAL	CC1CCC(N2C[C@H](C(=O)Nc3ccc4c(c3)S(=O)(=O)CC(=O)N4)CC2=O)CC1
vPhos-as1-113	PV-001821660404	-10.6	0.442	318.34	REAL	O=C(Cc1cc2ccccc2c(=O)[nH]1)Nc1nc2ccccc2[nH]1
vPhos-as1-114	PV-001847826059	-10.6	0.331	442.37	REAL	O=C(Nc1cccc(-c2n[nH]c(=O)[nH]2)c1)c1cc(F)ccc1-c1cccc(C(F)(F)F)c1
vPhos-as1-115	PV-001849946137	-10.6	0.393	381.82	REAL	C[C@@H](c1nc2cc(Cl)ccc2[nH]1)N(C)C(=O)c1cc2ccccc2c(=O)o1
vPhos-as1-116	PV-001850001199	-10.6	0.342	436.52	REAL	C[C@H]1C[C@@H](C(F)(F)F)CCN1C(=O)[C@H]1CCCC[C@H]1C(=O)Nc1c2ccccc2C[C@@H]1C
vPhos-as1-117	PV-001859056787	-10.6	0.331	446.43	REAL	Cc1noc2nc(C(C)C)cc(C(=O)N[C@H]3Cc4ccccc4N(C(=O)C(F)(F)F)C3)c12
vPhos-as1-118	PV-001859057531	-10.6	0.331	441.45	REAL	CC(C)c1cc(C(=O)N[C@H]2Cc3ccccc3N(C(=O)C(F)(F)F)C2)c2ccccc2n1
vPhos-as1-119	PV-001859058042	-10.6	0.353	418.35	REAL	O=C(N[C@H]1Cc2ccccc2N(C(=O)C(F)(F)F)C1)c1cc(F)cc2ncnc12
vPhos-as1-120	PV-001859059085	-10.6	0.353	417.39	REAL	Cc1cc(C(=O)N[C@H]2Cc3ccccc3N(C(=O)C(F)(F)F)C2)c2c(C)n[nH]c2n1
vPhos-as1-121	PV-001859059331	-10.6	0.331	447.39	REAL	Cc1cc(F)c2nc(O)cc(C(=O)N[C@H]3Cc4ccccc4N(C(=O)C(F)(F)F)C3)c2c1
vPhos-as1-122	PV-001859059693	-10.6	0.366	407.33	REAL	O=C(N[C@H]1Cc2ccccc2N(C(=O)C(F)(F)F)C1)c1cc(F)cc2[nH]nnc12
vPhos-as1-123	PV-001866302219	-10.6	0.366	404.50	REAL	C[C@H]1CC(F)(F)CCN1C(=O)[C@H]1CCCC[C@H]1C(=O)N1c2ccccc2C[C@@H]1C
vPhos-as1-124	PV-001867710843	-10.6	0.393	364.44	REAL	CC1(C)CC[C@@H](NC(=O)c2cccc3oc(=O)[nH]c23)[C@@H](c2ccccc2)C1
vPhos-as1-125	PV-001870662471	-10.6	0.353	405.45	REAL	Cc1cc(=O)[nH]c2cc(C(=O)Nc3ccccc3C(=O)N3CCC[C@H](O)C3)ccc12
vPhos-as1-126	PV-001874092663	-10.6	0.366	400.47	REAL	C[C@@H]1CCN(c2ccc(F)cc2F)CCN1C(=O)c1cc2c(cc1O)CCCC2
vPhos-as1-127	PV-001920948431	-10.6	0.342	430.43	REAL	Cc1cc2oc(=O)cc(CN[C@H]3Cc4ccccc4N(C(=O)C(F)(F)F)C3)c2cc1C
vPhos-as1-128	PV-001944142231	-10.6	0.342	434.37	REAL	CN1Cc2ccccc2[C@H](NC(=O)Nc2cc(C(F)(F)F)cc3c2OCC(=O)N3)C1=O
vPhos-as1-129	PV-001945993556	-10.6	0.379	381.45	REAL	C[C@H]1CCCc2ccccc2[C@H]1NC(=O)Nc1cc2c(cc1F)NC(=O)CC2
vPhos-as1-130	Z1014960404	-10.6	0.379	368.44	REAL	Cc1cc(C(=O)N2Cc3ccccc3-c3ccccc3C2)n2nc(C)cc2n1
vPhos-as1-131	Z1014963166	-10.6	0.393	355.44	REAL	O=C([C@H]1COc2ccccc2C1)N1Cc2ccccc2-c2ccccc2C1
vPhos-as1-132	Z1127073688	-10.6	0.331	431.53	REAL	C[C@@H]1Cc2ccccc2N1C(=O)[C@H]1CCCC[C@@H]1C(=O)Nc1ccc2c(c1)CCC(=O)N2
vPhos-as1-133	Z1127083015	-10.6	0.303	474.56	REAL	C[C@@H]1Cc2ccccc2N1C(=O)[C@H]1CCCC[C@@H]1C(=O)Nc1cccc([C@@]2(C)NC(=O)NC2=O)c1
vPhos-as1-134	Z1208157332	-10.6	0.393	375.45	REAL	O=S(=O)(c1cc[nH]c2ncccc12)N1Cc2ccccc2-c2ccccc2C1
vPhos-as1-135	Z1229867027	-10.6	0.366	388.51	REAL	Cc1cccc(NC[C@H]2CCCN2C(=O)c2ccc3[nH]c4c(c3c2)CCCC4)n1
vPhos-as1-136	Z1261350858	-10.6	0.331	434.58	REAL	O=C(NC[C@@H]1CCC[C@H](O)C1)[C@H]1C[C@H]2CCCC[C@H]2N1C(=O)c1ccc2ccccc2c1
vPhos-as1-137	Z1370788961	-10.6	0.321	446.55	REAL	O=C([C@H]1C[C@@H]2CCCC[C@H]2N1C(=O)c1ccc2ccccc2c1)N1CCN2C(=O)NC[C@H]2C1
vPhos-as1-138	Z1383803204	-10.6	0.331	424.46	REAL	O=C1c2ccccc2C(=O)c2cc(NC(=O)[C@H]3CCCN3C(=O)c3ccccc3)ccc21
vPhos-as1-139	Z1408711626	-10.6	0.379	378.40	REAL	O=C(N[C@@H]1CC2(CCC2)Oc2ccccc21)c1cc(=O)[nH]c2cc(F)ccc12
vPhos-as1-140	Z1546696527	-10.6	0.461	304.40	REAL	Cc1ccc([C@H]2CCCN2c2nc(N)c3ccccc3n2)cc1
vPhos-as1-141	Z1654923312	-10.6	0.342	416.44	REAL	O=C(c1cn[nH]c1-c1ccc2c(c1)OCO2)N1CCC[C@H](c2nnc3ccccn23)C1
vPhos-as1-142	Z1688101752	-10.6	0.379	377.49	REAL	CC(=O)N1CC[C@@H](NC(=O)N2CCCC[C@H]2c2ccccc2)c2ccccc21
vPhos-as1-143	Z1738588883	-10.6	0.342	410.48	REAL	Cc1n[nH]c(-c2ccccc2)c1NC(=O)[C@H]1CC(=O)N(c2cccc3ccccc23)C1
vPhos-as1-144	Z1739845677	-10.6	0.353	401.51	REAL	Cc1nc(-c2ccccc(NC(=O)N3C[C@H](c4ccccc4)[C@H]4CCCC[C@@H]43)c2)n[nH]1
vPhos-as1-145	Z1740680900	-10.6	0.353	403.52	REAL	C[C@H]1C(=O)Nc2cc(C(=O)N3C[C@@H](c4ccccc4)[C@H]4CCCC[C@@H]43)ccc2N1C
vPhos-as1-146	Z1744653995	-10.6	0.353	409.46	REAL	Cc1ccc(C(=O)N2CCC[C@@H](C(=O)Nc3ccc4c(cc3F)NC(=O)CC4)C2)cc1
vPhos-as1-147	Z1763699682	-10.6	0.353	408.36	REAL	NC(=O)Nc1ccccc(NC(=O)c2cc(F)cc3c(=O)c4cc(F)ccc4[nH]c23)c1
vPhos-as1-148	Z1764660517	-10.6	0.331	434.44	REAL	C[C@H]1CN(C(=O)c2cc(F)cc3c(=O)c4cc(F)ccc4[nH]c23)C[C@H](c2ccccc2)O1
vPhos-as1-149	Z1765704711	-10.6	0.393	449.28	REAL	O=C1CCc2cc(Br)c(S(=O)(=O)Nc3nnc(-c4ccccc4)o3)cc2N1
vPhos-as1-150	Z1767350224	-10.6	0.353	400.45	REAL	O=C(NC1(Cc2cccc(F)c2)CCC1)c1ccc2[nH]c3ccccc3c(=O)c2c1
vPhos-as1-151	Z1767371662	-10.6	0.366	390.37	REAL	O=C1CCc2cc(NC(=O)c3c[nH]nc3-c3cc4ccccc4o3)c(F)cc2N1
vPhos-as1-152	Z1819485203	-10.6	0.366	393.49	REAL	CC1CCC(N2C[C@H](C(=O)N3Cc4cnnn4Cc4ccccc43)CC2=O)CC1
vPhos-as1-153	Z1833941830	-10.6	0.342	420.55	REAL	O=C(NC[C@@H]1CC[C@H](O)C1)[C@H]1C[C@H]2CCCC[C@H]2N1C(=O)c1ccc2ccccc2c1
vPhos-as1-154	Z1863854981	-10.6	0.393	359.43	REAL	CCn1c([C@H]2CCCN2c2nc3ccccc3c(=O)[nH]2)nc2ccccc21
vPhos-as1-155	Z1870148279	-10.6	0.342	422.39	REAL	Cc1cc(C)c(C(=O)O)cc1NC(=O)c1cc(F)cc2c(=O)c3cc(F)ccc3[nH]c12
vPhos-as1-156	Z1883102035	-10.6	0.321	431.50	REAL	Cc1c(C(=O)N2C[C@@H](c3ccccc3)c3ccccc32)nnn1-c1ccccc2cnccc12
vPhos-as1-157	Z1888753158	-10.6	0.353	398.46	REAL	C[C@H]1CN(C(=O)c2cccc3c(=O)c4ccccc4[nH]c23)C[C@H](c2ccccc2)O1
vPhos-as1-158	Z1888854339	-10.6	0.342	408.46	REAL	Cc1cc(C)cc(-c2cc(NC(=O)c3cccc4c(=O)c5ccccc5[nH]c34)[nH]n2)c1
vPhos-as1-159	Z1889588641	-10.6	0.342	412.42	REAL	Cc1ccc(F)c(-c2cc(NC(=O)c3cccc4c(=O)c5ccccc5[nH]c34)[nH]n2)c1
vPhos-as1-160	Z1896312003	-10.6	0.366	399.47	REAL	O=C(c1cc2c(=O)[nH]c(S)nc2c1)N1C[C@@H](c2ccccc2)c2ccccc21
vPhos-as1-161	Z1897864320	-10.6	0.366	407.45	REAL	O=S(=O)(Nc1nnc(-c2ccc3ccccc3c2)o1)c1ccc2c(c1)CCCO2
vPhos-as1-162	Z1897865602	-10.6	0.366	407.45	REAL	C[C@H]1Cc2cc(S(=O)(=O)Nc3nnc(-c4ccc5ccccc5c4)o3)ccc2O1
vPhos-as1-163	Z1897888570	-10.6	0.379	395.44	REAL	O=S(=O)(Nc1nnc(-c2ccc3c(c2)CCC3)o1)C1=Cc2ccccc2OC1
vPhos-as1-164	Z1903256988	-10.6	0.366	391.45	REAL	Cn1c(=O)ccc2ccc(NC(=O)N[C@@H]3CC=C(c4ccc(F)cc4)CC3)cc21
vPhos-as1-165	Z1907876859	-10.6	0.366	385.47	REAL	NC(=O)N1CCCc2ccc(NC(=O)[C@@H]3C[C@@H]3c3ccc4ccccc4c3)cc21
vPhos-as1-166	Z1940274873	-10.6	0.408	391.30	REAL	NC(=O)c1ccccc1CCC(=O)NC1(c2c(Cl)cccc2Cl)CCC1
vPhos-as1-167	Z2000224831	-10.6	0.366	387.46	REAL	Cc1cc(F)cc2c1CN(c1nccc1C(=O)N1CCc3ccccc31)CC2
vPhos-as1-168	Z2001434849	-10.6	0.379	372.42	REAL	CN1C(=O)c2ccc(C(=O)N3[C@H]4C=C(c5ccccc5)C[C@H]3CC4)cc2C1=O
vPhos-as1-169	Z2003801839	-10.6	0.379	367.45	REAL	O=C1[C@@H]2[C@@H]3C[C@H]4[C@@H]2[C@@]2(C(=O)N5C[C@@H](c6ccccc6)c6ccccc65)[C@@H]1[C@@H]3[C@@H]42
vPhos-as1-170	Z2077108617	-10.6	0.321	441.42	REAL	O=C(Nc1cccc(-c2n[nH]c(=O)[nH]2)c1)c1ccccc1-c1ncc(-c2ccc(F)cc2)o1
vPhos-as1-171	Z2094108089	-10.6	0.353	402.43	REAL	O=C(NNc1cccc(F)n1)[C@@H]1CC(=O)N(c2ccc3c(c2)Cc2ccccc2-3)C1
vPhos-as1-172	Z2094243073	-10.6	0.342	416.52	REAL	C[C@@H]1C[C@@H](c2ccccc2)N(C(=O)[C@@H]2CCCN(C(=O)c3ccc4[nH]ncc4c3)C2)C1
vPhos-as1-173	Z2110433249	-10.6	0.379	377.49	REAL	O=C(Nc1ccn(C2CCCCC2)n1)N1CCCn2c(cc3ccccc32)C1
vPhos-as1-174	Z2207980461	-10.6	0.321	438.48	REAL	Cc1cc2cc(NC(=O)c3ccc4c(c3)C[C@H](c3ccccc3)OC4=O)ccc2n(C)c1=O
vPhos-as1-175	Z2233254854	-10.6	0.331	432.53	REAL	Cc1nnc2[nH]nc(NC(=O)[C@H]3CCCC[C@@H]3C(=O)N3c4ccccc4C[C@H]3C)c2c1C
vPhos-as1-176	Z228329578	-10.6	0.366	394.56	REAL	Cc1ccc(C23C[C@H]4C[C@@H](CC(C(=O)NCC(=O)N5CCCC5)(C4)C2)C3)cc1C
vPhos-as1-177	Z2299436853	-10.6	0.366	396.53	REAL	COc1ccc(C23C[C@H]4C[C@@H](CC(C(=O)NC[C@@]5(C)CCC(=O)N5)(C4)C2)C3)cc1
vPhos-as1-178	Z2362628506	-10.6	0.366	390.53	REAL	CC1(C)CC[C@@H]2C[C@@H](NC(=O)N3CCNC[C@H]3c3ccncc3)c3ccc1c32
vPhos-as1-179	Z240154694	-10.6	0.379	392.43	REAL	O=C1COc2ccc(S(=O)(=O)Nc3ccc4c(c3)Cc3ccccc3-4)cc2N1
vPhos-as1-180	Z2497462455	-10.6	0.379	377.48	REAL	O=C([C@@H]1CCO[C@H](c2ccccc2)O1)N1C[C@@H]2CCCC[C@@]21c1ccccc1
vPhos-as1-181	Z278904574	-10.6	0.321	458.42	REAL	O=C(c1c[nH]nc1-c1ccc(F)cc1)N1CCC[C@@H](c2nnc3ccc(C(F)(F)F)cn23)C1
vPhos-as1-182	Z28810677	-10.6	0.353	401.51	REAL	O=C(c1nn(Cc2ccccc2)c(=O)c2ccccc12)N1CC[C@H]2CCCC[C@@H]2C1
vPhos-as1-183	Z2952309486	-10.6	0.393	364.44	REAL	C[C@@H]1CO[C@H](c2ccccc2)CN1C(=O)C[C@@H]1CC(=O)Nc2ccccc21
vPhos-as1-184	Z295729120	-10.6	0.331	424.50	REAL	O=C(Nc1ccc(-c2cn3ccccc3n2)cc1)[C@H]1CCCCN1C(=O)c1ccccc1
vPhos-as1-185	Z346651904	-10.6	0.353	401.47	REAL	Cc1ccc2c(c1)C(=O)N([C@H](C)C(=O)N1CCc3[nH]c4ccc(C)cc4c3C1)C2=O
vPhos-as1-186	Z368083704	-10.6	0.321	466.56	REAL	O=C(Nc1cccc(N2CCCCC2=O)c1)C1CCN(C2=NS(=O)(=O)c3ccccc32)CC1
vPhos-as1-187	Z372557110	-10.6	0.331	440.43	REAL	O=C(c1c[nH]nc1-c1ccccc1)N1CCC[C@@H](c2nnc3ccc(C(F)(F)F)cn23)C1
vPhos-as1-188	Z442068238	-10.6	0.353	396.49	REAL	Cc1nc2c(c(C)nn2C)c(C)c1CC(=O)Nc1ccc2c(c1)Cc1ccccc1-2
vPhos-as1-189	Z738314028	-10.6	0.353	412.47	REAL	O=C1Nc2ccc(S(=O)(=O)N3Cc4ccccc4-c4ccccc43)c3ccnc1c23
vPhos-as1-190	ZINC000004660213	-10.6	0.331	419.53	ZINC	CCc1ccc2c(c1)C(c1c(C)[nH]c3ccccc31)c1c(C)[nH]c3ccccc31)C(=O)N2
vPhos-as1-191	ZINC000004747869	-10.6	0.393	361.48	ZINC	CC1(C)OC(=O)C2(c3ccccc3-c3ccccc32)[C@H]1NC1CCCCC1
vPhos-as1-192	ZINC000005013559	-10.6	0.342	409.46	ZINC	Cc1[nH]c2ccccc2c1C1(c2c(C)[nH]c3ccccc32)c2cc(F)ccc2NC1=O
vPhos-as1-193	ZINC000008845753	-10.6	0.379	374.40	ZINC	Cc1ccc(-c2n[nH]c3c2[C@@]2(c4ccccc4N(C)C2=O)N(C)C3=O)c(O)c1
vPhos-as1-194	ZINC000025546844	-10.6	0.353	394.47	ZINC	Cc1ccc2[nH]c3c(c2c1)CN(C(=O)c1ccccc1C(=O)c1ccccc1)CC3
vPhos-as1-195	ZINC000046046806	-10.6	0.312	471.46	ZINC	O=C(Nc1ccccc1C(F)(F)F)N1CCCN(c2nc3cc(F)ccc3n3cccc23)CC1
vPhos-as1-196	ZINC000075278522	-10.6	0.442	313.36	ZINC	O=C1c2ccccc2[C@H]2O[C@@H](c3ccccc3)c3ccccc3N12
vPhos-as1-197	ZINC000100737708	-10.6	0.321	431.45	ZINC	O=C(Nc1cccc2c1C(=O)[C@@H]1C=CC=C[C@@H]1C2=O)c1cccc2c1C(=O)c1ccccc1-2
vPhos-as1-198	ZINC000247411486	-10.6	0.379	369.46	ZINC	O=C(O)c1ccc2c(c1)[C@H]1[C@@H]([C@H]3CC[C@H]1C3)[C@@H](c1cccc3ccccc31)N2
vPhos-as1-199	ZINC000409046209	-10.6	0.312	465.98	ZINC	Cc1ccc(C(=C2[C@H]3C=C[C@H]2[C@@H]2C(=O)N(c4ccccc4Cl)C(=O)[C@H]32)c2ccc(C)cc2)cc1
vPhos-as1-200	ZINC000409333002	-10.6	0.353	464.31	ZINC	O=C(O)c1cccc2c1N[C@H](c1cc3c(cc1Br)OCO3)[C@H]1Cc3ccccc3[C@@H]21

Supplementary Table 20. Virtual screening hits 101 to 200 of the screen against the active site of the macrodomain in closed conformation (Screen ID: 10). Compounds were filtered so that hits had MW < 600 dalton, cLogP < 6, number of hydrogen bond acceptors < 11, and no reactive functional groups. The name of each compound consists of the initial letter 'v' for virtual hit, followed by the target protein name and the target site ('as' for active site, 1 for docking scenario 1). The score is the docking score given by QuickVina 2 in kcal/mol. The ligand efficiency (LE) is computed as LE = -score/#NonH, where #NonH is the number of heavy (i.e. non hydrogen) atoms.

Name	Catalog ID	Score	LE	MW	Library	SMILES
vPhos-as2-1	Z1069483432	-13.5	0.386	466.535	REAL	C[C@@H]1Oc2ccc(C(=O)C3CCN(C(=O)c4ccc5c(c4)-c4ccccc4C5)CC3)cc2NC1=O
vPhos-as2-2	Z1148472724	-13.5	0.365	497.641	REAL	O=C([C@H]1C[C@@H]2CCCC[C@H]2N1C(=O)c1ccc2ccccc2c1)N1CCC[C@@H](c2nnc3n2CCC3)C1
vPhos-as2-3	Z132917174	-13.4	0.394	467.875	REAL	O=C1/C(=C\Nc2nc3ccccc3n3nnnc23)c2ccccc2C(=O)N1c1ccccc1Cl
vPhos-as2-4	Z132917176	-13.2	0.388	447.457	REAL	Cc1ccc(N2C(=O)/C(=C/Nc3nc4ccccc4n4nnnc34)c3ccccc3C2=O)cc1
vPhos-as2-5	Z2902586015	-13.2	0.357	492.538	REAL	Cc1cc(C)n2ncc(-c3noc(C4[C@H]5[C@@H]6C=C[C@H]([C@H]7C(=O)N(Cc8ccccc8)C(=O)[C@@H]67)[C@H]45)n3)c2n1
vPhos-as2-6	Z228329578	-13.1	0.452	394.557	REAL	Cc1ccc(C23C[C@H]4C[C@@H](CC(C(=O)NCC(=O)N5CCCC5)(C4)C2)C3)cc1C
vPhos-as2-7	Z804205998	-13.1	0.374	469.496	REAL	O=C(NNC(=O)[C@@H]1CC(=O)N(c2ccc3c(c2)Cc2ccccc2-3)C1)c1ccc2c(c1)OCCO2
vPhos-as2-8	Z1147907130	-13	0.361	480.57	REAL	O=C(NCc1nnnn1-c1ccccc1)[C@H]1C[C@@H]2CCCC[C@H]2N1C(=O)c1ccc2ccccc2c1
vPhos-as2-9	Z2155695547	-13	0.433	402.453	REAL	C[C@@]1(c2ccc(-c3noc([C@H]4[C@@H]5[C@H]6C[C@H]7[C@H]8[C@H]6C[C@H]5[C@H]8[C@H]74)n3)cc2)NC(=O)NC1=O
vPhos-as2-10	Z1132505833	-12.9	0.461	385.506	REAL	CC(C)(C)OC(=O)Nc1ccc(NC(=O)N[C@H]2C[C@@H]3C[C@@H]2[C@H]2CCC[C@H]32)cc1
vPhos-as2-11	Z2155695080	-12.9	0.43	402.409	REAL	C[C@@]1(c2ccc(-c3noc([C@@]45[C@H]6C(=O)[C@H]7[C@H]8C[C@@H]([C@@H]74)[C@@H]5[C@H]86)n3)cc2)NC(=O)NC1=O
vPhos-as2-12	Z2167485420	-12.9	0.416	409.496	REAL	Cn1c(-c2ccc3ccccc3c2)nnc1N1CCC(c2nnc3ccccn23)CC1
vPhos-as2-13	Z805712270	-12.9	0.369	465.508	REAL	Cc1ccc(-c2nnc(COC(=O)[C@@H]3CC(=O)N(c4ccc5c(c4)Cc4ccccc4-5)C3)o2)cc1
vPhos-as2-14	ZINC000039754055	-12.9	0.391	434.454	ZINC	O=C(Nc1nnc(-c2ccccc2)o1)c1ccccc1NC(=O)c1ccc2ccccc21
vPhos-as2-15	Z1022496460	-12.8	0.346	495.621	REAL	O=C(NCC(=O)N1CCc2ccccc2C1)[C@@H]1C[C@@H]2CCCC[C@H]2N1C(=O)c1ccc2ccccc2c1
vPhos-as2-16	Z1983290694	-12.8	0.441	392.458	REAL	O=C1N[C@]2(C[C@H]3C[C@H]2[C@H]2CCC[C@H]32)C(=O)N1Cc1nc(Cc2ccccc2)no1
vPhos-as2-17	Z2002423492	-12.8	0.4	425.483	REAL	O=C1[C@@H]2[C@@H]3C[C@H]4[C@@H]2[C@]2(C(=O)Oc5cccc(C(=O)N6CCc7ccccc7C6)c5)[C@H]1[C@@H]3[C@@H]42
vPhos-as2-18	Z2003308006	-12.8	0.4	446.573	REAL	O=C(Nc1ccc2nc(N3CCOCC3)sc2c1)N1[C@H]2C=C(c3ccccc3)C[C@H]1CC2
vPhos-as2-19	Z2086931081	-12.8	0.427	407.444	REAL	O=C1CCc2cc(F)c(N3C(=O)N[C@H](C[C@H]4CCCc5ccccc54)C3=O)cc2N1
vPhos-as2-20	Z2175361627	-12.8	0.388	443.506	REAL	O=C(Nc1nnc2n1CCCC2)C1[C@H]2[C@@H]3C=C[C@H]([C@@H]4C(=O)N(Cc5ccccc5)C(=O)[C@H]34)[C@@H]12
vPhos-as2-21	Z2902742501	-12.8	0.388	461.541	REAL	CS(=O)(=O)c1ccc(-c2noc(C3CCN(C(=O)c4cccc5ccccc45)CC3)n2)cc1
vPhos-as2-22	Z29402875	-12.8	0.366	488.567	REAL	O=C(c1ccc2c(=O)n3c(nc2c1)CCC3)N1CCN(S(=O)(=O)c2ccc3ccccc3c2)CC1
vPhos-as2-23	Z847630838	-12.8	0.346	498.509	REAL	O=C1CCc2cc(C(=O)COC(=O)[C@@H]3CC(=O)N(c4ccc5c(c4)Cc4ccccc4-5)C3)c(F)cc2N1
vPhos-as2-24	ZINC000002776613	-12.8	0.376	458.442	ZINC	O=C(c1cnn2c1nc(-c1cccc3ccccc31)cc2C(F)(F)F)N1CCc2ccccc21
vPhos-as2-25	PV-001886592355	-12.7	0.423	411.411	REAL	Cc1cccc(C(=O)N2CCC[C@@H]2C(=O)Nc2nc(-c3c(F)cccc3F)n[nH]2)c1
vPhos-as2-26	Z1014269000	-12.7	0.353	481.594	REAL	O=C(NCC(=O)N1CCc2ccccc21)[C@@H]1C[C@@H]2CCCC[C@H]2N1C(=O)c1ccc2ccccc2c1
vPhos-as2-27	Z1014360770	-12.7	0.374	459.588	REAL	O=C(C1CC1)N1CCN(C(=O)[C@H]2C[C@@H]3CCCC[C@H]3N2C(=O)c2ccc3ccccc3c2)CC1
vPhos-as2-28	Z1682390335	-12.7	0.397	438.486	REAL	C[C@@]1(c2ccc(-c3noc(C4CCN(C(=O)N5CCCC5)CC4)n3)cc2)NC(=O)NC1=O
vPhos-as2-29	Z2007472842	-12.7	0.41	408.508	REAL	Cn1c(-c2ccc3ccccc3n2)nnc1N1CCC(c2c[nH]c3ccccc23)CC1
vPhos-as2-30	Z2166948166	-12.7	0.41	414.515	REAL	Cn1c(-c2ccc3ccccc3n2)nnc1N1CCC(c2nnc3n2CCCC3)CC1
vPhos-as2-31	Z2476204090	-12.7	0.438	393.402	REAL	C[C@@]1(c2ccc(-c3noc([C@@]45[C@H]6C[C@H](C(=O)N4)[C@H]5C6)n3)cc2)NC(=O)NC1=O
vPhos-as2-32	Z735270840	-12.7	0.363	467.524	REAL	Cc1ccc(N2C(=O)/C(=C/Nc3cccc(C(=O)N4CCOCC4)c3)c3ccccc3C2=O)cc1
vPhos-as2-33	Z847630072	-12.7	0.353	482.491	REAL	O=C1COc2ccc(C(=O)COC(=O)[C@@H]3CC(=O)N(c4ccc5c(c4)Cc4ccccc4-5)C3)cc2N1
vPhos-as2-34	PV-001943222490	-12.6	0.434	411.46	REAL	C[C@H]1C(=O)Nc2ccccc2CN1C(=O)Nc1nnc(Cc2ccc(F)cc2)s1
vPhos-as2-35	Z1054483432	-12.6	0.36	487.535	REAL	O=C(OCC1=Nc2ccccc2S(=O)(=O)N1)[C@@H]1CC(=O)N(c2ccc3c(c2)Cc2ccccc2-3)C1
vPhos-as2-36	Z1069482964	-12.6	0.382	445.517	REAL	Cc1[nH]c2ccc(C(=O)N3CCC(C(=O)c4ccc5c(c4)NC(=O)[C@H](C)O5)CC3)cc2c1C
vPhos-as2-37	Z1101835780	-12.6	0.35	478.507	REAL	O=C(Nc1ccc(N2C(=O)c3ccccc3C2=O)cc1)c1ccc2c(=O)n3c(nc2c1)CCCCC3
vPhos-as2-38	Z1448270388	-12.6	0.382	445.493	REAL	O=C1CCc2cc(C(=O)N3CCC[C@H](NC(=O)c4ccc5ccccc5c4)C3)c(F)cc2N1
vPhos-as2-39	Z1497615927	-12.6	0.406	421.543	REAL	C[C@@H](N[C@@H]1CCCC[C@H](N2C(=O)c3ccccc3C2=O)C1)c1nnc2n1CCCCC2
vPhos-as2-40	Z1682390413	-12.6	0.382	440.458	REAL	C[C@@]1(c2ccc(-c3noc(-c4cc(Cc5ccccc5)ccc4O)n3)cc2)NC(=O)NC1=O
vPhos-as2-41	Z1682390709	-12.6	0.434	391.361	REAL	C[C@@]1(c2ccc(-c3noc(-c4cc5cc(F)ccc5[nH]4)n3)cc2)NC(=O)NC1=O
vPhos-as2-42	Z1682391166	-12.6	0.42	399.409	REAL	Cc1cc(-c2nc(-c3ccc([C@]4(C)NC(=O)NC4=O)cc3)no2)nc2ccccc12
vPhos-as2-43	Z1682392301	-12.6	0.406	434.838	REAL	C[C@@]1(c2ccc(-c3noc(-c4cc(Cl)c5ccccc5c4O)n3)cc2)NC(=O)NC1=O
vPhos-as2-44	Z1684063173	-12.6	0.394	430.467	REAL	Cc1cccc(N2N=C(c3nc(-c4ccc(N5CCNC(=O)C5)cc4)no3)CCC2=O)c1
vPhos-as2-45	Z2182937357	-12.6	0.371	448.529	REAL	CN(c1nnc(-c2n[nH]c(=O)c3ccccc23)n1Cc1ccccc1)C1Cc2ccccc2C1
vPhos-as2-46	Z2902676334	-12.6	0.36	464.484	REAL	C[C@]1(c2ccc(-c3nc(-c4cccc(Cn5cnc6ccccc65)c4)no3)cc2)NC(=O)NC1=O
vPhos-as2-47	Z364958852	-12.6	0.36	483.591	REAL	Cc1cnc2c(S(=O)(=O)N3CCN(C(=O)c4ccc5c(c4)-c4ccccc4C5)CC3)ccce2c1
vPhos-as2-48	Z803556816	-12.6	0.394	429.45	REAL	O=C(NNC(=O)[C@@H]1CC(=O)N(c2ccc3c(c2)Cc2ccccc2-3)C1)c1ccccc1F
vPhos-as2-49	Z980288212	-12.6	0.36	469.539	REAL	O=C(CN1C(=O)[C@H]2[C@@H]3C=C[C@@H](C3)[C@@H]2C1=O)Nc1ccc(CC(=O)N2CCCc3ccccc32)cc1
vPhos-as2-50	ZINC000012100057	-12.6	0.36	468.555	ZINC	C[C@]1(C2CCN(C(=O)c3cce4ccccc4n3)CC2)NC(=O)N(C2Cc3ccccc3C2)C1=O
vPhos-as2-51	ZINC000253396823	-12.6	0.394	419.435	ZINC	O=C1C[C@@H](c2ccnc3ccccc32)c2c(ccc3c(=O)c(-c4ccccc4)coc32)O1
vPhos-as2-52	PV-001828571388	-12.5	0.391	431.538	REAL	Cc1ccc(N2C[C@H](C(=O)Nc3nnc(-c4ccc(C(C)(C)C)cc4)[nH]3)CC2=O)cc1C
vPhos-as2-53	PV-001828571480	-12.5	0.403	423.559	REAL	CC1CCC(N2C[C@H](C(=O)Nc3nnc(-c4ccc(C(C)(C)C)cc4)[nH]3)CC2=O)CC1
vPhos-as2-54	Z1010365726	-12.5	0.338	495.577	REAL	Cc1ccn2c(=O)ccc(COC(=O)[C@H]3C[C@H]4CCCC[C@H]4N3C(=O)c3ccc4ccccc4c3)nc2c1
vPhos-as2-55	Z1028449292	-12.5	0.357	467.567	REAL	O=C1Nc2ccccc2[C@@H]1C1CCN(C(=O)NCc2ccc(-c3ccc4c(c3)CCO4)cc2)CC1
vPhos-as2-56	Z1095049546	-12.5	0.403	416.415	REAL	O=C(Nc1nc(-c2ccc3ccccc3n2)n[nH]1)[C@@H]1CC(=O)N(c2ccccc2F)C1
vPhos-as2-57	Z1095049928	-12.5	0.391	434.405	REAL	O=C(Nc1nc(-c2ccc3ccccc3n2)n[nH]1)[C@@H]1CC(=O)N(c2ccc(F)cc2F)C1
vPhos-as2-58	Z1101972428	-12.5	0.379	441.529	REAL	O=C1CCCc2cc(NC(=O)[C@@H]3CCCN(C(=O)c4ccce5ccccc45)C3)ccc2N1
vPhos-as2-59	Z1224678717	-12.5	0.431	393.485	REAL	COc1cccc(C[C@]2(C(=O)NNC(=O)Cc3ccccn3)C[C@H]3CC[C@H]2C3)c1
vPhos-as2-60	Z132927926	-12.5	0.347	492.46	REAL	Cc1ccc(N2C(=O)/C(=C/Nc3cc(C)n4nc(C(F)(F)F)nc4n3)c3ccccc3C2=O)cc1C
vPhos-as2-61	Z132927986	-12.5	0.357	478.433	REAL	Cc1ccc(N2C(=O)/C(=C\Nc3cc(C)n4nc(C(F)(F)F)nc4n3)c3ccccc3C2=O)cc1
vPhos-as2-62	Z1331817052	-12.5	0.379	442.517	REAL	C[C@@]1(c2ccc(C(=O)N3CCN(Cc4cccc5ccccc45)CC3)cc2)NC(=O)NC1=O
vPhos-as2-63	Z1452691933	-12.5	0.379	445.493	REAL	O=C(NC[C@H]1[C@@H]2Cc3ccccc3[C@H]12)NNC(=O)c1ccccc1OCc1ccc(F)cc1
vPhos-as2-64	Z1504184600	-12.5	0.403	415.452	REAL	O=C1c2ccccc2C(=O)N1[C@@H]1CCCC/C(=N/Nc2nc3ccccc3c(=O)[nH]2)C1
vPhos-as2-65	Z1622690677	-12.5	0.379	445.521	REAL	Cc1ccc2[nH]c3c(c2c1)C[C@@H](NC(=O)NCc1cccc([C@]2(C)NC(=O)NC2=O)c1)CC3
vPhos-as2-66	Z1682391561	-12.5	0.431	385.382	REAL	C[C@@]1(c2ccc(-c3noc(-c4ccc5ccccc5n4)n3)cc2)NC(=O)NC1=O
vPhos-as2-67	Z1682391564	-12.5	0.431	384.394	REAL	C[C@@]1(c2ccc(-c3noc(-c4ccc5ccccc5c4)n3)cc2)NC(=O)NC1=O
vPhos-as2-68	Z1766440663	-12.5	0.403	422.365	REAL	O=C(Nc1nc2cc(C(F)(F)F)ccc2[nH]1)c1ccc2[nH]c3ccccc3c(=O)c2c1
vPhos-as2-69	Z1890645172	-12.5	0.403	414.464	REAL	Cc1ccc(-c2noc(C3CCN(C(=O)c4cccc5ccccc45)CC3)n2)c(=O)[nH]1
vPhos-as2-70	Z2089217145	-12.5	0.403	408.504	REAL	O=C(c1cnn2c(-c3ccccc3)ccnc12)N1C[C@H](c2ccccc2)[C@@H]2CCC[C@H]21
vPhos-as2-71	Z2155693156	-12.5	0.431	386.41	REAL	C[C@@]1(c2ccc(-c3noc(-c4ccc5c(c4)CCC=C5)n3)cc2)NC(=O)NC1=O
vPhos-as2-72	Z2155693869	-12.5	0.403	438.463	REAL	C[C@@]1(c2ccc(-c3noc([C@H]4CCS(=O)(=O)c5ccccc54)n3)cc2)NC(=O)NC1=O
vPhos-as2-73	Z2155695127	-12.5	0.403	415.408	REAL	Cn1cc(-c2nc(-c3ccc([C@]4(C)NC(=O)NC4=O)cc3)no2)c2ccccc2c1=O
vPhos-as2-74	Z2157387828	-12.5	0.391	425.447	REAL	O=C1[C@H]2CC=CC[C@@H]2C(=O)N1Nc1cccc(-c2nc(-c3ccc4cc[nH]c4c3)no2)c1
vPhos-as2-75	Z2158627109	-12.5	0.379	441.49	REAL	O=C1[C@H]2CC=CC[C@@H]2C(=O)N1Nc1cccc(-c2nc(-c3ccc4c(n3)CCCC4)no2)c1
vPhos-as2-76	Z2159473541	-12.5	0.379	440.458	REAL	Cc1c(-c2noc(-c3cccc(NN4C(=O)[C@H]5CC=CC[C@@H]5C4=O)c3)n2)oc2ccccc12
vPhos-as2-77	Z2166176296	-12.5	0.379	436.518	REAL	C[C@H](c1ccc(-c2ccccc2)cc1)N(C)c1nnc(-c2n[nH]c(=O)c3ccccc23)n1C
vPhos-as2-78	Z2188051281	-12.5	0.403	416.48	REAL	O=C(Nc1cc2c(cn1)CCCC2)c1cccc(NN2C(=O)[C@@H]3CC=CC[C@H]3C2=O)c1
vPhos-as2-79	Z2220064481	-12.5	0.379	443.502	REAL	Cc1ccc2nc(C(=O)N3CCC(C(=O)c4ccc5c(c4)NC(=O)[C@@H](C)O5)CC3)cc2c1
vPhos-as2-80	Z245217624	-12.5	0.391	448.55	REAL	Cc1ccc(-c2nnc(NC(=O)CCc3nc4sc5c(c4c(=O)[nH]3)CC[C@@H](C)C5)[nH]2)cc1
vPhos-as2-81	Z2940819846	-12.5	0.357	462.508	REAL	O=C(CN1CCc2c(ncn2-c2ccccc2)C1)Nc1ccc2c1C(=O)c1ccccc1C2=O
vPhos-as2-82	Z31286715	-12.5	0.403	427.385	REAL	Cc1ccc(N2C(=O)/C(=C/Nc3nnc(C(F)(F)F)[nH]3)c3ccccc3C2=O)cc1C
vPhos-as2-83	Z417128784	-12.5	0.403	447.554	REAL	CCOc1ccc(-c2noc(CS(=O)(=O)CC(=O)N[C@H](C)[C@@H]3C[C@@H]4CC[C@@H]3C4)n2)cc1
vPhos-as2-84	Z685909856	-12.5	0.338	488.506	REAL	O=c1c2ccccc2c(-c2nnc(-c3ccc4c(=O)n5c(nc4c3)CCC5)o2)nn1Cc1ccccc1
vPhos-as2-85	Z744862882	-12.5	0.403	411.464	REAL	O=C(NNC(=O)N1CC=C(c2c[nH]c3ncccc23)CC1)c1ccc2ccccc2c1
vPhos-as2-86	Z803315646	-12.5	0.391	445.905	REAL	O=C(NNC(=O)[C@@H]1CC(=O)N(c2ccc3c(c2)Cc2ccccc2-3)C1)c1ccccc1Cl
vPhos-as2-87	Z822869632	-12.5	0.357	465.508	REAL	Cc1ccc2nc(COC(=O)[C@@H]3CC(=O)N(c4ccc5c(c4)Cc4ccccc4-5)C3)cc(=O)n2c1
vPhos-as2-88	ZINC000002780891	-12.5	0.357	472.469	ZINC	C[C@@H]1Cc2ccccc2N1C(=O)c1cnn2c1nc(-c1cccc3ccccc31)cc2C(F)(F)F
vPhos-as2-89	ZINC000006610219	-12.5	0.403	401.468	ZINC	O=c1[nH]c(-c2cn(Cc3ccc4ccccc43)c3ccccc23)nc2ccccc12
vPhos-as2-90	ZINC000007063806	-12.5	0.403	410.436	ZINC	Cc1ccc(N2C(=O)c3ccccc3/C(=C/Nc3ncnc4[nH]cnc43)C2=O)cc1C
vPhos-as2-91	ZINC000065113794	-12.5	0.338	498.556	ZINC	Cc1ccc(NC(=O)c2ccc(-c3noc(C4CCN(C(=O)c5ccccc5C)CC4)n3)cc2)cc1F
vPhos-as2-92	ZINC000105321466	-12.5	0.403	410.436	ZINC	Cc1ccc(N2C(=O)c3ccccc3/C(=C\Nc3ncnc4[nH]cnc43)C2=O)cc1C
vPhos-as2-93	ZINC000253405232	-12.5	0.391	422.435	ZINC	O=C1C[C@@H](C2=Cc3ccccc3OC2)c2c(ccc3c(=O)c(-c4ccccc4)coc32)O1
vPhos-as2-94	PV-001795949494	-12.4	0.428	409.876	REAL	Cc1cccc(C(=O)N2CCC[C@@H]2C(=O)Nc2nnc(-c3cccc(Cl)c3)[nH]2)c1
vPhos-as2-95	PV-001866030056	-12.4	0.443	384.518	REAL	CC(C)(C)OC(=O)N1C[C@@H](CCNC(=O)[C@H]2C[C@@H]3CC[C@@H]2C3)c2ccccc21
vPhos-as2-96	PV-001883684517	-12.4	0.428	393.421	REAL	Cc1cccc(C(=O)N2CCC[C@@H]2C(=O)Nc2nc(-c3ccccc3F)n[nH]2)c1
vPhos-as2-97	PV-001943341190	-12.4	0.428	411.46	REAL	C[C@H]1C(=O)Nc2ccccc2CN1C(=O)Nc1nnc(Cc2ccccc2F)s1
vPhos-as2-98	PV-001944829044	-12.4	0.428	393.398	REAL	O=C1CC(c2ccc(NC(=O)Nc3cccc4c3OCCC4=O)cc2)CC(=O)N1
vPhos-as2-99	PV-001948473130	-12.4	0.413	405.453	REAL	O=C1CC(c2ccc(NC(=O)Nc3ccc4c(c3)C(=O)CCCC4)cc2)CC(=O)N1
vPhos-as2-100	PV-001952232485	-12.4	0.428	414.485	REAL	C[C@@]1(c2ccccc2)CCCN(C(=O)Nc2nc3cc(S(N)(=O)=O)ccc3o2)C1

Supplementary Table 21. Top 100 virtual hits of the screen against the active site of the macrodomain in open conformation (Screen ID: 11). Compounds were filtered so that hits had MW < 600 dalton, cLogP < 6, number of hydrogen bond acceptors < 11, and no reactive functional groups. The name of each compound consists of the initial letter 'v' for virtual hit, followed by the target protein name and the target site ('as' for active site, 2 for docking scenario 2). The score is the docking score given by QuickVina 2 in kcal/mol. The ligand efficiency (LE) is computed as LE = -score/#NonH, where #NonH is the number of heavy (i.e. non hydrogen) atoms.

Name	Catalog ID	Score	LE	MW	Library	SMILES
vPhos-as2-101	Z1010365500	-12.4	0.344	488.54	REAL	O=C(COC(=O)[C@H]1C[C@H]2CCCC[C@H]2N1C(=O)c1ccc2ccccc2c1)Nc1nnc(C2CC2)o1
vPhos-as2-102	Z1015402018	-12.4	0.413	397.48	REAL	O=C(NCCN1C(=O)Cc2ccccc21)N1Cc2ccccc2-c2ccccc2C1
vPhos-as2-103	Z1030514170	-12.4	0.344	479.58	REAL	O=C(NCc1nc(-c2ccccc2)n[nH]1)[C@@H]1C[C@H]2CCCC[C@H]2N1C(=O)c1ccc2ccccc2c1
vPhos-as2-104	Z1033218530	-12.4	0.365	455.47	REAL	O=C(Cn1cnc2c(oc3ccccc32)c1=O)N1CCCC[C@H]1c1nc(-c2ccccc2)no1
vPhos-as2-105	Z103993068	-12.4	0.365	468.54	REAL	O=S(=O)(c1cccc(-c2nnc(-c3ccc4ccccc4n3)o2)c1)N1CCc2ccccc2C1
vPhos-as2-106	Z1069484644	-12.4	0.387	428.49	REAL	C[C@@H]1Oc2ccc(C(=O)C3CCN(C(=O)c4ccc5ccccc5c4)CC3)ccc2NC1=O
vPhos-as2-107	Z1069527436	-12.4	0.376	445.56	REAL	Cc1ccc(C(=O)N2CCC(NC(=O)[C@@H]3CC(=O)N(c4ccc5c(c4)CCC5)C3)CC2)cc1
vPhos-as2-108	Z1072590256	-12.4	0.376	448.52	REAL	C[C@@H]1Oc2ccc(C(=O)C3CCN(C(=O)c4cc5c(cc4O)CCCC5)CC3)cc2NC1=O
vPhos-as2-109	Z1080964630	-12.4	0.354	483.91	REAL	O=C(Nc1ccc2nc3n(c(=O)c2c1)CCC3)c1ccccc1-c1nc(-c2cccc(Cl)c2)no1
vPhos-as2-110	Z1082329362	-12.4	0.387	423.43	REAL	O=C(Nc1nc2ccccc2c(=O)[nH]1)c1nn(Cc2ccccc2)c(=O)c2ccccc12
vPhos-as2-111	Z1095049948	-12.4	0.387	426.48	REAL	Cc1cccc(N2C[C@H](C(=O)Nc3nc(-c4ccc5ccccc5n4)n[nH]3)CC2=O)c1C
vPhos-as2-112	Z1099281343	-12.4	0.413	403.44	REAL	O=C(NNC(=O)N1CCC[C@H]1c1ccc2c(c1)OCO2)c1ccc2ccccc2c1
vPhos-as2-113	Z1167665994	-12.4	0.376	436.45	REAL	O=C(Nc1cccc(-c2ccc3ccccc3c2)n1)c1nn(-c2ccc(F)cc2)ccc1=O
vPhos-as2-114	Z1168208061	-12.4	0.400	415.50	REAL	CCc1cc(=O)[nH]c(-c2ccc(N3CCC([C@H]4C(=O)Nc5ccccc54)CC3)nc2)n1
vPhos-as2-115	Z132917118	-12.4	0.376	434.42	REAL	O=C1/C(=C/Nc2nc3ccccc3n3nnnc23)c2ccccc2C(=O)N1c1ccccn1
vPhos-as2-116	Z1370788961	-12.4	0.376	446.55	REAL	O=C([C@H]1C[C@@H]2CCCC[C@H]2N1C(=O)c1ccc2ccccc2c1)N1CCN2C(=O)NC[C@H]2C1
vPhos-as2-117	Z1383818019	-12.4	0.354	463.45	REAL	O=C(CCc1nnc(-c2cc3ccccc3o2)o1)Nc1ccc2c(c1)C(=O)c1ccccc12=O
vPhos-as2-118	Z1456519582	-12.4	0.428	386.50	REAL	O=C([C@H]1C[C@H]1c1ccc2ccccc2c1)N1CCn2c(nnc2C2CCCC2)C1
vPhos-as2-119	Z1470503096	-12.4	0.376	437.50	REAL	Cc1ccc(N2C(=O)/C(=C\Nc3cccc([C@H]4CNC(=O)C4)c3)c3ccccc3C2=O)cc1
vPhos-as2-120	Z1497614501	-12.4	0.413	407.52	REAL	O=C1c2ccccc2C(=O)N1[C@H]1CCCC[C@@H](NCc2nnc3n2CCCCC3)C1
vPhos-as2-121	Z1576646261	-12.4	0.428	406.50	REAL	CC(C)(C)OC(=O)N1[C@@H]2CC[C@@H]1CC(CC(=O)N[C@H](CO)c1ccc(F)cc1)C2
vPhos-as2-122	Z1616913493	-12.4	0.376	436.51	REAL	Cc1cccc(C(=O)Nc2ccccc2C(=O)N2CCc3c(ncn3-c3ccccc3)C2)c1
vPhos-as2-123	Z1641119041	-12.4	0.387	432.48	REAL	O=C(NN1Cc2ccccc2C1=O)[C@@H]1CCCC[C@H]1C(=O)NN1Cc2ccccc2C1=O
vPhos-as2-124	Z1646997646	-12.4	0.376	442.52	REAL	Cn1c(COC(=O)[C@@H]2CC(=O)N(c3ccc4c(c3)Cc3ccccc3-4)C2)nnc1C1CCC1
vPhos-as2-125	Z1682391507	-12.4	0.387	425.45	REAL	Cc1cccc(-c2cncc(-c3nc(-c4ccc([C@]5(C)NC(=O)NC5=O)cc4)no3)c2)c1
vPhos-as2-126	Z1682391523	-12.4	0.387	445.50	REAL	Cc1ccc(Cc2nc(-c3nc(-c4ccc([C@]5(C)NC(=O)NC5=O)cc4)no3)cs2)cc1
vPhos-as2-127	Z1682393317	-12.4	0.387	438.49	REAL	C[C@@]1(c2ccc(-c3noc([C@@H]4CCCN(C(=O)N5CCCC5)C4)n3)cc2)NC(=O)NC1=O
vPhos-as2-128	Z1688449394	-12.4	0.387	423.43	REAL	Cc1ccc(-c2cnc(-c3ccccc3C(=O)NN3C(=O)c4ccccc4C3=O)o2)cc1
vPhos-as2-129	Z18301479	-12.4	0.344	486.44	REAL	O=C(COC(=O)c1ccc2c1C(=O)c1ccccc1C2=O)NC(=O)Nc1ccc2c(c1)OCCO2
vPhos-as2-130	Z1891988670	-12.4	0.428	389.45	REAL	O=C1CCc2ccc(N3C(=O)N[C@H]([C[C@@H]4CCCc5ccccc54)C3=O)cc2N1
vPhos-as2-131	Z1907685565	-12.4	0.387	448.42	REAL	O=C(NC[C@]1(O)[C@H]2[C@@H]3C[C@@H]4[C@@H]5[C@@H]3C[C@@H]2[C@@H]5[C@@H]41)c1nnn(-c2ccccc2F)c1C(F)(F)F
vPhos-as2-132	Z1984803456	-12.4	0.376	436.47	REAL	O=C(OCc1nnc2ccccc2n1)[C@@H]1CC(=O)N(c2ccc3c(c2)Cc2ccccc2-3)C1
vPhos-as2-133	Z2003779354	-12.4	0.387	430.51	REAL	O=C(Nc1ccc2nc(N3CCOCC3)oc2c1)N1[C@H]2C=C(c3ccccc3)C[C@H]1CC2
vPhos-as2-134	Z2086931231	-12.4	0.413	403.41	REAL	O=C1CCc2cc(F)c(N3C(=O)N[C@H](Cc4cccc5ccccc45)C3=O)cc2N1
vPhos-as2-135	Z2091512148	-12.4	0.400	412.44	REAL	Cc1ccc2c(c1)CN(C(=O)c1cccc(N3C(=O)c4ccccc4C3=O)c1)CCO2
vPhos-as2-136	Z2154232659	-12.4	0.387	424.46	REAL	Cc1ccc(N2C(=O)/C(=C/Nc3ccc4c3COC4=O)c3ccccc3C2=O)cc1C
vPhos-as2-137	Z2155691650	-12.4	0.443	380.45	REAL	C[C@@]1(c2ccc(-c3noc(C4C[C@@H]5CCC[C@@H](C4)C5)n3)cc2)NC(=O)NC1=O
vPhos-as2-138	Z2155693725	-12.4	0.413	399.41	REAL	Cc1ccnc2ccc(-c3nc(-c4ccc([C@]5(C)NC(=O)NC5=O)cc4)no3)cc12
vPhos-as2-139	Z2159748972	-12.4	0.387	426.44	REAL	O=C1[C@H]2CC=CC[C@@H]2C(=O)N1Nc1cccc(-c2nc(-c3ccc4cc[nH]c4n3)no2)c1
vPhos-as2-140	Z2169733839	-12.4	0.376	438.49	REAL	O=C(Nc1n[nH]c2ccccc12)C1[C@H]2[C@@H]3C=C[C@H]([C@@H]4C(=O)N(Cc5ccccc5)C(=O)[C@H]34)[C@@H]12
vPhos-as2-141	Z2171889700	-12.4	0.376	437.50	REAL	Cc1ccccc1-c1noc(C2[C@H]3[C@@H]4C=C[C@H]([C@H]5C(=O)N(Cc6ccccc6)C(=O)[C@@H]45)[C@H]23)n1
vPhos-as2-142	Z2640091421	-12.4	0.428	383.41	REAL	O=C1[C@@H]2[C@@H]3C[C@H]4[C@@H]2[C@@]2(C(=O)Nc5nc(-c6ccc7cccc7n6)n[nH]5)[C@@H]1[C@@H]3[C@@H]42
vPhos-as2-143	Z2785110607	-12.4	0.459	365.43	REAL	CCCOc1ccccc1C(=O)CNC(=O)[C@]12[C@@H]3C(=O)[C@@H]4[C@H]5C[C@@H]([C@@H]41)[C@@H]2[C@H]53
vPhos-as2-144	Z2869537515	-12.4	0.443	376.42	REAL	O=C(Nc1cc2ccccc2nn1)N1CCC[C@H]1c1cc2c(c1)OCCO2
vPhos-as2-145	Z2902700571	-12.4	0.344	481.52	REAL	Cc1cc(C)n(-c2ccc(-c3noc(-c4ccc(NN5C(=O)[C@@H]6CC=CC[C@H]6C5=O)c4)n3)cn2)n1
vPhos-as2-146	Z2902742937	-12.4	0.376	479.48	REAL	CS(=O)(=O)c1ccc(-c2noc(C3CCN(C(=O)c4ccc(C(F)(F)F)cc4)CC3)n2)cc1
vPhos-as2-147	Z2903521762	-12.4	0.400	442.86	REAL	Cc1c(-c2noc(C3CCN(c4noc5ccc(Cl)cc45)CC3)n2)c(=O)[nH]c(=O)n1C
vPhos-as2-148	Z325118426	-12.4	0.428	395.50	REAL	Cc1ccc(C23C[C@H]4C[C@@H](CC(C(=O)OCCN5C(=O)CCC5=O)(C4)C2)C3)cc1
vPhos-as2-149	Z336594384	-12.4	0.400	421.45	REAL	O=C(NNC(=O)[C@H]1COc2ccccc2O1)[C@@H]1CC(=O)N(c2ccc3c(c2)CCC3)C1
vPhos-as2-150	Z365097060	-12.4	0.365	455.49	REAL	Cc1ccc(N2C(=O)/C(=C\Nc3cc4c(cc3F)CCC(=O)N4)c3ccccc3C2=O)cc1C
vPhos-as2-151	Z448673858	-12.4	0.354	465.51	REAL	O=C(NC[C@H]1CC2c3ccccc3C1c1ccccc12)NNC(=O)c1n[nH]c(=O)c2ccccc12
vPhos-as2-152	Z735258948	-12.4	0.365	452.51	REAL	Cc1ccc(N2C(=O)/C(=C/Nc3cccc(N4CCNC4=O)c3)c3ccccc3C2=O)cc1C
vPhos-as2-153	Z735279662	-12.4	0.365	453.54	REAL	Cc1ccc(N2C(=O)/C(=C\N[C@@H]3CCCN(c4ncccn4)C3)c3ccccc3C2=O)cc1C
vPhos-as2-154	Z804128848	-12.4	0.365	470.55	REAL	Cc1sc2ncn(NC(=O)[C@H]3CC(=O)N(c4ccc5c(c4)Cc4ccccc4-5)C3)c(=O)c2c1C
vPhos-as2-155	Z805712366	-12.4	0.344	481.51	REAL	COc1ccc(-c2nnc(COC(=O)[C@@H]3CC(=O)N(c4ccc5c(c4)Cc4ccccc4-5)C3)o2)cc1
vPhos-as2-156	Z805712484	-12.4	0.365	451.48	REAL	O=C(OCc1nnc(-c2ccccc2)o1)[C@@H]1CC(=O)N(c2ccc3c(c2)Cc2ccccc2-3)C1
vPhos-as2-157	Z805712572	-12.4	0.354	465.51	REAL	Cc1ccn2c(=O)cc(COC(=O)[C@@H]3CC(=O)N(c4ccc5c(c4)Cc4ccccc4-5)C3)nc2c1
vPhos-as2-158	Z826853494	-12.4	0.365	471.58	REAL	O=C(c1ccc2[nH]cnc2c1)N1CCN(C(=O)[C@@H]2CC=CC[C@H]2c2nc3ccccc3s2)CC1
vPhos-as2-159	Z924351782	-12.4	0.400	433.49	REAL	O=c1[nH]c(=O)c2cc(S(=O)(=O)N3CC=C(c4ccc5ccccc45)CC3)ccc2[nH]1
vPhos-as2-160	ZINC000005209194	-12.4	0.459	351.36	ZINC	Cc1nc2oc3c4ccccc4ccc3c(=O)c2c2nc3ccccc3n21
vPhos-as2-161	ZINC000009225450	-12.4	0.443	368.44	ZINC	Cc1nn2c(nnc3c2C[C@@H](c2ccc(C)cc2)CC3=O)c1-c1ccccc1
vPhos-as2-162	ZINC000033014745	-12.4	0.344	498.46	ZINC	O=C1NC2(CCCCC2)C(=O)N1N/C=C1\C(=O)N(c2ccccc(C(F)(F)F)c2)C(=O)c2ccccc21
vPhos-as2-163	ZINC000100698767	-12.4	0.387	428.49	ZINC	CC1=C[C@H]2C[C@H]1[C@H]1C(=O)N(c3cccc(N4C(=O)[C@H]5[C@H]6C=C(C)[C@@H](C6)[C@@H]5C4=O)c3)C(=O)[C@H]21
vPhos-as2-164	ZINC000102664280	-12.4	0.413	408.41	ZINC	C[C@H]1CC(O)=C2C(=NC(Nc3nc4ccccc4o3)=N[C@@H]2c2cc(F)cc(F)c2)C1
vPhos-as2-165	PV-001795673861	-12.3	0.424	409.88	REAL	Cc1cccc(C(=O)N2CCC[C@@H]2C(=O)Nc2nnc(-c3ccccc3Cl)[nH]2)c1
vPhos-as2-166	PV-001820538056	-12.3	0.397	419.52	REAL	CC(C)(C)c1ccc(C(=O)NNC(=O)[C@@H]2CC(=O)N(c3ccc4c(c3)CCC4)C2)cc1
vPhos-as2-167	PV-001828571076	-12.3	0.384	435.50	REAL	Cc1cc(N2C[C@H](C(=O)Nc3nnc(-c4ccc(C(C)(C)C)cc4)[nH]3)CC2=O)ccc1F
vPhos-as2-168	PV-001869139157	-12.3	0.410	408.54	REAL	Cc1cc(C)c(-c2cc(NC(=O)[C@@H]3CC(=O)N(C4CCC(C)CC4)C3)[nH]n2)cc1C
vPhos-as2-169	PV-001884142835	-12.3	0.424	409.88	REAL	Cc1cccc(C(=O)N2CCC[C@@H]2C(=O)Nc2nc(-c3ccc(Cl)cc3)n[nH]2)c1
vPhos-as2-170	PV-001907370542	-12.3	0.424	393.44	REAL	Cc1cccc(C(=O)NNC(=O)[C@@H]2CC(=O)N(c3ccc4c(c3)CCC4)C2)cc1O
vPhos-as2-171	PV-001948778849	-12.3	0.456	360.46	REAL	Cc1cccc(C[C@]2(C)CCCN2C(=O)Nc2cc3ccccc3nn2)c1
vPhos-as2-172	PV-001948779114	-12.3	0.439	382.41	REAL	C[C@@]1(Cc2ccc(F)c(F)c2)CCCN1C(=O)Nc1cc2ccccc2nn1
vPhos-as2-173	Z1014394788	-12.3	0.373	443.55	REAL	O=C(NCc1nnc2n1CCC2)[C@H]1C[C@@H]2CCCC[C@H]2N1C(=O)c1ccc2ccccc2c1
vPhos-as2-174	Z1069479596	-12.3	0.373	446.50	REAL	Cc1c(C(=O)N2CCC(C(=O)c3ccc4c(c3)NC(=O)[C@H](C)O4)CC2)oc2c(C)cccc12
vPhos-as2-175	Z1069482914	-12.3	0.373	443.50	REAL	Cc1nc2ccccc2cc1C(=O)N1CCC(C(=O)c2ccc3c(c2)NC(=O)[C@H](C)O3)CC1
vPhos-as2-176	Z1069483960	-12.3	0.384	432.52	REAL	C[C@@H]1Oc2ccc(C(=O)C3CCN(C(=O)c4ccc5c(c4)CCCC5)CC3)cc2NC1=O
vPhos-as2-177	Z1128817091	-12.3	0.373	464.95	REAL	CC(=O)N1Cc2ccccc2C[C@@H]1C(=O)N1CCC[C@@H](c2nc(-c3ccc(Cl)cc3)no2)C1
vPhos-as2-178	Z1190798510	-12.3	0.373	449.60	REAL	C[C@@H](NC(=O)[C@H]1CCCC[C@H]1C(=O)N1c2ccccc2C[C@H]1C)c1nnc2n1CCCCC2
vPhos-as2-179	Z1265332074	-12.3	0.373	440.50	REAL	Cc1ccccc1[C@H]1CN(C(=O)c2ccc(N3C(=O)c4ccccc4C3=O)cc2)[C@H](C)CO1
vPhos-as2-180	Z1267442045	-12.3	0.384	428.46	REAL	C[C@H]1C[C@@H](c2cccc(F)c2)N(C(=O)c2cccc(N3C(=O)c4ccccc4C3=O)c2)C1
vPhos-as2-181	Z1268242982	-12.3	0.373	448.47	REAL	O=C1O[C@H](C(=O)N2CCCN(C(=O)[C@@H]3Cc4ccccc4C(=O)O3)CC2)Cc2ccccc21
vPhos-as2-182	Z1280733585	-12.3	0.397	432.95	REAL	O=C1Nc2cc(Cl)ccc2C1=C1CCN(C(=O)[C@H]2C[C@]23CCCc2ccccc23)CC1
vPhos-as2-183	Z1373972850	-12.3	0.410	402.54	REAL	C[C@@H](C(=O)N1CCC[C@@H](c2nnc3n2CCCC3)C1)c1ccc2ccccc2c1
vPhos-as2-184	Z1384020225	-12.3	0.439	379.39	REAL	O=C(Nc1nc2ccc(F)cn2n1)[C@@H]1CC(=O)N(c2ccc3c(c2)CCC3)C1
vPhos-as2-185	Z1391609427	-12.3	0.384	424.54	REAL	O=C(N[C@@H]1CCCN(C(=O)[C@@H]2C[C@]23CCc2ccccc23)C1)c1ccc2ccccc2c1
vPhos-as2-186	Z1407895940	-12.3	0.424	401.49	REAL	Cc1ccc(-c2nc3c(s2)/C(=N/Nc2nc4ccccc4c(=O)[nH]2)CCC3)cc1
vPhos-as2-187	Z1451813869	-12.3	0.384	423.52	REAL	O=C(NC[C@H]1[C@H]2Cc3ccccc3[C@H]12)Nc1ccc(C(=O)N2CCc3ccccc32)c1
vPhos-as2-188	Z1531044259	-12.3	0.384	430.55	REAL	C[C@H]1C[C@H](C)CN(C(=O)c2ccccc2NC(=O)N2CCc3c([nH]c4ccccc34)C2)C1
vPhos-as2-189	Z1533926291	-12.3	0.373	448.52	REAL	Cc1ccc(N2C[C@H](C(=O)O[C@H](C)C(=O)c3ccc4c(c3)CC(=O)N4C)CCC2=O)cc1C
vPhos-as2-190	Z1553096181	-12.3	0.373	445.56	REAL	O=C([C@H]1C[C@@H]2CCCC[C@H]2N1C(=O)c1ccc2ccccc2c1)N1CCN2C(=O)CC[C@H]2C1
vPhos-as2-191	Z1595360070	-12.3	0.424	413.50	REAL	Cc1ccc(Cc2nnc(NC(=O)N3CC(=O)NC(=O)C34CCCC4)s2)cc1
vPhos-as2-192	Z1610572428	-12.3	0.397	415.50	REAL	O=C1c2ccccc2C(=O)N1[C@H]1CCCC[C@H](NCc2nc(-c3ccccc3)n[nH]2)C1
vPhos-as2-193	Z1614129232	-12.3	0.384	426.52	REAL	O=c1cc(CN2CCC[C@@H](c3n[nH]c(-c4ccccc4)n3)C2)c2cc3c(cc2o1)CCC3
vPhos-as2-194	Z1614243159	-12.3	0.410	408.50	REAL	O=C1O[C@H](C(=O)N2CCC[C@@H](c3n[nH]c(C4CCCCC4)n3)C2)Cc2ccccc21
vPhos-as2-195	Z1614248143	-12.3	0.397	412.54	REAL	O=C([C@@H]1C[C@]12CCCc1ccccc12)N1CCC[C@@H](c2n[nH]c(-c3ccccc3)n2)C1
vPhos-as2-196	Z1643361093	-12.3	0.397	412.44	REAL	C[C@H]1COc2ccccc2CN1C(=O)c1cccc(N2C(=O)c3ccccc3C2=O)c1
vPhos-as2-197	Z1682390649	-12.3	0.424	388.38	REAL	C[C@@]1(c2ccc(-c3noc(C4=Cc5ccccc5OC4)n3)cc2)NC(=O)NC1=O
vPhos-as2-198	Z1682390900	-12.3	0.410	402.45	REAL	C[C@@]1(c2ccc(-c3noc(C[C@H]4CCc5ccccc5C4)n3)cc2)NC(=O)NC1=O
vPhos-as2-199	Z1682391231	-12.3	0.397	417.40	REAL	Cc1cc(-c2nc(-c3ccc([C@]4(C)NC(=O)NC4=O)cc3)no2)c2ccc(F)cc2n1
vPhos-as2-200	Z1682391536	-12.3	0.424	389.37	REAL	Cn1nnc2ccc(-c3nc(-c4ccc([C@]5(C)NC(=O)NC5=O)cc4)no3)ccc21

Supplementary Table 22. Virtual screening hits 101 to 200 of the screen against the active site of the macrodomain in open conformation (Screen ID: 11). Compounds were filtered so that hits had MW < 600 dalton, cLogP < 6, number of hydrogen bond acceptors < 11, and no reactive functional groups. The name of each compound consists of the initial letter 'v' for virtual hit, followed by the target protein name and the target site ('as' for active site, 2 for docking scenario 2). The score is the docking score given by QuickVina 2 in kcal/mol. The ligand efficiency (LE) is computed as LE = -score/#NonH, where #NonH is the number of heavy (i.e. non hydrogen) atoms.

Name	Catalog ID	Score	LE	MW	Library	SMILES
vPlpro-as1-1	ZINC000004625770	-9.8	0.316	408.46	ZINC	CNC(=O)C1=C(C)Nc2nc3ccccc3n2[C@@H]1c1ccc2oc3ccccc3c2c1
vPlpro-as1-2	Z1580134599	-9.2	0.279	437.502	REAL	Cc1ccc(/C=C2/CCc3c2nc2ccccc2c3C(=O)Nc2nn(C)cc2C(N)=O)cc1
vPlpro-as1-3	Z1588380887	-9.2	0.307	398.421	REAL	O=C(OCc1nc(=O)[nH][nH]1)c1c2c(nc3ccccc13)/C(=C\c1ccccc1)CC2
vPlpro-as1-4	Z2608120210	-9.2	0.329	379.379	REAL	C[C@]1(c2cccc(-c3noc([C@@H]4CCCc5[nH]nnc54)n3)c2)NC(=O)NC1=O
vPlpro-as1-5	ZINC000239338793	-9.2	0.271	472.564	ZINC	Cc1ccc2c(c1)[C@H]1CN(C)CC[C@H]1N2C(=O)c1ccc2c(c1)S(=O)(=O)c1ccccc1C2=O
vPlpro-as1-6	ZINC000588226487	-9.1	0.294	422.511	ZINC	CSC1=NC(=O)C2=c3ccccc3=N[C@@H](c3c4ccccc4cc4ccccc43)N2N1
vPlpro-as1-7	Z1162534781	-9	0.29	431.427	REAL	O=C(Nc1nc2ccccc2c(=O)[nH]1)c1ccc2c(c1)S(=O)(=O)c1ccccc1C2=O
vPlpro-as1-8	Z1313223611	-9	0.321	368.395	REAL	O=C(CCC(=O)c1ccc2ccc3ccccc4ccc1c2c34)Nc1nnc[nH]1
vPlpro-as1-9	Z1381945046	-9	0.281	449.872	REAL	O=C(NCc1n[nH]c(=O)[nH]1)c1c2c(nc3ccccc13)/C(=C/c1c(F)cccc1Cl)CC2
vPlpro-as1-10	Z2227159520	-9	0.273	431.458	REAL	O=C(Nc1nnc2[nH]cnn12)c1cc(-c2ccc(-c3ccccc3)cc2)nc2ccccc12
vPlpro-as1-11	Z2476256758	-9	0.31	393.402	REAL	C[C@]1(c2cccc(-c3noc([C@]45C[C@H]6C[C@@H](C(=O)N4)[C@@H]5C6)n3)c2)NC(=O)NC1=O
vPlpro-as1-12	ZINC000101076130	-9	0.237	499.521	ZINC	O=C1c2ccccc2C(=O)C12O[C@@H](c1cccc1)[C@@H]1C(=O)N(c3ccc(-c4cccc4)cc3)C(=O)[C@@H]12
vPlpro-as1-13	Z1329937673	-8.9	0.297	398.421	REAL	Cc1cc(C(=O)N(C)C2c3ccccc3-c3ccccc32)nc2nc(O)[nH]c(=O)c12
vPlpro-as1-14	Z2002423492	-8.9	0.278	425.483	REAL	O=C1[C@@H]2[C@@H]3C[C@H]4[C@@H]2[C@]2(C(=O)Oc5cccc(C(=O)N6CCCc7ccccc7C6)c5)[C@H]1[C@@H]3[C@@H]42
vPlpro-as1-15	Z2221930705	-8.9	0.287	421.412	REAL	C[C@]1(c2cccc(-c3noc(CN4C(=O)[C@H]5CC=CC[C@H]5C4=O)n3)c2)NC(=O)NC1=O
vPlpro-as1-16	Z2608004674	-8.9	0.318	379.379	REAL	C[C@]1(c2ccc(-c3noc([C@@H]4CCCc5[nH]nnc54)n3)cc2)NC(=O)NC1=O
vPlpro-as1-17	Z2902754635	-8.9	0.342	339.357	REAL	c1ccc(-c2ccc(-c3noc(-c4cccc5nn[nH]c45)n3)cc2)cc1
vPlpro-as1-18	Z298859774	-8.9	0.241	491.546	REAL	O=C(N[C@H]1CCCc2[nH]c(=O)ccc21)c1c2c(nc3ccccc13)/C(=C/c1ccc3c(c1)OCO3)CC2
vPlpro-as1-19	ZINC000002751243	-8.9	0.254	455.468	ZINC	O=C1c2cc3oc4ccccc4c4ccccc4oc3cc2C(=O)N1c1ccccc2ccccc21
vPlpro-as1-20	ZINC000100504092	-8.9	0.287	404.512	ZINC	O=c1ccccc2n1C[C@H]1C[C@H]2CN(Cc2ccc3ccc4ccccc5ccc2c3c45)C1
vPlpro-as1-21	PV-001843557134	-8.8	0.293	403.485	REAL	CNC(=O)Nc1cccc(C(=O)N2CCCC[C@H]2c2nc(-c3cccc3)c[nH]2)c1
vPlpro-as1-22	PV-001866698351	-8.8	0.275	446.428	REAL	Cc1cc(C(=O)N2CC[C@@H](c3cccc(C(F)(F)F)c3)C2(C)C)nc2nc(O)[nH]c(=O)c12
vPlpro-as1-23	Z1348802091	-8.8	0.284	431.467	REAL	O=C(Nc1ccc2c(c1)C(=O)CCC2)c1ccc2c(c1)S(=O)(=O)c1ccccc1C2=O
vPlpro-as1-24	Z1418327339	-8.8	0.314	393.869	REAL	O=C(c1cc(Cl)c2ccccc2c1O)N1CCC2(CC1)OCc1ccccc12
vPlpro-as1-25	Z1451423747	-8.8	0.275	425.487	REAL	C[C@]1(c2cccc(C(=O)N3Cc4ccccc4[C@@H](c4ccccc4)C3)c2)NC(=O)NC1=O
vPlpro-as1-26	Z1479461244	-8.8	0.259	449.556	REAL	Cn1ccnc1N1CCN(C(=O)c2c3c(nc4ccccc24)/C(=C\c2ccccc2)CC3)CC1
vPlpro-as1-27	Z1683018400	-8.8	0.284	436.345	REAL	CC(=O)Nc1ccc(-c2noc(-c3cc(NC(=O)OCC(F)(F)F)ccc3O)n2)cc1
vPlpro-as1-28	Z1701868735	-8.8	0.267	440.502	REAL	C[C@]1(c2cccc(CNC(=O)N3CCc4c(-c5ccccc5)cccc43)c2)NC(=O)NC1=O
vPlpro-as1-29	Z1841450164	-8.8	0.284	429.495	REAL	O=C1c2ccccc2S(=O)(=O)c2cc(C(=O)N3CC4(CCC4)c4ccccc43)ccc21
vPlpro-as1-30	Z1975306154	-8.8	0.275	438.433	REAL	NC(=O)CCNC(=O)Nc1cccc(NC(=O)c2cccc(-c3c(F)cccc3F)c2)c1
vPlpro-as1-31	Z2028189624	-8.8	0.275	433.51	REAL	O=C(c1cccc2ccccc12)N1CCC[C@@H](C(=O)N2CCC[C@@H](c3nc(=O)[nH][nH]3)C2)C1
vPlpro-as1-32	Z2225986698	-8.8	0.275	427.507	REAL	Cc1ccc(-c2cc(C(=O)N3CCC[C@@H](c4nc(=O)[nH][nH]4)C3)c3ccccc3n2)c(C)c1
vPlpro-as1-33	Z2371494791	-8.8	0.303	389.458	REAL	N#Cc1cccnc1N1CCN(C(=O)Nc2ccc3c(c2)C(=O)CCCC3)CC1
vPlpro-as1-34	Z2905434948	-8.8	0.367	320.391	REAL	O=C1CC[C@@H](c2ccc(-c3cccc([C@H]4CCNC4=O)c3)cc2)N1
vPlpro-as1-35	Z433472214	-8.8	0.284	412.492	REAL	O=C(Nc1cccc(N2CCNC2=O)c1)N1CCc2ccccc2[C@@H](c2ccccc2)C1
vPlpro-as1-36	Z734855420	-8.8	0.367	312.335	REAL	c1ccc2c(c1)C(=NNc1ncnc3nc[nH]c13)c1ccccc1-2
vPlpro-as1-37	Z806245950	-8.8	0.244	481.554	REAL	NC(=O)c1ccc(N2CCN(C(=O)[C@@H]3CC(=O)N(c4ccc5c(c4)Cc4ccccc4-5)C3)CC2)nc1
vPlpro-as1-38	Z98335468	-8.8	0.267	435.486	REAL	NC1=Nc2nc3cc4c(cc3n2[C@H](c2c3ccccc3cc3ccccc23)N1)OCCCO4
vPlpro-as1-39	Z993685582	-8.8	0.244	485.626	REAL	Cc1ccc(C23C[C@@H]4C[C@H](CC(C(=O)NCc5ccccc5[C@@]6(C)NC(=O)NC6=O)c5)(C4)C2)C3)cc1C
vPlpro-as1-40	ZINC000001588361	-8.8	0.259	440.509	ZINC	Nc1nc(-c2cc(-c3cccc4ccccc43)nc(N)n2)cc(-c2cccc3ccccc32)n1
vPlpro-as1-41	ZINC000001664790	-8.8	0.244	468.574	ZINC	O=C1c2ccc3ccccc3c2CC[C@H]1[C@@]1([n+]2ccccc2)CCc2c3ccccc3ccc2C1=O
vPlpro-as1-42	ZINC000006045805	-8.8	0.338	338.369	ZINC	O=C1Nc2ccccc2/C1=N\Nc1nc2ccccc2c2ccccc21
vPlpro-as1-43	ZINC000011612116	-8.8	0.275	418.407	ZINC	Cn1c(=O)c2ccc3c4ccc5c6c(ccc(c7ccc(c2c37)c1=O)c46)c(=O)n(C)c5=O
vPlpro-as1-44	ZINC000100485510	-8.8	0.275	410.431	ZINC	O=C1c2ccc3c4c(ccc(c24)C2=Nc4ccccc4[C@H]21)C1=Nc2ccccc2[C@H]1C3=O
vPlpro-as1-45	ZINC000104879883	-8.8	0.251	466.543	ZINC	C[C@@H](OC(=O)c1c2c(nc3ccccc31)/C(=C\c1ccccc1)CC2)c1nc(N)nc(N(C)C)n1
vPlpro-as1-46	ZINC000408563977	-8.8	0.251	473.503	ZINC	O=C1Nc2ccccc2[C@]12[C@H](/[N+](=O)[O-])[C@@H](c1ccc(OCc3ccccc3F)cc1)[C@@H]1CCCN12
vPlpro-as1-47	PV-001944164475	-8.7	0.322	368.392	REAL	O=C1CCCc2ccc(NC(=O)N3CC[C@H](c4cc(=O)[nH]c(=O)[nH]4)C3)cc21
vPlpro-as1-48	PV-001944178908	-8.7	0.3	390.446	REAL	Cc1nc(-c2ccc(C)c(NC(=O)N3CC(=O)N(C)c4ccccc4C3)c2)n[nH]1
vPlpro-as1-49	Z1000943544	-8.7	0.272	430.506	REAL	C[C@H]1CCc2[nH]c3ccc(C(=O)NCc4cccc([C@@]5(C)NC(=O)NC5=O)c4)cc3c2C1
vPlpro-as1-50	Z109881682	-8.7	0.272	450.441	REAL	C[C@H]1CC(=O)c2c(OC(=O)c3ccc4c(c3)S(=O)(=O)c3ccccc3C4=O)ccc(F)c21
vPlpro-as1-51	Z1284391841	-8.7	0.29	397.477	REAL	CNC(=O)Cn1ccc2ccc(NC(=O)[C@@H]3C[C@H]3c3cccc4ccccc34)cc21
vPlpro-as1-52	Z1411897194	-8.7	0.29	424.476	REAL	O=C1CN(C(=O)c2ccc3c(c2)S(=O)(=O)c2ccccc2C3=O)[C@H]2CCCC[C@@H]2N1
vPlpro-as1-53	Z1460469899	-8.7	0.3	388.422	REAL	O=C(O[C@H]1CCNC1=O)c1c2c(nc3ccccc13)/C(=C/c1ccco1)CCC2
vPlpro-as1-54	Z1462140008	-8.7	0.272	425.53	REAL	Cc1ccc2c(c1)[C@H]1CN(C)CC[C@H]1N2C(=O)c1cncc(-c2ccc3c(c2)CCO3)c1
vPlpro-as1-55	Z1511588001	-8.7	0.281	449.55	REAL	C[C@@H]1CSc2ccccc2N(C(=O)c2ccc3c(c2)S(=O)(=O)c2ccccc2C3=O)C1
vPlpro-as1-56	Z1684579508	-8.7	0.281	417.424	REAL	CN1C(=O)C[C@H](c2nc(-c3cccc([C@@]4(C)NC(=O)NC4=O)c3)no2)c2ccccc21
vPlpro-as1-57	Z1684582706	-8.7	0.281	417.424	REAL	C[C@]1(c2cccc(-c3noc(CN4C(=O)CCc5ccccc54)n3)c2)NC(=O)NC1=O
vPlpro-as1-58	Z1842627070	-8.7	0.29	413.394	REAL	O=C(CCC(=O)c1ccc2ccc3cccc4ccc1c2c34)NC[C@@H](O)C(F)(F)F
vPlpro-as1-59	Z1907872359	-8.7	0.3	398.368	REAL	NC(=O)N1CCCc2ccc(NC(=O)c3cnc4c(F)cc(F)cc4c3O)cc21
vPlpro-as1-60	Z1907890376	-8.7	0.311	375.471	REAL	NC(=O)N1CCCc2ccc(NC(=O)[C@@H]3C[C@]34CCCc3ccccc34)cc21
vPlpro-as1-61	Z1907890391	-8.7	0.311	376.415	REAL	Cc1c(C(=O)Nc2ccc3c(c2)N(C(N)=O)CCC3)c(O)nc2ccccc12
vPlpro-as1-62	Z1943459592	-8.7	0.322	361.4	REAL	NC(=O)N1CCCc2ccc(NC(=O)c3cc(O)c4ccccc4c3)cc21
vPlpro-as1-63	Z1963612202	-8.7	0.272	425.53	REAL	Cc1ccc2c(c1)[C@H]1CN(C)CC[C@H]1N2C(=O)c1cncc(-c2ccc3c(c2)CCO3)c1
vPlpro-as1-64	Z1997870618	-8.7	0.29	405.496	REAL	CC1(C)CCc2ccccc2[C@H](NC(=O)c2cccc([C@@]3(C)NC(=O)NC3=O)c2)C1
vPlpro-as1-65	Z2156918190	-8.7	0.3	392.389	REAL	Cc1cc(C(=O)N[C@@H](C)c2ccc(F)c3ccccc23)nc2nc(O)[nH]c(=O)c12
vPlpro-as1-66	Z2157920095	-8.7	0.3	388.382	REAL	C[C@]1(c2cccc(-c3noc([C@H]4CC(=O)c5ccccc54)n3)c2)NC(=O)NC1=O
vPlpro-as1-67	Z2159455872	-8.7	0.281	412.412	REAL	O=C(Cc1noc(-c2nn[nH]c2-c2ccccc2)n1)N1CCn2c1nc1ccccc12
vPlpro-as1-68	Z2233225149	-8.7	0.264	445.478	REAL	Cc1ccc(C)c(N2C(=O)c3ccc(C(=O)N4CCC[C@@H](c5nc(=O)[nH][nH]5)C4)cc3C2=O)c1
vPlpro-as1-69	Z226811652	-8.7	0.272	446.478	REAL	Cc1ccc(OC(=O)c2ccc3c(c2)S(=O)(=O)c2ccccc2C3=O)c2c1[C@@H](C)CC2=O
vPlpro-as1-70	Z2651925511	-8.7	0.235	492.577	REAL	O=C(c1c2c(nc3ccccc13)/C(=C\c1ccco1)CCC2)N1Cc2ccnc2N2C[C@H](O)C[C@H]2C1
vPlpro-as1-71	Z283995916	-8.7	0.281	414.46	REAL	O=C(N[C@H]1CCCc2[nH]c(=O)ccc21)c1ccc2c(c1)C[C@@H](c1ccccc1)OC2=O
vPlpro-as1-72	Z2877665446	-8.7	0.3	386.454	REAL	Cc1nc2cc(C(=O)N3CCC(c4c[nH]c5ccccc45)CC3)ccc2c(=O)[nH]1
vPlpro-as1-73	Z2903061099	-8.7	0.281	410.432	REAL	O=C1N=CC=C[C@H]1c1noc([C@H]2CC(=O)N(c3ccc4c(c3)Cc3ccccc3-4)C2)n1
vPlpro-as1-74	Z2990878377	-8.7	0.322	383.842	REAL	Cc1nc([C@@H]2CCN(c3nnnn3[C@H]3[C@H]4Cc5c(Cl)cccc5[C@@H]43)C2)no1
vPlpro-as1-75	Z2991040225	-8.7	0.363	323.347	REAL	O=C1CC[C@@H](c2ccc(-c3ccc4c(c3)[C@H](C(=O)O)CO4)cc2)N1
vPlpro-as1-76	Z56769338	-8.7	0.3	380.454	REAL	CCn1c2ccccc2c2cc([C@@H]3NC(N)=Nc4nc5ccccc5n43)ccc21
vPlpro-as1-77	Z806008328	-8.7	0.281	416.44	REAL	Cc1nnc(NNC(=O)[C@@H]2CC(=O)N(c3ccc4c(c3)Cc3ccccc3-4)C2)[nH]c1=O
vPlpro-as1-78	Z852301160	-8.7	0.242	480.562	REAL	O=C1O[C@H](c2ccccc2)Cc2cc(C(=O)N3CCC(C(=O)N4CCc5ccccc54)CC3)ccc21
vPlpro-as1-79	Z858524370	-8.7	0.311	369.379	REAL	O=C(Nc1ccc2c(c1)Cc1ccccc1-2)Nc1ccc2c(c1)C(=O)NC2=O
vPlpro-as1-80	ZINC000000988780	-8.7	0.272	415.407	ZINC	O=c1c2ccc3c(=O)n(-c4ccccc4)c(=O)c4ccc(c5nc6ccccc6n51)c2c43
vPlpro-as1-81	ZINC000004265433	-8.7	0.249	473.551	ZINC	COC(=O)C1=N[C@]2(SC23c2ccccc2-c2ccccc23)C2(O1)c1ccccc1-c1ccccc12
vPlpro-as1-82	ZINC000005387000	-8.7	0.229	496.477	ZINC	COc1ccc(-n2c(=O)c3cc4c5ccc6c(=O)[nH]c(=O)c7ccc(c8ccc(c2=O)c3c48)c5c67)cc1
vPlpro-as1-83	ZINC000005389365	-8.7	0.281	409.484	ZINC	O=C(/C=C1\NCCc2cc3c(cc21)OCCCO3)C1c2ccccc2-c2ccccc21
vPlpro-as1-84	ZINC000009251328	-8.7	0.272	439.506	ZINC	Cc1c(C(=O)N2CCC3(CC2)OCCO3)oc2ccc3c(c12)C(=O)CC1(CCCCC1)O3
vPlpro-as1-85	ZINC000016919178	-8.7	0.256	448.517	ZINC	O=C1c2ccccc2C(=O)[C@H]2CC3=C(CC4=C(C3)C[C@@H]3C(=O)c5ccccc5C(=O)[C@@H]3C4)C[C@@H]12
vPlpro-as1-86	ZINC000020569790	-8.7	0.242	486.61	ZINC	C[C@@H]1CCC[C@H](n2c(=O)c3ccc4c5c(ccc(c35)c2=O)c(=O)n([C@@H]2CCC[C@@H](C)[C@@H]2C)c4=O)[C@@H]1C
vPlpro-as1-87	ZINC000022418719	-8.7	0.281	407.432	ZINC	O=c1[nH]c2ccccc2c2c1[C@@H](c1ccccc1)N/C(=N\c1nc3ccccc3o1)N2
vPlpro-as1-88	ZINC000036370631	-8.7	0.242	464.563	ZINC	O=C1[C@@H]2C3c4ccccc4C(c4ccccc43)[C@H]2C(=O)[C@H]2C3c4ccccc4C(c4ccccc43)[C@@H]12
vPlpro-as1-89	ZINC000102319789	-8.7	0.272	414.463	ZINC	O=C1Nc2ccccc2/C1=C\c1ccc2ccc(/C=C3/C(=O)Nc4ccccc43)cc2c1
vPlpro-as1-90	ZINC000103904797	-8.7	0.29	392.457	ZINC	Cc1cc2c(cc1C)NC1=C(O)[C@H](c3c4ccccc4cc4ccccc43)OC1=N2
vPlpro-as1-91	ZINC000104480052	-8.7	0.242	490.945	ZINC	O=C(NC1=CC=C[C@@H]2C(=O)c3ccccc3C(=O)[C@H]12)c1cc(-c2ccccc2Cl)nc2ccccc21
vPlpro-as1-92	ZINC000104480060	-8.7	0.242	490.945	ZINC	O=C(NC1=CC=C[C@@H]2C(=O)c3ccccc3C(=O)[C@@H]12)c1cc(-c2ccccc2Cl)nc2ccccc21
vPlpro-as1-93	ZINC000408675227	-8.7	0.229	498.58	ZINC	Cc1cccc(NC(=O)c2ccc(N3C(=O)[C@H]4[C@H](C3=O)C3c5ccccc5C4c4ccccc43)c2)c1C
vPlpro-as1-94	PV-001792855242	-8.6	0.277	413.436	REAL	Cc1ccc(-c2cc(NC(=O)c3[nH]c(=O)[nH]c(=O)c3N)nc(-c3ccccc3)c2)cc1
vPlpro-as1-95	PV-001804466420	-8.6	0.253	459.495	REAL	CNC(=O)CN(C)C(=O)c1c(C)c(-c2ccc(-c3ccccc3F)cc2)nc2ccc(F)cc12
vPlpro-as1-96	PV-001812862555	-8.6	0.277	416.48	REAL	CC(=O)NCC(=O)N1CCC[C@@H]1C(=O)Nc1cc(-c2ccccc2)nc2ccccc12
vPlpro-as1-97	PV-001813622296	-8.6	0.319	387.786	REAL	Cn1ncc2c(=O)nc(NC(=O)c3ccc(Cl)c(N4CCNC4=O)c3)[nH]c21
vPlpro-as1-98	PV-001851509350	-8.6	0.307	446.275	REAL	C[C@@]1(c2cccc(C(=O)N3CCc4c(F)ccc(Br)c4C3)c2)NC(=O)NC1=O
vPlpro-as1-99	PV-001857869184	-8.6	0.344	339.354	REAL	O=C(c1cc(-c2ccccc2O)[nH]n1)N1CC[C@@H](c2cc(O)[nH]n2)C1
vPlpro-as1-100	PV-001874412850	-8.6	0.297	389.41	REAL	C[C@@]1(c2cccc(C(=O)NCc3c(O)ccc4ccccc34)c2)NC(=O)NC1=O

Supplementary Table 23. Top 100 virtual hits of the screen against the active site of PL^{pro} (Screen ID: 12). Compounds were filtered so that hits had MW < 600 dalton, cLogP < 6, number of hydrogen bond acceptors < 11, and no reactive functional groups. A few compounds unsuitable for drug discovery were removed by visual inspection. The name of each compound consists of the initial letter 'v' for virtual hit, followed by the target protein name and the target site ('as' for active site, 1 for docking scenario 1). The score is the docking score given by QuickVina 2 in kcal/mol. The ligand efficiency (LE) is computed as LE = -score/#NonH, where #NonH is the number of heavy (i.e. non hydrogen) atoms.

Name	Catalog ID	Score	LE	MW	Library	SMILES
vPlpro-as1-101	PV-001875408549	-8.6	0.307	386.41	REAL	C[C@]1(c2ccc(C(=O)N3CCC4(CCNC(=O)O4)CC3)cc2)NC(=O)NC1=O
vPlpro-as1-102	PV-001878878021	-8.6	0.297	390.40	REAL	Cc1ccc(-c2c(C)n[nH]c2NC(=O)c2cc(C)c3c(=O)[nH]c(O)nc3n2)cc1
vPlpro-as1-103	PV-001878955056	-8.6	0.297	410.82	REAL	Cc1n[nH]c(NC(=O)c2cc(C)c3c(=O)[nH]c(O)nc3n2)c1-c1cccc(Cl)c1
vPlpro-as1-104	PV-001900498784	-8.6	0.277	410.48	REAL	NC(=O)NCCNC(=O)c1ccc(-c2ccc(-c3ccccc3)cc2)nc2ccccc12
vPlpro-as1-105	Z1014363782	-8.6	0.239	480.57	REAL	O=C(NNC(=O)[C@@H]1C[C@H]2CCCC[C@@H]2N1C(=O)c1ccc2ccccc2c1)c1c[nH]c2ccccc12
vPlpro-as1-106	Z1014641074	-8.6	0.232	492.58	REAL	O=C(NNC(=O)[C@@H]1C[C@H]2CCCC[C@@H]2N1C(=O)c1ccc2ccccc2c1)c1cccc2ccenc12
vPlpro-as1-107	Z1015254072	-8.6	0.287	418.52	REAL	CC(=O)N1CCc2cc(S(=O)(=O)N3CCc4ccccc4-c4ccccc4C3)ccc21
vPlpro-as1-108	Z1031611182	-8.6	0.269	421.50	REAL	O=C1CN(C(=O)c2cc(-c3ccc(-c4ccccc4)cc3)nc3ccccc23)CCCN1
vPlpro-as1-109	Z112144674	-8.6	0.246	483.45	REAL	O=C(COC(=O)c1c2c(nc3ccccc13)/C(=C\c1ccccc1)CC2)NC(=O)NCC(F)(F)F
vPlpro-as1-110	Z1135059810	-8.6	0.269	425.49	REAL	Cc1ccccc1-c1cccc([C@@H]2NC(N)=Nc3nc4cc5c(cc4n32)OCCCO5)c1
vPlpro-as1-111	Z1167318249	-8.6	0.277	417.44	REAL	O=C(N[C@H]1CCOc2ccc(F)cc21)c1ccc2c(c1)C[C@@H](c1ccccc1)OC2=O
vPlpro-as1-112	Z1174754345	-8.6	0.269	430.47	REAL	O=C([C@H]1CC(=O)N(c2ccc3c(c2)Cc2ccccc2-3)C1)N1CCO[C@H](c2nnn[nH]2)C1
vPlpro-as1-113	Z1195478438	-8.6	0.277	411.46	REAL	Cn1nnnc1COC(=O)c1c2c(nc3ccccc13)/C(=C\c1ccccc1)CCC2
vPlpro-as1-114	Z1229730348	-8.6	0.277	438.59	REAL	C[C@H]1C[C@@H]2CCCC[C@H]2N1C(=O)c1cccc(S(=O)(=O)N2c3ccccc3C[C@@H]2C)c1
vPlpro-as1-115	Z1232080198	-8.6	0.277	412.41	REAL	O=C(Nc1nnn[nH]1)c1c2c(nc3ccccc13)/C(=C\c1ccc3c(c1)OCO3)CC2
vPlpro-as1-116	Z1250584790	-8.6	0.307	374.40	REAL	Cc1cc(C(=O)N[C@@H](C)c2cccc3ccccc23)nc2nc(O)[nH]c(=O)c12
vPlpro-as1-117	Z1278192764	-8.6	0.297	394.45	REAL	CNC(=O)Cn1ccc2ccc(NC(=O)N3CCc4cccc(F)c4[C@H]3C)cc21
vPlpro-as1-118	Z1311761303	-8.6	0.261	447.49	REAL	O=C(NC[C@H]1CCC[C@]12NC(=O)NC2=O)Nc1cccc(C(=O)N2CCc3ccccc32)c1
vPlpro-as1-119	Z1312740018	-8.6	0.307	378.39	REAL	Cc1cc(C(=O)N2CC=C(c3ccc(O)cc3)CC2)nc2nc(O)[nH]c(=O)c12
vPlpro-as1-120	Z1313109499	-8.6	0.287	402.41	REAL	Cc1cc(C(=O)N2CCc3c(cnn3-c3ccccc3)C2)nc2nc(O)[nH]c(=O)c12
vPlpro-as1-121	Z1330295941	-8.6	0.331	348.36	REAL	CN(C(=O)c1[nH]c(=O)[nH]c(=O)c1N)C1c2ccccc2-c2ccccc21
vPlpro-as1-122	Z1330520607	-8.6	0.307	371.40	REAL	Cc1nc(C(=O)N(C)C2c3ccccc3-c3ccccc32)nn1-c1nnc[nH]1
vPlpro-as1-123	Z1333926093	-8.6	0.358	316.36	REAL	O=C(c1ccc2c(c1)-c1ccccc1C2)N1CCc2nn[nH]c2C1
vPlpro-as1-124	Z1369936592	-8.6	0.287	401.47	REAL	O=C(Nc1cccc(C(=O)N2CCc3cc(-c4ccccc4)oc3C2)c1)NC1CC1
vPlpro-as1-125	Z1417811909	-8.6	0.297	392.41	REAL	Cc1cc(C(=O)N2CCC3(CC2)OCc2ccccc23)nc2nc(O)[nH]c(=O)c12
vPlpro-as1-126	Z1417819669	-8.6	0.297	392.41	REAL	Cn1c(=O)[nH]c(=O)c2cc(C(=O)N3CCC4(CC3)OCc3ccccc34)cnc21
vPlpro-as1-127	Z1434566780	-8.6	0.269	423.52	REAL	CC(=O)N1CCN(C(=O)c2cc(-c3cccc4ccccc34)nc3ccccc23)[C@@H](C)C1
vPlpro-as1-128	Z1452101750	-8.6	0.319	363.42	REAL	Cc1cccc2c1CCN(C(=O)c1cccc([C@@]3(C)NC(=O)NC3=O)c1)C2
vPlpro-as1-129	Z1452804926	-8.6	0.277	423.43	REAL	C[C@]1(c2cccc(C(=O)N3CCN(C(=O)c4ccc(=O)[nH]c4)CC3)c2)NC(=O)NC1=O
vPlpro-as1-130	Z1452857456	-8.6	0.307	385.37	REAL	C[C@]1(c2cccc(C(=O)N3CCc4c(F)ccc(F)c4C3)c2)NC(=O)NC1=O
vPlpro-as1-131	Z1452890997	-8.6	0.287	405.50	REAL	Cc1ccc([C@@H]2[C@@H](C)CCCN2C(=O)c2cccc([C@@]3(C)NC(=O)NC3=O)c2)cc1
vPlpro-as1-132	Z1462331687	-8.6	0.269	432.43	REAL	C[C@@]1(c2cccc(C(=O)OCc3cc(=O)oc4cc5c(cc34)CCC5)c2)NC(=O)NC1=O
vPlpro-as1-133	Z148143666	-8.6	0.287	400.43	REAL	O=C1NC[C@@H](COC(=O)c2c3c(nc4ccccc24)/C(=C/c2ccccc2)CC3)O1
vPlpro-as1-134	Z1481746626	-8.6	0.287	404.43	REAL	Cc1ccc(C)c(-n2ncc(NC(=O)c3cc(C)c4c(=O)[nH]c(O)nc4n3)c2C)c1
vPlpro-as1-135	Z1506002348	-8.6	0.307	369.38	REAL	O=C(Cc1cc2c(ccc3ccccc32)o1)Nc1nc2ccccc2c(=O)[nH]1
vPlpro-as1-136	Z1515530361	-8.6	0.277	437.52	REAL	O=C(N[C@H]1[C@H]2CCO[C@@H]2C12CCCC2)c1ccc2c(c1)S(=O)(=O)c1ccccc1C2=O
vPlpro-as1-137	Z1521921304	-8.6	0.269	435.43	REAL	C[C@]1(c2cccc(CNC(=O)c3cccc(-c4c(F)cccc4F)c3)c2)NC(=O)NC1=O
vPlpro-as1-138	Z1531873572	-8.6	0.277	440.52	REAL	CC1(C)CCC(NC(=O)c2ccc3c(c2)S(=O)(=O)c2ccccc2C3=O)C(N)=O)CC1
vPlpro-as1-139	Z1552640130	-8.6	0.277	419.48	REAL	CNC(=O)[C@@H]1CCC[C@@H]1NC(=O)c1ccc2c(c1)C(=O)N(c1cc(C)ccc1C)C2=O
vPlpro-as1-140	Z1576137061	-8.6	0.261	437.46	REAL	Cc1ccc(C)c(N2C(=O)c3ccc(C(=O)Nc4ccccc4-c4nnc[nH]4)cc3C2=O)c1
vPlpro-as1-141	Z1667075702	-8.6	0.277	410.48	REAL	Cn1ncnc1COC(=O)c1c2c(nc3ccccc13)/C(=C\c1ccccc1)CCC2
vPlpro-as1-142	Z1669361714	-8.6	0.319	363.46	REAL	O=C(c1ccc2c(c1O)CCCC2)N1CCC2(CC1)OCc1ccccc12
vPlpro-as1-143	Z1682711662	-8.6	0.319	362.34	REAL	O=C1CCCN1c1ccc(-c2noc(-c3ccccc4[nH]c(=O)oc34)n2)cc1
vPlpro-as1-144	Z1684579693	-8.6	0.287	404.43	REAL	C[C@]1(c2cccc(-c3noc(-c4cc5c(cc4O)CCCC5)n3)c2)NC(=O)NC1=O
vPlpro-as1-145	Z1684579932	-8.6	0.287	400.39	REAL	C[C@]1(c2cccc(-c3noc(-c4cc5ccccc5cc4O)n3)c2)NC(=O)NC1=O
vPlpro-as1-146	Z1684580686	-8.6	0.277	417.42	REAL	CC(=O)N1c2ccccc2C[C@H]1c1nc(-c2cccc([C@@]3(C)NC(=O)NC3=O)c2)no1
vPlpro-as1-147	Z1684582157	-8.6	0.269	432.48	REAL	Cc1ccccc1C1(c2nc(-c3cccc([C@]4(C)NC(=O)NC4=O)c3)no2)CCOCC1
vPlpro-as1-148	Z1720488958	-8.6	0.287	411.41	REAL	C[C@]1(c2cccc(C(=O)N3CC=C(c4c(F)ccc4F)CC3)c2)NC(=O)NC1=O
vPlpro-as1-149	Z1752153169	-8.6	0.269	433.51	REAL	C[C@H](NC(=O)N1CC[C@]2(C1)C(=O)Nc1ccccc12)c1ccc(NC(=O)NC2CC2)cc1
vPlpro-as1-150	Z1834416322	-8.6	0.261	448.46	REAL	Cc1cc(C(=O)N2CCCC[C@H]2c2nc(-c3cccc(F)c3)c[nH]2)nc2nc(O)[nH]c(=O)c12
vPlpro-as1-151	Z1852536067	-8.6	0.307	378.43	REAL	Cc1cc(C(=O)N[C@H]2CCC[C@H](c3ccccc3)C2)nc2nc(O)[nH]c(=O)c12
vPlpro-as1-152	Z1867099401	-8.6	0.319	363.42	REAL	Cc1cccc2c1CN(C(=O)c1cccc([C@]3(C)NC(=O)NC3=O)c1)CC2
vPlpro-as1-153	Z1907889335	-8.6	0.269	428.49	REAL	NC(=O)N1CCCc2ccc(NC(=O)[C@H]3CC(=O)N(c4cccc5cccc45)C3)cc21
vPlpro-as1-154	Z1953102765	-8.6	0.269	430.47	REAL	Cc1cc(C(=O)N2CCCC[C@H]2c2nc(-c3ccccc3)c[nH]2)nc2nc(O)[nH]c(=O)c12
vPlpro-as1-155	Z1954532933	-8.6	0.307	382.39	REAL	Cc1cc(C(=O)N[C@@H]2CC[C@H](c3cccc(F)c3)C2)nc2nc(O)[nH]c(=O)c12
vPlpro-as1-156	Z1983291199	-8.6	0.269	436.51	REAL	O=C(CN1C(=O)N[C@]2(C[C@@H]3C[C@@H]2[C@H]2CCC[C@H]32)C1=O)Nc1cccc(N2CCCC2=O)c1
vPlpro-as1-157	Z1985378426	-8.6	0.277	412.44	REAL	O=C1CC[C@H](OC(=O)c2c3c(nc4ccccc24)/C(=C\c2ccccc2)CC3)C(=O)N1
vPlpro-as1-158	Z1995499474	-8.6	0.297	411.84	REAL	C[C@@H]1CCNC(=O)[C@@H]1NC(=O)c1ccc2c(c1)C(=O)N(c1cccc1Cl)C2=O
vPlpro-as1-159	Z203231200	-8.6	0.253	464.52	REAL	Cc1cc(NC(=O)CN2CCN(C(=O)c3ccc4c(=O)n5c(nc4c3)CCCCC5)CC2)no1
vPlpro-as1-160	Z2077116289	-8.6	0.307	368.40	REAL	O=C(Nc1cccc(-c2n[nH]c(=O)[nH]2)c1)c1ccc2c(c1)Cc1ccccc1-2
vPlpro-as1-161	Z2157919690	-8.6	0.287	402.41	REAL	C[C@]1(c2cccc(-c3noc([C@@]45[C@H]6C(=O)[C@@H]7[C@@H]8C[C@@H]([C@@H]74)[C@@H]5[C@H]86)n3)c2)NC(=O)NC1=O
vPlpro-as1-162	Z2193371631	-8.6	0.319	366.38	REAL	Cc1cccc2c1OC[C@H](NC(=O)c1cc(C)c3c(=O)[nH]c(O)nc3n1)C2
vPlpro-as1-163	Z2221930694	-8.6	0.277	421.36	REAL	C[C@]1(c2cccc(-c3noc(-c4cnc5c(F)ccc(F)c5c4)n3)c2)NC(=O)NC1=O
vPlpro-as1-164	Z2226903034	-8.6	0.331	349.35	REAL	O=C(NNc1nnc[nH]1)c1ccc2c(c1)C[C@@H](c1ccccc1)OC2=O
vPlpro-as1-165	Z2229128118	-8.6	0.287	402.46	REAL	CN(C(=O)c1nc(N)nc(N2CCOCC2)n1)C1c2ccccc2-c2ccccc21
vPlpro-as1-166	Z2233384834	-8.6	0.261	442.52	REAL	Nc1nnc(C2CCN(C(=O)[C@H]3CC(=O)N(c4ccc5c(c4)Cc4ccccc4-5)C3)CC2)[nH]1
vPlpro-as1-167	Z226196772	-8.6	0.261	471.93	REAL	O=C(CSc1ccc2c3c(cccc13)C(=O)c1ccccc1-2)Nc1nnc2ccc(Cl)nn12
vPlpro-as1-168	Z226395670	-8.6	0.253	475.57	REAL	NC(=O)[C@@H]1Cc2ccccc2CN1C(=O)c1ccc(S(=O)(=O)N2CCCc3ccccc32)c1
vPlpro-as1-169	Z237114998	-8.6	0.253	448.49	REAL	Cc1nnc(NNC(=O)c2cc(-c3ccc(-c4ccccc4)cc3)nc3ccccc23)[nH]c1=O
vPlpro-as1-170	Z2439188373	-8.6	0.307	396.47	REAL	O=C1c2ccccc2S(=O)(=O)c2cc(C(=O)N3C[C@@H]4CCC[C@@H](C3)N4)ccc21
vPlpro-as1-171	Z2444377924	-8.6	0.297	388.43	REAL	C[C@]1(c2cccc(-c3noc([C@@]4(C)CCc5ccccc54)n3)c2)NC(=O)NC1=O
vPlpro-as1-172	Z2621676662	-8.6	0.297	388.47	REAL	O=C1CCCc2ccc(NC(=O)N3CCC4(C=Cc5ccccc5O4)CC3)cc21
vPlpro-as1-173	Z2636421396	-8.6	0.297	398.47	REAL	C[C@@H]1CN(C(=O)[C@@H]2CCCc3[nH]nnc32)CCN1C(=O)[C@H]1CCCc2[nH]nnc21
vPlpro-as1-174	Z2709567915	-8.6	0.297	388.47	REAL	O=C1CCCc2ccc(NC(=O)N3CCN(c4ccccc5[nH]ccc45)CC3)cc21
vPlpro-as1-175	Z28263645	-8.6	0.261	435.53	REAL	CC(=O)N1CCN(C(=O)c2cc(-c3ccc(-c4ccccc4)cc3)nc3ccccc23)CC1
vPlpro-as1-176	Z2902754744	-8.6	0.319	354.37	REAL	O=c1[nH]c2cccc(-c3nc(-c4ccc(-c5ccccc5)cc4)no3)c2[nH]1
vPlpro-as1-177	Z2903525227	-8.6	0.297	417.45	REAL	Cc1cc(N2CCCS2(=O)=O)ccc1-c1nc(-c2c(C)n(C)c(=O)[nH]c2=O)no1
vPlpro-as1-178	Z2905434901	-8.6	0.344	334.37	REAL	O=C1C[C@H](c2ccccc(-c3ccc([C@@H]4CCC(=O)N4)cc3)c2)C(=O)N1
vPlpro-as1-179	Z29293949	-8.6	0.253	488.54	REAL	NC(=O)c1cc(-c2ccccc2)sc1NC(=O)c1ccc2c(c1)S(=O)(=O)c1ccccc1C2=O
vPlpro-as1-180	Z2962557287	-8.6	0.307	376.46	REAL	O=C(c1ccc2c(c1)-c1ccccc1C2)N1CCC2(CC1)C[C@@H](O)CNC2=O
vPlpro-as1-181	Z2991040262	-8.6	0.344	337.37	REAL	O=C1CC[C@@H](c2ccc(-c3ccc4c(c3)[C@H](C(=O)O)CCO4)cc2)N1
vPlpro-as1-182	Z3009936908	-8.6	0.307	382.38	REAL	C[C@@H]1c2cc(F)cc(F)c2CCN1c1nnc(-c2ncnc3nc[nH]c23)n1C
vPlpro-as1-183	Z325118426	-8.6	0.297	395.50	REAL	Cc1ccc(C23C[C@H]4C[C@@H](CC(C(=O)OCCN5C(=O)CCC5=O)(C4)C2)C3)cc1
vPlpro-as1-184	Z372498794	-8.6	0.253	449.47	REAL	O=C(CC1c2ccccc2Oc2ccccc21)Nc1ccc(-n2ncc3c(=O)[nH]cnc32)cc1
vPlpro-as1-185	Z393909394	-8.6	0.277	438.59	REAL	C[C@@H]1CCN(C(=O)c2cccc(S(=O)(=O)N3CCc4ccccc43)c2)[C@@H]2CCCC[C@H]12
vPlpro-as1-186	Z56768780	-8.6	0.307	363.42	REAL	NC1=Nc2nc3ccccc3n2[C@H](c2c3ccccc3cc3ccccc23)N1
vPlpro-as1-187	Z731266442	-8.6	0.232	487.52	REAL	Cn1ncc2c(=O)[nH]c(COC(=O)c3cc(-c4ccc(-c5ccccc5)cc4)nc4ccccc34)nc21
vPlpro-as1-188	Z731270762	-8.6	0.239	477.52	REAL	Cn1ncc2c(=O)[nH]c(COC(=O)c3c4c(nc5ccccc35)/C(=C/c3ccccc3)CCC4)nc21
vPlpro-as1-189	Z941454500	-8.6	0.287	418.43	REAL	O=C(Nc1ccc2c(c1)C(=O)NC2)c1ccc2c(c1)S(=O)(=O)c1ccccc1C2=O
vPlpro-as1-190	ZINC000001588362	-8.6	0.253	440.51	ZINC	Nc1nc(-c2ccc3ccccc3c2)cc(-c2cc(-c3cc4ccccc4c3)nc(N)n2)n1
vPlpro-as1-191	ZINC000008763747	-8.6	0.239	473.53	ZINC	COc1cccc2c1O[C@@H](c1ccc3noc(-c4ccccc4)c3c1)N1N=C(c3ccccc3)C[C@H]21
vPlpro-as1-192	ZINC000009612292	-8.6	0.232	496.58	ZINC	CC1CCN(c2cc(N3CCN(c4ccc(F)cc4)CC3)c3noc4c3c2C(=O)c2ccccc2-4)CC1
vPlpro-as1-193	ZINC000012895162	-8.6	0.253	476.90	ZINC	Nc1nc(N)nc(COC(=O)c2c3c(nc4ccccc42)/C(=C/c2c(F)cccc2Cl)CC3)n1
vPlpro-as1-194	ZINC000013304715	-8.6	0.253	472.56	ZINC	Cc1ccc2c(c1)[C@@H]1CN(C)CC[C@@H]1N2C(=O)c1ccc2c(c1)S(=O)(=O)c1ccccc1C2=O
vPlpro-as1-195	ZINC000018200371	-8.6	0.307	375.43	ZINC	Cc1nc2ccccc2nc1[C@@H]1c2c(O)n[nH]c2NC2=C1C(=O)CC(C)(C)C2
vPlpro-as1-196	ZINC000020464723	-8.6	0.269	429.51	ZINC	Cc1c(C(=O)N2CCc3ccccc3C2)oc2ccc3c(c12)C(=O)CC1(CCCCC1)O3
vPlpro-as1-197	ZINC000022528214	-8.6	0.253	449.51	ZINC	CC(C)c1ccc([C@H]2N/C(=N\c3nc4ccccc4o3)Nc3c4ccccc4[nH]c(=O)c32)cc1
vPlpro-as1-198	ZINC000026780145	-8.6	0.239	490.95	ZINC	O=C(NC1=CC=C[C@H]2C(=O)c3ccccc3C(=O)[C@@H]12)c1cc(-c2ccccc2Cl)nc2ccccc21
vPlpro-as1-199	ZINC000072389463	-8.6	0.269	429.52	ZINC	Cc1cc2nc([C@H]3CCCCN3C(=O)[C@@H](C)c3n[nH]c(=O)c4ccccc43)[nH]c2cc1C
vPlpro-as1-200	ZINC000092077956	-8.6	0.307	379.42	ZINC	Cc1cc(N2CCN(C(=O)c3cc(-c4ccccc4O)n[nH]3)CC2)nc(N)n

Supplementary Table 24. Virtual screening hits 101 to 200 of the screen against the active site of PL^{pro} (Screen ID: 12). Compounds were filtered so that hits had MW < 600 dalton, cLogP < 6, number of hydrogen bond acceptors < 11, and no reactive functional groups. A few compounds unsuitable for drug discovery were removed by visual inspection. The name of each compound consists of the initial letter 'v' for virtual hit, followed by the target protein name and the target site ('as' for active site, 1 for docking scenario 1). The score is the docking score given by QuickVina 2 in kcal/mol. The ligand efficiency (LE) is computed as LE = -score/#NonH, where #NonH is the number of heavy (i.e. non hydrogen) atoms.

Name	Catalog ID	Score	LE	MW	Library	SMILES
vPlpro-as2-1	Z1476773581	-10.1	0.337	421.839	REAL	NC(=O)c1nc(Cl)ccc1NC(=O)c1ccc2c(c1)C[C@@H](c1ccccc1)OC2=O
vPlpro-as2-2	Z1555227240	-9.9	0.341	411.848	REAL	NC(=O)c1nc(Cl)ccc1NC(=O)c1ccc2c(=O)n3c(nc2c1)CCCCC3
vPlpro-as2-3	Z1132505833	-9.8	0.35	385.506	REAL	CC(C)(C)OC(=O)Nc1ccc(NC(=O)N[C@H]2C[C@@H]3C[C@@H]2[C@H]2CCC[C@H]32)cc1
vPlpro-as2-4	Z2178142149	-9.8	0.306	425.443	REAL	O=C(Nc1cccc2[nH]c(=O)oc12)[C@H]1CC(=O)N(c2ccc3c(c2)Cc2ccccc2-3)C1
vPlpro-as2-5	Z812555872	-9.8	0.28	468.559	REAL	O=C(CC12C[C@H]3C[C@@H](C1)CC(C(=O)Nc1nc4ccccc4[nH]1)(C3)C2)Nc1nc2ccccc2[nH]1
vPlpro-as2-6	Z1555223912	-9.7	0.323	441.85	REAL	NC(=O)c1nc(Cl)ccc1NC(=O)c1ccc2c(c1)S(=O)(=O)c1ccccc1C2=O
vPlpro-as2-7	Z1915736221	-9.7	0.303	426.435	REAL	O=C(NNc1ccc(-n2ccnc2)nn1)c1ccc2c(c1)C[C@@H](c1ccccc1)OC2=O
vPlpro-as2-8	Z24206233	-9.7	0.269	482.447	REAL	C[C@@H](OC(=O)c1ccc2c(c1)C(=O)N(C)C2=O)C(=O)Nc1ccc2c(c1)C(=O)c1ccccc1C2=O
vPlpro-as2-9	Z1306303559	-9.6	0.3	431.451	REAL	C[C@@]1(c2cccc(CNC(=O)NNC(=O)c3ccce4ccccc34)e2)NC(=O)NC1=O
vPlpro-as2-10	Z1383548864	-9.6	0.291	436.47	REAL	O=C(NNc1ccc(-c2ccccc2)nn1)c1ccc2c(c1)C[C@@H](c1ccccc1)OC2=O
vPlpro-as2-11	Z1908699121	-9.6	0.291	443.51	REAL	Cc1ccnc(-c2n[nH]c([C@@H](C)NC(=O)c3ccc4c(=O)n5c(nc4c3)CCCCC5)n2)c1
vPlpro-as2-12	Z810119250	-9.6	0.3	429.45	REAL	NC(=O)c1ccc(F)c(NC(=O)[C@H]2CC(=O)N(c3ccc4c(c3)Cc3ccccc3-4)C2)c1
vPlpro-as2-13	Z92394424	-9.6	0.267	479.491	REAL	Cc1nc2ccc(C(=O)O[C@H](C)C(=O)Nc3ccc4c(c3)C(=O)c3ccccc3C4=O)cc2nc1C
vPlpro-as2-14	ZINC000408567169	-9.6	0.274	473.503	ZINC	O=C1Nc2ccccc2[C@]12[C@H](/[N+](=O)/[O-])[C@@H](c1ccc(OCc3ccc(F)c3)cc1)[C@@H]1CCCN12
vPlpro-as2-15	Z1095049106	-9.5	0.264	473.495	REAL	O=C(Nc1nc(-c2ccc3ccccc3n2)n[nH]1)c1nn(Cc2ccccc2)c(=O)c2ccccc12
vPlpro-as2-16	Z1233511775	-9.5	0.306	438.434	REAL	Cc1cc(NC(=O)c2ccc3c(c2)S(=O)(=O)c2ccccc2C3=O)c(C(N)=O)cc1F
vPlpro-as2-17	Z1311051704	-9.5	0.297	439.471	REAL	C[C@@]1(C2CCN(C(=O)CN3C(=O)N[C@@]4(CCc5ccccc54)C3=O)CC2)NC(=O)NC1=O
vPlpro-as2-18	Z1341825286	-9.5	0.317	405.457	REAL	NC(=O)[C@H]1CCCC[C@@H]1NC(=O)c1cccc(NC(=O)c2ccc3[nH]cnc3c2)c1
vPlpro-as2-19	Z1342001023	-9.5	0.328	403.413	REAL	C[C@@]1(C2CCN(C(=O)Nc3cc4c(cc3F)CCC(=O)N4)CC2)NC(=O)NC1=O
vPlpro-as2-20	Z1555220899	-9.5	0.339	394.817	REAL	NC(=O)c1nc(Cl)ccc1NC(=O)c1cncc(-c2ccc3c(c2)CCO3)c1
vPlpro-as2-21	Z1555221295	-9.5	0.317	420.811	REAL	NC(=O)c1nc(Cl)ccc1NC(=O)c1cccc(N2C(=O)c3ccccc3C2=O)c1
vPlpro-as2-22	Z1555224002	-9.5	0.317	420.811	REAL	NC(=O)c1nc(Cl)ccc1NC(=O)c1ccc(N2C(=O)c3ccccc3C2=O)cc1
vPlpro-as2-23	Z1555233322	-9.5	0.365	363.803	REAL	NC(=O)c1nc(Cl)ccc1NC(=O)c1ccc2c(c1)-c1ccccc1C2
vPlpro-as2-24	Z1576368580	-9.5	0.288	440.462	REAL	Cc1ccccc1Cn1c(NC(=O)c2cc(C)c3c(=O)[nH]c(O)nc3n2)nc2ccccc21
vPlpro-as2-25	Z1843805410	-9.5	0.297	448.502	REAL	O=C(NS(=O)(=O)c1cnc2ccccc2c1)c1ccc2c(=O)n3c(nc2c1)CCCCC3
vPlpro-as2-26	Z1846547768	-9.5	0.297	428.407	REAL	O=C(Nc1nnc(-c2cc3ccccc3o2)[nH]1)c1c[nH]nc1-c1ccc2c(c1)OCCO2
vPlpro-as2-27	Z1891420891	-9.5	0.297	431.451	REAL	COc1ccc(C(C)(C)c2noc(-c3c[nH]n4c3nc(=O)c3ccccc34)n2)cc1OC
vPlpro-as2-28	Z3094324441	-9.5	0.328	393.421	REAL	Cn1c([C@H]2Cc3cc(F)ccc3NC2=O)nnc1N1CCc2ccc(O)cc2C1
vPlpro-as2-29	Z66691734	-9.5	0.279	455.509	REAL	C[C@@H](OC(=O)c1ccc2c(c1)C[C@@H](c1ccccc1)OC2=O)C(=O)N1c2ccccc2C[C@H]1C
vPlpro-as2-30	Z787493126	-9.5	0.257	486.538	REAL	O=C(N[C@H](c1ccccc1)c1nnn[nH]1)c1cc(-c2ccccc2)nc2c1cnn2Cc1ccccc1
vPlpro-as2-31	Z96789853	-9.5	0.257	499.525	REAL	CC[C@]1(c2ccccc2)NC(=O)N(NC(=O)CN2C(=O)N[C@@](C)(c3cccc4ccccc34)C2=O)C1=O
vPlpro-as2-32	ZINC000009111256	-9.5	0.306	413.476	ZINC	C[C@@H](c1ccccc1)N1C(=O)NC(=O)[C@@]2(Cc3c4ccccc4ccc3N(C)C2)C1=O
vPlpro-as2-33	ZINC000408563977	-9.5	0.271	473.503	ZINC	O=C1Nc2ccccc2[C@]12[C@H](/[N+](=O)/[O-])[C@@H](c1ccc(OCc3cccc3F)cc1)[C@@H]1CCCN12
vPlpro-as2-34	PV-001798547283	-9.4	0.276	458.492	REAL	CCOc1ccc(NC(=O)c2cn(-c3ccc(F)cc3)nc2-c2cccc(C)c2)c(C(N)=O)c1
vPlpro-as2-35	PV-001801548796	-9.4	0.324	434.257	REAL	NC(=O)c1nc(Cl)ccc1NC(=O)c1nn(-c2cccc(Cl)c2F)c2c1CCC2
vPlpro-as2-36	PV-001801549308	-9.4	0.324	450.712	REAL	NC(=O)c1nc(Cl)ccc1NC(=O)c1nn(-c2ccc(Cl)cc2Cl)c2c1CCC2
vPlpro-as2-37	PV-001806954558	-9.4	0.303	442.397	REAL	NC(=O)c1cc(F)c(F)cc1NC(=O)c1ccc2c(c1)S(=O)(=O)c1ccccc1C2=O
vPlpro-as2-38	PV-001817117737	-9.4	0.313	409.391	REAL	Cc1ccc2c(c1)C(=O)O[C@](C)(C(=O)Nc1nccc(-c3ccc(F)c(F)c3)n1)C2
vPlpro-as2-39	PV-001826077043	-9.4	0.285	454.432	REAL	O=C(Nc1cccc(CNC(=O)[C@H](CO)NC(=O)c2ccccc(F)n2)c1)c1ccc(F)cc1
vPlpro-as2-40	PV-001829757973	-9.4	0.285	444.498	REAL	CN(C)c1nc(COc2ccccc(NC(=O)c3cccc(-c4cnn(C)c4)c3)c2)nc(=N)[nH]1
vPlpro-as2-41	PV-001834388437	-9.4	0.336	386.407	REAL	C[C@@]1(C(=O)N2CCC([C@]3(C)NC(=O)NC3=O)CC2)Oc2ccccc2NC1=O
vPlpro-as2-42	PV-001850780549	-9.4	0.324	394.342	REAL	Cn1c(=O)oc2c(C(=O)NNC(=O)[C@H]3C(=O)Nc4ccccc4C3=O)cccc21
vPlpro-as2-43	PV-001871635223	-9.4	0.313	410.472	REAL	Cc1ccc2c(c1)C(=O)O[C@](C)(C(=O)N[C@H]1CCCN(c3nc(C)cc(=O)[nH]3)C1)C2
vPlpro-as2-44	PV-001880465236	-9.4	0.294	448.546	REAL	O=C(Cc1nc(-c2ccccc2)cs1)NNC(=O)c1cccc(C(=O)N2CCCCC2)c1
vPlpro-as2-45	PV-001914591406	-9.4	0.348	397.787	REAL	C[C@]1(c2ccc(C(F)(F)F)cc2)CCCN1c1nc(Cl)nc2nc(O)[nH]c12
vPlpro-as2-46	PV-001950481491	-9.4	0.285	451.481	REAL	CC1(C)COc2ccc(NC(=O)NCc3cccc([C@]4(C)NC(=O)NC4=O)c3)cc2NC1=O
vPlpro-as2-47	PV-001950692474	-9.4	0.348	432.233	REAL	O=C1COc2ccccc(NC(=O)N[C@@H]3Cc4cc(Br)cnc4NC3=O)c2N1
vPlpro-as2-48	PV-001950837724	-9.4	0.324	399.406	REAL	C[C@]1(c2cccc(NC(=O)N3CC[C@H](c4ccc(=O)[nH]c(=O)[nH]4)C3)c2)COC(=O)N1
vPlpro-as2-49	Z1004366854	-9.4	0.269	467.528	REAL	Cc1ccc(C(=O)Nc2cccc(CNC(=O)NCC(=O)Nc3cccc4ccccc34)c2)cc1
vPlpro-as2-50	Z1014390962	-9.4	0.254	499.609	REAL	O=C(NC1CCN(C(=O)c2ccco2)CC1)[C@H]1C[C@@H]2CCCC[C@H]2N1C(=O)c1ccc2ccccc2c1
vPlpro-as2-51	Z1074810042	-9.4	0.269	469.539	REAL	C[C@H]1Oc2ccc(C(=O)C3CCN(C(=O)Nc4ccc5c6c(cccc46)CC5)CC3)cc2NC1=O
vPlpro-as2-52	Z1074879778	-9.4	0.261	487.558	REAL	Cc1cc(C)n(-c2ccccc(NC(=O)N3CCC(C(=O)c4ccc5c(c4)NC(=O)[C@H](C)O5)CC3)c2)n1
vPlpro-as2-53	Z1116925916	-9.4	0.261	479.491	REAL	Cc1[nH]c(-c2ccccc2)nc1C(=O)O[C@H](C)C(=O)Nc1ccc2c(c1)C(=O)c1ccccc1C2=O
vPlpro-as2-54	Z1132160593	-9.4	0.294	433.467	REAL	C[C@@H]1Oc2ccc(NC(=O)N3CCC(c4nc(-c5ccccc5)no4)CC3)cc2NC1=O
vPlpro-as2-55	Z1242104040	-9.4	0.336	378.366	REAL	Cc1oc(-c2ccccc2F)nc1C(=O)N[C@H](c1ccccc1)c1nnn[nH]1
vPlpro-as2-56	Z1270029508	-9.4	0.285	449.445	REAL	Cc1cc(C(=O)Nc2cc(-c3nnc4n3CCCCC4)ccc2F)nc2nc(O)[nH]c(=O)c12
vPlpro-as2-57	Z1333760456	-9.4	0.313	397.481	REAL	O=C(NNc1nc(-c2ccccn2)nc2c1CCC2)[C@H]1C[C@]12CCCc1ccccc12
vPlpro-as2-58	Z1410595931	-9.4	0.303	419.484	REAL	NC(=O)[C@H]1CCCCC[C@@H]1NC(=O)c1cccc(NC(=O)c2ccc3[nH]cnc3c2)c1
vPlpro-as2-59	Z1413476503	-9.4	0.285	445.453	REAL	Cn1c(NC(=O)CN2C(=O)N[C@@](C)(c3cccc4ccccc4c3)C2=O)nc2c(F)cccc21
vPlpro-as2-60	Z1613253586	-9.4	0.294	434.455	REAL	C[C@@]1(C2CCN(C(=O)Nc3ccc4nc(-c5ccccn5)oc4c3)CC2)NC(=O)NC1=O
vPlpro-as2-61	Z1681528804	-9.4	0.285	434.458	REAL	O=C(CCC(=O)c1ccc2ccc3cccc4ccc1c2c34)NNc1ncnc2nc[nH]c12
vPlpro-as2-62	Z1723439126	-9.4	0.294	446.897	REAL	C[C@@H](NC(=O)c1cccc(-c2cnc3[nH]c(=O)n(C)c3c2)c1)c1nc2cc(Cl)ccc2[nH]1
vPlpro-as2-63	Z1723442805	-9.4	0.285	440.462	REAL	C[C@@H](NC(=O)c1cccc(-c2cnc3[nH]c(=O)n(C)c3c2)c1)c1noc(-c2ccccc2)n1
vPlpro-as2-64	Z17235122	-9.4	0.261	480.475	REAL	Cc1oc(-c2ccccc2)nc1C(=O)O[C@H](C)C(=O)Nc1ccc2c(c1)C(=O)c1ccccc1C2=O
vPlpro-as2-65	Z1768170280	-9.4	0.294	446.446	REAL	O=C(NS(=O)(=O)c1cccc(-n2cnnn2)c1)c1ccc2[nH]c3ccccc3c(=O)c2c1
vPlpro-as2-66	Z1843807546	-9.4	0.303	429.455	REAL	O=C(NS(=O)(=O)c1cnc2ccccc2c1)c1ccc2[nH]c3ccccc3c(=O)c2c1
vPlpro-as2-67	Z2167347380	-9.4	0.303	424.431	REAL	C[C@@H]1Oc2ccc(NC(=O)N3CCC(c4noc5cc(F)ccc45)CC3)cc2NC1=O
vPlpro-as2-68	Z2196044717	-9.4	0.285	445.482	REAL	Cc1cc(=O)[nH]c2cc(C(=O)Nc3cccc(OCc4nc(N)nc(N(C)C)n4)c3)ccc12
vPlpro-as2-69	Z2233592864	-9.4	0.324	385.382	REAL	O=C1O[C@@H](C(=O)Nc2nc(-c3ccc4ccccc4n3)n[nH]2)Cc2ccccc21
vPlpro-as2-70	Z2524828114	-9.4	0.276	458.56	REAL	C[C@]1(c2cccc(C(=O)N3C[C@@H]4CC[C@H]3[C@H]3CN(Cc5ccccc5)C[C@@H]43)c2)NC(=O)NC1=O
vPlpro-as2-71	Z3094324410	-9.4	0.324	395.412	REAL	Cn1c([C@H]2Cc3cc(F)ccc3NC2=O)nnc1N1CCc2ccc(F)cc2C1
vPlpro-as2-72	Z804197044	-9.4	0.285	436.474	REAL	O=C(Nc1cccc(-c2nnn[nH]2)c1)[C@H]1CC(=O)N(c2ccc3c(c2)Cc2ccccc2-3)C1
vPlpro-as2-73	Z817512642	-9.4	0.261	493.546	REAL	C[C@]1(c2cccc(NC(=O)c3cc(-c4nc5ccccc5s4)nc4ccccc34)c2)NC(=O)NC1=O
vPlpro-as2-74	Z827905556	-9.4	0.313	440.862	REAL	NC(=O)c1cc(Cl)ccc1NC(=O)c1ccc2c(c1)S(=O)(=O)c1ccccc1C2=O
vPlpro-as2-75	Z828086234	-9.4	0.285	443.51	REAL	C[C@@H](NC(=O)c1cccc(NC(=O)c2ccc3[nH]cnc3c2)c1)c1nnc2n1CCCCC2
vPlpro-as2-76	Z89989485	-9.4	0.269	486.547	REAL	CCN(C(=O)COC(=O)c1ccc2c(c1)C[C@@H](c1ccccc1)OC2=O)c1nc2ccccc2s1
vPlpro-as2-77	Z920840756	-9.4	0.313	397.433	REAL	Cc1ccc(NC(=O)c2ccc3c(c2)C[C@@H](c2ccccc2)OC3=O)c2[nH]ncc12
vPlpro-as2-78	Z929407976	-9.4	0.294	425.487	REAL	Cc1ccc(C(N)=O)cc1NC(=O)[C@H]1CC(=O)N(c2ccc3c(c2)Cc2ccccc2-3)C1
vPlpro-as2-79	Z941828156	-9.4	0.303	415.456	REAL	C[C@@H](NC(=O)c1cccc(NC(=O)c2ccc3[nH]cnc3c2)c1)c1nnc2n1CCC2
vPlpro-as2-80	Z956278970	-9.4	0.348	363.38	REAL	O=C(N[C@H](c1ccccc1)c1nnn[nH]1)c1cccc(N2CCNC2=O)c1
vPlpro-as2-81	Z956279018	-9.4	0.336	442.251	REAL	O=C(N[C@H](c1ccccc1)c1nnn[nH]1)c1nn(-c2ccccc2F)cc1Br
vPlpro-as2-82	ZINC000008444419	-9.4	0.324	390.37	ZINC	C/C(=N/Nc1nnc2c3ccccc3[nH]c2n1)c1nnn(-c2nonc2N)c1C
vPlpro-as2-83	ZINC000012360280	-9.4	0.285	431.45	ZINC	O=C1Nc2ccccc2[C@]12Nc1ccccc1C(=O)N2c1ccc2c(c1)oc1ccccc12
vPlpro-as2-84	ZINC000107176340	-9.4	0.276	451.525	ZINC	Cc1ccc2c(c1C)NC(=O)[C@@]21[C@@H]2C(=O)N(c3ccc4ccccc4c3)C(=O)[C@H]2[C@H]2CCCN21
vPlpro-as2-85	ZINC000408569802	-9.4	0.269	473.503	ZINC	O=C1Nc2ccccc2[C@]12[C@H](/[N+](=O)/[O-])[C@@H](c1ccc(OCc3ccc(F)cc3)cc1)[C@@H]1CCCN12
vPlpro-as2-86	PV-001798358790	-9.3	0.31	430.841	REAL	Cc1cc(NC(=O)c2nn(-c3cccc(Cl)c3F)c3c2CCC3)c(C(N)=O)cc1F
vPlpro-as2-87	PV-001801549732	-9.3	0.3	456.909	REAL	NC(=O)c1nc(Cl)ccc1NC(=O)c1cccc(S(=O)(=O)N2CCc3ccccc32)c1
vPlpro-as2-88	PV-001808957571	-9.3	0.291	450.493	REAL	Cc1nc(NC(=O)c2cc3ccccc3cc2NS(C)(=O)=O)cc(-c2ccc(F)cc2)n1
vPlpro-as2-89	PV-001810356674	-9.3	0.31	420.444	REAL	Cc1ccc(NC(=O)c2ccc3c(c2)S(=O)(=O)c2ccccc2C3=O)c(C(N)=O)c1
vPlpro-as2-90	PV-001810357670	-9.3	0.321	396.396	REAL	Cc1ccc(NC(=O)c2nn(-c3ccc(F)c(F)c3)c3c2CCC3)c(C(N)=O)c1
vPlpro-as2-91	PV-001810731842	-9.3	0.31	420.444	REAL	Cc1ccc(C(N)=O)c(NC(=O)c2ccc3c(c2)S(=O)(=O)c2ccccc2C3=O)c1
vPlpro-as2-92	PV-001829124324	-9.3	0.3	421.452	REAL	Cc1ccc2c(c1)C(=O)O[C@@](C)(C(=O)NCc1cccc([C@]3(C)NC(=O)NC3=O)c1)C2
vPlpro-as2-93	PV-001829759358	-9.3	0.291	451.51	REAL	CN(C)c1nc(COc2cccc(NC(=O)c3ccc4c(c3)SCC(=O)N4)c2)nc(=N)[nH]1
vPlpro-as2-94	PV-001829760146	-9.3	0.291	444.397	REAL	CN(C)c1nc(COc2cccc(NC(=O)c3cccc4c3OC(F)(F)O4)c2)nc(=N)[nH]1
vPlpro-as2-95	PV-001834243815	-9.3	0.332	391.817	REAL	NC(=O)c1cc(Cl)ccc1NC(=O)c1cc(-c2cnc3[nH]ccc3c2)ccn1
vPlpro-as2-96	PV-001852481239	-9.3	0.282	456.541	REAL	C[C@@H](O)[C@H](NC(=O)C1CCCC1)C(=O)NCc1cccc(N2C(=O)NC3(CCCC3)C2=O)c1
vPlpro-as2-97	PV-001863327318	-9.3	0.358	347.341	REAL	O=C(N[C@H](c1ccccc1)c1nnn[nH]1)c1cccc(-n2cncn2)n1
vPlpro-as2-98	PV-001863327977	-9.3	0.291	429.483	REAL	CC(C)c1ncc(OCc2ccccc2)c(C(=O)N[C@H](c2ccccc2)c2nnn[nH]2)n1
vPlpro-as2-99	PV-001942086262	-9.3	0.282	455.557	REAL	Cc1cc(C(=O)N2CCC(C)CC2)ccc1NC(=O)N1CCC([C@]2(C)NC(=O)NC2=O)CC1
vPlpro-as2-100	PV-001942703233	-9.3	0.282	455.557	REAL	Cc1cc(C(=O)N2CCCC[C@@H]2C)ccc1NC(=O)N1CCC([C@]2(C)NC(=O)NC2=O)CC1

Supplementary Table 25. Top 100 virtual hits of the screen against the accessory pocked besides the active site of PL^{pro} (Screen ID: 13). Compounds were filtered so that hits had MW < 600 dalton, cLogP < 6, number of hydrogen bond acceptors < 11, and no reactive functional groups. The name of each compound consists of the initial letter 'v' for virtual hit, followed by the target protein name and the target site ('as' for active site, 2 for docking scenario 2). The score is the docking score given by QuickVina 2 in kcal/mol. The ligand efficiency (LE) is computed as LE = -score/#NonH, where #NonH is the number of heavy (i.e. non hydrogen) atoms.

Name	Catalog ID	Score	LE	MW	Library	SMILES
vPlpro-as2-101	PV-001945992639	-9.3	0.321	403.41	REAL	C[C@@]1(C2CCN(C(=O)Nc3cc4c(cc3F)NC(=O)CC4)CC2)NC(=O)NC1=O
vPlpro-as2-102	PV-001947486420	-9.3	0.321	398.47	REAL	Cc1nc(NC(=O)N2CCC[C@H]([C@@]3(C)COC(=O)N3)C2)ccc1-c1cnn(C)c1
vPlpro-as2-103	PV-001955705986	-9.3	0.300	420.51	REAL	CC1(C)CN(C(=O)NCc2cccc([C@@]3(C)NC(=O)NC3=O)c2)CCc2ccccc21
vPlpro-as2-104	PV-001968759769	-9.3	0.372	336.35	REAL	O=C(NCc1noc2ccccc12)N[C@@H]1Cc2ccccc2NC1=O
vPlpro-as2-105	Z1018321982	-9.3	0.291	455.54	REAL	C[C@@H]1CCc2sc(C(=O)NNC(=O)NCc3cccc([C@]4(C)NC(=O)NC4=O)c3)cc2C1
vPlpro-as2-106	Z1094919884	-9.3	0.291	435.49	REAL	Cc1c(C(=O)Nc2cccc(OCc3nc(N)nc(N(C)C)n3)c2)[nH]c2c1C(=O)CCC2
vPlpro-as2-107	Z1153782123	-9.3	0.300	433.49	REAL	Cn1nnnc1-c1cccc(S(=O)(=O)NC(=O)[C@@H]2C[C@@H]2c2ccc3ccccc23)c1
vPlpro-as2-108	Z1175272016	-9.3	0.291	445.91	REAL	NC(=O)c1ccc(Cl)c(NC(=O)[C@H]2CC(=O)N(c3ccc4c(c3)Cc3ccccc3-4)C2)c1
vPlpro-as2-109	Z1241736262	-9.3	0.282	444.47	REAL	Cc1cc(C)n2nc(NC(=O)Nc3ccc(-c4nc5cc(F)ccc5n4C)cc3C)nc2n1
vPlpro-as2-110	Z1244364839	-9.3	0.310	410.45	REAL	C[C@@H]1c2c(F)cccc2CCN1C(=O)NCc1cccc([C@]2(C)NC(=O)NC2=O)c1
vPlpro-as2-111	Z1250586272	-9.3	0.282	438.49	REAL	Cc1cc(C(=O)NC[C@H]2CC3c4ccccc4C2c2ccccc23)nc2nc(O)[nH]c(=O)c12
vPlpro-as2-112	Z1266545027	-9.3	0.310	421.84	REAL	O=C(Nc1nnc(-c2ccccc2Cl)[nH]1)c1c[nH]cc1-c1ccc2c(c1)OCCO2
vPlpro-as2-113	Z1309241095	-9.3	0.300	421.46	REAL	CC[C@@H]1Oc2cc([C@@H](C)NC(=O)NNC(=O)c3c[nH]c4ccccc34)ccc2NC1=O
vPlpro-as2-114	Z1309244936	-9.3	0.291	436.47	REAL	CC[C@@H]1Oc2cc([C@@H](C)NC(=O)NNC(=O)c3c(C)nc4ccccn34)ccc2NC1=O
vPlpro-as2-115	Z1313180586	-9.3	0.282	447.49	REAL	C[C@@H](NC(=O)[C@H]1CN(Cc2nc3ccccc3c(=O)[nH]2)CCO1)c1ccc2c(c1)CC(=O)N2
vPlpro-as2-116	Z131523858	-9.3	0.282	440.48	REAL	Cc1cccc(-c2nn(-c3ccc(F)cc3)cc2C(=O)N[C@H](C)c2nnc3ccccn23)c1
vPlpro-as2-117	Z1334110618	-9.3	0.310	414.46	REAL	Cc1nc2[nH]n(C)c(=O)c2c(C)c1CC(=O)N1CCC([C@]2(C)NC(=O)NC2=O)CC1
vPlpro-as2-118	Z1334905606	-9.3	0.291	425.49	REAL	C[C@@]1(c2ccc(C(=O)N3Cc4ccccc4[C@H](c4ccccc4)C3)cc2)NC(=O)NC1=O
vPlpro-as2-119	Z1348687747	-9.3	0.332	407.45	REAL	C[C@@]1(C2CCN(C(=O)[C@@H]3Nc4ccccc4S(=O)(=O)N3)CC2)NC(=O)NC1=O
vPlpro-as2-120	Z1414031655	-9.3	0.321	385.43	REAL	C/C(=N/Nc1ncnc2c1oc1ccccc12)c1ccc2c(c1)C(C)(C)C(=O)N2
vPlpro-as2-121	Z1461440103	-9.3	0.291	427.46	REAL	O=C(NC1(c2ccc3c(c2)OCO3)CC1)c1ccc2c(c1)C[C@@H](c1ccccc1)OC2=O
vPlpro-as2-122	Z1462387367	-9.3	0.332	438.28	REAL	NC(=O)c1cc(Br)ccc1NC(=O)c1cncc(-c2ccc3c(c2)CCO3)c1
vPlpro-as2-123	Z1462451153	-9.3	0.332	393.83	REAL	NC(=O)c1cc(Cl)ccc1NC(=O)c1cncc(-c2ccc3c(c2)CCO3)c1
vPlpro-as2-124	Z146471890	-9.3	0.332	373.46	REAL	C[C@H]1CCc2[nH]c3ccc(C(=O)N[C@H](C)c4nnc5ccccn45)cc3c2C1
vPlpro-as2-125	Z1472745582	-9.3	0.291	423.47	REAL	Cc1n[nH]c(NC(=O)c2ccc3c(c2)-c2ccccc2C3)c1-c1ccc2c(c1)OCCO2
vPlpro-as2-126	Z1523753148	-9.3	0.332	373.42	REAL	Cc1cccc(-c2nc(C(=O)N[C@H](c3ccccc3)c3nnn[nH]3)c(C)[nH]2)c1
vPlpro-as2-127	Z1527328078	-9.3	0.291	431.50	REAL	Cc1ccc([C@]2(C)CC(=O)NC(C(=O)Nc3cc(C)ccc3-c3nnc(C)[nH]3)C2=O)cc1
vPlpro-as2-128	Z1531684313	-9.3	0.291	434.46	REAL	C[C@@]1(C2CCN(C(=O)Nc3cnn(-c4cnc5ccccc5n4)c3)CC2)NC(=O)NC1=O
vPlpro-as2-129	Z153971468	-9.3	0.266	472.50	REAL	Cc1cccc(NC(=O)NC(=O)COC(=O)c2ccc3c(c2)C[C@@H](c2ccccc2)OC3=O)c1C
vPlpro-as2-130	Z1549989310	-9.3	0.291	428.50	REAL	O=C([C@H]1CC(=O)N(c2ccc3c(c2)Cc2ccccc2-3)C1)N1CCC[C@H](c2nnn[nH]2)C1
vPlpro-as2-131	Z1567340539	-9.3	0.300	419.48	REAL	CN(C)c1ccc(NC(=O)c2ccc3c(=O)n4c(nc3c2)CCCCC4)c(C(N)=O)c1
vPlpro-as2-132	Z1592201701	-9.3	0.291	423.47	REAL	N#Cc1cc2c(nc1NC(=O)c1ccc3c(c1)C[C@@H](c1ccccc1)OC3=O)CCCC2
vPlpro-as2-133	Z1595928473	-9.3	0.282	448.52	REAL	C[C@H]1Oc2ccc(C(=O)C3CCN(C(=O)Nc4ccc5c(c4)N(C)CC5)CC3)cc2NC1=O
vPlpro-as2-134	Z1652520760	-9.3	0.344	365.43	REAL	C[C@H]1OCC[C@]1(C)NC(=O)c1ccc2c(c1)C[C@@H](c1ccccc1)OC2=O
vPlpro-as2-135	Z1677885341	-9.3	0.291	434.46	REAL	C[C@@H]1Oc2ccc(C(=O)C3CCN(C(=O)Nc4nc5ccccn5n4)CC3)cc2NC1=O
vPlpro-as2-136	Z1686057337	-9.3	0.291	426.44	REAL	O=C1C[C@@H](c2noc(-c3c[nH]n4c3nc(=O)c3ccccc34)n2)CN1Cc1ccccc1
vPlpro-as2-137	Z1723441352	-9.3	0.274	474.91	REAL	C[C@@H](NC(=O)c1cccc(-c2cnc3[nH]c(=O)n(C)c3c2)c1)c1nc(-c2ccc(Cl)cc2)no1
vPlpro-as2-138	Z1723442076	-9.3	0.274	474.91	REAL	C[C@@H](NC(=O)c1cccc(-c2cnc3[nH]c(=O)n(C)c3c2)c1)c1noc(-c2ccc(Cl)cc2)n1
vPlpro-as2-139	Z1723442824	-9.3	0.282	439.48	REAL	C[C@@H](NC(=O)c1cccc(-c2cnc3[nH]c(=O)n(C)c3c2)c1)c1cn(-c2ccccc2)nn1
vPlpro-as2-140	Z1765586707	-9.3	0.310	416.87	REAL	C[C@@H](NC(=O)c1ccc2[nH]c3ccccc3c(=O)c2c1)c1nc2cc(Cl)ccc2[nH]1
vPlpro-as2-141	Z1768179492	-9.3	0.300	433.44	REAL	O=C(NS(=O)(=O)Cc1noc2ccccc12)c1ccc2[nH]c3ccccc3c(=O)c2c1
vPlpro-as2-142	Z1771146907	-9.3	0.300	407.43	REAL	O=C(NNc1ccc(-c2ccccc2)nn1)c1ccc2[nH]c3ccccc3c(=O)c2c1
vPlpro-as2-143	Z1843801530	-9.3	0.300	431.47	REAL	O=C(NS(=O)(=O)c1cnc2ccccc2c1)c1cncc(-c2ccc3c(c2)CCO3)c1
vPlpro-as2-144	Z1882361007	-9.3	0.321	426.26	REAL	NC(=O)c1nc(Cl)ccc1NC(=O)c1ccc(-n2nce3ccccc32)cc1Cl
vPlpro-as2-145	Z1890998351	-9.3	0.300	414.42	REAL	Cc1ccc(CNC(=O)Cc2noc(-c3c[nH]n4c3nc(=O)c3ccccc34)n2)cc1
vPlpro-as2-146	Z1937475593	-9.3	0.291	428.42	REAL	O=C(Nc1cc(-c2nc[nH]n2)ccc1F)c1ccc2c(c1)C[C@@H](c1ccccc1)OC2=O
vPlpro-as2-147	Z2091794012	-9.3	0.300	418.45	REAL	C[C@@]1(C[C@@H]2CCCN2C(=O)c2ccc3[nH]c4ccccc4c(=O)c3c2)NC(=O)NC1=O
vPlpro-as2-148	Z2147290607	-9.3	0.321	389.45	REAL	C[C@@H]1Oc2ccccc2[C@@H]1NC(=O)c1ccc2c(=O)n3c(nc2c1)CCCCC3
vPlpro-as2-149	Z2147308727	-9.3	0.310	399.45	REAL	C[C@@H]1Oc2ccccc2[C@@H]1NC(=O)c1ccc2c(c1)C[C@@H](c1ccccc1)OC2=O
vPlpro-as2-150	Z2148315940	-9.3	0.321	402.84	REAL	NC(=O)c1nc(Cl)ccc1NC(=O)c1ccc(-c2cccc3ccenc23)cc1
vPlpro-as2-151	Z2167247853	-9.3	0.310	408.46	REAL	Cc1c(-c2nnc(N3CCC([C@]4(C)NC(=O)NC4=O)CC3)n2C)oc2ccccc12
vPlpro-as2-152	Z2177640273	-9.3	0.300	412.45	REAL	C[C@@H]1Oc2ccccc2[C@@H]1NC(=O)c1ccc(NC(=O)c2ccc3[nH]cnc3c2)c1
vPlpro-as2-153	Z2227147910	-9.3	0.291	424.46	REAL	O=C(Nc1cccc2[nH]c(=O)[nH]c12)[C@H]1CC(=O)N(c2ccc3c(c2)Cc2ccccc2-3)C1
vPlpro-as2-154	Z269521258	-9.3	0.310	402.41	REAL	Cc1ccc(-c2nnc(NC(=O)c3c[nH]nc3-c3ccc4c(c3)OCCO4)[nH]2)cc1
vPlpro-as2-155	Z31289584	-9.3	0.258	479.50	REAL	Cc1ccc(N2C(=O)/C(=C/NNC(=O)Cn3nnc(-c4ccccc4)n3)c3ccccc3C2=O)cc1
vPlpro-as2-156	Z333044520	-9.3	0.282	439.47	REAL	C[C@@]1(c2ccc3ccccc3c2)NC(=O)N(CC(=O)N2CCn3c2nc2ccccc23)C1=O
vPlpro-as2-157	Z364929980	-9.3	0.310	440.86	REAL	NC(=O)c1ccc(Cl)cc1NC(=O)c1ccc2c(c1)S(=O)(=O)c1ccccc1C2=O
vPlpro-as2-158	Z385016388	-9.3	0.291	427.51	REAL	Cc1cc(C)n(-c2cccc(NC(=O)c3ccc4c(=O)n5c(nc4c3)CCCCC5)c2)n1
vPlpro-as2-159	Z419535712	-9.3	0.258	489.53	REAL	O=C(COC(=O)C1CCN(C(=O)N2CCCC2)CC1)Nc1ccc2c(c1)C(=O)c1ccccc1C2=O
vPlpro-as2-160	Z610950654	-9.3	0.291	447.51	REAL	O=C(NS(=O)(=O)c1ccc2ccccc2c1)c1ccc2c(=O)n3c(nc2c1)CCCCC3
vPlpro-as2-161	Z804787346	-9.3	0.291	429.45	REAL	NC(=O)c1cc(NC(=O)[C@H]2CC(=O)N(c3ccc4c(c3)Cc3ccccc3-4)C2)ccc1F
vPlpro-as2-162	Z851465882	-9.3	0.291	434.49	REAL	C[C@@H]1Oc2ccc(NC(=O)N3CCC(C(=O)N4CCc5ccccc54)CC3)cc2NC1=O
vPlpro-as2-163	Z92394118	-9.3	0.258	479.49	REAL	Cc1nc2ccc(C(=O)O[C@H](C)C(=O)Nc3cccc4c3C(=O)c3ccccc3C4=O)cc2nc1C
vPlpro-as2-164	Z942851496	-9.3	0.291	427.51	REAL	Cc1nc(-c2cccc(NC(=O)c3ccc4c(=O)n5c(nc4c3)CCCCC5)c2)[nH]c1C
vPlpro-as2-165	Z956278810	-9.3	0.344	364.36	REAL	O=C(N[C@H](c1ccccc1)c1nnn[nH]1)c1cccc(N2CCOC2=O)c1
vPlpro-as2-166	Z981481022	-9.3	0.266	468.56	REAL	Cc1[nH]c(-c2ccccc2)nc1C(=O)NC[C@H](NC(=O)c1nc(-c2ccccc2)[nH]c1C)C1CC1
vPlpro-as2-167	Z993685702	-9.3	0.310	407.43	REAL	C[C@@]1(C(=O)NCc2cccc([C@@]3(C)NC(=O)NC3=O)c2)Cc2ccccc2C(=O)O1
vPlpro-as2-168	Z995711582	-9.3	0.251	495.62	REAL	O=C(c1ccccc1)N1CCN(C(=O)[C@H]2C[C@@H]3CCCC[C@H]3N2C(=O)c2ccc3ccccc3c2)CC1
vPlpro-as2-169	ZINC000001355405	-9.3	0.258	484.55	ZINC	COc1cccc(C(=O)CN2c3cc(C(=O)N4CCCc5ccccc54)ccc3OC(C)(C)C2=O)c1
vPlpro-as2-170	ZINC000001355433	-9.3	0.258	484.55	ZINC	COc1cccc(C(=O)CN2c3cc(C(=O)N4CCc5ccccc5C4)ccc3OC(C)(C)C2=O)c1
vPlpro-as2-171	ZINC000017862766	-9.3	0.233	520.59	ZINC	O=C(Nc1ccc2ccccc2c1)c1cccc(N2C(=O)[C@H]3[C@@H](C2=O)C2c4ccccc4C3c3ccccc32)c1
vPlpro-as2-172	ZINC000261361409	-9.3	0.332	382.30	ZINC	O=C1[C@H]2[C@@H](C(=O)N1c1nnn[nH]1)[C@@H]1C=C[C@H]2[C@@H]2C(=O)N(c3nnn[nH]3)C(=O)[C@H]21
vPlpro-as2-173	ZINC000408566848	-9.3	0.310	399.45	ZINC	O=C1Nc2ccccc2[C@]12[C@H]([N+](=O)[O-])[C@@H](c1cccc3ccccc31)[C@@H]1CCCN12
vPlpro-as2-174	ZINC000408679811	-9.3	0.245	498.58	ZINC	Cc1ccc(C)cc(NC(=O)c2cccc(N3C(=O)[C@H]4[C@@H](C3=O)C3c5ccccc5C4c4ccccc43)c2)c1
vPlpro-as2-175	ZINC000408688101	-9.3	0.245	498.58	ZINC	Cc1ccc(NC(=O)c2cccc(N3C(=O)[C@H]4[C@@H](C3=O)C3c5ccccc5C4c4ccccc43)c2)cc1C
vPlpro-as2-176	PV-001792571772	-9.2	0.329	379.34	REAL	Cc1cc(F)c2nc(O)cc(C(=O)Oc3ccc4c(C)cc(=O)oc4c3)c2c1
vPlpro-as2-177	PV-001801548821	-9.2	0.317	434.26	REAL	NC(=O)c1nc(Cl)ccc1NC(=O)c1nn(-c2cec(Cl)cc2F)c2c1CCC2
vPlpro-as2-178	PV-001801549440	-9.2	0.329	411.73	REAL	NC(=O)c1nc(Cl)ccc1NC(=O)c1cccc(-c2noc(C(F)(F)F)n2)c1
vPlpro-as2-179	PV-001801549447	-9.2	0.317	426.26	REAL	NC(=O)c1nc(Cl)ccc1NC(=O)c1ccc2ncn(-c3ccc(Cl)cc3)c2c1
vPlpro-as2-180	PV-001803452932	-9.2	0.354	350.42	REAL	Cc1ccc(-c2cc(C(=O)N[C@@]3(C)CCO[C@H]3C)c3ccccc3n2)o1
vPlpro-as2-181	PV-001804115083	-9.2	0.317	431.87	REAL	Cc1ccc2c(c1)C(=O)O[C@](C)(C(=O)Nc1nnc(-c3c(F)cccc3Cl)s1)C2
vPlpro-as2-182	PV-001805948340	-9.2	0.341	362.39	REAL	NC(=O)c1[nH]nnc1NC(=O)c1ccc(N2CCCc3ccccc32)cc1
vPlpro-as2-183	PV-001808268561	-9.2	0.354	352.35	REAL	Cc1cc(=O)n2nc(NC(=O)C[C@H]3CC(=O)Nc4ccccc43)[nH]c2n1
vPlpro-as2-184	PV-001810360017	-9.2	0.317	396.40	REAL	Cc1ccc(NC(=O)c2nn(-c3cccc(F)c3F)c3c2CCC3)c(C(N)=O)c1
vPlpro-as2-185	PV-001814247474	-9.2	0.317	448.33	REAL	Cc1ccc2c(c1)C(=O)O[C@](C)(C(=O)Nc1nnc(-c3c(Cl)cccc3Cl)s1)C2
vPlpro-as2-186	PV-001814661898	-9.2	0.307	407.49	REAL	Cc1cccc(-c2nn(-c3ccc(F)cc3)cc2C(=O)N[C@@H]2[C@H](C)O[C@H](C)[C@H]2C)c1
vPlpro-as2-187	PV-001850781803	-9.2	0.317	391.38	REAL	O=C1CCc2ccccc2C(=O)NNC(=O)[C@H]3C(=O)Nc4ccccc4C3=O)c2C1
vPlpro-as2-188	PV-001863325713	-9.2	0.329	379.35	REAL	O=C(N[C@H](c1ccccc1)c1nnn[nH]1)c1nn(-c2ccccc2F)cc1O
vPlpro-as2-189	PV-001863326253	-9.2	0.354	392.83	REAL	CS(=O)(=O)c1ccc(Cl)c(C(=O)N[C@H](c2ccccc2)c2nnn[nH]2)n1
vPlpro-as2-190	PV-001864151216	-9.2	0.341	362.39	REAL	Cc1ccc(C)c(C2=NO[C@@H](C(=O)Nc3ccccc3-c3nn[nH]n3)C2)c1
vPlpro-as2-191	PV-001865194497	-9.2	0.329	397.86	REAL	CC1(C)CN(C(=O)c2ccccc([C@]3(C)NC(=O)NC3=O)c2)c2ccc(Cl)cc21
vPlpro-as2-192	PV-001872243742	-9.2	0.341	437.29	REAL	C[C@]1(C2CCN(C(=O)[C@@H]3Cc4ccc(Br)cc4C(=O)O3)CC2)COC(=O)N1
vPlpro-as2-193	PV-001905849046	-9.2	0.317	389.50	REAL	C[C@H]1O[C@@H](C)[C@@H](NC(=O)c2cc(NCc3ccccc3)nc3ccccc23)[C@@H]1C
vPlpro-as2-194	PV-001948929830	-9.2	0.329	391.36	REAL	C[C@@]1(C2CCN(C(=O)Nc3cc4oc(=O)[nH]c4cc3F)CC2)NC(=O)NC1=O
vPlpro-as2-195	PV-001952078834	-9.2	0.341	372.38	REAL	C[C@@]1(C2CCN(C(=O)Nc3cnc4c(c3)CNC4=O)CC2)NC(=O)NC1=O
vPlpro-as2-196	PV-001955708029	-9.2	0.317	394.43	REAL	C[C@@]1(c2cccc(CNC(=O)N[C@@H]3Cc4ccccc4[C@H]3O)c2)NC(=O)NC1=O
vPlpro-as2-197	PV-001964845439	-9.2	0.329	444.29	REAL	O=C(N[C@H]1CCc2ccccc2NC1=O)N[C@@H]1Cc2cc(Br)cnc2NC1=O
vPlpro-as2-198	PV-001966449898	-9.2	0.317	390.40	REAL	C[C@@H](NC(=O)NNC(=O)c1cccc2ccccc12)c1ccc2[nH]c(=O)oc2c1
vPlpro-as2-199	PV-001966453658	-9.2	0.329	392.32	REAL	C[C@@H](NC(=O)NNc1cccc2c1OC(F)(F)O2)c1ccc2[nH]c(=O)oc2c1
vPlpro-as2-200	Z1280088302	-9.2	0.329	382.35	REAL	O=C(N[C@H](c1ccccc1)c1nnn[nH]1)c1cc(N2CCOC2=O)ccc1F

Supplementary Table 26. Virtual screening hits 101 to 200 of the screen against the accessory pocked besides the active site of PL^{pro} (Screen ID: 13). Compounds were filtered so that hits had MW < 600 dalton, cLogP < 6, number of hydrogen bond acceptors < 11, and no reactive functional groups. The name of each compound consists of the initial letter 'v' for virtual hit, followed by the target protein name and the target site ('as' for active site, 2 for docking scenario 2). The score is the docking score given by QuickVina 2 in kcal/mol. The ligand efficiency (LE) is computed as LE = -score/#NonH, where #NonH is the number of heavy (i.e. non hydrogen) atoms.

Name	Catalog ID	Score	LE	MW	Library	SMILES
vMpro-mpro1-1	Z735794618	-9.1	0.303	415.516	REAL	O=C(C[C@H]1S/C(=N\c2ccc3c(c2)CCC3)NC1=O)Nc1ccc2ccccc2c1
vMpro-mpro1-2	Z1957164301	-8.8	0.267	444.486	REAL	CC1(C)C/C(=C/c2ccc3c(c2)NC(=O)CO3)C(=O)/C(=C/c2ccc3c(c2)NC(=O)CO3)C1
vMpro-mpro1-3	Z1449094151	-8.7	0.256	448.564	REAL	O=C(NC[C@H]1[C@@H]2Cc3ccccc3[C@H]12)c1ccc(C(=O)NC[C@H]2[C@@H]3Cc4ccccc4[C@@H]23)cc1
vMpro-mpro1-4	Z1739548330	-8.7	0.272	428.534	REAL	Cc1nc(-c2ccc(NC(=O)N3C[C@@H](c4ccccc4)[C@@H]4CCCC[C@H]43)cc2)cc(=O)[nH]1
vMpro-mpro1-5	Z1839408167	-8.7	0.264	448.478	REAL	C[C@H]1Oc2ccc(C(=O)C3CCN(C(=O)[C@@H]4CC(c5ccccn5)=NO4)CC3)cc2NC1=O
vMpro-mpro1-6	Z2093731375	-8.7	0.264	446.462	REAL	O=C1NC(=O)C2(CCC(NC(=O)c3cccc(CN4C(=O)c5ccccc5C4=O)c3)CC2)N1
vMpro-mpro1-7	Z744861644	-8.7	0.256	457.532	REAL	O=C(NNC(=O)N1CCN(CC(=O)N2CCc3ccccc32)CC1)c1ccc2ccccc2c1
vMpro-mpro1-8	Z995807442	-8.7	0.235	499.565	REAL	O=C(NNC(=O)[C@@H]1C[C@H]2CCCC[C@@H]2N1C(=O)c1ccc2ccccc2c1)c1ccc2c(c1)OCCO2
vMpro-mpro1-9	Z1069485244	-8.6	0.239	488.582	REAL	C[C@H]1Oc2ccc(C(=O)C3CCN(C(=O)CCC(=O)c4ccc5c(c4)CCCC5)CC3)cc2NC1=O
vMpro-mpro1-10	Z1161081819	-8.6	0.232	494.553	REAL	C[C@]1(c2ccc3ccccc3c2)NC(=O)N(CC(=O)Nc2ccc(-c3nnc4n3CCCC4)cc2)C1=O
vMpro-mpro1-11	Z1170164505	-8.6	0.253	448.485	REAL	O=c1[nH]c(CCc2nc(-c3cccc(Cn4cnc5ccccc54)c3)no2)nc2ccccc12
vMpro-mpro1-12	Z1312817858	-8.6	0.277	411.504	REAL	CN1CCC(=O)Nc2cc(C(=O)N3Cc4ccccc4[C@H](c4ccccc4)C3)ccc21
vMpro-mpro1-13	Z1329925738	-8.6	0.287	403.481	REAL	Cc1ccc2c(c1)N(C(=O)c1ccc3c(=O)n4c(nc3c1)CCCCC4)C[C@@H](C)O2
vMpro-mpro1-14	Z1631362590	-8.6	0.269	435.433	REAL	Cc1cc(F)c2nc(O)cc(C(=O)N[C@H]3CCc4nnc(-c5ccc(F)cc5)n4C3)c2c1
vMpro-mpro1-15	Z1733801359	-8.6	0.269	427.55	REAL	Cc1nc([C@H]2CCCN(C(=O)NC[C@H]3CC4c5ccccc5C3c3ccccc34)C2)n[nH]1
vMpro-mpro1-16	Z1983285517	-8.6	0.297	395.433	REAL	O=C1N[C@]2(C[C@H]3C[C@@H]2[C@H]2CCC[C@H]32)C(=O)N1Cc1coc(-c2cccc(F)c2)n1
vMpro-mpro1-17	Z2233377075	-8.6	0.261	446.456	REAL	C[C@@]1(NC(=O)c2cc(F)cc3ccenc23)CCN(C(=O)c2cc(F)cc3ccenc23)C1
vMpro-mpro1-18	Z428167628	-8.6	0.239	492.524	REAL	C[C@]1(c2cc(F)ccc2F)NC(=O)N(CC(=O)N2CCN(Cc3cccc4ccccc34)CC2)C1=O
vMpro-mpro1-19	Z70913644	-8.6	0.239	482.578	REAL	CN1CCC2(CC1)C[C@H](NC(=O)c1ccc3c(c1)C[C@H](c1ccccc1)OC3=O)c1ccccc1O2
vMpro-mpro1-20	Z735794652	-8.6	0.297	407.493	REAL	CC(=O)c1ccc(NC(=O)C[C@H]2S/C(=N/c3ccc4c(c3)CCC4)NC2=O)cc1
vMpro-mpro1-21	ZINC000002256624	-8.6	0.261	459.911	ZINC	Cc1ccc(/C(O)=N/C2=NN3C(=NC(c4ccc(Cl)cc4)=C[C@@H]3c3ccc(F)cc3)N2)cc1
vMpro-mpro1-22	ZINC000017988176	-8.6	0.215	521.571	ZINC	O=C(Oc1ccc2ccccc2c1)c1ccc(N2C(=O)[C@H]3[C@@H](C2=O)C2c4ccccc4C3c3ccccc32)c1
vMpro-mpro1-23	ZINC000019782240	-8.6	0.253	461.648	ZINC	CC1(C)C[C@]2(CCCN(Cc3nc4c(c(=O)[nH]3)C3(CCCCC3)Cc3ccccc3-4)C2)CCO1
vMpro-mpro1-24	ZINC000101835312	-8.6	0.269	421.503	ZINC	Cc1ccc(C(=O)Nc2nc3n(n2)[C@@H](c2ccccc2)C=C(c2ccc(C)cc2)N3)cc1
vMpro-mpro1-25	ZINC000101836350	-8.6	0.261	439.493	ZINC	Cc1ccc(C(=O)Nc2nc3n(n2)[C@@H](c2ccc(F)cc2)C=C(c2ccc(C)cc2)N3)cc1
vMpro-mpro1-26	ZINC000408966831	-8.6	0.253	445.521	ZINC	Cn1cc(/C=C/NN2C(=O)[C@H]3[C@@H](C2=O)C2c4ccccc4C3c3ccccc32)c2ccccc21
vMpro-mpro1-27	PV-001813621319	-8.5	0.274	434.377	REAL	Cn1ncc2c(=O)nc(NC(=O)[C@H]3CC(=O)N(Cc4cccc(C(F)(F)F)c4C3)[nH]c21
vMpro-mpro1-28	PV-001841355465	-8.5	0.266	430.482	REAL	Cc1ccc(-c2cc(C(=O)NNC(=O)CCc3ccc(F)c4ccccc34)[nH]n2)cc1C
vMpro-mpro1-29	PV-001866699826	-8.5	0.283	418.458	REAL	CC1(C)[C@H](c2ccccc(C(F)(F)F)c2)CCN1C(=O)c1cc(=O)[nH]c2c1CCCC2
vMpro-mpro1-30	PV-001880912833	-8.5	0.315	359.388	REAL	Cc1ccc(-c2nnc(NC(=O)Cc3cc4ccccc4c(=O)[nH]3)[nH]2)cc1
vMpro-mpro1-31	Z1007201180	-8.5	0.236	486.526	REAL	C[C@@]1(c2ccccc(CNC(=O)[C@@H]3CCCN3C(=O)c3ccc4ccccc4c3O)c2)NC(=O)NC1=O
vMpro-mpro1-32	Z1210043489	-8.5	0.266	433.546	REAL	C[C@H]1c2cc3c(cc2C2(CCCC2)CN1C(=O)C[C@@H]1OCCc2ccccc21)OCCO3
vMpro-mpro1-33	Z1251851504	-8.5	0.304	373.426	REAL	O=C([C@H]1Cc2cc(F)ccc2O1)N1CC=C(c2cccc3ccccc23)CC1
vMpro-mpro1-34	Z1274012075	-8.5	0.258	448.517	REAL	Cc1cc2c(cc1C)O[C@H](C(=O)N1CCC(C(=O)c3ccc4c(c3)NC(=O)[C@@H](C)O4)CC1)C2
vMpro-mpro1-35	Z1282626410	-8.5	0.266	428.491	REAL	O=C(NNC(=O)c1ccc2ccccc2c1)N[C@H]1CC(=O)N([C@H]2C[C@@H]2c2ccccc2)C1
vMpro-mpro1-36	Z1450310091	-8.5	0.266	427.546	REAL	Cc1ccc(CNC(=O)C2CCN(C(=O)c3cncc(-c4cccc(C)c4)c3)CC2)cc1
vMpro-mpro1-37	Z1466534626	-8.5	0.274	419.531	REAL	C[C@H]1CN(C(=O)N[C@@H]2CCC(C)(C)c3ccccc32)CCN1c1ncen2cnnc12
vMpro-mpro1-38	Z1682770450	-8.5	0.274	415.456	REAL	Nc1nc(Cc2noc(-c3ccc4c(c3O)CCCC4)n2)nc(Nc2ccccc2)n1
vMpro-mpro1-39	Z1682772382	-8.5	0.266	429.483	REAL	Nc1nc(Cc2noc(-c3cccc([C@H]4CCCOC4)c3)n2)nc(Nc2ccccc2)n1
vMpro-mpro1-40	Z1685085222	-8.5	0.25	449.469	REAL	O=C1C[C@H](c2nc(-c3ccc4[nH]c(=O)[nH]c4c3)no2)CN1c1ccc2c(c1)Cc1ccccc1-2
vMpro-mpro1-41	Z1704439649	-8.5	0.266	428.53	REAL	C[C@H]1CCN(C(=O)C2CCN(C(=O)c3cccc4ccccc34)CC2)c2c(O)cccc21
vMpro-mpro1-42	Z1723445137	-8.5	0.236	479.542	REAL	Cn1c(=O)[nH]c2ncc(-c3cccc(C(=O)N4CCC[C@@H](c5n[nH]c(-c6ccccc6n5)C4)c3)cc21
vMpro-mpro1-43	Z1739749623	-8.5	0.266	423.435	REAL	Cn1c(=O)[nH]c2ncc(-c3cccc(-c4nc(Cc5c[nH]c6ncccc56)no4)c3)cc21
vMpro-mpro1-44	Z2001060769	-8.5	0.25	447.497	REAL	O=C1C[C@@H](c2nc(Cc3ccc4[nH]ncc4c3)no2)CN1c1ccc2c(c1)Cc1ccccc1-2
vMpro-mpro1-45	Z2087242474	-8.5	0.266	436.392	REAL	O=C1N[C@@H](c2ccc3ccccc3c2)C(=O)N1c1ccn(-c2cccc(C(F)(F)F)c2)n1
vMpro-mpro1-46	Z2233591161	-8.5	0.304	371.399	REAL	O=C(Nc1nc(-c2ccc3ccccc3n2)n[nH]1)[C@H]1COc2ccccc2C1
vMpro-mpro1-47	Z2370152275	-8.5	0.293	387.442	REAL	CC1(C)C[C@H](c2nc(Cc3nc(-c4ccccc4)n[nH]3)no2)c2ccccc2O1
vMpro-mpro1-48	Z3094405269	-8.5	0.283	399.453	REAL	Cn1c(-c2ccc3cc[nH]c3c2)nnc1N1CC[C@@]2(CC(=O)c3ccccc3O2)C1
vMpro-mpro1-49	Z806191076	-8.5	0.243	471.52	REAL	O=C(Cn1cnnn1)N1CCN(C(=O)[C@@H]2CC(=O)N(c3ccc4c(c3)Cc3ccccc3-4)C2)CC1
vMpro-mpro1-50	Z920796942	-8.5	0.25	451.525	REAL	O=C(CN1C(=O)N[C@]2(CCc3ccccc32)C1=O)N1CC=C(c2cccc3ccccc23)CC1
vMpro-mpro1-51	Z924791026	-8.5	0.283	402.496	REAL	Cc1nc(-c2ccc(NC(=O)N[C@@H]3CCC(C)(C)c4ccccc43)cc2)cc(=O)[nH]1
vMpro-mpro1-52	Z961874654	-8.5	0.236	477.527	REAL	Cc1ccccc1-c1cc(NC(=O)c2cncc(C(=O)Nc3cc(-c4ccccc4C)n[nH]3)c2)[nH]n1
vMpro-mpro1-53	ZINC000002249520	-8.5	0.243	489.912	ZINC	OC(/C=C/c1ccc(F)cc1)=N\C1=NN2C(=NC(c3ccc(Cl)cc3)=C[C@@H]2c2ccc(F)cc2)N1
vMpro-mpro1-54	ZINC000100891431	-8.5	0.266	445.884	ZINC	O=C(Nc1nc2n(n1)[C@@H](c1ccccc1)C=C(c1ccc(Cl)cc1)N2)c1ccc(F)cc1
vMpro-mpro1-55	PV-001795683452	-8.4	0.255	449.549	REAL	Cc1ccc(C)c(C2=NO[C@H](C(=O)NCc3ccc(C(=O)N4C[C@H](C)O[C@H](C)C4)cc3)C2)c1
vMpro-mpro1-56	PV-001795949565	-8.4	0.323	366.851	REAL	O=C(C[C@@H]1CCc2ccccc2C1)Nc1nnc(-c2cccc(Cl)c2)[nH]1
vMpro-mpro1-57	PV-001816830401	-8.4	0.311	423.309	REAL	Cc1ccc(C2=NO[C@H](C(=O)NCc3cc(Br)c4ccccc4c3)C2)cc1
vMpro-mpro1-58	PV-001817114279	-8.4	0.262	432.429	REAL	O=C(CCNC(=O)c1ccc2ccccc2c1)Nc1nccc(-c2ccc(F)c(F)c2)n1
vMpro-mpro1-59	PV-001827574151	-8.4	0.271	435.953	REAL	O=C(NCC(=O)N1CCC(c2cccc3ccccc23)CC1)NCc1ccc(Cl)cc1
vMpro-mpro1-60	PV-001852481517	-8.4	0.262	445.44	REAL	Cc1ccc(C(=O)NCc2cccc(N3C(=O)NC4(CCCC4)C3=O)c2)cc1C(F)(F)F
vMpro-mpro1-61	PV-001867454921	-8.4	0.255	444.505	REAL	O=C(CNC(=O)C1CCN(C(=O)/C=C/c2ccccc2)CC1)c1ccc(F)c2ccccc12
vMpro-mpro1-62	PV-001880913380	-8.4	0.271	412.492	REAL	Cc1ccc(-c2nnc(NC(=O)Cc3cccc(OCc4cccc(C)c4)c3)[nH]2)cc1
vMpro-mpro1-63	PV-001884141760	-8.4	0.323	362.819	REAL	O=C(Cc1cccc2ccccc12)Nc1nc(-c2ccc(Cl)cc2)n[nH]1
vMpro-mpro1-64	PV-001893362365	-8.4	0.3	413.263	REAL	O=C(Cc1cc(Cl)cc2ccccc12)Nc1nnc(-c2ccc(O)c(Cl)c2)[nH]1
vMpro-mpro1-65	PV-001918402502	-8.4	0.28	400.528	REAL	Cc1cc(C)cc(C2=CCN([C@@H](C)c3nc(N)nc(Nc4ccccc4)n3)CC2)c1
vMpro-mpro1-66	PV-001943424279	-8.4	0.255	458.439	REAL	O=C(Nc1cc(-c2ccccc2)on1)N[C@H]1CCCN(Cc2cccc(C(F)(F)F)c2)C1=O
vMpro-mpro1-67	PV-001945276015	-8.4	0.29	388.43	REAL	Cc1cc(C)c(-c2cc(NC(=O)Nc3nc(-c4ccccc4)no3)[nH]n2)cc1C
vMpro-mpro1-68	PV-001955706252	-8.4	0.255	455.42	REAL	C[C@]1(c2cccc(CNC(=O)NCc3cc(-c4ccc(F)cc4F)on3)c2)NC(=O)NC1=O
vMpro-mpro1-69	Z1014458650	-8.4	0.233	484.598	REAL	C[C@H](NC(=O)[C@H]1C[C@@H]2CCCC[C@H]2N1C(=O)c1ccc2ccccc2c1)c1ccc(NC(N)=O)cc1
vMpro-mpro1-70	Z1091072178	-8.4	0.311	425.245	REAL	O=C(Cc1n[nH]c(=O)c2ccccc12)Nc1nnc(-c2ccc(Br)cc2)[nH]1
vMpro-mpro1-71	Z1097147018	-8.4	0.24	479.417	REAL	O=C(Nc1nnc(C(F)(F)F)[nH]1)c1c2c(nc3ccccc13)/C(=C/c1ccc3c(c1)OCO3)CC2
vMpro-mpro1-72	Z1129712783	-8.4	0.29	403.447	REAL	Cc1cccc2c1CC[C@H]2NC(=O)[C@@H]1CCCN(c2nccc2C(F)(F)F)C1
vMpro-mpro1-73	Z1173530296	-8.4	0.28	399.445	REAL	C[C@@H]1CN(C(=O)c2ccc3c(c2)C[C@@H](c2ccccc2)OC3=O)c2ccccc2O1
vMpro-mpro1-74	Z1322887690	-8.4	0.262	426.558	REAL	Cc1ccc(CNC(=O)C2CCN(C(=O)[C@@H]3C[C@H]3c3cccc4ccccc34)CC2)cc1
vMpro-mpro1-75	Z1438518877	-8.4	0.28	399.453	REAL	Cc1ccc(-c2cc(C(=O)NNC(=O)Nc3cccc4ccccc34)[nH]n2)cc1C
vMpro-mpro1-76	Z148969640	-8.4	0.24	489.551	REAL	Cc1cccc2c(=O)[nH]c(COC(=O)c3cccc(S(=O)(=O)N4CCc5ccccc5C4)c3)nc12
vMpro-mpro1-77	Z1544877647	-8.4	0.336	330.39	REAL	O=c1[nH]c(N/N=C2\C[C@H]3CCCc4ccccc2c43)nc2ccccc12
vMpro-mpro1-78	Z1563969320	-8.4	0.311	356.384	REAL	O=C(Cc1cc2c(ccc3ccccc32)o1)NNc1nc2ccccc2[nH]1
vMpro-mpro1-79	Z1612409440	-8.4	0.255	442.517	REAL	O=C1[C@H]2c3ccccc3CCN2C(=O)N1C1CCN(Cc2coc(-c3ccccc3)n2)CC1
vMpro-mpro1-80	Z1667259234	-8.4	0.255	441.486	REAL	O=C(NCc1ccc2c(c1)C(=O)NCC2)c1ccc(NC(=O)[C@@H]2Cc3ccccc3O2)c1
vMpro-mpro1-81	Z1671353188	-8.4	0.255	444.533	REAL	O=C(Cc1cccc2ccccc12)NNC(=O)Nc1cccc(NC(=O)C2CCCCC2)c1
vMpro-mpro1-82	Z1671628574	-8.4	0.262	426.475	REAL	Cc1ccc(Cn2cccc(NC(=O)NNC(=O)c3ccc4ccccc4c3)c2=O)cc1
vMpro-mpro1-83	Z1674151959	-8.4	0.262	430.51	REAL	O=C1NCCc2ccc(CNC(=O)N3CCC[C@H](c4n[nH]c(-c5ccccc5)n4)C3)cc21
vMpro-mpro1-84	Z1676450116	-8.4	0.255	441.49	REAL	Cn1nc(CNC(=O)CN2C(=O)N[C@]1(C)c3ccc4ccccc4c3)C2=O)c2ccccc21
vMpro-mpro1-85	Z1682409982	-8.4	0.262	444.514	REAL	Cc1sc2nc(Cc3noc(-c4cc(Cc5ccccc5)ccc4O)n3)[nH]c(=O)c2c1C
vMpro-mpro1-86	Z1682771434	-8.4	0.28	399.413	REAL	Cc1cccc2cc(-c3nc(Cc4nc(N)nc(Nc5ccccc5)n4)no3)oc12
vMpro-mpro1-87	Z1715973129	-8.4	0.29	402.375	REAL	Cc1cc2c(cc1C)[C@H](C(=O)Nc1ccn(-c3nccnc3C(F)(F)F)n1)CO2
vMpro-mpro1-88	Z1719399387	-8.4	0.255	448.517	REAL	Cc1cc2c(cc1C)[C@H](C(=O)N1CCC(C(=O)c3ccc4c(c3)NC(=O)[C@@H](C)O4)CC1)CO2
vMpro-mpro1-89	Z1723430646	-8.4	0.247	453.457	REAL	Cn1c(=O)[nH]c2ncc(-c3cccc(C(=O)NNC(=O)c4cc5ccccc5cc4O)c3)cc21
vMpro-mpro1-90	Z1723437952	-8.4	0.262	429.41	REAL	Cn1c(=O)[nH]c2ncc(-c3cccc(C(=O)Nc4cc(-c5ccccc5F)no4)c3)cc21
vMpro-mpro1-91	Z1723445065	-8.4	0.271	410.436	REAL	Cn1c(=O)[nH]c2ncc(-c3cccc(C(=O)NNc4ccc5ccccc5n4)c3)cc21
vMpro-mpro1-92	Z1765050171	-8.4	0.247	449.513	REAL	O=C(c1ccc2[nH]c3ccccc3c(=O)c2c1)N1CCC(c2nc(-c3ccccc3)n[nH]2)CC1
vMpro-mpro1-93	Z1787248753	-8.4	0.255	441.577	REAL	Cc1cc(N2CCC(NC(=O)NC[C@@H]3CC4c5ccccc5C3c3ccccc34)CC2)[nH]n1
vMpro-mpro1-94	Z1869802407	-8.4	0.262	427.503	REAL	O=C(CCc1ccccc1)N1CC[C@@H](N2C(=O)N[C@H](c3ccc4ccccc4c3)C2=O)C1
vMpro-mpro1-95	Z1883096891	-8.4	0.255	437.498	REAL	O=C1N[C@]2(CCc3ccccc32)C(=O)N1CC(=O)N1C[C@@H](c2ccccc2)c2ccccc21
vMpro-mpro1-96	Z1891911863	-8.4	0.28	397.433	REAL	Cc1nc(-c2cccc(N3C(=O)N[C@H](c4ccc5ccccc5c4)C3=O)c2)oc1C
vMpro-mpro1-97	Z1892034646	-8.4	0.3	371.395	REAL	O=C1N[C@H](c2cccnc2)C(=O)N1c1ccccc(-c2ccc3c(c2)CCO3)c1
vMpro-mpro1-98	Z1897868293	-8.4	0.271	432.459	REAL	O=c1ccc2cc(S(=O)(=O)Nc3nnc(Cc4cccc5ccccc45)o3)ccc2[nH]1
vMpro-mpro1-99	Z2008406872	-8.4	0.255	440.549	REAL	Cc1ccccc(NC(=O)[C@@H]2CCCN(c3nnc(Cc4ccc5ccccc5c4)n3)C2)n1
vMpro-mpro1-100	Z2014787080	-8.4	0.3	383.401	REAL	O=C(c1cc2[nH]nnc2cc1F)N1CCC(N2CCc3cc(F)ccc32)CC1

Supplementary Table 27. Top 100 virtual hits of the screen against the dimerization interface of M^{pro} (Screen ID: 18). Compounds were filtered so that hits had MW < 600 dalton, cLogP < 6, number of hydrogen bond acceptors < 11, and no reactive functional groups. A few compounds unsuitable for drug discovery were removed by visual inspection. The name of each compound consists of the initial letter 'v' for virtual hit, followed by the target protein name and the target site ('mpro' for the M^{pro} binding site, 1 for docking scenario 1). The score is the docking score given by QuickVina 2 in kcal/mol. The ligand efficiency (LE) is computed as LE = -score/#NonH, where #NonH is the number of heavy (i.e. non hydrogen) atoms.

Name	Catalog ID	Score	LE	MW	Library	SMILES
vMpro-mpro1-101	Z2066206380	-8.4	0.271	430.43	REAL	Cc1onc(-c2cccnc2)c1C(=O)N1CCN(Cc2cccc(C(F)(F)F)c2)CC1
vMpro-mpro1-102	Z2071462070	-8.4	0.271	414.51	REAL	Cc1nc(-c2ccc(NC(=O)N3C[C@@H](c4ccccc4)[C@@H]4CCC[C@H]43)cc2)cc(=O)[nH]1
vMpro-mpro1-103	Z2145998018	-8.4	0.255	449.51	REAL	C[C@H]1Oc2ccc(C(=O)C3CCN(C(=O)N[C@H]4c5ccccc5O[C@H]4C)CC3)cc2NC1=O
vMpro-mpro1-104	Z2166666151	-8.4	0.300	375.45	REAL	C[C@@H]1c2c(F)cccc2CCN1c1nnc(Cn2ccc3ccccc32)n1C
vMpro-mpro1-105	Z2166788903	-8.4	0.255	434.50	REAL	Cn1c(-c2n[nH]c(=O)c3ccccc23)nnc1N1Cc2ccccc2[C@@H](c2ccccc2)C1
vMpro-mpro1-106	Z2222904009	-8.4	0.262	423.52	REAL	Cc1ccc2nc(C(=O)N3CCC[C@@H](NC(=O)c4ccc5ccccc5c4)C3)ccc2c1
vMpro-mpro1-107	Z2227194367	-8.4	0.280	400.48	REAL	Cc1c(NC(=O)c2ccc3c(c2)CCC3)n[nH]c1NC(=O)c1ccc2c(c1)CCC2
vMpro-mpro1-108	Z273919386	-8.4	0.247	451.48	REAL	O=C(Nc1ccc2nc3n(c(=O)c2c1)CCC3)c1ccc(COc2ccc3ccccc3c2)o1
vMpro-mpro1-109	Z2749929283	-8.4	0.280	395.46	REAL	O=C1C[C@@H](c2ccc(NCc3c4ccccc4cc4ccccc34)cc2)NC(=O)N1
vMpro-mpro1-110	Z298859774	-8.4	0.227	491.55	REAL	O=C(N[C@H]1CCCc2[nH]c(=O)ccc21)c1c2c(nc3ccccc13)/C(=C/c1ccc3c(c1)OCO3)CC2
vMpro-mpro1-111	Z3136368895	-8.4	0.290	389.50	REAL	Cc1ccc2c(CC(=O)N3CCC4(CC3)C[C@H](N)c3ccccc3O4)c[nH]c12
vMpro-mpro1-112	Z3214715191	-8.4	0.240	469.55	REAL	Cc1ccc(C(=O)NCCn2nnnc2N2CCN(C(=O)c3cccc4ccccc34)CC2)cc1
vMpro-mpro1-113	Z365380428	-8.4	0.262	447.43	REAL	Cc1onc(-c2ccc(F)cc2)c1C(=O)N1CCN(Cc2cccc(C(F)(F)F)c2)CC1
vMpro-mpro1-114	Z424332426	-8.4	0.240	470.53	REAL	C[C@]1(c2ccccc(NC(=O)[C@@H]3CCCN(C(=O)c4cccc5ccccc45)C3)c2)NC(=O)NC1=O
vMpro-mpro1-115	Z48966018	-8.4	0.290	403.51	REAL	Cc1ccc(/N=C2\NC(=O)[C@@H](CC(=O)Nc3cccc4ccccc34)S2)cc1C
vMpro-mpro1-116	Z641838178	-8.4	0.280	398.42	REAL	O=C(c1cnc2[nH]c(=O)[nH]c(=O)c2c1)N1Cc2ccccc2[C@H](c2ccccc2)C1
vMpro-mpro1-117	Z650301094	-8.4	0.240	465.55	REAL	O=C(CN1C(=O)N[C@]2(CCc3ccccc3C2)C1=O)N1Cc2ccccc2[C@@H](c2ccccc2)C1
vMpro-mpro1-118	Z735794490	-8.4	0.290	429.93	REAL	COc1ccc(Cl)cc1NC(=O)C[C@H]1S/C(=N\c2ccc3c(c2)CCC3)NC1=O
vMpro-mpro1-119	Z819321846	-8.4	0.240	470.57	REAL	NC(=O)c1ccc(/C=C/C(=O)N2CCC[C@H]2C(=O)N2CCC(c3c[nH]c4ccccc34)CC2)cc1
vMpro-mpro1-120	Z968517082	-8.4	0.247	454.49	REAL	Cc1n[nH]c(-c2ccc(NC(=O)CN3C(=O)N[C@](C)(c4ccc5ccccc5c4)C3=O)cc2)n1
vMpro-mpro1-121	Z997744568	-8.4	0.227	494.55	REAL	Cc1ccc(N2C(=O)/C(=C/NCc3cccc([C@@]4(C)NC(=O)NC4=O)c3)c3ccccc3C2=O)cc1C
vMpro-mpro1-122	ZINC000000659882	-8.4	0.221	496.57	ZINC	O=C(c1ccccc1)c1ccc2c(c1)NC1=C(C(=O)C[C@@H](c3ccccc3)C1)[C@H]1c3ccccc3C(=O)N21
vMpro-mpro1-123	ZINC000001714466	-8.4	0.205	560.59	ZINC	O=C1C=C(Nc2ccc(S(=O)(=O)c3ccc(NC4=CC(=O)C(=O)c5ccccc54)cc3)cc2)c2ccccc21=O
vMpro-mpro1-124	ZINC000002256453	-8.4	0.247	471.92	ZINC	OC(/C=C/c1ccccc1)=N\C1=NN2C(=NC(c3ccc(Cl)cc3)=C[C@H]2c2ccc(F)cc2)N1
vMpro-mpro1-125	ZINC000002401785	-8.4	0.227	489.51	ZINC	O=C(c1ccc(F)cc1)[C@@H]1[C@@H]2C(=O)N(c3ccc4ccccc4c3)C(=O)[C@@H]2[C@@H]2c3ccccc3C=NN21
vMpro-mpro1-126	ZINC000008449797	-8.4	0.221	493.56	ZINC	O=C1[C@H]2[C@H](C(=O)N1c1ccc(Oc3ccc4ccccc4c3)cc1)C1c3ccccc3C2c2ccccc21
vMpro-mpro1-127	ZINC000011838457	-8.4	0.271	435.91	ZINC	O=C(/C=C/c1cccc(Cl)c1)N1CCc2nnc(CNC(=O)c3ccccc3)n2CC1
vMpro-mpro1-128	ZINC000013018541	-8.4	0.227	489.49	ZINC	O=C(NNC(=O)c1ccc(-n2cnnn2)cc1)c1ccc(CN2C(=O)c3cccc4cccc2c34)cc1
vMpro-mpro1-129	ZINC000017057457	-8.4	0.255	447.62	ZINC	CC1(C)C[C@]2(CCCN(Cc3nc4c(c(=O)[nH]3)C3(CCCC3)Cc3ccccc3-4)C2)CCO1
vMpro-mpro1-130	ZINC000021867163	-8.4	0.233	482.52	ZINC	Cc1cccc(-c2nnn3c2nc(O)c2ccc(C(=O)N4CCN(c5ccc(F)cc5)CC4)ce23)c1
vMpro-mpro1-131	ZINC000024967363	-8.4	0.240	494.57	ZINC	Cc1cc(C)cc(-c2nnc(SCC(=O)N3CCN(C(=O)[C@@H]4COc5ccccc5O4)CC3)o2)c1
vMpro-mpro1-132	ZINC000032848695	-8.4	0.271	430.50	ZINC	C[C@H](Sc1nnc(-c2c[nH]c3ccccc32)o1)c1nc(N)nc(Nc2ccccc2)n1
vMpro-mpro1-133	ZINC000100847054	-8.4	0.262	462.34	ZINC	O=C(Nc1nc2n(n1)[C@@H](c1ccccc1)C=C(c1ccc(Cl)cc1)N2)c1ccc(Cl)cc1
vMpro-mpro1-134	ZINC000100861439	-8.4	0.247	471.92	ZINC	O=C(/C=C/c1ccc(F)cc1)Nc1nc2n(n1)[C@@H](c1ccccc1)C=C(c1ccc(Cl)cc1)N2
vMpro-mpro1-135	ZINC000101016697	-8.4	0.262	441.92	ZINC	Cc1ccc(C(=O)Nc2nc3n(n2)[C@@H](c2ccccc2)C=C(c2ccc(Cl)cc2)N3)cc1
vMpro-mpro1-136	ZINC000101262733	-8.4	0.262	428.45	ZINC	Cc1ccc(-c2noc(CN3N=N[C@@H]4C(=O)N(c5ccc6c(c5)CCC6)C(=O)[C@@H]43)n2)cc1
vMpro-mpro1-137	ZINC000101262738	-8.4	0.262	428.45	ZINC	Cc1ccc(-c2noc(CN3N=N[C@@H]4C(=O)N(c5ccc6c(c5)CCC6)C(=O)[C@@H]43)n2)cc1
vMpro-mpro1-138	ZINC000101835650	-8.4	0.233	493.59	ZINC	Cc1ccc([C@H]2C=C(c3ccccc3)Nc3nc(NS(=O)(=O)c4ccc5ccccc5c4)nn32)cc1
vMpro-mpro1-139	ZINC000101835741	-8.4	0.255	459.91	ZINC	Cc1ccc([C@H]2C=C(c3ccc(Cl)cc3)Nc3nc(NC(=O)c4ccc(F)cc4)nn32)cc1
vMpro-mpro1-140	ZINC000101835965	-8.4	0.271	411.46	ZINC	Cc1ccc(C2=C[C@H](c3ccc(C)cc3)n3nc(NC(=O)c4ccco4)nc3N2)cc1
vMpro-mpro1-141	ZINC000101836019	-8.4	0.262	441.92	ZINC	Cc1ccc(C(=O)Nc2nc3n(n2)[C@@H](c2ccc(Cl)cc2)C=C(c2ccccc2)N3)c1
vMpro-mpro1-142	ZINC000245377192	-8.4	0.227	488.54	ZINC	O=C1[C@@H]2[C@H]3C=C[C@@H](C3)[C@H]2C(=O)N1c1ccc2c(c1)-c1cc(N3C(=O)[C@@H]4[C@H]5C=C[C@@H](C5)[C@@H]4C3=O)ccc1C2
vMpro-mpro1-143	ZINC000253412163	-8.4	0.227	489.48	ZINC	Cn1cc(/C=C2\Oc3c(ccc4c3[C@H](c3coc5ccccc5c3=O)CC(=O)O4)C2=O)c2ccccc21
vMpro-mpro1-144	ZINC000257219292	-8.4	0.262	427.51	ZINC	Cc1cccc2[nH]c(C(=O)N3CCO[C@H](c4ccc(Nc5nccc5C)cn4)C3)cc21
vMpro-mpro1-145	ZINC000408688101	-8.4	0.221	498.58	ZINC	Cc1ccc(NC(=O)c2cccc(N3C(=O)[C@H]4[C@@H](C3=O)C3c5ccccc5C4c4ccccc43)c2)cc1C
vMpro-mpro1-146	PV-001825233883	-8.3	0.277	416.40	REAL	Cc1ccc2[nH]ncc2c1C(=O)N1CCN(C(=O)c2cccc(C(F)(F)F)c2)CC1
vMpro-mpro1-147	PV-001828294963	-8.3	0.296	405.56	REAL	CC(C)(C)OC(=O)NCCc1nc(C(=O)N[C@@H]2C[C@@H]3C[C@@H]2[C@@H]2CCC[C@@H]32)cs1
vMpro-mpro1-148	PV-001828578687	-8.3	0.319	407.27	REAL	O=C(Cc1cccc2ccccc12)Nc1nnc(-c2ccc(Br)cc2)[nH]1
vMpro-mpro1-149	PV-001841353548	-8.3	0.268	416.48	REAL	Cc1ccc(-c2cc(C(=O)NNC(=O)c3ccc4c(c3)CCCCC4=O)[nH]n2)cc1C
vMpro-mpro1-150	PV-001944455366	-8.3	0.259	455.34	REAL	O=C(NCCc1cccc2c1OC(F)(F)O2)Nc1ccn(-c2ncccc2C(F)(F)F)n1
vMpro-mpro1-151	PV-001949905716	-8.3	0.252	446.51	REAL	Cc1ccc(-c2cc(C(=O)NNC(=O)Nc3ccc4c(c3)[C@@H](C)CC(=O)N4C)[nH]n2)cc1C
vMpro-mpro1-152	PV-001950141570	-8.3	0.244	456.54	REAL	COc1cccc([C@H](Cc2cc(C)cc(C)c2)NC(=O)Nc2ccc3[nH]c(C(N)=O)cc3c2)c1
vMpro-mpro1-153	PV-001957986730	-8.3	0.252	457.41	REAL	O=C(NNC(=O)c1ccc2ccccc2n1)N[C@@H]1CC(=O)N(c2cccc(C(F)(F)F)c2)C1
vMpro-mpro1-154	PV-001969232762	-8.3	0.268	416.44	REAL	Cc1ccc(-c2cc(C(=O)NNC(=O)NCc3c[nH]c(=O)c4ccccc34)[nH]n2)cc1
vMpro-mpro1-155	Z1000936770	-8.3	0.231	484.51	REAL	C[C@]1(c2cccc(CNC(=O)c3cccc(NC(=O)[C@H]4Cc5ccccc5O4)c3)c2)NC(=O)NC1=O
vMpro-mpro1-156	Z1000940884	-8.3	0.231	481.51	REAL	Cc1ccc(-c2nnc(-c3ccc(C(=O)NCc4cccc([C@@]5(C)NC(=O)NC5=O)c4)ce3)o2)cc1
vMpro-mpro1-157	Z1000941172	-8.3	0.231	481.51	REAL	Cc1nc2ccccc2c(=O)n1-c1ccc(C(=O)NCc2cccc([C@@]3(C)NC(=O)NC3=O)c2)cc1
vMpro-mpro1-158	Z1014558476	-8.3	0.252	450.49	REAL	O=C(Nc1ccc(-c2cc[nH]n2)cc1)[C@@H]1C[C@@H]2CCCC[C@H]2N1C(=O)c1ccc(F)cc1F
vMpro-mpro1-159	Z1021036848	-8.3	0.277	434.84	REAL	O=C1Nc2cc(Cl)ccc2C1=C1CCN(C(=O)Cc2cccc(C(F)(F)F)c2)CC1
vMpro-mpro1-160	Z1022496460	-8.3	0.224	495.62	REAL	O=C(NCC(=O)N1CCc2ccccc2C1)[C@@H]1C[C@@H]2CCCC[C@H]2N1C(=O)c1ccc2ccccc2c1
vMpro-mpro1-161	Z1022503832	-8.3	0.259	430.51	REAL	O=C(NCC(=O)N1CCc2ccccc2C1)c1ccc2c(=O)n3c(nc2c1)CCCCC3
vMpro-mpro1-162	Z1028479320	-8.3	0.231	492.51	REAL	C[C@@]1(c2cccc(CNC(=O)N3CCC[C@H](c4nc(-c5cccc(F)c5)no4)C3)c2)NC(=O)NC1=O
vMpro-mpro1-163	Z1039646216	-8.3	0.231	483.57	REAL	O=C(c1ccc2[nH]ncc2c1)N1CCC[C@H](C(=O)N2CCC(c3nc(-c4ccccc4)n[nH]3)CC2)C1
vMpro-mpro1-164	Z1069480524	-8.3	0.231	487.51	REAL	C[C@H]1Oc2ccc(C(=O)C3CCN(C(=O)c4cccc(NC(=O)c5ccco5)c4)CC3)cc2NC1=O
vMpro-mpro1-165	Z1069481792	-8.3	0.231	485.58	REAL	C[C@H]1Oc2ccc(C(=O)C3CCN(C(=O)c4ccc5[nH]c6c(c5c4)CCCCC6)CC3)cc2NC1=O
vMpro-mpro1-166	Z1069482782	-8.3	0.244	465.48	REAL	C[C@@H]1Oc2ccc(C(=O)C3CCN(C(=O)[C@@H]4CC(c5cccc(F)c5)=NO4)CC3)cc2NC1=O
vMpro-mpro1-167	Z1069483370	-8.3	0.259	454.91	REAL	C[C@H]1Oc2ccc(C(=O)C3CCN(C(=O)[C@@H]4Cc5cc(Cl)ccc5O4)CC3)cc2NC1=O
vMpro-mpro1-168	Z1069484924	-8.3	0.231	490.51	REAL	Cc1cc(=O)oc2cc(OCC(=O)N3CCC(C(=O)c4ccc5c(c4)NC(=O)[C@@H](C)O5)CC3)ccc12
vMpro-mpro1-169	Z1103945220	-8.3	0.231	494.44	REAL	O=C(CCc1nc2c(cnn2-c2ccccc2)c(=O)[nH]1)Nc1nc(-c2cccc(C(F)(F)F)c2)n[nH]1
vMpro-mpro1-170	Z1117098552	-8.3	0.231	488.57	REAL	O=C1Nc2ccccc2[C@H]1C1CCN(C(=O)Nc2cc(-c3nnc4n3CCCCC4)ccc2F)CC1
vMpro-mpro1-171	Z1122829524	-8.3	0.231	482.59	REAL	O=C(NC[C@@H]1CC2c3ccccc3C1c1ccccc12)NNC(=O)C1CCN(c2nccnc2)CC1
vMpro-mpro1-172	Z1128863346	-8.3	0.244	453.50	REAL	CC(C)c1nnc(NC(=O)c2c3c(nc4ccccc24)/C(=C\c2ccc4c(c2)OCO4)CC3)[nH]1
vMpro-mpro1-173	Z1249275940	-8.3	0.259	432.52	REAL	Cc1ccc(C(=O)N2CCC(NC(=O)N[C@H](C)c3ncc(-c4ccccc4)o3)CC2)cc1
vMpro-mpro1-174	Z1251877223	-8.3	0.259	438.45	REAL	C[C@H]1Oc2ccc(C(=O)C3CCN(C(=O)[C@@H]4Cc5cc(F)ccc5O4)CC3)cc2NC1=O
vMpro-mpro1-175	Z1283506798	-8.3	0.259	428.49	REAL	O=C(NNC(=O)c1ccc2ccccc12)N[C@H]1CC(=O)N([C@H]2C[C@H]2c2ccccc2)C1
vMpro-mpro1-176	Z1301415790	-8.3	0.268	412.46	REAL	Cn1c(=O)c2ccccc2n2c(CN3CCn4c(nnc4-c4ccccc4)C3)nnc12
vMpro-mpro1-177	Z1394794482	-8.3	0.252	440.50	REAL	Cc1ccc2c(O)c(C(=O)N3CCC[C@@H](NC(=O)c4ccc5ccccc5c4)C3)cnc2n1
vMpro-mpro1-178	Z14009835	-8.3	0.244	461.52	REAL	O=C(CN1C(=O)N[C@@]2(CCCCc3ccccc32)C1=O)Nc1ccc2c(c1)OC1(CCCC1)O2
vMpro-mpro1-179	Z14136476	-8.3	0.252	438.48	REAL	C[C@]1(c2ccc3ccccc3c2)NC(=O)N(Cc2cc(=O)oc3cc4c(cc23)CCC4)C1=O
vMpro-mpro1-180	Z1437003676	-8.3	0.268	430.43	REAL	Cc1onc(-c2cccen2)c1C(=O)N1CCN(Cc2ccccc(C(F)(F)F)c2)CC1
vMpro-mpro1-181	Z1437003689	-8.3	0.268	430.43	REAL	Cc1onc(-c2ccncc2)c1C(=O)N1CCN(Cc2ccccc(C(F)(F)F)c2)CC1
vMpro-mpro1-182	Z1446847326	-8.3	0.252	445.45	REAL	C[C@]1(c2cccc3ccccc23)NC(=O)N(CC(=O)c2cc3c(cc2F)NC(=O)CC3)C1=O
vMpro-mpro1-183	Z1446853476	-8.3	0.252	445.45	REAL	C[C@@]1(c2ccc3ccccc3c2)NC(=O)N(CC(=O)c2cc3c(cc2F)NC(=O)CC3)C1=O
vMpro-mpro1-184	Z1449091094	-8.3	0.244	449.55	REAL	O=C(NC[C@@H]1[C@H]2Cc3ccccc3[C@@H]12)c1cccc(C(=O)NC[C@@H]2[C@H]3Cc4ccccc4[C@@H]23)n1
vMpro-mpro1-185	Z1449095738	-8.3	0.252	439.51	REAL	C[C@]1(c2ccc3ccccc3c2)NC(=O)N(CC(=O)NC[C@H]2[C@H]3Cc4ccccc4[C@H]23)C1=O
vMpro-mpro1-186	Z1522533358	-8.3	0.259	433.51	REAL	C[C@@H]1Cc2cc(-c3ccc(CNC(=O)C4CCC5(CC4)NC(=O)NC5=O)cc3)ccc2O1
vMpro-mpro1-187	Z1553127176	-8.3	0.268	420.44	REAL	Cc1n[nH]c(C)c1[C@@H]1COCCN1C(=O)c1ccc2noc(-c3ccc(F)cc3)c2c1
vMpro-mpro1-188	Z1614241915	-8.3	0.268	421.54	REAL	CN1C(=O)C[C@@H](C(=O)N2CCC[C@@H](c3n[nH]c(C4CCCCC4)n3)C2)c2ccccc21
vMpro-mpro1-189	Z1614248130	-8.3	0.268	409.49	REAL	O=C(/C=C/c1ccnc2ccccc12)N1CCC[C@H](c2n[nH]c(-c3ccccc3)n2)C1
vMpro-mpro1-190	Z1618474375	-8.3	0.252	446.48	REAL	Cc1cc(F)c2nc(O)cc(C(=O)N3CCN(C(=O)Cc4c[nH]c5ccccc45)CC3)c2c1
vMpro-mpro1-191	Z1626782479	-8.3	0.252	435.53	REAL	O=C(c1ccc2c(=O)n3c(nc2c1)CCCCC3)N1CC=C(c2ccccc3ccccc23)C1
vMpro-mpro1-192	Z1631990546	-8.3	0.252	448.46	REAL	C[C@@]1(c2cccc(C(=O)N[C@H]3CCc4nnc(-c5ccc(F)cc5)n4C3)c2)NC(=O)NC1=O
vMpro-mpro1-193	Z1678212354	-8.3	0.259	424.51	REAL	Cn1nc(CNC(=O)NCc2cccc(Cn3cnc4ccccc43)c2)c2ccccc21
vMpro-mpro1-194	Z1682560636	-8.3	0.259	433.49	REAL	Cc1ccc(-c2noc(Cc3noc([C@H]4CCCN(Cc5cccc(F)c5)C4)n3)n2)cc1
vMpro-mpro1-195	Z1684581792	-8.3	0.252	438.44	REAL	C[C@]1(c2cccc(-c3noc(Cc4cc5c(cccc6ccccc65)o4)n3)c2)NC(=O)NC1=O
vMpro-mpro1-196	Z1723432865	-8.3	0.244	456.46	REAL	Cn1c(=O)[nH]c2ncc(-c3cccc(C(=O)Nc4ccc([C@@]5(C)NC(=O)NC5=O)cc4)c3)cc21
vMpro-mpro1-197	Z1723433311	-8.3	0.259	445.87	REAL	Cn1c(=O)[nH]c2ncc(-c3cccc(C(=O)Nc4nnc(-c5ccccc5Cl)[nH]4)c3)cc21
vMpro-mpro1-198	Z1723439192	-8.3	0.259	490.32	REAL	Cn1c(=O)[nH]c2ncc(-c3cccc(C(=O)Nc4cc(-c5ccccc5Br)no4)c3)cc21
vMpro-mpro1-199	Z1723439439	-8.3	0.224	490.52	REAL	Cn1c(=O)[nH]c2ncc(-c3cccc(C(=O)Nc4ccc5c(c4)CCN5C(=O)c4ccnc4)c3)cc21
vMpro-mpro1-200	Z1723440722	-8.3	0.252	446.48	REAL	C[C@@H]1CN(C(=O)c2cccc(-c3cnc4[nH]c(=O)n(C)c4c3)c2)C[C@@H](c2ccc(F)cc2)O1

Supplementary Table 28. Virtual screening hits 101 to 200 of the screen against the dimerization interface of M^{pro} (Screen ID: 18). Compounds were filtered so that hits had MW < 600 dalton, cLogP < 6, number of hydrogen bond acceptors < 11, and no reactive functional groups. A few compounds unsuitable for drug discovery were removed by visual inspection. The name of each compound consists of the initial letter 'v' for virtual hit, followed by the target protein name and the target site ('mpro' for the M^{pro} binding site, 1 for docking scenario 1). The score is the docking score given by QuickVina 2 in kcal/mol. The ligand efficiency (LE) is computed as LE = -score/#NonH, where #NonH is the number of heavy (i.e. non hydrogen) atoms.

Name	Catalog ID	Score	LE	MW	Library	SMILES
vPlpro-dub1-1	PV-001940740368	-10	0.313	456.609	REAL	C[C@H](CNC(=O)Nc1ccc(S(=O)(=O)N[C@H](C)[C@@H]2C[C@H]3CC[C@H]2C3)cc1)c1ccncc1
vPlpro-dub1-2	Z804255824	-9.9	0.268	494.593	REAL	O=C(NC1CCN(C(=O)Nc2ccccc2)CC1)[C@@H]1CC(=O)N(c2ccc3c(c2)Cc2ccccc2-3)C1
vPlpro-dub1-3	ZINC000008449795	-9.8	0.258	493.561	ZINC	O=C1[C@@H]2[C@@H](C(=O)N1c1ccc(Oc3ccc4ccccc4c3)cc1)C1c3ccccc3C2c2ccccc21
vPlpro-dub1-4	Z2902674503	-9.6	0.274	459.468	REAL	O=c1nc2c(-c3nc(-c4cccc(Cn5cnc6ccccc65)c4)no3)c[nH]n2c2ccccc12
vPlpro-dub1-5	Z1663725990	-9.5	0.288	440.437	REAL	Fc1ccc2c(c1)C[C@@H](c1nnc(-c3ccc(Cn4nnc(-c5ccccc5)n4)cc3)o1)O2
vPlpro-dub1-6	Z1663728734	-9.5	0.279	449.473	REAL	O=C1Nc2ccccc2[C@H]1Cc1nnc(-c2ccc(Cn3nnc(-c4ccccc4)n3)cc2)o1
vPlpro-dub1-7	Z804171530	-9.5	0.264	479.578	REAL	O=C(NC1CCN(C(=O)c2ccccc2)CC1)[C@H]1CC(=O)N(c2ccc3c(c2)Cc2ccccc2-3)C1
vPlpro-dub1-8	ZINC000033354415	-9.5	0.226	568.62	ZINC	O=C(c1ccccc1)c1ccc2c(c1)OCCOCCOc1ccc(C(=O)c3ccccc3)cc1OCCOCCO2
vPlpro-dub1-9	ZINC000097947962	-9.5	0.232	547.522	ZINC	Cc1cc(NC(=O)COC(=O)c2ccc3c(c2)C(=O)N(c2ccc(Oc4ccc5ccccc5c4)cc2)C3=O)no1
vPlpro-dub1-10	Z1161204097	-9.4	0.261	473.539	REAL	Cc1c(C(=O)NCc2cccc(Cn3cnc4ccccc43)c2)nnn1-c1ccc2ncccc2c1
vPlpro-dub1-11	Z1276059047	-9.4	0.294	449.465	REAL	Cn1c(NC(=O)c2ccc(NC3=NS(=O)(=O)c4ccccc43)cc2)nc2cc(F)ccc21
vPlpro-dub1-12	Z1411816259	-9.4	0.294	449.465	REAL	Cn1c(NC(=O)c2ccc(NC3=NS(=O)(=O)c4ccccc43)cc2)nc2c(F)ccc21
vPlpro-dub1-13	Z1872620962	-9.4	0.285	447.545	REAL	O=C(Nc1nc(C23CC4CC(CC(C4)C2)C3)c[nH]1)C1CCN(c2ccc3nnnn3n2)CC1
vPlpro-dub1-14	Z2524829917	-9.4	0.254	493.609	REAL	Cn1c(=O)[nH]c2ncc(-c3ccc(C(=O)N4C[C@H]5CC[C@H]4[C@H]4CN(Cc6ccccc6)C[C@H]54)c3)cc21
vPlpro-dub1-15	Z2902663617	-9.4	0.269	467.488	REAL	Cn1c(=O)c2cc(-c3nc(-c4ccc(Cn5cnc6ccccc65)cc4)no3)n(C)c2n(C)c1=O
vPlpro-dub1-16	Z511008034	-9.4	0.261	479.582	REAL	O=C(NCc1ccc(N2CCc3ccccc3C2)nc1)c1ccc2c(=O)n3c(nc2c1)CCCCC3
vPlpro-dub1-17	Z966271352	-9.4	0.269	468.52	REAL	O=C(Nc1cccc(C(=O)N2CCc3ccccc32)c1)C1CCN(c2ccc3nnnn3n2)CC1
vPlpro-dub1-18	Z1092439300	-9.3	0.291	426.431	REAL	O=C(NNc1nc(-c2ccccc2no1)c1ccc2c(c1)C[C@@H](c1ccccc1)OC2=O
vPlpro-dub1-19	Z1177635971	-9.3	0.344	371.386	REAL	O=C(NCC(=O)N1CCc2cc(F)c(F)cc21)N1CCc2ccccc2C1
vPlpro-dub1-20	Z1663728900	-9.3	0.282	436.474	REAL	c1ccc(-c2nnn(Cc3ccc(-c4nnc([C@H]5COc6ccccc6C5)o4)cc3)n2)cc1
vPlpro-dub1-21	Z1785570864	-9.3	0.282	436.43	REAL	Cn1c(-c2nc(-c3ccc(Oc4ccenc4)cc3)no2)cc2c(=O)n3ccccc3nc21
vPlpro-dub1-22	Z2159901371	-9.3	0.291	424.459	REAL	Cc1cccc(CNC(=O)Cc2noc(-c3ccc4[nH]c5ccccc5c(=O)c4c3)n2)c1
vPlpro-dub1-23	Z2193901914	-9.3	0.282	434.458	REAL	O=C1C[C@@H](c2nc(-c3ccc4[nH]nnc4c3)no2)CN1c1ccc2c(c1)Cc1ccccc1-2
vPlpro-dub1-24	Z2902663063	-9.3	0.258	477.483	REAL	O=c1[nH]c(=O)n(C2CC2)c2ncc(-c3nc(-c4ccc(Cn5cnc6ccccc65)cc4)no3)cc12
vPlpro-dub1-25	Z2902663552	-9.3	0.274	451.445	REAL	Cn1c(=O)[nH]c(=O)c2cc(-c3nc(-c4ccc(Cn5cnc6ccccc65)cc4)no3)cnc21
vPlpro-dub1-26	Z2902663689	-9.3	0.251	492.538	REAL	CC(=O)NCC(=O)N1CCc2cc(-c3nc(-c4ccc(Cn5cnc6ccccc65)cc4)no3)ccc21
vPlpro-dub1-27	Z2902666487	-9.3	0.291	423.431	REAL	O=C1Nc2ccc(-c3nc(-c4ccc(Cn5cnc6ccccc65)cc4)no3)cc2CO1
vPlpro-dub1-28	Z426089174	-9.3	0.258	482.518	REAL	O=C(CCc1nc2c(cnn2-c2ccccc2)c(=O)[nH]1)N1CC=C(c2c[nH]c3cc(F)ccc23)CC1
vPlpro-dub1-29	Z651461636	-9.3	0.282	448.565	REAL	Cc1cc(C)cc(C(=O)N2CCC[C@H](C(=O)NC3CCN(C(=O)c4ccncc4)CC3)C2)c1
vPlpro-dub1-30	Z770166350	-9.3	0.291	430.514	REAL	O=C(C1CCN(c2ccc3nnnn3n2)CC1)N1CCC[C@H](c2ec3ccccc3[nH]2)C1
vPlpro-dub1-31	Z804222766	-9.3	0.258	479.578	REAL	O=C(NC1CCN(C(=O)[C@@H]2CC(=O)N(c3cec4c(c3)Cc3ccccc3-4)C2)CC1)c1ccccc1
vPlpro-dub1-32	Z983351314	-9.3	0.291	428.447	REAL	O=C(NCc1ccc(-c2ccc3c(c2)CCCO3)cc1)c1cnc2[nH]c(=O)[nH]c(=O)c2c1
vPlpro-dub1-33	Z997042574	-9.3	0.258	481.55	REAL	O=C(Oc1cccc(C(=O)N2CCc3ccccc3C2)c1)C1CCN(c2nc3ccccc3o2)CC1
vPlpro-dub1-34	ZINC000006161704	-9.3	0.227	564.625	ZINC	Cc1ccc(-c2nnc(Nc3ccc4c(c3)OCO4)c3ccccc32)cc1S(=O)(=O)NCc1nc2ccccc2[nH]1
vPlpro-dub1-35	ZINC000065113756	-9.3	0.251	498.556	ZINC	Cc1ccc(C(=O)N2CCC(c3nc(-c4ccc(C(=O)NCc5ccc(F)cc5)cc4)no3)CC2)cc1
vPlpro-dub1-36	ZINC000104480052	-9.3	0.258	490.945	ZINC	O=C(NC1=CC=C[C@@H]2C(=O)c3ccccc3C(=O)[C@H]12)c1cc(-c2ccccc2Cl)nc2ccccc21
vPlpro-dub1-37	ZINC000104480060	-9.3	0.258	490.945	ZINC	O=C(NC1=CC=C[C@@H]2C(=O)c3ccccc3C(=O)[C@@H]12)c1cc(-c2ccccc2Cl)nc2ccccc21
vPlpro-dub1-38	PV-001847908068	-9.2	0.287	459.451	REAL	O=C1CCSc2ccc(C(=O)NNc3ccc(-c4cccc(C(F)(F)F)c4)nn3)cc2N1
vPlpro-dub1-39	PV-001905679643	-9.2	0.329	405.399	REAL	O=C(c1ccc2c(=O)[nH]c(S)nc2c1)N1CCc2ccc(C(F)(F)F)cc2C1
vPlpro-dub1-40	Z1037996148	-9.2	0.263	485.421	REAL	C[C@@]12CCC(=O)N1c1ccccc1C(=O)N2CC(=O)Nc1ccc(-c2noc(C(F)(F)F)n2)cc1
vPlpro-dub1-41	Z1067526278	-9.2	0.249	497.593	REAL	Cc1cc(C(=O)NC2CCN(C(=O)[C@H]3CC(=O)N(c4ccc5c(c4)Cc4ccccc4-5)C3)CC2)c(C)o1
vPlpro-dub1-42	Z1103945698	-9.2	0.263	498.44	REAL	O=C(Nc1nc(-c2cccc(C(F)(F)F)c2)n[nH]1)c1ccc2c(c1)S(=O)(=O)c1ccccc1C2=O
vPlpro-dub1-43	Z1119585351	-9.2	0.256	483.531	REAL	Cc1ccc(-c2nnc(-c3ccc(C(=O)NNC(=O)C4CCN(c5ncccn5)CC4)cc3)o2)cc1
vPlpro-dub1-44	Z1155217220	-9.2	0.271	463.526	REAL	NC(=O)[C@H]1CCCN(Cc2ccccc(CNC(=O)c3ccc(-c4ccc(F)cc4)cc3F)c2)C1
vPlpro-dub1-45	Z1158447919	-9.2	0.263	468.551	REAL	C[C@H]1Oc2ccc(C(=O)C3CCN(C(=O)[C@H]4C[C@@H]4c4ccc5ccccc5c4)CC3)cc2NC1=O
vPlpro-dub1-46	Z1161075056	-9.2	0.256	499.59	REAL	O=C(Oc1ccc(C(=O)N2CCc3sccc3C2)cc1)c1ccc2c(=O)n3c(nc2c1)CCCCC3
vPlpro-dub1-47	Z1162537090	-9.2	0.279	436.47	REAL	O=C(Nc1nc2ccccc2c(=O)[nH]1)[C@H]1CC(=O)N(c2ccc3c(c2)Cc2ccccc2-3)C1
vPlpro-dub1-48	Z1170164200	-9.2	0.287	420.427	REAL	O=c1oc2ccccc2cc1-c1nc(-c2cccc(Cn3cnc4ccccc43)c2)no1
vPlpro-dub1-49	Z1197754387	-9.2	0.287	421.459	REAL	O=C1CCc2cc(-c3nc(-c4ccc(Cn5cnc6ccccc65)cc4)no3)ccc2N1
vPlpro-dub1-50	Z1244070312	-9.2	0.287	431.47	REAL	Cc1cc(-c2nc3cc(F)ccc3n2C)ccc1NC(=O)NCc1cccc(C(N)=O)c1
vPlpro-dub1-51	Z1374245548	-9.2	0.287	429.562	REAL	O=C(C1CCN(c2nc3ccccc3o2)CC1)N1CCC[C@@]2(CCCc3ccccc32)C1
vPlpro-dub1-52	Z1646973064	-9.2	0.297	429.401	REAL	CC(=O)N1Cc2ccc(NC(=O)Nc3ccn(-c4cccc(C(F)(F)F)c4)n3)cc2C1
vPlpro-dub1-53	Z1663725968	-9.2	0.279	436.474	REAL	c1ccc(-c2nnn(Cc3ccc(-c4nnc([C@@H]5CCOc6ccccc65)o4)cc3)n2)cc1
vPlpro-dub1-54	Z1663726628	-9.2	0.279	435.45	REAL	Cc1nnc2ccc(-c3nnc(-c4ccc(Cn5nnc(-c6ccccc6)n5)cc4)o3)cn12
vPlpro-dub1-55	Z1663726895	-9.2	0.279	434.462	REAL	Cn1cnc2cc(-c3nnc(-c4ccc(Cn5nnc(-c6ccccc6)n5)cc4)o3)ccc21
vPlpro-dub1-56	Z1663728550	-9.2	0.279	434.462	REAL	Cc1c(-c2nnc(-c3ccc(Cn4nnc(-c5ccccc5)n4)cc3)o2)ccc2cncn12
vPlpro-dub1-57	Z1684581770	-9.2	0.279	441.45	REAL	Cc1ccc(Nc2ccc(-c3nc(-c4cccc([C@]5(C)NC(=O)NC5=O)c4)no3)c2)nn1
vPlpro-dub1-58	Z1685223609	-9.2	0.279	438.446	REAL	O=c1[nH]c2ccc(NCc3ccc(-c4noc(Cc5noc6ccccc56)n4)cc3)cc2[nH]1
vPlpro-dub1-59	Z183399140	-9.2	0.263	495.602	REAL	O=C(NC[C@H]1COc2ccccc2O1)N1CCN(Cc2nc3sc4c(c3c(=O)[nH]2)CCCC4)CC1
vPlpro-dub1-60	Z285524048	-9.2	0.287	448.554	REAL	O=C(C1CCN(c2ccc3nnnn3n2)CC1)N1CCC[C@H](c2nc3ccccc3s2)C1
vPlpro-dub1-61	Z288540894	-9.2	0.263	484.579	REAL	Cc1c(NC(=O)c2ccc3c(=O)n4c(nc3c2)CCC4)cccc1C(=O)N1CCc2scc2C1
vPlpro-dub1-62	Z2902665079	-9.2	0.263	464.484	REAL	C[C@@]1(c2ccc(-c3nc(-c4ccc(Cn5cnc6ccccc65)cc4)no3)cc2)NC(=O)NC1=O
vPlpro-dub1-63	Z2902665187	-9.2	0.263	464.484	REAL	C[C@]1(c2ccccc(-c3nc(-c4ccc(Cn5cnc6ccccc65)cc4)no3)c2)NC(=O)NC1=O
vPlpro-dub1-64	Z606625330	-9.2	0.256	478.515	REAL	Cc1[nH]c(-c2ccccc2)nc1C(=O)NNC(=O)c1ccc(Cn2nnc(-c3ccccc3)n2)cc1
vPlpro-dub1-65	Z615610854	-9.2	0.263	491.523	REAL	O=C1CCc2cc(S(=O)(=O)NC(=O)c3cccc(NC(=O)[C@@H]4Cc5ccccc5O4)c3)ccc2N1
vPlpro-dub1-66	Z685870398	-9.2	0.279	434.462	REAL	Cc1ccn2cc(-c3nnc(-c4ccc(Cn5nnc(-c6ccccc6)n5)cc4)o3)nc2c1
vPlpro-dub1-67	Z751929890	-9.2	0.256	476.495	REAL	Cc1[nH]nc2ncc(C(=O)NNC(=O)c3ccc(CN4C(=O)c5cccc6cccc4c56)cc3)cc12
vPlpro-dub1-68	Z770162890	-9.2	0.263	463.536	REAL	O=C(c1cccc(CN2C(=O)c3ccccc3C2=O)c1)N1CCC[C@H](c2cc3ccccc3[nH]2)C1
vPlpro-dub1-69	Z806433234	-9.2	0.271	451.529	REAL	O=C(c1ccc(OCc2cn3ccccc3n2)cc1)N1CCC(c2c[nH]c3ncccc23)CC1
vPlpro-dub1-70	Z828027642	-9.2	0.263	467.528	REAL	O=C(Nc1cccc(C(=O)NC2CCN(C(=O)c3ccccc3)CC2)c1)c1ccc2[nH]cnc2c1
vPlpro-dub1-71	Z920795534	-9.2	0.256	475.551	REAL	O=C(CCc1nc2c(cnn2-c2ccccc2)c(=O)[nH]1)N1CC=C(c2ccccc3ccccc23)CC1
vPlpro-dub1-72	Z932165648	-9.2	0.287	465.92	REAL	Cn1c(NC(=O)c2ccc(NC3=NS(=O)(=O)c4ccccc43)cc2)nc2cc(Cl)ccc21
vPlpro-dub1-73	Z954163544	-9.2	0.263	469.5	REAL	Cn1nc(C(=O)NNC(=O)NCc2ccc(-c3ccc4c(c3)CCO4)cc2)c2ccccc2c1=O
vPlpro-dub1-74	ZINC000002908937	-9.2	0.249	494.452	ZINC	O=c1oc(-c2cccc(F)c2)nc2cc(Cc3ccc4nc(-c5cccc(F)c5)oc(=O)c4c3)ccc12
vPlpro-dub1-75	ZINC000004804591	-9.2	0.249	499.649	ZINC	C[C@]12CC[C@H]3[C@@H](CCC4=CC(=O)CC[C@@]43C)[C@@H]1C[C@H]1[C@H]3C(=O)N(C4ccccc4)C(=O)[C@@H]3CC(=O)[C@@H]12
vPlpro-dub1-76	ZINC000021171142	-9.2	0.263	492.922	ZINC	O=C(c1ccc2c(c1)OCO2)N1CCC(c2nc3c(nnn3Cc3cccc(Cl)c3)c(=O)[nH]2)CC1
vPlpro-dub1-77	ZINC000065113760	-9.2	0.256	480.566	ZINC	Cc1ccc(C(=O)N2CCC(c3nc(-c4ccc(C(=O)NCc5ccccc5)cc4)no3)CC2)cc1
vPlpro-dub1-78	ZINC000065113778	-9.2	0.256	484.53	ZINC	O=C(NCc1ccccc1)c1ccc(-c2noc(C3CCN(C(=O)c4ccc(F)cc4)CC3)n2)cc1
vPlpro-dub1-79	PV-001806848564	-9.1	0.276	455.503	REAL	C[C@@H](NC(=O)C1CCN(C(=O)c2ccc(F)cc2F)CC1)C(=O)N1c2ccccc2C[C@H]1C
vPlpro-dub1-80	PV-001847908228	-9.1	0.276	458.378	REAL	Cc1nnnn1-c1ccc(C(=O)NNc2ccc(-c3cccc(C(F)(F)F)c3)nn2)c(F)c1
vPlpro-dub1-81	PV-001941100205	-9.1	0.284	454.553	REAL	C[C@H]1C[C@H](C)CN(S(=O)(=O)c2ccc(NC(=O)NNc3cnc4ccccc4n3)cc2)C1
vPlpro-dub1-82	Z1071336660	-9.1	0.268	461.473	REAL	C[C@H]1Oc2ccc(C(=O)C3CCN(C(=O)Nc4ccc5oc(=O)ccc5c4)CC3)cc2NC1=O
vPlpro-dub1-83	Z1072131206	-9.1	0.253	499.593	REAL	Cc1ccc2[nH]c([C@H]3CCCN(C(=O)c4ccc(NC5=NS(=O)(=O)c6ccccc65)cc4)C3)nc2c1
vPlpro-dub1-84	Z1099420375	-9.1	0.276	466.967	REAL	C[C@@H](NC(=O)N1CCC([C@H]2C(=O)Nc3cc(Cl)ccc32)CC1)c1ccc2c(c1)CC(=O)N2C
vPlpro-dub1-85	Z1100832889	-9.1	0.26	475.566	REAL	Cc1ccc2c(c1C)OC[C@@H]2NC(=O)NCc1ccnc(N2CCN(c3ccc(F)cc3)CC2)c1
vPlpro-dub1-86	Z1155214904	-9.1	0.26	491.658	REAL	NC(=O)[C@H]1CCCN(Cc2ccccc(CNC(=O)[C@H]3CCCN(c4nc5ccccc5s4)C3)c2)C1
vPlpro-dub1-87	Z1158361686	-9.1	0.26	491.934	REAL	Cc1cc(C(=O)NC2CCN(C(=O)c3ccccc3-c3nc(-c4cccc(Cl)c4)no3)CC2)no1
vPlpro-dub1-88	Z1161212068	-9.1	0.26	464.532	REAL	Cc1c(C(=O)N2CCC(c3nc(-c4ccccc4)n[nH]3)CC2)nnn1-c1ccc2ncccc2c1
vPlpro-dub1-89	Z1170158405	-9.1	0.276	435.442	REAL	CN1C(=O)c2ccc(-c3nc(-c4ccc(Cn5cnc6ccccc65)cc4)no3)cc2C1=O
vPlpro-dub1-90	Z1197754175	-9.1	0.276	436.474	REAL	O=C1NCCN1c1ccc(-c2nc(-c3ccc(Cn4cnc5ccccc54)cc3)no2)cc1
vPlpro-dub1-91	Z1240805966	-9.1	0.276	446.445	REAL	Cc1cc(-c2nc3cc(F)ccc3n2C)ccc1NC(=O)CCc1nc(-c2nnc[nH]2)no1
vPlpro-dub1-92	Z1416535113	-9.1	0.276	433.474	REAL	Cc1nnc(-c2ccc(-c3nc(-c4cccc(Cn5cnc6ccccc65)c4)no3)cc2)[nH]1
vPlpro-dub1-93	Z1565301025	-9.1	0.276	442.497	REAL	O=C(Nc1ccc(CCn2nnc(-c3ccccc3)n2)cc1)N1CCc2cc(F)ccc2C1
vPlpro-dub1-94	Z1632303440	-9.1	0.276	447.473	REAL	C[C@@H](NC(=O)N1CCC[C@H]1c1nc(-c2ccccc2)n[nH]1)c1nc(-c2cccc(F)c2)no1
vPlpro-dub1-95	Z1663726902	-9.1	0.303	398.469	REAL	c1ccc(-c2nnn(Cc3ccc(-c4nnc([C@H]5CC56CCCC6)o4)cc3)n2)cc1
vPlpro-dub1-96	Z1663728246	-9.1	0.284	429.483	REAL	CC(=O)N1CCC[C@@H](c2nnc(-c3ccc(Cn4nnc(-c5ccccc5)n4)cc3)o2)C1
vPlpro-dub1-97	Z1663729930	-9.1	0.284	422.447	REAL	c1ccc(-c2nnn(Cc3ccc(-c4nnc(-c5ccc6c(c5)COC6)o4)cc3)n2)cc1
vPlpro-dub1-98	Z1663730093	-9.1	0.276	440.506	REAL	O=C1[C@H]2CCC[C@@H]1CC(c1nnc(-c3ccc(Cn4nnc(-c5ccccc5)n4)cc3)o1)C2
vPlpro-dub1-99	Z1664137504	-9.1	0.276	441.494	REAL	C[C@H](Oc1ccc2ccccc2c1)c1nnc(C2CCN(c3ccc4nncn4n3)CC2)o1
vPlpro-dub1-100	Z1685223316	-9.1	0.276	437.462	REAL	O=c1[nH]c2ccc(NCc3ccc(-c4noc(Cc5n[nH]c6ccccc56)n4)cc3)cc2[nH]1

Supplementary Table 29. Top 100 virtual hits of the screen against the DUB binding site of PL^{pro} (Screen ID: 14). Compounds were filtered so that hits had MW < 600 dalton, cLogP < 6, number of hydrogen bond acceptors < 11, and no reactive functional groups. A few compounds unsuitable for drug discovery were removed by visual inspection. The name of each compound consists of the initial letter 'v' for virtual hit, followed by the target protein name and the target site ('dub' for DUB binding site, 1 for docking scenario 1). The score is the docking score given by QuickVina 2 in kcal/mol. The ligand efficiency (LE) is computed as LE = -score/#NonH, where #NonH is the number of heavy (i.e. non hydrogen) atoms.

Name	Catalog ID	Score	LE	MW	Library	SMILES
vPlpro-dub1-101	Z1685438116	-9.1	0.276	437.45	REAL	O=C1CCc2cc(-c3noc(-c4ccc5c(c4)C[C@H](c4ccccc4)OC5=O)n3)ccc2N1
vPlpro-dub1-102	Z1703807856	-9.1	0.284	449.47	REAL	Cn1c(NC(=O)c2ccc(NC3=NS(=O)(=O)c4ccccc43)cc2)nc2ccc(F)cc21
vPlpro-dub1-103	Z1733398265	-9.1	0.294	419.49	REAL	O=C(C1CCN(c2ccc3nnnn3n2)CC1)N1CCC[C@]2(C1)OCc1ccccc12
vPlpro-dub1-104	Z184820682	-9.1	0.268	471.50	REAL	O=C(NNC(=O)c1ccc2ccccc2n1)c1ccc(NC2=NS(=O)(=O)c3ccccc32)cc1
vPlpro-dub1-105	Z1936480527	-9.1	0.294	421.47	REAL	C[C@@H](C(=O)NC1CCN(C(=O)c2ccccc2F)CC1)n1ccc2ccccc2c1=O
vPlpro-dub1-106	Z198667882	-9.1	0.284	462.55	REAL	CCc1ccc2nc(NC(=O)c3ccc(NC4=NS(=O)(=O)c5ccccc54)cc3)sc2c1
vPlpro-dub1-107	Z2041545958	-9.1	0.284	448.51	REAL	Cc1nc2c(-c3noc(C4CCN(C5=NS(=O)(=O)c6ccccc65)CC4)n3)cccc2[nH]1
vPlpro-dub1-108	Z2107458903	-9.1	0.284	428.47	REAL	Cc1cc(-c2nc3cc(F)ccc3n2C)ccc1NC(=O)NCc1cnn2ccccc12
vPlpro-dub1-109	Z2156411824	-9.1	0.284	420.43	REAL	O=c1c2ccccc2[nH]c2ccc(-c3nc(-c4ccc(Cn5cncn5)cc4)no3)cc12
vPlpro-dub1-110	Z2157310224	-9.1	0.276	437.46	REAL	O=C1CN(c2ccc(-c3noc(-c4ccc5[nH]c6ccccc6c(=O)c5c4)n3)cc2)CCN1
vPlpro-dub1-111	Z2158784959	-9.1	0.276	442.45	REAL	O=c1c2ccccc2[nH]c2ccc(-c3nc(-c4ccc(N5CCOCC5)c(F)c4)no3)cc12
vPlpro-dub1-112	Z2159873762	-9.1	0.284	444.88	REAL	O=C(Cc1noc(-c2ccc3[nH]c4ccccc4c(=O)c3c2)n1)NCc1cccc(Cl)c1
vPlpro-dub1-113	Z2180030189	-9.1	0.284	432.45	REAL	O=C(NNC(=O)N1CCC(c2noc3ccc(F)ccc23)CC1)c1ccc2ccccc2c1
vPlpro-dub1-114	Z2902659410	-9.1	0.260	461.48	REAL	Cc1c(-c2nc(-c3ccc(OCc4ccenc4)cc3)no2)nnn1-c1ccc2ncccc2c1
vPlpro-dub1-115	Z2902663274	-9.1	0.260	459.47	REAL	O=c1nc2c(-c3nc(-c4ccc(Cn5cnc6ccccc65)cc4)no3)c[nH]n2c2ccccc12
vPlpro-dub1-116	Z2902665125	-9.1	0.260	463.50	REAL	O=C1C[C@@H](Cc2ccc(-c3nc(-c4ccc(Cn5cnc6ccccc65)cc4)no3)cc2)C(=O)N1
vPlpro-dub1-117	Z2902675641	-9.1	0.268	446.47	REAL	O=C(c1ccccc1)c1nc[nH]c1-c1nc(-c2cccc(Cn3cnc4ccccc43)c2)no1
vPlpro-dub1-118	Z2902677365	-9.1	0.294	408.46	REAL	c1cc(Cn2cnc3ccccc32)cc(-c2noc(C[C@H]3Cc4ccccc4O3)n2)c1
vPlpro-dub1-119	Z2902891095	-9.1	0.268	453.52	REAL	Fc1ccc(N2CCN(c3ccc(-c4noc([C@H]5[C@H]6Cc7ccccc7[C@@H]65)n4)cn3)CC2)cc1
vPlpro-dub1-120	Z2902950191	-9.1	0.276	435.48	REAL	O=C1C[C@@H](c2nc(-c3ccc4c(c3)CCO4)no2)CN1c1ccc2c(c1)Cc1ccccc1-2
vPlpro-dub1-121	Z393496026	-9.1	0.246	496.57	REAL	O=C(Nc1ccc(CC(=O)N2CCN(c3ccccc3)CC2)cc1)c1ccc(N2C(=O)CCC2=O)c1
vPlpro-dub1-122	Z396724670	-9.1	0.268	451.48	REAL	O=C(c1ccc(N2C(=O)c3ccccc3C2=O)c1)N1CCC[C@@H](c2nc3ccccc3o2)C1
vPlpro-dub1-123	Z402807448	-9.1	0.268	450.54	REAL	C[C@@H](c1nc(-c2ccccc2)no1)N1CCN(C(=O)c2ccc3c(c2)-c2ccccc2C3)CC1
vPlpro-dub1-124	Z402809840	-9.1	0.268	450.54	REAL	C[C@@H](c1nc(-c2ccccc2)no1)N1CCN(C(=O)c2ccc3c(c2)Cc2ccccc2-3)CC1
vPlpro-dub1-125	Z413441340	-9.1	0.253	484.60	REAL	O=C(Cc1ccc(NC(=O)N2CCO[C@H](c3ccccc3)C2)cc1)N1CCN(c2ccccc2)CC1
vPlpro-dub1-126	Z503753174	-9.1	0.260	487.54	REAL	O=C(Nc1nc2cc3c(cc2s1)OCCCO3)c1ccc(NC(=O)[C@@H]2Cc3ccccc3O2)c1
vPlpro-dub1-127	Z604030594	-9.1	0.276	445.57	REAL	C[C@H]1CCCCN1C(=O)c1ccc(NC(=O)N2CCC[C@H](c3nc4ccccc4[nH]3)C2)cc1
vPlpro-dub1-128	Z685869690	-9.1	0.284	422.45	REAL	c1ccc(-c2nnn(Cc3ccc(-c4nnc(-c5ccc6c(c5)CCO6)o4)cc3)n2)cc1
vPlpro-dub1-129	Z685869976	-9.1	0.276	434.46	REAL	C1=C(c2nnc(-c3ccc(Cn4nnc(-c5ccccc5)n4)cc3)o2)COc2ccccc21
vPlpro-dub1-130	Z757782482	-9.1	0.268	455.47	REAL	C[C@@]12CCC(=O)N1c1ccccc1C(=O)N2CC(=O)Nc1ccc2[nH]c(-c3ccco3)nc2c1
vPlpro-dub1-131	Z770162286	-9.1	0.268	449.51	REAL	O=C(c1ccc(N2C(=O)c3ccccc3C2=O)c1)N1CCC[C@@H](c2cc3ccccc3[nH]2)C1
vPlpro-dub1-132	Z806333512	-9.1	0.260	465.55	REAL	C[C@H](NC(=O)[C@@H]1CC(=O)N(c2ccc3c(c2)Cc2ccccc2-3)C1)c1ccc2c(c1)CCC(=O)N2
vPlpro-dub1-133	Z806363806	-9.1	0.260	467.52	REAL	O=C(NCc1ccnc(N2CCOC2=O)c1)[C@H]1CC(=O)N(c2ccc3c(c2)Cc2ccccc2-3)C1
vPlpro-dub1-134	Z806434386	-9.1	0.260	485.57	REAL	O=C(c1ccc(NC2=NS(=O)(=O)c3ccccc32)cc1)N1CCC(c2c[nH]c3ncccc23)CC1
vPlpro-dub1-135	Z806888942	-9.1	0.260	469.54	REAL	O=C(NCc1ccc(N2CCCCC2=O)cc1)c1ccc(NC(=O)[C@@H]2Cc3ccccc3O2)c1
vPlpro-dub1-136	Z855225378	-9.1	0.268	489.58	REAL	Cc1ccc(-c2nnc(NC(=O)c3ccc(NC4=NS(=O)(=O)c5ccccc54)cc3)s2)c(C)c1
vPlpro-dub1-137	Z982689964	-9.1	0.276	440.46	REAL	O=C1COc2ccc(C(=O)Nc3ccc(CCn4nnc(-c5ccccc5)n4)cc3)cc2N1
vPlpro-dub1-138	ZINC000001714466	-9.1	0.222	560.59	ZINC	O=C1C=C(Nc2ccc(S(=O)(=O)c3ccc(NC4=CC(=O)C(=O)c5ccccc54)cc3)cc2)c2ccccc2C1=O
vPlpro-dub1-139	ZINC000002079077	-9.1	0.228	528.56	ZINC	Cc1ccc(N2C(=O)c3ccc(C(=O)c4ccc5c(c4)C(=O)N(c4ccc(C)cc4C)C5=O)cc3C2=O)c(C)c1
vPlpro-dub1-140	ZINC000012890378	-9.1	0.253	484.55	ZINC	Cc1c2cc3c(cc2oc(=O)c1CC(=O)N1C[C@H]2C[C@@H](C1)c1ccccc(=O)n1C2)oc1c3CCCC1
vPlpro-dub1-141	ZINC000013735971	-9.1	0.276	460.41	ZINC	O=C(c1ccc2ncC(F)(F)F)[nH]c2c1)N1CCN(C(=O)[C@@H]2COc3ccccc3O2)CC1
vPlpro-dub1-142	ZINC000019877423	-9.1	0.253	484.51	ZINC	O=C(c1ccc(N2CCN([C@@H]3CC(=O)N(c4ccc5c(c4)OCO5)C3=O)CC2)cc1)c1ccncn1
vPlpro-dub1-143	ZINC000021867256	-9.1	0.246	492.58	ZINC	Cc1ccc(-c2nnn3c2nc(O)c2ccc(C(=O)N4CCN(c5cc(C)ccc5C)CC4)cc23)cc1
vPlpro-dub1-144	ZINC000026780145	-9.1	0.253	490.95	ZINC	O=C(NC1=CC=C[C@H]2C(=O)c3ccccc3C(=O)[C@@H]12)c1cc(-c2ccccc2Cl)nc2ccccc21
vPlpro-dub1-145	ZINC000065113766	-9.1	0.246	494.59	ZINC	Cc1ccc(C(=O)N2CCC(c3nc(-c4ccc(C(=O)NCc5ccccc5C)cc4)no3)CC2)cc1
vPlpro-dub1-146	ZINC000070691633	-9.1	0.276	455.68	ZINC	CC(=O)N1C[C@H](C)CC[C@]12O[C@H]1C[C@H]3[C@@H]4CC=C5C[C@@H](O)CC[C@]5(C)[C@@H]4CC[C@]3(C)[C@H]1[C@@H]2C
vPlpro-dub1-147	ZINC000146057035	-9.1	0.217	566.64	ZINC	CCc1cc(O)c(F)cc1-c1ccc2c(c1)[nH]nc2-c1nc2c([nH]1)CCN(C(=O)c1cnc(N3CCCC3)cn1)C2
vPlpro-dub1-148	ZINC000208172338	-9.1	0.246	498.58	ZINC	Cc1c2cc3c(cc2oc(=O)c1CCC(=O)N1C[C@H]2C[C@@H](C1)Cn1c(=O)ccce12)oc1c3CCCC1
vPlpro-dub1-149	ZINC000408684129	-9.1	0.253	485.58	ZINC	CC1=CC[C@@H]2C(=O)N(c3cccc(C(=O)Nc4cccc(C(=O)N5CCC(C)CC5)c4)c3)C(=O)[C@@H]2C1
vPlpro-dub1-150	PV-001806344634	-9.0	0.281	448.46	REAL	Cc1cc(N2C[C@H](C(=O)N3CCC[C@H](c4cccc(C(F)(F)F)c4)C3)CC2=O)ccc1F
vPlpro-dub1-151	PV-001807670206	-9.0	0.290	418.58	REAL	Cc1cc(C)cc(C(=O)N2CCC[C@H](C(=O)N3Cc4cc(C)ccc4CC3(C)C)C2)c1
vPlpro-dub1-152	PV-001822709578	-9.0	0.265	458.50	REAL	C[C@H](CC(=O)NNC(=O)c1ccc(Cn2nnc(-c3cccc3)n2)cc1)c1cccc(F)c1
vPlpro-dub1-153	PV-001829134206	-9.0	0.273	441.53	REAL	NC(=O)[C@H]1CCCN(Cc2ccc(NC(=O)c3ccc(-c4ccc(C=O)cc4)cc3)cc2)C1
vPlpro-dub1-154	PV-001838186275	-9.0	0.273	451.50	REAL	Cc1cc(-c2noc([C@@H](C)NC(=O)C3CCN(C(=O)Nc4ccccc4)CC3)n2)ccc1F
vPlpro-dub1-155	PV-001861984223	-9.0	0.310	409.80	REAL	O=C(Nc1nc2cc(F)c(Cl)cc2[nH]1)c1ccc(C(=O)c2ccco[O]c2)cc1
vPlpro-dub1-156	PV-001941456637	-9.0	0.290	411.46	REAL	Cc1cc(-c2ccccc2)ccc1NC(=O)NNC(=O)c1cc2ccccc2cc1O
vPlpro-dub1-157	PV-001958808597	-9.0	0.281	440.41	REAL	Cc1ccc(-c2noc([C@H](C)NC(=O)NCc3nc(-c4cccc(F)c4no3)n2)cc1F
vPlpro-dub1-158	PV-001970374134	-9.0	0.265	459.55	REAL	O=C(NC[C@H]1CCC=CCCC1)NNC(=O)c1ccc(Cn2nnc(-c3cccc3)n2)cc1
vPlpro-dub1-159	PV-001970461401	-9.0	0.265	456.51	REAL	Cc1ccccnc1[C@H](C)NC(=O)NNC(=O)c1ccc(Cn2nnc(-c3cccc3)n2)cc1
vPlpro-dub1-160	Z1004161580	-9.0	0.265	461.50	REAL	Cc1cc(C)n(-c2ccc(NC(=O)N3CCC[C@H](c4nc(-c5cccc(F)c5)no4)C3)cn2)n1
vPlpro-dub1-161	Z1028466884	-9.0	0.250	492.55	REAL	O=C(CNC(=O)N1CCC[C@@H](c2nc(-c3cccc(F)c3no2)C1)N1CCN(c2ccccc2)CC1
vPlpro-dub1-162	Z104124248	-9.0	0.273	434.46	REAL	Cc1cccc2nc(-c3nnc(-c4ccc(Cn5nnc(-c6ccccc6)n5)cc4)o3)cn12
vPlpro-dub1-163	Z1071975926	-9.0	0.265	474.59	REAL	O=C(c1ccc2[nH]cnc2c1)N1CCN(C(=O)C2CCN(c3nc4ccccc4s3)CC2)CC1
vPlpro-dub1-164	Z1074948108	-9.0	0.250	490.51	REAL	O=C(Nc1ccc(CCn2nnc(-c3ccccc3)n2)cc1)N1CCO[C@H](c2cccc(F)c(F)c2)C1
vPlpro-dub1-165	Z1081850494	-9.0	0.273	495.97	REAL	O=C(Nc1nnc(-c2cccc(Cl)c2)s1)c1ccc(NC2=NS(=O)(=O)c3ccccc32)cc1
vPlpro-dub1-166	Z1093587674	-9.0	0.257	471.46	REAL	C[C@@H]1Oc2ccc(C(=O)COC(=O)c3ccc4c(c3)C[C@H](c3cccc3)OC4=O)cc2NC1=O
vPlpro-dub1-167	Z1095050516	-9.0	0.265	462.46	REAL	O=C(Nc1nc(-c2ccc3ccccc3n2)n[nH]1)C1CCN(C(=O)c2ccc(F)cc2F)CC1
vPlpro-dub1-168	Z1101778747	-9.0	0.243	497.55	REAL	NC(=O)[C@H]1CCCN(Cc2ccc(NC(=O)c3ccc4c(=O)n(-c5ccccc5)c(=O)[nH]c4c3)cc2)C1
vPlpro-dub1-169	Z1104835324	-9.0	0.257	476.53	REAL	C[C@H]1Oc2ccc(C(=O)C3CCN(C(=O)Nc4ccc5c(c4)CCCC(=O)N5)CC3)cc2NC1=O
vPlpro-dub1-170	Z1118913902	-9.0	0.257	471.52	REAL	O=C(NNC(=O)C1CCN(c2ncccn2)CC1)c1ccc(COc2ccc3ccccc3c2)o1
vPlpro-dub1-171	Z1130447974	-9.0	0.265	459.57	REAL	Cc1ccc2c1CC[C@@H]2NC(=O)NCc1ccnc(N2CCN(c3ccc(F)cc3)CC2)c1
vPlpro-dub1-172	Z1130974395	-9.0	0.250	499.45	REAL	C[C@H](c1nc(-c2cccc(C(F)(F)F)c2)no1)N1CCN(C(=O)c2ccc3c(c2)C(=O)NC3=O)CC1
vPlpro-dub1-173	Z1155700234	-9.0	0.265	458.52	REAL	O=C(Nc1cccc(-c2ccc3c(c2)OCCO3)n1)C1CCN(C(=O)Nc2ccccc2)CC1
vPlpro-dub1-174	Z1155808619	-9.0	0.273	464.57	REAL	NC(=O)[C@H]1CCCN(Cc2cccc(CNc3nn4cc(-c5ccc(F)cc5)nc4s3)c2)C1
vPlpro-dub1-175	Z1157951829	-9.0	0.243	491.59	REAL	O=C(Nc1ccc(CC(=O)N2CCN(c3nccn3)CC2)cc1)[C@@H]1C[C@H]1c1ccc2ccccc2c1
vPlpro-dub1-176	Z1160465879	-9.0	0.250	483.53	REAL	O=C(NC[C@@H]1CCOc2ccccc21)NNC(=O)c1ccc(Cn2nnc(-c3cccc3)n2)cc1
vPlpro-dub1-177	Z1170158949	-9.0	0.281	423.43	REAL	O=C1COc2cc(-c3nc(-c4ccc(Cn5cnc6ccccc65)cc4)no3)ccc2N1
vPlpro-dub1-178	Z1197755822	-9.0	0.273	436.47	REAL	O=C1NCCN1c1ccc(-c2nc(-c3cccc(Cn4cnc5ccccc54)c3)no2)cc1
vPlpro-dub1-179	Z1279497653	-9.0	0.273	442.56	REAL	Cc1ccc(-c2noc([C@H](C)N3CCN(C(=O)[C@H]4C[C@@]45CCc4ccccc45)CC3)n2)cc1
vPlpro-dub1-180	Z1302752921	-9.0	0.273	445.47	REAL	Cn1ccc(N2CCC[C@H](OC(=O)c3ccc4c(c3)C[C@H](c3cccc3)OC4=O)C2=O)n1
vPlpro-dub1-181	Z1304751151	-9.0	0.273	449.51	REAL	COc1cccc(-c2noc([C@H](C)NC(=O)NC3CCN(C(=O)c4ccccc4)CC3)n2)c1
vPlpro-dub1-182	Z1382450133	-9.0	0.273	440.46	REAL	Cc1cc2nc(-c3ccc(CNC(=O)c4cnc5[nH]c(=O)[nH]c(=O)c5c4)cc3)[nH]c2cc1C
vPlpro-dub1-183	Z1395804888	-9.0	0.273	444.49	REAL	O=C(N[C@H]1CCCN(C(=O)NCc2coc(-c3cccc3)n2)C1)c1cc2ccccc2o1
vPlpro-dub1-184	Z1424139941	-9.0	0.281	438.51	REAL	Cc1nc([C@@H]2CCCN(C(=O)Nc3cc(-c4nnc5n4CCCCC5)cccc3F)C2)n[nH]1
vPlpro-dub1-185	Z1447552358	-9.0	0.281	438.43	REAL	O=C1CCc2cc(C(=O)N3CCC[C@H](c4nc(-c5cccc(F)c5)no4)C3)c(F)cc2N1
vPlpro-dub1-186	Z1458999179	-9.0	0.265	448.56	REAL	O=C(NC[C@@H]1[C@H]2Cc3ccccc3[C@@H]12)c1cccc(C(=O)NC[C@H]2[C@H]3Cc4ccccc4[C@@H]23)c1
vPlpro-dub1-187	Z1570191269	-9.0	0.281	435.50	REAL	C[C@@H](NC(=O)NC1CCN(C(=O)c2ccco2)CC1)c1ccc(-c2ccc(F)cc2)cc1
vPlpro-dub1-188	Z1571477946	-9.0	0.273	446.60	REAL	CC1CCN(CCc2ccccc(NC(=O)N3CCC(c4nnc5ccccn45)CC3)c2)CC1
vPlpro-dub1-189	Z1571944414	-9.0	0.290	431.42	REAL	Cc1cc(C)cc(C2=CCN(C(=O)c3nc(C)n(-c4nnc(C(F)(F)F)[nH]4)n3)CC2)c1
vPlpro-dub1-190	Z1578175778	-9.0	0.273	449.55	REAL	Cc1ccc(Oc2ccc(NC(=O)N3CCC4(CC3)C[C@H]4C(=O)N3CCCC3)cc2)nn1
vPlpro-dub1-191	Z1611841199	-9.0	0.290	425.51	REAL	O=C1NC2(Cc3ccccc3C2)C(=O)N1c1ccc(Cc2nc3ccccc3s2)cc1
vPlpro-dub1-192	Z1619661413	-9.0	0.281	427.47	REAL	O=C(/C=C\C(=O)N1CCC[C@H]1c1nc(-c2ccccc2)n[nH]1)Nc1ccc2[nH]ncc2c1
vPlpro-dub1-193	Z1632355327	-9.0	0.290	417.49	REAL	O=C(N[C@H]1CCc2nnc(-c3ccc(F)cc3)n2C1)N[C@@H]1[C@H]2CCc3ccccc3[C@H]21
vPlpro-dub1-194	Z1658286589	-9.0	0.290	413.52	REAL	O=C(N[C@@H]1[C@H]2CCc3ccccc3[C@H]21)N1CCC[C@H](c2n[nH]c(-c3cccc3)n2)C1
vPlpro-dub1-195	Z1663727278	-9.0	0.273	438.45	REAL	c1ccc(-c2nnn(Cc3ccc(-c4nnc(-c5cccc6c5OCCO6)o4)cc3)n2)cc1
vPlpro-dub1-196	Z1663729142	-9.0	0.273	438.45	REAL	c1ccc(-c2nnn(Cc3ccc(-c4nnc([C@H]5CCo6ccccc6O5)o4)cc3)n2)cc1
vPlpro-dub1-197	Z1684079466	-9.0	0.265	449.47	REAL	Nc1nc(Cc2noc(-c3ccc4c(c3)C[C@@H](c3cccc3)OC4=O)n2)nc2ccccc12
vPlpro-dub1-198	Z1764154579	-9.0	0.281	426.47	REAL	O=C(c1ccc(C(=O)N2CCC[C@@H](c3nc4ccccc4o3)C2)cc1)c1ccccc(O)c1
vPlpro-dub1-199	Z1766451513	-9.0	0.273	436.51	REAL	Cc1ccc2[nH]c([C@H]3CCCN(C(=O)c4ccc5[nH]c6ccccc6c(=O)c5c4)C3)nc2c1
vPlpro-dub1-200	Z1770982996	-9.0	0.290	417.37	REAL	O=C(Nc1nc(-c2c(F)cccc2F)n[nH]1)c1ccc2[nH]c3ccccc3c(=O)c2c1

Supplementary Table 30. Virtual screening hits 101 to 200 of the screen against the DUB binding site of PL^{pro} (Screen ID: 14). Compounds were filtered so that hits had MW < 600 dalton, cLogP < 6, number of hydrogen bond acceptors < 11, and no reactive functional groups. A few compounds unsuitable for drug discovery were removed by visual inspection. The name of each compound consists of the initial letter 'v' for virtual hit, followed by the target protein name and the target site ('dub' for DUB binding site, 1 for docking scenario 1). The score is the docking score given by QuickVina 2 in kcal/mol. The ligand efficiency (LE) is computed as LE = -score/#NonH, where #NonH is the number of heavy (i.e. non hydrogen) atoms.

Name	Catalog ID	Score	LE	MW	Library	SMILES
vMpro-mpro2-1	ZINC000017862766	-11.4	0.285	520.587	ZINC	O=C(Nc1ccc2ccccc2c1)c1cccc(N2C(=O)[C@H]3[C@@H](C2=O)C2c4ccccc4C3c3ccccc32)c1
vMpro-mpro2-2	Z2785110607	-11.1	0.411	365.428	REAL	CCCOc1ccccc1C(=O)CNC(=O)[C@]12[C@@H]3C(=O)[C@@H]4[C@H]5C[C@@H]([C@@H]41)[C@@H]2[C@H]53
vMpro-mpro2-3	ZINC000240824838	-10.8	0.277	516.556	ZINC	O=C1[C@@H]2[C@H]3C=C[C@@H](C3)[C@H]2C(=O)N1c1ccc(-c2nc3ccc(N4C(=O)[C@@H]5[C@H]6C=C[C@@H](C6)[C@@H]5C4=O)cc3[nH]2)cc1
vMpro-mpro2-4	Z1082363914	-10.7	0.345	426.515	REAL	C[C@H]1CC(C)(C)C[C@@]2(C1)NC(=O)N(CC(=O)N1C[C@@H](C(N)=O)Cc3ccccc31)C2=O
vMpro-mpro2-5	Z1531172578	-10.7	0.334	444.495	REAL	CN1C(=O)CC[C@H](C(=O)N2Cc3ccccc3C(C)(C)C2)[C@H]1c1ccc(C(F)(F)F)cc1
vMpro-mpro2-6	ZINC000017988176	-10.7	0.268	521.571	ZINC	O=C(Oc1ccc2ccccc2c1)c1cccc(N2C(=O)[C@H]3[C@@H](C2=O)C2c4ccccc4C3c3ccccc32)c1
vMpro-mpro2-7	Z1147822896	-10.6	0.312	470.45	REAL	O=C(c1ccc(-c2noc(C(F)(F)F)n2)cc1)N1CCC(C(=O)N2CCc3ccccc32)CC1
vMpro-mpro2-8	ZINC000100505727	-10.6	0.286	488.542	ZINC	O=C1[C@@H]2[C@H]3C=C[C@@H](C3)[C@@H]2C(=O)N1c1ccc2c(c1)-c1cc(N3C(=O)[C@H]4[C@H]5C=C[C@H](C5)[C@@H]4C3=O)ccc1C2
vMpro-mpro2-9	ZINC000101343712	-10.6	0.303	460.488	ZINC	O=C(c1ccco1)[C@@H]1[C@@H]2C(=O)N(c3ccc4ccccc4c3)C(=O)[C@H]2[C@H]2c3ccccc3C=CN12
vMpro-mpro2-10	Z1072127096	-10.5	0.292	482.582	REAL	Cc1ccc2[nH]c([C@@H]3CCCN(C(=O)[C@@H]4CCCN4C(=O)c4ccc5ccccc5c4O)C3)nc2c1
vMpro-mpro2-11	Z1250586272	-10.5	0.318	438.486	REAL	Cc1cc(C(=O)NC[C@H]2CC3c4ccccc4C2c2ccccc23)nc2nc(O)[nH]c(=O)c12
vMpro-mpro2-12	Z1323884037	-10.5	0.339	425.373	REAL	Cc1nc(C(=O)Nc2ccc3c(c2)Cc2ccccc2-3)nn1-c1nnc(C(F)(F)F)[nH]1
vMpro-mpro2-13	Z1766229415	-10.5	0.339	410.472	REAL	O=C(N[C@@H]1CC2(CCC2)Oc2ccccc21)c1ccc2[nH]c3ccccc3c(=O)c2c1
vMpro-mpro2-14	ZINC000011880144	-10.5	0.292	489.593	ZINC	Cc1nc(N2CCC(C(=O)N3CCNC(=O)[C@@H]3c3cccc(F)c3)CC2)nc2ccc(C(C)C)cc12
vMpro-mpro2-15	ZINC000101421018	-10.5	0.284	488.542	ZINC	O=C(Nc1ccc2c(c1)C(=O)c1ccccc1-2)[C@H](Cc1ccccc1)N1C(=O)[C@@H]2[C@H]3C=C[C@@H](C3)[C@@H]2C1=O
vMpro-mpro2-16	PV-001801086753	-10.4	0.347	413.516	REAL	C[C@H]1CC(C)(C)C[C@@]2(C1)NC(=O)N(CC(=O)N1CC(C)(C)Oc3ccccc31)C2=O
vMpro-mpro2-17	PV-001801233687	-10.4	0.325	442.4	REAL	CCNC(=O)c1cc(NC(=O)c2cc3ncc(C)cc(C(F)(F)F)n3n2)nc2ccccc12
vMpro-mpro2-18	PV-001815343469	-10.4	0.359	459.295	REAL	CC1(C)COc2ccc(NC(=O)[C@@H]3Cc4ccc(Br)cc4C(=O)O3)cc2NC1=O
vMpro-mpro2-19	PV-001942447235	-10.4	0.325	447.456	REAL	Cc1c(NC(=O)N2CCc3cc(C(F)(F)F)ccc3C2)ccc1C(=O)N1CCOCC1
vMpro-mpro2-20	PV-001950485965	-10.4	0.335	433.41	REAL	CN(Cc1ccc2c(c1)OC(F)(F)O2)C(=O)Nc1ccc2c(c1)NC(=O)C(C)(C)CO2
vMpro-mpro2-21	Z1091251226	-10.4	0.297	480.405	REAL	O=C(Nc1nc2ccccc2n1Cc1cccc(C(F)(F)F)c1)c1cnc2[nH]c(=O)[nH]c(=O)c2c1
vMpro-mpro2-22	Z1095050586	-10.4	0.297	465.472	REAL	Cc1cc(-c2cc(C(=O)Nc3nc(-c4ccc5ccccc5n4)n[nH]3)c3c(C)noc3n2)c(C)o1
vMpro-mpro2-23	Z3121383986	-10.4	0.4	371.504	REAL	Cc1sc(=O)n(CC(=O)N[C@@H]2CCNC3(CCC3)C2)c1-c1ccccc1
vMpro-mpro2-24	Z806293372	-10.4	0.289	480.523	REAL	C[C@]1(c2ccccc(NC(=O)[C@@H]3CC(=O)N(c4ccc5c(c4)Cc4ccccc4-5)C3)c2)NC(=O)NC1=O
vMpro-mpro2-25	Z979337174	-10.4	0.315	439.561	REAL	Cc1ccc(-n2nc(C(=O)N3CCC[C@@H](c4nc5cc(C)ccc5[nH]4)C3)c2CCC3)cc1
vMpro-mpro2-26	ZINC000008449797	-10.4	0.274	493.561	ZINC	O=C1[C@H]2[C@H](C(=O)N1c1ccc(Oc3ccc4ccccc4c3)cc1)C1c3ccccc3C2c2ccccc21
vMpro-mpro2-27	ZINC000013036826	-10.4	0.281	489.538	ZINC	O=C(C1c2ccccc2Oc2ccccc21)N1CCN(c2ncnc3c2nnn3-c2ccccc2)CC1
vMpro-mpro2-28	ZINC000020464531	-10.4	0.281	491.506	ZINC	O=C(c1ccc(-c2ccccc2)cc1)N1Cc2nc[nH]c2C[C@H]1c1nc(-c2ccc3c(c2)OCO3)no1
vMpro-mpro2-29	ZINC000101094105	-10.4	0.306	444.485	ZINC	O=C1c2cc3ccccc3cc2C(=O)[C@@H]2C[C@@H]3C(=O)c4cc5ccccc5cc4C(=O)[C@@H]3C[C@@H]12
vMpro-mpro2-30	ZINC000230202081	-10.4	0.297	478.425	ZINC	O=C(c1ccco1)[C@@H]1[C@@H]2C(=O)N(c3ccccC(F)(F)F)c3)C(=O)[C@@H]2[C@H]2c3ccccc3C=CN12
vMpro-mpro2-31	ZINC000252021496	-10.4	0.297	493.582	ZINC	Cc1nc(NS(=O)(=O)c2ccc3c(c2)[C@H]2[C@@H]([C@H]4CC[C@H]2C4)[C@@H](c2ccccC(C=O)O)c2)N3)oc1C
vMpro-mpro2-32	PV-001814171865	-10.3	0.355	404.362	REAL	Cc1cc(F)c2nc(O)cc(C(=O)N3CCc4cc(C(F)(F)F)ccc4C3)c2c1
vMpro-mpro2-33	PV-002009801064	-10.3	0.312	478.436	REAL	Cc1cc(C(F)(F)F)ccc1Cn1c([C@@H]2CCCCO2)nnc1N1CCO[C@@H](C(F)(F)F)C1
vMpro-mpro2-34	Z1014751880	-10.3	0.312	459.467	REAL	C[C@@]1(c2ccc(CNC(=O)C3(c4cccc(C(F)(F)F)c4)CCCC3)cc2)NC(=O)NC1=O
vMpro-mpro2-35	Z1069482880	-10.3	0.286	492.574	REAL	C[C@H]1CN(c2ccc(C(=O)N3CCC(C(=O)c4ccc5c(c4)NC(=O)[C@H](C)O5)CC3)cn2)C[C@@H](C)O1
vMpro-mpro2-36	Z1166685113	-10.3	0.343	438.454	REAL	O=C(Nc1nc2cc3c(cc2s1)OC(F)(F)O3)N1CCC(C(=O)N2CCCC2)CC1
vMpro-mpro2-37	Z1232342590	-10.3	0.322	424.467	REAL	CCc1nnnn1-c1ccccc1NC(=O)c1ccc2c(C)nn(-c3ccccc3)c2n1
vMpro-mpro2-38	Z1274039105	-10.3	0.322	439.44	REAL	O=C(Nc1nc2ccccc2n1Cc1cccc(C(F)(F)F)c1)[C@@H]1CCc2cn[nH]c2C1
vMpro-mpro2-39	Z1324964303	-10.3	0.332	427.345	REAL	Cc1nc(C(=O)Nc2ccc3c(c2)oc2ccccc23)nn1-c1nnc(C(F)(F)F)[nH]1
vMpro-mpro2-40	Z1325401657	-10.3	0.355	406.327	REAL	Cc1nc(C(=O)Nc2ccc3c(c2)NC(=O)CC3)nn1-c1nnc(C(F)(F)F)[nH]1
vMpro-mpro2-41	Z1452514506	-10.3	0.343	397.433	REAL	C[C@@]1(c2cccc(C(=O)N3Cc4ccccc4-c4ccccc43)c2)NC(=O)NC1=O
vMpro-mpro2-42	Z1488358401	-10.3	0.332	443.35	REAL	Cc1nc2c(c(C(F)(F)F)n1)C[C@H](C(=O)Nc1nc3ccc(C(F)(F)F)ccc3[nH]1)CC2
vMpro-mpro2-43	Z1521653481	-10.3	0.355	405.453	REAL	C[C@H]1C[C@H](C)CC2(C1)NC(=O)N(CC(=O)N1CCC3(CC1)NC(=O)NC3=O)C2=O
vMpro-mpro2-44	Z1546785129	-10.3	0.322	433.558	REAL	C[C@@H]1CN(c2nc3ccccc3nc2N2CCC[C@H](c3nnc4n3CCC4)C2)C[C@@H](C)O1
vMpro-mpro2-45	Z1673511399	-10.3	0.312	440.502	REAL	C[C@]1(c2cccc(CNC(=O)N3CC=C(c4ccc5ccccc45)C3)c2)NC(=O)NC1=O
vMpro-mpro2-46	Z1685438116	-10.3	0.312	437.454	REAL	O=C1CCc2cc(-c3noc(-c4ccc5c(c4)C[C@@H](c4cccc4)OC5=O)n3)ccc2N1
vMpro-mpro2-47	Z2157918107	-10.3	0.322	428.447	REAL	C[C@H](Oc1ccc2ccccc2c1)c1nc(-c2cccc([C@]3(C)NC(=O)NC3=O)c2)no1
vMpro-mpro2-48	Z2207852801	-10.3	0.343	416.366	REAL	Cc1nc(C(=O)N2CCn3c(cc4ccccc43)C2)nn1-c1nnc(C(F)(F)F)[nH]1
vMpro-mpro2-49	Z2209929430	-10.3	0.332	432.441	REAL	C[C@@H]1CO[C@H](c2cccc(C(F)(F)F)c2)CN1C(=O)[C@@H]1CN(C)C(=O)c2ccccc21
vMpro-mpro2-50	Z2708374981	-10.3	0.368	391.348	REAL	O=C1COc2ccc(NC(=O)N3CCc4cc(C(F)(F)F)ccc4C3)cc2N1
vMpro-mpro2-51	Z3046818953	-10.3	0.368	382.506	REAL	O=C(N[C@@H]1C[C@]2(CCNC2)Oc2ccccc21)N1C[C@H]2[C@H]3CC[C@H](NC3)[C@@H]2C1
vMpro-mpro2-52	Z358867962	-10.3	0.343	415.532	REAL	Cc1cccc([C@@H](CC(=O)O[C@@H](C)C(=O)N[C@@H](C)[C@H]2C[C@H]3CC[C@H]2C3)NC(N)=O)c1
vMpro-mpro2-53	Z767247218	-10.3	0.303	471.409	REAL	C[C@@]1(c2ccc(NC(=O)c3cc(F)ccc3-c3cccc(C(F)(F)F)c3)cc2)NC(=O)NC1=O
vMpro-mpro2-54	Z804312190	-10.3	0.355	390.402	REAL	O=C(Nc1ccc2c(c1)nc1n2CCCC1)c1cnc2[nH]c(=O)[nH]c(=O)c2c1
vMpro-mpro2-55	Z805930424	-10.3	0.312	439.47	REAL	Cc1c(C(=O)NN2C(=O)NC(c3ccccc3)(c3ccccc3)C2=O)oc2c(C)cccc12
vMpro-mpro2-56	Z956280640	-10.3	0.303	474.544	REAL	O=C(N[C@@H](c1ccccc1)c1nnn[nH]1)c1cccc(S(=O)(=O)N2CCc3ccccc3C2)c1
vMpro-mpro2-57	ZINC000003178975	-10.3	0.264	525.529	ZINC	CCn1c2ccccc2c2cc(N/C=C3/c4ccccc4C(=O)N(c4cccc(C(F)(F)F)c4)C3=O)ccc21
vMpro-mpro2-58	ZINC000018181098	-10.3	0.278	487.51	ZINC	Cc1cccc([C@@H]2OC3(C(=O)c4ccccc4C3=O)[C@@H]3C(=O)N(c4cccc5ccccc54)C(=O)[C@@H]23)c1
vMpro-mpro2-59	ZINC000020366657	-10.3	0.271	503.608	ZINC	Cc1ccc(C(=O)N2CCN(c3ccc(Nc4cc(C)nc5nc(-c6ccccc6)nn54)cc3)CC2)cc1
vMpro-mpro2-60	ZINC000034812740	-10.3	0.322	433.457	ZINC	Cc1ccc2c(c1)Oc1ccccc1C(N1CCN(C(=O)c3cc(F)cc(F)c3)CC1)=N2
vMpro-mpro2-61	ZINC000064980242	-10.3	0.294	479.515	ZINC	O=c1oc2ccccc2cc1-c1nc(-c2ccc3c(c2)Sc2ccccc2C(=O)N3C2CC2)no1
vMpro-mpro2-62	ZINC000100415678	-10.3	0.278	487.51	ZINC	Cc1cccc([C@H]2OC3(C(=O)c4ccccc4C3=O)[C@@H]3C(=O)N(c4cccc5ccccc54)C(=O)[C@@H]32)c1
vMpro-mpro2-63	ZINC000229904975	-10.3	0.286	486.53	ZINC	O=c1[nH]c2cc3c(cc2cc1[C@H](c1nnnn1C[C@H]1CCCO1)N1CCc2ccccc21)OCCO3
vMpro-mpro2-64	ZINC000229930169	-10.3	0.24	589.046	ZINC	CC1=C[C@@H]2N(c3ccccc31)[C@H](C(=O)c1ccc(Cl)cc1)[C@@H](C(=O)c1ccc3c(c1)OCO3)[C@@]21C(=O)Nc2ccccc21
vMpro-mpro2-65	ZINC000231657553	-10.3	0.294	472.504	ZINC	O=c1[nH]c2cc3c(cc2cc1[C@H](c1nnnn1C[C@H]1CCCO1)N1CCc2ccccc21)OCO3
vMpro-mpro2-66	ZINC000245254646	-10.3	0.303	479.556	ZINC	Cc1cc(NS(=O)(=O)c2ccc3c(c2)[C@H]2[C@@H]([C@H]4CC[C@H]2C4)[C@@H](c2ccccC(=O)O)c2)N3)no1
vMpro-mpro2-67	ZINC000253414049	-10.3	0.286	478.455	ZINC	O=C(O)c1cccc(-c2ccc([C@@H]3CC(=O)Oc4ccc5c(c43)O/C(=C\c3ccccc3)C5=O)o2)cc1
vMpro-mpro2-68	ZINC000408674312	-10.3	0.286	476.574	ZINC	CC1CCN(C(=O)c2cccc(N3C(=O)[C@@H]4[C@@H](C3=O)C3c5ccccc5C4c4ccccc43)c2)CC1
vMpro-mpro2-69	ZINC000408674316	-10.3	0.286	476.574	ZINC	CC1CCN(C(=O)c2cccc(N3C(=O)[C@H]4[C@@H](C3=O)C3c5ccccc5C4c4ccccc43)c2)CC1
vMpro-mpro2-70	ZINC000408679811	-10.3	0.271	498.58	ZINC	Cc1cc(C)cc(NC(=O)c2cccc(N3C(=O)[C@H]4[C@@H](C3=O)C3c5ccccc5C4c4ccccc43)c2)c1
vMpro-mpro2-71	ZINC000408974666	-10.3	0.286	465.515	ZINC	CN(C(=O)c1ccc2nc3c4ccnc4c4nccc4c3nc2c1)c1ccc2ccccc2c1
vMpro-mpro2-72	ZINC000409205109	-10.3	0.303	452.465	ZINC	O=C(O)c1ccc(NC(=O)CN2C(=O)[C@H]3[C@@H](C2=O)C2c4ccccc4C3c3ccccc32)cc1
vMpro-mpro2-73	PV-001794027686	-10.2	0.309	449.549	REAL	CC(C)(C)OC(=O)[C@]1(C(=O)NCc2ccccc(NC(=O)c3ccenc3)c2)C[C@@H]2CC[C@@H]1C2
vMpro-mpro2-74	PV-001796088840	-10.2	0.319	434.534	REAL	Cc1ccc2c(c1)C(=O)O[C@]1(C)C(=O)Nc1ccc(C(=O)N3CCC[C@@H](C)C3)cc1C)C2
vMpro-mpro2-75	PV-001796254702	-10.2	0.319	434.534	REAL	Cc1ccc2c(c1)C(=O)O[C@](C)(C(=O)Nc1ccc(C(=O)N3CCCC[C@@H]3C)cc1C)C2
vMpro-mpro2-76	PV-001829216634	-10.2	0.392	354.536	REAL	CN(C)c1cccc(CCC(=O)N2CCC[C@@H]2C[C@H]2C[C@H]3CC[C@H]2C3)c1
vMpro-mpro2-77	PV-001861981057	-10.2	0.352	429.725	REAL	Cc1nc(C(=O)Nc2nc3ccc(F)c(Cl)cc3[nH]2)nn1-c1nnc(C(F)(F)F)[nH]1
vMpro-mpro2-78	PV-001878966052	-10.2	0.329	441.55	REAL	C[C@@H]1C[C@H](C)CN(S(=O)(=O)c2cccc(C(=O)N3NC(=O)C[C@@H]3c3ccccc3)c2)C1
vMpro-mpro2-79	PV-001942555097	-10.2	0.319	449.475	REAL	C[C@@H]1CN(c2ccc(NC(=O)N3CC[C@H](c4nccc(C(F)(F)F)n4C3)cc2)C[C@@H](C)O1
vMpro-mpro2-80	PV-001945739492	-10.2	0.34	410.387	REAL	Cc1cc(C)nc(-n2ncc2NC(=O)Nc2cc(-c3cccc(F)c3F)n[nH]2)n1
vMpro-mpro2-81	PV-001946523931	-10.2	0.319	450.463	REAL	C[C@@H]1CN(c2ccc(NC(=O)N3CC[C@H](c4nccc(C(F)(F)F)n4C3)cn2)C[C@@H](C)O1
vMpro-mpro2-82	Z1021035700	-10.2	0.319	456.972	REAL	O=C1Nc2cc(Cl)ccc2C1=C1CCN(C(=O)[C@H]2CCCN(C(=O)N3CCCC3)C2)CC1
vMpro-mpro2-83	Z1071464848	-10.2	0.291	475.587	REAL	C[C@H]1Oc2ccc(C(=O)C3CCN(C(=O)N[C@@H]4CCCC[C@@H]4c4ccccc4)CC3)cc2NC1=O
vMpro-mpro2-84	Z1090590728	-10.2	0.3	466.418	REAL	O=C1COc2ccc(C(=O)Nc3nc4ccccc4n3Cc3cccc(C(F)(F)F)c3)cc2N1
vMpro-mpro2-85	Z1172231620	-10.2	0.352	379.462	REAL	O=c1[nH]c(NC[C@@H]2CC3c4ccccc4C2c2ccccc23)nc2ccccc12
vMpro-mpro2-86	Z1280619910	-10.2	0.34	400.481	REAL	Cc1ccc(-c2ocnc2C(=O)N2CCC[C@@H](c3nc4cc(C)ccc4[nH]3)C2)cc1
vMpro-mpro2-87	Z1451755722	-10.2	0.34	403.441	REAL	Cc1cc(NC(=O)c2cccc([C@]3(C)NC(=O)NC3=O)c2)n(Cc2ccccc2)n1
vMpro-mpro2-88	Z1452691933	-10.2	0.309	445.493	REAL	O=C(NC[C@H]1[C@@H]2Cc3ccccc3[C@H]12)NNC(=O)c1ccccc1OCc1ccc(F)cc1
vMpro-mpro2-89	Z1506513321	-10.2	0.319	434.474	REAL	O=C(Nc1ccc(F)c(-n2nnnc2C2CC2)c1)N1CCO[C@@]2(CCc3ccccc32)C1
vMpro-mpro2-90	Z1668772547	-10.2	0.319	437.384	REAL	O=C(Nc1nc2ccccc2n1Cc1cccc(C(F)(F)F)c1)c1cnc2[nH]nnc2c1
vMpro-mpro2-91	Z1684581535	-10.2	0.329	418.452	REAL	C[C@H](Oc1ccc2c(c1)CCC2)c1nc(-c2cccc([C@]3(C)NC(=O)NC3=O)c2)no1
vMpro-mpro2-92	Z1684582500	-10.2	0.319	430.423	REAL	Cc1noc2nc(C3CC3)cc(-c3nc(-c4cccc([C@@]5(C)NC(=O)NC5=O)c4)no3)c12
vMpro-mpro2-93	Z1684583182	-10.2	0.309	439.474	REAL	Cc1ccc2nc(C3CC3)cc(-c3nc(-c4cccc([C@@]5(C)NC(=O)NC5=O)c4)no3)c2c1
vMpro-mpro2-94	Z1685380263	-10.2	0.329	410.392	REAL	COc1ccc(-c2noc(-c3c[nH]n4c3nc(=O)c3ccccc34)n2)c2ccccc2n1
vMpro-mpro2-95	Z1685666242	-10.2	0.319	427.463	REAL	Cc1ccc(-c2noc(-c3c[nH]n4c3nc(=O)c3ccccc34)n2)c(OC2CCCC2)c1
vMpro-mpro2-96	Z1770657082	-10.2	0.329	408.46	REAL	Cc1cc(C)cc(-c2cc(NC(=O)c3ccc4[nH]c5ccccc5c(=O)c4c3)[nH]n2)c1
vMpro-mpro2-97	Z1832420013	-10.2	0.34	393.485	REAL	O=C1C[C@@H](C(=O)NC[C@H]2CC3c4ccccc4C2c2ccccc23)c2ccccc21
vMpro-mpro2-98	Z1844670808	-10.2	0.329	415.539	REAL	Cc1ccc2c(c1)CCN(C(=O)Nc1ccc(-c3nnc4n3CCCCCC4)cc1)C2
vMpro-mpro2-99	Z1907687348	-10.2	0.364	412.577	REAL	C[C@H](Sc1nc2ccccc2s1)C(=O)NC[C@]1(O)C[C@H]2[C@H]3C[C@H]4[C@H]5[C@H]3C[C@H]2[C@@H]5[C@@H]41
vMpro-mpro2-100	Z1919302648	-10.2	0.319	427.503	REAL	C[C@H]1Cc2cc(-c3ccc(CNC(=O)Nc4ccc5c(c4)CC(=O)N5C)cc3)ccc2O1

Supplementary Table 31. Top 100 virtual hits of the screen against the α-helix 5 association site on the dimerization interface of M^{pro} (Screen ID: 19). Compounds were filtered so that hits had MW < 600 dalton, cLogP < 6, number of hydrogen bond acceptors < 11, and no reactive functional groups. The name of each compound consists of the initial letter 'v' for virtual hit, followed by the target protein name and the target site ('mpro' for the M^{pro} binding site, 2 for docking scenario 2). The score is the docking score given by QuickVina 2 in kcal/mol. The ligand efficiency (LE) is computed as LE = -score/#NonH, where #NonH is the number of heavy (i.e. non hydrogen) atoms.

Name	Catalog ID	Score	LE	MW	Library	SMILES
vMpro-mpro2-101	Z196866182	-10.2	0.309	438.49	REAL	Cc1cc(C)c2cc(C(=O)NN3C(=O)NC(c4ccccc4)(c4ccccc4)C3=O)[nH]c2c1
vMpro-mpro2-102	Z2047258400	-10.2	0.329	431.46	REAL	C[C@@]1(c2ccc(CN[C@H]3CCC[C@@H]3c3cccc(C(F)(F)F)c3)cc2)NC(=O)NC1=O
vMpro-mpro2-103	Z2087916333	-10.2	0.329	433.44	REAL	Cc1nc(C(=O)N2CCC[C@@](C)(c3ccccc3)CC2)nn1-c1nnc(C(F)(F)F)[nH]1
vMpro-mpro2-104	Z2157917276	-10.2	0.309	445.48	REAL	Cc1ccc(CN2C(=O)CC[C@H]2c2nc(-c3cccc([C@]4(C)NC(=O)NC4=O)c3)no2)cc1
vMpro-mpro2-105	Z2157919912	-10.2	0.319	431.45	REAL	C[C@]1(c2ccccc(-c3noc([C@@H]4CCCN4C(=O)c4ccccc4)n3)c2)NC(=O)NC1=O
vMpro-mpro2-106	Z2159562280	-10.2	0.352	401.31	REAL	Cc1nc(-c2nc(-c3c[nH]c4ccccc34)no2)nn1-c1nnc(C(F)(F)F)[nH]1
vMpro-mpro2-107	Z2188326028	-10.2	0.340	396.45	REAL	O=C(c1ccc2[nH]c3ccccc3c(=O)c2c1)N1Cc2ccc(O)cc2C2(CC2)C1
vMpro-mpro2-108	Z2204274720	-10.2	0.329	432.41	REAL	Cc1nc(C(=O)N2CCCN3c4ccccc4C[C@@H]3C2)nn1-c1nnc(C(F)(F)F)[nH]1
vMpro-mpro2-109	Z2226172543	-10.2	0.309	445.54	REAL	O=C(c1cccc2ccccc12)N1CCC[C@H](C(=O)N2CCC(F)(c3ccccn3)CC2)C1
vMpro-mpro2-110	Z2228534062	-10.2	0.329	421.54	REAL	O=C1CC[C@@](C(=O)N2CCC[C@H](c3nnc4n3CCCCC4)C2)(c2ccccc2)CN1
vMpro-mpro2-111	Z2233590891	-10.2	0.329	406.45	REAL	O=C(Nc1nc(-c2ccc3ccccc3n2)n[nH]1)c1cc(C2CC2)nc2ccccc12
vMpro-mpro2-112	Z2233591800	-10.2	0.340	399.41	REAL	C[C@@]1(C(=O)Nc2nc(-c3ccc4ccccc4n3)n[nH]2)Cc2ccccc2C(=O)O1
vMpro-mpro2-113	Z229366068	-10.2	0.329	409.49	REAL	Cc1cc(C(=O)NC[C@H]2CC3c4ccccc4C2c2ccccc23)c2c(C)noc2n1
vMpro-mpro2-114	Z2495853746	-10.2	0.364	377.44	REAL	O=C1CN(C(=O)N[C@@H]2CC3(CCC3)Oc3ccccc32)Cc2ccccc2N1
vMpro-mpro2-115	Z2807002010	-10.2	0.364	385.46	REAL	COC(=O)[C@H]1C[C@H]2CC[C@H]1N2C(=O)N[C@H](CN1CCCC1=O)c1ccccc1
vMpro-mpro2-116	Z2902677787	-10.2	0.309	435.49	REAL	CC(=O)N/C(=C/c1ccccc1)c1nc(-c2cccc(Cn3cnc4ccccc43)c2)no1
vMpro-mpro2-117	Z3046819374	-10.2	0.352	392.46	REAL	O=C1CN(C(=O)N[C@@H]2C[C@]3(CCNC3)Oc3ccccc32)Cc2ccccc2N1
vMpro-mpro2-118	Z653342672	-10.2	0.276	490.50	REAL	O=C(Nc1nnc(-c2ccccn2)[nH]1)c1cc(-c2ccccc2)nc2c1cnn2Cc1ccccc(F)c1
vMpro-mpro2-119	Z66708984	-10.2	0.291	467.52	REAL	CC(C)N(Cc1nc2ccccc2c(=O)[nH]1)C(=O)c1ccc2c(c1)C[C@H](c1ccccc1)OC2=O
vMpro-mpro2-120	Z741366052	-10.2	0.276	490.52	REAL	Cc1cc(C(=O)NNC(=O)c2ccc(CN3C(=O)c4cccc5cccc3c45)cc2)n2nc(C)cc2n1
vMpro-mpro2-121	Z764564012	-10.2	0.340	397.47	REAL	O=C(NC1(c2ccccc2)CCC1)c1ccc2c(c1)C[C@H](c1ccccc1)OC2=O
vMpro-mpro2-122	Z852303526	-10.2	0.283	499.53	REAL	O=C1C[C@H](C(=O)N2CCC(C(=O)N3CCc4ccccc43)CC2)CN1Cc1cccc(C(F)(F)F)c1
vMpro-mpro2-123	ZINC000001009635	-10.2	0.309	456.42	ZINC	O=C(c1ccccc1)[C@H]1[C@@H](c2cccc(Oc3ccccc3)c2)NC(=O)N[C@]1(O)C(F)(F)F
vMpro-mpro2-124	ZINC000001380527	-10.2	0.319	460.48	ZINC	O=S(=O)(c1cccc2ccccc21)N1CCC(n2nnc3cc(C(F)(F)F)ccc32)CC1
vMpro-mpro2-125	ZINC000008449795	-10.2	0.268	493.56	ZINC	O=C1[C@@H]2[C@@H](C(=O)N1c1ccc(Oc3ccc4ccccc4c3)cc1)C1c3ccccc3C2c2ccccc21
vMpro-mpro2-126	ZINC000008915312	-10.2	0.300	470.45	ZINC	Cc1ccc(C(=O)[C@H]2[C@@H](c3ccccc(Oc4ccccc4)c3)NC(=O)N[C@]2(O)C(F)(F)F)cc1
vMpro-mpro2-127	ZINC000012888000	-10.2	0.283	478.55	ZINC	C[C@H](NC(=O)[C@@H]1Cc2c3ccccc3[nH]c2[C@H]2c3ccccc3C(=O)N21)C(=O)N(Cc1ccccc1
vMpro-mpro2-128	ZINC000015822408	-10.2	0.309	447.46	ZINC	CC12c3ccccc3C(C)(c3ccccc31)[C@H]1C(=O)N(c3ccccc(C(F)(F)F)c3)C(=O)[C@H]12
vMpro-mpro2-129	ZINC000019738999	-10.2	0.309	446.59	ZINC	Cc1cc(C)cc(C2(C(=O)N3CC[C@H](c4nc(C)c5c(n4)N(C)C(=O)CC5)C3)CCCC2)c1
vMpro-mpro2-130	ZINC000034788670	-10.2	0.268	527.66	ZINC	O=C(CN1CCc2sccc2[C@H]1c1cccc(F)c1)N1CCCN(C(=O)c2ccc3ccccc3c2)CC1
vMpro-mpro2-131	ZINC000034814026	-10.2	0.276	508.54	ZINC	Cc1cccc(CNC(=O)N2CCN(C3=Nc4ccc(C(F)(F)F)cc4Oc4ccccc43)C[C@@H]2C)c1
vMpro-mpro2-132	ZINC000057506062	-10.2	0.300	454.53	ZINC	Cc1cc2nn(CC(=O)N[C@H]3CCc4ccccc43)c(=O)n2c(N2CCc3ccccc3C2)n1
vMpro-mpro2-133	ZINC000096402886	-10.2	0.300	452.47	ZINC	CC(=O)c1ccc(N2C(=O)[C@@H]3[C@@H](C2=O)[C@H]2c4ccccc4C=CN2[C@@H]3C(=O)c2ccco2)cc1
vMpro-mpro2-134	ZINC000097945321	-10.2	0.255	522.56	ZINC	O=C(Oc1cccc2ccncc21)c1cccc(N2C(=O)[C@H]3[C@@H](C2=O)C2c4ccccc4C3c3ccccc32)c1
vMpro-mpro2-135	ZINC000097945322	-10.2	0.255	522.56	ZINC	O=C(Oc1cccc2ccncc21)c1cccc(N2C(=O)[C@@H]3[C@@H](C2=O)C2c4ccccc4C3c3ccccc32)c1
vMpro-mpro2-136	ZINC000097945639	-10.2	0.262	533.03	ZINC	O=C(Nc1cccc(Cl)c1)[C@@H](Cc1ccccc1)N1C(=O)[C@H]2[C@@H](C1=O)C1c3ccccc3C2c2ccccc21
vMpro-mpro2-137	ZINC000100504092	-10.2	0.329	404.51	ZINC	O=c1cccc2n1C[C@H]1C[C@H]2CN(Cc2ccc3ccc4cccc5ccc2c3c45)C1
vMpro-mpro2-138	ZINC000101094110	-10.2	0.300	444.49	ZINC	O=C1c2cc3ccccc3cc2C(=O)[C@H]2C[C@@H]3C(=O)c4cc5ccccc5cc4C(=O)[C@H]3C[C@@H]12
vMpro-mpro2-139	ZINC000104094576	-10.2	0.268	538.71	ZINC	COc1ccc(S(=O)(=O)/N=C(\[C@@H]2CC3=CC[C@H]4[C@H]5CCC(=O)[C@]5(C)CC(=O)[C@@H]4[C@@]3(C)C2)N2CCCC2)cc1
vMpro-mpro2-140	ZINC000408688101	-10.2	0.268	498.58	ZINC	Cc1ccc(NC(=O)c2ccccc(N3C(=O)[C@H]4[C@@H](C3=O)C3c5ccccc5C4c4ccccc43)c2)cc1C
vMpro-mpro2-141	PV-001795236883	-10.1	0.326	420.51	REAL	Cc1ccc2c(c1)C(=O)O[C@](C)(C(=O)Nc1ccc(C(=O)N3CCCC[C@@H]3C)cc1)C2
vMpro-mpro2-142	PV-001795272695	-10.1	0.316	454.95	REAL	Cc1ccc2c(c1)C(=O)O[C@](C)(C(=O)Nc1ccc(C(=O)N3CCCC[C@@H]3C)c(Cl)c1)C2
vMpro-mpro2-143	PV-001799987153	-10.1	0.337	413.52	REAL	Cc1ccc2c(c1)N(C(=O)CN1C(=O)N[C@@]3(C[C@@H](C)CC(C)(C)C3)C1=O)C[C@@H](C)O2
vMpro-mpro2-144	PV-001801235018	-10.1	0.337	401.43	REAL	CCNC(=O)c1cc(NC(=O)c2ccc3c(=O)[nH]c(C)nc3c2)nc2ccccc12
vMpro-mpro2-145	PV-001811282366	-10.1	0.348	390.53	REAL	Cc1ccc(C2(NC(=O)[C@H]3CCC(=O)N(c4ccc(C)c(C)c4)C3)CCC2)cc1
vMpro-mpro2-146	PV-001836502928	-10.1	0.316	444.50	REAL	CCN1C(=O)C[C@H](C(=O)N2CC(Cc3ccccc3C(F)(F)F)C2)[C@H]1c1ccccc(C)c1
vMpro-mpro2-147	PV-001850234138	-10.1	0.326	427.36	REAL	O=C(Nc1nc(-c2ccc3ccccc3n2)n[nH]1)/C(F)=C\c1ccc(C(F)(F)F)cc1
vMpro-mpro2-148	PV-001860070711	-10.1	0.337	428.27	REAL	O=C(NNc1ccccc2c1OC(F)(F)O2)c1ccccc(-c2noc(C(F)(F)F)n2)c1
vMpro-mpro2-149	PV-001863481024	-10.1	0.326	426.52	REAL	C[C@H]1CC(C)(C)C[C@@]2(C1)NC(=O)N(CC(=O)Nc1ccccc1[C@H]1CCC(=O)N1)C2=O
vMpro-mpro2-150	PV-001868003022	-10.1	0.326	436.54	REAL	Cc1ccc(N(C)S(=O)(=O)c2ccccc(C(=O)N3Cc4cncnc4[C@H](C)C3)c2)cc1
vMpro-mpro2-151	PV-001871675063	-10.1	0.337	438.43	REAL	Cn1c(S)nc2cc(C(=O)NCc3nnc4n3CC[C@H](C(F)(F)F)C4)ccc2c1=O
vMpro-mpro2-152	PV-001873656926	-10.1	0.326	428.38	REAL	Cc1ccc(-c2cccc(NC(=O)c3nc(C)n(-c4nnc(C(F)(F)F)[nH]4)n3)n2)cc1
vMpro-mpro2-153	PV-001878089193	-10.1	0.337	429.28	REAL	Cc1cc(C(F)(F)F)n2nc(C(=O)Nc3n[nH]c4nc(C(F)(F)F)ccc34)cc2n1
vMpro-mpro2-154	PV-001941139141	-10.1	0.388	429.19	REAL	O=C(Nc1ccc2c(c1)OC(F)(F)O2)N1CCc2cc(Br)c(F)cc2C1
vMpro-mpro2-155	PV-001941447160	-10.1	0.348	407.35	REAL	CN(Cc1ccc2c(c1)OC(F)(F)O2)C(=O)Nc1cc2c(cc1F)CCC(=O)N2
vMpro-mpro2-156	PV-001945739486	-10.1	0.337	410.39	REAL	Cc1cc(C)nc(-n2nccc2NC(=O)Nc2cc(-c3cc(F)cc(F)c3)[nH]n2)n1
vMpro-mpro2-157	PV-001960225091	-10.1	0.326	416.52	REAL	C[C@@H]1CCCc2ccccc2[C@@H]1NC(=O)N[C@H]1CCCN(c2ccc(C#N)cc2)C1=O
vMpro-mpro2-158	PV-001962079864	-10.1	0.326	440.47	REAL	O=C(N[C@H]1CCCN(C(=O)N2CCCC2)C1)N1CC[C@H](c2ncec(C(F)(F)F)n2)C1
vMpro-mpro2-159	PV-002045827939	-10.1	0.316	463.38	REAL	O=C1CC[C@@H](c2nnc(N3CCO[C@@H](C(F)(F)F)C3)n2Cc2ccc(C(F)(F)F)c2)N1
vMpro-mpro2-160	Z1002304722	-10.1	0.337	400.44	REAL	Cc1cc2nc(NCc3ccc([C@]4(C)NC(=O)NC4=O)c3)c3ccccc3n2n1
vMpro-mpro2-161	Z1015092982	-10.1	0.337	415.37	REAL	C[C@@]1(c2ccc(CNc3nc(C(F)(F)F)nc4ccccc34)cc2)NC(=O)NC1=O
vMpro-mpro2-162	Z1177489688	-10.1	0.316	430.47	REAL	O=C(Nc1ccc(-c2nnc3n2CCCCCC3)cc1)c1ccc(-c2noc(=O)[nH]2)cc1
vMpro-mpro2-163	Z1177859618	-10.1	0.316	426.43	REAL	O=C(Nc1ccccc(C(=O)N2CCc3ccccc32)c1)c1ccc(-c2noc(=O)[nH]2)cc1
vMpro-mpro2-164	Z1197861618	-10.1	0.316	421.42	REAL	O=c1nc2c(-c3nc(-c4cccc(Oc5ccccc5)c4)no3)c[nH]n2c2ccccc12
vMpro-mpro2-165	Z1232342434	-10.1	0.316	439.52	REAL	CCc1nnnn1-c1ccccc1NC(=O)CN1C(=O)N[C@]2(C[C@@H](C)CC(C)(C)C2)C1=O
vMpro-mpro2-166	Z1267642839	-10.1	0.316	445.44	REAL	Cc1c(C(=O)NC2(c3cccc(C(F)(F)F)c3)CCCCC2)cnn1-c1ccc(=O)[nH]n1
vMpro-mpro2-167	Z1273237869	-10.1	0.316	430.48	REAL	O=C(c1cc(C2CC2)nc2ccc(F)cc12)N1CCC(n2c(=O)[nH]c3ccccc32)CC1
vMpro-mpro2-168	Z1278119438	-10.1	0.316	423.52	REAL	O=C1CCc2ccc(NC(=O)NC[C@H]3CC4c5ccccc5C3c3ccccc34)cc2N1
vMpro-mpro2-169	Z1322647598	-10.1	0.316	426.52	REAL	Cc1ccc2nc(C3CC3)cc(C(=O)N3CCC(n4c(=O)[nH]c5ccccc54)CC3)c2c1
vMpro-mpro2-170	Z1323928843	-10.1	0.316	444.38	REAL	Cc1ccc(Oc2ccc(NC(=O)c3nc(C)n(-c4nnc(C(F)(F)F)[nH]4)n3)cn2)cc1
vMpro-mpro2-171	Z1323941631	-10.1	0.348	405.30	REAL	Cc1nc(C(=O)Nc2ccc3oc(=O)ccc3c2)nn1-c1nnc(C(F)(F)F)[nH]1
vMpro-mpro2-172	Z1324988134	-10.1	0.316	444.42	REAL	Cc1nc(C(=O)N2CCC[C@@H](c3cc4ccccc4[nH]3)C2)nn1-c1nnc(C(F)(F)F)[nH]1
vMpro-mpro2-173	Z1325183705	-10.1	0.361	395.28	REAL	Cc1nc(C(=O)Nc2n[nH]c3ccc(F)cc23)nn1-c1nnc(C(F)(F)F)[nH]1
vMpro-mpro2-174	Z1360029906	-10.1	0.316	446.94	REAL	O=C(c1cc(C2CC2)nc2ccc(Cl)cc12)N1CCC(n2c(=O)[nH]c3ccccc32)CC1
vMpro-mpro2-175	Z1488353027	-10.1	0.326	445.29	REAL	Cc1nc(C(=O)Nc2nc3ccc(C(F)(F)F)ccc3[nH]2)nn1-c1nnc(C(F)(F)F)[nH]1
vMpro-mpro2-176	Z1521947912	-10.1	0.316	439.44	REAL	O=C(Nc1nc2ccccc2n1Cc1cccc(C(F)(F)F)c1)[C@@H]1CCc2[nH]ncc2C1
vMpro-mpro2-177	Z1544509723	-10.1	0.337	419.46	REAL	CCNC(=O)c1cc(NC(=O)c2ccc3c(=O)[nH]c(S)nc3c2)nc2ccccc12
vMpro-mpro2-178	Z1555089581	-10.1	0.326	438.41	REAL	C[C@H]1C[C@H](C)CC2(C1)NC(=O)N(CC(=O)Nc1cccc3oc(C(F)(F)F)nc13)C2=O
vMpro-mpro2-179	Z1611904366	-10.1	0.316	434.44	REAL	O=C1NC2(Cc3ccccc3C2)C(=O)N1c1ccc(OC(F)F)c(Cc2ccccc2)c1
vMpro-mpro2-180	Z1657462730	-10.1	0.316	428.50	REAL	CC(C)n1nnnc1-c1ccccc1NC(=O)N1CC=C(c2c[nH]c3ncccc23)CC1
vMpro-mpro2-181	Z1683106796	-10.1	0.361	372.34	REAL	NC(=O)c1ccc(-c2noc(-c3c[nH]n4c3nc(=O)c3ccccc34)n2)cc1
vMpro-mpro2-182	Z1685436255	-10.1	0.316	427.46	REAL	O=C1CCc2cc(-c3noc(-c4ccc5c(=O)n6c(nc5c4)CCCCC6)n3)ccc2N1
vMpro-mpro2-183	Z1731791665	-10.1	0.316	434.47	REAL	O=C(Nc1ccc(F)c(-n2nnnc2C2CC2)c1)N1CCC[C@]2(C1)OCc1ccccc12
vMpro-mpro2-184	Z1733801330	-10.1	0.316	442.48	REAL	O=C(NC[C@@H]1CC2c3ccccc3C1c1ccccc12)N1CCC(C(=O)C(F)(F)F)CC1
vMpro-mpro2-185	Z1904663859	-10.1	0.348	392.50	REAL	O=C(NCCCn1cnc2ccccc21)NC[C@@]1(O)[C@H]2[C@@H]3C[C@H]4[C@H]5[C@H]3C[C@H]2[C@H]5[C@@H]41
vMpro-mpro2-186	Z1907741698	-10.1	0.361	395.28	REAL	Cc1nc(C(=O)Nc2nc3ccc(F)cc3[nH]2)nn1-c1nnc(C(F)(F)F)[nH]1
vMpro-mpro2-187	Z2003311939	-10.1	0.348	389.45	REAL	CCc1ccc(-c2noc([C@@H](C)NC(=O)[C@@]34[C@@H]5C(=O)[C@H]6[C@H]7C[C@@H]([C@@H]63)[C@@H]4[C@@H]75)n2)cc1
vMpro-mpro2-188	Z2015459306	-10.1	0.316	449.40	REAL	C[C@@]1(c2cccc(C(=O)N3CC[C@](F)(c4cccc(C(F)(F)F)c4)C3)c2)NC(=O)NC1=O
vMpro-mpro2-189	Z2041582288	-10.1	0.326	415.43	REAL	O=c1nc2c(-c3nc(C4(c5ccccc5F)CCCC4)no3)c[nH]n2c2ccccc12
vMpro-mpro2-190	Z2117484922	-10.1	0.326	418.54	REAL	O=C(N[C@@H]1CC2(CCC2)Oc2ccccc21)N1C[C@H](c2ccccc2)[C@@H]2COCC[C@H]21
vMpro-mpro2-191	Z2157858933	-10.1	0.326	429.37	REAL	Cc1ccc2c(Cc3noc(-c4nc(C)n(-c5nnc(C(F)(F)F)[nH]5)n4)n3)c[nH]c2c1
vMpro-mpro2-192	Z2157917567	-10.1	0.326	420.44	REAL	C[C@@]1(c2cccc(-c3noc(C4(Cc5cccc(F)c5)CCC4)n3)c2)NC(=O)NC1=O
vMpro-mpro2-193	Z2158231042	-10.1	0.337	418.34	REAL	Cc1nc(-c2nc([C@H]3CCOc4ccccc43)no2)nn1-c1nnc(C(F)(F)F)[nH]1
vMpro-mpro2-194	Z2158588243	-10.1	0.316	420.43	REAL	COc1cc(-c2noc(-c3ccc4[nH]c5ccccc5c(=O)c4c3)n2)c2ccccc2n1
vMpro-mpro2-195	Z2160729392	-10.1	0.316	447.37	REAL	O=C1NC(=O)C2(CCC(c3nc(-c4ncoc4-c4cccc(C(F)(F)F)c4)no3)CC2)N1
vMpro-mpro2-196	Z2222082585	-10.1	0.316	442.40	REAL	O=C1CNC(=O)c2ccc(-c3nc(C4(c5cccc(C(F)(F)F)c5)CCC4)no3)cc2N1
vMpro-mpro2-197	Z2229149086	-10.1	0.337	403.49	REAL	O=C1CC[C@@](C(=O)N2CCC[C@H](c3nnc4ccccn34)C2)(c2ccccc2)CN1
vMpro-mpro2-198	Z2229741353	-10.1	0.348	389.50	REAL	C[C@H]1CN(C(=O)c2ccc3[nH]c4ccccc4c(=O)c3c2)CCN(C2CCC2)C1
vMpro-mpro2-199	Z225722654	-10.1	0.316	432.44	REAL	O=C1NC(=O)C2(CCN(C(=O)c3cccc(CN4C(=O)c5ccccc5C4=O)c3)CC2)N1
vMpro-mpro2-200	Z243556424	-10.1	0.316	426.49	REAL	O=C1C[C@@H](C(=O)NC[C@H]2CC3c4ccccc4C2c2ccccc23)c2ccc(F)cc2N1

Supplementary Table 32. Virtual screening hits 101 to 200 of the α-helix 5 association site on the dimerization interface of M^{pro} (Screen ID: 19). Compounds were filtered so that hits had MW < 600 dalton, cLogP < 6, number of hydrogen bond acceptors < 11, and no reactive functional groups. The name of each compound consists of the initial letter 'v' for virtual hit, followed by the target protein name and the target site ('mpro' for the M^{pro} binding site, 2 for docking scenario 2). The score is the docking score given by QuickVina 2 in kcal/mol. The ligand efficiency (LE) is computed as LE = -score/#NonH, where #NonH is the number of heavy (i.e. non hydrogen) atoms.

Name	Catalog ID	Score	LE	MW	Library	SMILES
vPlpro-as3-1	PV-001961056574	-10.6	0.424	360.299	REAL	O=C(NCc1nc(C(F)(F)F)n[nH]1)N1CCC[C@@H](c2nc(=O)[nH][nH]2)C1
vPlpro-as3-2	PV-000673056873	-10.5	0.42	348.449	REAL	CCCNC(=O)CN[C@H]1C[C@H]2CC[C@H]1N(C=O)CCc1nnc[nH]1)C2
vPlpro-as3-3	PV-001874653455	-10.4	0.4333333	343.308	REAL	C[C@@H](NC(=O)[C@]12C[C@H]3C[C@@H](C(=O)N1)[C@@H]2C3)c1nnc(C(F)(F)F)[nH]1
vPlpro-as3-4	Z2091798621	-10.4	0.3354839	437.377	REAL	C[C@@]1(C[C@H]2CCCN2C(=O)c2cccc(-c3noc(C(F)(F)F)n3)c2)NC(=O)NC1=O
vPlpro-as3-5	Z2496599416	-10.4	0.3586207	391.438	REAL	CC1=C(C(=O)Nc2cccc(-c3nc(C4CC4)n[nH]3)c2)[C@@H](C)n2nnnc2N1C
vPlpro-as3-6	PV-001799414339	-10.3	0.3551724	388.422	REAL	C[C@@H]1CN(C(=O)c2cccc(C(=O)c3ccco3)c2)c2ccccc2N(C)C1=O
vPlpro-as3-7	PV-001948844490	-10.3	0.4291667	346.391	REAL	O=C(NC[C@H]1C[C@H]2C[C@H]1[C@H]1C[C@H]21)N[C@H](C[C@H]1CCCO1)C(F)(F)F
vPlpro-as3-8	Z2497441024	-10.3	0.3551724	392.422	REAL	CC1=C(C(=O)Nc2cccc(-c3noc(C4CC4)n3)c2)[C@@H](C)n2nnnc2N1C
vPlpro-as3-9	PV-001941691598	-10.2	0.3777778	381.321	REAL	Cc1nnnn1-c1cccc(NC(=O)N[C@@H](C)c2nnc(C(F)(F)F)[nH]2)c1
vPlpro-as3-10	PV-001943088205	-10.2	0.3777778	380.333	REAL	Cc1nc(-c2cccc(NC(=O)N[C@H](C)c3nnc(C(F)(F)F)[nH]3)c2)n[nH]1
vPlpro-as3-11	Z1447261755	-10.2	0.31875	423.519	REAL	Cc1ccc(-c2nnc(C)[nH]2)c(NC(=O)CN2Cc3ccccc3-c3ccccc3C2)c1
vPlpro-as3-12	Z2119836411	-10.2	0.3777778	389.337	REAL	C[C@@]1(C[C@@H]2CCCN2C(=O)NCc2nc(C(F)(F)F)n[nH]2)NC(=O)NC1=O
vPlpro-as3-13	PV-001835127023	-10.1	0.3607143	378.387	REAL	C[C@@H]1CN(C(=O)c2cccc(-c3noc(O)n3)c2)c2ccccc2N(C)C1=O
vPlpro-as3-14	PV-001874645511	-10.1	0.404	352.279	REAL	C[C@H](NC(=O)c1cccc(-n2cnnn2)c1)c1nnc(C(F)(F)F)[nH]1
vPlpro-as3-15	PV-001874650759	-10.1	0.404	351.291	REAL	C[C@H](NC(=O)c1cccc(-c2ncn[nH]2)c1)c1nnc(C(F)(F)F)[nH]1
vPlpro-as3-16	PV-001943013145	-10.1	0.3740741	379.345	REAL	C[C@@H](NC(=O)Nc1cccc(-c2ncnc2C)c1)c1nnc(C(F)(F)F)[nH]1
vPlpro-as3-17	PV-001945388926	-10.1	0.3884616	365.318	REAL	C[C@H](NC(=O)Nc1cccc(-c2cc[nH]n2)c1)c1nnc(C(F)(F)F)[nH]1
vPlpro-as3-18	PV-001950837730	-10.1	0.3607143	398.344	REAL	C[C@H](NC(=O)Nc1cccc([C@@]2(C)COC(=O)N2)c1)c1nnc(C(F)(F)F)[nH]1
vPlpro-as3-19	Z1552980360	-10.1	0.3366667	409.496	REAL	Cc1nc2nc(N)nn2c(C)c1CCC(=O)N1CCC[C@H](c2n[nH]c(C3CC3)n2)C1
vPlpro-as3-20	Z1669951931	-10.1	0.3607143	377.403	REAL	Cc1nc(-c2ccccc2NC(=O)NCc2ccc3c(c2)C(=O)NCC3)no1
vPlpro-as3-21	Z2183518056	-10.1	0.3884616	369.346	REAL	CC1(C)CN(C(=O)NCc2nc(C(F)(F)F)n[nH]2)Cc2ccccc2O1
vPlpro-as3-22	Z2221875786	-10.1	0.3607143	375.427	REAL	COc1cccc2c1[C@@H](c1nc(-c3ccccc3NC(=O)C3CC3)no1)CC2
vPlpro-as3-23	Z2480806289	-10.1	0.4391305	329.281	REAL	O=C1N[C@]2(C(=O)NCc3nc(C(F)(F)F)n[nH]3)C[C@H]3C[C@@H]1[C@@H]2C3
vPlpro-as3-24	Z2497385957	-10.1	0.3482759	394.438	REAL	CCc1noc(-c2ccc(C)c(NC(=O)C3=C(C)N(C)c4nnnn4[C@@H]3C)c2)n1
vPlpro-as3-25	Z3177240398	-10.1	0.3607143	375.431	REAL	O=C(Nc1ccccc1-c1noc(C2CC2)n1)N[C@H]1CCCc2ccnc21
vPlpro-as3-26	PV-000382958414	-10	0.3846154	355.401	REAL	O=C(N[C@]12CCC[C@H]1CN(C(=O)c1cc(C3CC3)[nH]n1)C2)c1c[nH]nn1
vPlpro-as3-27	PV-000383417016	-10	0.3846154	355.401	REAL	O=C(N[C@]12CCC[C@H]1CN(C(=O)c1cc(C3CC3)[nH]n1)C2)c1nc[nH]n1
vPlpro-as3-28	PV-000432843358	-10	0.4	346.386	REAL	Cc1cc(C)c(C(=O)N2C[C@@H]3CC[C@H](C2)N3C(=O)[C@H]2COC(=O)N2)[nH]1
vPlpro-as3-29	PV-001798531197	-10	0.3571429	374.395	REAL	C[C@@H]1CN(C(=O)c2cccc(C(=O)c3ccco3)c2)c2ccccc2NC1=O
vPlpro-as3-30	PV-001806516802	-10	0.3571429	387.36	REAL	Cc1cc(CNC(=O)C(F)(F)F)cc(NC(=O)c2cccc3ccenc23)c1
vPlpro-as3-31	PV-001860282783	-10	0.3448276	405.383	REAL	Cc1nc(C(=O)N2c3ccccc3C(C)(C)[C@H]2C)nn1-c1nnc(C(F)(F)F)[nH]1
vPlpro-as3-32	PV-001874653373	-10	0.4166667	341.252	REAL	C[C@@H](NC(=O)c1ccnc2[nH]c(O)nc12)c1nnc(C(F)(F)F)[nH]1
vPlpro-as3-33	PV-001945397668	-10	0.3703704	381.317	REAL	C[C@@H](NC(=O)Nc1cccc(-c2ncn(C)n2)c1)c1nc(C(F)(F)F)no1
vPlpro-as3-34	PV-001966447882	-10	0.3225806	434.417	REAL	C[C@@H](NC(=O)N1CCN(c2cccc(C(F)(F)F)c2)CC1)c1ccc2[nH]c(=O)oc2c1
vPlpro-as3-35	PV-001969303142	-10	0.3225806	437.449	REAL	O=C(Nc1c[nH]nc1[C@@H]1CCCN(C(=O)NCc2nc(C(F)F)no2)C1)C1CCCC1
vPlpro-as3-36	Z1622502464	-10	0.3448276	397.449	REAL	O=C(NCc1cccc(C(=O)NC2CC2)c1)N[C@@H]1CCCOc2c(F)cccc21
vPlpro-as3-37	Z1663741468	-10	0.3703704	363.355	REAL	O=C(Nc1cccc(-c2nc(C3CC3)n[nH]2)c1)c1cc2[nH]nnc2cc1F
vPlpro-as3-38	Z1690282109	-10	0.3571429	380.49	REAL	C[C@H]1C[C@@H]1c1ccc(CNC(=O)[C@H]2C[C@H]3CCCC[C@H]3N2c2ncccn2)o1
vPlpro-as3-39	Z1734186392	-10	0.3571429	399.391	REAL	O=C(NCc1nc(C(F)(F)F)n[nH]1)NCC1(c2cccc(F)c2)CCCCC1
vPlpro-as3-40	Z1856527055	-10	0.3846154	354.369	REAL	O=C(Nc1ccc(C[C@H]2NC(=O)NC2=O)cc1)Nc1cc(C2CC2)n[nH]1
vPlpro-as3-41	Z1857230786	-10	0.3225806	429.513	REAL	O=C(NCC1(c2cccc(F)c2F)CCCC1)N1CCC[C@H](c2n[nH]c(C3CC3)n2)C1
vPlpro-as3-42	Z2077132778	-10	0.3333333	416.318	REAL	O=C(Nc1cccc(-c2n[nH]c(=O)[nH]2)c1)c1cccc(-c2noc(C(F)(F)F)n2)c1
vPlpro-as3-43	Z2140796505	-10	0.3125	449.363	REAL	O=C(Nc1ccc(F)c(N2CCCNC2=O)c1)c1cccc(-c2noc(C(F)(F)F)n2)c1
vPlpro-as3-44	Z2229067221	-10	0.3703704	399.377	REAL	O=C(NC1(c2noc(C(F)F)n2)CCC1)[C@H]1Nc2ccccc2S(=O)(=O)N1
vPlpro-as3-45	Z2608162531	-10	0.3703704	375.353	REAL	FC(F)(F)c1cccc(C2(c3noc([C@H]4CCCc5[nH]nnc54)n3)CC2)c1
vPlpro-as3-46	Z2870121956	-10	0.3846154	352.393	REAL	O=C1CC[C@@H](c2ccccc2NC(=O)N2CCOc3ncccc3C2)N1
vPlpro-as3-47	Z2871037532	-10	0.3571429	392.405	REAL	C[C@]1(CNC(=O)NC2(c3noc(C(F)F)n3)CCC2)OCCc2ccccc21
vPlpro-as3-48	Z2949745095	-10	0.3448276	387.442	REAL	CC(C)c1n[nH]c(-c2ccccc2NC(=O)[C@@H]2C[C@]23C(=O)Nc2ccccc23)n1
vPlpro-as3-49	PV-000383559386	-9.9	0.3666667	370.416	REAL	O=C(N[C@]12CCC[C@H]1CN(C(=O)c1c[nH]nn1)C2)[C@H]1CCCc2[nH]nnc21
vPlpro-as3-50	PV-001244123461	-9.9	0.396	348.406	REAL	CCC(=O)N[C@@H](C)C(=O)N1C[C@H]2CCN(C(=O)c3c[nH]nn3)C[C@H]2C1
vPlpro-as3-51	PV-001288696185	-9.9	0.3807692	367.399	REAL	CC(F)(F)CC(=O)N[C@@H]1C[C@H]2CC[C@@H]1N2C(=O)[C@@H]1CCCc2[nH]nnc21
vPlpro-as3-52	PV-001812572154	-9.9	0.3666667	427.341	REAL	C[C@H]1C[C@@H]1C(=O)Nc1cccc(C(=O)N2CC(C)(C)c3ccc(Br)cc32)c1
vPlpro-as3-53	PV-001814145740	-9.9	0.33	423.365	REAL	CN1C(=O)C[C@@H](C(=O)Nc2cc(F)cc(CNC(=O)C(F)(F)F)c2)c2ccccc21
vPlpro-as3-54	PV-001825447919	-9.9	0.3666667	362.348	REAL	Cc1nccn1-c1ncccc1NC(=O)c1cccc(-c2noc(O)n2)c1
vPlpro-as3-55	PV-001826101798	-9.9	0.396	335.326	REAL	Cc1nc(-c2cccc(NC(=O)c3ccnc4[nH]c(O)nc34)c2)n[nH]1
vPlpro-as3-56	PV-001831156391	-9.9	0.3	452.391	REAL	O=C(Nc1cccc(NC(=O)c2cccc3nc[nH]c(=O)c23)c1)c1cccc(C(F)(F)F)c1
vPlpro-as3-57	PV-001835969753	-9.9	0.3666667	365.392	REAL	Cc1nc(-c2ccc(C)c(NC(=O)c3coc4c3C(=O)NCCC4)c2)n[nH]1
vPlpro-as3-58	PV-001855136767	-9.9	0.3193548	432.357	REAL	O=C(c1cccc(-c2noc(O)n2)c1)N1c2ccccc2C[C@H]1CNC(=O)C(F)(F)F
vPlpro-as3-59	PV-001855733037	-9.9	0.3535714	397.312	REAL	C[C@@H](NC(=O)c1ccc([C@@]2(C)NC(=O)NC2=O)cc1)c1noc(C(F)(F)F)n1
vPlpro-as3-60	PV-001855733991	-9.9	0.3535714	397.312	REAL	C[C@H](NC(=O)c1cccc([C@]2(C)NC(=O)NC2=O)c1)c1noc(C(F)(F)F)n1
vPlpro-as3-61	PV-001857870809	-9.9	0.396	340.346	REAL	O=C(c1cccc(Nc2nnn[nH]2)c1)N1CC[C@@H](c2cc(O)[nH]n2)C1
vPlpro-as3-62	PV-001861212350	-9.9	0.33	413.398	REAL	O=C(N[C@H]1CCc2ccc(O)cc21)c1cccnc1Nc1cccc(C(F)(F)F)c1
vPlpro-as3-63	PV-001874647474	-9.9	0.396	357.291	REAL	C[C@H](NC(=O)c1cccc(OCC(N)=O)c1)c1nnc(C(F)(F)F)[nH]1
vPlpro-as3-64	PV-001874649401	-9.9	0.3807692	366.302	REAL	Cc1nnc(-c2cccc(C(=O)N[C@@H](C)c3nnc(C(F)(F)F)[nH]3)c2)o1
vPlpro-as3-65	PV-001874652242	-9.9	0.4125	340.264	REAL	C[C@@H](NC(=O)c1cccc2[nH]c(=O)[nH]c12)c1nnc(C(F)(F)F)[nH]1
vPlpro-as3-66	PV-001901041694	-9.9	0.33	405.417	REAL	Cc1cc(=O)[nH]c(CNC(=O)CCc2nc3c(cnn3-c3ccccc3)c(=O)[nH]2)n1
vPlpro-as3-67	PV-001945139178	-9.9	0.3807692	366.302	REAL	C[C@@H](NC(=O)Nc1cccc(-c2ncco2)c1)c1nnc(C(F)(F)F)[nH]1
vPlpro-as3-68	PV-001945387951	-9.9	0.3807692	366.302	REAL	C[C@@H](NC(=O)Nc1cccc(-c2cc[nH]n2)c1)c1nc(C(F)(F)F)no1
vPlpro-as3-69	PV-001947454901	-9.9	0.3807692	375.285	REAL	C[C@H](NC(=O)Nc1ccc(F)c(NC(N)=O)c1)c1nnc(C(F)(F)F)[nH]1
vPlpro-as3-70	PV-001954600664	-9.9	0.309375	432.479	REAL	CN1Cc2ccccc2[C@H](NC(=O)NCc2cccc(C(=O)NCc3ccco3)c2)C1=O
vPlpro-as3-71	PV-001955708126	-9.9	0.33	426.354	REAL	C[C@@H](NC(=O)NCc1cccc([C@]2(C)NC(=O)NC2=O)c1)c1nc(C(F)(F)F)no1
vPlpro-as3-72	PV-001961988559	-9.9	0.3666667	390.321	REAL	C[C@H](NC(=O)NC1CCC2(CC1)NC(=O)NC2=O)c1nc(C(F)(F)F)no1
vPlpro-as3-73	Z1228768887	-9.9	0.3413793	410.824	REAL	O=C(CCc1nc2c(cnn2-c2ccccc2)c(=O)[nH]1)NNc1ccc(Cl)nn1
vPlpro-as3-74	Z1303408920	-9.9	0.309375	427.467	REAL	Cc1ccc2[nH]c(CNC(=O)CCc3nc4c(cnn4-c4ccccc4)c(=O)[nH]3)nc2c1
vPlpro-as3-75	Z1335413755	-9.9	0.3666667	384.321	REAL	Cc1nc(C(=O)N2[C@H]3CC[C@H]2CC(=O)NC3)nn1-c1nnc(C(F)(F)F)[nH]1
vPlpro-as3-76	Z1337298200	-9.9	0.3535714	379.394	REAL	Cc1nc(-c2ccc(C)c(NC(=O)[C@@H]3CC(=O)Nc4cc(F)ccc43)c2)n[nH]1
vPlpro-as3-77	Z1453182959	-9.9	0.3535714	382.423	REAL	Cc1nc([C@@H]2CCCN(C(=O)c3cccc([C@]4(C)NC(=O)NC4=O)c3)C2)n[nH]1
vPlpro-as3-78	Z1649061081	-9.9	0.309375	444.416	REAL	Cc1nc2cc(O)nn2c(C)c1CCC(=O)Nc1ccn(-c2cccc(C(F)(F)F)c2)n1
vPlpro-as3-79	Z1663741430	-9.9	0.3807692	346.353	REAL	O=C(Nc1cccc(-c2nc(C3CC3)n[nH]2)c1)c1ccc2[nH]nnc2n1
vPlpro-as3-80	Z1683604007	-9.9	0.3535714	370.411	REAL	O=C(Nc1ccccc1-c1noc(Cc2cccc3cccnc23)n1)C1CC1
vPlpro-as3-81	Z1685319232	-9.9	0.3413793	389.433	REAL	Cc1nnc(-c2cccc(-c3noc(C4(c5cccc(F)c5)CCCC4)n3)c2)[nH]1
vPlpro-as3-82	Z1724925028	-9.9	0.3193548	443.425	REAL	C[C@H](OC(=O)[C@H]1C[C@H]2CCCC[C@H]2N1c1nccn1)C(=O)NC(=O)NCC(F)(F)F
vPlpro-as3-83	Z1731343178	-9.9	0.3535714	408.269	REAL	FC(F)(F)c1n[nH]c(CNc2nccnc2NCc2nc(C(F)(F)F)n[nH]2)n1
vPlpro-as3-84	Z1732872617	-9.9	0.4125	338.252	REAL	O=C(NCc1nc(C(F)(F)F)n[nH]1)c1cccc(-n2cnnn2)c1
vPlpro-as3-85	Z1873403528	-9.9	0.309375	446.384	REAL	C[C@H](NC(=O)c1cccc(-c2noc(C(F)(F)F)n2)c1)c1cccc(N2CCOC2=O)c1
vPlpro-as3-86	Z1987085945	-9.9	0.3535714	379.423	REAL	CCc1nnc(-c2cccc(NC(=O)C3=C(C)N(C)c4ncnn4[C@@H]3C)c2)o1
vPlpro-as3-87	Z2053024196	-9.9	0.396	366.804	REAL	Cc1noc(C(C)(C)NC(=O)Nc2cc3c(cc2Cl)OCCCO3)n1
vPlpro-as3-88	Z2156853430	-9.9	0.3413793	409.465	REAL	O=C(Nc1ccccc1-c1noc([C@@H]2CCS(=O)(=O)c3ccccc32)n1)C1CC1
vPlpro-as3-89	Z2160585963	-9.9	0.33	415.37	REAL	C[C@@H]1Oc2c(cccc2-c2nc(C3(c4cccc(C(F)(F)F)c4)CC3)no2)NC1=O
vPlpro-as3-90	Z2174767061	-9.9	0.3193548	424.439	REAL	Cc1nnnn1/C(=C\c1cccc(F)c1)C(=O)O[C@H]1CCCN(c2ccnc(N)n2)C1
vPlpro-as3-91	Z2174768941	-9.9	0.3413793	395.462	REAL	C[C@H]1C[C@@H]1C(=O)Nc1cccc(C(=O)O[C@H]2CCCN(c3ccnc(N)n3)C2)c1
vPlpro-as3-92	Z2200386183	-9.9	0.3413793	412.396	REAL	CN1C(=O)N[C@@]2(CCC[C@H]2CNC(=O)NC2(c3noc(C(F)F)n3)CCC2)C1=O
vPlpro-as3-93	Z2409932038	-9.9	0.3535714	385.379	REAL	C[C@@]1(c2ccccc(C(=O)N3CCC[C@H](c4n[nH]c(=O)o4)C3)c2)NC(=O)NC1=O
vPlpro-as3-94	Z2601586378	-9.9	0.3535714	382.466	REAL	CCNC(=O)N1CC[C@H](NC(=O)N[C@@H]2CCc3ccccc3-n3ccnc32)C1
vPlpro-as3-95	Z2608156635	-9.9	0.3535714	389.38	REAL	FC(F)(F)c1cccc(C2(c3noc([C@H]4CCCc5[nH]nnc54)n3)CCC2)c1
vPlpro-as3-96	Z2624341781	-9.9	0.3666667	378.353	REAL	O=C(N[C@@H]1[C@H]2Cc3cc(F)ccc3[C@H]21)NC1(c2noc(C(F)(F)F)n2)CCC1
vPlpro-as3-97	Z2626796376	-9.9	0.3666667	364.412	REAL	CN1NN=C2C1=NCC[C@@H]2C(=O)Nc1cccc(-c2nc(C3CC3)n[nH]2)c1
vPlpro-as3-98	Z2638287826	-9.9	0.396	339.358	REAL	Cc1ccc(-c2n[nH]c(=O)[nH]2)cc1NC(=O)[C@H]1CCCc2[nH]nnc21
vPlpro-as3-99	Z2638287841	-9.9	0.3807692	354.373	REAL	Cc1ccc(-c2n[nH]c(=O)[nH]2)cc1NC(=O)[C@H]1CCN=C2C1=NNN2C
vPlpro-as3-100	Z2640851556	-9.9	0.4125	326.315	REAL	O=C(NCc1nc(C2CC2)n[nH]1)c1cccc(-c2noc(O)n2)c1

Supplementary Table 33. Top 100 virtual hits of the screen against the active site of PL^{pro} (Screen ID: 15). Compounds were filtered so that hits had MW < 600 dalton, cLogP < 6, number of hydrogen bond acceptors < 11, and no reactive functional groups. The name of each compound consists of the initial letter 'v' for virtual hit, followed by the target protein name and the target site ('as' for active site, 3 for docking scenario 3). The score is the docking score given by QuickVina 2 in kcal/mol. The ligand efficiency (LE) is computed as LE = -score/#NonH, where #NonH is the number of heavy (i.e. non hydrogen) atoms.

Name	Catalog ID	Score	LE	MW	Library	SMILES
vPlpro-as3-101	Z2892912342	-9.9	0.381	350.43	REAL	Cc1nc(-c2ccc(C)c(NC(=O)[C@H]3C[C@@H](C)Cc4cn[nH]c43)c2)n[nH]1
vPlpro-as3-102	Z2927634465	-9.9	0.354	386.47	REAL	Cc1cc(F)ccc1[C@@H](C)NC(=O)N1CCCC[C@@H]1c1nnc(C2CCC2)o1
vPlpro-as3-103	Z775751440	-9.9	0.354	380.46	REAL	CC(=O)Nc1ccnc2c1CCN(C(=O)C1(c3cccc(F)c3)CCCC1)C2
vPlpro-as3-104	PV-000345756551	-9.8	0.363	369.38	REAL	NC(=O)c1cccc(C(=O)N2C[C@H]3CCN(C(=O)c4c[nH]nn4)C[C@H]3C2)n1
vPlpro-as3-105	PV-000346551724	-9.8	0.363	365.40	REAL	O=C(c1c[nH]nn1)N1CC[C@@H]2CN(C(=O)c3cccc4cn[nH]c34)C[C@@H]2C1
vPlpro-as3-106	PV-000376279830	-9.8	0.377	357.41	REAL	CCc1cccc(C(=O)N2[C@H]3CC[C@@H]2C[C@@H]3NC(=O)[C@@H]2CNC(=O)N2)n1
vPlpro-as3-107	PV-000383496402	-9.8	0.377	356.39	REAL	O=C(N[C@]12CCC[C@H]1CN(C(=O)c1cc(C3CC3)[nH]n1)C2)c1cnon1
vPlpro-as3-108	PV-000494867227	-9.8	0.392	343.39	REAL	Cc1n[nH]nc1C(=O)N1CC(NC(=O)[C@H]2C[C@H](C)Cc3cn[nH]c32)C1
vPlpro-as3-109	PV-001795357298	-9.8	0.377	351.37	REAL	Cc1nc(-c2cccc(NC(=O)c3coc4c3C(=O)NCCC4)c2)n[nH]1
vPlpro-as3-110	PV-001814148911	-9.8	0.338	409.34	REAL	O=C1NC[C@@H](C(=O)Nc2cc(F)cc(CNC(=O)C(F)(F)F)c2)c2ccccc21
vPlpro-as3-111	PV-001829370115	-9.8	0.408	326.32	REAL	O=C(Cc1n[nH]c(C2CC2)n1)Nc1cccc(-c2noc(=O)[nH]2)c1
vPlpro-as3-112	PV-001836990918	-9.8	0.408	324.35	REAL	O=C(N[C@H]1CCCc2cn[nH]c21)c1cccc(Nc2nnn[nH]2)c1
vPlpro-as3-113	PV-001841744670	-9.8	0.392	341.38	REAL	CC(C)c1nc([C@@H](C)NC(=O)c2cccc(Nc3nnn[nH]3)c2)n[nH]1
vPlpro-as3-114	PV-001843003305	-9.8	0.306	455.39	REAL	Cc1nc(C(=O)NCC2(c3cccc(F)c3F)CCCC2)nn1-c1nnc(C(F)(F)F)n[nH]1
vPlpro-as3-115	PV-001843115882	-9.8	0.327	416.36	REAL	O=C(c1cccc(Nc2nccc(C(F)(F)F)n2)c1)N1CCc2c(nc[nH]c2=O)C1
vPlpro-as3-116	PV-001847827789	-9.8	0.408	325.33	REAL	O=C(Cc1n[nH]c(C2CC2)n1)Nc1cccc(-c2n[nH]c(=O)[nH]2)c1
vPlpro-as3-117	PV-001847828947	-9.8	0.377	366.30	REAL	C[C@@H](C(=O)Nc1cccc(-c2n[nH]c(=O)[nH]2)c1)n1ccc(C(F)(F)F)n1
vPlpro-as3-118	PV-001850705881	-9.8	0.306	442.40	REAL	Cc1noc2nc(-c3cccc(C(F)(F)F)c3)cc(C(=O)N[C@@H](C)c3ncnc(N)n3)c12
vPlpro-as3-119	PV-001853043386	-9.8	0.408	334.29	REAL	C[C@@H](NC(=O)c1cccc(-c2ncn[nH]2)c1)c1noc(C(F)F)n1
vPlpro-as3-120	PV-001853044875	-9.8	0.392	350.29	REAL	C[C@H](NC(=O)c1cccc(Nc2nnn[nH]2)c1)c1noc(C(F)F)n1
vPlpro-as3-121	PV-001856495070	-9.8	0.377	348.41	REAL	Cc1cccnc1Oc1ccc(C(=O)Nc2cc([C@H]3C[C@@H]3C)n[nH]2)cc1
vPlpro-as3-122	PV-001857212520	-9.8	0.392	343.39	REAL	C[C@@H]1[C@H](C)N(C(=O)c2cccc(Nc3nnn[nH]3)c2)[C@@H](C)C(=O)N1C
vPlpro-as3-123	PV-001857871519	-9.8	0.392	341.33	REAL	O=C(c1cccc(-c2noc(O)n2)c1)N1CC[C@H](c2ccc(O)[nH]n2)C1
vPlpro-as3-124	PV-001869312792	-9.8	0.363	368.40	REAL	C[C@@]1(c2cccc(C(=O)N3CCC[C@H](c4nnc[nH]4)C3)c2)NC(=O)NC1=O
vPlpro-as3-125	PV-001872939571	-9.8	0.338	408.34	REAL	CNC(=O)c1cccc(N(C)C(=O)c2nc(C)n(-c3nnc(C(F)(F)F)[nH]3)n2)c1
vPlpro-as3-126	PV-001873780308	-9.8	0.392	371.42	REAL	O=C1NC(=O)C2(CCC(C(=O)N3CCN4[C@H](CNS4(=O)=O)C3)CC2)N1
vPlpro-as3-127	PV-001874419837	-9.8	0.377	354.32	REAL	Cc1n[nH]c(NC(=O)c2cc3[nH]nnc3cc2F)c1-c1ccc(F)cc1
vPlpro-as3-128	PV-001874648437	-9.8	0.338	408.38	REAL	C[C@@H](NC(=O)c1ccc2c(c1)[nH]c(=O)n2C1CCCC1)c1nnc(C(F)(F)F)[nH]1
vPlpro-as3-129	PV-001874649165	-9.8	0.363	377.33	REAL	C[C@H](NC(=O)c1cccc(Oc2ccncc2)c1)c1nnc(C(F)(F)F)[nH]1
vPlpro-as3-130	PV-001874655431	-9.8	0.377	374.27	REAL	C[C@@H](NC(=O)c1cccc2[nH]c(C(F)F)nc12)c1nnc(C(F)(F)F)[nH]1
vPlpro-as3-131	PV-001878888213	-9.8	0.377	354.32	REAL	Cc1n[nH]c(NC(=O)c2cc3[nH]nnc3cc2F)c1-c1cccc(F)c1
vPlpro-as3-132	PV-001921894140	-9.8	0.338	398.47	REAL	Cc1ccc(-c2nnc(C)[nH]2)c(NC(=O)CN2CCC[C@@H]3OCCNC(=O)[C@H]32)c1
vPlpro-as3-133	PV-001921932433	-9.8	0.350	382.47	REAL	Cc1ccc(-c2nnc(C)[nH]2)c(NC(=O)CN2CCC[C@@H]3CCNC(=O)[C@H]32)c1
vPlpro-as3-134	PV-001939722912	-9.8	0.363	402.36	REAL	C[C@H](NS(=O)(=O)c1cccc(-c2nnnn2C)c1)c1nnc(C(F)(F)F)[nH]1
vPlpro-as3-135	PV-001940784048	-9.8	0.377	370.33	REAL	C[C@@H](NC(=O)Nc1cccc(C(=O)N(C)C)c1)c1nnc(C(F)(F)F)[nH]1
vPlpro-as3-136	PV-001941153508	-9.8	0.363	384.32	REAL	C[C@@H]1Oc2ccc(NC(=O)N[C@@H](C)c3nnc(C(F)(F)F)n[nH]3)cc2NC1=O
vPlpro-as3-137	PV-001941765741	-9.8	0.377	357.37	REAL	Cc1ccc(NC(=O)C2CC2)cc1NC(=O)NCc1cc(=O)[nH]c(=O)[nH]1
vPlpro-as3-138	PV-001941922120	-9.8	0.350	408.89	REAL	CCC(=O)Nc1ccc(Cl)c(NC(=O)N2CCC[C@@H]([C@]3(C)COC(=O)N3)C2)c1
vPlpro-as3-139	PV-001942156821	-9.8	0.350	382.42	REAL	C[C@@H]1C(=O)Nc2ccccc2CN1C(=O)Nc1ccccc1OCCC(N)=O
vPlpro-as3-140	PV-001943086967	-9.8	0.363	365.39	REAL	Cc1nc(-c2cccc(NC(=O)N3CCOc4ccc(O)cc4C3)c2)n[nH]1
vPlpro-as3-141	PV-001947993018	-9.8	0.338	416.33	REAL	C[C@@H](NC(=O)Nc1ccc(F)c(N2CCCNC2=O)c1)c1nc(C(F)(F)F)no1
vPlpro-as3-142	PV-001951172065	-9.8	0.338	409.34	REAL	C[C@H](NC(=O)Nc1cccc(Oc2ccccc2F)c1)c1nnc(C(F)(F)F)[nH]1
vPlpro-as3-143	PV-001951457308	-9.8	0.377	366.30	REAL	C[C@H](NC(=O)Nc1cccc(-c2ccon2)c1)c1nnc(C(F)(F)F)[nH]1
vPlpro-as3-144	PV-001951768748	-9.8	0.350	407.32	REAL	C[C@H](NC(=O)N[C@@]1(C(F)(F)F)CCc2ccccc21)c1nnc(C(F)(F)F)[nH]1
vPlpro-as3-145	PV-001952096489	-9.8	0.350	383.41	REAL	O=C(NCC(=O)N1CCCc2ccccc21)Nc1[nH]nnc1C(=O)NC1CC1
vPlpro-as3-146	PV-001961056361	-9.8	0.377	371.32	REAL	C[C@@]1(CNC(=O)NCc2nc(C(F)(F)F)n[nH]2)COc2ccccc2O1
vPlpro-as3-147	PV-001961058042	-9.8	0.392	354.29	REAL	O=C(NCc1nc(C(F)(F)F)n[nH]1)N[C@H]1Cc2ccccc2NC1=O
vPlpro-as3-148	PV-001969244620	-9.8	0.327	425.37	REAL	CN1Cc2ccccc2[C@H](NC(=O)NCc2cn(CC(F)(F)F)c(=O)[nH]c2=O)C1=O
vPlpro-as3-149	PV-001969897094	-9.8	0.363	375.39	REAL	O=C(N[C@H]1CCCc2ccncc21)NC1(c2cccc(C(F)(F)F)c2)CC1
vPlpro-as3-150	PV-001970703762	-9.8	0.338	416.33	REAL	COC(=O)c1ccc(F)c2c1CN(C(=O)N[C@H](C)c1nc(C(F)(F)F)no1)CC2
vPlpro-as3-151	Z1029998890	-9.8	0.350	380.41	REAL	Cc1[nH]c(=O)[nH]c(=O)c1CCC(=O)Nc1cccc(-c2nc(C3CC3)n[nH]2)c1
vPlpro-as3-152	Z1030062256	-9.8	0.338	408.45	REAL	O=S(=O)(Nc1cccc(-c2nc(C3CC3)n[nH]2)c1)c1cccc(-n2cnnn2)c1
vPlpro-as3-153	Z1030835064	-9.8	0.377	345.37	REAL	O=C(Nc1cccc(-c2nc(C3CC3)n[nH]2)c1)c1ccc2[nH]nnc2c1
vPlpro-as3-154	Z1185263457	-9.8	0.306	430.51	REAL	C[C@@H]1Cc2ccccc2N1C(=O)[C@@H]1CCCC[C@H]1C(=O)Nc1cccc(-c2nnn[nH]2)c1
vPlpro-as3-155	Z1230348379	-9.8	0.363	367.41	REAL	Cc1nc(-c2cccc(NC(=O)NC3(c4noc(C)n4)CCCC3)c2)n[nH]1
vPlpro-as3-156	Z1274548713	-9.8	0.327	402.45	REAL	CC(=O)N1CCCN(C(=O)c2cccc(-c3noc(C4CC4)n3)c2)c2ccccc21
vPlpro-as3-157	Z1518693764	-9.8	0.338	389.46	REAL	CCc1n[nH]c(-c2ccccc2NC(=O)CCN2C(=O)CCc3ccccc32)n1
vPlpro-as3-158	Z1560165569	-9.8	0.377	353.39	REAL	Cc1nc(-c2ccccc2NC(=O)N2CCC[C@H]2c2nncn2C)no1
vPlpro-as3-159	Z1632177538	-9.8	0.327	411.50	REAL	CC(C)(CNC(=O)N1CCC[C@H](c2n[nH]c(C3CC3)n2)C1)c1ccc2c(c1)OCO2
vPlpro-as3-160	Z1683397791	-9.8	0.350	393.30	REAL	O=C1C[C@@H](c2nc(-c3ccccc3OC(F)(F)F)no2)c2ccc(F)cc2N1
vPlpro-as3-161	Z1683600676	-9.8	0.350	373.37	REAL	O=C(Nc1ccccc1-c1noc(-c2n[nH]c(=O)c3ccccc23)n1)C1CC1
vPlpro-as3-162	Z1684855351	-9.8	0.316	435.36	REAL	O=C(Nc1ccc(O)c(-c2nc([C@H]3CCOc4ccccc43)no2)c1)OCC(F)(F)F
vPlpro-as3-163	Z1733332091	-9.8	0.316	443.35	REAL	O=C(N[C@@H](c1ccccc1)c1nnc[nH]1)N[C@@H](c1cccc(C(F)(F)F)c1)C(F)(F)F
vPlpro-as3-164	Z1817771669	-9.8	0.350	382.47	REAL	Cc1ccc(-c2nnc(C)[nH]2)c(NC(=O)CN2C[C@H]3CCC[C@@H]3[C@@H]2C(N)=O)c1
vPlpro-as3-165	Z1839824388	-9.8	0.338	393.49	REAL	Cc1c([C@H](C)NC(=O)N2CCC[C@H](c3n[nH]c(C4CC4)n3)C2)oc2ccccc12
vPlpro-as3-166	Z1864182400	-9.8	0.392	358.28	REAL	CC(C)(NC(=O)C(F)(F)F)C(=O)Nc1cccc(-c2noc(=O)[nH]2)c1
vPlpro-as3-167	Z1873449022	-9.8	0.363	363.36	REAL	O=C(Nc1cccc(-c2nc(C3CC3)n[nH]2)c1)c1cc(F)cc2[nH]nnc12
vPlpro-as3-168	Z1873545213	-9.8	0.363	365.40	REAL	CC1=C(C(=O)Nc2cccc(-c3nnc(C)o3)c2)[C@@H](C)n2ncnc2N1C
vPlpro-as3-169	Z2003649444	-9.8	0.408	338.29	REAL	O=C1[C@@H]2[C@@H]3C[C@@H]4[C@H]2[C@]2(C(=O)NCc5nc(C(F)(F)F)n[nH]5)[C@H]1[C@H]3[C@H]42
vPlpro-as3-170	Z2077110526	-9.8	0.392	341.37	REAL	O=C(Nc1cccc(-c2n[nH]c(=O)[nH]2)c1)C1(C(=O)NC2CC2)CCC1
vPlpro-as3-171	Z2199193912	-9.8	0.363	365.43	REAL	Cc1cccc1C1(C(=O)Nc2cccc(C(=O)NC(N)=O)c2)CCCC1
vPlpro-as3-172	Z2229065761	-9.8	0.377	361.35	REAL	O=C1[C@H]2[C@H]3C[C@@H]4[C@H]2[C@]2(C(=O)NC5(c6noc(C(F)F)n6)CCC5)[C@H]1[C@H]3[C@H]42
vPlpro-as3-173	Z227662740	-9.8	0.288	471.46	REAL	CC(=O)c1ccc(N2CCN(C(=O)COC(=O)[C@H]3CC(=O)Nc4cc(F)ccc43)CC2)c(F)c1
vPlpro-as3-174	Z2293400827	-9.8	0.363	374.35	REAL	O=C(Nc1cccc(-c2cc[nH]n2)c1)NC1(c2noc(C(F)F)n2)CCC1
vPlpro-as3-175	Z2615013860	-9.8	0.338	398.47	REAL	COC(=O)[C@@H]1CCN(C(=O)Nc2cc(-n3cnnn3)ccc2C)[C@@H]2CCCC[C@H]12
vPlpro-as3-176	Z2623174272	-9.8	0.408	323.36	REAL	Cc1nc(-c2cccc(NC(=O)[C@H]3CCCc4[nH]nnc43)c2)n[nH]1
vPlpro-as3-177	Z2639159836	-9.8	0.350	385.38	REAL	C[C@@]1(C[C@H]2CCCN2C(=O)c2cccc(-c3noc(O)n3)c2)NC(=O)NC1=O
vPlpro-as3-178	Z2816347136	-9.8	0.350	394.38	REAL	C[C@@]1(CNC(=O)NC2(c3noc(C(F)F)n3)CCC2)COc2ccccc2O1
vPlpro-as3-179	Z3204024303	-9.8	0.350	388.35	REAL	O=C(c1cc(-c2cccc(C(F)(F)F)c2)ccn1)N1CC[C@H](c2nn[nH]n2)C1
vPlpro-as3-180	Z495438910	-9.8	0.338	395.42	REAL	Cc1nc(-c2ccccc2NC(=O)NC2CCN(C(=O)c3ccco3)CC2)no1
vPlpro-as3-181	Z998534512	-9.8	0.316	421.50	REAL	Cc1nc2cc(O)nn2c(C)c1CCC(=O)NCc1ccnc(NC(=O)C2CCC2)c1
vPlpro-as3-182	ZINC000020086595	-9.8	0.288	456.46	ZINC	Cc1n[nH]c2c1[C@@H](c1ccc([C@H]3c4c(C)n[nH]c4NC4=C3C(=O)OC4)cc1)C1=C(COC1=O)N2
vPlpro-as3-183	ZINC000171230450	-9.8	0.377	345.37	ZINC	O=C(Nc1cccc(-c2nc(C3CC3)n[nH]2)c1)c1ccc2[nH]nnc2c1
vPlpro-as3-184	PV-001822112387	-9.7	0.404	323.36	REAL	C[C@H]1Cc2cn[nH]c2[C@@H](C(=O)Nc2cccc(-c3nnn[nH]3)c2)C1
vPlpro-as3-185	PV-001824311454	-9.7	0.404	324.35	REAL	Cc1nnnn1-c1cccc(NC(=O)Cc2n[nH]c(C3CC3)n2)c1
vPlpro-as3-186	PV-001841384344	-9.7	0.404	327.35	REAL	CCc1nc([C@@H](C)NC(=O)c2cccc(Nc3nnn[nH]3)c2)n[nH]1
vPlpro-as3-187	PV-001844598731	-9.7	0.422	327.23	REAL	O=C(NCc1nc(C(F)(F)F)n[nH]1)c1ccnc2[nH]c(O)nc12
vPlpro-as3-188	PV-001853427240	-9.7	0.404	328.31	REAL	O=C(Nc1cc(-c2nnn[nH]2)ccc1F)[C@H]1CCCc2[nH]nnc21
vPlpro-as3-189	PV-001874653316	-9.7	0.404	342.32	REAL	C[C@@H]1Cc2cn[nH]c2[C@@H](C(=O)N[C@H](C)c2nnc(C(F)(F)F)[nH]2)C1
vPlpro-as3-190	PV-001941995790	-9.7	0.388	337.38	REAL	Cc1nc(-c2ccccc2NC(=O)N[C@H](C)Cc2cccn2)no1
vPlpro-as3-191	PV-001945532557	-9.7	0.388	357.29	REAL	Cc1cc2c(cc1NC(=O)N[C@@H](C)c1nnc(C(F)(F)F)[nH]1)OCO2
vPlpro-as3-192	PV-001947122567	-9.7	0.422	323.36	REAL	CCn1nnnc1NC(=O)N1CCC[C@@H]([C@@]2(C)COC(=O)N2)C1
vPlpro-as3-193	PV-001952102732	-9.7	0.404	338.28	REAL	O=C(NNc1ncc(F)cc1F)Nc1[nH]nnc1C(=O)NC1CC1
vPlpro-as3-194	PV-001961058063	-9.7	0.404	348.28	REAL	O=C1N[C@@H]2CN(C(=O)NCc3nc(C(F)(F)F)n[nH]3)C[C@H]2CO1
vPlpro-as3-195	PV-001963004891	-9.7	0.404	332.37	REAL	O=C(NCc1nc(C2CC2)n[nH]1)N1CCC[C@H](c2nc(=O)[nH][nH]2)C1
vPlpro-as3-196	Z1272834829	-9.7	0.388	329.37	REAL	NC1=Nc2nc3ccccc3n2[C@H](c2c[nH]c(-c3ccccc3)n2)N1
vPlpro-as3-197	Z1389646089	-9.7	0.404	334.35	REAL	Cc1noc([C@@H](C)NC(=O)N[C@H]2CCN(c3nccnc3F)C2)n1
vPlpro-as3-198	Z1511812731	-9.7	0.388	335.33	REAL	Cc1nc(-c2cccc(NC(=O)c3ccc4n[nH]c(=O)n4c3)c2)n[nH]1
vPlpro-as3-199	Z1545959498	-9.7	0.388	364.79	REAL	O=C(NCc1noc(C2CC2)n1)Nc1cc2c(cc1Cl)OCCCO2
vPlpro-as3-200	Z1623080921	-9.7	0.422	319.34	REAL	C[C@@H](NC(=O)N[C@H]1CCN(c2nccc2F)C1)c1nc[nH]n1

Supplementary Table 34. Virtual screening hits 101 to 200 of the screen against the active site of PL^{pro} (Screen ID: 15). Compounds were filtered so that hits had MW < 600 dalton, cLogP < 6, number of hydrogen bond acceptors < 11, and no reactive functional groups. The name of each compound consists of the initial letter 'v' for virtual hit, followed by the target protein name and the target site ('as' for active site, 3 for docking scenario 3). The score is the docking score given by QuickVina 2 in kcal/mol. The ligand efficiency (LE) is computed as LE = -score/#NonH, where #NonH is the number of heavy (i.e. non hydrogen) atoms.

Name	Catalog ID	Score	LE	MW	Library	SMILES
vNsp7-ppi1-1	Z1162537090	-9.1	0.276	436.47	REAL	O=C(Nc1nc2ccccc2c(=O)[nH]1)[C@H]1CC(=O)N(c2ccc3c(c2)Cc2ccccc2-3)C1
vNsp7-ppi1-2	Z2087363989	-8.9	0.278	420.427	REAL	O=C1N[C@H](c2ccc3ccccc3c2)C(=O)N1c1cc(-c2ccc3nccnc3c2)on1
vNsp7-ppi1-3	ZINC000001717023	-8.9	0.278	417.419	ZINC	O=c1oc2ccc(-n3c(=O)c4ccccc4c4ccccc4c3=O)cc2c2ccccc12
vNsp7-ppi1-4	ZINC000097945321	-8.9	0.222	522.559	ZINC	O=C(Oc1cccc2ccenc21)c1cccc(N2C(=O)[C@H]3[C@@H](C2=O)C2c4ccccc4C3c3ccccc32)c1
vNsp7-ppi1-5	ZINC000409334997	-8.9	0.247	466.503	ZINC	O=C(Nc1ccc2ccccc2c1)Nc1ccc2nc3c4cccnc4c4nccc4c3nc2c1
vNsp7-ppi1-6	Z1697483552	-8.8	0.275	423.467	REAL	O=C1O[C@H](c2ccccc2)Cc2cc(C(=O)N3C[C@H]4CCC(=O)c5ccec3c54)ccc21
vNsp7-ppi1-7	Z1766655795	-8.8	0.259	449.513	REAL	O=C(c1ccc2[nH]c3ccccc3c(=O)c2c1)N1CCC[C@@H](c2n[nH]c(-c3ccccc3)n2)C1
vNsp7-ppi1-8	Z426104010	-8.8	0.251	486.522	REAL	O=C1c2ccccc2S(=O)(=O)c2cc(C(=O)N3CC=C(c4c[nH]c5cc(F)ccc45)CC3)ccc21
vNsp7-ppi1-9	Z804128572	-8.8	0.244	496.59	REAL	O=C(Nn1cnc2sc3c(c2c1=O)CCCC3)[C@@H]1CC(=O)N(c2ccc3c(c2)Cc2ccccc2-3)C1
vNsp7-ppi1-10	ZINC000003845263	-8.8	0.267	444.465	ZINC	O=C1c2cccc3cccc(c23)/C1=C1\Sc2ccc3c(c2C1=O)C(=O)c1ccccc1C3=O
vNsp7-ppi1-11	ZINC000003960761	-8.8	0.232	494.64	ZINC	c1ccc2c(c1)c1cc[n+]2Cc2cccc(c2)C[n+]2ccc(c3ccccc32)NCc2ccc(cc2)CN1
vNsp7-ppi1-12	ZINC000006779972	-8.8	0.275	424.542	ZINC	Cc1cc2nc(-c3cc4cc(C56CC7CC(CC(C7)C5)C6)ccc4oc3=O)[nH]c2cc1C
vNsp7-ppi1-13	ZINC000100983474	-8.8	0.259	443.505	ZINC	O=C1[C@@H]2[C@H]3C=C[C@@H](C3)[C@@H]2C(=O)N1c1ccc(-c2nc(-c3ccccc3)nc3ccccc32)cc1
vNsp7-ppi1-14	ZINC000408674312	-8.8	0.244	476.574	ZINC	CC1CCN(C(=O)c2cccc(N3C(=O)[C@@H]4[C@@H](C3=O)C3c5ccccc5C4c4ccccc43)c2)CC1
vNsp7-ppi1-15	ZINC000408674316	-8.8	0.244	476.574	ZINC	CC1CCN(C(=O)c2cccc(N3C(=O)[C@H]4[C@@H](C3=O)C3c5ccccc5C4c4ccccc43)c2)CC1
vNsp7-ppi1-16	PV-001940740368	-8.7	0.272	456.609	REAL	C[C@H](CNC(=O)Nc1ccc(S(=O)(=O)N[C@H](C)[C@@H]2C[C@H]3CC[C@H]2C3)cc1)c1ccncc1
vNsp7-ppi1-17	Z1104727050	-8.7	0.242	498.605	REAL	O=C(Nc1ccc2c(c1)Cc1ccccc1-2)N1CCCN(S(=O)(=O)c2cccc3cnccc23)CC1
vNsp7-ppi1-18	Z1144203593	-8.7	0.29	402.468	REAL	Cc1ccc(-c2ccc(C(=O)NCC(=O)N3CCc4ccccc4C3)c(F)c2)cc1
vNsp7-ppi1-19	Z1663815549	-8.7	0.256	447.497	REAL	Cc1nc2ceccn2c1-c1nnc([C@H]2CC(=O)N(c3ccc4c(c3)Cc3ccccc3-4)C2)o1
vNsp7-ppi1-20	Z1891946720	-8.7	0.256	447.493	REAL	O=C(c1cccc(N2C(=O)N[C@@H](c3cccc4ccccc34)C2=O)c1)N1CCc2ccccc21
vNsp7-ppi1-21	Z2141647691	-8.7	0.281	407.472	REAL	O=C(c1cccc2c(=O)c3ccccc3[nH]c12)N1CCCn2c(cc3ccccc32)C1
vNsp7-ppi1-22	Z2212498002	-8.7	0.29	400.437	REAL	O=C1CNC(=O)c2ccc(C(=O)N3CC=C(c4c[nH]c5ccccc45)CC3)cc2N1
vNsp7-ppi1-23	ZINC000000659879	-8.7	0.229	496.565	ZINC	O=C(c1ccccc1)c1ccc2c(c1)NC1=C(C(=O)C[C@H](c3ccccc3)C1)[C@@H]1c3ccccc3C(=O)N21
vNsp7-ppi1-24	ZINC000003954537	-8.7	0.235	481.466	ZINC	O=C(Nc1ccc2c1C(=O)c1ccccc1C2=O)c1ccc2c3c1ncnc3-c1ccccc1C2=O
vNsp7-ppi1-25	ZINC000006664340	-8.7	0.281	410.515	ZINC	Cc1ccc2nc(-c3cc4cc(C56CC7CC(CC(C7)C5)C6)ccc4oc3=O)[nH]c2c1
vNsp7-ppi1-26	ZINC000245310675	-8.7	0.235	484.554	ZINC	CC(=O)[C@@H]1[C@H](C(=O)c2ccccc2)[C@@]2(C(=O)Nc3ccccc32)[C@H]2C=Cc3c4ccccc4ccc3N21
vNsp7-ppi1-27	Z1024049768	-8.6	0.246	492.598	REAL	O=C1Nc2ccccc2[C@H]1C1CCN(C(=O)C2CCN(C3=NS(=O)(=O)c4ccccc43)CC2)CC1
vNsp7-ppi1-28	Z1139907512	-8.6	0.287	406.431	REAL	O=C(NCC(=O)N1CCc2ccccc2C1)c1ccc(-c2ccc(F)cc2)cc1F
vNsp7-ppi1-29	Z1147872580	-8.6	0.277	416.495	REAL	Cc1ccc(-c2ccc(C(=O)NCC(=O)N3CCc4ccccc4C3)c(F)c2)cc1C
vNsp7-ppi1-30	Z1723444755	-8.6	0.261	438.529	REAL	Cc1cc(C)cc(C2=CCN(C(=O)c3cccc(-c4cnc5[nH]c(=O)n(C)c5c4)c3)CC2)c1
vNsp7-ppi1-31	Z2087363247	-8.6	0.287	398.421	REAL	Cc1cccc([C@H]2NC(=O)N(c3cc(-c4ccc5nccc5c4)on3)C2=O)c1C
vNsp7-ppi1-32	Z2162739490	-8.6	0.287	394.473	REAL	Cc1cc(=O)[nH]c2cc(C(=O)N3CC=C(c4ccccc5ccccc45)CC3)ccc12
vNsp7-ppi1-33	Z2178344697	-8.6	0.277	409.488	REAL	O=C(c1ccccc2c(=O)c3ccccc3[nH]c12)N1CCCN2c3ccccc3C[C@H]2C1
vNsp7-ppi1-34	Z745825910	-8.6	0.246	493.522	REAL	O=C1COc2ccc(NC(=O)N3CCN(c4nn5cc(-c6ccc(F)cc6)nc5s4)CC3)cc2N1
vNsp7-ppi1-35	Z806445912	-8.6	0.239	485.626	REAL	CC1CCN(C(=O)C2CCN(C(=O)[C@@H]3CC(=O)N(c4ccc5c(c4)Cc4ccccc4-5)C3)CC2)CC1
vNsp7-ppi1-36	Z826657018	-8.6	0.269	421.455	REAL	O=C(CN1C(=O)Cn2c(cc3ccccc32)C1=O)Nc1ccc2c(c1)Cc1ccccc1-2
vNsp7-ppi1-37	Z996454780	-8.6	0.261	451.451	REAL	O=C(c1cn(-c2ccc(C(F)(F)F)cn2)nn1)N1CCC(c2cccc3ccccc23)CC1
vNsp7-ppi1-38	ZINC000002078775	-8.6	0.253	444.489	ZINC	Cc1ccc(C)c(C(=O)COC(=O)c2ccc3nc4c(nc3c2)-c2cccc3cccc-4c23)c1
vNsp7-ppi1-39	ZINC000002439597	-8.6	0.277	406.448	ZINC	Cc1ccc(-n2ncc3c4nnc(-c5cc6ccccc6cc5O)n4cnc32)cc1C
vNsp7-ppi1-40	ZINC000004015296	-8.6	0.226	493.477	ZINC	O=c1nc2c3cccc4cccc(c(=O)n2c2cc(N5C(=O)c6cccc7cccc(c76)C5=O)ccc12)c43
vNsp7-ppi1-41	ZINC000008424887	-8.6	0.269	433.384	ZINC	O=C1OC(c2ccc3ccccc3c2)=N/C1=C\c1ccc(-c2cccc(C(F)(F)F)c2)o1
vNsp7-ppi1-42	ZINC000016038076	-8.6	0.226	519.987	ZINC	O=C(Nc1ccc(Cl)cc1)[C@@H]1[C@@H]2C(=O)N(c3ccc4ccccc4c3)C(=O)[C@@H]2[C@H]2c3ccccc3C=CN12
vNsp7-ppi1-43	ZINC000017988176	-8.6	0.215	521.571	ZINC	O=C(Oc1ccc2ccccc2c1)c1cccc(N2C(=O)[C@H]3[C@@H](C2=O)C2c4ccccc4C3c3ccccc32)c1
vNsp7-ppi1-44	ZINC000049114528	-8.6	0.297	389.454	ZINC	Cc1cc2c(cc1C)C(=O)CC1(CCN(C(=O)c3cccc4cn[nH]c43)CC1)O2
vNsp7-ppi1-45	ZINC000065026956	-8.6	0.253	453.584	ZINC	CC(=O)N1CCc2cc(-c3ccc(C(=O)N4CCN(c5cc(C)ccc5C)CC4)cc3)cccc21
vNsp7-ppi1-46	ZINC000408731313	-8.6	0.226	499.565	ZINC	Cc1ccc(C)c(N2C(=O)[C@@H]3[C@H](C2=O)[C@@H]2C(=O)Oc4c5ccccc5ccc4C2=C[C@H]3c2ccccc2)c1
vNsp7-ppi1-47	ZINC000409044391	-8.6	0.232	481.593	ZINC	Cc1ccc(C(=C2[C@H]3C=C[C@H]2[C@@H]2C(=O)N(c4cccc5ccccc54)C(=O)[C@H]32)c2ccc(C)cc2)cc1
vNsp7-ppi1-48	ZINC000409044397	-8.6	0.232	481.593	ZINC	Cc1ccc(C(=C2[C@H]3C=C[C@H]2[C@H]2C(=O)N(c4cccc5ccccc54)C(=O)[C@@H]23)c2ccc(C)cc2)cc1
vNsp7-ppi1-49	Z1408725850	-8.5	0.266	425.491	REAL	Cc1c(C(=O)N[C@@H]2CC3(CCC3)Oc3ccccc32)nnn1-c1ccc2ncccc2c1
vNsp7-ppi1-50	Z1452705446	-8.5	0.293	403.549	REAL	O=C(NC[C@@H]1[C@H]2Cc3ccccc3[C@H]12)N1CCC(c2nc3ccccc3s2)CC1
vNsp7-ppi1-51	Z1751240507	-8.5	0.274	419.43	REAL	O=C(Nc1ccc(-c2ccc(F)c2c)F)c1)N1CC[C@]2(C1)C(=O)Nc1ccccc12
vNsp7-ppi1-52	Z1763694538	-8.5	0.283	397.481	REAL	Cc1ccc(-c2cc(C(=O)N3CC=C(c4c[nH]c5ncccc45)CC3)[nH]n2)cc1C
vNsp7-ppi1-53	Z1889500448	-8.5	0.274	409.444	REAL	O=C(c1cccc2c(=O)c3ccccc3[nH]c12)N1CC[C@@]2(C1)C(=O)Nc1ccccc12
vNsp7-ppi1-54	Z1892022362	-8.5	0.25	449.509	REAL	O=C(NCc1ccccc1)c1cccc(N2C(=O)N[C@@H](Cc3cccc4ccccc34)C2=O)c1
vNsp7-ppi1-55	Z1892039329	-8.5	0.266	420.427	REAL	O=C1N[C@H](c2ccc3ccccc3c2)C(=O)N1c1ccc2nc(-c3cccn3)oc2c1
vNsp7-ppi1-56	Z1894486130	-8.5	0.266	446.937	REAL	O=C(c1ccc2c(=O)n3c(nc2c1)CCCCC3)N1CCN2c(cc3ccc(Cl)cc32)C1
vNsp7-ppi1-57	Z2143205901	-8.5	0.274	413.436	REAL	Cc1nnc2[nH]nc(NC(=O)c3ccc4c(c3)C[C@@H](c3ccccc3)OC4=O)c2c1C
vNsp7-ppi1-58	Z2157007880	-8.5	0.258	436.47	REAL	Cc1ccc(CNC(=O)c2cccc(-c3noc(-c4c[nH]c(=O)c5ccccc45)n3)c2)cc1
vNsp7-ppi1-59	Z2213277017	-8.5	0.274	418.427	REAL	O=C1CNC(=O)c2ccc(C(=O)N3CC=C(c4c[nH]c5cc(F)ccc45)CC3)cc2N1
vNsp7-ppi1-60	Z2963801868	-8.5	0.304	380.486	REAL	COc1ccc(C[C@]2(C(=O)N(C)Cc3ccccc3)C(=O)[nH]3)C[C@@H]3CC[C@@H]2C3)c1
vNsp7-ppi1-61	Z804235270	-8.5	0.236	481.511	REAL	Cn1c(=O)c2cc(NC(=O)[C@@H]3CC(=O)N(c4ccc5c(c4)Cc4ccccc4-5)C3)cnc2n(C)c1=O
vNsp7-ppi1-62	Z806435092	-8.5	0.25	471.536	REAL	O=C1c2ccccc2S(=O)(=O)c2cc(C(=O)N3CCC(c4c[nH]c5ncccc45)CC3)ccc21
vNsp7-ppi1-63	Z931884850	-8.5	0.243	465.551	REAL	C[C@@]12CCCC(=O)N1c1ccccc1C(=O)N2CC(=O)N1CC=C(c2cccc3ccccc23)CC1
vNsp7-ppi1-64	Z996181132	-8.5	0.266	450.921	REAL	O=C(Nc1ccc2oc(=O)ccc2c1)[C@@H]1C[C@@H]2CCCC[C@H]2N1C(=O)c1ccc(Cl)cc1
vNsp7-ppi1-65	Z998554428	-8.5	0.258	442.493	REAL	O=C(Nc1ccc(-c2ccccc2)cc1F)[C@H]1CCCN(C(=O)c2ccc3[nH]ncc3c2)C1
vNsp7-ppi1-66	ZINC000000659876	-8.5	0.224	496.565	ZINC	O=C(c1ccccc1)c1ccc2c(c1)NC1=C(C(=O)C[C@@H](c3ccccc3)C1)[C@@H]1c3ccccc3C(=O)N21
vNsp7-ppi1-67	ZINC000001641985	-8.5	0.236	495.929	ZINC	O=C1C(/C=C/c2ccc(Cl)cc2)=NN[C@@H]2N1N=C1N=C(O)C3(NN12)c1ccccc1-c1ccccc13
vNsp7-ppi1-68	ZINC000006142778	-8.5	0.25	471.532	ZINC	C[C@@H]1CCc2oc3ccc(NS(=O)(=O)c4ccc5c(c4)C(=O)c4ccccc4C5=O)cc3c2C1
vNsp7-ppi1-69	ZINC000006664337	-8.5	0.283	396.489	ZINC	O=c1oc2ccc(C34CC5CC(CC(C5)C3)C4)cc2cc1-c1nc2ccccc2[nH]1
vNsp7-ppi1-70	ZINC000071782681	-8.5	0.266	406.527	ZINC	c1ccc2c(c1)C1C=C(C3=CC4c5ccccc5C3c3ccccc34)C2c2ccccc21
vNsp7-ppi1-71	ZINC000239438991	-8.5	0.25	452.552	ZINC	O=C(NCc1ccc2c(c1)OCO2)c1ccc2c(c1)[C@H]1[C@@H]([C@H]3CC[C@H]1C3)[C@H](c1ccccc1)N2
vNsp7-ppi1-72	ZINC000408730040	-8.5	0.23	485.538	ZINC	Cc1ccc(N2C(=O)[C@H]3[C@H](C2=O)[C@@H]2C(=O)Oc4c5ccccc5ccc4C2=C[C@H]3c2ccccc2)cc1
vNsp7-ppi1-73	ZINC000408974528	-8.5	0.236	471.523	ZINC	O=C(c1ccc2nc3c4ncccc4c4ccnc4c3nc2c1)N1CCN(c2ccccn2)CC1
vNsp7-ppi1-74	PV-001795146017	-8.4	0.271	420.458	REAL	Cc1ccc(C(=O)N2CCN(C(=O)/C=C/c3ccc(F)c4ccccc34)CC2)cc1F
vNsp7-ppi1-75	PV-001900759447	-8.4	0.29	424.784	REAL	O=C(Nc1nn(-c2ccc(F)cc2)c2c1CCC2)c1cc(C(F)(F)F)cc(Cl)n1
vNsp7-ppi1-76	Z1024049228	-8.4	0.24	486.547	REAL	O=C1c2ccccc2S(=O)(=O)c2cc(C(=O)N3CCC([C@@H]4C(=O)Nc5ccccc54)CC3)ccc21
vNsp7-ppi1-77	Z1048772960	-8.4	0.247	449.556	REAL	Cc1nc2n(n1)C[C@@H](NC(=O)c1c3c(nc4ccccc14)/C(=C\c1ccccc1)CCC3)CC2
vNsp7-ppi1-78	Z1129472770	-8.4	0.28	397.473	REAL	C[C@@H]1Cc2ccccc2N(C(=O)c2ccc3c(c2)C[C@@H](c2ccccc2)OC3=O)C1
vNsp7-ppi1-79	Z1157905514	-8.4	0.247	450.58	REAL	O=C(NC[C@@H]1CC2c3ccccc3C1c1ccccc12)[C@@H]1CCCN(C(=O)c2ccccc2)C1
vNsp7-ppi1-80	Z1233596958	-8.4	0.271	439.51	REAL	NS(=O)(=O)c1cc(C(=O)N2CC=C(c3c[nH]c4cc(F)ccc34)CC2)cc2c1CCC2
vNsp7-ppi1-81	Z14136476	-8.4	0.255	438.482	REAL	C[C@@]1(c2ccc3ccccc3c2)NC(=O)N(Cc2cc(=O)oc3cc4c(cc23)CCC4)C1=O
vNsp7-ppi1-82	Z1541651173	-8.4	0.271	409.448	REAL	O=C(Nc1nc2ccccn2n1)[C@H]1CC(=O)N(c2ccc3c(c2)Cc2ccccc2-3)C1
vNsp7-ppi1-83	Z1613880891	-8.4	0.262	424.499	REAL	Cc1ccc(C2=CCN(C(=O)c3ccc4c(c3)C[C@H](c3ccccc3)OC4=O)CC2)cn1
vNsp7-ppi1-84	Z1685438116	-8.4	0.255	437.454	REAL	O=C1CCc2cc(-c3noc(-c4ccc5c(c4)C[C@@H](c4ccccc4)OC5=O)n3)ccc2N1
vNsp7-ppi1-85	Z1750693056	-8.4	0.28	401.44	REAL	O=C(Nc1ccc(-c2ccccc2)cc1F)N1CC[C@]2(C1)C(=O)Nc1ccccc12
vNsp7-ppi1-86	Z1763678964	-8.4	0.262	422.487	REAL	O=C(c1ccc2[nH]c3ccccc3c(=O)c2c1)N1CCC[C@@H](c2nc3ccccc3[nH]2)C1
vNsp7-ppi1-87	Z1763694714	-8.4	0.262	420.471	REAL	O=C(c1ccc2[nH]c3ccccc3c(=O)c2c1)N1CC=C(c2c[nH]c3ncccc23)CC1
vNsp7-ppi1-88	Z1764154851	-8.4	0.262	423.471	REAL	O=C(c1ccc2[nH]c3ccccc3c(=O)c2c1)N1CCC[C@@H](c2nc3ccccc3o2)C1
vNsp7-ppi1-89	Z1764585143	-8.4	0.28	399.497	REAL	Cc1ccc(-c2cc(C(=O)N3CCC(c4c[nH]c5ncccc45)CC3)[nH]n2)cc1C
vNsp7-ppi1-90	Z1764585304	-8.4	0.262	422.487	REAL	O=C(c1ccc2[nH]c3ccccc3c(=O)c2c1)N1CCC(c2c[nH]c3ncccc23)CC1
vNsp7-ppi1-91	Z1870462902	-8.4	0.255	441.465	REAL	O=C1N[C@H](c2ccc3ccccc3c2)C(=O)N1[C@@H]1CCc2nnc(-c3ccc(F)cc3)n2C1
vNsp7-ppi1-92	Z1888539547	-8.4	0.262	420.471	REAL	O=C(c1ccccc2c(=O)c3ccccc3[nH]c12)N1CC=C(c2c[nH]c3ncccc23)CC1
vNsp7-ppi1-93	Z1889191826	-8.4	0.271	410.472	REAL	O=C(c1ccccc2c(=O)c3ccccc3[nH]c12)N1CCC2(CC1)OCc1ccccc12
vNsp7-ppi1-94	Z193319398	-8.4	0.271	409.488	REAL	O=C(Nc1ccc2c3c(cccc13)CC2)c1ccc2c(=O)n3c(nc2c1)CCCCC3
vNsp7-ppi1-95	Z1972351420	-8.4	0.255	444.442	REAL	C[C@H]1CN(C(=O)c2cc3ccccc3c(=O)o2)CCN1C(=O)c1cc2ccccc2c(=O)o1
vNsp7-ppi1-96	Z2087363339	-8.4	0.262	420.427	REAL	O=C1N[C@H](c2cccc3ccccc23)C(=O)N1c1ccc(-c2ccc3nccnc3c2)on1
vNsp7-ppi1-97	Z2090583813	-8.4	0.255	437.541	REAL	Cc1nc2cc(C(=O)N3C[C@@H](c4ccccc4)[C@@H]4COCC[C@@H]43)ccc2n1-c1ccccc1
vNsp7-ppi1-98	Z228707972	-8.4	0.255	439.557	REAL	CC(=O)N1CCN(C(=O)c2c3c(nc4ccccc24)/C(=C/c2ccccc2)C[C@H](C)C3)CC1
vNsp7-ppi1-99	Z318479386	-8.4	0.227	490.557	REAL	O=C1O[C@@H](c2ccccc2)Cc2cc(C(=O)N3CCN(C(=O)c4ccc5ccccc45)CC3)ccc21
vNsp7-ppi1-100	Z344018212	-8.4	0.24	468.551	REAL	CCc1ccc(C(=O)N2CCN(C(=O)c3ccc4c(c3)C[C@H](c3ccccc3)OC4=O)CC2)cc1

Supplementary Table 35. Top 100 virtual hits of the screen against the surface of nsp7 (Screen ID: 20). Compounds were filtered so that hits had MW < 600 dalton, cLogP < 6, number of hydrogen bond acceptors < 11, and no reactive functional groups. A few compounds unsuitable for drug discovery were removed by visual inspection. The name of each compound consists of the initial letter 'v' for virtual hit, followed by the target protein name and the target site ('ppi' for protein-protein interface, 1 for docking scenario 1). The score is the docking score given by QuickVina 2 in kcal/mol. The ligand efficiency (LE) is computed as LE = -score/#NonH, where #NonH is the number of heavy (i.e. non hydrogen) atoms.

Name	Catalog ID	Score	LE	MW	Library	SMILES
vNsp7-ppi1-101	Z426085800	-8.4	0.280	400.46	REAL	Cc1ccc(-c2cc(C(=O)N3CC=C(c4c[nH]c5cc(F)ccc45)CC3)[nH]n2)cc1
vNsp7-ppi1-102	Z426093840	-8.4	0.247	456.52	REAL	O=C(c1ccc2c(=O)n3c(nc2c1)CCCCC3)N1CC=C(c2c[nH]c3cc(F)ccc23)CC1
vNsp7-ppi1-103	Z453950058	-8.4	0.255	450.46	REAL	O=C(c1cccc(C(F)(F)F)c1)N1CCN(C(=O)c2ccc3c(c2)Cc2ccccc2-3)CC1
vNsp7-ppi1-104	Z737751942	-8.4	0.240	492.53	REAL	Cc1ccc(C(=O)N2CCN(C(=O)c3ccc4c(c3)S(=O)(=O)c3ccccc3C4=O)CC2)cc1F
vNsp7-ppi1-105	Z739010590	-8.4	0.233	480.61	REAL	C[C@H]1C/C(=C/c2ccccc2)c2nc3ccccc3c(C(=O)N3CCC(N4CCNC4=O)CC3)c2C1
vNsp7-ppi1-106	Z750259636	-8.4	0.247	455.56	REAL	C[C@H]1CCc2[nH]c3ccc(C(=O)N4CCC(CN5C(=O)c6ccccc6C5=O)CC4)cc3c2C1
vNsp7-ppi1-107	Z803815148	-8.4	0.247	451.53	REAL	CC(=O)N1CCc2cc(NC(=O)[C@@H]3CC(=O)N(c4ccc5c(c4)Cc4ccccc4-5)C3)ccc21
vNsp7-ppi1-108	Z803944988	-8.4	0.247	453.43	REAL	O=C(NNC(=O)c1n[nH]c(=O)c2ccccc12)c1cc(-c2ccccc2)nc2cc(F)ccc12
vNsp7-ppi1-109	Z804800684	-8.4	0.247	455.49	REAL	O=C1CCc2cc(F)c(NC(=O)[C@@H]3CC(=O)N(c4ccc5c(c4)Cc4ccccc4-5)C3)cc2N1
vNsp7-ppi1-110	Z909185838	-8.4	0.247	479.64	REAL	C[C@@H]1C[C@H](C)CN(S(=O)(=O)c2ccc(C(=O)N3CCC(c4cc5ccccc5[nH]4)CC3)cc2)C1
vNsp7-ppi1-111	Z920795958	-8.4	0.262	446.57	REAL	CS(=O)(=O)N1CCCc2cc(C(=O)N3CC=C(c4ccccc5ccccc45)CC3)ccc21
vNsp7-ppi1-112	Z961874410	-8.4	0.271	416.52	REAL	Cc1cc(C)cc(C(=O)N2CCC[C@H](C(=O)Nc3cc(-c4ccccc4C)n[nH]3)C2)c1
vNsp7-ppi1-113	Z980023660	-8.4	0.233	492.52	REAL	O=C(Nc1ccc2nc3n(c(=O)c2c1)CCC3)[C@@H]1C[C@@H]2CCCC[C@H]2N1C(=O)c1ccc(F)cc1F
vNsp7-ppi1-114	Z999683352	-8.4	0.240	464.57	REAL	O=C(c1ccc2[nH]ncc2c1)N1CCC[C@H](C(=O)N2CC=C(c3cccc4ccccc34)CC2)C1
vNsp7-ppi1-115	ZINC000001714466	-8.4	0.205	560.59	ZINC	O=C1C=C(Nc2ccc(S(=O)(=O)c3ccc(NC4=CC(=O)C(=O)c5ccccc54)cc3)cc2)c2ccccc2C1=O
vNsp7-ppi1-116	ZINC000002267002	-8.4	0.271	406.40	ZINC	O=c1oc2ccc3ccccc3c2cc1-c1nnc(-c2cc3ccccc3cc2O)o1
vNsp7-ppi1-117	ZINC000003649621	-8.4	0.262	426.56	ZINC	Cc1c(C)n(C)c2ccc(C(=O)Nc3ccc4nc(N5CCCCC5)cc(C)c4c3)cc12
vNsp7-ppi1-118	ZINC000004522763	-8.4	0.233	472.46	ZINC	Nc1c(C(=O)Nc2cccc3c2C(=O)c2ccccc2C3=O)ccc2c1C(=O)c1ccccc1C2=O
vNsp7-ppi1-119	ZINC000005955034	-8.4	0.233	495.93	ZINC	O=C1NC2=NN3C(=O)C(/C=C\c4ccc(Cl)cc4)=NN[C@H]3N2NC12c1ccccc1-c1ccccc12
vNsp7-ppi1-120	ZINC000008449797	-8.4	0.221	493.56	ZINC	O=C1[C@H]2[C@H](C(=O)N1c1ccc(Oc3ccc4ccccc4c3)cc1)C1c3ccccc3C2c2ccccc21
vNsp7-ppi1-121	ZINC000009419595	-8.4	0.271	415.45	ZINC	Cc1cc(C)c2oc(C(=O)Nc3nonc3-c3ccc4c(c3)CCCC4)cc(=O)c2c1
vNsp7-ppi1-122	ZINC000012330018	-8.4	0.227	497.64	ZINC	O=C(c1ccc2[nH]c3c(c2c1)CCCC3)N1CCC2(C[C@@H]2C(=O)N2CCN(c3ccccn3)CC2)CC1
vNsp7-ppi1-123	ZINC000014272522	-8.4	0.233	472.50	ZINC	Cc1ccc(-c2nc3cc(NC(=O)c4cccc(-c5cc6ccccc6oc5=O)c4)ccc3o2)cc1
vNsp7-ppi1-124	ZINC000016689618	-8.4	0.262	425.48	ZINC	O=C(C1c2ccccc2Oc2ccccc21)N1CCC2(CC1)CC(=O)c1ccccc1O2
vNsp7-ppi1-125	ZINC000017862766	-8.4	0.210	520.59	ZINC	O=C(Nc1ccc2ccccc2c1)c1cccc(N2C(=O)[C@H]3[C@@H](C2=O)C2c4ccccc4C3c3ccccc32)c1
vNsp7-ppi1-126	ZINC000017988183	-8.4	0.221	501.54	ZINC	COc1ccc(OC(=O)c2ccccc(N3C(=O)[C@H]4[C@@H](C3=O)C3c5ccccc5C4c4ccccc43)c2)cc1
vNsp7-ppi1-127	ZINC000019925957	-8.4	0.280	394.45	ZINC	Fc1cccc([C@@H]2Oc3ccccc3[C@H]3CC(c4ccc5ccccc5c4)=NN32)c1
vNsp7-ppi1-128	ZINC000021090895	-8.4	0.280	392.46	ZINC	CC(=O)N1N=C(c2ccc(-c3ccccc3)cc2)O[C@H]1c1ccc2ccccc2c1
vNsp7-ppi1-129	ZINC000035843219	-8.4	0.247	471.94	ZINC	Cc1c2c(ccc1Cl)[C@]1(C(=O)N2)[C@H]2C(=O)N(c3ccc4ccccc4c3)C(=O)[C@@H]2[C@H]2CCCN21
vNsp7-ppi1-130	ZINC000100414118	-8.4	0.240	465.50	ZINC	Cc1ccc([C@H]2OC3(C(=O)c4ccccc4C3=O)[C@@H]3C(=O)N(c4cc(C)cc(C)c4)C(=O)[C@@H]2)cc1
vNsp7-ppi1-131	ZINC000100414422	-8.4	0.221	499.52	ZINC	O=C1c2ccccc2C(=O)C12O[C@@H](c1ccccc1)[C@@H]1C(=O)N(c3ccc(-c4ccccc4)cc3)C(=O)[C@H]12
vNsp7-ppi1-132	ZINC000100968105	-8.4	0.233	491.53	ZINC	C[C@@H]1CCc2cc(F)cc3c(O)c(CCC4=C(O)c5cc(F)cc6c5[C@H](C4=O)[C@@H](C)CC6)c(=O)n1c23
vNsp7-ppi1-133	ZINC000100982519	-8.4	0.227	499.53	ZINC	Cc1ccc(C(=C2[C@H]3C=C[C@H]2[C@H]2C(=O)N(c4cccc(C(F)(F)F)c4)C(=O)[C@@H]23)c2ccc(C)cc2)cc1
vNsp7-ppi1-134	ZINC000101076130	-8.4	0.221	499.52	ZINC	O=C1c2ccccc2C(=O)C12O[C@@H](c1ccccc1)[C@@H]1C(=O)N(c3ccc(-c4ccccc4)cc3)C(=O)[C@@H]12
vNsp7-ppi1-135	ZINC000101344120	-8.4	0.227	489.51	ZINC	O=C(c1ccc(F)cc1)[C@@H]1[C@@H]2C(=O)N(c3ccc4ccccc4c3)C(=O)[C@H]2[C@H]2c3ccccc3C=NN12
vNsp7-ppi1-136	ZINC000102334618	-8.4	0.271	412.46	ZINC	Cc1nn2c([nH]cc(-c3nc(Nc4nc(C)cc(C)n4)n[nH]3)c2=N)c1-c1ccccc1
vNsp7-ppi1-137	ZINC000146057035	-8.4	0.200	566.64	ZINC	CCc1cc(O)c(F)cc1-c1ccc2c(c1)[nH]nc2-c1nc2c([nH]1)CCN(C(=O)c1cnc(N3CCCCC3)cn1)C2
vNsp7-ppi1-138	ZINC000245226645	-8.4	0.227	499.53	ZINC	Cc1ccc(C(=C2[C@H]3C=C[C@H]2[C@@H]2C(=O)N(c4cccc(C(F)(F)F)c4)C(=O)[C@H]32)c2ccc(C)cc2)cc1
vNsp7-ppi1-139	ZINC000408733661	-8.4	0.227	485.54	ZINC	Cc1ccccc1N1C(=O)[C@@H]2[C@H](C1=O)[C@@H]1C(=O)Oc3c4ccccc4ccc3C1=C[C@H]2c1ccccc1
vNsp7-ppi1-140	ZINC000408975099	-8.4	0.240	451.49	ZINC	O=C(Nc1ccc2ccccc2c1)c1ccc2nc3c4ccccnc4c4ncccc4c3nc2c1
vNsp7-ppi1-141	ZINC000408977147	-8.4	0.233	470.54	ZINC	O=C(c1ccc2nc3c4ncccc4c4ccccnc4c3nc2c1)N1CCN(c2ccccc2)CC1
vNsp7-ppi1-142	ZINC000524730934	-8.4	0.233	496.95	ZINC	O=C(CN1C(=O)c2ccccc2N2C(=O)c3ccccc3[C@@H]21)N1CCc2[nH]c3ccc(Cl)cc3c2C1
vNsp7-ppi1-143	PV-001800958561	-8.3	0.277	406.50	REAL	Cc1cccc(N2C[C@@H](C(=O)N3CCC(=Cc4ccccc4F)CC3)CC2=O)c1C
vNsp7-ppi1-144	PV-001800958777	-8.3	0.268	420.53	REAL	Cc1cc(C)c(N2C[C@@H](C(=O)N3CCC(=Cc4ccccc4F)CC3)CC2=O)c(C)c1
vNsp7-ppi1-145	PV-001804646457	-8.3	0.277	420.41	REAL	Cc1ccc(C2=NO[C@@H](C(=O)N3CC[C@@](F)(c4ccccc(C(F)(F)F)c4)C3)C2)cc1
vNsp7-ppi1-146	PV-001829951574	-8.3	0.277	398.50	REAL	Cc1cc(C)c2c(c1)N(C(=O)CNC(=O)c1ccc(-c3ccccc3)cc1)CCC2
vNsp7-ppi1-147	PV-001844587946	-8.3	0.259	438.52	REAL	Cc1cc(C)c(N2C[C@@H](C(=O)N3CCC(=Cc4ccc(F)c(F)c4)CC3)CC2=O)c(C)c1
vNsp7-ppi1-148	PV-001856344731	-8.3	0.286	395.45	REAL	Cc1ccc(-c2cc(C(=O)N3CCC(c4cccc(F)c4F)CC3)[nH]n2)cc1C
vNsp7-ppi1-149	PV-001945951347	-8.3	0.286	407.50	REAL	Cc1cc(C)cc(-c2nnc(NC(=O)N[C@@H]3CCc4ccccc4NC3=O)s2)c1
vNsp7-ppi1-150	PV-002027835936	-8.3	0.277	438.64	REAL	CCN1C[C@@H](C)N(c2nnc([C@H](C)NS(C)(=O)=O)n2C[C@@H]2C[C@H]3CC[C@H]2C3)C[C@@H]1C
vNsp7-ppi1-151	Z1014754282	-8.3	0.268	411.46	REAL	C[C@]1(c2ccc(CNC(=O)c3ccc4c(c3)-c3ccccc3C4)cc2)NC(=O)NC1=O
vNsp7-ppi1-152	Z1066763888	-8.3	0.259	435.50	REAL	O=C1CCc2cc(F)c(NC(=O)[C@@H]3C[C@H]4CCCC[C@H]4N3C(=O)c3ccccc3)cc2N1
vNsp7-ppi1-153	Z1144203620	-8.3	0.277	422.89	REAL	O=C(NCC(=O)N1CCc2ccccc2C1)c1ccc(-c2ccc(Cl)cc2)cc1F
vNsp7-ppi1-154	Z1144328868	-8.3	0.286	387.48	REAL	C[C@@H]1c2ccccc2CCN1C(=O)c1ccc2c(=O)n3c(nc2c1)CCCCC3
vNsp7-ppi1-155	Z1172231620	-8.3	0.286	379.46	REAL	O=c1[nH]c(NC[C@H]2CC3c4ccccc4C2c2ccccc23)nc2ccccc12
vNsp7-ppi1-156	Z119762844	-8.3	0.268	406.45	REAL	Cc1ccc(-c2nnc(NC(=O)c3cc(-c4cccn4)nc4ccccc34)[nH]2)cc1
vNsp7-ppi1-157	Z1212625353	-8.3	0.252	440.51	REAL	CCc1nn(C)c2[nH]nc(NC(=O)[C@H]3CC(=O)N(c4ccc5c(c4)Cc4ccccc4-5)C3)c12
vNsp7-ppi1-158	Z1246447783	-8.3	0.259	437.42	REAL	O=C(c1cn(-c2cccc(C(F)(F)F)c2)nn1)N1CC=C(c2c[nH]c3ccccc23)CC1
vNsp7-ppi1-159	Z1260292725	-8.3	0.296	377.48	REAL	C[C@@H]1CCC[C@@H](C)N(C(=O)c2ccc3c(c2)C[C@@H](c2ccccc2)OC3=O)C1
vNsp7-ppi1-160	Z1282626410	-8.3	0.259	428.49	REAL	O=C(NNC(=O)c1ccc2ccccc2c1)N[C@H]1CC(=O)N([C@@H]2C[C@H]2c2ccccc2)C1
vNsp7-ppi1-161	Z1311458970	-8.3	0.259	426.51	REAL	CNC(=O)[C@H]1CCCN(C(=O)CCC(=O)c2ccc3ccc4ccccc5ccc2c3c45)C1
vNsp7-ppi1-162	Z1312757240	-8.3	0.277	400.48	REAL	CN1CCC(=O)Nc2cc(C(=O)N3CC=C(c4c[nH]c5ccccc45)CC3)ccc21
vNsp7-ppi1-163	Z1347775753	-8.3	0.277	400.48	REAL	C[C@@H]1C(=O)Nc2cc(C(=O)N3CC=C(c4c[nH]c5ccccc45)CC3)ccc2N1C
vNsp7-ppi1-164	Z1374564897	-8.3	0.286	389.45	REAL	O=C(c1ccc(-c2noc(=O)[nH]2)cc1)N1CCC[C@]2(CCCc3ccccc32)C1
vNsp7-ppi1-165	Z1410520849	-8.3	0.259	428.53	REAL	Cc1ccc(C23C[C@@H]4C[C@@H](CC(C(=O)NNc5nc6ccccc6c(=O)[nH]5)(C4)C2)C3)cc1
vNsp7-ppi1-166	Z1418328206	-8.3	0.277	397.47	REAL	O=C(C1c2ccccc2Oc2ccccc21)N1CCC2(CC1)OCc1ccccc12
vNsp7-ppi1-167	Z145039644	-8.3	0.259	426.45	REAL	O=C(c1cccc(N2C(=O)c3ccccc3C2=O)c1)N1CC=C(c2ccc(F)cc2)CC1
vNsp7-ppi1-168	Z1451642807	-8.3	0.277	404.51	REAL	CN1CC[C@@H]2[C@H](CCCN2C(=O)c2ccc3c(c2)C[C@@H](c2ccccc2)OC3=O)C1
vNsp7-ppi1-169	Z1473413185	-8.3	0.259	443.47	REAL	O=C(N[C@@H]1[C@H]2CCc3ccccc3[C@H]21)N1CCN(C(=O)c2cccc(C(F)(F)F)c2)CC1
vNsp7-ppi1-170	Z1473415434	-8.3	0.286	386.50	REAL	O=C(N[C@@H]1[C@H]2CCc3ccccc3[C@@H]21)N1CCC(c2c[nH]c3ncccc23)CC1
vNsp7-ppi1-171	Z1494833866	-8.3	0.286	384.43	REAL	O=C1O[C@@H](c2ccccc2)Cc2cc(C(=O)N3CCc4ncccc4C3)ccc21
vNsp7-ppi1-172	Z1498283742	-8.3	0.277	394.48	REAL	O=c1[nH]c(N2CCN(C3c4ccccc4-c4ccccc43)CC2)nc2ccccc12
vNsp7-ppi1-173	Z1531742412	-8.3	0.259	428.42	REAL	O=C(Nc1ccn(-c2ncccc2F)n1)c1ccc2c(c1)C[C@@H](c1ccccc1)OC2=O
vNsp7-ppi1-174	Z1549989310	-8.3	0.259	428.50	REAL	O=C([C@@H]1CC(=O)N(c2ccc3c(c2)Cc2ccccc2-3)C1)N1CCC[C@H](c2nnn[nH]2)C1
vNsp7-ppi1-175	Z1580556063	-8.3	0.259	423.47	REAL	Cc1cc(NC(=O)c2ccc3c(c2)C[C@@H](c2ccccc2)OC3=O)nn1-c1ccccc1
vNsp7-ppi1-176	Z1626782605	-8.3	0.286	382.46	REAL	O=C1CCCc2cc(C(=O)N3CC=C(c4cccc5ccccc45)C3)ccc2N1
vNsp7-ppi1-177	Z1626784252	-8.3	0.286	380.45	REAL	Cc1ccc(-n2cc(C(=O)N3CC=C(c4cccc5ccccc45)C3)nn2)cc1
vNsp7-ppi1-178	Z1626784363	-8.3	0.286	380.45	REAL	Cc1ccccc(-n2cc(C(=O)N3CC=C(c4cccc5ccccc45)C3)nn2)c1
vNsp7-ppi1-179	Z1661273043	-8.3	0.259	446.44	REAL	O=C1c2ccccc2S(=O)(=O)c2cc(-c3nnc([C@@H]4CCc5ccccc5O4)o3)ccc21
vNsp7-ppi1-180	Z1664497612	-8.3	0.259	422.41	REAL	Cc1c(-c2nnc(-c3nnc(-c4ccccc4)o3)o2)nnn1-c1ccc2ncccc2c1
vNsp7-ppi1-181	Z1682437294	-8.3	0.259	449.46	REAL	Cc1ccc(-c2ccc(-c3nc(CN4C(=O)c5ccccc5S4(=O)=O)no3)c(F)c2)cc1
vNsp7-ppi1-182	Z1682439470	-8.3	0.268	449.51	REAL	O=C1c2ccccc2S(=O)(=O)N1Cc1noc(-c2cc3c(s2)-c2ccccc2CC3)n1
vNsp7-ppi1-183	Z1763670220	-8.3	0.277	399.50	REAL	Cc1ccc(-c2cc(C(=O)N3CCC(c4nc5ccccc5[nH]4)CC3)[nH]n2)cc1C
vNsp7-ppi1-184	Z1763729289	-8.3	0.286	382.46	REAL	O=C(c1ccc2[nH]c3ccccc3c(=O)c2c1)N1CCC(c2ccccc2)CC1
vNsp7-ppi1-185	Z1764002120	-8.3	0.268	424.45	REAL	Cc1ccc(-c2cc(C(=O)N3CCN(C(=O)c4ccc(F)c(F)c4)CC3)[nH]n2)cc1C
vNsp7-ppi1-186	Z1764441773	-8.3	0.268	420.49	REAL	Cc1ccc(-c2cc(C(=O)N3CCN(C(=O)c4ccc(C)c(F)c4)CC3)[nH]n2)cc1C
vNsp7-ppi1-187	Z1764513585	-8.3	0.277	391.43	REAL	O=C(Nc1ccc(-c2ccccc2)cn1)c1ccc2[nH]c3ccccc3c(=O)c2c1
vNsp7-ppi1-188	Z1831291812	-8.3	0.268	410.48	REAL	Cc1cc(C)nc(-n2nccc2NC(=O)N2CC=C(c3cccc4ccccc34)C2)n1
vNsp7-ppi1-189	Z1832420013	-8.3	0.277	393.49	REAL	O=C1C[C@H](C(=O)NC[C@H]2CC3c4ccccc4C2c2ccccc23)c2ccccc21
vNsp7-ppi1-190	Z1835896344	-8.3	0.277	400.44	REAL	Nc1ncc2c(n1)CCN(C(=O)c1ccc3c(c1)C[C@H](c1ccccc1)OC3=O)C2
vNsp7-ppi1-191	Z1888706491	-8.3	0.259	422.49	REAL	O=C(c1cccc2c(=O)c3ccccc3[nH]c12)N1CCC(c2c[nH]c3ncccc23)CC1
vNsp7-ppi1-192	Z1889210072	-8.3	0.268	411.50	REAL	Cc1ccc(C)c(N2CCN(C(=O)c3cccc4c(=O)c5ccccc5[nH]c34)CC2)c1
vNsp7-ppi1-193	Z1890552818	-8.3	0.268	411.42	REAL	O=C(Cc1noc(-c2cc3ccccc3cc2O)n1)N1CCn2c1nc1ccccc12
vNsp7-ppi1-194	Z1893430104	-8.3	0.268	427.89	REAL	O=C(c1ccc2[nH]c3ccccc3c(=O)c2c1)N1CCn2c(cc3c(Cl)cccc32)C1
vNsp7-ppi1-195	Z1895496278	-8.3	0.268	436.54	REAL	C[C@H](C(=O)N1CCc2ccccc2C1)S(=O)(=O)c1nc(-c2ccc3c(c2)CCC3)n[nH]1
vNsp7-ppi1-196	Z1902963039	-8.3	0.277	406.46	REAL	O=C(Nc1nc2ccc(F)cc2[nH]1)[C@@H]1C[C@H]2CCCC[C@H]2N1C(=O)c1ccccc1
vNsp7-ppi1-197	Z191742546	-8.3	0.252	461.52	REAL	O=C(c1ccc(NC2=NS(=O)(=O)c3ccccc32)cc1)N1CC=C(c2ccc(F)cc2)CC1
vNsp7-ppi1-198	Z1917776029	-8.3	0.268	431.47	REAL	O=C1CCCc2cc(-c3nc4cc(-c5ccc6c(c5)OCCO6)sc4c(=O)[nH]3)cnc21
vNsp7-ppi1-199	Z1952653684	-8.3	0.252	444.44	REAL	O=C(Nc1ccc2[nH]nc(NC(=O)[C@H]3Cc4ccc(F)cc43)c2c1)[C@H]1Cc2ccc(F)cc21
vNsp7-ppi1-200	Z1952918351	-8.3	0.252	438.45	REAL	O=C(NCc1ccc2c(c1)CN(C(=O)c1ccc3[nH]nnc3c1)C2)c1ccc2[nH]nnc2c1

Supplementary Table 36. Virtual screening hits 101 to 200 of the screen against the surface of nsp7 (Screen ID: 20). Compounds were filtered so that hits had MW < 600 dalton, cLogP < 6, number of hydrogen bond acceptors < 11, and no reactive functional groups. A few compounds unsuitable for drug discovery were removed by visual inspection. The name of each compound consists of the initial letter 'v' for virtual hit, followed by the target protein name and the target site ('ppi' for protein-protein interface, 1 for docking scenario 1). The score is the docking score given by QuickVina 2 in kcal/mol. The ligand efficiency (LE) is computed as LE = -score/#NonH, where #NonH is the number of heavy (i.e. non hydrogen) atoms.

Name	Catalog ID	Score	LE	MW	Library	SMILES
vNsp8-nsp7.1-1	ZINC000017862766	-10.5	0.262	520.587	ZINC	O=C(Nc1ccc2ccccc2c1)c1cccc(N2C(=O)[C@H]3[C@@H](C2=O)C2c4ccccc4C3c3ccccc32)c1
vNsp8-nsp7.1-2	ZINC000226404692	-10	0.227	586.642	ZINC	O=C(Oc1ccc(N2C(=O)[C@@H]3[C@H]4C=C[C@@H](C4)[C@@H]3C2=O)cc1)c1ccnc(N2C(=O)[C@@H]3CC[C@@H](c4ccccc4)C[C@@H]3C2=O)c1
vNsp8-nsp7.1-3	ZINC000017988176	-9.9	0.248	521.571	ZINC	O=C(Oc1ccc2ccccc2c1)c1cccc(N2C(=O)[C@H]3[C@@H](C2=O)C2c4ccccc4C3c3ccccc32)c1
vNsp8-nsp7.1-4	PV-001940740368	-9.7	0.303	456.609	REAL	C[C@H](CNC(=O)Nc1ccc(S(=O)(=O)N[C@H](C)[C@@H]2C[C@H]3CC[C@H]2C3)cc1)c1ccncc1
vNsp8-nsp7.1-5	ZINC000013382161	-9.7	0.255	518.999	ZINC	O=C(Cc1ccccc1)Nc1ccc(N2C(=O)[C@H]3[C@@H](C2=O)C2c4ccccc4C3c3ccccc32)cc1Cl
vNsp8-nsp7.1-6	ZINC000100505724	-9.7	0.262	488.542	ZINC	O=C1[C@@H]2[C@H]3C=C[C@@H](C3)[C@@H]2C(=O)N1c1ccc2c(c1)-c1cc(N3C(=O)[C@@H]4[C@H]5C=C[C@@H](C5)[C@@H]4C3=O)ccc1C2
vNsp8-nsp7.1-7	ZINC000017988472	-9.6	0.24	533.666	ZINC	CC(C)(C)c1ccc(OC(=O)C2CCC(N3C(=O)[C@H]4[C@@H](C3=O)C3c5ccccc5C4c4ccccc43)CC2)cc1
vNsp8-nsp7.1-8	ZINC000408961266	-9.6	0.274	473.599	ZINC	Cc1ccc(N=C2NC(=O)/C(=C\c3cn(Cc4ccc5ccccc5c4)c4ccccc34)S2)cc1
vNsp8-nsp7.1-9	PV-001936962679	-9.5	0.352	412.573	REAL	CCCCS(=O)(=O)Nc1ccc(S(=O)(=O)NC[C@H]2C[C@H]3C=C[C@H]2CC3)cc1
vNsp8-nsp7.1-10	Z1239620028	-9.5	0.288	445.493	REAL	C[C@H]1c2ccc(F)cc2CCN1C(=O)CN1C(=O)N[C@@](C)(c2ccc3ccccc3c2)C1=O
vNsp8-nsp7.1-11	ZINC000015972085	-9.5	0.257	490.561	ZINC	Cc1ccc2c(c1C)NC(=O)[C@]21N[C@@H](Cc2c[nH]c3ccccc23)[C@H]2C(=O)N(c3ccccc3)C(=O)[C@H]21
vNsp8-nsp7.1-12	Z239283838	-9.4	0.261	483.541	REAL	C[C@@]1(c2ccc(F)cc2)NC(=O)N(CC(=O)NC[C@H]2CC3c4ccccc4C2c2ccccc23)C1=O
vNsp8-nsp7.1-13	ZINC000000659879	-9.4	0.247	496.565	ZINC	O=C(c1ccccc1)c1ccc2c(c1)NC1=C(C(=O)C[C@H](c3ccccc3)C1)[C@@H]1c3ccccc3C(=O)N21
vNsp8-nsp7.1-14	ZINC000001588361	-9.4	0.276	440.509	ZINC	Nc1nc(-c2cc(-c3ccc4ccccc43)nc(N)n2)cc(-c2cccc3ccccc32)n1
vNsp8-nsp7.1-15	ZINC000004293490	-9.4	0.261	558.818	ZINC	O=C(C1=NN(c2ccc(Cl)cc2)[C@@H]2C(=O)N(c3ccc(Br)cc3)C(=O)[C@@H]12)c1ccc2ccccc2c1
vNsp8-nsp7.1-16	ZINC000018246982	-9.4	0.241	513.548	ZINC	O=C(COC(=O)c1ccc(N2C(=O)[C@H]3[C@@H](C2=O)C2c4ccccc4C3c3ccccc32)c1)c1ccccc1
vNsp8-nsp7.1-17	ZINC000100505726	-9.4	0.254	488.542	ZINC	O=C1[C@@H]2[C@H]3C=C[C@@H](C3)[C@@H]2C(=O)N1c1ccc2c(c1)-c1cc(N3C(=O)[C@@H]4[C@@H]5C=C[C@@H](C5)[C@@H]4C3=O)ccc1C2
vNsp8-nsp7.1-18	Z1472861059	-9.3	0.282	439.514	REAL	C[C@@]1(c2ccc3ccccc3c2)NC(=O)N(CC(=O)N[C@H]2[C@H]3CCc4ccccc4[C@H]32)C1=O
vNsp8-nsp7.1-19	Z448671386	-9.3	0.266	471.643	REAL	C[C@@H]1CCCN(C(=O)C2CCN(C(=O)NC[C@@H]3CC4c5ccccc5C3c3ccccc34)CC2)C1
vNsp8-nsp7.1-20	ZINC000000990509	-9.3	0.233	547.993	ZINC	O=C(COC(=O)c1cccc(N2C(=O)[C@H]3[C@H](C2=O)C2c4ccccc4C3c3ccccc32)c1)c1ccc(Cl)cc1
vNsp8-nsp7.1-21	ZINC000000990510	-9.3	0.233	547.993	ZINC	O=C(COC(=O)c1ccc(N2C(=O)[C@H]3[C@@H](C2=O)C2c4ccccc4C3c3ccccc32)c1)c1ccc(Cl)cc1
vNsp8-nsp7.1-22	ZINC000097945320	-9.3	0.233	522.559	ZINC	O=C(Oc1cccc2ccccn21)c1cccc(N2C(=O)[C@H]3[C@H](C2=O)C2c4ccccc4C3c3ccccc32)c1
vNsp8-nsp7.1-23	ZINC000097945321	-9.3	0.233	522.559	ZINC	O=C(Oc1cccc2ccccn21)c1cccc(N2C(=O)[C@H]3[C@@H](C2=O)C2c4ccccc4C3c3ccccc32)c1
vNsp8-nsp7.1-24	ZINC000100505727	-9.3	0.251	488.542	ZINC	O=C1[C@@H]2[C@H]3C=C[C@@H](C3)[C@@H]2C(=O)N1c1ccc2c(c1)-c1cc(N3C(=O)[C@H]4[C@H]5C=C[C@H](C5)[C@@H]4C3=O)ccc1C2
vNsp8-nsp7.1-25	ZINC000100694082	-9.3	0.291	416.606	ZINC	C1=CC2C3C=CC(C4C5C6C7C=CC(C=CC76)C5C43)C2C2C1C1C2C2C3C=CC1C=CC32
vNsp8-nsp7.1-26	Z1038827768	-9.2	0.341	367.491	REAL	O=C1NCCN1c1cccc(C(=O)N2CCC[C@H]2C[C@H]2C[C@H]3CC[C@H]2C3)c1
vNsp8-nsp7.1-27	Z1090158730	-9.2	0.279	443.458	REAL	C[C@@H]1Oc2ccc(C(=O)CN3C(=O)N[C@@](C)(c4ccc5ccccc5c4)C3=O)cc2NC1=O
vNsp8-nsp7.1-28	Z1158447919	-9.2	0.263	468.551	REAL	C[C@H]1Oc2ccc(C(=O)C3CCN(C(=O)[C@@H]4C[C@H]4c4ccc5ccccc5c4)CC3)cc2NC1=O
vNsp8-nsp7.1-29	Z1204289470	-9.2	0.279	441.529	REAL	CC[C@H]1c2ccccc2CCN1C(=O)CN1C(=O)N[C@@](C)(c2ccc3ccccc3c2)C1=O
vNsp8-nsp7.1-30	Z1643374763	-9.2	0.279	443.502	REAL	C[C@H]1COc2ccccc2CN1C(=O)CN1C(=O)N[C@@](C)(c2ccc3ccccc3c2)C1=O
vNsp8-nsp7.1-31	Z1725944097	-9.2	0.279	444.581	REAL	Cc1ccc(-n2nc(C(=O)N3CCC(c4nnc5n4CCCC5)CC3)c3c2CCC3)c(C)c1
vNsp8-nsp7.1-32	Z1744199641	-9.2	0.279	438.482	REAL	O=C1O[C@@H](c2ccccc2)Cc2cc(C(=O)N3CC[C@@]4(C3)C(=O)Nc3ccccc34)ccc21
vNsp8-nsp7.1-33	Z1828838268	-9.2	0.307	432.381	REAL	O=C1Nc2ccc(S(=O)(=O)Nc3n[nH]c4ccc(C(F)(F)F)cc34)c3cccc1c23
vNsp8-nsp7.1-34	Z2187203011	-9.2	0.287	422.483	REAL	O=C1O[C@@H](c2ccccc2)Cc2cc(C(=O)N3CCn4c(cc5ccccc54)C3)ccc21
vNsp8-nsp7.1-35	Z2286275921	-9.2	0.341	380.874	REAL	CC(C)(Cc1ccc(Cl)cc1)c1noc([C@]23[C@H]4C(=O)[C@H]5[C@@H]6C[C@@H](C[C@@H](C[C@H]52)[C@H]3[C@@H]64)n1
vNsp8-nsp7.1-36	Z362739648	-9.2	0.256	475.551	REAL	O=C(c1ccccc(C(=O)N2CCc3[nH]c4ccccc4c3C2)n1)N1CCc2[nH]c3ccccc3c2C1
vNsp8-nsp7.1-37	Z973896126	-9.2	0.271	448.525	REAL	Cc1n[nH]c(NC(=O)[C@H]2CC(=O)N(c3ccc4c(c3)Cc3ccccc3-4)C2)c1-c1ccccc1
vNsp8-nsp7.1-38	Z997317242	-9.2	0.249	498.581	REAL	Cc1ccc(CC(=O)N2CCN(C(=O)CN3C(=O)N[C@@](C)(c4ccc5ccccc5c4)C3=O)CC2)cc1
vNsp8-nsp7.1-39	ZINC000008887245	-9.2	0.279	434.494	ZINC	C[C@@]1(c2ccc3ccccc3c2)NC(=O)N(CC(=O)c2ccc(-c3ccccc3)cc2)C1=O
vNsp8-nsp7.1-40	ZINC000015971911	-9.2	0.249	490.561	ZINC	Cc1ccc(N2C(=O)[C@@H]3[C@H](C2=O)[C@H](Cc2c[nH]c4ccccc24)N[C@]32C(=O)Nc3c2cccc3C)cc1
vNsp8-nsp7.1-41	ZINC000015972405	-9.2	0.249	494.525	ZINC	Cc1cccc2c1NC(=O)[C@]21N[C@@H](Cc2c[nH]c3ccccc23)[C@H]2C(=O)N(c3ccc(F)cc3)C(=O)[C@H]21
vNsp8-nsp7.1-42	ZINC000018120083	-9.2	0.297	401.464	ZINC	O=C1[C@H]2[C@@H](C(=O)N1c1ccc3ccccc3c1)C1c3ccccc3C2c2ccccc21
vNsp8-nsp7.1-43	ZINC000095918522	-9.2	0.256	464.563	ZINC	O=C1[C@@H]2C(c3ccccc3)=C(c3ccccc3)[C@H]2C(=O)[C@H]2C3c4ccccc4C(c4ccccc43)[C@@H]12
vNsp8-nsp7.1-44	ZINC000100237612	-9.2	0.249	490.557	ZINC	O=C1[C@@H]2[C@H]3C=C[C@@H](C3)[C@@H]2C(=O)N1c1ccc(Cc2ccc(N3C(=O)[C@@H]4[C@H]5C=C[C@@H](C5)[C@@H]4C3=O)cc2)cc1
vNsp8-nsp7.1-45	ZINC000102921683	-9.2	0.256	473.535	ZINC	Cc1cn2nc(N/C=C3\c4ccccc4C(=O)N(c4ccc(C)cc4C)C3=O)c3ccccc3c2n1
vNsp8-nsp7.1-46	ZINC000222376525	-9.2	0.256	481.613	ZINC	O=C(c1ccc2c(c1)[C@@H]1[C@H]3CC[C@@H](C3)[C@@H]1[C@@H](c1ccccc1)N2)N1CCN(c2ccccc2F)CC1
vNsp8-nsp7.1-47	ZINC000245377192	-9.2	0.249	488.542	ZINC	O=C1[C@@H]2[C@H]3C=C[C@@H](C3)[C@H]2C(=O)N1c1ccc2c(c1)-c1cc(N3C(=O)[C@@H]4[C@H]5C=C[C@@H](C5)[C@@H]4C3=O)ccc1C2
vNsp8-nsp7.1-48	ZINC000408688101	-9.2	0.242	498.58	ZINC	Cc1ccc(NC(=O)c2cccc(N3C(=O)[C@H]4[C@@H](C3=O)C3c5ccccc5C4c4ccccc43)c2)cc1C
vNsp8-nsp7.1-49	ZINC000408730073	-9.2	0.249	485.538	ZINC	Cc1ccc(N2C(=O)[C@H]3[C@H](C2=O)[C@@H]2C(=O)Oc4ccc5ccccc5c4C2=C[C@@H]3c2ccccc2)cc1
vNsp8-nsp7.1-50	ZINC000409336222	-9.2	0.242	499.565	ZINC	Cc1ccc(N2C(=O)[C@H]3[C@H](C2=O)[C@@H]2C(=O)Oc4ccc5ccccc5c4C2=C[C@@H]3c2ccccc2)cc1C
vNsp8-nsp7.1-51	PV-001802120353	-9.1	0.294	425.409	REAL	C[C@@H]1CN(C(=O)c2cc(-c3cccc(C(F)(F)F)c3)ccn2)c2ccccc2C(=O)N1
vNsp8-nsp7.1-52	Z1239620241	-9.1	0.294	434.432	REAL	C[C@@H]1c2ccc(F)cc2CCN1C(=O)[C@@H]1CC(=O)N(Cc2ccc(C(F)(F)F)c2)C1
vNsp8-nsp7.1-53	Z1280012976	-9.1	0.294	409.531	REAL	O=C(N[C@@H]1CCc2nc(-c3ccccc3)ncc2C1)[C@H]1C[C@@]12CCCc1ccccc12
vNsp8-nsp7.1-54	Z1391353159	-9.1	0.276	445.493	REAL	C[C@@]1(c2ccc3ccccc3c2)NC(=O)N(CC(=O)N2CC[C@@H](c3ccc(F)cc3)C2)C1=O
vNsp8-nsp7.1-55	Z1417271037	-9.1	0.284	427.546	REAL	Cc1ccc(-n2nc(C(=O)N3CCC4(CC3)OCc3ccccc34)c3c2CCC3)c(C)c1
vNsp8-nsp7.1-56	Z1585182982	-9.1	0.276	439.561	REAL	O=C(Nc1cccc(C#Cc2ccccc2)c1)N1CCC[C@H](c2nnc3n2CCCCC3)C1
vNsp8-nsp7.1-57	Z167447042	-9.1	0.268	453.54	REAL	Cc1ccc(C2=CCN(C(=O)CN3C(=O)N[C@@](C)(c4ccc5ccccc5c4)C3=O)CC2)cc1
vNsp8-nsp7.1-58	Z1869157732	-9.1	0.294	413.476	REAL	O=C(c1ccccc1)N1CCC[C@H](N2C(=O)N[C@@H](c3ccc4ccccc4c3)C2=O)C1
vNsp8-nsp7.1-59	Z1870102572	-9.1	0.284	425.487	REAL	O=C1C[C@@H](N2C(=O)N[C@@H](c3ccc4ccccc4c3)C2=O)CN1[C@@H]1C[C@@H]1c1ccccc1
vNsp8-nsp7.1-60	Z1891946784	-9.1	0.268	447.493	REAL	O=C(c1ccccc(N2C(=O)N[C@@H](c3ccc4ccccc4c3)C2=O)c1)N1CCc2ccccc21
vNsp8-nsp7.1-61	Z1952432369	-9.1	0.294	416.519	REAL	O=C(N[C@@H]1CCCN(C(=O)[C@@H]2[C@H]3[C@@H]4C[C@@H]5[C@@H]6[C@H]4C[C@H]3[C@@H]6[C@@H]52)C1)c1cc2ccccc2o1
vNsp8-nsp7.1-62	Z1952716655	-9.1	0.303	400.524	REAL	O=C([C@@H]1[C@H]2[C@H]3C[C@@H]4[C@@H]5[C@H]3C[C@H]2[C@@H]5[C@@H]4)N1CCC[C@@H](c2n[nH]c(-c3ccccc3)n2)C1
vNsp8-nsp7.1-63	Z2201098239	-9.1	0.325	385.506	REAL	C[C@H]1[C@H](NC(=O)NCC[C@@]2(O)C[C@H]3CC[C@H]2C3)CC(=O)N1Cc1ccccc1
vNsp8-nsp7.1-64	Z225649522	-9.1	0.268	449.509	REAL	Cc1ccc(C)c(N2C(=O)c3ccc(C(=O)N4CCc5[nH]c6ccccc6c5C4)cc3C2=O)c1
vNsp8-nsp7.1-65	Z271073804	-9.1	0.253	474.519	REAL	C[C@@]1(c2ccc3ccccc3c2)NC(=O)N(CC(=O)Nc2cccc(C#Cc3ccccn3)c2)C1=O
vNsp8-nsp7.1-66	Z650281252	-9.1	0.26	486.958	REAL	C[C@@]1(c2ccc3ccccc3c2)NC(=O)N(CC(=O)N2CCc3[nH]c4ccc(Cl)cc4c3C2)C1=O
vNsp8-nsp7.1-67	Z970816588	-9.1	0.253	479.578	REAL	Cc1c(NC(=O)[C@H]2CC(=O)N(c3ccc4c(c3)Cc3ccccc3-4)C2)ccc1C(=O)N1CCCC1
vNsp8-nsp7.1-68	ZINC000000629966	-9.1	0.284	415.491	ZINC	C[C@@]12C(=O)N(c3ccc4ccccc4c3)C(=O)[C@@H]1C1c3ccccc3C2c2ccccc21
vNsp8-nsp7.1-69	ZINC000001266504	-9.1	0.26	456.456	ZINC	O=C1c2cc3oc4ccccc4c4ccccc4oc3cc2C(=O)N1c1cccc2ccenc21
vNsp8-nsp7.1-70	ZINC000001588362	-9.1	0.268	440.509	ZINC	Nc1nc(-c2ccc3ccccc3c2)cc(-c2cc(-c3ccc4ccccc4c3)nc(N)n2)n1
vNsp8-nsp7.1-71	ZINC000004235914	-9.1	0.26	479.457	ZINC	O=C(c1ccccc1)N1CCN2C(=O)c3cc(-c4cccc(C(F)(F)F)c4)ccc3NC(=O)[C@H]2C1
vNsp8-nsp7.1-72	ZINC000004235924	-9.1	0.253	497.447	ZINC	O=C(c1cccc(F)c1)N1CCN2C(=O)c3cc(-c4cccc(C(F)(F)F)c4)ccc3NC(=O)[C@H]2C1
vNsp8-nsp7.1-73	ZINC000007777873	-9.1	0.284	414.507	ZINC	Cc1ccc(-c2nn(-c3ccccc3)cc2[C@H]2CC(=O)c3ccc4cccc2c43)cc1
vNsp8-nsp7.1-74	ZINC000008449797	-9.1	0.239	493.561	ZINC	O=C1[C@H]2[C@H](C(=O)N1c1ccc(Oc3ccc4ccccc4c3)cc1)C1c3ccccc3C2c2ccccc21
vNsp8-nsp7.1-75	ZINC000013154493	-9.1	0.284	434.518	ZINC	O=C1[C@H]2[C@@H](C(=O)N1c1nc(-c3ccccc3)cs1)C1c3ccccc3C2c2ccccc21
vNsp8-nsp7.1-76	ZINC000013857706	-9.1	0.228	533.666	ZINC	CC(C)[C@H]1CC[C@@H](C)C[C@@H]1OC(=O)c1ccc(N2C(=O)[C@H]3[C@@H](C2=O)C2c4ccccc4C3c3ccccc32)c1
vNsp8-nsp7.1-77	ZINC000015971657	-9.1	0.253	476.535	ZINC	Cc1ccc(N2C(=O)[C@@H]3[C@H](C2=O)[C@H](Cc2c[nH]c4ccccc24)N[C@]32C(=O)Nc3ccccc32)cc1
vNsp8-nsp7.1-78	ZINC000016362633	-9.1	0.268	448.477	ZINC	Cc1ccccc1C1=N/C(=C/c2ccc(/C=C3\N=C(c4ccccc4C)OC3=O)cc2)C(=O)O1
vNsp8-nsp7.1-79	ZINC000017988475	-9.1	0.228	533.666	ZINC	Cc1ccc(C(C)C)c(OC(=O)C2CCC(N3C(=O)[C@H]4[C@@H](C3=O)C3c5ccccc5C4c4ccccc43)CC2)c1
vNsp8-nsp7.1-80	ZINC000018067970	-9.1	0.239	518.999	ZINC	Cc1ccc(NC(=O)c2cccc(N3C(=O)[C@H]4[C@@H](C3=O)C3c5ccccc5C4c4ccccc43)c2)cc1Cl
vNsp8-nsp7.1-81	ZINC000018247105	-9.1	0.239	501.537	ZINC	COc1ccccc(C(=O)Oc2cccc(N3C(=O)[C@H]4[C@@H](C3=O)C3c5ccccc5C4c4ccccc43)c2)c1
vNsp8-nsp7.1-82	ZINC000033509726	-9.1	0.268	441.493	ZINC	C[C@H]1Cc2ccccc2N1C(=O)c1ccc2nc3c4cccnc4c4nccc4c3nc2c1
vNsp8-nsp7.1-83	ZINC000097945493	-9.1	0.228	529.547	ZINC	COC(=O)c1ccc(OC(=O)c2cccc(N3C(=O)[C@H]4[C@@H](C3=O)C3c5ccccc5C4c4ccccc43)c2)cc1
vNsp8-nsp7.1-84	ZINC000101026429	-9.1	0.217	550.668	ZINC	c1ccc(N2CN(c3ccccc3)NC(c3cccc(C4=NN(c5ccccc5)CN(c5ccccc5)N4)c3)=N2)cc1
vNsp8-nsp7.1-85	ZINC000138991166	-9.1	0.268	453.536	ZINC	Cc1ccc(OC(=O)c2cccc(N3C(=O)[C@@H]4CC[C@@H](c5ccccc5)C[C@@H]4C3=O)c2)c(C)c1
vNsp8-nsp7.1-86	ZINC000223268229	-9.1	0.294	432.543	ZINC	C[C@@H]1Cc2cc(S(=O)(=O)N3CCc4ccccc4C3)ccc2N1C(=O)c1ccccc1
vNsp8-nsp7.1-87	ZINC000245310077	-9.1	0.222	539.633	ZINC	Cc1ccc(C(=O)[C@@H]2[C@H](C(=O)c3ccccn3)[C@]3(c4ccccc4NC3=O)[C@@H]3C=C(C)c4cc(C)ccc4N32)cc1
vNsp8-nsp7.1-88	ZINC000253623932	-9.1	0.26	463.488	ZINC	Cc1ccc2cc([C@H]3CC(=O)Oc4c5c(cc(C)c43)oc(=O)cc5-c3ccccc3)c(O)nc2c1
vNsp8-nsp7.1-89	ZINC000257315129	-9.1	0.26	478.517	ZINC	Cc1nn(C)c2ccc(C(=O)N3CCC[C@@H](c4cccc(-c5cccc(C(F)(F)F)c5)n4)C3)cc12
vNsp8-nsp7.1-90	ZINC000408686158	-9.1	0.239	498.58	ZINC	Cc1cc(C)cc(NC(=O)c2ccc(N3C(=O)[C@H]4[C@@H](C3=O)C3c5ccccc5C4c4ccccc43)cc2)c1
vNsp8-nsp7.1-91	ZINC000408978119	-9.1	0.239	495.493	ZINC	O=C(Oc1ccc2nc3c4ccccc4c4ccccc4c3nc2c1)c1ccc(N2C(=O)C=CC2=O)cc1
vNsp8-nsp7.1-92	PV-000321157727	-9	0.3	402.492	REAL	O=C([C@@H]1C[C@@H]2O[C@H]1[C@H]1C[C@@H]21)N1CC[C@@H]2CN(C(=O)c3ccc4ccccc4c3)[C@@H]2C1
vNsp8-nsp7.1-93	PV-001800072315	-9	0.3	416.442	REAL	C[C@@H]1c2ccccc2CCN1C(=O)[C@@H]1CC(=O)N(Cc2ccc(C(F)(F)F)c2)C1
vNsp8-nsp7.1-94	PV-001849072825	-9	0.3	405.54	REAL	Cc1cccc(NC(=O)N2CCC[C@H](C(=O)N3CCCc4ccccc4CC3)C2)c1
vNsp8-nsp7.1-95	PV-001940788457	-9	0.273	437.541	REAL	O=C(NC[C@H]1CCCN(C(=O)Nc2cccc(C#Cc3ccccc3)c2)C1)c1ccccc1
vNsp8-nsp7.1-96	PV-001956482772	-9	0.3	413.604	REAL	COCCN1[C@@H]2CC[C@@H]1CC(N(C)C(=O)NCC1CCC(c3ccccc3)CC1)C2
vNsp8-nsp7.1-97	Z1134736654	-9	0.281	425.53	REAL	C[C@H]1Cc2ccccc2N(C(=O)c2cncc(C(=O)N3C[C@@H](C)Cc4ccccc43)c2)C1
vNsp8-nsp7.1-98	Z1144561143	-9	0.281	430.554	REAL	Cc1ccc(-n2nc(C(=O)N3CCC(c4nnc5n4CCC5)CC3)c3c2CCC3)c(C)c1
vNsp8-nsp7.1-99	Z1144584568	-9	0.273	439.561	REAL	Cc1ccc(-n2nc(C(=O)N3CCC(c4c[nH]c5nccc45)CC3)c3c2CCC3)c(C)c1
vNsp8-nsp7.1-100	Z1177635971	-9	0.333	371.386	REAL	O=C(NCC(=O)N1CCc2cc(F)c(F)cc21)N1CCc2ccccc2C1

Supplementary Table 37. Top 100 virtual hits of the screen against the nsp7 binding site of nsp8 (Screen ID: 21). Compounds were filtered so that hits had MW < 600 dalton, cLogP < 6, number of hydrogen bond acceptors < 11, and no reactive functional groups. A few compounds unsuitable for drug discovery were removed by visual inspection. The name of each compound consists of the initial letter 'v' for virtual hit, followed by the target protein name and the target site ('nsp7' for nsp7 binding site, 1 for docking scenario 1). The score is the docking score given by QuickVina 2 in kcal/mol. The ligand efficiency (LE) is computed as LE = -score/#NonH, where #NonH is the number of heavy (i.e. non hydrogen) atoms.

Name	Catalog ID	Score	LE	MW	Library	SMILES
vNsp8-nsp7.1-101	Z1229730875	-9.0	0.290	419.52	REAL	C[C@@H]1C[C@H]2CCCC[C@H]2N1C(=O)CN1C(=O)N[C@@](C)(c2ccc3ccccc3c2)C1=O
vNsp8-nsp7.1-102	Z1239623610	-9.0	0.290	434.43	REAL	C[C@@H]1c2c(F)cccc2CCN1C(=O)[C@@H]1CC(=O)N(Cc2cccc(C(F)(F)F)c2)C1
vNsp8-nsp7.1-103	Z1266331370	-9.0	0.281	419.48	REAL	O=C(Nc1ccc2nc(NC(=O)[C@H]3Cc4ccccc43)ccc2c1)[C@@H]1Cc2ccccc21
vNsp8-nsp7.1-104	Z1449095738	-9.0	0.273	439.51	REAL	C[C@@]1(c2ccc3ccccc3c2)NC(=O)N(CC(=O)NC[C@@H]2[C@H]3Cc4ccccc4[C@H]23)C1=O
vNsp8-nsp7.1-105	Z1555037598	-9.0	0.273	442.56	REAL	O=C(N[C@@H]1CCCN(C(=O)c2cccc([C@H]3CCOC3)c2)C1)c1ccc2ccccc2c1
vNsp8-nsp7.1-106	Z1568124094	-9.0	0.281	427.50	REAL	CC1(NC(=O)CN2C(=O)N[C@@](C)(c3ccc4ccccc4c3)C2=O)Cc2ccccc2C1
vNsp8-nsp7.1-107	Z1662365797	-9.0	0.281	418.46	REAL	Cc1c(-c2nnc(Cc3ccc4ccccc4c3)o2)nnn1-c1cccc2cnccc12
vNsp8-nsp7.1-108	Z1662368152	-9.0	0.281	418.46	REAL	Cc1c(-c2nnc(Cc3ccc4ccccc4c3)o2)nnn1-c1cccc2ncccc12
vNsp8-nsp7.1-109	Z1684579932	-9.0	0.300	400.39	REAL	C[C@]1(c2cccc(-c3noc(-c4cc5ccccc5cc4O)n3)c2)NC(=O)NC1=O
vNsp8-nsp7.1-110	Z1716066358	-9.0	0.281	425.48	REAL	O=C1O[C@@H](c2ccccc2)Cc2cc(C(=O)N3CC[C@@]4(C3)OCc3ccccc34)ccc21
vNsp8-nsp7.1-111	Z1891946663	-9.0	0.273	443.55	REAL	O=C(c1cccc(N2C(=O)[C@@H]3C[C@H](C4CCCC4)CN3C2=O)c1)N1CCc2ccccc21
vNsp8-nsp7.1-112	Z1907680005	-9.0	0.321	444.37	REAL	C[C@H](CC(=O)c1cccc(Br)c1)C(=O)NC[C@]1(O)[C@H]2[C@H]3C[C@@H]4[C@@H]5[C@H]3C[C@H]2[C@H]5[C@H]41
vNsp8-nsp7.1-113	Z1949016388	-9.0	0.281	442.48	REAL	O=C([C@H]1[C@@H]2[C@@H]3C[C@H]4[C@H]5[C@@H]3C[C@@H]2[C@H]5[C@H]41)N1CCC[C@H](c2nnc3ccc(C(F)(F)F)cn23)C1
vNsp8-nsp7.1-114	Z1951487061	-9.0	0.290	419.50	REAL	O=C([C@@H]1[C@H]2[C@H]3C[C@@H]4[C@@H]5[C@H]3C[C@H]2[C@@H]5[C@@H]41)N1CCC[C@@H](c2nc(-c3ccc(F)cc3)no2)C1
vNsp8-nsp7.1-115	Z1952432406	-9.0	0.300	402.47	REAL	O=C(N[C@@H]1CCCN(C(=O)[C@H]2Cc3ccc(F)cc32)C1)c1ccc2ccccc2c1
vNsp8-nsp7.1-116	Z2026749975	-9.0	0.273	440.46	REAL	C[C@@]1(c2ccc3ccccc3c2)NC(=O)N(CC(=O)Nc2nc(-c3ccccc3)co2)C1=O
vNsp8-nsp7.1-117	Z2087376571	-9.0	0.310	382.42	REAL	COc1ccc2cc(N3C(=O)N[C@@H](c4ccc5ccccc5c4)C3=O)ccc2c1
vNsp8-nsp7.1-118	Z2157032951	-9.0	0.333	361.44	REAL	CN(C)C(=O)c1cccc(-c2noc([C@@H]3[C@H]4[C@@H]5C[C@H]6[C@H]7[C@@H]5C[C@@H]4[C@H]7[C@H]63)n2)c1
vNsp8-nsp7.1-119	Z2902490588	-9.0	0.250	491.47	REAL	O=C1[C@@H]2[C@@H]3C=C[C@H]([C@@H]2C(=O)N1Cc1ccccc1)[C@@H]1C(c2nc(-c4cccc(C(F)(F)F)c4)no2)[C@H]31
vNsp8-nsp7.1-120	Z2964220498	-9.0	0.310	386.45	REAL	O=C([C@H]1C[C@@]12C(=O)Nc1ccccc12)N1CCC[C@]2(C=Cc3ccccc3O2)C1
vNsp8-nsp7.1-121	Z364181486	-9.0	0.273	468.52	REAL	C[C@H]1Cc2ccccc2N1S(=O)(=O)c1cccc(C(=O)N[C@@H]3CC4c5ccccc5C3c3ccccc34)C2=O)cc1
vNsp8-nsp7.1-122	Z394510666	-9.0	0.250	490.60	REAL	C[C@H]1CCCN(C(=O)C2CCN(C(=O)CN3C(=O)N[C@@](C)(c4ccc5ccccc5c4)C3=O)CC2)C1
vNsp8-nsp7.1-123	Z424332728	-9.0	0.300	397.43	REAL	C[C@@]1(c2cccc(NC(=O)c3ccc4c(c3)-c3ccccc3C4)c2)NC(=O)NC1=O
vNsp8-nsp7.1-124	Z62471841	-9.0	0.250	493.49	REAL	O=C(Nc1ccc2c(c1)C(=O)c1ccccc1C2=O)c1ccc2c(c1)S(=O)(=O)c1ccccc1C2=O
vNsp8-nsp7.1-125	Z654032508	-9.0	0.250	480.52	REAL	C[C@@]1(c2ccc3ccccc3c2)NC(=O)N(CC(=O)NNC(=O)Cc2ccc3ccccc3c2)C1=O
vNsp8-nsp7.1-126	Z71169942	-9.0	0.243	495.58	REAL	COc1ccc([C@]2(C)NC(=O)N(CC(=O)NC[C@@H]3CC4c5ccccc5C3c3ccccc34)C2=O)cc1
vNsp8-nsp7.1-127	Z728497534	-9.0	0.257	490.60	REAL	O=C(c1cccc(S(=O)(=O)N2CCc3ccccc3C2)c1)N1CCC(=Cc2ccccc(F)c2)CC1
vNsp8-nsp7.1-128	Z804787624	-9.0	0.273	437.50	REAL	O=C1CCc2ccc(NC(=O)[C@H]3CC(=O)N(c4ccc5c(c4)Cc4ccccc4-5)C3)ccc2N1
vNsp8-nsp7.1-129	Z806333512	-9.0	0.257	465.55	REAL	C[C@H](NC(=O)[C@@H]1CC(=O)N(c2ccc3c(c2)Cc2ccccc2-3)C1)c1ccc2c(c1)CCC(=O)N2
vNsp8-nsp7.1-130	Z87765160	-9.0	0.250	477.52	REAL	C[C@@]1(c2ccc3ccccc3c2)NC(=O)N(CC(=O)c2ccc(NC(=O)c3ccccc3)cc2)C1=O
vNsp8-nsp7.1-131	Z905886434	-9.0	0.281	432.61	REAL	O=C(c1cccc(C(=O)N2CC3C[C@H]4CC2C[C@@H](C3)C4)c1)N1CC2C[C@H]3CC1C[C@@H](C2)C3
vNsp8-nsp7.1-132	ZINC000000991032	-9.0	0.250	478.55	ZINC	O=C(NC[C@@H]1CCCO1)c1ccc(N2C(=O)[C@H]3[C@@H](C2=O)C2c4ccccc4C3c3ccccc32)cc1
vNsp8-nsp7.1-133	ZINC000002412360	-9.0	0.243	485.49	ZINC	O=C(Nc1ccc(-c2ccc3ccccc3oc2=O)cc1)c1ccc(-c2cc3ccccc3oc2=O)c1
vNsp8-nsp7.1-134	ZINC000003415059	-9.0	0.220	577.58	ZINC	Cc1ccc(S(=O)(=O)c2ccc(NN/C=C3/c4ccccc4C(=O)N(c4cccc(C(F)(F)F)c4)C3=O)cc2)cc1
vNsp8-nsp7.1-135	ZINC000003672765	-9.0	0.243	486.62	ZINC	Cc1cc(N2CCN(c3nc(N4CCc5ccccc5C4)nc4ccccc43)CC2)c2ccccc2n1
vNsp8-nsp7.1-136	ZINC000008901217	-9.0	0.237	499.52	ZINC	Cc1cc(NC(=O)c2cccc(-c3cc4ccccc4oc3=O)c2)ccc1-c1cc2ccccc2oc1=O
vNsp8-nsp7.1-137	ZINC000008920335	-9.0	0.281	434.52	ZINC	O=C1[C@H]2[C@H](C(=O)N1c1nc(-c3ccccc3)cs1)C1c3ccccc3C2c2ccccc21
vNsp8-nsp7.1-138	ZINC000008921453	-9.0	0.237	498.54	ZINC	O=C(NN1C(=O)[C@@H]2[C@@H](C1=O)C1c3ccccc3C2c2ccccc21)C1(O)c2ccccc2-c2ccccc21
vNsp8-nsp7.1-139	ZINC000009009890	-9.0	0.250	488.46	ZINC	O=C(c1ccccc1)[C@@H]1[C@@H]2C(=O)N(c3cccc(C(F)(F)F)c3)C(=O)[C@@H]2[C@H]2C=Cc3ccccc3N21
vNsp8-nsp7.1-140	ZINC000010215018	-9.0	0.250	477.52	ZINC	C[C@@]1(c2ccc3ccccc3c2)NC(=O)N(CC(=O)c2ccc(NC(=O)c3ccccc3)cc2)C1=O
vNsp8-nsp7.1-141	ZINC000015972608	-9.0	0.243	490.56	ZINC	Cc1ccc(N2C(=O)[C@@H]3[C@H](C2=O)[C@H](Cc2c[nH]c4ccccc24)N[C@]32C(=O)Nc3ccccc32)cc1C
vNsp8-nsp7.1-142	ZINC000016034752	-9.0	0.250	488.46	ZINC	O=C(c1ccccc1)[C@H]1[C@H]2C(=O)N(c3cccc(C(F)(F)F)c3)C(=O)[C@@H]2[C@H]2C=Cc3ccccc3N21
vNsp8-nsp7.1-143	ZINC000018021374	-9.0	0.237	498.54	ZINC	O=C(NN1C(=O)[C@@H]2[C@@H](C1=O)C1c3ccccc3C2c2ccccc21)C1(O)c2ccccc2-c2ccccc21
vNsp8-nsp7.1-144	ZINC000018043517	-9.0	0.265	441.53	ZINC	O=C1[C@H]2[C@@H](C(=O)N1c1ccc(Cc3ccccc3)cc1)C1c3ccccc3C2c2ccccc21
vNsp8-nsp7.1-145	ZINC000018125166	-9.0	0.300	408.48	ZINC	O=C1[C@H]2[C@@H](C(=O)N1c1nc3ccccc3s1)C1c3ccccc3C2c2ccccc21
vNsp8-nsp7.1-146	ZINC000018246985	-9.0	0.231	513.55	ZINC	O=C(COC(=O)c1ccc(N2C(=O)[C@H]3[C@@H](C2=O)C2c4ccccc4C3c3ccccc32)cc1)c1ccccc1
vNsp8-nsp7.1-147	ZINC000019863151	-9.0	0.265	450.49	ZINC	Cc1ccc(-c2cc(-c3ccc4c(c3)NC(=O)CO4)nc(-c3ccc4c(c3)OCCO4)c2)cc1
vNsp8-nsp7.1-148	ZINC000020100563	-9.0	0.243	504.97	ZINC	O=C(c1ccc(Cl)cc1)[C@@H]1[C@@H]2C(=O)N(c3ccc4ccccc43)C(=O)[C@@H]2[C@@H]2c3ccccc3C=CN21
vNsp8-nsp7.1-149	ZINC000037546025	-9.0	0.257	484.49	ZINC	O=C(NCc1ccccc(C(F)(F)F)c1)[C@H]1CC[C@H](c2ccc(F)cc2)N(C(=O)c2ccccc2)C1
vNsp8-nsp7.1-150	ZINC000097945495	-9.0	0.225	529.55	ZINC	COC(=O)c1ccc(OC(=O)c2cccc(N3C(=O)[C@H]4[C@H](C3=O)C3c5ccccc5C4c4ccccc43)c2)cc1
vNsp8-nsp7.1-151	ZINC000101835219	-9.0	0.257	479.56	ZINC	O=S(=O)(Nc1nc2n(n1)[C@@H](c1ccccc1)C=C(c1ccccc1)N2)c1ccc2ccccc2c1
vNsp8-nsp7.1-152	ZINC000101965949	-9.0	0.257	475.57	ZINC	O=S1(=O)c2ccccc2-c2cc(-c3nc(C4=CN[C@@H]5C=CC=C[C@@H]45)[nH]c3-c3ccccc3)ccc21
vNsp8-nsp7.1-153	ZINC000169684224	-9.0	0.243	487.51	ZINC	Cc1ccccc[C@H]2OC3(C(=O)c4ccccc4C3=O)[C@H]3C(=O)N(c4ccc5ccccc54)C(=O)[C@@H]23)c1
vNsp8-nsp7.1-154	ZINC000216312311	-9.0	0.237	497.55	ZINC	O=C(c1ccc(-c2ccccc2)cc1)[C@@H]1[C@@H]2C(=O)N(c3cccc3)C(=O)[C@@H]2[C@@H]2c3ccccc3C=NN21
vNsp8-nsp7.1-155	ZINC000229930169	-9.0	0.209	589.05	ZINC	CC1=C[C@@H]2N(c3cccc31)[C@H](C(=O)c1ccc(Cl)cc1)[C@@H](C(=O)c1ccc3c(c1)OCO3)[C@@]21C(=O)Nc2ccccc21
vNsp8-nsp7.1-156	ZINC000253623870	-9.0	0.243	488.50	ZINC	Cn1cc(/C=C2/Oc3c(ccc4c3[C@@H](c3cc5ccccc5nc3O)CC(=O)O4)C2=O)c2ccccc21
vNsp8-nsp7.1-157	ZINC000263586231	-9.0	0.243	488.50	ZINC	Cn1cc(/C=C2\Oc3c(ccc4c3[C@@H](c3cc5ccccc5nc3O)CC(=O)O4)C2=O)c2ccccc21
vNsp8-nsp7.1-158	ZINC000408668687	-9.0	0.243	484.55	ZINC	O=C(CN1C(=O)[C@H]2[C@@H](C1=O)C1c3ccccc3C2c2ccccc21)Nc1ccc(-c2ccccc2)cc1
vNsp8-nsp7.1-159	ZINC000408675226	-9.0	0.237	498.58	ZINC	Cc1cccc(NC(=O)c2cccc(N3C(=O)[C@H]4[C@@H](C3=O)C3c5ccccc5C4c4ccccc43)c2)c1C
vNsp8-nsp7.1-160	ZINC000408730071	-9.0	0.243	485.54	ZINC	Cc1ccc(N2C(=O)[C@@H]3[C@H](C2=O)[C@@H]2C(=O)Oc4ccc5ccccc5c4C2=C[C@H]3c2ccccc2)cc1
vNsp8-nsp7.1-161	ZINC000408730080	-9.0	0.237	499.57	ZINC	Cc1ccc(N2C(=O)[C@H]3[C@H](C2=O)[C@@H]2C(=O)Oc4c5ccccc5ccc4C2=C[C@H]3c2ccccc2)c(C)c1
vNsp8-nsp7.1-162	ZINC000408731315	-9.0	0.237	499.57	ZINC	Cc1ccc(C)c(N2C(=O)[C@H]3[C@H](C2=O)[C@@H]2C(=O)Oc4c5ccccc5ccc4C2=C[C@H]3c2ccccc2)c1
vNsp8-nsp7.1-163	ZINC000408731989	-9.0	0.243	493.56	ZINC	COc1ccc([C@@H]2C=C3c4ccc(C)cc4OC(=O)[C@@H]3[C@@H]3C(=O)N(c4ccc(C)ccc4C)C(=O)[C@@H]32)cc1
vNsp8-nsp7.1-164	ZINC000408965224	-9.0	0.250	489.60	ZINC	COc1ccc(N=C2NC(=O)/C(=C\c3cn(Cc4ccc5ccccc5c4)c4ccccc34)S2)cc1
vNsp8-nsp7.1-165	ZINC000409333198	-9.0	0.250	476.58	ZINC	C[C@@]12C[C@H](CC(C)(C)C1)N(C(=O)Nc1ccc3nc4c5cccnc5c5ncccc5c4nc3c1)C2
vNsp8-nsp7.1-166	ZINC000409337254	-9.0	0.237	499.57	ZINC	Cc1ccc(N2C(=O)[C@H]3[C@H](C2=O)[C@@H]2C(=O)Oc4ccc5ccccc5c4C2=C[C@@H]3c2ccccc2)c(C)c1
vNsp8-nsp7.1-167	ZINC000409337264	-9.0	0.237	499.57	ZINC	Cc1ccc(N2C(=O)[C@@H]3[C@H](C2=O)[C@@H]2C(=O)Oc4ccc5ccccc5c4C2=C[C@H]3c2ccccc2)c(C)c1
vNsp8-nsp7.1-168	PV-000319693283	-8.9	0.287	421.50	REAL	O=C1CCc2cc(C(=O)N3C[C@H]4CCN(C(=O)[C@@H]5C[C@@H]6O[C@H]5[C@H]5C[C@@H]65)C[C@H]43)ccc2N1
vNsp8-nsp7.1-169	PV-001801321307	-8.9	0.278	448.46	REAL	C[C@H]1Cc2cc(F)ccc2[C@H](C)N1C(=O)[C@@H]1CC(=O)N(Cc2cccc(C(F)(F)F)c2)C1
vNsp8-nsp7.1-170	PV-001819927408	-8.9	0.287	430.47	REAL	Cc1cc(C)c2c(c1)CCN(C(=O)[C@@H]1CC(=O)N(Cc3ccccc(C(F)(F)F)c3)C1)C2
vNsp8-nsp7.1-171	PV-001828045390	-8.9	0.262	457.53	REAL	Cc1cc(C)cc(Oc2ccc(CNC(=O)c3cccc([C@]4(C)NC(=O)NC4=O)c3)cc2C)c1
vNsp8-nsp7.1-172	PV-001838758079	-8.9	0.297	407.49	REAL	CC(C)c1cccc(-n2cc(O)c(C(=O)N3[C@@H](C)Cc4cc(F)ccc4[C@@H]3C)n2)c1
vNsp8-nsp7.1-173	PV-001848618322	-8.9	0.287	430.47	REAL	Cc1ccc(C(=O)N2CCC[C@@H](C(=O)N3CC(c4cccc(C(F)(F)F)c4)C3)C2)cc1
vNsp8-nsp7.1-174	Z1014266774	-8.9	0.278	426.45	REAL	O=C(c1cccc(N2C(=O)c3ccccc3C2=O)c1)N1CC2(CCC2)c2c(F)ccc21
vNsp8-nsp7.1-175	Z1020942096	-8.9	0.262	468.48	REAL	Cc1ccc(-n2ncc(C(=O)N3CCC([C@H]4C(=O)Nc5ccccc54)CC3)c2C(F)(F)F)cc1
vNsp8-nsp7.1-176	Z1028232342	-8.9	0.287	424.52	REAL	O=C(N[C@@H]1C[C@H]2C[C@H]1[C@H]1CCC[C@H]21)N1CCC[C@@H](c2nc(-c3cccc(F)c3)no2)C1
vNsp8-nsp7.1-177	Z1084980652	-8.9	0.307	420.58	REAL	CNS(=O)(=O)c1ccccc1N1CCN(C(=O)NCC[C@H]2C[C@H]3CC[C@H]2C3)CC1
vNsp8-nsp7.1-178	Z1090165298	-8.9	0.278	433.46	REAL	C[C@@H]1Oc2ccc(C(=O)CN3C(=O)N[C@@](C)(c4ccc5c(c4)CCC5)C3=O)cc2NC1=O
vNsp8-nsp7.1-179	Z1144328999	-8.9	0.278	425.53	REAL	C[C@H]1c2cccc2CCN1C(=O)c1ccc(C(=O)N2CCc3cccc3[C@H]2C)nc1
vNsp8-nsp7.1-180	Z1148134425	-8.9	0.262	459.52	REAL	Cc1ccc(-n2nc(C(=O)N3CCC(n4c(=O)[nH]c5ccccc54)CC3)c3c2CCC3)c(F)c1
vNsp8-nsp7.1-181	Z1148246559	-8.9	0.278	434.52	REAL	Cc1ccc(-n2nc(C(=O)N3CCC(c4nnc5n4CCC5)CC3)c3c2CCC3)c(F)c1
vNsp8-nsp7.1-182	Z1157985985	-8.9	0.278	424.54	REAL	O=C([C@@H]1C[C@H]1c1ccc2ccccc2c1)N1CCC(C(=O)N2CCc3ccccc32)CC1
vNsp8-nsp7.1-183	Z1160611324	-8.9	0.254	487.54	REAL	Cc1c(C(=O)NS(=O)(=O)c2ccc3c(c2)CCC(=O)N3)nnn1-c1ccc(-c2ccccc2)cc1
vNsp8-nsp7.1-184	Z1173241422	-8.9	0.278	427.50	REAL	C[C@@]1(c2ccc3ccccc3c2)NC(=O)N(CC(=O)NC[C@H]2CCc3ccccc32)C1=O
vNsp8-nsp7.1-185	Z1194138033	-8.9	0.297	409.49	REAL	Cc1ccc2[nH]c([C@@H]3CCCN(C(=O)C4CCC5(CC4)NC(=O)NC5=O)C3)nc2c1
vNsp8-nsp7.1-186	Z1204215146	-8.9	0.270	441.53	REAL	CN(C(=O)CN1C(=O)N[C@@](C)(c2ccc3ccccc3c2)C1=O)[C@H]1CCc2ccccc2C1
vNsp8-nsp7.1-187	Z1247051650	-8.9	0.318	376.50	REAL	Cc1ccccc1C(=O)N[C@H](CC(C)C)C(=O)N1[C@H]2CC[C@H]1c1ccccc12
vNsp8-nsp7.1-188	Z1281678770	-8.9	0.270	445.52	REAL	C[C@@]1(c2ccc3ccccc3c2)NC(=O)N(CC(=O)Nc2cc(C3CCCCC3)[nH]n2)C1=O
vNsp8-nsp7.1-189	Z1315354037	-8.9	0.278	421.50	REAL	O=C(c1ccnc(C(=O)N2CC3(CC3)c3ccccc32)c1)N1CC2(CC2)c2ccccc21
vNsp8-nsp7.1-190	Z1371209381	-8.9	0.278	430.51	REAL	CC(C)c1cccc(-n2cc(O)c(C(=O)N3CCC(c4nnc5ccccn45)CC3)n2)c1
vNsp8-nsp7.1-191	Z1389965473	-8.9	0.270	441.53	REAL	O=C(NCCN1C(=O)[C@H]2[C@H]3C=C[C@@H](C3)[C@H]2C1=O)N1CC=C(c2cccc3ccccc23)CC1
vNsp8-nsp7.1-192	Z14133109	-8.9	0.278	427.50	REAL	C[C@@]1(c2ccc3ccccc3c2)NC(=O)N(CC(=O)N[C@H]2CCCc3ccccc32)C1=O
vNsp8-nsp7.1-193	Z14138603	-8.9	0.287	413.48	REAL	C[C@@H]1Cc2ccccc2N1C(=O)CN1C(=O)N[C@@](C)(c2ccc3ccccc3c2)C1=O
vNsp8-nsp7.1-194	Z1452018654	-8.9	0.270	436.47	REAL	C[C@@]1(c2cccc(C(=O)Nc3cccc(-c4ccc5ccccc5c4)n3)c2)NC(=O)NC1=O
vNsp8-nsp7.1-195	Z1452691933	-8.9	0.270	445.49	REAL	O=C(NC[C@H]1[C@@H]2Cc3ccccc3[C@H]12)NNC(=O)c1ccccc1OCc1ccc(F)cc1
vNsp8-nsp7.1-196	Z1453804507	-8.9	0.262	449.55	REAL	O=C(NC[C@@H]1[C@H]2Cc3ccccc3[C@@H]12)c1ccnc(C(=O)NC[C@H]2[C@H]3Cc4ccccc4[C@H]23)c1
vNsp8-nsp7.1-197	Z1458999179	-8.9	0.262	448.56	REAL	O=C(NC[C@@H]1[C@H]2Cc3ccccc3[C@@H]12)c1cccc(C(=O)NC[C@@H]2[C@H]3Cc4ccccc4[C@H]23)c1
vNsp8-nsp7.1-198	Z1522381998	-8.9	0.278	441.45	REAL	Cc1[nH]c(-c2cccc(C(F)(F)F)c2)nc1C(=O)N1CCO[C@]2(CCc3ccccc32)C1
vNsp8-nsp7.1-199	Z1562578406	-8.9	0.262	449.55	REAL	N#Cc1ccc(C2=CCN(C(=O)[C@@H]3CCCN(C(=O)c4ccc5ccccc45)C3)CC2)cc1
vNsp8-nsp7.1-200	Z1628669968	-8.9	0.330	371.52	REAL	COc1cccc(C[C@@]2(C(=O)N[C@@H](C)[C@@H]3CCCOC3)C[C@H]3CC[C@H]2C3)c1

Supplementary Table 38. Virtual screening hits 101 to 200 of the screen against the nsp7 binding site of nsp8 (Screen ID: 21). Compounds were filtered so that hits had MW < 600 dalton, cLogP < 6, number of hydrogen bond acceptors < 11, and no reactive functional groups. A few compounds unsuitable for drug discovery were removed by visual inspection. The name of each compound consists of the initial letter 'v' for virtual hit, followed by the target protein name and the target site ('nsp7' for nsp7 binding site, 1 for docking scenario 1). The score is the docking score given by QuickVina 2 in kcal/mol. The ligand efficiency (LE) is computed as LE = -score/#NonH, where #NonH is the number of heavy (i.e. non hydrogen) atoms.

Name	Catalog ID	Score	LE	MW	Library	SMILES
vNsp8-nsp12.1-1	Z1024051824	-10.7	0.289	491.589	REAL	O=C1Nc2ccccc2[C@H]1C1CCN(C(=O)[C@H]2CC(=O)N(c3ccc4c(c3)Cc3ccccc3-4)C2)CC1
vNsp8-nsp12.1-2	Z1452691933	-10.6	0.321	445.493	REAL	O=C(NC[C@H]1[C@@H]2Cc3ccccc3[C@H]12)NNC(=O)c1ccccc1OCc1ccc(F)cc1
vNsp8-nsp12.1-3	PV-001960106277	-10.5	0.35	399.493	REAL	C[C@@H]1C(=O)Nc2ccccc2CN1C(=O)N[C@@H](C)c1ccc(-c2ccccc2)cc1
vNsp8-nsp12.1-4	Z1716062271	-10.5	0.328	424.455	REAL	O=C(c1cccc(N2C(=O)c3ccccc3C2=O)c1)N1CC[C@@]2(C1)OCc1ccccc12
vNsp8-nsp12.1-5	Z685930754	-10.5	0.309	449.425	REAL	Cn1nc(-c2nnc(-c3cccc(N4C(=O)c5ccccc5C4=O)c3)o2)c2ccccc2c1=O
vNsp8-nsp12.1-6	PV-001960115042	-10.4	0.385	363.46	REAL	C[C@@H]1C(=O)Nc2ccccc2CN1C(=O)N[C@H](C)c1ccc2c(c1)CCC2
vNsp8-nsp12.1-7	PV-001960430807	-10.3	0.322	424.503	REAL	C[C@H](NC(=O)N1Cc2ccccc2NC(=O)[C@H]1C)c1ccc(-c2cccc(C#N)c2)cc1
vNsp8-nsp12.1-8	Z272412450	-10.3	0.294	491.546	REAL	O=C(CN1c2cccc3cccc(c23)S1(=O)=O)Nc1ccc(F)c(-c2nnc3n2CCCCC3)c1
vNsp8-nsp12.1-9	Z29556548	-10.3	0.303	455.473	REAL	Cn1nc(C(=O)NNC(=O)[C@H]2CC(=O)N(c3cccc4ccccc34)C2)c2ccccc2c1=O
vNsp8-nsp12.1-10	ZINC000000659883	-10.3	0.271	496.565	ZINC	O=C(c1ccccc1)c1ccc2c(c1)NC1=C(C(=O)C[C@H](c3ccccc3)C1)[C@H]1c3ccccc3C(=O)N21
vNsp8-nsp12.1-11	ZINC000012863900	-10.3	0.286	482.514	ZINC	C[C@]12C(=O)N(c3cccc(C(=O)NCc4ccc(F)cc4)c3)C(=O)N1CCc1c3ccccc3[nH]c12
vNsp8-nsp12.1-12	Z1025125890	-10.2	0.319	428.491	REAL	O=C(NNC(=O)N1CCC([C@H]2C(=O)Nc3ccccc32)CC1)c1ccc2ccccc2c1
vNsp8-nsp12.1-13	Z1742390315	-10.2	0.329	411.46	REAL	O=C1C[C@@H](N2CC[C@]3(C2)C(=O)Nc2ccccc23)C(=O)N1c1ccc2ccccc2c1
vNsp8-nsp12.1-14	Z2198667042	-10.2	0.319	433.377	REAL	O=C(Nc1n[nH]c2ccc(F)ccc12)c1cncc(C(=O)Nc2n[nH]c3cc(F)ccc23)c1
vNsp8-nsp12.1-15	Z2495736500	-10.2	0.392	349.433	REAL	O=C1CN(C(=O)NC[C@@H]2CCc3ccccc3C2)Cc2ccccc2N1
vNsp8-nsp12.1-16	ZINC000002250011	-10.2	0.309	459.911	ZINC	O/C(Cc1ccccc1)=N\C1=NN2C(=NC(c3ccc(Cl)cc3)=C[C@H]2c2ccc(F)cc2)N1
vNsp8-nsp12.1-17	ZINC000408668686	-10.2	0.276	484.554	ZINC	O=C(CN1C(=O)[C@@H]2[C@@H](C1=O)C1c3ccccc3C2c2ccccc21)Nc1ccc(-c2ccccc2)cc1
vNsp8-nsp12.1-18	PV-001957989977	-10.1	0.326	432.401	REAL	O=C1CN(C(=O)N[C@H]2CC(=O)Nc3cccc(C(F)(F)F)c3)C2)Cc2ccccc2N1
vNsp8-nsp12.1-19	PV-001958169076	-10.1	0.337	400.481	REAL	C[C@H](NC(=O)N1Cc2ccccc2NC(=O)[C@H]1C)c1ccc(-c2ccnc2)cc1
vNsp8-nsp12.1-20	PV-001959107578	-10.1	0.337	403.456	REAL	C[C@@H](NC(=O)N1CC(=O)Nc2ccccc2C1)c1ccc(-c2ccc(F)cc2)cc1
vNsp8-nsp12.1-21	PV-001960283614	-10.1	0.361	377.486	REAL	C[C@@H]1C(=O)Nc2ccccc2CN1C(=O)N[C@H](C)c1ccc2c(c1)CCCC2
vNsp8-nsp12.1-22	PV-001960695773	-10.1	0.374	379.483	REAL	C[C@H](NC(=O)N1Cc2ccccc2NC(=O)[C@H]1C)c1cc2ccccc2s1
vNsp8-nsp12.1-23	Z1014269000	-10.1	0.281	481.594	REAL	O=C(NCC(=O)N1CCc2ccccc21)[C@@H]1C[C@H]2CCCC[C@H]2N1C(=O)c1ccc2ccccc2c1
vNsp8-nsp12.1-24	Z1099605356	-10.1	0.316	433.377	REAL	O=C(Nc1n[nH]c2ccc(F)cc12)c1cncc(C(=O)Nc2n[nH]c3ccc(F)ccc23)c1
vNsp8-nsp12.1-25	Z1217455627	-10.1	0.306	443.506	REAL	Cc1ncc2c(n1)CCC[C@@H]2NC(=O)CN1C(=O)N[C@]1(C)(c2ccc3ccccc3c2)C1=O
vNsp8-nsp12.1-26	Z1383818315	-10.1	0.289	458.472	REAL	O=C(Cn1c2ccccc2c(=O)c2ccccc21)Nc1ccc2c(c1)C(=O)c1ccccc1C2=O
vNsp8-nsp12.1-27	Z1411891150	-10.1	0.326	434.417	REAL	Cc1cc(=O)c(C(=O)N2CC(=O)N[C@H]3CCCC[C@H]32)nn1-c1ccccc(C(F)(F)F)c1
vNsp8-nsp12.1-28	Z1472861059	-10.1	0.306	439.514	REAL	C[C@]1(c2ccc3ccccc3c2)NC(=O)N(CC(=O)N[C@@H]2[C@@H]3CCc4ccccc4[C@@H]32)C1=O
vNsp8-nsp12.1-29	Z1688896240	-10.1	0.337	413.354	REAL	O=C(Cc1noc(-c2cc3ccccc3cc2O)n1)Nc1cccc(C(F)(F)F)c1
vNsp8-nsp12.1-30	Z2008725225	-10.1	0.306	437.545	REAL	Cn1c(-c2cccc3ccccc23)nnc1N1CCC(C(=O)N2CCc3ccccc32)CC1
vNsp8-nsp12.1-31	Z2154912715	-10.1	0.374	358.396	REAL	C[C@H]1Oc2ccccc2[C@@H]1N1C(=O)N[C@H](c2ccc3ccccc3c2)C1=O
vNsp8-nsp12.1-32	Z2500778670	-10.1	0.374	360.412	REAL	O=C1CN(C(=O)Cc2coc3cc4c(cc23)CCC4)Cc2ccccc2N1
vNsp8-nsp12.1-33	ZINC000034757525	-10.1	0.266	509.583	ZINC	Cc1ccc(NC(=O)N2CCc3nc(N4CCc5ccccc5C4)nc(Oc4cccc(F)c4)c3C2)cc1
vNsp8-nsp12.1-34	ZINC000040374174	-10.1	0.297	470.595	ZINC	O=S(=O)(c1ccc2ccccc2c1)N1CCc2nc(-c3ccccc3)nc(N3CCCC3)c2C1
vNsp8-nsp12.1-35	ZINC000408760211	-10.1	0.289	455.512	ZINC	O=CC12c3ccccc3C(c3ccccc31)[C@@H]1C(=O)N(c3ccccc3-c3ccccc3)C(=O)[C@H]12
vNsp8-nsp12.1-36	ZINC000408760214	-10.1	0.289	455.512	ZINC	O=CC12c3ccccc3C(c3ccccc31)[C@@H]1C(=O)N(c3ccccc3-c3ccccc3)C(=O)[C@@H]12
vNsp8-nsp12.1-37	PV-001918438386	-10	0.323	413.519	REAL	Cc1ccc(NC(=O)NC(=O)CN2Cc3ccccc3C[C@H]2c2ccccc2)cc1C
vNsp8-nsp12.1-38	PV-001960283431	-10	0.37	363.46	REAL	C[C@@H](NC(=O)N1CC(=O)Nc2ccccc2C1)c1ccc2c(c1)CCCC2
vNsp8-nsp12.1-39	PV-001960567229	-10	0.303	463.474	REAL	CN1C(=O)C[C@H](NC(=O)NCC2(c3cccc(F)c3F)CCCC2)[C@H]1c1ccc(F)c(F)c1
vNsp8-nsp12.1-40	Z1020941934	-10	0.303	443.545	REAL	O=C1Nc2ccccc2[C@@H]1C1CCN(C(=O)[C@@H]2CC(=O)N(c3ccc4c(c3)CCC4)C2)CC1
vNsp8-nsp12.1-41	Z1070219674	-10	0.278	499.953	REAL	O=C1Nc2cc(Cl)ccc2[C@H]1C1CCN(C(=O)c2cccc(N3C(=O)c4ccccc4C3=O)c2)CC1
vNsp8-nsp12.1-42	Z1117336200	-10	0.294	461.564	REAL	C[C@H]1Cc2ccccc2N1C1CCN(C(=O)NCc2ccc([C@@]3(C)NC(=O)NC3=O)cc2)CC1
vNsp8-nsp12.1-43	Z1192942893	-10	0.313	427.463	REAL	Cn1c(NNC(=O)[C@H]2CC(=O)N(c3cccc4ccccc34)C2)nc2ccccc2c1=O
vNsp8-nsp12.1-44	Z14134091	-10	0.294	449.509	REAL	C[C@]1(c2ccc3ccccc3c2)NC(=O)N(CC(=O)Nc2ccccc2-c2ccccc2)C1=O
vNsp8-nsp12.1-45	Z1473414262	-10	0.294	448.525	REAL	O=C(NNC(=O)c1cc(-c2ccccc2)nc2ccccc12)N[C@H]1[C@H]2CCc3ccccc3[C@H]21
vNsp8-nsp12.1-46	Z1507813901	-10	0.333	394.473	REAL	O=C(c1cc2ccccc2c2cccnc12)N1CCO[C@]2(CCc3ccccc32)C1
vNsp8-nsp12.1-47	Z1580995160	-10	0.345	386.45	REAL	O=C(Nc1cccc(-c2ccc3c(c2)CCO3)c1)N1CCOc2ccccc2C1
vNsp8-nsp12.1-48	Z1581009374	-10	0.303	447.577	REAL	CC1CCN(C(=O)C2CCN(C(=O)Nc3cccc(-c4ccc5c(c4)CCO5)c3)CC2)CC1
vNsp8-nsp12.1-49	Z1620029751	-10	0.313	431.47	REAL	Cc1cc(F)c2nc(O)cc(C(=O)N3CCC[C@H](c4n[nH]c(-c5ccccc5)n4)C3)c2c1
vNsp8-nsp12.1-50	Z1742966054	-10	0.357	373.455	REAL	O=C(NC[C@@H]1[C@H]2Cc3ccccc3[C@H]12)N1CC[C@]2(C1)C(=O)Nc1ccccc12
vNsp8-nsp12.1-51	Z1903496763	-10	0.303	441.529	REAL	Cc1ccc(NC(=O)N(C)C2c3ccccc3-c3ccccc32)cc1C(=O)N1CCOCC1
vNsp8-nsp12.1-52	Z1983282088	-10	0.313	435.479	REAL	O=C(CCN1C(=O)c2ccccc2C1=O)CN1C(=O)N[C@@]2(C[C@H]3C[C@H]2[C@H]2CCC[C@H]32)C1=O
vNsp8-nsp12.1-53	Z2008683668	-10	0.303	436.518	REAL	Cn1c(-c2cccc3ccccc23)nnc1N1CCN(C(=O)c2cc3ccccc3[nH]2)CC1
vNsp8-nsp12.1-54	Z2016870234	-10	0.345	394.449	REAL	Cc1cc(C)cc(-n2nc(NC(=O)N3CCOc4ccccc4C3)cc2C)c1
vNsp8-nsp12.1-55	Z2109647986	-10	0.345	390.525	REAL	O=C(NC[C@@H]1CCCc2ccccc21)N1C[C@@H](c2ccccc2)[C@@H]2COCC[C@H]21
vNsp8-nsp12.1-56	Z2175485383	-10	0.313	435.425	REAL	O=C(N[C@H]1COc2c(F)cc(F)cc2C1)c1ccc2c(c1)C[C@@H](c1ccccc1)OC2=O
vNsp8-nsp12.1-57	Z2231284919	-10	0.313	448.415	REAL	CC1(C)CN(C(=O)c2cc(=O)[nH]c3cc(F)ccc23)C[C@H](c2ccccc(C(F)(F)F)c2)O1
vNsp8-nsp12.1-58	Z284415450	-10	0.286	491.546	REAL	O=C(CN1c2cccc3cccc(c23)S1(=O)=O)Nc1ccc(-c2nnc3n2CCCCC3)ccc1F
vNsp8-nsp12.1-59	Z289110610	-10	0.286	487.583	REAL	Cc1ccc(-c2nnc3n2CCCCC3)cc1NC(=O)CN1c2cccc3ccccc(c23)S1(=O)=O
vNsp8-nsp12.1-60	Z3045322725	-10	0.345	389.497	REAL	O=C(N[C@H]1C[C@]2(CCNC2)Oc2ccccc21)N[C@@H]1[C@H]2CCc3ccccc3[C@H]21
vNsp8-nsp12.1-61	Z736933500	-10	0.286	491.567	REAL	C[C@]1(c2ccc3ccccc3c2)NC(=O)N(CC(=O)N2CCCc3cc(S(C)(=O)=O)ccc32)C1=O
vNsp8-nsp12.1-62	Z804128572	-10	0.278	496.59	REAL	O=C(Nn1cnc2sc3c(c2c1=O)CCCC3)[C@H]1CC(=O)N(c2ccc3c(c2)Cc2ccccc2-3)C1
vNsp8-nsp12.1-63	Z992474436	-10	0.323	411.504	REAL	O=C(Nc1ccc2c(c1)Cc1ccccc1-2)N[C@@H]1CCCN(C(=O)c2ccccc2)C1
vNsp8-nsp12.1-64	Z996704354	-10	0.278	487.573	REAL	O=C(Nc1cccc(F)c1)C1CCN(C(=O)[C@H]2CCCN(C(=O)c3cccc4ccccc34)C2)CC1
vNsp8-nsp12.1-65	Z999727030	-10	0.278	481.554	REAL	NC(=O)c1cccnc1N1CCN(C(=O)[C@@H]2CC(=O)N(c3ccc4c(c3)Cc3ccccc3-4)C2)CC1
vNsp8-nsp12.1-66	ZINC000000781557	-10	0.286	482.515	ZINC	O=C1Nc2ccc(S(=O)(=O)Nc3ccc(O)c(-c4c(O)ccc5ccccc54)c3)c3ccccc1c23
vNsp8-nsp12.1-67	ZINC000005604654	-10	0.323	398.464	ZINC	c1ccc2c(c1)-c1ccccc1C2c1nnc(C2c3ccccc3-c3ccccc32)o1
vNsp8-nsp12.1-68	ZINC000008815915	-10	0.303	439.557	ZINC	O=C(Nc1cccc(NC(=O)C23CC4CC(CC(C4)C2)C3)c1)Nc1ccc2ccccc21
vNsp8-nsp12.1-69	ZINC000008918388	-10	0.278	498.969	ZINC	C[C@]12C(=O)N(c3cccc(C(=O)NCc4ccccc4Cl)c3)C(=O)N1CCc1c3ccccc3[nH]c12
vNsp8-nsp12.1-70	ZINC000008990006	-10	0.294	456.524	ZINC	N#C/C(=C/c1ccc2ccccc12)c1nc(-c2cc3c(ccc4ccccc43)oc2=O)os1
vNsp8-nsp12.1-71	ZINC000012100055	-10	0.286	468.555	ZINC	C[C@@]1(C2CCN(C(=O)c3cce4ccccc4n3)CC2)NC(=O)N(C2Cc3ccccc3C2)C1=O
vNsp8-nsp12.1-72	ZINC000043214914	-10	0.294	444.485	ZINC	O=C1c2cc3ccccc3cc2C(=O)[C@H]2C[C@H]3C(=O)c4cc5ccccc5cc4C(=O)[C@H]3C[C@@H]12
vNsp8-nsp12.1-73	ZINC000059796308	-10	0.256	513.595	ZINC	Cc1cccc2c1NC(=O)[C@@]21N2CCC[C@@H]2[C@@H](C(=O)c2ccc3ccccc3c2)[C@]12c1ccccc1NC2=O
vNsp8-nsp12.1-74	ZINC000059932650	-10	0.25	527.622	ZINC	Cc1ccc2c(c1C)NC(=O)[C@@]21N2CCC[C@@H]2[C@@H](C(=O)c2ccc3ccccc3c2)[C@]12c1ccccc1NC2=O
vNsp8-nsp12.1-75	ZINC000096116418	-10	0.27	491.498	ZINC	O=c1cc(-c2ccccc2)oc2c1c(O)cc1c2[C@@H](c2cc3cccc4c3n(c2=O)CCC4)CC(=O)O1
vNsp8-nsp12.1-76	ZINC000100505727	-10	0.27	488.542	ZINC	O=C1[C@@H]2[C@H]3C=C[C@@H](C3)[C@@H]2C(=O)N1c1ccc2c(c1)-c1cc(N3C(=O)[C@H]4[C@H]5C=C[C@H](C5)[C@@H]4C3=O)ccc1C2
vNsp8-nsp12.1-77	ZINC000253623870	-10	0.27	488.498	ZINC	Cn1cc(/C=C2/Oc3c(ccc4c3[C@@H](c3cc5ccccc5nc3O)CC(=O)O4)C2=O)c2ccccc21
vNsp8-nsp12.1-78	ZINC000263586231	-10	0.27	488.498	ZINC	Cn1cc(/C=C2\Oc3c(ccc4c3[C@@H](c3cc5ccccc5nc3O)CC(=O)O4)C2=O)c2ccccc21
vNsp8-nsp12.1-79	PV-001801798049	-9.9	0.341	406.407	REAL	O=C1C[C@@H](C(=O)Nc2ccn(-c3cccc(C(F)(F)F)c3)n2)[C@H]2CCCC[C@@H]2N1
vNsp8-nsp12.1-80	PV-001806921196	-9.9	0.291	459.505	REAL	CN(C)C(=O)Nc1cccc(NC(=O)CN2C(=O)N[C@](C)(c3ccc4ccccc4c3)C2=O)c1
vNsp8-nsp12.1-81	PV-001944971855	-9.9	0.341	389.458	REAL	Cc1cc(C)cc(-n2nc(NC(=O)N3CC(=O)Nc4ccccc4C3)cc2C)c1
vNsp8-nsp12.1-82	PV-001946570502	-9.9	0.341	397.384	REAL	Cn1nc(-c2ccc(F)cc2F)cc1NC(=O)N1CC(=O)Nc2ccccc2C1
vNsp8-nsp12.1-83	PV-001954630926	-9.9	0.354	377.443	REAL	Cc1c([C@@H](C)NC(=O)N2Cc3ccccc3NC(=O)[C@H]2C)oc2ccccc12
vNsp8-nsp12.1-84	PV-001955868254	-9.9	0.3	463.474	REAL	CN1C(=O)C[C@H](NC(=O)NCC2(c3c(F)cccc3F)CCCC2)[C@H]1c1ccc(F)c(F)c1
vNsp8-nsp12.1-85	PV-001956054547	-9.9	0.354	377.486	REAL	O=C1CN(C(=O)N[C@@H]2CCCC[C@H]2Cc2ccccc2)Cc2ccccc2N1
vNsp8-nsp12.1-86	PV-001957670919	-9.9	0.33	405.54	REAL	Cc1ccc(N2CCC[C@@H](NC(=O)N[C@H]3c4ccccc4CCC[C@H]3C)C2=O)cc1
vNsp8-nsp12.1-87	PV-001957970907	-9.9	0.319	423.53	REAL	Cc1cccc(C(=O)NC2CCN(C(=O)N[C@H]3c4cccc(F)c4CC[C@H]3C)CC2)c1
vNsp8-nsp12.1-88	PV-001958877663	-9.9	0.319	423.447	REAL	Cc1cc(-c2noc([C@H](C)NC(=O)N3Cc4ccccc4NC(=O)[C@H]3C)n2)ccc1F
vNsp8-nsp12.1-89	PV-001959311545	-9.9	0.354	384.45	REAL	Cc1ccc2c1C[C@@H](NC(=O)N[C@H]1CC(C)(C)Oc3cc(F)ccc31)CO2
vNsp8-nsp12.1-90	PV-001959729887	-9.9	0.367	362.515	REAL	C[C@H]1CCCc2ccccc2[C@H]1NC(=O)NC[C@@H]1CCc2ccccc2C1
vNsp8-nsp12.1-91	PV-001960547630	-9.9	0.354	377.443	REAL	Cc1c([C@@H](C)NC(=O)N2Cc3ccccc3NC(=O)[C@H]2C)oc2ccccc12
vNsp8-nsp12.1-92	PV-001961059778	-9.9	0.309	453.933	REAL	C[C@@H](NC(=O)NNc1nc2c(cnn2C(C)(C)C)c(=O)[nH]1)c1ccc(Cl)c2ccccc12
vNsp8-nsp12.1-93	PV-001961963419	-9.9	0.341	406.422	REAL	O=C(NCC(F)(F)c1ccc(F)cc1F)NC1[C@H]2CC[C@@H]1Cc1ccccc1C2
vNsp8-nsp12.1-94	PV-001963137338	-9.9	0.319	421.499	REAL	C[C@H](NC(=O)N1Cc2ccccc2NC(=O)[C@H]1C)c1ccc(N2CCCNC2=O)cc1
vNsp8-nsp12.1-95	PV-001963311729	-9.9	0.341	391.445	REAL	C[C@H](NC(=O)N1Cc2ccccc2NC(=O)[C@H]1C)c1ccc(F)c2ccccc12
vNsp8-nsp12.1-96	PV-001965045343	-9.9	0.354	384.45	REAL	Cc1ccc2c1C[C@@H](NC(=O)N[C@H]1CC(C)(C)Oc3ccc(F)cc31)CO2
vNsp8-nsp12.1-97	Z1014236248	-9.9	0.283	498.577	REAL	O=C(Nc1ccc(F)cc1)C1CCN(C(=O)C2CCN(C3=NS(=O)(=O)c4ccccc43)CC2)CC1
vNsp8-nsp12.1-98	Z1014397762	-9.9	0.283	469.583	REAL	O=C(N[C@@H]1CCCc2[nH]c(=O)ccc21)[C@@H]1C[C@@H]2CCCC[C@@H]2N1C(=O)c1ccc2ccccc2c1
vNsp8-nsp12.1-99	Z1014965352	-9.9	0.3	460.596	REAL	Cc1ccc(S(=O)(=O)N2CCC[C@H](C(=O)N3Cc4ccccc4-c4ccccc4C3)C2)cc1
vNsp8-nsp12.1-100	Z1147996353	-9.9	0.319	415.463	REAL	O=C1O[C@H](c2ccccc2)Cc2cc(C(=O)N3CC[C@@H](c4ccccc4F)C3)ccc21

Supplementary Table 39. Top 100 virtual hits of the screen against the nsp12 binding site on nsp8 (Screen ID: 22). The name of each compound consists of the initial letter 'v' for virtual hit, followed by the target protein name and the target site ('nsp12' for nsp12 binding site, 1 for docking scenario 1). The score is the docking score given by QuickVina 2 in kcal/mol. The ligand efficiency (LE) is computed as LE = -score/#NonH, where #NonH is the number of heavy (i.e. non hydrogen) atoms.

Name	Catalog ID	Score	LE	MW	Library	SMILES
vNsp8-nsp12.1-101	Z1151714823	-9.9	0.300	439.51	REAL	Cc1cccc(N2C(=O)N[C@@H](CCC(=O)N3Cc4ccccc4-c4ccccc4C3)C2=O)c1
vNsp8-nsp12.1-102	Z1157915550	-9.9	0.330	394.47	REAL	O=C(Cc1cccc2ccccc12)NNC(=O)[C@@H]1C[C@H]1c1ccc2ccccc2c1
vNsp8-nsp12.1-103	Z1239253310	-9.9	0.300	442.45	REAL	O=C(Oc1cccc(C(=O)N2CCc3ccccc3C2)c1)c1cc(=O)[nH]c2ccc(F)cc12
vNsp8-nsp12.1-104	Z1313928483	-9.9	0.300	441.53	REAL	O=C(NNC(=O)C1(O)Cc2ccccc2C1)[C@@H]1Cc2ccccc2CN1Cc1ccccc1
vNsp8-nsp12.1-105	Z1391613386	-9.9	0.300	439.51	REAL	Cc1ccc(-c2ocnc2C(=O)N2CCC[C@H](NC(=O)c3ccc4ccccc4c3)C2)cc1
vNsp8-nsp12.1-106	Z1392038003	-9.9	0.309	426.44	REAL	Cc1ccn2c(NC(=O)c3cccc(C(=O)Nc4nnc5cc(C)ccn45)c3)nnc2c1
vNsp8-nsp12.1-107	Z1471726242	-9.9	0.291	449.55	REAL	Cc1cc(=O)c(C(=O)N2CCc3ccccc3[C@@H](c3ccccc3)[C@@H]2C)nn1-c1ccccc1
vNsp8-nsp12.1-108	Z1572375518	-9.9	0.396	341.45	REAL	CC1(CNC(=O)N2CC(=O)N[C@H]3CCCC[C@H]32)Cc2ccccc2C1
vNsp8-nsp12.1-109	Z1581473271	-9.9	0.300	440.59	REAL	O=C(NC[C@H]1CCCN1C(=O)[C@H]1C[C@@]12CCc1ccccc12)[C@H]1C[C@]12CCc1ccccc12
vNsp8-nsp12.1-110	Z1626782290	-9.9	0.319	411.46	REAL	C[C@@]1(c2ccc(C(=O)N3CC=C(c4ccccc5ccccc45)C3)cc2)NC(=O)NC1=O
vNsp8-nsp12.1-111	Z1688127865	-9.9	0.300	436.51	REAL	Cc1ccc(-c2cc(C(=O)NNC(=O)NC3Cc4ccccc4C3)c3ccccc3n2)cc1
vNsp8-nsp12.1-112	Z1688207416	-9.9	0.300	442.47	REAL	C[C@]1(c2ccc3ccccc3c2)NC(=O)N(CC(=O)N2CCNC(=O)c3ccccc32)C1=O
vNsp8-nsp12.1-113	Z1715941472	-9.9	0.300	443.48	REAL	O=C(N[C@H]1CCCN(C(=O)c2ncoc2-c2ccc(F)cc2)C1)c1ccc2ccccc2c1
vNsp8-nsp12.1-114	Z1741002788	-9.9	0.309	431.58	REAL	O=C(c1ccccc1)N1CCC(NC(=O)N2C[C@@H](c3ccccc3)[C@H]3CCCC[C@H]32)CC1
vNsp8-nsp12.1-115	Z1766471540	-9.9	0.341	387.48	REAL	Cc1ccc(-c2cc(C(=O)N3CCO[C@@]4(CCc5ccccc54)C3)[nH]n2)cc1C
vNsp8-nsp12.1-116	Z1869176890	-9.9	0.330	399.45	REAL	O=C(CN1C(=O)N[C@@H](c2ccc3ccccc3c2)C1=O)N1CCc2ccccc2C1
vNsp8-nsp12.1-117	Z1905093647	-9.9	0.319	411.46	REAL	CN1C[C@H](C(=O)OCC(=O)c2ccc3c(c2)Cc2ccccc2-3)c2ccccc2C1=O
vNsp8-nsp12.1-118	Z1906392261	-9.9	0.309	428.47	REAL	O=C(NCc1nc(-c2cccc(F)c2)no1)N1Cc2ccccc2C[C@H]1c1ccccc1
vNsp8-nsp12.1-119	Z2090589879	-9.9	0.354	373.49	REAL	O=C([C@H]1C[C@@]12CCc1ccccc12)N1C[C@@H](c2ccccc2)[C@@H]2COCC[C@H]21
vNsp8-nsp12.1-120	Z2180030269	-9.9	0.319	415.49	REAL	O=C(NNC(=O)c1ccc2ccccc2c1)N[C@H]1c2ccccc2CC12CCOCC2
vNsp8-nsp12.1-121	Z218028876	-9.9	0.283	466.50	REAL	C[C@@H]1Oc2ccccc2N(CC(=O)NNC(=O)c2cc(-c3ccccc3)nc3ccccc23)C1=O
vNsp8-nsp12.1-122	Z2187138452	-9.9	0.309	438.54	REAL	CN(C(=O)N[C@@H]1c2ccccc2CC12CCOCC2)[C@H]1CCO[C@@H](c2ccc(F)cc2)C1
vNsp8-nsp12.1-123	Z2231283323	-9.9	0.309	448.42	REAL	CC1(C)CN(C(=O)c2cc(=O)[nH]c3ccc(F)cc23)C[C@H](c2ccccc(C(F)(F)F)c2)O1
vNsp8-nsp12.1-124	Z2233376677	-9.9	0.319	410.48	REAL	C[C@@]1(NC(=O)c2ccc3ccccc3n2)CCN(C(=O)c2ccc3ccccc3n2)C1
vNsp8-nsp12.1-125	Z2495480410	-9.9	0.396	335.41	REAL	O=C1CN(C(=O)NCc2ccc3c(c2)CCC3)Cc2ccccc2N1
vNsp8-nsp12.1-126	Z2712646699	-9.9	0.354	375.51	REAL	O=C(C1CCc2ccccc2CC1)N1C[C@@H](c2ccccc2)[C@@H]2COCC[C@H]21
vNsp8-nsp12.1-127	Z2852204389	-9.9	0.341	393.48	REAL	Cc1ec2c(cc1C)O[C@@H](C(=O)N[C@H]1CC3(CCOCC3)Oc3ccccc31)C2
vNsp8-nsp12.1-128	Z2878463306	-9.9	0.341	391.45	REAL	CN1C(=O)C[C@H](c2nc([C@H]3CCCc4ccccc43)no2)[C@H]1c1ccc(F)cc1
vNsp8-nsp12.1-129	Z2920380486	-9.9	0.341	397.45	REAL	C[C@H]1C(=O)Nc2ccccc2CN1C(=O)N[C@@H]1CCO[C@H](c2ccc(F)cc2)C1
vNsp8-nsp12.1-130	Z2940921742	-9.9	0.283	468.51	REAL	O=C(NCc1ccc(C(=O)N2CCc3nc[nH]c3C2)o1)OCC1c2ccccc2-c2ccccc21
vNsp8-nsp12.1-131	Z29554437	-9.9	0.283	469.50	REAL	CCn1nc(C(=O)NNC(=O)[C@H]2CC(=O)N(c3cccc4ccccc34)C2)c2ccccc2c1=O
vNsp8-nsp12.1-132	Z3046166282	-9.9	0.341	392.50	REAL	O=C(NC[C@@H]1Cc2ccccc2CN1)N[C@H]1C[C@]2(CCNC2)Oc2ccccc21
vNsp8-nsp12.1-133	Z3093345685	-9.9	0.354	379.46	REAL	Cc1cc2c(cc1C)O[C@@H](C(=O)N[C@H]1C[C@]3(CCOC3)Oc3ccccc31)C2
vNsp8-nsp12.1-134	Z31939470	-9.9	0.300	466.56	REAL	O=C(c1ccccc1)N1CCN(C(=O)C2CCN(C3=NS(=O)(=O)c4ccccc43)CC2)CC1
vNsp8-nsp12.1-135	Z365661428	-9.9	0.275	499.47	REAL	Cc1cc(C(=O)N2CCN(Cc3nc(-c4cccc(C(F)(F)F)c4)no3)CC2)c2ccc(F)cc2n1
vNsp8-nsp12.1-136	Z804800684	-9.9	0.291	455.49	REAL	O=C1CCc2cc(F)c(NC(=O)[C@H]3CC(=O)N(c4ccc5c(c4)Cc4ccccc4-5)C3)cc2N1
vNsp8-nsp12.1-137	Z87589679	-9.9	0.275	477.52	REAL	Cc1ccc(-c2cc(C(=O)NNC(=O)Cc3nn(C)c(=O)c4ccccc34)c3ccccc3n2)cc1
vNsp8-nsp12.1-138	Z997042788	-9.9	0.283	465.51	REAL	Cc1cc(=O)c(C(=O)Oc2ccccc(C(=O)N3CCc4ccccc4C3)c2)nn1-c1ccccc1
vNsp8-nsp12.1-139	ZINC000013564332	-9.9	0.268	504.97	ZINC	O=C(c1ccc(Cl)cc1)[C@@H]1[C@@H]2C(=O)N(c3ccc4ccccc4c3)C(=O)[C@@H]2[C@@H]2c3ccccc3C=CN21
vNsp8-nsp12.1-140	ZINC000101835211	-9.9	0.283	479.56	ZINC	O=S(=O)(Nc1nc2n(n1)[C@H](c1ccccc1)C=C(c1ccccc1)N2)c1ccc2ccccc2c1
vNsp8-nsp12.1-141	ZINC000101835646	-9.9	0.275	493.59	ZINC	Cc1ccc([C@@H]2C=C(c3ccccc3)Nc3nc(NS(=O)(=O)c4ccc5ccccc5c4)nn32)cc1
vNsp8-nsp12.1-142	ZINC000101893793	-9.9	0.300	456.38	ZINC	Cc1ccc(N2C(=O)[C@@H]3N=NN(Cc4nc(-c5ccccc(C(F)(F)F)c5)no4)[C@H]3C2=O)cc1
vNsp8-nsp12.1-143	ZINC000181176531	-9.9	0.341	384.43	ZINC	O=C(Nc1ccccc1-c2ccc3c(c2)CCO3)c1)[C@H]1CC(=O)Nc2ccccc21
vNsp8-nsp12.1-144	ZINC000263588750	-9.9	0.268	509.51	ZINC	O=C1C[C@H](c2ccc(-c3nc4ccccc4s3)o2)c2c(ccc3c(=O)c(-c4ccccc4F)coc32)O1
vNsp8-nsp12.1-145	ZINC000408674321	-9.9	0.268	494.55	ZINC	CC1=CC[C@@H]2C(=O)N(c3cccc(OC(=O)[C@@H]4CC(=O)N(c5cccc6ccccc65)C4)c3)C(=O)[C@@H]2C1
vNsp8-nsp12.1-146	PV-001809252235	-9.8	0.350	378.45	REAL	C[C@@H]1C[C@H](NC(=O)c2cc(=O)[nH]c3cc(F)ccc23)C[C@H](c2ccccc2)C1
vNsp8-nsp12.1-147	PV-001809252240	-9.8	0.350	378.45	REAL	C[C@@H]1C[C@H](NC(=O)c2cc(=O)[nH]c3ccc(F)cc23)C[C@H](c2ccccc2)C1
vNsp8-nsp12.1-148	PV-001838045179	-9.8	0.377	355.44	REAL	Cc1ccc(C)c(C2=NO[C@H](C(=O)N3CC(=O)N[C@H]4CCCC[C@H]43)C2)c1
vNsp8-nsp12.1-149	PV-001918438385	-9.8	0.316	413.52	REAL	Cc1cccc(NC(=O)NC(=O)CN2Cc3ccccc3C[C@H]2c2ccccc2)c1C
vNsp8-nsp12.1-150	PV-001944908065	-9.8	0.350	375.43	REAL	Cc1ccc(-n2nc(NC(=O)N3CC(=O)Nc4ccccc4C3)cc2C)cc1
vNsp8-nsp12.1-151	PV-001947214685	-9.8	0.338	393.39	REAL	O=C1CN(C(=O)Nc2cccc(-c3ccc(F)c(F)c3)c2)Cc2ccccc2N1
vNsp8-nsp12.1-152	PV-001949082297	-9.8	0.327	416.40	REAL	Cc1cc(NC(=O)N2CCOc3ccccc3C2)nn1-c1cccc(C(F)(F)F)c1
vNsp8-nsp12.1-153	PV-001949085151	-9.8	0.316	429.40	REAL	Cc1cc(NC(=O)N2CC(=O)Nc3ccccc3C2)nn1-c1cccc(C(F)(F)F)c1
vNsp8-nsp12.1-154	PV-001955510765	-9.8	0.350	379.46	REAL	CCc1cccc2c1OCC[C@@H]2NC(=O)N1Cc2ccccc2NC(=O)[C@H]1C
vNsp8-nsp12.1-155	PV-001956056488	-9.8	0.338	391.51	REAL	C[C@H]1C(=O)Nc2ccccc2CN1C(=O)N[C@@H]1CCCC[C@H]1Cc1ccccc1
vNsp8-nsp12.1-156	PV-001957335688	-9.8	0.363	363.46	REAL	O=C1CN(C(=O)N[C@@H]2CCC[C@@H]2Cc2ccccc2)Cc2ccccc2N1
vNsp8-nsp12.1-157	PV-001957968779	-9.8	0.306	457.98	REAL	C[C@@H]1CCc2c(F)cccc2[C@@H]1NC(=O)N1CCN(C(=O)Cc2cccc(Cl)c2)[C@H](C)C1
vNsp8-nsp12.1-158	PV-001958455872	-9.8	0.338	385.47	REAL	O=C1CN(C(=O)NCCc2ccc(-c3ccccc3)cc2)Cc2ccccc2N1
vNsp8-nsp12.1-159	PV-001960275433	-9.8	0.350	377.49	REAL	C[C@@H]1C(=O)Nc2ccccc2CN1C(=O)N[C@@H](C)c1ccc2c(c1)CCCC2
vNsp8-nsp12.1-160	PV-001960919069	-9.8	0.297	463.47	REAL	CN1C(=O)C[C@H](NC(=O)NCC2(c3ccc(F)cc3F)CCCC2)[C@H]1c1ccc(F)c(F)c1
vNsp8-nsp12.1-161	PV-001961137748	-9.8	0.327	406.48	REAL	O=C1CN(C(=O)N[C@@H]2CCCN(C(=O)Cc3ccccc3)C2)Cc2ccccc2N1
vNsp8-nsp12.1-162	PV-001962810693	-9.8	0.350	377.49	REAL	O=C1CN(C(=O)NCc2ccc(C3CCCCC3)cc2)Cc2ccccc2N1
vNsp8-nsp12.1-163	PV-001963249370	-9.8	0.316	420.51	REAL	C[C@H](NC(=O)N1Cc2ccccc2NC(=O)[C@H]1C)c1ccc(N2CCCCC2=O)cc1
vNsp8-nsp12.1-164	Z1023497304	-9.8	0.316	418.43	REAL	O=C(c1cc(=O)c2ccccc2[nH]1)N1CCC[C@@H](c2nc(-c3ccc(F)cc3)no2)C1
vNsp8-nsp12.1-165	Z1024896812	-9.8	0.297	439.51	REAL	O=C1Nc2ccccc2[C@H]1C1CCN([C@@H]2CC(=O)N(c3ccc4ccccc4c3)C2=O)CC1
vNsp8-nsp12.1-166	Z1027495642	-9.8	0.316	411.46	REAL	CC(=O)N1c2ccccc2C[C@H]1C(=O)OCC(=O)c1ccc2c(c1)Cc1ccccc1-2
vNsp8-nsp12.1-167	Z1067033518	-9.8	0.306	444.56	REAL	O=C(CNC(=O)C1CCN(c2nc3ccccc3s2)CC1)Nc1ccccc2ccccc12
vNsp8-nsp12.1-168	Z1099605958	-9.8	0.306	433.38	REAL	O=C(Nc1n[nH]c2ccc(F)cc12)c1cccc(C(=O)Nc2n[nH]c3ccc(F)cc23)n1
vNsp8-nsp12.1-169	Z1103621774	-9.8	0.297	439.51	REAL	C[C@@H]1Cc2ccccc2N1Cc1ccoc1C(=O)NNC(=O)Cc1ccc2ccccc2c1
vNsp8-nsp12.1-170	Z1128821654	-9.8	0.316	417.51	REAL	CC(=O)N1Cc2ccccc2C[C@H]1C(=O)N1CCC([C@H]2C(=O)Nc3ccccc32)CC1
vNsp8-nsp12.1-171	Z1181376000	-9.8	0.297	436.51	REAL	C[C@@H]1Cc2ccccc2[C@@H]1NC(=O)NNC(=O)c1cc(-c2ccccc2)nc2ccccc12
vNsp8-nsp12.1-172	Z1212622998	-9.8	0.306	428.50	REAL	CC(=O)N1CCc2ccccc2[C@H]1CC(=O)Nc1n[nH]c2c1c(-c1ccccc1)nn2C
vNsp8-nsp12.1-173	Z1212623288	-9.8	0.327	398.43	REAL	Cc1ccc(-c2cc(C(=O)Nc3n[nH]c4c3c(-c3ccccc3)nn4C)on2)cc1
vNsp8-nsp12.1-174	Z1232916804	-9.8	0.327	402.47	REAL	O=C1C[C@@H](N2CCC(c3ccccc3F)CC2)C(=O)N1c1ccc2ccccc2c1
vNsp8-nsp12.1-175	Z1239889878	-9.8	0.350	375.40	REAL	Cc1ccc2[nH]c3c(c2c1)CN(C(=O)c1cc(=O)[nH]c2ccc(F)cc12)CC3
vNsp8-nsp12.1-176	Z1260483075	-9.8	0.316	412.53	REAL	C[C@H]1Cc2ccccc2CN1C(=O)C1CCN(C(=O)c2cccc3ccccc23)CC1
vNsp8-nsp12.1-177	Z1263165231	-9.8	0.306	437.51	REAL	C[C@@H]1CN(CC(=O)N2c3ccccc3NC(=O)C23CCCC3)C[C@@H](c2ccc(F)cc2)O1
vNsp8-nsp12.1-178	Z1279182018	-9.8	0.316	428.50	REAL	O=C([C@H]1C[C@@]12CCc1ccccc12)N1CCCN(Cc2ccc(C(F)(F)F)cc2)CC1
vNsp8-nsp12.1-179	Z1279472282	-9.8	0.306	424.54	REAL	O=C(c1cccc2ccccc12)N1CCN(C(=O)[C@H]2C[C@@]23CCCc2ccccc23)CC1
vNsp8-nsp12.1-180	Z1283488639	-9.8	0.306	428.49	REAL	O=C(NNC(=O)N1CCC([C@@H]2C(=O)Nc3ccccc32)CC1)c1cccc2ccccc12
vNsp8-nsp12.1-181	Z1312645830	-9.8	0.306	425.53	REAL	C[C@@H]1CN(C(=O)c2ccnc(C(=O)N3Cc4ccccc4[C@@H](C)C3)c2)Cc2ccccc21
vNsp8-nsp12.1-182	Z1313725294	-9.8	0.297	449.55	REAL	O=C([C@@H]1CCCCN1C(=O)c1ccc(=O)[nH]n1)N1CCC(N2CCc3ccccc3C2)CC1
vNsp8-nsp12.1-183	Z1314453644	-9.8	0.306	425.53	REAL	Cc1cccc2c1CCN(C(=O)c1ccnc(C(=O)N3CCc4c(C)cccc4C3)c1)C2
vNsp8-nsp12.1-184	Z1357118605	-9.8	0.316	419.50	REAL	C[C@@H]1CCc2c(F)cccc2[C@@H]1NC(=O)N1CCn2c(Cc3ccccc3)nnc2C1
vNsp8-nsp12.1-185	Z1368707600	-9.8	0.306	434.49	REAL	O=C(c1cccc2ccccc12)N1CCC[C@@H](C(=O)N2CCc3c(F)ccc(F)c3C2)C1
vNsp8-nsp12.1-186	Z1375389621	-9.8	0.297	446.59	REAL	CN1CCN(C(=O)c2ccccc2NC(=O)N2CCC[C@]3(CCCc4ccccc43)C2)CC1
vNsp8-nsp12.1-187	Z1408677299	-9.8	0.316	415.49	REAL	O=C(Cc1ccc2ccccc2c1)NNC(=O)N[C@H]1CC2(CCC2)Oc2ccccc21
vNsp8-nsp12.1-188	Z1410522214	-9.8	0.297	441.49	REAL	O=C(NNc1nc2ccccc2c(=O)[nH]1)[C@@H]1CCCN(C(=O)c2cccc3ccccc23)C1
vNsp8-nsp12.1-189	Z1413768132	-9.8	0.306	433.44	REAL	C[C@]1(c2ccc3ccccc3c2)NC(=O)N(CC(=O)N2CCOc3ccccc(F)c32)C1=O
vNsp8-nsp12.1-190	Z1431636041	-9.8	0.297	441.49	REAL	CC1(C)C(=O)Nc2ccc(C(=O)CN3C(=O)N[C@]1(C)c4ccc5ccccc5c4)C3=O)cc21
vNsp8-nsp12.1-191	Z1446807423	-9.8	0.350	371.42	REAL	Fc1ccccc1-c1nnc2ccc(NC[C@H]3[C@H]4Cc5ccccc5[C@H]34)nn12
vNsp8-nsp12.1-192	Z1452372791	-9.8	0.316	408.46	REAL	Cc1cccc(-c2cncc(C(=O)Nc3n[nH]c4c3c(-c3ccccc3)nn4C)c2)c1
vNsp8-nsp12.1-193	Z1471454329	-9.8	0.306	422.53	REAL	Cc1nc(C(=O)N2CCc3ccccc3[C@@H](c3ccccc3)[C@@H]2C)nn1-c1ccccc1
vNsp8-nsp12.1-194	Z1472908284	-9.8	0.306	422.53	REAL	C[C@@H]1[C@H](c2ccccc2)c2ccccc2CCN1C(=O)Cc1cc2ccccc2[nH]c1=O
vNsp8-nsp12.1-195	Z1503246681	-9.8	0.306	427.55	REAL	O=C(NCc1cc2c([nH]c1=O)CCC2)N[C@@H](c1ccccc1)[C@@H]1CCCc2ccccc21
vNsp8-nsp12.1-196	Z1506264384	-9.8	0.377	343.43	REAL	O=C(c1ccc2ccccc2c1)N1CCO[C@]2(CCc3ccccc32)C1
vNsp8-nsp12.1-197	Z1507105069	-9.8	0.316	412.49	REAL	O=C1C[C@@H](N2CCO[C@]3(CCc4ccccc43)C2)C(=O)N1c1ccc2ccccc2c1
vNsp8-nsp12.1-198	Z1507811661	-9.8	0.338	382.46	REAL	O=C(c1cc2c(ccc3ccccc32)[nH]1)N1CCO[C@]2(CCc3ccccc32)C1
vNsp8-nsp12.1-199	Z1515148618	-9.8	0.338	422.89	REAL	CN1C(=O)C[C@@H](NC(=O)N2CCC(=O)N[C@H]3CCCC[C@H]32)[C@@H]1c1ccc(Cl)c(F)c1
vNsp8-nsp12.1-200	Z1579619188	-9.8	0.327	402.42	REAL	O=C1C[C@H](C(=O)Nc2cccc(-c3ccc4c(c3)CCO4)c2)c2ccc(F)cc2N1

Supplementary Table 40. Virtual screening hits 101 to 200 of the screen against the nsp12 binding site on nsp8 (Screen ID: 22). Compounds were filtered so that hits had MW < 600 dalton, cLogP < 6, number of hydrogen bond acceptors < 11, and no reactive functional groups. The name of each compound consists of the initial letter 'v' for virtual hit, followed by the target protein name and the target site ('nsp12' for nsp12 binding site, 1 for docking scenario 1). The score is the docking score given by QuickVina 2 in kcal/mol. The ligand efficiency (LE) is computed as LE = -score/#NonH, where #NonH is the number of heavy (i.e. non hydrogen) atoms.

Name	Catalog ID	Score	LE	MW	Library	SMILES
vNsp9-nsp9.1-1	Z996744910	-9	0.243	494.593	REAL	O=C(c1cc2ccccc2[nH]1)N1CCN(C(=O)C2CCN(C(=O)c3cccc4ccccc34)CC2)CC1
vNsp9-nsp9.1-2	Z743656142	-8.8	0.314	389.446	REAL	COC(=O)COc1cccc(C(=O)OCC(=O)N[C@@H](C)[C@H]2C[C@@H]3CC[C@@H]2C3)c1
vNsp9-nsp9.1-3	Z1025324518	-8.6	0.253	455.56	REAL	O=C(NCC(=O)N1CCc2ccccc2C1)NCc1ccc(N2CCc3ccccc3C2)nc1
vNsp9-nsp9.1-4	Z1458999179	-8.6	0.253	448.564	REAL	O=C(NC[C@@H]1[C@H]2Cc3ccccc3[C@@H]12)c1cccc(C(=O)NC[C@@H]2[C@H]3Cc4ccccc4[C@@H]23)c1
vNsp9-nsp9.1-5	Z397588902	-8.6	0.246	463.536	REAL	O=C1O[C@@H](c2ccccc2)Cc2cc(C(=O)N3CCN(c4ccc5ccccc5n4)CC3)ccc21
vNsp9-nsp9.1-6	Z402807448	-8.6	0.253	450.54	REAL	C[C@@H](c1nc(-c2ccccc2)no1)N1CCN(C(=O)c2ccc3c(c2)-c2ccccc2C3)CC1
vNsp9-nsp9.1-7	PV-001952969357	-8.5	0.258	441.573	REAL	Cc1ccc(CNC(=O)c2cccc(CNC(=O)N3CCCc4ccccc4CC3)c2)cc1
vNsp9-nsp9.1-8	Z1019375078	-8.5	0.23	494.549	REAL	O=C(NCC(=O)N1CCc2ccccc21)NNC(=O)c1ccc(COc2ccc3ccccc3c2)cc1
vNsp9-nsp9.1-9	Z1023498194	-8.5	0.23	496.497	REAL	O=C(c1cccc(N2C(=O)c3ccccc3C2=O)c1)N1CCC[C@@H](c2nc(-c3ccc(F)cc3)no2)C1
vNsp9-nsp9.1-10	Z1095050508	-8.5	0.243	488.502	REAL	O=C(Nc1nc(-c2ccc3ccccc3n2)n[nH]1)c1ccccc(S(=O)(=O)Nc2ccccc2F)c1
vNsp9-nsp9.1-11	Z1156365264	-8.5	0.25	453.497	REAL	O=C(CCNC(=O)c1ccc2ccccc2c1)Nc1cccc(-c2ccc3c(c2)OCCO3)n1
vNsp9-nsp9.1-12	Z1279860846	-8.5	0.293	390.485	REAL	C[C@]1(C(=O)Nc2ccc3[nH]c(N4CCOCC4)nc3c2)CCc2ccccc2C1
vNsp9-nsp9.1-13	Z1685539403	-8.5	0.283	400.481	REAL	c1ccc2c(c1)CC[C@H](c1noc(C3CCN(c4nc5ccccc5o4)CC3)n1)C2
vNsp9-nsp9.1-14	Z2174896855	-8.5	0.258	439.51	REAL	O=C1O[C@H](c2ccccc2)Cc2cc(C(=O)N3CC[C@@]4(CCc5ccccc5O4)C3)ccc21
vNsp9-nsp9.1-15	Z230413636	-8.5	0.25	450.54	REAL	Cc1ccc(-c2noc(CN3CCN(C(=O)c4ccc5c(c4)-c4ccccc4C5)CC3)n2)cc1
vNsp9-nsp9.1-16	Z2651942379	-8.5	0.236	480.566	REAL	O=C([C@@H]1CC(=O)N(c2ccc3c(c2)Cc2ccccc2-3)C1)N1CCc2ccnc2N2C[C@H](O)C[C@H]2C1
vNsp9-nsp9.1-17	Z409843976	-8.5	0.243	487.583	REAL	Cc1sc2nc(CN3CCN(C(=O)Nc4ccc5oc6ccccc6c5c4)CC3)[nH]c(=O)c2c1C
vNsp9-nsp9.1-18	Z448668286	-8.5	0.236	479.586	REAL	Cn1ncc2c(N3CCN(C(=O)NC[C@H]4CC5c6ccccc6C4c4ccccc45)CC3)ncnc21
vNsp9-nsp9.1-19	Z448918604	-8.5	0.236	479.539	REAL	C[C@H](NC(=O)NNC(=O)c1ccc(COc2ccc3ccccc3c2)cc1)c1nc2ccccc2[nH]1
vNsp9-nsp9.1-20	Z758711278	-8.5	0.23	494.597	REAL	CCc1cccc2c(C3CCN(C(=O)CCc4nc5c(cnn5-c5ccccc5)c(=O)[nH]4)CC3)c[nH]c12
vNsp9-nsp9.1-21	ZINC000408976120	-8.5	0.243	451.488	ZINC	O=C(Nc1cccc2ccccc21)c1ccc2nc3c4ccccnc4c4nccc4c3nc2c1
vNsp9-nsp9.1-22	Z1148372350	-8.4	0.227	497.549	REAL	O=C(Nc1ccc(CC(=O)N2CCc3ccccc32)cc1)[C@H]1CCN(c2ccc3c(c2)OCCO3)C1=O
vNsp9-nsp9.1-23	Z1153384088	-8.4	0.233	494.476	REAL	O=C(NCc1ccc(-n2ccnc2)nc1)Nc1ccc(CNC(=O)c2ccc(C(F)(F)F)cc2)cc1
vNsp9-nsp9.1-24	Z1158348688	-8.4	0.247	452.556	REAL	C[C@H](c1nc(-c2ccccc2)no1)N1CCN(C(=O)[C@H]2C[C@@H]2c2cc3ccccc3c2)CC1
vNsp9-nsp9.1-25	Z1602294442	-8.4	0.262	433.55	REAL	CC1(C)CC[C@H]2C[C@H](NC(=O)Nc3ccc(C(=O)N4CCOCC4)cc3)c3cccc1c32
vNsp9-nsp9.1-26	Z1890552278	-8.4	0.247	449.469	REAL	O=C(Cc1noc(Cc2cc3c(ccc4ccccc43)o2)n1)N1CCn2c1nc1ccccc12
vNsp9-nsp9.1-27	Z1976164250	-8.4	0.255	441.509	REAL	O=C(N[C@H]1CCc2nnc(-c3ccc(F)cc3)n2C1)N[C@@H]1C[C@H]1c1ccc2ccccc2c1
vNsp9-nsp9.1-28	Z226664332	-8.4	0.227	493.565	REAL	Nc1nc(CN2CCN(C(=O)c3ccc4c(c3)C[C@@H](c3ccccc3)OC4=O)CC2)nc2ccccc12
vNsp9-nsp9.1-29	Z2624532205	-8.4	0.29	391.517	REAL	O=C(Nc1ccc2c(c1)CCCCC2)N1CCc2nnc(N3CCC3)cc2C1
vNsp9-nsp9.1-30	Z315128454	-8.4	0.233	489.485	REAL	C/C(=N/Nc1nc2cc(F)c(F)cc2[nH]1)c1ccc(NC(=O)C[C@@H]2Nc3ccccc3NC2=O)cc1
vNsp9-nsp9.1-31	Z383457526	-8.4	0.247	458.524	REAL	Cc1cc(N2CCN(C(=O)c3ccc4c(=O)n5c(nc4c3)CCCCC5)CC2)n2ncnc2n1
vNsp9-nsp9.1-32	Z654854304	-8.4	0.233	485.586	REAL	O=C(c1ccc2c(=O)n3c(nc2c1)CCCCC3)N1CCN(CC(=O)N2CCc3ccccc32)CC1
vNsp9-nsp9.1-33	Z908875862	-8.4	0.233	481.594	REAL	O=C(Nc1cccc(C(=O)N2CCC(N3CCc4ccccc4C3)CC2)c1)[C@H]1Cc2ccccc2O1
vNsp9-nsp9.1-34	Z92055821	-8.4	0.233	499.502	REAL	O=C(CSc1nnc([C@H]2COc3ccccc3O2)o1)Nc1ccc2c(c1)C(=O)c1ccccc1C2=O
vNsp9-nsp9.1-35	Z988060630	-8.4	0.247	453.544	REAL	Cc1ccn2cc(CNC(=O)Nc3ccc(CC(=O)N4CCCc5ccccc54)cc3)nc2c1
vNsp9-nsp9.1-36	Z1022495902	-8.3	0.237	465.551	REAL	O=C(NCC(=O)N1CCc2ccccc2C1)[C@H]1CC(=O)N(c2ccc3c(c2)Cc2ccccc2-3)C1
vNsp9-nsp9.1-37	Z1025321958	-8.3	0.252	448.609	REAL	CC(C)(C)c1ccc(N2CCC(NC(=O)NCCC(=O)N3CCc4ccccc4C3)CC2)cc1
vNsp9-nsp9.1-38	Z1027916538	-8.3	0.231	482.582	REAL	O=C(NCCC(=O)N1CCc2ccccc2C1)Nc1ccc(CC(=O)N2CCCc3ccccc32)cc1
vNsp9-nsp9.1-39	Z1101912653	-8.3	0.231	479.535	REAL	O=C(Nc1cccc(N2C(=O)c3ccccc3C2=O)c1)C1CCN(C(=O)/C=C\c2ccccc2)CC1
vNsp9-nsp9.1-40	Z1152269316	-8.3	0.244	471.434	REAL	O=C(NCc1ccc2c(c1)OCO2)Nc1ccc(CNC(=O)c2ccc(C(F)(F)F)cc2)cc1
vNsp9-nsp9.1-41	Z1157896444	-8.3	0.231	498.649	REAL	O=C([C@H]1C[C@@H]1c1ccc2ccccc2c1)N1CCN(Cc2nc3sc4c(c3c(=O)[nH]2)CCCC4)CC1
vNsp9-nsp9.1-42	Z1160969640	-8.3	0.237	484.579	REAL	O=C(NCc1ccc(N2CCc3ccccc3C2)nc1)c1csc(-c2ccc3c(c2)OCCO3)n1
vNsp9-nsp9.1-43	Z1250586272	-8.3	0.252	438.486	REAL	Cc1cc(C(=O)NC[C@H]2CC3c4ccccc4C2c2ccccc23)nc2nc(O)[nH]c(=O)c12
vNsp9-nsp9.1-44	Z1273268389	-8.3	0.268	433.574	REAL	C[C@]1(C(=O)Nc2ccc(-c3csc(N4CCOCC4)n3)cc2)CCc2ccccc2C1
vNsp9-nsp9.1-45	Z1323784801	-8.3	0.259	421.459	REAL	O=C(NCc1nc(NC(=O)c2ccc3ccccc3c2)n[nH]1)c1ccc2ccccc2c1
vNsp9-nsp9.1-46	Z1449091094	-8.3	0.244	449.552	REAL	O=C(NC[C@@H]1[C@H]2Cc3ccccc3[C@@H]12)c1cccc(C(=O)NC[C@H]2[C@@H]3Cc4ccccc4[C@H]23)n1
vNsp9-nsp9.1-47	Z1449094151	-8.3	0.244	448.564	REAL	O=C(NC[C@@H]1[C@@H]2Cc3ccccc3[C@@H]12)c1ccc(C(=O)NC[C@H]2[C@@H]3Cc4ccccc4[C@@H]23)cc1
vNsp9-nsp9.1-48	Z1685085222	-8.3	0.244	449.469	REAL	O=C1C[C@H](c2nc(-c3ccc4[nH]c(=O)[nH]c4c3)no2)CN1c1ccc2c(c1)Cc1ccccc1-2
vNsp9-nsp9.1-49	Z17183268	-8.3	0.296	398.573	REAL	CCn1c(Cc2ccccc2)nnc1SCC(=O)N[C@@H](C)[C@H]1C[C@H]2CC[C@H]1C2
vNsp9-nsp9.1-50	Z2014845245	-8.3	0.259	447.514	REAL	O=C(N[C@@H]1CCc2ccccc2OC1)c1ccc(NC2=NS(=O)(=O)c3ccccc32)cc1
vNsp9-nsp9.1-51	Z2108705053	-8.3	0.259	435.541	REAL	O=C(NC1CCN(C(=O)c2ccccc2F)CC1)NC1[C@@H]2CC[C@@H]1Cc1ccccc1C2
vNsp9-nsp9.1-52	Z230394528	-8.3	0.244	455.56	REAL	Cc1ccc(-c2noc(CN3CCN(C(=O)c4ccc5[nH]c6c(c5c4)CCCC6)CC3)n2)cc1
vNsp9-nsp9.1-53	Z2590314585	-8.3	0.307	371.44	REAL	Cc1cnc2nc(C(=O)O[C@@H](C)C(=O)N[C@H](C)[C@@H]3C[C@H]4CC[C@H]3C4)nn2c1
vNsp9-nsp9.1-54	Z2902585873	-8.3	0.244	455.477	REAL	Cc1ccc(C)n2ncc(-c3noc(-c4cccc(NN5C(=O)[C@@H]6CC=CC[C@@H]6C5=O)c4)n3)c2n1
vNsp9-nsp9.1-55	Z33016959	-8.3	0.231	498.562	REAL	Cc1ccc(C(=O)NCC(=O)NNC(=O)c2ccc(CN3C(=O)c4ccc5ccc3c45)cc2)s1
vNsp9-nsp9.1-56	Z383455608	-8.3	0.231	498.468	REAL	Cc1cc(N2CCN(C(=O)c3nn(-c4cccc(C(F)(F)F)c4)c(C)cc3=O)CC2)n2ncnc2n1
vNsp9-nsp9.1-57	Z494517906	-8.3	0.231	483.523	REAL	C[C@@H](NC(=O)NNC(=O)c1ccc(COc2ccc3ccccc3c2)cc1)c1ccc2c(c1)OCO2
vNsp9-nsp9.1-58	Z495834056	-8.3	0.231	499.957	REAL	O=C(NCc1cn2cc(Cl)ccc2n1)NNC(=O)c1ccc(COc2ccc3ccccc3c2)cc1
vNsp9-nsp9.1-59	Z654861696	-8.3	0.252	437.541	REAL	O=C(c1ccc2c(c1)-c1ccccc1C2)N1CCN(CC(=O)N2CCc3ccccc32)CC1
vNsp9-nsp9.1-60	Z741365778	-8.3	0.224	490.518	REAL	O=C(NNC(=O)[C@H]1CC(c2ccccc2)=NO1)c1ccc(CN2C(=O)c3ccc4cccc2c34)cc1
vNsp9-nsp9.1-61	Z743981502	-8.3	0.231	495.606	REAL	O=C(CSc1nnc(-c2ccc3ccccc3c2)o1)N1CCN(Cc2cccc3ccnc23)CC1
vNsp9-nsp9.1-62	Z744367702	-8.3	0.244	455.604	REAL	C[C@H](CNC(=O)NCc1ccc(N2CCc3ccccc3C2)nc1)N1CCc2ccccc2C1
vNsp9-nsp9.1-63	Z746548344	-8.3	0.237	490.558	REAL	O=C(c1cccc(S(=O)(=O)Nc2ccccc2F)c1)N1CCN(c2ccc3ccccc3n2)CC1
vNsp9-nsp9.1-64	Z793728496	-8.3	0.231	489.526	REAL	O=C(COC(=O)[C@@H]1CCCN(C(=O)N2CCCC2)C1)Nc1ccc2c(c1)C(=O)c1ccccc1C2=O
vNsp9-nsp9.1-65	Z937715906	-8.3	0.231	478.546	REAL	O=C(CCC(=O)c1ccc2c(c1)-c1ccccc1C2)OCC(=O)N1CCc2[nH]c3ccccc3c2C1
vNsp9-nsp9.1-66	Z954105534	-8.3	0.224	488.593	REAL	O=C(CNCc1ccc(-n2cnc3ccccc32)cc1)NCc1ccc(N2CCc3ccccc3C2)nc1
vNsp9-nsp9.1-67	Z980286566	-8.3	0.237	464.524	REAL	O=C(Nc1ccc(CC(=O)N2CCCc3ccccc32)cc1)c1ccc(=O)n(-c2ccccc2)n1
vNsp9-nsp9.1-68	Z992139876	-8.3	0.237	472.519	REAL	O=C(NCCCC(=O)N1CCC[C@@H](c2nc(-c3cccc(F)c3)no2)C1)c1ccc2ccccc2c1
vNsp9-nsp9.1-69	ZINC000016292162	-8.3	0.244	448.477	ZINC	Cc1ccc(C2=N/C(=C3ccc(/C=C4\N=C(c5ccc(C)cc5)OC4=O)cc3)C(=O)O2)cc1
vNsp9-nsp9.1-70	ZINC000223098740	-8.3	0.259	460.988	ZINC	O=C(Nc1nnc(-c2ccc(Cl)cc2)s1)c1ccc(CN2CCc3ccccc3C2)cc1
vNsp9-nsp9.1-71	PV-001946409651	-8.2	0.241	456.505	REAL	CN(C)c1ccc(NC(=O)NNC(=O)c2ccc(COc3ccc4ccccc4c3)cc2)ncn1
vNsp9-nsp9.1-72	Z1027916486	-8.2	0.241	459.548	REAL	Cc1noc([C@@H]2CCCN(C(=O)Nc3ccc(CC(=O)N4CCCc5ccccc54)cc3)C2)n1
vNsp9-nsp9.1-73	Z1074947666	-8.2	0.234	473.546	REAL	O=C(Nc1ccc(CC(=O)N2CCCc3ccccc32)cc1)N1CCO[C@H](c2ccccc2)C1
vNsp9-nsp9.1-74	Z1075913880	-8.2	0.222	497.549	REAL	O=C(NCc1ccc2c(c1)OCCCO2)NNC(=O)c1ccc(COc2ccc3ccccc3c2)cc1
vNsp9-nsp9.1-75	Z1094011376	-8.2	0.228	489.574	REAL	COc1ccc(NC(=O)N2CCN(C(=O)N3CCCC3)CC2)cc1OCc1ccc2ccccc2n1
vNsp9-nsp9.1-76	Z1095049898	-8.2	0.241	452.517	REAL	O=C(Nc1nc(-c2ccc3ccccc3n2)n[nH]1)C1CCN(C(=O)/C=C/c2ccccc2)CC1
vNsp9-nsp9.1-77	Z1132550717	-8.2	0.241	456.544	REAL	Cc1ccc(CNC(=O)c2cccc(CNC(=O)Nc3ccc4c(c3)CCC(=O)N4C)c2)cc1
vNsp9-nsp9.1-78	Z1153383902	-8.2	0.228	497.519	REAL	O=C(NCc1ccnc(N2CCCC2)c1)Nc1ccc(CNC(=O)c2ccc(C(F)(F)F)cc2)cc1
vNsp9-nsp9.1-79	Z1160217482	-8.2	0.241	460.485	REAL	O=C(COC(=O)[C@H]1C[C@@H]1c1ccc2ccccc2c1)NC(=O)Nc1ccc2c(c1)OCCCO2
vNsp9-nsp9.1-80	Z1222907927	-8.2	0.256	445.542	REAL	O=C(NC[C@H]1CCc2ccccc2C1)c1ccc(NC2=NS(=O)(=O)c3ccccc32)cc1
vNsp9-nsp9.1-81	Z1262345314	-8.2	0.248	437.541	REAL	CN1CCC(=O)Nc2cc(C(=O)NC[C@H]3CC4c5ccccc5C3c3ccccc34)ccc21
vNsp9-nsp9.1-82	Z1315796391	-8.2	0.241	449.509	REAL	Cn1nc2c(cc1=O)CN(C(=O)CCC(=O)c1ccc3ccc4ccc5ccc1c3c45)CC2
vNsp9-nsp9.1-83	Z131821778	-8.2	0.228	496.633	REAL	O=C(c1ccc2c(c1)-c1ccccc1C2)N1CCN(Cc2nc3sc4c(c3c(=O)[nH]2)CCCC4)CC1
vNsp9-nsp9.1-84	Z135713990	-8.2	0.222	489.534	REAL	O=C(CCc1nc2ccccc2[nH]1)NNC(=O)c1ccc(CN2C(=O)c3cccc4cccc2c34)cc1
vNsp9-nsp9.1-85	Z1373694948	-8.2	0.256	449.573	REAL	C[C@@H](C(=O)Nc1ccc(S(=O)(=O)/N=C2\CCCCCN2)cc1)c1ccc2ccccc2c1
vNsp9-nsp9.1-86	Z1374832514	-8.2	0.248	446.549	REAL	C[C@@]1(c2ccc(CNC(=O)N3CCC[C@@]4(CCCc5ccccc54)C3)cc2)NC(=O)NC1=O
vNsp9-nsp9.1-87	Z1472866131	-8.2	0.241	449.552	REAL	O=C(N[C@H]1[C@H]2CCc3ccccc3[C@@H]21)c1cncc(C(=O)N[C@H]2[C@@H]3CCc4ccccc4[C@H]32)c1
vNsp9-nsp9.1-88	Z1473258230	-8.2	0.273	418.563	REAL	O=C(NC1CCN(c2nc3ccccc3s2)CC1)N[C@H]1[C@@H]2CCc3ccccc3[C@@H]21
vNsp9-nsp9.1-89	Z1474433863	-8.2	0.248	438.525	REAL	O=C(N[C@H]1[C@H]2CCc3ccccc3[C@@H]21)c1ccc(C(=O)N[C@@H]2[C@@H]3CCc4ccccc4[C@H]32)o1
vNsp9-nsp9.1-90	Z1546798785	-8.2	0.256	442.404	REAL	Cc1cc(C)nc(-n2nc(C(=O)Nc3nc(-c4cccc(C(F)(F)F)c4)n[nH]3)cc2C)n1
vNsp9-nsp9.1-91	Z1610577213	-8.2	0.256	441.514	REAL	Cc1cc2ccccc2nc1NNC(=O)CSc1nnc(-c2ccc3ccccc3c2)o1
vNsp9-nsp9.1-92	Z1664538010	-8.2	0.273	397.441	REAL	c1ccc2cc(-c3nnc(C4CCN(c5ccc6nncn6n5)CC4)o3)ccc2c1
vNsp9-nsp9.1-93	Z1684580724	-8.2	0.256	424.459	REAL	C[C@@]1(c2cccc(-c3noc([C@H]4C[C@@H]4c4ccc5ccccc5c4)n3)c2)NC(=O)NC1=O
vNsp9-nsp9.1-94	Z1723443504	-8.2	0.265	410.476	REAL	Cn1c(=O)[nH]c2ncc(-c3cccc(C(=O)N[C@H]4[C@@H]5CCc6ccccc6[C@@H]54)c3)cc21
vNsp9-nsp9.1-95	Z1915932083	-8.2	0.248	447.581	REAL	O=C(N[C@@H]1CCc2[nH]c(C3CCCCC3)nc2C1)C1CCN(c2nc3ccccc3o2)CC1
vNsp9-nsp9.1-96	Z203542340	-8.2	0.248	478.596	REAL	O=C1CC[C@@]2(C(=O)Nc3ccc(-c4csc(N5CCOCC5)n4)cc3)Sc3ccccc3N12
vNsp9-nsp9.1-97	Z2090581018	-8.2	0.273	397.516	REAL	O=C([C@H]1C[C@@H]1c1ccc2ccccc2c1)N1C[C@H](c2ccccc2)[C@@H]2COCC[C@H]21
vNsp9-nsp9.1-98	Z2146048613	-8.2	0.248	447.581	REAL	CC(=O)N1C[C@@H]2CCC[C@H](NC(=O)NCc3ccc(N4CCc5ccccc5C4)nc3)[C@H]2C1
vNsp9-nsp9.1-99	Z2160220603	-8.2	0.248	440.462	REAL	Cc1nc2c(-c3noc(-c4cccc(NN5C(=O)[C@@H]6CC=CC[C@@H]6C5=O)c4)n3)cccc2[nH]1
vNsp9-nsp9.1-100	Z2167605163	-8.2	0.256	434.494	REAL	O=C(Nc1ccc2nc(N3CCOCC3)oc2c1)N1CC[C@]2(CCc3ccccc3O2)C1

Supplementary Table 41. Top 100 virtual hits of the screen against the dimerization site of nsp9 (Screen ID: 23). The name of each compound consists of the initial letter 'v' for virtual hit, followed by the target protein name and the target site ('nsp9' for nsp9 binding site, 1 for docking scenario 1). The score is the docking score given by QuickVina 2 in kcal/mol. The ligand efficiency (LE) is computed as LE = -score/#NonH, where #NonH is the number of heavy (i.e. non hydrogen) atoms.

Name	Catalog ID	Score	LE	MW	Library	SMILES
vNsp9-nsp9.1-101	Z2182524186	-8.2	0.256	448.59	REAL	O=C(NC1CCN(c2nc3ccccc3s2)CC1)N1CC[C@@]2(CCc3ccccc3O2)C1
vNsp9-nsp9.1-102	Z2204561306	-8.2	0.265	412.42	REAL	O=C1/C(=C/c2ccc(Oc3cccc(F)c3)cc2)CCc2c1cnn2-c1ncccn1
vNsp9-nsp9.1-103	Z226646826	-8.2	0.228	483.57	REAL	Nc1nc(CN2CCN(C(=O)c3ccc4c(=O)n5c(nc4c3)CCCCC5)CC2)nc2ccccc12
vNsp9-nsp9.1-104	Z242688088	-8.2	0.241	489.99	REAL	C[C@@H](NC(=O)CSc1nc(=O)c2cnn(-c3cccc(Cl)c3)c2[nH]1)c1ccc2ccccc2c1
vNsp9-nsp9.1-105	Z27148941	-8.2	0.222	492.53	REAL	C[C@@H](NC(=O)c1ccccc1)C(=O)NNC(=O)c1ccc(CN2C(=O)c3cccc4cccc2c34)cc1
vNsp9-nsp9.1-106	Z2843319202	-8.2	0.283	388.51	REAL	O=C1CC[C@H](c2ccc(C(=O)N3CCC4(CCc5ccccc5C4)CC3)cc2)N1
vNsp9-nsp9.1-107	Z301270256	-8.2	0.273	419.55	REAL	O=C(Nc1ccc(-c2csc(N3CCOCC3)n2)cc1)[C@H]1CCCc2ccccc21
vNsp9-nsp9.1-108	Z316831972	-8.2	0.256	445.54	REAL	C[C@H]1Sc2ccc(C(=O)N3CCN(C(=O)c4cccc5ccccc45)CC3)cc2NC1=O
vNsp9-nsp9.1-109	Z340407600	-8.2	0.234	489.64	REAL	CC(C)c1ccc2cc(C(=O)N3CCN(Cc4nc5sc6c(c5c(=O)[nH]4)CCCC6)CC3)[nH]c2c1
vNsp9-nsp9.1-110	Z383112800	-8.2	0.241	450.54	REAL	Cc1ccc(-c2noc(CN3CCN(C(=O)c4ccc5c(c4)Cc4ccccc4-5)CC3)n2)cc1
vNsp9-nsp9.1-111	Z383452882	-8.2	0.256	429.53	REAL	Cc1cc(N2CCN(C(=O)c3ccc4[nH]c5c(c4c3)CCCCC5)CC2)n2ncnc2n1
vNsp9-nsp9.1-112	Z407184134	-8.2	0.241	446.51	REAL	O=C(NCc1ccc2ccccc2n1)c1ccc(C(=O)NCc2ccc3ccccc3n2)cc1
vNsp9-nsp9.1-113	Z424118300	-8.2	0.315	352.38	REAL	Cc1nc2ccccc2c(C)c1CC(=O)N1CCc2cc(F)c(F)cc21
vNsp9-nsp9.1-114	Z486313780	-8.2	0.228	488.56	REAL	O=C(NCc1ccc(C(=O)N2CCCCC2)cc1)Nc1ccc(C(=O)NCc2ccc(F)cc2)cc1
vNsp9-nsp9.1-115	Z499064874	-8.2	0.248	465.58	REAL	Cc1ncc2c(n1)CC[C@H](NC(=O)N1CCN(S(=O)(=O)c3ccc4ccccc4c3)CC1)C2
vNsp9-nsp9.1-116	Z499114828	-8.2	0.234	493.63	REAL	Cc1ncc2c(n1)CC[C@@H](NC(=O)N1CCN(Cc3nc4sc5c(c4c(=O)[nH]3)CCCC5)CC1)C2
vNsp9-nsp9.1-117	Z507908380	-8.2	0.222	495.58	REAL	O=C(NCc1ccc(N2CCCC2)nc1)NNC(=O)c1ccc(COc2ccc3ccccc3c2)cc1
vNsp9-nsp9.1-118	Z510529426	-8.2	0.241	455.56	REAL	C[C@H](NC(=O)NCc1ccc(N2CCc3ccccc3C2)nc1)c1ccc2c(c1)CCC(=O)N2
vNsp9-nsp9.1-119	Z511018740	-8.2	0.234	467.57	REAL	O=C(NCc1ccc(N2CCc3ccccc3C2)nc1)C1CCN(c2nc3ccccc3o2)CC1
vNsp9-nsp9.1-120	Z51914030	-8.2	0.265	431.52	REAL	O=C(N[C@H]1CCc2ccccc2C1)c1ccc(NC2=NS(=O)(=O)c3ccccc32)cc1
vNsp9-nsp9.1-121	Z741366036	-8.2	0.234	466.50	REAL	O=C(NNC(=O)c1noc2c1CCCC2)c1ccc(CN2C(=O)c3cccc4cccc2c34)cc1
vNsp9-nsp9.1-122	Z752463526	-8.2	0.222	499.61	REAL	Cc1ccc(CNC(=O)c2cccc(CNC(=O)N3CCC[C@H](C(=O)Nc4ccc(C)cn4)C3)c2)cc1
vNsp9-nsp9.1-123	Z804171530	-8.2	0.228	479.58	REAL	O=C(NC1CCN(C(=O)c2ccccc2)CC1)[C@@H]1CC(=O)N(c2ccc3c(c2)Cc2ccccc2-3)C1
vNsp9-nsp9.1-124	Z812723786	-8.2	0.222	493.61	REAL	O=C(Nc1ccc(CCC(=O)N2CCCC2)cc1)[C@H]1CC(=O)N(c2ccc3c(c2)Cc2ccccc2-3)C1
vNsp9-nsp9.1-125	Z899145384	-8.2	0.228	479.49	REAL	O=C(NNC(=O)c1cccc2c1OCCO2)c1ccc(CN2C(=O)c3cccc4cccc2c34)cc1
vNsp9-nsp9.1-126	Z988062996	-8.2	0.228	482.63	REAL	O=C(NCCCN1CCc2ccccc2C1)Nc1ccc(CC(=O)N2CCCc3ccccc32)cc1
vNsp9-nsp9.1-127	ZINC000034711653	-8.2	0.228	512.51	ZINC	O=C(NCc1ccc2c(c1)OCO2)c1csc(-c2ccc(OCc3ccc(C(F)(F)F)cc3)cc2)n1
vNsp9-nsp9.1-128	ZINC000034711978	-8.2	0.228	512.51	ZINC	O=C(NCc1ccc2c(c1)OCO2)c1csc(-c2ccc(OCc3cccc(C(F)(F)F)c3)cc2)n1
vNsp9-nsp9.1-129	ZINC000408640899	-8.2	0.241	450.54	ZINC	Cc1ccc(N2C[C@@H](C(=O)Nc3ccc(Oc4ccc5ccccc5c4)cc3)CC2=O)cc1C
vNsp9-nsp9.1-130	PV-000249168010	-8.1	0.312	354.45	REAL	C=C1CC(C)(C(=O)N2C[C@@H]3C(CNC(=O)[C@@H]4C[C@H]4c4ccco4)[C@H]3C2)C1
vNsp9-nsp9.1-131	PV-001820093546	-8.1	0.261	417.48	REAL	Cc1cccc(-c2cccc(C(=O)N3CCN(C(=O)Nc4ccc(F)cc4)CC3)c2)c1
vNsp9-nsp9.1-132	PV-001825197417	-8.1	0.245	445.54	REAL	Cc1cccc(-c2cccc(C(=O)N3CCN([C@@H](C)C(=O)Nc4ccc(F)c4)CC3)c2)c1
vNsp9-nsp9.1-133	PV-001943488888	-8.1	0.245	458.44	REAL	C[C@H]1C[C@H](NC(=O)Nc2ccc(CNC(=O)c3ccc(C(F)(F)F)cc3)cc2)c2ncnn21
vNsp9-nsp9.1-134	PV-001944080597	-8.1	0.253	446.89	REAL	O=C(NNC(=O)c1ccc(COc2ccc3ccccc3c2)cc1)Nc1cccc(Cl)n1
vNsp9-nsp9.1-135	PV-001945333845	-8.1	0.253	430.44	REAL	O=C(NNC(=O)c1ccc(COc2ccc3ccccc3c2)cc1)Nc1cccc(F)n1
vNsp9-nsp9.1-136	PV-001948123031	-8.1	0.245	445.48	REAL	CC(C)c1noc(NC(=O)NNC(=O)c2ccc(COc3ccc4ccccc4c3)cc2)n1
vNsp9-nsp9.1-137	PV-001955902609	-8.1	0.253	433.59	REAL	Cc1ccc(C(=O)N2CCC(NC(=O)N[C@H]3C[C@@H](C)C[C@@H](c4ccccc4)C3)CC2)cc1
vNsp9-nsp9.1-138	PV-001962078169	-8.1	0.253	440.63	REAL	CC(C)c1ccc(CC2CCN(C(=O)N[C@H]3CCCN(C(=O)N4CCCC4)C3)CC2)cc1
vNsp9-nsp9.1-139	PV-001970435868	-8.1	0.261	440.41	REAL	O=C(N[C@@H]1COc2c(F)cc(F)cc2C1)N1CCC[C@H](c2cccc(C(F)(F)F)c2)C1
vNsp9-nsp9.1-140	Z1003146774	-8.1	0.261	439.49	REAL	Cc1nn(C)c2ncc(S(=O)(=O)Oc3ccc4c5c(c(=O)oc4c3)CCCCC5)cc12
vNsp9-nsp9.1-141	Z1015438138	-8.1	0.245	441.53	REAL	O=C(NCC(=O)N1CCc2ccccc21)NCc1ccc(N2CCc3ccccc3C2)nc1
vNsp9-nsp9.1-142	Z1039648604	-8.1	0.253	435.53	REAL	C[C@@H](C(=O)N1CCC(c2nc(-c3ccccc3)n[nH]2)CC1)N1C(=O)[C@@H]2CCCC[C@@H]2C1=O
vNsp9-nsp9.1-143	Z1067528868	-8.1	0.261	414.50	REAL	Cc1cc(C(=O)NC2CCN(C(=O)c3ccc4c(c3)Cc3ccccc3-4)CC2)c(C)o1
vNsp9-nsp9.1-144	Z1070573146	-8.1	0.245	447.53	REAL	C[C@@H]1Oc2ccc(C(=O)C3CCN([C@@H](C)C(=O)N4CCc5ccccc54)CC3)cc2NC1=O
vNsp9-nsp9.1-145	Z1128836946	-8.1	0.245	432.48	REAL	O=C(Nc1ccccc(-c2ccc3ccccc3c2)n1)c1ccc2c(=O)n3c(nc2c1)CCC3
vNsp9-nsp9.1-146	Z1128836973	-8.1	0.253	423.47	REAL	CC(=O)N1C[C@@H](C(=O)Nc2ccccc(-c3ccc4ccccc4c3)n2)Oc2ccccc21
vNsp9-nsp9.1-147	Z1128852876	-8.1	0.245	442.52	REAL	O=C(c1ccc(N2CCc3ccccc3C2)cc1)N1CCN(C(=O)c2ccc(=O)[nH]c2)CC1
vNsp9-nsp9.1-148	Z1137567349	-8.1	0.245	442.45	REAL	O=C(NCc1nc(-c2ccc(F)cc2)n[nH]1)c1ccc(COc2ccc3ccccc3c2)o1
vNsp9-nsp9.1-149	Z1151633265	-8.1	0.238	452.56	REAL	C[C@@H](c1nc(-c2ccccc2)no1)N1CCN(C(=O)[C@@H]2C[C@H]2c2ccc3ccccc23)CC1
vNsp9-nsp9.1-150	Z1157881954	-8.1	0.238	472.57	REAL	Cc1cc(NS(=O)(=O)c2ccc(NC(=O)[C@H]3C[C@@H]3c3ccc4ccccc4c3)cc2)nc(C)n1
vNsp9-nsp9.1-151	Z1157905028	-8.1	0.245	438.57	REAL	Cc1ccn2c(CN3CCN(C(=O)[C@H]4C[C@@H]4c4ccc5ccccc5c4)CC3)c(C)nc2c1
vNsp9-nsp9.1-152	Z1157954700	-8.1	0.245	434.50	REAL	O=C(Nc1ccccc(Cn2nc3ccccn3c2=O)c1)[C@H]1C[C@@H]1c1ccc2ccccc2c1
vNsp9-nsp9.1-153	Z1158237548	-8.1	0.238	452.56	REAL	Cc1ccc(-c2noc(CN3CCN(C(=O)[C@H]4C[C@@H]4c4ccc5ccccc5c4)CC3)n2)cc1
vNsp9-nsp9.1-154	Z1177519426	-8.1	0.253	431.54	REAL	O=C(CCNC(=O)N1CCc2ccccc2C1)Nc1ccc2c(c1)nc1n2CCCC1
vNsp9-nsp9.1-155	Z1206462936	-8.1	0.270	420.58	REAL	CN(C(=O)NC1CCN(c2nc3ccccc3s2)CC1)[C@@H]1CCc2ccccc2C1
vNsp9-nsp9.1-156	Z1278117353	-8.1	0.253	427.51	REAL	O=C1CCc2ccc(NC(=O)NCc3ccc(N4CCc5ccccc5C4)nc3)cc2N1
vNsp9-nsp9.1-157	Z1304563904	-8.1	0.253	426.52	REAL	Cn1nc2c(cc1=O)CN(C(=O)NC[C@H]1CC3c4ccccc4C1c1ccccc13)CC2
vNsp9-nsp9.1-158	Z1313096566	-8.1	0.238	447.50	REAL	O=C(NCc1ccc2ccccc2n1)c1ccnc(C(=O)NCc2ccc3ccccc3n2)c1
vNsp9-nsp9.1-159	Z131389876	-8.1	0.245	436.56	REAL	Cc1ccn2c(CN3CCN(C(=O)c4ccc5c(c4)-c4ccccc4C5)CC3)c(C)nc2c1
vNsp9-nsp9.1-160	Z1314149838	-8.1	0.253	423.43	REAL	Cc1cc(C(=O)Nc2cccc(-c3ccc4ccccc4c3)n2)nc2nc(O)[nH]c(=O)c12
vNsp9-nsp9.1-161	Z1314149843	-8.1	0.253	422.49	REAL	CN1CCC(=O)Nc2cc(C(=O)Nc3cccc(-c4ccc5ccccc5c4)n3)ccc21
vNsp9-nsp9.1-162	Z133656968	-8.1	0.245	467.54	REAL	CC(=O)N1CCCc2cc(S(=O)(=O)Oc3ccc4c5c(c(=O)oc4c3)CCCCC5)ccc21
vNsp9-nsp9.1-163	Z137251570	-8.1	0.245	440.46	REAL	Cn1c(NNC(=O)c2ccc(COc3ccc4ccccc4c3)o2)nc2ccccc2c1=O
vNsp9-nsp9.1-164	Z1373795450	-8.1	0.245	445.57	REAL	C[C@H](C(=O)N[C@H]1CCCN(c2cc(N3CCOCC3)ncn2)C1)c1ccc2ccccc2c1
vNsp9-nsp9.1-165	Z1383810146	-8.1	0.253	440.48	REAL	O=C1c2ccccc2C(=O)c2cc(NC(=O)[C@]34CCC(=O)N3c3ccccc3S4)ccc21
vNsp9-nsp9.1-166	Z1402437962	-8.1	0.245	449.55	REAL	O=C(Nc1ccc(CC(=O)N2CCCc3ccccc32)cc1)N1CCO[C@H]([C@@H]2CCCO2)C1
vNsp9-nsp9.1-167	Z1420802165	-8.1	0.245	446.55	REAL	O=C(N[C@H]1CCN(C(=O)C2CCCCC2)C1)c1ccc(COc2ccc3ccccc3c2)o1
vNsp9-nsp9.1-168	Z1437573219	-8.1	0.245	436.47	REAL	O=C(NCc1ccc2ccccc2n1)c1ccc(C(=O)NCc2ccc3ccccc3n2)o1
vNsp9-nsp9.1-169	Z1439421335	-8.1	0.245	442.56	REAL	O=C(c1ccc2c(=O)n3c(nc2c1)CCC3)N1CC[C@@H]2[C@@H](CCCN2Cc2ccccc2)C1
vNsp9-nsp9.1-170	Z1449090022	-8.1	0.253	443.53	REAL	O=C(N[C@@H]1[C@H]2Cc3ccccc3[C@@H]12)c1ccc(NC2=NS(=O)(=O)c3ccccc32)cc1
vNsp9-nsp9.1-171	Z1449094407	-8.1	0.238	449.55	REAL	O=C(N[C@@H]1[C@H]2Cc3ccccc3[C@@H]12)c1cncc(C(=O)N[C@H]2[C@@H]3Cc4ccccc4[C@H]23)c1
vNsp9-nsp9.1-172	Z1453808091	-8.1	0.261	408.46	REAL	O=C(N[C@H]1[C@@H]2Cc3ccccc3[C@@H]12)c1cccc(N2C(=O)c3ccccc3C2=O)c1
vNsp9-nsp9.1-173	Z1470610307	-8.1	0.279	386.45	REAL	Cc1nc(-c2ccc(NC(=O)N[C@H]3[C@H]4CCc5ccccc5[C@@H]43)cc2)cc(=O)[nH]1
vNsp9-nsp9.1-174	Z1506267234	-8.1	0.245	439.51	REAL	O=C1O[C@H](c2ccccc2)Cc2cc(C(=O)N3CCO[C@@]4(CCc5ccccc54)C3)ccc21
vNsp9-nsp9.1-175	Z1545306425	-8.1	0.238	449.56	REAL	Cc1cc(C)nc(-n2nc(C(=O)NC[C@@H]3CC4c5ccccc5C3c3ccccc34)cc2C)n1
vNsp9-nsp9.1-176	Z1560099094	-8.1	0.261	438.53	REAL	O=C(Nc1ccc(-c2csc(N3CCOCC3)n2)cc1)N1CCc2ccc(F)c2C1
vNsp9-nsp9.1-177	Z1607819863	-8.1	0.279	413.88	REAL	O=C(N[C@H]1[C@@H]2Cc3ccccc3[C@@H]12)N[C@@H]1CCN(c2ccc(F)c(Cl)c2)C1=O
vNsp9-nsp9.1-178	Z16226326	-8.1	0.245	453.48	REAL	O=C(CSc1nnc2[nH]c3ccccc3n12)Nc1ccc2c(c1)C(=O)c1ccccc1C2=O
vNsp9-nsp9.1-179	Z1662366531	-8.1	0.270	396.45	REAL	Cc1cc(C)nc(-n2nc(-c3nnc(Cc4ccc5ccccc5c4)o3)cc2C)n1
vNsp9-nsp9.1-180	Z166952536	-8.1	0.261	417.46	REAL	CC(=O)N1CCc2cc(C(=O)Oc3ccc4c5c(c(=O)oc4c3)CCCCC5)ccc21
vNsp9-nsp9.1-181	Z1671603539	-8.1	0.253	429.48	REAL	Cc1cc(NC(=O)NNC(=O)c2ccc(COc3ccc4ccccc4c3)cc2)nn1C
vNsp9-nsp9.1-182	Z1683536670	-8.1	0.238	448.48	REAL	O=C(Nc1cccc(-c2nc(Cc3ccc4ccccc4n3)no2)c1)[C@@H]1Cc2ccccc2O1
vNsp9-nsp9.1-183	Z1684693925	-8.1	0.253	442.50	REAL	O=S1(=O)N=C(Nc2ccc(-c3nc(C4Cc5ccccc5C4)no3)cc2)c2ccccc21
vNsp9-nsp9.1-184	Z1685090849	-8.1	0.245	433.47	REAL	O=C1C[C@H](c2nc(-c3ccc4[nH]cnc4c3)no2)CN1c1ccc2c(c1)Cc1ccccc1-2
vNsp9-nsp9.1-185	Z1685539349	-8.1	0.270	402.46	REAL	c1ccc2c(c1)CC[C@H](c1noc(C3CCN(c4ccc5nnnn5n4)CC3)n1)C2
vNsp9-nsp9.1-186	Z1693555389	-8.1	0.245	442.56	REAL	O=C(NCc1ccc(N2CCc3ccccc3C2)nc1)N[C@H]1CCO[C@@H](c2ccccc2)C1
vNsp9-nsp9.1-187	Z1731314567	-8.1	0.261	419.52	REAL	O=C(Nc1cccc(C(=O)N2CCCCC2)c1)N1CCC[C@]2(C1)OCc1ccccc12
vNsp9-nsp9.1-188	Z1734363530	-8.1	0.253	434.49	REAL	C[C@@]1(c2ccc(CNC(=O)N3CCC[C@]4(C3)OCc3ccccc34)cc2)NC(=O)NC1=O
vNsp9-nsp9.1-189	Z1739745081	-8.1	0.245	439.48	REAL	Oc1cccc2ccc(N3CCC(c4nc(-c5cccc(-n6ccnc6)n5)no4)CC3)nc12
vNsp9-nsp9.1-190	Z1763866145	-8.1	0.245	444.47	REAL	O=C(Nc1ccc(F)cc1)N1CCN(C(=O)c2ccc3[nH]c4ccccc4c(=O)c3c2)CC1
vNsp9-nsp9.1-191	Z1766154647	-8.1	0.279	382.46	REAL	C[C@@H]1[C@H](c2ccccc2)CCN1C(=O)c1ccc2[nH]c3ccccc3c(=O)c2c1
vNsp9-nsp9.1-192	Z1865790844	-8.1	0.261	434.56	REAL	Cc1cccc2c1CN(C(=O)Nc1ccc(-c3csc(N4CCOCC4)n3)cc1)CC2
vNsp9-nsp9.1-193	Z1890551640	-8.1	0.245	441.49	REAL	O=C(CCc1nc(CC(=O)N2CCn3c2nc2ccccc23)no1)c1ccc2c(c1)CCC2
vNsp9-nsp9.1-194	Z1890553561	-8.1	0.245	435.49	REAL	O=C(Cc1noc([C@H]2C[C@@H]2c2ccc3ccccc3c2)n1)N1CCn2c1nc1ccccc12
vNsp9-nsp9.1-195	Z1904991998	-8.1	0.279	396.53	REAL	C[C@H](CNC(=O)NC[C@]1(O)[C@H]2[C@H]3C[C@H]4[C@@H]5[C@@H]3C[C@@H]2[C@H]5[C@H]41)COCc1ccccc1
vNsp9-nsp9.1-196	Z1927956105	-8.1	0.253	425.49	REAL	Nc1ncc2c(n1)CCN(C(=O)[C@@H]1CC(=O)N(c3ccc4c(c3)Cc3ccccc3-4)C1)C2
vNsp9-nsp9.1-197	Z1948607584	-8.1	0.245	445.52	REAL	Cc1ncc2c(n1)CC[C@H](NC(=O)N1CC=C(CCN3C(=O)c4ccccc4C3=O)CC1)C2
vNsp9-nsp9.1-198	Z1952500303	-8.1	0.245	445.52	REAL	Cc1ccnc(N2CCN(C(=O)c3cccc(NN4C(=O)[C@@H]5CC=CC[C@@H]5C4=O)c3)CC2)c1
vNsp9-nsp9.1-199	Z1975428318	-8.1	0.245	445.54	REAL	O=C(NCc1ccc(F)cc1)C1CCN(C(=O)N[C@@H]2C[C@H]2c2ccc3ccccc3c2)CC1
vNsp9-nsp9.1-200	Z1983290694	-8.1	0.279	392.46	REAL	O=C1N[C@]2(C[C@H]3C[C@H]2[C@H]2CCC[C@H]32)C(=O)N1Cc1nc(Cc2ccccc2)no1

Supplementary Table 42. Virtual screening hits 101 to 200 of the screen against the dimerization site of nsp9 (Screen ID: 23). Compounds were filtered so that hits had MW < 600 dalton, cLogP < 6, number of hydrogen bond acceptors < 11, and no reactive functional groups. The name of each compound consists of the initial letter 'v' for virtual hit, followed by the target protein name and the target site ('nsp9' for nsp binding site, 1 for docking scenario 1). The score is the docking score given by QuickVina 2 in kcal/mol. The ligand efficiency (LE) is computed as LE = -score/#NonH, where #NonH is the number of heavy (i.e. non hydrogen) atoms.

Name	Catalog ID	Score	LE	MW	Library	SMILES
vNsp9-nsp9.2-101	PV-001916081528	-8.4	0.311	365.38	REAL	Cc1ccc2c(CN3C(=O)c4ccccc4C(F)(F)C3=O)c(C)ccc2c1
vNsp9-nsp9.2-102	PV-001948929647	-8.4	0.280	419.33	REAL	O=C(Nc1cc2oc(=O)[nH]c2cc1F)N[C@H](c1cccc2ccccc12)C(F)(F)F
vNsp9-nsp9.2-103	PV-001949369524	-8.4	0.290	404.39	REAL	Cc1ccc(C(F)(F)F)c(NC(=O)N2CC[C@@]3(CC(=O)c4ccccc4O3)C2)c1
vNsp9-nsp9.2-104	PV-001950730589	-8.4	0.311	430.30	REAL	Cc1ccc2c(c1)[C@@H](NC(=O)Nc1cc(Br)cc3c1NC(=O)CO3)CCC2
vNsp9-nsp9.2-105	PV-001956522418	-8.4	0.290	399.53	REAL	Cc1ccccc1[C@@H](NC(=O)N1CC[C@H]2OCC(=O)N[C@@H]2C1)[C@H]1CCC[C@@H](C)C1
vNsp9-nsp9.2-106	PV-001959013187	-8.4	0.300	377.49	REAL	CC(=O)N1CC[C@@H](NC(=O)N[C@@H]2c3cc(C)ccc3C[C@H]2C)c2ccccc21
vNsp9-nsp9.2-107	Z1005853866	-8.4	0.247	485.49	REAL	O=C(c1ccc2[nH]cnc2c1)N1CCN(C(=O)c2csc(-c3cccc(C(F)(F)F)c3)n2)CC1
vNsp9-nsp9.2-108	Z1023118894	-8.4	0.262	426.52	REAL	O=C([C@H]1CC(=O)N(c2ccc3c(c2)Cc2ccccc2-3)C1)N1CCC[C@H](c2ccn[nH]2)C1
vNsp9-nsp9.2-109	Z1096470735	-8.4	0.247	470.49	REAL	O=C(c1ccc2[nH]cnc2c1)N1CCN(C(=O)C2(c3cccc(C(F)(F)F)c3)CCCC2)CC1
vNsp9-nsp9.2-110	Z1127340552	-8.4	0.271	408.46	REAL	O=C(NC[C@@H]1CC2c3ccccc3C1c1ccccc12)c1ccc2c(c1)C(=O)NC2=O
vNsp9-nsp9.2-111	Z1136007076	-8.4	0.255	441.49	REAL	O=C1CCNc2ccc(C(=O)OCC(=O)N3c4ccccc4CCc4ccccc43)cc2N1
vNsp9-nsp9.2-112	Z1148590295	-8.4	0.247	447.50	REAL	Cc1c(C(=O)Nc2ccccc2-c2ccc(-c3cccc3)cc2)cnn1-c1ccc(=O)[nH]n1
vNsp9-nsp9.2-113	Z1151723422	-8.4	0.240	468.55	REAL	C[C@H]1Oc2ccc(C(=O)C3CCN(C(=O)[C@H]4C[C@@H]4c4cccc5ccccc45)CC3)cc2NC1=O
vNsp9-nsp9.2-114	Z1173672108	-8.4	0.290	386.41	REAL	O=C(c1nn(Cc2ccccc2)c(=O)c2ccccc12)N1CCn2cnnc2C1
vNsp9-nsp9.2-115	Z1250586272	-8.4	0.255	438.49	REAL	Cc1cc(C(=O)NC[C@H]2CC3c4ccccc4C2c2ccccc23)nc2nc(O)[nH]c(=O)c12
vNsp9-nsp9.2-116	Z1261987068	-8.4	0.255	437.50	REAL	O=C1CCc2ccc(NC(=O)[C@H]3CC(=O)N(c4ccc5c(c4)Cc4ccccc4-5)C3)cc2N1
vNsp9-nsp9.2-117	Z1265173172	-8.4	0.262	446.53	REAL	C[C@@H]1CN(C)c2ccccc2N(C(=O)c2ccc3c(c2)S(=O)(=O)c2ccccc2C3=O)C1
vNsp9-nsp9.2-118	Z1273281560	-8.4	0.255	442.51	REAL	O=C(CN1C(=O)[C@@H]2[C@@H]3CC[C@@H](O3)[C@H]2C1=O)NC[C@@H]1CC2c3ccccc3C1c1ccccc12
vNsp9-nsp9.2-119	Z1279246712	-8.4	0.290	385.51	REAL	O=C([C@H]1C[C@@]12CCCc1ccccc12)N1CCC[C@H](c2nc3ccccc3[nH]2)C1
vNsp9-nsp9.2-120	Z1303048763	-8.4	0.271	411.42	REAL	O=C1CN(C(=O)c2nn(Cc3ccccc3)c(=O)c3ccccc23)c2ccncc2N1
vNsp9-nsp9.2-121	Z1304563798	-8.4	0.290	389.50	REAL	C[C@@H]1CC(=O)NCCN1C(=O)NC[C@@H]1CC2c3ccccc3C1c1ccccc12
vNsp9-nsp9.2-122	Z1330296988	-8.4	0.280	398.42	REAL	CN(C(=O)c1cnc2c(c1)c(=O)[nH]c(=O)n2C)C1c2ccccc2-c2ccccc21
vNsp9-nsp9.2-123	Z1333122870	-8.4	0.350	326.33	REAL	C[C@@H]1CCc2c(F)cccc2/C1=N/Nc1nc2[nH]ncc2c(=O)[nH]1
vNsp9-nsp9.2-124	Z1333930318	-8.4	0.280	399.45	REAL	O=C([C@H]1CC(=O)N(c2ccc3c(c2)Cc2ccccc2-3)C1)N1CCc2nn[nH]c2C1
vNsp9-nsp9.2-125	Z1335192709	-8.4	0.247	449.51	REAL	C[C@@]1(c2ccc(C(=O)N[C@H](c3ccccc3)c3cccc4ccccc34)cc2)NC(=O)NC1=O
vNsp9-nsp9.2-126	Z1335281960	-8.4	0.255	448.57	REAL	NC(=O)NC1CCN(C(=O)[C@H]2C[C@H]3CCCC[C@H]3N2C(=O)c2ccc3ccccc3c2)CC1
vNsp9-nsp9.2-127	Z1360455696	-8.4	0.290	403.45	REAL	O=C(NCc1ccccc1-n1ccnc1)C12C[C@@H]3C[C@@H](C1)CC(C(F)(F)F)(C3)C2
vNsp9-nsp9.2-128	Z1367042156	-8.4	0.323	372.40	REAL	C[C@H]1CCc2ccccc2N1S(=O)(=O)c1cnc2[nH]c(=O)[nH]c(=O)c2c1
vNsp9-nsp9.2-129	Z1367045995	-8.4	0.323	372.40	REAL	O=c1[nH]c(=O)c2cc(S(=O)(=O)N3CCCCc4ccccc43)cnc2[nH]1
vNsp9-nsp9.2-130	Z1439449847	-8.4	0.262	429.57	REAL	Cc1nc(-c2ccc(N3CC[C@H]4[C@@H](CCCN4Cc4ccccc4)C3)nc2)[nH]c(=O)c1C
vNsp9-nsp9.2-131	Z1448252267	-8.4	0.290	392.47	REAL	O=C1CCc2cc(C(=O)N3CCC[C@@]4(CCCc5ccccc54)C3)c(F)cc2N1
vNsp9-nsp9.2-132	Z1453162889	-8.4	0.311	363.42	REAL	C[C@H]1Cc2ccccc2CN1C(=O)c1cccc[C@@]2(C)NC(=O)NC2=O)c1
vNsp9-nsp9.2-133	Z1471597646	-8.4	0.323	346.43	REAL	O=C1C[C@@H](c2cccc(NC(=O)[C@@H]3C[C@@]34CCc3ccccc34)c2)CN1
vNsp9-nsp9.2-134	Z1472020813	-8.4	0.290	384.43	REAL	O=C1C[C@@H](c2cccc(NC(=O)C3c4ccccc4Oc4ccccc43)c2)CN1
vNsp9-nsp9.2-135	Z1472743415	-8.4	0.271	415.49	REAL	Cc1n[nH]c(NC(=O)[C@@H]2C[C@]23CCCc2ccccc23)c1-c1ccc2c(c1)OCCO2
vNsp9-nsp9.2-136	Z1495097302	-8.4	0.280	398.47	REAL	O=C([C@H]1CC(=O)N(c2ccc3c(c2)Cc2ccccc2-3)C1)N1CCc2cn[nH]c2C1
vNsp9-nsp9.2-137	Z1495101820	-8.4	0.262	428.53	REAL	O=C([C@H]1C[C@@H]2CCCC[C@@H]2N1C(=O)c1ccc2ccccc2c1)N1CCc2cn[nH]c2C1
vNsp9-nsp9.2-138	Z1544063703	-8.4	0.300	378.43	REAL	CC(C)c1ccc2c(c1)[C@@H](NC(=O)c1cnc3[nH]c(=O)[nH]c(=O)c3c1)CCC2
vNsp9-nsp9.2-139	Z1575433873	-8.4	0.271	411.46	REAL	O=C1COc2ncc(C(=O)NC[C@@H]3CC4c5ccccc5C3c3ccccc34)cc2N1
vNsp9-nsp9.2-140	Z1602168597	-8.4	0.280	407.49	REAL	CC1(C)CC[C@H]2C[C@@H](NC(=O)c3cc(N4CCNC4=O)ccc3F)c3ccccc1c32
vNsp9-nsp9.2-141	Z1614159859	-8.4	0.271	415.50	REAL	O=C1CCCc2ccc(NC(=O)N3CCC[C@H](c4n[nH]c(-c5ccccc5)n4)C3)cc21
vNsp9-nsp9.2-142	Z1619862679	-8.4	0.271	434.52	REAL	O=C(c1ccccc(S(=O)(=O)N2CCc3ccccc32)c1)N1CCCc2ccccc(O)c21
vNsp9-nsp9.2-143	Z1619868538	-8.4	0.262	448.54	REAL	O=C(c1ccccc(S(=O)(=O)N2CCCc3ccccc32)c1)N1CCCc2ccccc(O)c21
vNsp9-nsp9.2-144	Z1636458725	-8.4	0.280	408.54	REAL	Cc1noc(C2(C)CCN(C(=O)N[C@@H]3C[C@H]4CCC(C)(C)c5ccccc5C4)CC2)n1
vNsp9-nsp9.2-145	Z1657984819	-8.4	0.255	440.50	REAL	O=C1NC2(CCN(C(=O)CCC(=O)c3ccc4ccc5cccc6ccc3c4c56)CC2)CO1
vNsp9-nsp9.2-146	Z1659785962	-8.4	0.255	432.48	REAL	O=C(c1cc(-c2cccc3ccccc23)nc2ccccc12)N1CCc2c(nc[nH]c2=O)C1
vNsp9-nsp9.2-147	Z167420156	-8.4	0.262	451.55	REAL	Cc1noc(C)c1S(=O)(=O)N1CCCN(C(=O)c2ccc3c(c2)-c2ccccc2C3)CC1
vNsp9-nsp9.2-148	Z1682393043	-8.4	0.290	394.47	REAL	C[C@]1(c2cccc(-c3noc([C@@H]4CC[C@H]5CCCC[C@H]5C4)n3)cc2)NC(=O)NC1=O
vNsp9-nsp9.2-149	Z1684582679	-8.4	0.280	402.45	REAL	C[C@]1(c2cccc(-c3noc([C@]4(C)CCCc5ccccc54)n3)c2)NC(=O)NC1=O
vNsp9-nsp9.2-150	Z1685085314	-8.4	0.300	368.40	REAL	O=c1[nH]c2ccc(-c3noc([C@H]4C[C@H]4c4ccc5ccccc5c4)n3)cc2[nH]1
vNsp9-nsp9.2-151	Z1685100348	-8.4	0.255	440.46	REAL	Cc1cc(C)nc(-c2noc(-c3cc(CN4C(=O)c5ccccc5C4=O)cc(C)c3O)n2)c1
vNsp9-nsp9.2-152	Z1685223830	-8.4	0.247	449.51	REAL	O=c1[nH]c2ccc(NCc3ccc(-c4noc([C@@H]5C[C@@]56CCc5ccccc56)n4)cc3)cc2[nH]1
vNsp9-nsp9.2-153	Z1685323917	-8.4	0.300	371.44	REAL	Cc1nnc(-c2cccc(-c3noc([C@]4(C)CCc5ccccc5C4)n3)c2)[nH]1
vNsp9-nsp9.2-154	Z1685540802	-8.4	0.300	374.44	REAL	CN1CCC(=O)Nc2cc(-c3nc([C@@H]4CCc5ccccc5C4)no3)ccc21
vNsp9-nsp9.2-155	Z1689460084	-8.4	0.290	395.36	REAL	O=C1c2ccccc2C(F)(F)C(=O)N1Cc1cc(=O)oc2cc3c(cc12)CCC3
vNsp9-nsp9.2-156	Z1693220059	-8.4	0.290	413.50	REAL	CC(C)[C@@H]1CCc2ccccc2[C@H]1NS(=O)(=O)c1ccc2[nH]c(=O)[nH]c(=O)c2c1
vNsp9-nsp9.2-157	Z1694321769	-8.4	0.290	392.46	REAL	CC(C)[C@@H]1CCc2ccccc2[C@@H]1NC(=O)c1cnc2c(c1)c(=O)[nH]c(=O)n2C
vNsp9-nsp9.2-158	Z1698774339	-8.4	0.255	438.53	REAL	O=C1CCc2cc(C(=O)CCC(=O)N3Cc4ccccc4C[C@H]3c3ccccc3)ccc2N1
vNsp9-nsp9.2-159	Z1723440953	-8.4	0.262	430.48	REAL	C[C@H]1C[C@H](c2cccc(F)c2)N(C(=O)c2cccc(-c3cnc4[nH]c(=O)n(C)c4c3)c2)C1
vNsp9-nsp9.2-160	Z1723441592	-8.4	0.262	430.48	REAL	C[C@@H]1CCN(C(=O)c2cccc(-c3cnc4[nH]c(=O)n(C)c4c3)c2)[C@H]1c1cccc(F)c1
vNsp9-nsp9.2-161	Z1723442888	-8.4	0.262	426.52	REAL	Cc1ccc(C)c([C@H]2CCCN2C(=O)c2cccc(-c3cnc4[nH]c(=O)n(C)c4c3)c2)c1
vNsp9-nsp9.2-162	Z1734957928	-8.4	0.262	433.60	REAL	CC1(C)CC[C@@H]2C[C@@H](NC(=O)N3CCC(c4nnc5n4CCCC5)CC3)c3cccc1c32
vNsp9-nsp9.2-163	Z1752851838	-8.4	0.300	375.47	REAL	O=C1C[C@H]2CC[C@@H](CN1)N2C(=O)N[C@@H]1CCc2ccc(-c3ccccc3)cc21
vNsp9-nsp9.2-164	Z1763467989	-8.4	0.271	417.51	REAL	O=C1NCC2(CCN(C(=O)NC[C@@H]3CC4c5ccccc5C3c3ccccc34)CC2)O1
vNsp9-nsp9.2-165	Z1816708572	-8.4	0.280	424.52	REAL	O=C1CCCc2cc(S(=O)(=O)NC(=O)[C@H]3C[C@]34CCCc3ccccc34)ccc2N1
vNsp9-nsp9.2-166	Z1842765125	-8.4	0.262	424.46	REAL	O=C(NNc1nc2ccccn2n1)[C@H]1CC(=O)N(c2ccc3c(c2)Cc2ccccc2-3)C1
vNsp9-nsp9.2-167	Z1903831541	-8.4	0.271	418.54	REAL	Cc1ccc(N2CCNC2=O)cc1NC(=O)N[C@@H]1C[C@@H]2CCC(C)(C)c3cccc1c32
vNsp9-nsp9.2-168	Z1907866233	-8.4	0.271	412.45	REAL	NC(=O)N1CCCc2ccc(NC(=O)c3ccc4[nH]c5ccccc5c(=O)c4c3)cc21
vNsp9-nsp9.2-169	Z1993952823	-8.4	0.300	376.50	REAL	O=C(CN1CC[C@H]2OCCC[C@@H]2C1)N1c2ccccc2CCc2ccccc21
vNsp9-nsp9.2-170	Z2001523460	-8.4	0.262	430.52	REAL	Cc1cc(F)cc2c1CN(C(=O)[C@@H]1CCCN(C(=O)c3ccc4ccccc34)C1)CC2
vNsp9-nsp9.2-171	Z2003604215	-8.4	0.262	437.49	REAL	Cc1cc(F)cc2c1CN(C(=O)Nc1cc(-c3nnc4n3CCCCC4)ccc1F)CC2
vNsp9-nsp9.2-172	Z2016706505	-8.4	0.280	421.39	REAL	O=C1CCc2ccc(NC(=O)N3CC[C@@](F)(c4cccc(C(F)(F)F)c4)C3)cc2N1
vNsp9-nsp9.2-173	Z2098619087	-8.4	0.323	352.36	REAL	O=C(c1ccc2oc(=O)[nH]c2c1)N1CC2(CCCC2)c2cccc(F)c21
vNsp9-nsp9.2-174	Z2099627854	-8.4	0.280	403.48	REAL	C[C@@]1(c2cccc(C(=O)NC3[C@@H]4CC[C@@H]3Cc3ccccc3C4)c2)NC(=O)NC1=O
vNsp9-nsp9.2-175	Z2105781658	-8.4	0.311	360.50	REAL	C[C@H](NC1[C@H]2CC[C@H]1Cc1ccccc1C2)c1ccc2c(c1)CCC(=O)N2
vNsp9-nsp9.2-176	Z2138237430	-8.4	0.262	446.93	REAL	O=C1COC[C@@H](C[C@@H]2CN(C(=O)c3cc(-c4ccccc4)ccc3Cl)c3ccccc32)N1
vNsp9-nsp9.2-177	Z2142506532	-8.4	0.300	372.47	REAL	Cn1c(N/N=C2\[C@H]3CCC[C@@H]2Cc2ccccc2C3)nc2ccccc2c1=O
vNsp9-nsp9.2-178	Z2142871386	-8.4	0.262	420.51	REAL	Cc1cc(=O)[nH]c2cc(C(=O)NC[C@@H]3CC4c5ccccc5C3c3ccccc34)ccc12
vNsp9-nsp9.2-179	Z2148626079	-8.4	0.255	438.48	REAL	Cc1cc(=O)[nH]c2cc(C(=O)OCC(=O)N3c4ccccc4CCc4ccccc43)ccc12
vNsp9-nsp9.2-180	Z2155754288	-8.4	0.255	440.54	REAL	CC(C(=O)N1C[C@H](C[C@@H]2COCC(=O)N2)c2ccccc21)(c1ccccc1)c1ccccc1
vNsp9-nsp9.2-181	Z2158235699	-8.4	0.350	316.36	REAL	O=C1C[C@H](c2nc([C@H]3CCc4ccccc43)no2)c2ccccc21
vNsp9-nsp9.2-182	Z219397242	-8.4	0.271	412.44	REAL	O=C1c2ccccc2N[C@@H](C2=Cc3ccccc3OC2)N1c1ccc2c(c1)OCCO2
vNsp9-nsp9.2-183	Z2198842959	-8.4	0.255	442.51	REAL	Cc1cc(C(=O)N2C[C@H](O)Cc3ccccc32)cc(C(=O)N2C[C@H](O)Cc3ccccc32)c1
vNsp9-nsp9.2-184	Z220420554	-8.4	0.311	354.42	REAL	c1ccc2c(c1)C1C[C@@H](CNc3ccc4nnnn4n3)C2c2ccccc21
vNsp9-nsp9.2-185	Z2214121349	-8.4	0.300	412.39	REAL	O=C1COc2ccc(S(=O)(=O)N3CC[C@H](C(F)(F)F)c4ccccc43)ccc2N1
vNsp9-nsp9.2-186	Z2222215913	-8.4	0.280	399.41	REAL	CC(C)(c1noc(-c2cnc3[nH]c(=O)[nH]c(=O)c3c2)n1)c1ccccc2ccccc12
vNsp9-nsp9.2-187	Z2225645671	-8.4	0.255	444.49	REAL	O=C([C@H]1CC(=O)N(c2ccc3c(c2)Cc2ccccc2-3)C1)N1CCC[C@H](c2n[nH]c(=O)o2)C1
vNsp9-nsp9.2-188	Z2225987667	-8.4	0.255	443.51	REAL	O=C([C@H]1CC(=O)N(c2ccc3c(c2)Cc2ccccc2-3)C1)N1CCC[C@H](c2nc(=O)[nH][nH]2)C1
vNsp9-nsp9.2-189	Z2227695484	-8.4	0.290	388.43	REAL	Cc1[nH][nH]c(=O)c1NC(=O)[C@H]1CC(=O)N(c2ccc3c(c2)Cc2ccccc2-3)C1
vNsp9-nsp9.2-190	Z2232120160	-8.4	0.262	425.49	REAL	C[C@@]1(c2cccc(C(=O)N3CCc4ccccc4[C@@H]3c3ccccc3)cc2)NC(=O)NC1=O
vNsp9-nsp9.2-191	Z2232121002	-8.4	0.280	398.42	REAL	O=C(c1cnc2[nH]c(=O)[nH]c(=O)c2c1)N1CCc2ccccc2[C@@H]1c1ccccc1
vNsp9-nsp9.2-192	Z238450370	-8.4	0.262	443.85	REAL	O=C1NC(=O)c2c(N/C=C3/C(=O)N(c4ccccc4Cl)C(=O)c4ccccc43)cccc21
vNsp9-nsp9.2-193	Z2497407953	-8.4	0.311	362.43	REAL	O=C(c1cccc2oc(=O)[nH]c12)N1CCC[C@@]2(CCCc3ccccc32)C1
vNsp9-nsp9.2-194	Z2524829917	-8.4	0.227	493.61	REAL	Cn1c(=O)[nH]c2ncc(-c3cccc(C(=O)N4C[C@@H]5CC[C@H]4[C@@H]4CN(Cc6ccccc6)C[C@H]54)c3)cc21
vNsp9-nsp9.2-195	Z2624532205	-8.4	0.290	391.52	REAL	O=C(Nc1ccc2c(c1)CCCCC2)N1CCc2nnc(N3CCCC3)cc2C1
vNsp9-nsp9.2-196	Z2635690034	-8.4	0.311	361.44	REAL	CC1(C)CC[C@H]2C[C@@H](NC(=O)c3cnc4c3CC(=O)N4)c3ccec1c32
vNsp9-nsp9.2-197	Z2642343808	-8.4	0.290	388.47	REAL	CN1CCc2[nH]c3ccc(C(=O)N[C@@H]4CCc5ccccc5NC4=O)cc3c2C1
vNsp9-nsp9.2-198	Z2711572347	-8.4	0.300	377.44	REAL	O=C(Nc1ccc2c(c1)COC(=O)N2)NC1[C@H]2CC[C@@H]1Cc1ccccc1C2
vNsp9-nsp9.2-199	Z2773532079	-8.4	0.300	377.45	REAL	Cc1nnc(-c2cccc(-c3noc(C4C[C@@H]5CCCC[C@@H](C4)C5=O)n3)c2)[nH]1
vNsp9-nsp9.2-200	Z28946042	-8.4	0.247	475.52	REAL	O=C1c2ccccc2S(=O)(=O)c2cc(C(=O)N3CCC[C@@H]3c3ccc4c(c3)OCCO4)ccc21

Supplementary Table 43. Top 100 virtual hits of the screen against the dimerization site of nsp9 (Screen ID: 24). The name of each compound consists of the initial letter 'v' for virtual hit, followed by the target protein name and the target site ('nsp9' for nsp9 binding site, 2 for docking scenario 2). The score is the docking score given by QuickVina 2 in kcal/mol. The ligand efficiency (LE) is computed as LE = -score/#NonH, where #NonH is the number of heavy (i.e. non hydrogen) atoms.

Name	Catalog ID	Score	LE	MW	Library	SMILES
vNsp9-nsp9.2-1	ZINC000100504092	-9.6	0.31	404.512	ZINC	O=c1cccc2n1C[C@H]1C[C@H]2CN(Cc2ccc3ccc4cccc5ccc2c3c45)C1
vNsp9-nsp9.2-2	ZINC000100572803	-9.2	0.329	368.479	ZINC	O=c1cccc2n1C[C@H]1C[C@H]2CN(Cc2ccc3c(c2)Cc2ccccc2-3)C1
vNsp9-nsp9.2-3	ZINC000001564229	-9	0.321	360.459	ZINC	c1ccc2c(c1)cc[n+]1c2-c2c3ccccc3cc[n+]2Cc2ccccc2C1
vNsp9-nsp9.2-4	ZINC000003772018	-9	0.281	414.463	ZINC	O=c1oc2ccccc2c2c1[C@@H](c1c[nH]c3ccccc31)Nc1ccc3ccccc3c1-2
vNsp9-nsp9.2-5	ZINC000048523764	-9	0.25	464.475	ZINC	O=C1c2ccccc2C(=O)C2=C3C=CC4=CC5=C(C(=O)c6ccccc6C5=O)C5=CC=C(C=C12)[C@@H]3[C@@H]45
vNsp9-nsp9.2-6	Z1245894026	-8.9	0.27	448.493	REAL	C[C@H]1c2cc3c(cc2C2(CCCC2)CN1C(=O)c1cc(=O)[nH]c2cc(F)ccc12)OCCO3
vNsp9-nsp9.2-7	Z1985082805	-8.9	0.27	437.498	REAL	O=C1N[C@H]2CCN(C(=O)c3cc(-c4cccc5ccccc45)nc4ccccc34)C[C@@H]2CO1
vNsp9-nsp9.2-8	Z448669214	-8.9	0.247	478.594	REAL	O=C(NC[C@@H]1CC2c3ccccc3C1c1ccccc12)N1CCC(n2c(=O)[nH]c3ccccc32)CC1
vNsp9-nsp9.2-9	ZINC000247702001	-8.9	0.247	470.527	ZINC	O=C(c1ccccc1)[C@@H]1[C@@H]2C(=O)N(c3cccc4ccccc43)C(=O)[C@@H]2[C@@H]2c3ccccc3C=CN21
vNsp9-nsp9.2-10	ZINC000247702004	-8.9	0.247	470.527	ZINC	O=C(c1ccccc1)[C@@H]1[C@@H]2C(=O)N(c3cccc4ccccc43)C(=O)[C@H]2[C@@H]2c3ccccc3C=CN21
vNsp9-nsp9.2-11	Z1280905646	-8.8	0.326	361.4	REAL	O=C(Nc1ccc(-c2noc(=O)[nH]2)cc1)[C@H]1C[C@]12CCCCc1ccccc12
vNsp9-nsp9.2-12	Z1356153550	-8.8	0.314	382.394	REAL	C[C@@H]1CCc2c(F)cccc2[C@@H]1NC(=O)c1cnc2c(c1)c(=O)[nH]c(=O)n2C
vNsp9-nsp9.2-13	Z1974384967	-8.8	0.352	336.434	REAL	CC1(C)CCc2ccccc2[C@@H](Nc2ccc3c(c2)NC(=O)CO3)C1
vNsp9-nsp9.2-14	ZINC000003120897	-8.8	0.338	333.433	ZINC	CN1c2ccccc2C=C/C1=C\C=C1c2ccccc2-c2ccccc21
vNsp9-nsp9.2-15	ZINC000006724167	-8.8	0.293	416.907	ZINC	Cc1ccc(NC(=O)[C@H]2c3ccccc3C(=O)N3CCc4ccccc4[C@H]23)c(Cl)c1
vNsp9-nsp9.2-16	ZINC000013774180	-8.8	0.275	415.451	ZINC	O=C1Nc2ccccc2/C1=C/c1nc2ccccc2c(=O)n1-c1cccc2ccccc21
vNsp9-nsp9.2-17	ZINC000059835301	-8.8	0.275	415.451	ZINC	O=C1Nc2ccccc2/C1=C\c1nc2ccccc2c(=O)n1-c1cccc2ccccc21
vNsp9-nsp9.2-18	Z1280799883	-8.7	0.264	444.529	REAL	C[C@@H]1Oc2ccc(C(=O)C3CCN(C(=O)[C@H]4C[C@]45CCc4ccccc45)CC3)cc2NC1=O
vNsp9-nsp9.2-19	Z1330295129	-8.7	0.3	384.394	REAL	CN(C(=O)c1cnc2[nH]c(=O)[nH]c(=O)c2c1)C1c2ccccc2-c2ccccc21
vNsp9-nsp9.2-20	Z1994150987	-8.7	0.311	393.514	REAL	CC1(C)CCc2ccccc2[C@@H](Nc2ccc(C(=O)Nc3nncs3)cn2)C1
vNsp9-nsp9.2-21	Z2027558239	-8.7	0.322	356.384	REAL	O=C(c1ccc2[nH]c(=O)[nH]c2n1)N1CCc2ccccc2-c2ccccc2C1
vNsp9-nsp9.2-22	Z2903522870	-8.7	0.264	469.928	REAL	Cc1c(-c2noc([C@H]3C[C@@H]4CCCC[C@H]4N3C(=O)c3cccc(Cl)c3)n2)c(=O)[nH]c(=O)n1C
vNsp9-nsp9.2-23	ZINC000002466527	-8.7	0.3	402.88	ZINC	O=C(Nc1ccc(Cl)c1)[C@H]1c2ccccc2C(=O)N2CCc3ccccc3[C@H]12
vNsp9-nsp9.2-24	ZINC000002466561	-8.7	0.3	386.425	ZINC	O=C(Nc1ccccc1F)[C@H]1c2ccccc2C(=O)N2CCc3ccccc3[C@H]12
vNsp9-nsp9.2-25	ZINC000003852220	-8.7	0.242	482.618	ZINC	CC1(C)c2ccccc2C(C)(C)c2c3c(c=O)oc4c(c3c(=O)oc21)C(C)(C)[C@@H]1C=CC=C[C@@H]1C4(C)C
vNsp9-nsp9.2-26	ZINC000102139627	-8.7	0.264	435.478	ZINC	O=C(Oc1ccc2ccccc2c1)c1cccc(N2C(=O)[C@H]3[C@@H](C2=O)[C@@H]2C=C[C@H]3[C@H]3C[C@@H]32)c1
vNsp9-nsp9.2-27	ZINC000102139631	-8.7	0.264	435.478	ZINC	O=C(Oc1ccc2ccccc2c1)c1cccc(N2C(=O)[C@@H]3[C@@H](C2=O)[C@@H]2C=C[C@H]3[C@H]3C[C@@H]32)c1
vNsp9-nsp9.2-28	ZINC000408733452	-8.7	0.235	485.538	ZINC	Cc1ccc2c(c1)OC(=O)[C@@H]1C2=C[C@H](c2ccccc2)[C@@H]2C(=O)N(c3cccc4ccccc43)C(=O)[C@@H]21
vNsp9-nsp9.2-29	Z1452691933	-8.6	0.261	445.493	REAL	O=C(NC[C@H]1[C@@H]2Cc3ccccc3[C@H]12)NNC(=O)c1ccccc1OCc1ccc(F)cc1
vNsp9-nsp9.2-30	Z1544043949	-8.6	0.331	350.377	REAL	C[C@@H]1CCc2ccccc2[C@@H]1NC(=O)c1cnc2[nH]c(=O)[nH]c(=O)c2c1
vNsp9-nsp9.2-31	Z1744517862	-8.6	0.261	437.454	REAL	O=C(c1ccccc(N2C(=O)c3ccccc3C2=O)c1)N1CC[C@]2(C1)C(=O)Nc1ccccc12
vNsp9-nsp9.2-32	Z1833387196	-8.6	0.319	353.42	REAL	O=C1C[C@H](C(=O)N2Cc3ccccc3-c3ccccc3C2)c2ccccc21
vNsp9-nsp9.2-33	Z2105986954	-8.6	0.307	375.471	REAL	O=C1CCc2cc(NC(=O)NC3[C@H]4CC[C@@H]3Cc3ccccc3C4)ccc2N1
vNsp9-nsp9.2-34	Z2158636017	-8.6	0.261	442.517	REAL	O=C1CCc2cc(-c3noc([C@H]4C[C@@H]5CCCC[C@@H]5N4C(=O)c4ccccc4)n3)ccc2N1
vNsp9-nsp9.2-35	Z2160287639	-8.6	0.261	440.502	REAL	O=C(c1ccccc1)N1[C@@H](c2nc(-c3cc(=O)[nH]c4ccccc34)no2)C[C@@H]2CCCC[C@@H]21
vNsp9-nsp9.2-36	Z431891148	-8.6	0.269	424.459	REAL	O=C(NC[C@@H]1CC2c3ccccc3C1c1ccccc12)c1cnc2[nH]c(=O)[nH]c(=O)c2c1
vNsp9-nsp9.2-37	ZINC000002336562	-8.6	0.287	390.485	ZINC	O=C1C=CC2=N[C@@]34c5ccccc5CC[C@@H]3CC3=C(c5ccccc5CC3)N4C2=C1
vNsp9-nsp9.2-38	ZINC000002336563	-8.6	0.287	390.485	ZINC	O=C1C=CC2=N[C@]34c5ccccc5CC[C@H]3CC3=C(c5ccccc5CC3)N4C2=C1
vNsp9-nsp9.2-39	ZINC000002466568	-8.6	0.287	420.87	ZINC	O=C(Nc1ccc(F)cc1Cl)[C@H]1c2ccccc2C(=O)N2CCc3ccccc3[C@H]12
vNsp9-nsp9.2-40	ZINC000004301341	-8.6	0.297	376.458	ZINC	c1ccc(C2=NN3[C@H](C2)c2ccccc2O[C@@H]3c2ccc3ccccc3c2)cc1
vNsp9-nsp9.2-41	ZINC000004563809	-8.6	0.287	396.489	ZINC	CCc1cccc(NC(=O)[C@H]2c3ccccc3C(=O)N3CCc4ccccc4[C@H]23)c1
vNsp9-nsp9.2-42	ZINC000006724159	-8.6	0.297	386.425	ZINC	O=C(Nc1ccc(F)cc1)[C@H]1c2ccccc2C(=O)N2CCc3ccccc3[C@H]12
vNsp9-nsp9.2-43	ZINC000009598516	-8.6	0.277	432.906	ZINC	COc1ccc(Cl)cc1NC(=O)[C@H]1c2ccccc2C(=O)N2CCc3ccccc3[C@H]12
vNsp9-nsp9.2-44	ZINC000012417037	-8.6	0.331	372.444	ZINC	C[C@H]1Oc2ccc(S(=O)(=O)N3CCCCc4ccccc43)cc2NC1=O
vNsp9-nsp9.2-45	ZINC000014198734	-8.6	0.319	358.396	ZINC	C[C@H]1Oc2ccc(NC(=O)c3ccc4c5c(cccc53)CC4)cc2NC1=O
vNsp9-nsp9.2-46	ZINC000257334714	-8.6	0.261	439.514	ZINC	O=C([C@@H]1CC(=O)Nc2ccccc21)N1CCNC(=O)[C@@H]1Cc1cccc(-c2ccccc2)c1
vNsp9-nsp9.2-47	PV-001875531671	-8.5	0.274	457.276	REAL	O=C(c1cccc(-c2noc(O)n2)c1)N1C[C@@H]2[C@H](C1)C(F)(F)C(F)(F)F)C(F)(F)C2(F)F
vNsp9-nsp9.2-48	PV-001948596877	-8.5	0.258	457.411	REAL	O=C1CC(c2ccc(NC(=O)Nc3ccn(-c4ccccc4C(F)(F)F)n3)cc2)CC(=O)N1
vNsp9-nsp9.2-49	Z1014383878	-8.5	0.258	452.464	REAL	O=C(Nc1cccc(-c2nnn[nH]2)c1)[C@@H]1C[C@H]2CCCC[C@H]2N1C(=O)c1ccc(F)cc1F
vNsp9-nsp9.2-50	Z1014397590	-8.5	0.243	474.559	REAL	O=C1NC(=O)C2(CCN(C(=O)[C@H]3C[C@H]4CCCC[C@@H]4N3C(=O)c3ccc4ccccc4c3)CC2)N1
vNsp9-nsp9.2-51	Z1042990360	-8.5	0.304	369.379	REAL	O=C(Nc1ccc(-c2noc(=O)[nH]2)cc1)c1ccc2c(c1)-c1ccccc1C2
vNsp9-nsp9.2-52	Z1098709950	-8.5	0.283	401.396	REAL	O=C(Nc1n[nH]c2ccc(F)cc12)c1ccc2c(c1)C[C@H](c1ccccc1)OC2=O
vNsp9-nsp9.2-53	Z1128758047	-8.5	0.315	353.384	REAL	O=C(Nc1ccc(-c2nnn[nH]2)cc1)c1ccc2c(c1)-c1ccccc1C2
vNsp9-nsp9.2-54	Z1171670002	-8.5	0.266	423.471	REAL	O=C(NC[C@@H]1CC2c3ccccc3C1c1ccccc12)c1ccc(-c2noc(=O)[nH]2)cc1
vNsp9-nsp9.2-55	Z1269872274	-8.5	0.266	420.515	REAL	Cc1nnc(-c2ccc(C(=O)NC[C@@H]3CC4c5ccccc5C3c3ccccc34)cc2)[nH]1
vNsp9-nsp9.2-56	Z1373819196	-8.5	0.283	402.492	REAL	CC[C@H]1Oc2cc([C@@H](C)NC(=O)[C@@H](C)c3ccc4ccccc4c3)ccc2NC1=O
vNsp9-nsp9.2-57	Z1374247583	-8.5	0.293	388.509	REAL	O=C1CCCc2cc(C(=O)N3CCC[C@@]4(CCCc5ccccc54)C3)ccc2N1
vNsp9-nsp9.2-58	Z1374247775	-8.5	0.274	417.507	REAL	C[C@@]1(c2ccc(C(=O)N3CCC[C@@]4(CCCc5ccccc54)C3)cc2)NC(=O)NC1=O
vNsp9-nsp9.2-59	Z1461741130	-8.5	0.283	420.458	REAL	CN1C(=O)N[C@@]2(CCC[C@@H]2CNC(=O)N2CCCC[C@@H]2c2ccc(F)cc2F)C1=O
vNsp9-nsp9.2-60	Z1499315551	-8.5	0.266	426.475	REAL	O=C(N[C@@H](c1ccccc1)[C@H]1CCCc2ccccc21)c1cnc2[nH]c(=O)[nH]c(=O)c2c1
vNsp9-nsp9.2-61	Z1506410084	-8.5	0.304	379.415	REAL	O=C1COc2cc(NC(=O)N3CCO[C@]4(CCc5ccccc54)C3)ccc2N1
vNsp9-nsp9.2-62	Z1544044328	-8.5	0.315	364.404	REAL	C[C@@H]1CCc2ccccc2[C@@H]1NC(=O)c1cnc2c(c1)c(=O)[nH]c(=O)n2C
vNsp9-nsp9.2-63	Z1581473271	-8.5	0.258	440.585	REAL	O=C(NC[C@H]1CCCN1C(=O)[C@H]1C[C@@]12CCCc1ccccc12)[C@@H]1C[C@@]12CCc1ccccc12
vNsp9-nsp9.2-64	Z1585178605	-8.5	0.274	415.539	REAL	O=C(Nc1ccc2c3c(cccc13)CC2)N1CCC[C@H](c2nnc3n2CCCCC3)C1
vNsp9-nsp9.2-65	Z1601677547	-8.5	0.283	404.512	REAL	CC1(C)CC[C@H]2C[C@@H](NC(=O)Nc3cccc(N4CCNC4=O)c3)c3cccc1c32
vNsp9-nsp9.2-66	Z1603534374	-8.5	0.274	424.543	REAL	CC1(C)CC[C@H]2C[C@@H](NC(=O)N3CCC([C@]4(C)NC(=O)NC4=O)CC3)c3cccc1c32
vNsp9-nsp9.2-67	Z1626782700	-8.5	0.274	411.46	REAL	O=C1CCC(=O)N(c2ccc(C(=O)N3CC=C(c4cccc5ccccc45)C3)cc2)N1
vNsp9-nsp9.2-68	Z1626784260	-8.5	0.293	384.394	REAL	O=C(c1cnc2[nH]c(=O)[nH]c(=O)c2c1)N1CC=C(c2ccccc3ccccc23)C1
vNsp9-nsp9.2-69	Z1637547541	-8.5	0.283	415.414	REAL	CNC(=O)c1cccc(NC(=O)N[C@H](c2cccc3ccccc23)C(F)(F)F)c1C
vNsp9-nsp9.2-70	Z1685323319	-8.5	0.304	369.427	REAL	Cc1nnc(-c2cccc(-c3noc([C@@H]4C[C@@]45CCc4ccccc45)n3)c2)[nH]1
vNsp9-nsp9.2-71	Z1693220356	-8.5	0.283	428.512	REAL	CC(C)[C@@H]1CCc2ccccc2[C@H]1NS(=O)(=O)c1cnc2c(c1)c(=O)[nH]c(=O)n2C
vNsp9-nsp9.2-72	Z1723441064	-8.5	0.266	430.482	REAL	C[C@H]1C[C@H](c2ccccc2F)N(C(=O)c2cccc(-c3cnc4[nH]c(=O)n(C)c4c3)c2)C1
vNsp9-nsp9.2-73	Z1902113203	-8.5	0.283	407.6	REAL	CN1CCC(N(C)c2ccccc2CNC[C@@]2(O)[C@H]3[C@@H]4C[C@@H]5[C@H]6[C@H]4C[C@H]3[C@H]6[C@@H]52)CC1
vNsp9-nsp9.2-74	Z2099253090	-8.5	0.293	396.529	REAL	O=C1COC[C@H](C[C@H]2CN(C(=O)[C@@H]3CCC[C@H]4CCCC[C@H]43)c3ccccc32)N1
vNsp9-nsp9.2-75	Z2159546797	-8.5	0.274	421.456	REAL	Cn1ccc(-c2noc([C@H]3C[C@@H]4CCCC[C@H]4N3C(=O)c3ccccc3)n2)c(=O)[nH]c1=O
vNsp9-nsp9.2-76	Z2219870566	-8.5	0.283	397.433	REAL	O=C1CNC(=O)c2ccc(C(=O)N3Cc4ccccc4-c4ccccc4C3)cc2N1
vNsp9-nsp9.2-77	Z2371498666	-8.5	0.293	393.489	REAL	O=C1CCCCc2ccc(NC(=O)N3CCC[C@H](c4nnc5n4CCC5)C3)cc21
vNsp9-nsp9.2-78	Z2619375941	-8.5	0.327	357.409	REAL	C[C@H]1Oc2ccc(NC(=O)[C@H]3CC(=O)N[C@@H]4CCCC[C@H]43)cc2NC1=O
vNsp9-nsp9.2-79	Z2793654732	-8.5	0.304	396.51	REAL	O=C(NC[C@@H]1CS(=O)(=O)c2ccccc21)N1CC[C@@]2(CCc3ccccc32)C1
vNsp9-nsp9.2-80	Z281604624	-8.5	0.258	438.533	REAL	Cc1nc2nc(N)nn2c(C)c1CC(=O)NC[C@@H]1CC2c3ccccc3C1c1ccccc12
vNsp9-nsp9.2-81	Z2964124784	-8.5	0.304	378.431	REAL	CC1(C)CCN(C(=O)c2cnc3[nH]c(=O)[nH]c(=O)c3c2)C[C@@H]1c1ccccc1
vNsp9-nsp9.2-82	Z33397808	-8.5	0.274	410.432	REAL	O=C1CN(C(=O)c2nn(Cc3ccccc3)c(=O)c3ccccc23)c2ccccc2N1
vNsp9-nsp9.2-83	Z358867962	-8.5	0.283	415.532	REAL	Cc1cccc([C@@H](CC(=O)O[C@@H](C)C(=O)N[C@@H](C)[C@H]2C[C@H]3CC[C@H]2C3)NC(N)=O)c1
vNsp9-nsp9.2-84	Z448674688	-8.5	0.243	463.583	REAL	O=C(NC[C@@H]1CC2c3ccccc3C1c1ccccc12)N1CCC(c2nnc3ccccn23)CC1
vNsp9-nsp9.2-85	Z73363218	-8.5	0.274	410.472	REAL	O=C1COc2ccc(C(=O)NC[C@@H]3CC4c5ccccc5C3c3ccccc34)cc2N1
vNsp9-nsp9.2-86	Z740884216	-8.5	0.34	358.417	REAL	O=C1COc2ccc(S(=O)(=O)N3CCCCc4ccccc43)cc2N1
vNsp9-nsp9.2-87	Z740884300	-8.5	0.327	371.416	REAL	O=c1[nH]c(=O)c2cc(S(=O)(=O)N3CCCCc4ccccc43)ccc2[nH]1
vNsp9-nsp9.2-88	Z803631308	-8.5	0.258	439.47	REAL	O=C1COc2ccc(NC(=O)[C@H]3CC(=O)N(c4ccc5c(c4)Cc4ccccc4-5)C3)cc2N1
vNsp9-nsp9.2-89	ZINC000000629970	-8.5	0.266	415.491	ZINC	C[C@@]12C(=O)N(c3ccc4ccccc4c3)C(=O)[C@H]1C1c3ccccc3C2c2ccccc21
vNsp9-nsp9.2-90	ZINC000000708552	-8.5	0.283	397.473	ZINC	CC1(C)CC(=O)C2=C(C1)[C@H](c1ccc3c(c1)OCO3)Nc1ccc3ccccc3c12
vNsp9-nsp9.2-91	ZINC000002466544	-8.5	0.283	420.87	ZINC	O=C(Nc1ccc(F)c(Cl)c1)[C@H]1c2ccccc2C(=O)N2CCc3ccccc3[C@H]12
vNsp9-nsp9.2-92	ZINC000004811935	-8.5	0.293	376.458	ZINC	c1ccc([C@H]2Oc3ccccc3[C@@H]3CC(c4cccc5ccccc54)=NN32)cc1
vNsp9-nsp9.2-93	ZINC000023399789	-8.5	0.304	371.483	ZINC	Cc1nc([C@@H]2CCCN(Cc3ccc4c(c3)Cc3ccccc3-4)C2)cc(=O)[nH]1
vNsp9-nsp9.2-94	ZINC000048523762	-8.5	0.236	464.475	ZINC	O=C1c2ccccc2C(=O)C2=C3C=CC4=CC5=C(C(=O)c6ccccc6C5=O)C5=CC=C(C=C12)[C@H]3[C@H]45
vNsp9-nsp9.2-95	ZINC000059475095	-8.5	0.266	412.535	ZINC	c1ccc2c(c1)ccc2N1Cc2cc3c(cc2C1)CN(c1ccccc2ccc21)C3
vNsp9-nsp9.2-96	ZINC000252602741	-8.5	0.283	394.433	ZINC	NC(=O)NN=C1c2ccccc2N(C2c3ccccc3C=Cc3ccccc32)C1=O
vNsp9-nsp9.2-97	PV-001830108148	-8.4	0.271	428.502	REAL	C[C@H]1Oc2ccc(C(=O)C3CCN(C(=O)/C(F)=C\C4CCCCC4)CC3)cc2NC1=O
vNsp9-nsp9.2-98	PV-001840979694	-8.4	0.28	418.414	REAL	O=C(N[C@@H]1CCCCC[C@@H]1c1ccccc1C(F)(F)F)c1ccc2oc(=O)[nH]c2c1
vNsp9-nsp9.2-99	PV-001864857702	-8.4	0.28	417.386	REAL	C[C@@]1(c2ccc(C(=O)N3CCc4cccc(C(F)(F)F)c4C3)cc2)NC(=O)NC1=O
vNsp9-nsp9.2-100	PV-001916080720	-8.4	0.323	371.769	REAL	O=C1c2ccccc2C(F)(F)C(=O)N1Cc1ccc(Cl)c2ccccc12

Supplementary Table 44. Virtual screening hits 101 to 200 of the screen against the dimerization site of nsp9 (Screen ID: 24). Compounds were filtered so that hits had MW < 600 dalton, cLogP < 6, number of hydrogen bond acceptors < 11, and no reactive functional groups. The name of each compound consists of the initial letter 'v' for virtual hit, followed by the target protein name and the target site ('nsp9' for the nsp9 binding site, 2 for docking scenario 2). The score is the docking score given by QuickVina 2 in kcal/mol. The ligand efficiency (LE) is computed as LE = -score/#NonH, where #NonH is the number of heavy (i.e. non hydrogen) atoms.

Name	Catalog ID	Score	LE	MW	Library	SMILES
vNsp10-ppi1-1	Z1554585254	-8.8	0.267	447.494	REAL	CN1C(=O)NC2(CCN(C(=O)Nc3cccc(C(=O)N4CCc5ccccc54)c3)CC2)C1=O
vNsp10-ppi1-2	Z2002423492	-8.8	0.275	425.483	REAL	O=C1[C@@H]2[C@@H]3C[C@H]4[C@@H]2[C@]2(C(=O)Oc5cccc(C(=O)N6CCc7ccccc7C6)c5)[C@H]1[C@@H]3[C@@H]42
vNsp10-ppi1-3	PV-001940740368	-8.7	0.272	456.609	REAL	C[C@H](CNC(=O)Nc1ccc(S(=O)(=O)N[C@H](C)[C@@H]2C[C@H]3CC[C@H]2C3)cc1)c1ccncc1
vNsp10-ppi1-4	Z1907681358	-8.7	0.3	414.524	REAL	C=CCNS(=O)(=O)c1ccc(C(=O)NC[C@]2(O)[C@H]3[C@@H]4C[C@@H]5[C@@H]6[C@H]4C[C@H]3[C@H]6[C@H]52)cc1
vNsp10-ppi1-5	Z1313212974	-8.6	0.297	384.394	REAL	Cc1cc(C(=O)N2Cc3ccccc3-c3ccccc32)nc2nc(O)[nH]c(=O)c12
vNsp10-ppi1-6	Z1684579926	-8.6	0.277	417.38	REAL	CN1C(=O)c2ccc(-c3nc(-c4cccc([C@]5(C)NC(=O)NC5=O)c4)no3)cc2C1=O
vNsp10-ppi1-7	Z1766126310	-8.6	0.277	418.398	REAL	O=C1CCCc2ccc(NC(=O)c3cc(F)cc4c(=O)c5cc(F)ccc5[nH]c34)cc21
vNsp10-ppi1-8	Z1769366525	-8.6	0.269	436.471	REAL	Cc1cccc2nc(C3CCN(C(=O)CCc4nc5c([nH]4)c(=O)[nH]c(=O)n5C)CC3)oc12
vNsp10-ppi1-9	ZINC000009211273	-8.6	0.246	472.547	ZINC15	Cc1cc(=O)oc2cc(NC(=O)C3CCN(c4ncnc5c4nc4n5CCCCC4)CC3)ccc12
vNsp10-ppi1-10	Z1018313090	-8.5	0.25	481.939	REAL	C[C@]1(c2cccc(CNC(=O)N3CCC(c4nc5cc(Cl)ccc5o4)CC3)c2)NC(=O)NC1=O
vNsp10-ppi1-11	Z1028479320	-8.5	0.236	492.51	REAL	C[C@@]1(c2cccc(CNC(=O)N3CCC[C@@H](c4nc(-c5cccc(F)c5)no4)C3)c2)NC(=O)NC1=O
vNsp10-ppi1-12	Z1165732158	-8.5	0.25	447.457	REAL	O=C(Nc1ccc2nc(NC(=O)c3n[nH]c4ccccc34)ccc2c1)c1n[nH]c2ccccc12
vNsp10-ppi1-13	Z1905519675	-8.5	0.293	394.557	REAL	CCC[C@@H](CCc1cccc1)NC(=O)NC[C@@]1(O)[C@@H]2[C@@H]3C[C@@H]4[C@H]5[C@@H]3C[C@@H]2[C@H]5[C@@H]41
vNsp10-ppi1-14	Z1907923722	-8.5	0.283	398.421	REAL	NC(=O)N1CCc2ccc(NC(=O)c3cccc4c(=O)c5ccccc5[nH]c34)cc21
vNsp10-ppi1-15	Z2140576210	-8.5	0.258	448.478	REAL	C[C@@]1(c2ccc(C(=O)N3C[C@@H](C[C@H]4COCC(=O)N4)c4ccccc43)cc2)NC(=O)NC1=O
vNsp10-ppi1-16	ZINC000001862466	-8.5	0.243	455.468	ZINC15	Cc1nc(-c2cc3c(ccc4ccccc43)oc2=O)cc2c1c(=O)oc1ccc3ccccc3c12
vNsp10-ppi1-17	PV-001941700947	-8.4	0.271	416.44	REAL	COC(=O)c1cccc(C#Cc2cccc(NC(=O)NNc3cc(C)nc(N)n3)c2)c1
vNsp10-ppi1-18	PV-001951422452	-8.4	0.28	415.449	REAL	CN1C(=O)C(C)(C)COc2ccc(NC(=O)N3CCC4(CC3)NC(=O)NC4=O)cc21
vNsp10-ppi1-19	Z1002304938	-8.4	0.24	484.583	REAL	C[C@@]1(c2cccc(CNc3nc(-c4ccenc4)nc4sc5c(c34)CCCC5)c2)NC(=O)NC1=O
vNsp10-ppi1-20	Z1018313560	-8.4	0.255	445.521	REAL	C[C@]1(c2cccc(CNC(=O)N3CCC(c4cc5ccccc5[nH]4)CC3)c2)NC(=O)NC1=O
vNsp10-ppi1-21	Z1027916398	-8.4	0.262	431.495	REAL	Cc1noc([C@@H]2CCCN(C(=O)Nc3cccc(C(=O)N4CCc5ccccc54)c3)C2)n1
vNsp10-ppi1-22	Z1333510772	-8.4	0.255	440.545	REAL	Cc1ccc2[nH]c(C(=O)N3C[C@@H]4CCCN(C(=O)c5cc6ccc(C)ccc6[nH]5)[C@@H]4C3)cc2c1
vNsp10-ppi1-23	Z1571381874	-8.4	0.262	446.49	REAL	Cn1ncc2c(=O)[nH]c(CCC(=O)Nc3ccc(O)c(-c4nc5ccccc5s4)c3)nc21
vNsp10-ppi1-24	Z1723430342	-8.4	0.227	499.525	REAL	Cn1c(=O)[nH]c2ncc(-c3cccc(C(=O)N4CCC(C(=O)Nc5ccc6c(c5)OCO6)CC4)c3)cc21
vNsp10-ppi1-25	Z1723433805	-8.4	0.24	487.946	REAL	Cn1c(=O)[nH]c2ncc(-c3cccc(C(=O)N4CCC(c5nc6cc(Cl)ccc6o5)CC4)c3)cc21
vNsp10-ppi1-26	Z1763864729	-8.4	0.255	443.477	REAL	O=C(c1ccc2[nH]c3ccccc3c(=O)c2c1)N1CCCN(C(=O)c2ccccc2F)CC1
vNsp10-ppi1-27	Z1765661123	-8.4	0.262	437.365	REAL	Cn1ncc2c(=O)[nH]c(NNC(=O)c3cc(F)cc4c(=O)c5cc(F)ccc5[nH]c34)nc21
vNsp10-ppi1-28	Z185218180	-8.4	0.255	459.485	REAL	O=C(NNC(=O)c1c[nH]c2ccccc12)c1ccc(NC2=NS(=O)(=O)c3ccccc32)cc1
vNsp10-ppi1-29	Z2138775241	-8.4	0.28	449.511	REAL	O=C1NC(=O)C2(CCC(NC(=O)c3ccc4c(c3)SC3=NS(=O)(=O)CCN34)CC2)N1
vNsp10-ppi1-30	Z2160288385	-8.4	0.271	416.396	REAL	Cc1cc(-c2nc(-c3cc(=O)[nH]c4ccccc34)no2)nc2c1c(=O)n(C)c(=O)n2C
vNsp10-ppi1-31	Z2178243476	-8.4	0.255	441.461	REAL	O=C(c1ccc2[nH]c3ccccc3c(=O)c2c1)N1CCC(c2noc3cc(F)ccc23)CC1
vNsp10-ppi1-32	Z228233828	-8.4	0.247	462.544	REAL	C[C@@H]1c2cc3c(cc2C2(CCCC2)CN1C(=O)CN1C(=O)[C@H]2[C@H]4C=C[C@@H](C4)[C@H]2C1=O)OCCO3
vNsp10-ppi1-33	Z240397980	-8.4	0.255	473.596	REAL	O=C(C1CCN(C2=NS(=O)(=O)c3ccccc32)CC1)N1CCN(C(=O)N2CCCCC2)CC1
vNsp10-ppi1-34	Z397589742	-8.4	0.24	483.547	REAL	O=C1c2ccccc2S(=O)(=O)c2cc(C(=O)N3CCN(c4ccc5ccccc5n4)CC3)ccc21
vNsp10-ppi1-35	Z511799576	-8.4	0.24	492.53	REAL	O=C(Nc1cccc(C(=O)N2CCN(C3=NS(=O)(=O)c4ccccc43)CC2)c1)c1ccc(F)cc1
vNsp10-ppi1-36	Z511805156	-8.4	0.24	497.525	REAL	O=C(c1nn(-c2ccc(F)c(F)c2)c2c1CCC2)N1CCN(C2=NS(=O)(=O)c3ccccc32)CC1
vNsp10-ppi1-37	Z651897218	-8.4	0.233	498.464	REAL	C[C@@H](c1nc(-c2cccc(C(F)(F)F)c2)no1)N1CCN(C(=O)c2n[nH]c(=O)c3ccccc23)CC1
vNsp10-ppi1-38	Z838336028	-8.4	0.24	475.547	REAL	Cc1nc(-c2ccc(NC(=O)NCc3ccc(C(=O)N4C[C@H](C)O[C@H](C)C4)cc3)cc2)cc(=O)[nH]1
vNsp10-ppi1-39	Z838768352	-8.4	0.227	497.549	REAL	C[C@H]1CN(C(=O)c2ccc(CNC(=O)c3cccc(N4C(=O)c5ccccc5C4=O)c3)cc2)C[C@@H](C)O1
vNsp10-ppi1-40	Z925888868	-8.4	0.262	456.889	REAL	Cn1c(=O)[nH]c(=O)c2[nH]c(CCC(=O)N3CCC(c4nc5cc(Cl)ccc5o4)CC3)nc21
vNsp10-ppi1-41	Z992145818	-8.4	0.227	493.609	REAL	O=C(c1cccc2ccccc12)N1CCC[C@H](C(=O)N2CCC(c3nc(-c4ccccc4)n[nH]3)CC2)C1
vNsp10-ppi1-42	Z992637882	-8.4	0.233	483.526	REAL	C[C@@]1(c2cccc(CNC(=O)Nc3cccc(C(=O)N4CCc5ccccc54)c3)c2)NC(=O)NC1=O
vNsp10-ppi1-43	ZINC000003371634	-8.4	0.24	480.591	ZINC15	Cc1ccc(N2C(=O)c3ccccc3/C(=C/Nc3ncnc4sc5c(c43)CCCC5)C2=O)c(C)c1
vNsp10-ppi1-44	ZINC000104854096	-8.4	0.24	480.591	ZINC15	Cc1ccc(N2C(=O)c3ccccc3/C(=C\Nc3ncnc4sc5c(c43)CCCC5)C2=O)c(C)c1
vNsp10-ppi1-45	PV-001810978558	-8.3	0.268	414.424	REAL	CNC(=O)c1ccc(NC(=O)c2ccc(-c3nnc(-c4cccc(C)c4)o3)cc2)nn1
vNsp10-ppi1-46	PV-001817755623	-8.3	0.286	456.251	REAL	Cn1c(=O)c2ccc(NC(=O)c3cc4ccc(Br)cc4c(=O)o3)cc2n(C)c1=O
vNsp10-ppi1-47	PV-001819607343	-8.3	0.259	428.422	REAL	NC(=O)NC(=O)c1cccc(NC(=O)c2cc(-c3cccc3)nc3cc(F)ccc23)c1
vNsp10-ppi1-48	PV-001819607724	-8.3	0.259	444.877	REAL	NC(=O)NC(=O)c1cccc(NC(=O)c2cc(-c3ccc(Cl)cc3)nc3ccccc23)c1
vNsp10-ppi1-49	PV-001862353769	-8.3	0.259	457.51	REAL	Cc1cc(C)nc(-n2[nH]c(C(=O)N3CCO[C@H](c4ccc(S(C)(=O)=O)cc4)C3)cc2=O)n1
vNsp10-ppi1-50	PV-001941699840	-8.3	0.252	454.407	REAL	COC(=O)c1cccc(C#Cc2cccc(NC(=O)NNc3cc(C(F)(F)F)ccn3)c2)c1
vNsp10-ppi1-51	PV-001941700374	-8.3	0.268	422.39	REAL	COC(=O)c1cccc(C#Cc2cccc(NC(=O)NNc3ncc(F)cc3F)c2)c1
vNsp10-ppi1-52	Z1000361640	-8.3	0.259	442.45	REAL	Cn1c(=O)[nH]c(=O)c2[nH]c(CCC(=O)N3CCC(C(=O)Nc4cccc(F)c4)CC3)nc21
vNsp10-ppi1-53	Z1000936108	-8.3	0.224	494.549	REAL	C[C@@]1(c2cccc(CNC(=O)[C@@H]3CC(=O)N(c4ccc5c(c4)Cc4ccccc4-5)C3)c2)NC(=O)NC1=O
vNsp10-ppi1-54	Z1000942970	-8.3	0.237	495.559	REAL	C[C@]1(c2cccc(CNC(=O)C3CCN(C4=NS(=O)(=O)c5ccccc54)CC3)c2)NC(=O)NC1=O
vNsp10-ppi1-55	Z1004161538	-8.3	0.237	474.495	REAL	Cc1nc(-c2ccc(NC(=O)N3CCC[C@@H](c4nc(-c5cccc(F)c5)no4)C3)cc2)cc(=O)[nH]1
vNsp10-ppi1-56	Z1018320010	-8.3	0.252	446.509	REAL	C[C@]1(c2cccc(CNC(=O)N3CCC(c4nc5ccccc5[nH]4)CC3)c2)NC(=O)NC1=O
vNsp10-ppi1-57	Z1018322170	-8.3	0.252	447.494	REAL	C[C@]1(c2cccc(CNC(=O)N3CCC(c4nc5ccccc5o4)CC3)c2)NC(=O)NC1=O
vNsp10-ppi1-58	Z1023595734	-8.3	0.252	481.963	REAL	Cn1c(S)nc2cc(C(=O)N3CCC[C@H](c4nc(-c5ccc(Cl)cc5)no4)C3)ccc2c1=O
vNsp10-ppi1-59	Z1024045698	-8.3	0.252	444.533	REAL	O=C1Nc2ccccc2[C@@H]1C1CCN(C(=O)C2CCN(c3nc4ccccc4o3)CC2)CC1
vNsp10-ppi1-60	Z1027885332	-8.3	0.252	448.457	REAL	Cc1nc(-c2ccc(NC(=O)N3CCC[C@H](c4nc(-c5cccc(F)c5)no4)C3)c2)no1
vNsp10-ppi1-61	Z1069479690	-8.3	0.237	474.515	REAL	Cc1c[nH]c(=O)n1-c1ccc(C(=O)N2CCC(C(=O)c3ccc4c(c3)NC(=O)[C@H](C)O4)CC2)cc1
vNsp10-ppi1-62	Z1071336810	-8.3	0.244	462.461	REAL	C[C@@H]1Oc2ccc(C(=O)C3CCN(C(=O)Nc4ccc5c(c4)C(=O)NC5=O)CC3)cc2NC1=O
vNsp10-ppi1-63	Z1092424798	-8.3	0.244	452.473	REAL	O=C(NNc1nc(-c2cccnc2)no1)[C@H]1CC(=O)N(c2ccc3c(c2)Cc2ccccc2-3)C1
vNsp10-ppi1-64	Z1098711166	-8.3	0.259	438.437	REAL	O=C(Nc1n[nH]c2ccc(F)cc12)[C@@H]1CCC[C@@H](C(=O)Nc2n[nH]c3ccc(F)cc23)C1
vNsp10-ppi1-65	Z1147771205	-8.3	0.237	493.562	REAL	Cc1ccc(-n2nc(C(=O)N3CCN(C4=NS(=O)(=O)c5ccccc54)CC3)c3c2CCC3)c(F)c1
vNsp10-ppi1-66	Z1270006322	-8.3	0.259	432.439	REAL	Cc1cc(C(=O)N2CCN(C(=O)c3cc4ccccc4[nH]3)CC2)nc2nc(O)[nH]c(=O)c12
vNsp10-ppi1-67	Z1278114934	-8.3	0.268	416.484	REAL	O=C1CCc2ccc(NC(=O)N3CCC(c4nc(-c5ccccc5)n[nH]4)CC3)cc2N1
vNsp10-ppi1-68	Z1281865420	-8.3	0.252	442.434	REAL	Cc1cc(=O)oc2cc(OCc3ccc(C(=O)NNc4ncnc5nc[nH]c45)cc3)ccc12
vNsp10-ppi1-69	Z1313999761	-8.3	0.252	447.425	REAL	Cc1cc(C(=O)NCc2ccc(NC(=O)c3ccc(F)cc3)cc2)nc2nc(O)[nH]c(=O)c12
vNsp10-ppi1-70	Z1391595476	-8.3	0.252	446.505	REAL	C[C@H]1C(=O)Nc2cc(C(=O)N3CCC[C@H](NC(=O)c4ac5ccccc5o4)C3)ccc2N1C
vNsp10-ppi1-71	Z1447722636	-8.3	0.259	429.522	REAL	O=C(NC[C@@H]1[C@H]2Cc3ccccc3[C@@H]12)N1CCN(Cc2nc3ccccc3c(=O)[nH]2)CC1
vNsp10-ppi1-72	Z1466232901	-8.3	0.277	427.488	REAL	C[C@H]1CN(C(=O)Nc2ccc3c(c2)S(=O)(=O)CC3)CCN1c1nccn2cnnc12
vNsp10-ppi1-73	Z1623725880	-8.3	0.277	409.488	REAL	Cc1ccc2[nH]c3c(c2c1)C[C@H](NC(=O)N1CCC2(CC1)NC(=O)N(C)C2=O)CC3
vNsp10-ppi1-74	Z1683766366	-8.3	0.259	426.431	REAL	NC(=O)c1cccc(-c2noc(-c3cccc(NC(=O)[C@H]4Cc5ccccc5O4)c3)n2)c1
vNsp10-ppi1-75	Z1685319763	-8.3	0.259	422.447	REAL	Cc1nnc(-c2cccc(-c3noc(-c4cncc(-c5ccc6c(c5)CCO6)c4n3)c2)[nH]1
vNsp10-ppi1-76	Z1685321741	-8.3	0.252	443.466	REAL	Cc1ccc([C@]2(C)NC(=O)N(Cc3nc(-c4cccc(-c5nnc(C)[nH]5)c4)no3)C2=O)cc1
vNsp10-ppi1-77	Z1723432535	-8.3	0.237	473.507	REAL	Cn1c(=O)[nH]c2ncc(-c3cccc(C(=O)N4CCC(NC(=O)c5ccc(F)cc5)CC4)c3)cc21
vNsp10-ppi1-78	Z1723433681	-8.3	0.224	496.569	REAL	Cn1c(=O)[nH]c2ncc(-c3cccc(C(=O)N4CCN(CC(=O)N5CCc6ccccc65)CC4)c3)cc21
vNsp10-ppi1-79	Z1723436102	-8.3	0.244	451.529	REAL	Cn1c(=O)[nH]c2ncc(-c3cccc(C(=O)N4CCC(c5cc6ccccc6[nH]5)CC4)c3)cc21
vNsp10-ppi1-80	Z1723437642	-8.3	0.237	473.531	REAL	Cc1cc(C(=O)NC2CCN(C(=O)c3cccc(-c4cnc5[nH]c(=O)n(C)c5c4)c3)CC2)c(C)o1
vNsp10-ppi1-81	Z1723438078	-8.3	0.231	480.527	REAL	Cn1c(=O)[nH]c2ncc(-c3cccc(C(=O)N4CCC(c5nc(-c6ccccc6)no5)CC4)c3)cc21
vNsp10-ppi1-82	Z1723445289	-8.3	0.244	446.509	REAL	Cn1c(=O)[nH]c2ncc(-c3cccc(C(=O)N4CC=C(c5cccc6ccccc56)C4)c3)cc21
vNsp10-ppi1-83	Z1728533456	-8.3	0.268	424.499	REAL	O=C(O)[C@@H]1C[C@H]2CCCC[C@H]2N1C(=O)[C@H]1CCCN(C(=O)c2ccc3[nH]ncc3c2)C1
vNsp10-ppi1-84	Z17955407	-8.3	0.237	498.918	REAL	Cc1cc(=O)oc2cc(OCC(=O)N3CCN(C(=O)[C@H]4COc5ccccc5O4)CC3)c(Cl)cc12
vNsp10-ppi1-85	Z1896762151	-8.3	0.259	431.455	REAL	O=C(NNc1cnc2ccccc2n1)[C@H]1CN(Cc2nc3ccccc3c(=O)[nH]2)CCO1
vNsp10-ppi1-86	Z2008564505	-8.3	0.252	444.513	REAL	Cc1cc(-c2nnc(N3CCC(C(=O)Nc4cccc(F)c4)CC3)n2C)c2ccccc2n1
vNsp10-ppi1-87	Z2032903082	-8.3	0.244	447.457	REAL	O=C(Nc1ccc2nc(NC(=O)c3ccc4cncn4c3)ccc2c1)c1ccc2cncn2c1
vNsp10-ppi1-88	Z203498158	-8.3	0.244	455.513	REAL	Cc1nc(NC(=O)c2ccc(COc3ccc4c(C)cc(=O)oc4c3)cc2)nc2c1CCCC2
vNsp10-ppi1-89	Z2087642860	-8.3	0.244	447.457	REAL	O=c1[nH]c(-c2nnc(-c3ccc(Cn4nnc(-c5cccc5)n4)cc3)o2)cc2ccccc12
vNsp10-ppi1-90	Z2099250020	-8.3	0.252	444.49	REAL	O=C1COC[C@H](C[C@@H]2CN(C(=O)c3ccc4c(=O)n5c(nc4c3)CCC5)c3ccccc32)N1
vNsp10-ppi1-91	Z2099940140	-8.3	0.268	437.435	REAL	Cc1cc(=O)oc2cc(N(C)C(=O)c3ccc4c(c3)S(=O)(=O)Nc3ncnn3-c4ccc12)c1
vNsp10-ppi1-92	Z2140567616	-8.3	0.252	448.478	REAL	C[C@@]1(c2cccc(C(=O)N3C[C@@H](C[C@H]4COCC(=O)N4)c4ccccc43)c2)NC(=O)NC1=O
vNsp10-ppi1-93	Z2147310569	-8.3	0.252	444.533	REAL	CC(=O)N1C[C@@H]2CCC[C@H](NC(=O)c3ccc(-c4nnc(-c5cccc(C)c5)o4)cc3)[C@H]2C1
vNsp10-ppi1-94	Z2157919690	-8.3	0.277	402.409	REAL	C[C@@]1(c2cccc(-c3noc([C@@]45[C@@H]6C(=O)[C@H]7[C@H]8C[C@H]([C@@H]74)[C@@H]5[C@H]86)n3)c2)NC(=O)NC1=O
vNsp10-ppi1-95	Z2177645584	-8.3	0.259	437.542	REAL	CC(=O)N1C[C@@H]2CCC[C@H](NC(=O)[C@H]3CCCN(C(=O)c4ccc5[nH]ncc5c4)C3)[C@H]2C1
vNsp10-ppi1-96	Z2185350395	-8.3	0.259	436.558	REAL	CC(=O)N1C[C@@H]2CCC[C@H](NC(=O)N3CCC[C@@H](c4n[nH]c(-c5cccc5)n4)C3)[C@H]2C1
vNsp10-ppi1-97	Z2224002803	-8.3	0.259	434.407	REAL	O=C1CNC(=O)c2ccc(C(=O)Oc3ccc(-c4noc([C@@H]5CCCO5)n4)cc3)cc2N1
vNsp10-ppi1-98	Z2227622484	-8.3	0.307	363.416	REAL	CC1(C)CCN(C(=O)c2ccc3c(c2)NC(=O)CNC3=O)c2ccccc21
vNsp10-ppi1-99	Z2234937502	-8.3	0.252	438.486	REAL	O=C(NCc1ccc2c(=O)cc[nH]c2c1)Nc1cccc(C(=O)N2CCc3ccccc32)c1
vNsp10-ppi1-100	Z225721138	-8.3	0.244	461.473	REAL	Cc1cc(=O)oc2cc(OCc3ccc(C(=O)N4CCC5(CC4)NC(=O)NC5=O)cc3)ccc12

Supplementary Table 45. Top 100 virtual hits of the screen against the nsp14/nsp16 binding site on nsp10 (Screen ID: 25). The name of each compound consists of the initial letter 'v' for virtual hit, followed by the target protein name and the target site ('ppi' for protein protein interface, 1 for docking scenario 1). The score is the docking score given by QuickVina 2 in kcal/mol. The ligand efficiency (LE) is computed as LE = -score/#NonH, where #NonH is the number of heavy (i.e. non hydrogen) atoms.

Name	Catalog ID	Score	LE	MW	Library	SMILES
vNsp10-ppi1-101	Z229624416	-8.3	0.224	491.51	REAL	O=C(NNC(=O)c1n[nH]c(=O)c2ccccc12)c1c2c(nc3ccccc13)/C(=C/c1ccco1)CCC2
vNsp10-ppi1-102	Z244096966	-8.3	0.237	488.57	REAL	O=C(Nc1cccc1C(=O)N1CCCCC1)c1ccc(NC2=NS(=O)(=O)c3ccccc32)cc1
vNsp10-ppi1-103	Z2830825415	-8.3	0.231	485.50	REAL	NC1=Nc2nc3cc4c(cc3n2[C@@H](c2cccc(OCc3ccccc3C(=O)O)c2)N1)OCCCO4
vNsp10-ppi1-104	Z2903528386	-8.3	0.268	415.41	REAL	Cc1c(-c2nooc(Cn3c4ccccc4c(=O)c4ccccc43)n2)c(=O)[nH]c(=O)n1C
vNsp10-ppi1-105	Z296159422	-8.3	0.244	451.49	REAL	Cc1nc2ccccc2c2c(NC(=O)CCc3nc4c(cnn4C)c(=O)[nH]3)c3ccccc3n12
vNsp10-ppi1-106	Z333313620	-8.3	0.231	497.62	REAL	O=C(c1cc2c(ccc3ccccc32)[nH]1)N1CCN(Cc2nc3sc4c(c3c(=O)[nH]2)CCCC4)CC1
vNsp10-ppi1-107	Z358867962	-8.3	0.277	415.53	REAL	Cc1cccc([C@@H](CC(=O)O[C@@H](C)C(=O)N[C@@H](C)[C@H]2C[C@H]3CC[C@H]2C3)NC(N)=O)c1
vNsp10-ppi1-108	Z512491668	-8.3	0.286	385.43	REAL	Cn1ncc2c(=O)[nH]c(CCC(=O)N3Cc4ccccc4-c4ccccc43)nc21
vNsp10-ppi1-109	Z651902802	-8.3	0.237	487.46	REAL	C[C@@H](c1nc(-c2cccc(C(F)(F)F)c2)no1)N1CCN(C(=O)c2cc3c(F)cccc3[nH]2)CC1
vNsp10-ppi1-110	Z757262012	-8.3	0.277	420.49	REAL	Cc1c(C(=O)N2CCC(C(=O)Nc3nncs3)CC2)oc2c1ccc1ccccc12
vNsp10-ppi1-111	Z767058602	-8.3	0.224	494.51	REAL	C[C@]1(c2cccc(NC(=O)c3cc(-c4ccc5c(c4)OCCO5)nc4ccccc34)c2)NC(=O)NC1=O
vNsp10-ppi1-112	Z806355354	-8.3	0.244	481.58	REAL	NC(=O)[C@H]1CCCN(c2ccc(C(=O)N3CCN(C4=NS(=O)(=O)c5ccccc54)CC3)cc2)C1
vNsp10-ppi1-113	Z847339404	-8.3	0.237	469.46	REAL	Cn1ncc2c(=O)[nH]c(COC(=O)c3cc(-c4ccc5c(c4)OCCO5)nc4ccccc34)nc21
vNsp10-ppi1-114	Z941404930	-8.3	0.252	441.54	REAL	O=C(C1CCN(c2ccc3nnnn3n2)CC1)N1CCC(c2cccc3ccccc23)CC1
vNsp10-ppi1-115	ZINC000001717023	-8.3	0.259	417.42	ZINC15	O=c1oc2ccc(-n3c(=O)c4ccccc4c4ccccc4c3=O)cc2c2ccccc12
vNsp10-ppi1-116	ZINC000003242561	-8.3	0.268	406.44	ZINC15	Cc1ccc(-c2cc(C(=O)Nc3nnc(-c4ccccc4)o3)c3ccccc3n2)cc1
vNsp10-ppi1-117	ZINC000017988176	-8.3	0.207	521.57	ZINC15	O=C(Oc1ccc2ccccc2c1)c1cccc(N2C(=O)[C@H]3[C@@H](C2=O)C2c4ccccc4C3c3ccccc32)c1
vNsp10-ppi1-118	PV-001813138008	-8.2	0.293	373.37	REAL	Cc1nc2cc(C(=O)Nc3cc(C(N)=O)c4ccccc4n3)ccc2c(=O)[nH]1
vNsp10-ppi1-119	PV-001826685592	-8.2	0.265	421.46	REAL	C[C@H]1CN(C(=O)c2ccc(NC(=O)c3cccc(Nc4nnn[nH]4)c3)cc2)C[C@@H](C)O1
vNsp10-ppi1-120	PV-001831825387	-8.2	0.248	454.46	REAL	Cc1cc(C(=O)N2CCN(CCNC(=O)c3ccccc3F)CC2)nc2nc(O)[nH]c(=O)c12
vNsp10-ppi1-121	PV-001833788668	-8.2	0.248	458.42	REAL	CN1C(=O)NC2(CCN(C(=O)c3ccc(NC(=O)c4cc(F)cc(F)c4)cc3O)CC2)C1=O
vNsp10-ppi1-122	PV-001853987759	-8.2	0.304	365.35	REAL	Cc1cc(C(=O)Nc2cccc3c2CCNC3=O)nc2nc(O)[nH]c(=O)c12
vNsp10-ppi1-123	PV-001857874292	-8.2	0.256	439.51	REAL	CN(Cc1ccccc1)C(=O)N1CCC(C(=O)N2CC[C@@H](c3cc(=O)[nH]c(=O)[nH]3)C2)CC1
vNsp10-ppi1-124	PV-001870339826	-8.2	0.273	406.44	REAL	CC(=O)Nc1ccc2c(c1)CN(C(=O)c1ccc([C@]3(C)NC(=O)NC3=O)cc1)CC2
vNsp10-ppi1-125	PV-001873640084	-8.2	0.265	423.43	REAL	Cc1cc(C(=O)Nc2ccc3c(c2)N(C)C(=O)C(C)(C)CO3)nc2nc(O)[nH]c(=O)c12
vNsp10-ppi1-126	PV-001903904524	-8.2	0.304	360.33	REAL	NC(=O)c1cc(NC(=O)c2ccc3c(c2)C(=O)NC3=O)nc2ccccc12
vNsp10-ppi1-127	PV-001950330373	-8.2	0.248	459.42	REAL	O=C(Nc1ccc(C(=O)C(F)(F)F)cc1)N1CCC(CN2C(=O)c3ccccc3C2=O)CC1
vNsp10-ppi1-128	PV-001951422344	-8.2	0.273	414.46	REAL	CN1C(=O)C(C)(C)COc2ccc(NC(=O)N3CCC(n4cn[nH]c4=O)CC3)cc21
vNsp10-ppi1-129	PV-001954437442	-8.2	0.256	459.54	REAL	C[C@@H](NC(=O)N1CC[C@H]2CC[C@H](C1)S2(=O)=O)c1ccc(NC(=O)c2ccc(F)cc2)cc1
vNsp10-ppi1-130	Z1004162744	-8.2	0.241	454.54	REAL	O=C(Nc1cccc(-c2nnc3n2CCC3)c1)N1CCC(c2nc(-c3ccccc3)n[nH]2)CC1
vNsp10-ppi1-131	Z1023505554	-8.2	0.241	476.39	REAL	O=C(c1cc2c(C(F)(F)F)cc(=O)[nH]c2o1)N1CCC[C@H](c2nc(-c3cccc(F)c3)no2)C1
vNsp10-ppi1-132	Z1072126168	-8.2	0.256	435.49	REAL	Cc1ccc2[nH]c([C@@H]3CCCN(C(=O)CCc4nc5c([nH]4)c(=O)[nH]c(=O)n5C)C3)nc2c1
vNsp10-ppi1-133	Z1083442292	-8.2	0.241	455.45	REAL	Cc1cccc(-c2nnc(-c3ccc(C(=O)Nc4ccc(F)c(-n5nnnc5C)c4)cc3)o2)c1
vNsp10-ppi1-134	Z1092356672	-8.2	0.241	452.47	REAL	O=C(NNc1nc(-c2ccncc2)no1)[C@H]1CC(=O)N(c2ccc3c(c2)Cc2ccccc2-3)C1
vNsp10-ppi1-135	Z1123536269	-8.2	0.248	448.43	REAL	CCn1c(=O)[nH]c2cc(C(=O)Oc3ccc(-c4noc([C@H]5CCCO5)n4)cc3)ccc2c1=O
vNsp10-ppi1-136	Z1132401381	-8.2	0.256	431.50	REAL	Cc1noc(C2CCN(C(=O)Nc3cccc(C(=O)N4CCc5ccccc54)c3)CC2)n1
vNsp10-ppi1-137	Z1132402333	-8.2	0.248	438.53	REAL	Cc1cccc2c1CCN(C(=O)Nc1ccc(CCn3nnc(-c4ccccc4)n3)cc1)C2
vNsp10-ppi1-138	Z1152477570	-8.2	0.265	412.49	REAL	O=C(Nc1ccc2[nH]c(N3CCOCC3)nc2c1)[C@@H]1C[C@H]1c1cccc2ccccc12
vNsp10-ppi1-139	Z1161074794	-8.2	0.241	496.56	REAL	CCN1C(=O)c2ccc(C(=O)Oc3ccc(C(=O)N4CCc5scc5C4)cc3)cc2S1(=O)=O
vNsp10-ppi1-140	Z1161168809	-8.2	0.248	447.54	REAL	Cc1c(C(=O)N2CCC(C(=O)N3CCN(C)CC3)CC2)nnn1-c1cccc2ncccc12
vNsp10-ppi1-141	Z1268273543	-8.2	0.248	436.47	REAL	Cc1cccc(-c2nnc(-c3ccc(C(=O)NCc4cc(=O)[nH]c5ccccc45)cc3)o2)c1
vNsp10-ppi1-142	Z1269955434	-8.2	0.256	438.49	REAL	Cc1noc(C2CCN(C(=O)[C@@H]3CN(Cc4nc5ccccc5c(=O)[nH]4)CCO3)CC2)n1
vNsp10-ppi1-143	Z1272302813	-8.2	0.256	429.44	REAL	C[C@@]1(c2cccc(CNc3nc4c(cnn4-c4ccccc4)c(=O)[nH]3)c2)NC(=O)NC1=O
vNsp10-ppi1-144	Z1274153640	-8.2	0.248	448.45	REAL	O=C(CCN1C(=O)[C@@H]2[C@@H]3CC[C@@H](O3)[C@@H]2C1=O)Nc1ccc(-c2nc3c(F)cccc3[nH]2)cc1
vNsp10-ppi1-145	Z1314668728	-8.2	0.256	442.52	REAL	Cc1cc(C(=O)N2CCN(CC(=O)N[C@@H]3CCC[C@@H](C)C3)CC2)nc2nc(O)[nH]c(=O)c12
vNsp10-ppi1-146	Z1315803654	-8.2	0.248	440.46	REAL	Cc1ccc(-n2c(NC(=O)c3cc(C)c4c(=O)[nH]c(O)nc4n3)nc3cc(C)ccc32)cc1
vNsp10-ppi1-147	Z1334977090	-8.2	0.273	406.44	REAL	CC(=O)Nc1cccc2c1CCCN2C(=O)c1ccc([C@]2(C)NC(=O)NC2=O)cc1
vNsp10-ppi1-148	Z1353324229	-8.2	0.256	434.45	REAL	C[C@H]1C(=O)Nc2cc(C(=O)Oc3ccc(-c4noc([C@H]5CCCO5)n4)cc3)ccc2N1C
vNsp10-ppi1-149	Z1355380163	-8.2	0.248	443.42	REAL	Cc1cc(N2C(=O)c3ccccc3C2=O)ccc1C(=O)OCc1nc2c(cnn2C)c(=O)[nH]1
vNsp10-ppi1-150	Z1357277549	-8.2	0.265	416.48	REAL	C[C@H]1C(=O)Nc2cc(C(=O)Nc3nc4ccccc4nc3N3CCCC3)ccc2N1C
vNsp10-ppi1-151	Z1366478637	-8.2	0.248	445.48	REAL	CCN1C(=O)[C@H]2CN(C(=O)c3ccc(-c4nnc(-c5ccc(C)cc5)o4)cc3)CCN2C1=O
vNsp10-ppi1-152	Z1382447358	-8.2	0.273	405.50	REAL	Cc1cc2nc(-c3ccc(CNC(=O)[C@H]4CCCN(C(N)=O)C4)cc3)[nH]c2cc1C
vNsp10-ppi1-153	Z1382933462	-8.2	0.248	449.45	REAL	O=C(Nc1nc(-c2ccccc2F)n[nH]1)[C@H]1CN(Cc2nc3ccccc3c(=O)[nH]2)CCO1
vNsp10-ppi1-154	Z1421222311	-8.2	0.248	447.48	REAL	O=C(CN1CCC(c2nc(-c3ccccc3)n[nH]2)CC1)Nc1cc(-n2cnnn2)ccc1F
vNsp10-ppi1-155	Z1507820863	-8.2	0.248	443.44	REAL	NC(=O)N1CCc2cc(NC(=O)c3ccc(-c4noc(-c5ccc(F)cc5)n4)cc3)ccc21
vNsp10-ppi1-156	Z1542971223	-8.2	0.304	391.31	REAL	O=C(Nc1nc2cc3c(cc2s1)OC(F)(F)O3)c1ccc2n[nH]c(=O)n2c1
vNsp10-ppi1-157	Z1570458486	-8.2	0.248	449.42	REAL	Cc1n[nH]c(-c2ccc(NC(=O)c3ccc(NC(=O)c4cc(F)cc(F)c4)cc3O)cc2)n1
vNsp10-ppi1-158	Z1575853900	-8.2	0.273	405.41	REAL	CC(=O)c1cccc(OCc2cc(C(=O)Nc3nc4cc(C)cc(C)c4o3)no2)c1
vNsp10-ppi1-159	Z1590125447	-8.2	0.256	433.47	REAL	CN1C(=O)NC2(CCN(C(=O)NCc3ccc(-n4cnc5ccccc54)nc3)CC2)C1=O
vNsp10-ppi1-160	Z1614159841	-8.2	0.248	442.53	REAL	Cc1nc(-c2ccc(C)c(NC(=O)N3CCC[C@H](c4n[nH]c(-c5ccccc5)n4)C3)c2)n[nH]1
vNsp10-ppi1-161	Z1614247255	-8.2	0.248	444.49	REAL	C[C@@]1(c2cccc(C(=O)N3CCC[C@H](c4n[nH]c(-c5ccccc5)n4)C3)cc2)NC(=O)NC1=O
vNsp10-ppi1-162	Z1622711383	-8.2	0.248	445.52	REAL	Cc1ccc2[nH]c3c(c2c1)C[C@H](NC(=O)NCc1ccc([C@]2(C)NC(=O)NC2=O)cc1)CC3
vNsp10-ppi1-163	Z1626781648	-8.2	0.256	443.49	REAL	O=C(c1ccc2c(c1)S(=O)(=O)Nc1ncnn1-2)N1CC=C(c2cccc3ccccc23)C1
vNsp10-ppi1-164	Z1631987088	-8.2	0.248	448.46	REAL	O=C1CCC(=O)N(c2ccc(C(=O)N[C@H]3CCc4nnc(-c5ccc(F)cc5)n4C3)cc2)N1
vNsp10-ppi1-165	Z1633130044	-8.2	0.256	427.46	REAL	O=C(Cc1cccc(O)c1)Nc1ccc2nc(NC(=O)Cc3cccc(O)c3)ccc2c1
vNsp10-ppi1-166	Z1682390413	-8.2	0.248	440.46	REAL	C[C@@]1(c2ccc(-c3noc(-c4cc(Cc5ccccc5)ccc4O)n3)cc2)NC(=O)NC1=O
vNsp10-ppi1-167	Z1682391338	-8.2	0.256	435.41	REAL	C[C@]1(c2ccc(-c3noc([C@@H]4CC(=O)N(c5ccc(F)cc5)C4)n3)cc2)NC(=O)NC1=O
vNsp10-ppi1-168	Z1683771859	-8.2	0.256	436.37	REAL	NC(=O)c1cccc(-c2noc(-c3ccc(NC(=O)c4cc(F)cc(F)c4)cc3O)n2)c1
vNsp10-ppi1-169	Z1684079864	-8.2	0.248	444.45	REAL	Nc1nc(Cc2noc([C@@H]3CCN(c4ccc5c(c4)OCCO5)C3=O)n2)nc2ccccc12
vNsp10-ppi1-170	Z1684080889	-8.2	0.241	448.49	REAL	Cc1nn(C)c2nc(-c3ccccc3)cc(-c3nc(Cc4nc(N)c5ccccc5n4)no3)c12
vNsp10-ppi1-171	Z1684081449	-8.2	0.248	434.46	REAL	Cc1ccc(-c2cc(-c3nc(Cc4nc(N)c5ccccc5n4)no3)c3ccccc3n2)o1
vNsp10-ppi1-172	Z1684580484	-8.2	0.248	443.42	REAL	C=CCN1C(=O)c2cccc(-c3nc(-c4cccc([C@]5(C)NC(=O)NC5=O)c4)no3)cc2C1=O
vNsp10-ppi1-173	Z1685322133	-8.2	0.256	444.47	REAL	Cc1nnc(-c2cccc(-c3noc(-c4cse(-c5cce6c(c5)OCCO6)n4)n3)c2)[nH]1
vNsp10-ppi1-174	Z1685322514	-8.2	0.248	441.45	REAL	Cc1nnc(-c2cccc(-c3noc(CN4C(=O)N[C@]5(CCc6ccccc65)C4=O)n3)c2)[nH]1
vNsp10-ppi1-175	Z1765570711	-8.2	0.248	443.47	REAL	CC(C)(C)n1ncc2c(=O)[nH]c(NNC(=O)c3ccc4[nH]c5ccccc5c(=O)c4c3)nc21
vNsp10-ppi1-176	Z1766726077	-8.2	0.273	402.45	REAL	Cc1noc(C2(C)CCN(C(=O)c3ccc4[nH]c5ccccc5c(=O)c4c3)CC2)n1
vNsp10-ppi1-177	Z1767880670	-8.2	0.256	437.36	REAL	Cn1ncc2c(=O)[nH]c(COC(=O)c3cc(F)cc4c(=O)c5cc(F)ccc5[nH]c34)nc21
vNsp10-ppi1-178	Z1769349321	-8.2	0.265	420.47	REAL	Cc1cccc2nc(C3CCN(C(=O)CCc4nc5c(cnn5C)c(=O)[nH]4)CC3)oc12
vNsp10-ppi1-179	Z1845468653	-8.2	0.248	446.51	REAL	COc1ccccc1-c1nc(C2CCN(C(=O)Nc3ccc4c(c3)C(=O)CCC4)CC2)no1
vNsp10-ppi1-180	Z1890714849	-8.2	0.248	443.42	REAL	Cn1cc(-c2noc(Cc3ccc(NC(=O)c4cc5ccccc5o4)cc3)n2)c(=O)[nH]c1=O
vNsp10-ppi1-181	Z1890715613	-8.2	0.248	441.45	REAL	Cn1cc(-c2noc([C@H]3CC(=O)N(c4ccc5c(c4)Cc4ccccc4-5)C3)n2)c(=O)[nH]c1=O
vNsp10-ppi1-182	Z1891232783	-8.2	0.328	334.30	REAL	Cc1nnc2ccc(-c3noc(-c4ccc5n[nH]c(=O)n5c4)n3)cn12
vNsp10-ppi1-183	Z1904663859	-8.2	0.283	392.50	REAL	O=C(NCCCn1cnc2ccccc21)NC[C@@]1(O)[C@H]2[C@@H]3C[C@H]4[C@H]5[C@H]3C[C@H]2[C@H]5[C@@H]41
vNsp10-ppi1-184	Z1907872362	-8.2	0.248	442.48	REAL	Cn1c(=O)[nH]c2ncc(-c3cccc(C(=O)Nc4ccc5c(c4)N(C(N)=O)CCC5)c3)cc21
vNsp10-ppi1-185	Z1920293768	-8.2	0.283	397.48	REAL	CCOC(=O)c1nc(-c2cccc(CNC(=O)NC[C@H]3C[C@H]4CC[C@H]3C4)c2)n[nH]1
vNsp10-ppi1-186	Z1929420146	-8.2	0.265	439.45	REAL	O=C1NC(=O)[C@@]2(CCCN(C(=O)c3ccc4c(c3)S(=O)(=O)c3ccccc3C4=O)C2)N1
vNsp10-ppi1-187	Z1931360674	-8.2	0.256	435.46	REAL	O=C(Nc1cccc(N2CCC2=O)c1)N1CCC[C@@H](c2nc(-c3cccc(F)c3)no2)C1
vNsp10-ppi1-188	Z1952918575	-8.2	0.265	430.36	REAL	O=C(NCc1ccc2c(c1)CN(C(=O)c1ncc(F)cc1F)C2)c1ncc(F)cc1F
vNsp10-ppi1-189	Z2021032753	-8.2	0.265	411.42	REAL	NC(=O)NC(=O)c1cccc(NC(=O)c2cc(-c3cccnc3)nc3ccccc23)c1
vNsp10-ppi1-190	Z2087363551	-8.2	0.248	438.49	REAL	O=C1N[C@@H](C[C@@H]2CCCc3ccccc32)C(=O)N1c1cc(-c2ccc3ncccc3c2)on1
vNsp10-ppi1-191	Z2090518029	-8.2	0.256	445.91	REAL	Cc1nnc2c3ccccc3c(N3CCC[C@H](c4nc(-c5ccc(Cl)cc5)no4)C3)nn12
vNsp10-ppi1-192	Z2099246103	-8.2	0.248	448.48	REAL	O=C1COC[C@H](C[C@@H]2CN(C(=O)c3cccc(CN4C(=O)CNC4=O)c3)c3ccccc32)N1
vNsp10-ppi1-193	Z2142490724	-8.2	0.248	445.48	REAL	O=C(NCc1ccc2c(=O)cc[nH]c2c1)[C@@H]1CN(Cc2nc3ccccc3c(=O)[nH]2)CCO1
vNsp10-ppi1-194	Z2143212618	-8.2	0.265	417.40	REAL	Cc1nnc2[nH]nc(NC(=O)c3cc(-c4ccc(F)cc4)nc4onc(C)c34)c2c1C
vNsp10-ppi1-195	Z2157441149	-8.2	0.248	447.53	REAL	CC(=O)N1C[C@@H]2CCC[C@H](NC(=O)c3cccc(NC(=O)[C@H]4Cc5ccccc5O4)c3)[C@H]2C1
vNsp10-ppi1-196	Z2161363258	-8.2	0.256	441.41	REAL	O=C(c1cccc2ccc(O)nc12)N1CCC[C@H](c2nnc3ccc(C(F)(F)F)cn23)C1
vNsp10-ppi1-197	Z2171975786	-8.2	0.256	420.47	REAL	O=C1CCc2cccc(-c3nc(-c4ccc(Cn5cnc6ccccc65)cc4)no3)c2C1
vNsp10-ppi1-198	Z2171979207	-8.2	0.273	402.41	REAL	C[C@@]1(c2ccccc(-c3noc(-c4cccc5c4CC(=O)CC5)n3)c2)NC(=O)NC1=O
vNsp10-ppi1-199	Z2172064780	-8.2	0.256	434.47	REAL	O=C1CCc2cccc(-c3nc(CC(=O)N4CCN(c5ccccc5F)CC4)no3)c2C1
vNsp10-ppi1-200	Z2189066470	-8.2	0.273	406.44	REAL	CC(=O)c1cccc(OCc2cc(C(=O)Nc3nc(C)c4c(n3)CCCC4)no2)c1

Supplementary Table 46. Virtual screening hits 101 to 200 of the the nsp14/nsp16 binding site on nsp10 (Screen ID: 25). Compounds were filtered so that hits had MW < 600 dalton, cLogP < 6, number of hydrogen bond acceptors < 11, and no reactive functional groups. The name of each compound consists of the initial letter 'v' for virtual hit, followed by the target protein name and the target site ('ppi' for protein-protein interface, 1 for docking scenario 1). The score is the docking score given by QuickVina 2 in kcal/mol. The ligand efficiency (LE) is computed as LE = -score/#NonH, where #NonH is the number of heavy (i.e. non hydrogen) atoms.

Name	Catalog ID	Score	LE	MW	Library	SMILES
vNsp10-ppi2-1	Z2998241729	-9.9	0.367	362.384	REAL	O=C1C[C@]2(CCc3cc(-c4ccc5c(c4)C(=O)NCCO5)ccc32)C(=O)N1
vNsp10-ppi2-2	Z1576646261	-9.8	0.338	406.496	REAL	CC(C)(C)OC(=O)N1[C@@H]2CC[C@@H]1CC(CC(=O)N[C@H](CO)c1ccc(F)cc1)C2
vNsp10-ppi2-3	Z2830825486	-9.8	0.288	469.422	REAL	NC1=Nc2nc3cc4c(cc3n2[C@@H](c2ccc(-c3cccc(C(F)(F)F)c3)o2)N1)OCCCO4
vNsp10-ppi2-4	Z997212184	-9.8	0.288	475.524	REAL	CS(=O)(=O)c1ccc2c(c1)N(C(=O)c1ccc3c(=O)n(-c4ccccc4)c(=O)[nH]c3c1)CCC2
vNsp10-ppi2-5	Z1730125512	-9.6	0.291	446.505	REAL	COc1ccc(C(=O)N2CCC[C@H](C(=O)N3CCc4n[nH]c(=O)cc4C3)C2)c2ccccc12
vNsp10-ppi2-6	Z1507824335	-9.5	0.297	432.483	REAL	NC(=O)N1CCc2cc(NC(=O)[C@H]3CCCN(C(=O)c4ccc5[nH]ncc5c4)C3)ccc21
vNsp10-ppi2-7	Z2160281895	-9.5	0.279	448.437	REAL	O=C1c2ccc(-c3nc(-c4cc(=O)[nH]c5ccccc45)no3)cc2C(=O)N1Cc1ccccc1
vNsp10-ppi2-8	Z2638095677	-9.5	0.339	386.45	REAL	C[C@H]1CC[C@@H](O)[C@@H]([C@@H]2CCCCN2C(=O)c2cnc3[nH]c(=O)[nH]c(=O)c3c2)C1
vNsp10-ppi2-9	Z2830825680	-9.5	0.271	477.47	REAL	NC1=Nc2nc3cc4c(cc3n2[C@@H](c2cccc(OCc3ccc(F)cc3F)c2)N1)OCCCO4
vNsp10-ppi2-10	Z98336011	-9.5	0.271	488.934	REAL	NC1=Nc2nc3cc4c(cc3n2[C@@H](c2cccc(NC(=O)c3ccc(Cl)cc3)c2)N1)OCCCO4
vNsp10-ppi2-11	Z1070824292	-9.4	0.276	483.544	REAL	C[C@@H]1Oc2ccc(C(=O)C3CCN(S(=O)(=O)c4ccc5c(c4)CCC(=O)N5)CC3)cc2NC1=O
vNsp10-ppi2-12	Z1213022201	-9.4	0.294	433.442	REAL	Cc1cc(F)ccc1-c1ccc([C@H]2NC(N)=Nc3nc4cc5c(cc4n32)OCCCO5)o1
vNsp10-ppi2-13	Z1837791861	-9.4	0.294	437.405	REAL	NC1=Nc2nc3cc4c(cc3n2[C@@H](c2ccc(-c3cccc(F)c3F)o2)N1)OCCCO4
vNsp10-ppi2-14	Z2077357332	-9.4	0.294	430.467	REAL	O=C(NNc1ccc2c(=O)[nH]ccc2c1)[C@@H]1CCCN(C(=O)c2ccc3[nH]ncc3c2)C1
vNsp10-ppi2-15	Z2160279884	-9.4	0.285	438.398	REAL	O=C1c2ccc(-c3nc(-c4cc(=O)[nH]c5ccccc45)no3)cc2C(=O)N1Cc1ccco1
vNsp10-ppi2-16	Z2160283311	-9.4	0.313	396.365	REAL	O=c1cc(-c2noc(-c3c[nH]n4c3nc(=O)c3ccccc34)n2)c2ccccc2[nH]1
vNsp10-ppi2-17	Z2466019156	-9.4	0.324	394.39	REAL	Cn1c(N2CCc3[nH]c4ccc(C(=O)O)cc4c3C2)nc2c1c(=O)[nH]c(=O)n2C
vNsp10-ppi2-18	Z98335822	-9.4	0.294	470.315	REAL	NC1=Nc2nc3cc4c(cc3n2[C@@H](c2ccc(-c3ccc(Cl)ccc3Cl)o2)N1)OCCCO4
vNsp10-ppi2-19	ZINC000012548283	-9.4	0.294	470.315	ZINC	NC1=Nc2nc3cc4c(cc3n2[C@@H](c2ccc(-c3ccc(Cl)c3Cl)o2)N1)OCCCO4
vNsp10-ppi2-20	PV-001811066172	-9.3	0.31	419.358	REAL	CCn1c(=O)[nH]c2cc(C(=O)N3CCOc4c3ccce4C(F)(F)F)ccc2c1=O
vNsp10-ppi2-21	PV-001872965615	-9.3	0.321	404.307	REAL	Cc1cc(C(=O)Nc2cc(C(F)(F)F)c3cn[nH]c3c2)nc2nc(O)[nH]c(=O)c12
vNsp10-ppi2-22	PV-001875532042	-9.3	0.3	454.316	REAL	Cc1nc2ccc(O)cc2cc1C(=O)N1C[C@H]2[C@H](C1)C(F)(F)C(F)(F)C(F)(F)C2(F)F
vNsp10-ppi2-23	PV-001950483714	-9.3	0.31	414.46	REAL	CC1(C)COc2ccc(NC(=O)N3CC(=O)NC(=O)C34CCCC4)cc2NC1=O
vNsp10-ppi2-24	Z1213022199	-9.3	0.291	433.442	REAL	Cc1c(F)cccc1-c1ccc([C@H]2NC(N)=Nc3nc4cc5c(cc4n32)OCCCO5)o1
vNsp10-ppi2-25	Z1264834677	-9.3	0.291	446.482	REAL	C[C@@H]1CN(C(=O)c2ccc3c(c2)S(=O)(=O)c2ccccc2C3=O)c2ccccc2NC1=O
vNsp10-ppi2-26	Z1356719911	-9.3	0.372	340.342	REAL	C[C@@]1(c2ccc(C(=O)N3CCc4nn[nH]c4C3)cc2)NC(=O)NC1=O
vNsp10-ppi2-27	Z1748294130	-9.3	0.332	373.415	REAL	Cc1nnc(-c2ccc(C(=O)N3CC[C@]4(C3)C(=O)Nc3ccccc34)cc2)[nH]1
vNsp10-ppi2-28	Z2157917520	-9.3	0.291	437.43	REAL	C[C@]1(c2cccc(-c3noc(-c4cc(F)ccc4N4COCC4)n3)c2)NC(=O)NC1=O
vNsp10-ppi2-29	Z2233642508	-9.3	0.3	415.492	REAL	O=C1CCN(C(=O)c2ccc3c(=O)n4c(nc3c2)CCCC4)[C@@H](c2ccccc2)C1
vNsp10-ppi2-30	Z237105524	-9.3	0.258	485.63	REAL	O=C(c1cccc2ccccc12)N1CCC[C@@H](C(=O)N2CCC[C@@H](c3nnc4n3CCCCC4)C2)C1
vNsp10-ppi2-31	Z2830825432	-9.3	0.3	480.325	REAL	NC1=Nc2nc3cc4c(cc3n2[C@@H](c2ncc(-c3cccc(Br)c3)[nH]2)N1)OCCCO4
vNsp10-ppi2-32	Z284317138	-9.3	0.258	499.957	REAL	C[C@@H]1c2[nH]c3ccccc3c2[C@H](c2ccccc2Cl)CN1C(=O)c1cnc2c(c1)c(=O)[nH]c(=O)n2C
vNsp10-ppi2-33	Z2924313672	-9.3	0.344	379.439	REAL	O=C1NCCOc2ccc(-c3nc([C@H]4CCSc5ccccc54)no3)cc21
vNsp10-ppi2-34	Z29638352	-9.3	0.266	472.496	REAL	O=C(CN1C(=O)N[C@]2(CCc3ccccc32)C1=O)Oc1ccc2c3c(c(=O)oc2c1)CCCCC3
vNsp10-ppi2-35	Z98335691	-9.3	0.3	419.415	REAL	NC1=Nc2nc3cc4c(cc3n2[C@@H](c2ccc(-c3ccc(F)cc3)o2)N1)OCCCO4
vNsp10-ppi2-36	Z98336398	-9.3	0.3	419.415	REAL	NC1=Nc2nc3cc4c(cc3n2[C@@H](c2ccc(-c3ccccc3F)o2)N1)OCCCO4
vNsp10-ppi2-37	ZINC000257203151	-9.3	0.3	422.44	ZINC	Cc1ccc2nc(O)cc(C(=O)N3CCC[C@]4(Cc5c(nc(O)nc5O)O4)CC3)c2c1
vNsp10-ppi2-38	PV-001834881599	-9.2	0.307	454.269	REAL	O=C1NC(=O)N2CCN(C(=O)CC[C@@H]3NC(=O)N(c4ccc(Cl)c(Cl)c4)C3=O)C[C@@H]12
vNsp10-ppi2-39	PV-001942320545	-9.2	0.307	433.571	REAL	CC1CCN(C(=O)c2ccc(NC(=O)N3CCC[C@]4(CCS(=O)(=O)C4)C3)cc2)CC1
vNsp10-ppi2-40	PV-001950487553	-9.2	0.317	401.422	REAL	CC1(C)COc2ccc(NC(=O)N3CCC[C@]4(C3)NC(=O)NC4=O)cc2NC1=O
vNsp10-ppi2-41	Z1014348548	-9.2	0.263	493.95	REAL	O=C(NNC(=O)[C@@H]1C[C@@H]2CCCC[C@@H]2N1C(=O)c1cccc(Cl)c1)c1n[nH]c(=O)c2ccccc12
vNsp10-ppi2-42	Z103379036	-9.2	0.297	480.321	REAL	NC1=Nc2nc3cc4c(cc3n2[C@@H](c2ccc(-c3cccc(Br)c3)o2)N1)OCCCO4
vNsp10-ppi2-43	Z1069484372	-9.2	0.263	474.515	REAL	C[C@H]1Oc2cccc(C(=O)C3CCN(C(=O)CCc4nc5ccccc5c(=O)[nH]4)CC3)cc2NC1=O
vNsp10-ppi2-44	Z1135059810	-9.2	0.287	425.491	REAL	Cc1ccccc1-c1cccc([C@H]2NC(N)=Nc3nc4cc5c(cc4n32)OCCCO5)c1
vNsp10-ppi2-45	Z1170211509	-9.2	0.317	379.378	REAL	O=c1nc2c(-c3nc(-c4cccc5ccccc45)no3)c[nH]n2c2ccccc12
vNsp10-ppi2-46	Z1213022197	-9.2	0.287	437.405	REAL	NC1=Nc2nc3cc4c(cc3n2[C@@H](c2ccc(-c3c(F)cccc3F)o2)N1)OCCCO4
vNsp10-ppi2-47	Z1313212974	-9.2	0.317	384.394	REAL	Cc1cc(C(=O)N2Cc3ccccc3-c3ccccc32)nc2nc(O)[nH]c(=O)c12
vNsp10-ppi2-48	Z1334956036	-9.2	0.307	397.433	REAL	C[C@@]1(c2ccc(C(=O)N3Cc4ccccc4-c4ccccc43)cc2)NC(=O)NC1=O
vNsp10-ppi2-49	Z1538679049	-9.2	0.287	426.475	REAL	Cc1cc(C(=O)N2CCc3ccccc3[C@@H]2Cc2ccccc2)nc2nc(O)[nH]c(=O)c12
vNsp10-ppi2-50	Z1647954397	-9.2	0.287	430.394	REAL	O=C1CN(C(=O)c2ccc3c(=O)n(-c4ccccc4)c(=O)[nH]c3c2)c2ccccc(F)c2N1
vNsp10-ppi2-51	Z1685380263	-9.2	0.297	410.392	REAL	COc1cc(-c2noc(-c3c[nH]n4c3nc(=O)c3ccccc34)n2)c2ccccc2n1
vNsp10-ppi2-52	Z1703928418	-9.2	0.287	428.491	REAL	O=C1CC[C@@H]2CN(C(=O)[C@H]3CCCN(C(=O)c4ccc5[nH]ncc5c4)C3)c3cccc1c32
vNsp10-ppi2-53	Z1723444485	-9.2	0.297	419.484	REAL	Cn1c(=O)[nH]c2ncc(-c3cccc(C(=O)N4CCCC[C@@H]4[C@H]4CNC(=O)C4)c3)cc21
vNsp10-ppi2-54	Z1741136260	-9.2	0.287	427.463	REAL	Cn1c(=O)[nH]c2ncc(-c3cccc(C(=O)N4C[C@H](C(N)=O)Cc5ccccc54)c3)cc21
vNsp10-ppi2-55	Z1929417160	-9.2	0.287	433.423	REAL	O=C1NC(=O)[C@@]2(CCCN(C(=O)c3ccc4c(=O)n(-c5ccccc5)c(=O)[nH]c4c3)C2)N1
vNsp10-ppi2-56	Z2041553691	-9.2	0.317	380.366	REAL	O=c1nc2c(-c3nc(-c4cccc5nccc45)no3)c[nH]n2c2ccccc12
vNsp10-ppi2-57	Z2105848333	-9.2	0.341	382.322	REAL	O=C(Nc1ccc2c(c1)OC(F)(F)O2)NC1CCC2(CC1)NC(=O)NC2=O
vNsp10-ppi2-58	Z2157920378	-9.2	0.287	431.451	REAL	CC(=O)N1Cc2ccccc2C[C@H]1c1nc(-c2cccc[C@]3(C)NC(=O)NC3=O)c2)no1
vNsp10-ppi2-59	Z2180397377	-9.2	0.297	427.45	REAL	O=C(N[C@@H]1CCCOc2ccc(F)cc21)N1CCC(c2noc3cc(F)ccc23)CC1
vNsp10-ppi2-60	Z220408526	-9.2	0.263	467.484	REAL	O=C(Nc1nc2ccccc2nc1N1CCCC1)c1ccc2c(c1)C(=O)N(Cc1ccco1)C2=O
vNsp10-ppi2-61	Z2223104085	-9.2	0.307	411.457	REAL	O=C1CNC(=O)c2ccc(C(=O)N3CCCCC[C@@H]3C[C@H](O)c3ccco3)cc2N1
vNsp10-ppi2-62	Z2227819160	-9.2	0.279	438.442	REAL	O=C(Nc1c(-c2ccccc2)[nH][nH]c1=O)c1ccc2c(c1)C(=O)N(Cc1ccccc1)C2=O
vNsp10-ppi2-63	Z226525548	-9.2	0.256	478.511	REAL	O=C(Nc1nc2ccccc2nc1N1CCCC1)c1ccc2c(c1)C(=O)N(Cc1ccnc1)C2=O
vNsp10-ppi2-64	Z2290738086	-9.2	0.317	395.505	REAL	O=C(Nc1cccc(-c2nnc3n2CCC3)c1)N1CCCC[C@H]1[C@H]1CCC[C@@H]1O
vNsp10-ppi2-65	Z2674896681	-9.2	0.317	393.402	REAL	CCn1c(=O)[nH]c2cc(C(=O)N3CCCc4ccc(C(N)=O)nc43)ccc2c1=O
vNsp10-ppi2-66	Z2830825686	-9.2	0.287	429.483	REAL	Cc1cccc(-n2cc([C@H]3NC(N)=Nc4nc5cc6c(cc5n43)OCCCO6)c(C)n2)c1
vNsp10-ppi2-67	Z2830825748	-9.2	0.279	446.441	REAL	NC1=Nc2nc3cc4c(cc3n2[C@@H](c2ccc(Oc3ccc(F)cc3)nc2)N1)OCCCO4
vNsp10-ppi2-68	Z2830825837	-9.2	0.271	464.524	REAL	CC(C)(C)OC(=O)NCc1cccc([C@H]2NC(N)=Nc3nc4cc5c(cc4n32)OCCCO5)c1
vNsp10-ppi2-69	Z335410572	-9.2	0.297	425.444	REAL	C[C@@]12CCC(=O)N1c1ccccc1C(=O)N2CC(=O)N1CCC2(CC1)NC(=O)NC2=O
vNsp10-ppi2-70	Z393676132	-9.2	0.279	464.505	REAL	C[C@@H]1Cc2cc(C(=O)Nc3cccc3-n3ncc4c(=O)[nH]cnc43)ccc2N1S(C)(=O)=O
vNsp10-ppi2-71	Z758227188	-9.2	0.263	484.575	REAL	Cc1[nH]c2ccccc2c1C1CCN(C(=O)c2ccc3c(c2)S(=O)(=O)c2ccccc2C3=O)CC1
vNsp10-ppi2-72	Z785732278	-9.2	0.279	482.951	REAL	NC1=Nc2nc3cc4c(cc3n2[C@@H](c2csc(COc3ccc(Cl)cc3)n2)N1)OCCCO4
vNsp10-ppi2-73	Z807847140	-9.2	0.307	409.464	REAL	O=C(N[C@@H]1CCCOc2ccc(F)cc21)N1CCC(c2nnc3cccn23)CC1
vNsp10-ppi2-74	Z839917398	-9.2	0.279	462.533	REAL	Cc1ccc(OCc2nc([C@H]3NC(N)=Nc4nc5cc6c(cc5n43)OCCCO6)cs2)cc1
vNsp10-ppi2-75	Z853015960	-9.2	0.307	404.469	REAL	CCn1c(=O)[nH]c2cc(C(=O)N3C[C@@H]4CCCN4Cc4ccccc43)ccc2c1=O
vNsp10-ppi2-76	Z98335813	-9.2	0.263	488.934	REAL	NC1=Nc2nc3cc4c(cc3n2[C@@H](c2cccc(NC(=O)c3ccccc3Cl)c2)N1)OCCCO4
vNsp10-ppi2-77	Z98335890	-9.2	0.287	470.315	REAL	NC1=Nc2nc3cc4c(cc3n2[C@@H](c2ccc(-c3ccc(Cl)c(Cl)c3)o2)N1)OCCCO4
vNsp10-ppi2-78	Z998823256	-9.2	0.271	468.502	REAL	O=C(c1ccc2[nH]ncc2c1)N1CCC[C@@H](C(=O)N2CCC(Oc3ccc(F)cc3F)CC2)C1
vNsp10-ppi2-79	ZINC000254513606	-9.2	0.271	473.552	ZINC	CN1c2ccccc2C(C)(C)[C@@]12CC(c1ccc3c(c1)S(=O)(=O)c1ccccc1C3=NO)=NO2
vNsp10-ppi2-80	PV-000277699505	-9.1	0.314	394.434	REAL	O=C(c1ccc2[nH]nnc2n1)N1CC2(CCN(C(=O)[C@@H]3C[C@@H]4O[C@H]3[C@H]3C[C@@H]43)C2)C1
vNsp10-ppi2-81	PV-001799899368	-9.1	0.284	448.356	REAL	CCn1c(=O)[nH]c2cc(C(=O)Nc3cc(C(F)(F)F)cc4c3OCC(=O)N4)ccc2c1=O
vNsp10-ppi2-82	PV-001814273301	-9.1	0.284	434.494	REAL	Cc1cccc(N2C(=O)N[C@@H](CCC(=O)N3c4ccccc4N(C)C(=O)C3(C)C)C2=O)c1
vNsp10-ppi2-83	PV-001820070350	-9.1	0.294	418.456	REAL	C[C@@H]1CC(=O)Nc2cccc2N1C(=O)CN(C)C(=O)c1ccc2c(N)ncnc2c1
vNsp10-ppi2-84	PV-001820070709	-9.1	0.284	433.467	REAL	Cc1nc2cc(C(=O)N(C)CC(=O)N3c4ccccc4NC(=O)C[C@H]3C)ccc2c(=O)[nH]1
vNsp10-ppi2-85	PV-001836138854	-9.1	0.35	349.345	REAL	O=C(Nc1ccc2c(c1)C(=O)CCC2)c1cccc(-c2noc(O)n2)c1
vNsp10-ppi2-86	PV-001844203226	-9.1	0.337	367.364	REAL	O=C1CCC(=O)N(c2ccc(C(=O)N3CCc4n[nH]c(=O)cc4C3)cc2)N1
vNsp10-ppi2-87	PV-001857872588	-9.1	0.325	384.391	REAL	CC(=O)N1C[C@H](C(=O)N2CC[C@@H](c3cc(=O)[nH]c(=O)[nH]3)C2)Oc2ccccc21
vNsp10-ppi2-88	Z1066143060	-9.1	0.276	475.548	REAL	O=C1COc2ccc(S(=O)(=O)Nc3nc(-c4ccc5c(c4)Cc4ccccc4-5)cs3)cc2N1
vNsp10-ppi2-89	Z1128937075	-9.1	0.268	463.489	REAL	C[C@@H]1Oc2ccc(C(=O)C3CCN(C(=O)c4cccc5c4O[C@@H](C)C(=O)N5)CC3)cc2NC1=O
vNsp10-ppi2-90	Z1147554284	-9.1	0.294	413.436	REAL	NC1=Nc2nc3ccccc3n2[C@H](c2cccc(OCc3cccc(C(=O)O)c3)c2)N1
vNsp10-ppi2-91	Z1161544373	-9.1	0.26	466.5	REAL	N\#Cc1ccccc1COc1cccc([C@H]2NC(N)=Nc3nc4cc5c(cc4n32)OCCCO5)c1
vNsp10-ppi2-92	Z1168445497	-9.1	0.294	413.436	REAL	NC1=Nc2nc3ccccc3n2[C@H](c2cccc(OCc3ccccc3C(=O)O)c2)N1
vNsp10-ppi2-93	Z1197769518	-9.1	0.325	371.355	REAL	Cn1c(=O)[nH]c(=O)c2cc(-c3nc(-c4cccc5ccccc45)no3)cnc21
vNsp10-ppi2-94	Z1231329722	-9.1	0.314	394.473	REAL	NC(=O)c1ccn(-c2ccccc2NC(=O)CC23C[C@@H]4C[C@H](CC(O)(C4)C2)C3)n1
vNsp10-ppi2-95	Z132909684	-9.1	0.314	408.8	REAL	O=C1/C(=C/Nc2nc(O)cc(O)n2)c2ccccc2C(=O)N1c1ccccc1Cl
vNsp10-ppi2-96	Z132917174	-9.1	0.268	467.875	REAL	O=C1/C(=C/Nc2nc3ccccc3n3nnnc23)c2ccccc2C(=O)N1c1ccccc1Cl
vNsp10-ppi2-97	Z1416052756	-9.1	0.337	371.352	REAL	C[C@@]1(c2ccc(C(=O)N3CCN4C(=O)NC(=O)[C@H]4C3)cc2)NC(=O)NC1=O
vNsp10-ppi2-98	Z1531888782	-9.1	0.276	439.47	REAL	NC(=O)[C@H]1CCN(C(=O)c2ccc3c(c2)C(=O)N(Cc2ccccc2)C3=O)c2ccccc21
vNsp10-ppi2-99	Z154278062	-9.1	0.284	442.4	REAL	O=C(c1n[nH]c(=O)c2ccccc12)N1CCC[C@H](c2nnc3ccc(C(F)(F)F)cn23)C1
vNsp10-ppi2-100	Z154279844	-9.1	0.284	448.487	REAL	O=C(N1CCC[C@H](c2nnc3ccc(C(F)(F)F)cn23)C1)C12C[C@@H]3C[C@H](CC(O)(C3)C1)C2

Supplementary Table 47. Top 100 virtual hits of the screen against the nsp14/nsp16 binding site on nsp10 (Screen ID: 26). The name of each compound consists of the initial letter 'v' for virtual hit, followed by the target protein name and the target site ('ppi' for protein-protein interface, 2 for docking scenario 2). The score is the docking score given by QuickVina 2 in kcal/mol. The ligand efficiency (LE) is computed as LE = -score/#NonH, where #NonH is the number of heavy (i.e. non hydrogen) atoms.

Name	Catalog ID	Score	LE	MW	Library	SMILES
vNsp10-ppi2-101	Z1548457952	-9.1	0.314	419.82	REAL	O=C1NC(=O)N2CCN(C(=O)CC[C@@H]3NC(=O)N(c4ccc(Cl)cc4)C3=O)C[C@@H]12
vNsp10-ppi2-102	Z1550949660	-9.1	0.284	432.48	REAL	O=C1CCCc2cc(OC(=O)[C@@H]3CCCN(C(=O)c4ccc5[nH]ncc5c4)C3)ccc2N1
vNsp10-ppi2-103	Z1657566126	-9.1	0.276	438.49	REAL	C[C@H](NC(=O)c1ccc2[nH]ncc2c1)c1ccc(CNC(=O)c2ccc3[nH]ncc3c2)cc1
vNsp10-ppi2-104	Z1682390101	-9.1	0.303	404.43	REAL	C[C@@]1(c2ccc(-c3noc(-c4ccc5c(c4O)CCCC5)n3)cc2)NC(=O)NC1=O
vNsp10-ppi2-105	Z1683264317	-9.1	0.337	361.40	REAL	O=C1CCCc2[nH]c(=O)c(-c3nc([C@H]4CCCc5ccccc54)no3)cc21
vNsp10-ppi2-106	Z1684366656	-9.1	0.276	442.48	REAL	Cc1c[nH]c(=O)n1-c1cccc(-c2noc(C3CCN(c4nc5ccccc5o4)CC3)n2)c1
vNsp10-ppi2-107	Z1684579919	-9.1	0.303	404.43	REAL	C[C@]1(c2cccc(-c3noc(-c4ccc5c(c4O)CCCC5)n3)c2)NC(=O)NC1=O
vNsp10-ppi2-108	Z1684581556	-9.1	0.294	419.40	REAL	C[C@@]1(c2cccc(-c3noc(C[C@@H]4Oc5ccccc5NC4=O)n3)c2)NC(=O)NC1=O
vNsp10-ppi2-109	Z1685321589	-9.1	0.337	360.33	REAL	Cc1nnc(-c2cccc(-c3noc(-c4ccc5[nH]c(=O)oc45)n3)c2)[nH]1
vNsp10-ppi2-110	Z1685374493	-9.1	0.294	415.41	REAL	CN(C)c1cc(-c2noc(-c3cnc4c(c3)c(=O)[nH]c(=O)n4C)n2)c2ccccc2n1
vNsp10-ppi2-111	Z1716064262	-9.1	0.294	411.46	REAL	Cc1c(C(=O)N2CC[C@]3(C2)OCc2ccccc23)nnn1-c1cccc2ncccc12
vNsp10-ppi2-112	Z1729312784	-9.1	0.337	383.47	REAL	Cc1cc(-c2nc([C@H]3CCCc4ccccc43)no2)cc(S(N)(=O)=O)c1C
vNsp10-ppi2-113	Z1730125238	-9.1	0.294	414.42	REAL	O=C(c1ccc2c(c1)C(=O)N(Cc1ccccc1)C2=O)N1CCc2n[nH]c(=O)cc2C1
vNsp10-ppi2-114	Z1730540337	-9.1	0.294	424.43	REAL	C[C@@H]1CN(C(=O)c2ccc3c(c2)C(=O)N(C[C@@H]2CCCO2)C3=O)c2cccc(F)c2O1
vNsp10-ppi2-115	Z1731722057	-9.1	0.364	339.35	REAL	O=C1NCCc2ccc(NC(=O)N3CCc4n[nH]c(=O)cc4C3)cc21
vNsp10-ppi2-116	Z1744194755	-9.1	0.325	376.42	REAL	O=C(c1ccc(N2CCNC2=O)cc1)N1CC[C@]2(C1)C(=O)Nc1ccccc12
vNsp10-ppi2-117	Z1819919761	-9.1	0.303	402.41	REAL	CCn1c(=O)[nH]c2cc(C(=O)N3Cc4cnnn4Cc4ccccc43)ccc2c1=O
vNsp10-ppi2-118	Z1846568199	-9.1	0.284	442.40	REAL	Cc1nc2c(c(C(F)(F)F)n1)C[C@H](C(=O)Nc1nnc(-c3cc4ccccc4o3)[nH]1)CC2
vNsp10-ppi2-119	Z1866978403	-9.1	0.303	406.39	REAL	O=C(N[C@@H]1Cc2ccccc(O)c2C1)c1ccc(F)cc2c(=O)c3cc(F)ccc3[nH]c12
vNsp10-ppi2-120	Z1879021149	-9.1	0.325	395.48	REAL	NS(=O)(=O)c1cc(-c2nc([C@H]3CCCc4ccccc43)no2)cc2c1CCC2
vNsp10-ppi2-121	Z1957155428	-9.1	0.364	398.22	REAL	O=C1COc2ccc(/C=C\c3nc(O)c4cc(Br)ccc4n3)cc2N1
vNsp10-ppi2-122	Z197423910	-9.1	0.294	436.47	REAL	NC1=Nc2nc3cc4c(cc3n2[C@@H](c2csc(-c3ccc(F)cc3)n2)N1)OCCCO4
vNsp10-ppi2-123	Z197423918	-9.1	0.268	459.48	REAL	NC1=Nc2nc3cc4c(cc3n2[C@@H](c2ccc(OCc3cccc(F)c3)cc2)N1)OCCCO4
vNsp10-ppi2-124	Z2090896559	-9.1	0.325	374.45	REAL	Cc1nnc2c3ccccc3c(N3CCC[C@@H](c4nnc5n4CCC5)C3)nn12
vNsp10-ppi2-125	Z2091794012	-9.1	0.294	418.45	REAL	C[C@@]1(C[C@H]2CCCN2C(=O)c2ccc3[nH]c4ccccc4c(=O)c3c2)NC(=O)NC1=O
vNsp10-ppi2-126	Z2126407583	-9.1	0.314	409.32	REAL	O=C1NC(=O)[C@]2(CCCN(C(=O)c3cccc(-c4noc(C(F)(F)F)n4)c3)C2)N1
vNsp10-ppi2-127	Z2157916870	-9.1	0.294	417.47	REAL	C[C@]1(c2cccc(-c3noc(-c4ccccc4N4CCCCC4)n3)c2)NC(=O)NC1=O
vNsp10-ppi2-128	Z2157917506	-9.1	0.303	405.42	REAL	C[C@@]1(c2cccc(-c3noc([C@H]4CCCN4c4ncccn4)n3)c2)NC(=O)NC1=O
vNsp10-ppi2-129	Z2159014087	-9.1	0.303	425.51	REAL	COc1ccc2c(c1)CCC[C@@H]2c1noc(-c2cc3c(c(S(N)(=O)=O)c2)CCC3)n1
vNsp10-ppi2-130	Z2160280486	-9.1	0.294	406.40	REAL	O=c1cc(-c2noc(-c3ccc4[nH]c5ccccc5c(=O)c4c3)n2)c2ccccc2[nH]1
vNsp10-ppi2-131	Z2161933778	-9.1	0.337	362.34	REAL	O=C(Nc1cccc(N2C(=O)CNC2=O)c1)c1ccc2ccc(O)nc12
vNsp10-ppi2-132	Z2164955025	-9.1	0.276	441.49	REAL	O=C(Nc1c[nH]nc1[C@@H]1CCCN(C(=O)c2cccc3ccc(O)nc23)C1)c1ccccc1
vNsp10-ppi2-133	Z2184179620	-9.1	0.337	362.39	REAL	Cc1c(NC(=O)c2cccc3c2CC(=O)CC3)cccc1-n1cn[nH]c1=O
vNsp10-ppi2-134	Z2230502519	-9.1	0.294	416.44	REAL	C[C@]1(c2cccc(C(=O)N3CCc4c(nnn4-c4ccccc4)C3)c2)NC(=O)NC1=O
vNsp10-ppi2-135	Z2458313126	-9.1	0.350	359.38	REAL	CC(=O)N1C[C@H](C(=O)N2CC[C@@H]3COC(=O)N[C@H]3C2)Oc2ccccc21
vNsp10-ppi2-136	Z2621674330	-9.1	0.325	379.42	REAL	Cc1nc(-c2ccc(C)c(NC(=O)N3CCOc4ccc(O)cc4C3)c2)n[nH]1
vNsp10-ppi2-137	Z2803219509	-9.1	0.314	393.45	REAL	Cc1nc(C2C[C@@H]3CC[C@H](C2)N3C(=O)c2ccc(-n3c(C)c[nH]c3=O)cc2)no1
vNsp10-ppi2-138	Z2830825448	-9.1	0.284	454.85	REAL	NC1=Nc2nc3cc4c(cc3n2[C@@H](c2cn(-c3ccc(F)cc3Cl)nn2)N1)OCCCO4
vNsp10-ppi2-139	Z2830825472	-9.1	0.268	459.48	REAL	NC1=Nc2nc3cc4c(cc3n2[C@@H](c2ccccc(OCc3ccc(F)cc3)c2)N1)OCCCO4
vNsp10-ppi2-140	Z2830825496	-9.1	0.276	445.45	REAL	NC1=Nc2nc3cc4c(cc3n2[C@@H](c2ccc(Oc3cccc(F)c3)cc2)N1)OCCCO4
vNsp10-ppi2-141	Z2830825693	-9.1	0.284	433.45	REAL	Cc1nn(-c2cccc(F)c2)cc1[C@H]1NC(N)=Nc2nc3cc4c(cc3n21)OCCCO4
vNsp10-ppi2-142	Z286720458	-9.1	0.253	477.53	REAL	Cc1nc2ccccc2c2c(NC(=O)C3CCN(c4ccc5nnnn5n4)CC3)c3ccccc3n12
vNsp10-ppi2-143	Z2959277079	-9.1	0.337	372.46	REAL	O=C1NCCOc2ccc(C(=O)N3CCCC[C@H]3[C@H]3CCCC[C@H]3O)cc21
vNsp10-ppi2-144	Z3203804723	-9.1	0.303	397.44	REAL	Cc1c(C(=O)N2[C@@H]3CC[C@H]2c2cncnc2C3)nnn1-c1cccc2ncccc12
vNsp10-ppi2-145	Z381165816	-9.1	0.276	464.51	REAL	CS(=O)(=O)N1CCCc2cc(C(=O)Nc3ccccc3-n3ncc4c(=O)[nH]cnc43)ccc21
vNsp10-ppi2-146	Z393471410	-9.1	0.284	432.43	REAL	O=C1c2ccc(C(=O)N3CCCc4c(F)cc(F)cc43)cc2C(=O)N1Cc1ccccc1
vNsp10-ppi2-147	Z424331808	-9.1	0.303	408.41	REAL	CC(=O)N1C[C@@H](C(=O)Nc2ccccc([C@]3(C)NC(=O)NC3=O)c2)Oc2ccccc21
vNsp10-ppi2-148	Z70955293	-9.1	0.246	487.52	REAL	Cc1cccn2c(NC(=O)c3ccc4c(c3)C(=O)N(Cc3ccncc3)C4=O)c(-c3ccccc3)nc12
vNsp10-ppi2-149	Z70955889	-9.1	0.253	476.49	REAL	Cc1cccn2c(NC(=O)c3ccc4c(c3)C(=O)N(Cc3ccco3)C4=O)c(-c3ccccc3)nc12
vNsp10-ppi2-150	Z759696940	-9.1	0.276	440.46	REAL	Cc1nn(-c2ccccc2)c2nc(C(=O)Nc3cccc([C@]4(C)NC(=O)NC4=O)c3)ccc12
vNsp10-ppi2-151	Z785732276	-9.1	0.268	486.48	REAL	NC1=Nc2nc3cc4c(cc3n2[C@@H](c2csc(-c3ccc(C(F)(F)F)cc3)n2)N1)OCCCO4
vNsp10-ppi2-152	Z804787624	-9.1	0.276	437.50	REAL	O=C1CCc2cc(NC(=O)[C@@H]3CC(=O)N(c4ccc5c(c4)Cc4ccccc4-5)C3)ccc2N1
vNsp10-ppi2-153	Z804874408	-9.1	0.294	421.46	REAL	C[C@@H]1C[C@H](C)CN(C(=O)c2ccccc2NC(=O)c2cnc3[nH]c(=O)[nH]c(=O)c3c2)C1
vNsp10-ppi2-154	Z806473494	-9.1	0.276	439.47	REAL	O=C1COc2cc(NC(=O)[C@H]3CC(=O)N(c4ccc5c(c4)Cc4ccccc4-5)C3)ccc2N1
vNsp10-ppi2-155	Z806909574	-9.1	0.294	421.47	REAL	O=C(N[C@@H]1CCCOc2ccc(F)cc21)c1ccc2c(=O)n3c(nc2c1)CCCCC3
vNsp10-ppi2-156	Z839917374	-9.1	0.268	459.48	REAL	NC1=Nc2nc3cc4c(cc3n2[C@@H](c2cccc(OCc3cccc3F)c2)N1)OCCCO4
vNsp10-ppi2-157	Z852852030	-9.1	0.268	462.46	REAL	CCn1c(=O)[nH]c2cc(C(=O)Nc3c(C(=O)N4CCOCC4)oc4ccccc34)ccc2c1=O
vNsp10-ppi2-158	Z900461148	-9.1	0.268	463.44	REAL	NC1=Nc2nc3cc4c(cc3n2[C@@H](c2ccc(Oc3cc(F)cc(F)c3)cc2)N1)OCCCO4
vNsp10-ppi2-159	Z914309960	-9.1	0.246	495.54	REAL	Cc1cccn2cc(COc3ccc([C@H]4NC(N)=Nc5nc6cc7c(cc6n54)OCCCO7)cc3)nc12
vNsp10-ppi2-160	Z98336196	-9.1	0.294	497.38	REAL	NC1=Nc2nc3cc4c(cc3n2[C@@H](c2csc(-c3cccc(Br)c3)n2)N1)OCCCO4
vNsp10-ppi2-161	Z998266280	-9.1	0.260	475.60	REAL	O=C(c1ccc2[nH]ncc2c1)N1CCC[C@@H](C(=O)N2CCC[C@@H](c3nnc4n3CCCCC4)C2)C1
vNsp10-ppi2-162	ZINC000008582204	-9.1	0.276	434.45	ZINC	O=C(O)c1ccccc1-c1ccccc1C(=O)Nc1ccc2c(c1)nc(O)c1ccccc12
vNsp10-ppi2-163	ZINC000012548239	-9.1	0.268	459.48	ZINC	NC1=Nc2nc3cc4c(cc3n2[C@@H](c2ccc(OCc3cccc(F)c3)cc2)N1)OCCCO4
vNsp10-ppi2-164	ZINC000071769572	-9.1	0.350	350.29	ZINC	O=C(c1ccc2c(=O)[nH]nc(O)c2c1)c1ccc2c(O)n[nH]c(=O)c2c1
vNsp10-ppi2-165	ZINC000104854096	-9.1	0.260	480.59	ZINC	Cc1ccc(N2C(=O)c3cccc3/C(=C\Nc3ncnc4sc5c(c43)CCCC5)C2=O)c(C)c1
vNsp10-ppi2-166	ZINC000253623870	-9.1	0.246	488.50	ZINC	Cn1cc(/C=C2/Oc3c(ccc4c3[C@@H](c3cc5cccc5nc3O)CC(=O)O4)C2=O)c2ccccc21
vNsp10-ppi2-167	ZINC000534664670	-9.1	0.325	373.46	ZINC	N=c1cc2ccc(-c3cccc(C(=O)N4CCC5(CCO5)CC4)c3)ccc2c[nH]1
vNsp10-ppi2-168	PV-000380451420	-9.0	0.346	356.39	REAL	O=C(N[C@@H]1C[C@H]2CC[C@@H]1N2C(=O)[C@@H]1CCCc2[nH]nnc21)c1nc[nH]n1
vNsp10-ppi2-169	PV-001809144491	-9.0	0.321	419.31	REAL	CC(=O)N1C[C@@H](C(=O)N2CCCc3c2cc(Cl)c(C)c3Cl)Oc2ccccc21
vNsp10-ppi2-170	PV-001817734716	-9.0	0.321	387.36	REAL	O=C(Nc1nnc(C(F)(F)F)[nH]1)c1ccc(N2CCCc3ccccc32)cc1
vNsp10-ppi2-171	PV-001832222190	-9.0	0.321	382.38	REAL	Cc1ccc2c(c1)C(=O)O[C@](C)(C(=O)NNc1nc3c(cnn3C)c(=O)[nH]1)C2
vNsp10-ppi2-172	PV-001853195817	-9.0	0.321	407.45	REAL	C[C@@]1(c2cccc(C(=O)N3CCS(=O)(=O)[C@@H]4COCC[C@H]43)c2)NC(=O)NC1=O
vNsp10-ppi2-173	PV-001865527676	-9.0	0.321	384.39	REAL	C[C@@]1(c2cccc(C(=O)N3C[C@@]4(C)C(=O)NC(=O)[C@]4(C)C3)c2)NC(=O)NC1=O
vNsp10-ppi2-174	PV-001943428163	-9.0	0.333	362.39	REAL	O=C1CN(C(=O)Nc2cc(-c3cccc3)on2)[C@H](c2ccccc2)CN1
vNsp10-ppi2-175	PV-001944177619	-9.0	0.321	376.42	REAL	Cc1nc(-c2ccc(C)c(NC(=O)N3CC(=O)Nc4ccccc4C3)c2)n[nH]1
vNsp10-ppi2-176	Z1250598570	-9.0	0.321	372.38	REAL	Cc1cc(C(=O)Nc2ccc3c4c(cccc24)CC3)nc2nc(O)[nH]c(=O)c12
vNsp10-ppi2-177	Z1335192400	-9.0	0.333	363.42	REAL	Cc1ccc2c(c1)N(C(=O)c1ccc([C@]3(C)NC(=O)NC3=O)cc1)CCC2
vNsp10-ppi2-178	Z1480903585	-9.0	0.321	366.38	REAL	O=c1[nH]c(/C=C/c2cccc3ccccc23)nc2c1cnn2-c1ncccn1
vNsp10-ppi2-179	Z1521778328	-9.0	0.321	399.47	REAL	O=C([C@H]1CCc2[nH]ncc2C1)N1CCN(C2=NS(=O)(=O)c3ccccc32)CC1
vNsp10-ppi2-180	Z1531888758	-9.0	0.321	398.44	REAL	NC(=O)[C@@H]1CCN(C(=O)CNC2=NS(=O)(=O)c3ccccc32)c2ccccc21
vNsp10-ppi2-181	Z1685242716	-9.0	0.333	363.35	REAL	Cc1cc(-c2noc([C@@H]3CC(=O)Nc4cc(F)ccc43)n2)cc2nc[nH]c12
vNsp10-ppi2-182	Z1685323848	-9.0	0.321	372.39	REAL	Cc1cc(-c2nc(-c3cccc(-c4nnc(C)[nH]4)c3)no2)c2c(C)n[nH]c2n1
vNsp10-ppi2-183	Z1725312648	-9.0	0.321	377.41	REAL	Nc1nc(CN2CCN(c3nc(=O)c4cn[nH]c4[nH]3)CC2)nc2ccccc12
vNsp10-ppi2-184	Z1766237442	-9.0	0.321	375.43	REAL	O=C1CN(C(=O)c2ccc3[nH]c4ccccc4c(=O)c3c2)[C@H]2CCCC[C@@H]2N1
vNsp10-ppi2-185	Z2033272386	-9.0	0.333	360.42	REAL	Cc1nc(-c2ccc(C)c(NC(=O)[C@H]3CCC(=O)c4ccccc43)c2)n[nH]1
vNsp10-ppi2-186	Z2059629190	-9.0	0.321	389.47	REAL	C[C@H]1CC[C@@H](O)[C@@H]([C@@H]2CCCN2C(=O)Nc2ccc3c(c2F)CCNC3=O)C1
vNsp10-ppi2-187	Z2154662864	-9.0	0.321	372.43	REAL	O=C(c1cccc2ccc(O)nc12)N1CCC[C@@H]1Cn1cnc2ccccc21
vNsp10-ppi2-188	Z2162770105	-9.0	0.321	377.40	REAL	NC(=O)c1cccnc1N1CCN(C(=O)c2cccc3ccc(O)nc23)CC1
vNsp10-ppi2-189	Z2164938115	-9.0	0.333	378.82	REAL	Cc1cc2ccc(Cl)cc2nc1NNC(=O)c1cccc2ccc(O)nc12
vNsp10-ppi2-190	Z2165306038	-9.0	0.346	368.41	REAL	O=C(c1cccc2ccc(O)nc12)N1CCS(=O)(=O)c2ccccc2C1
vNsp10-ppi2-191	Z2184176467	-9.0	0.333	362.43	REAL	Cc1c(NC(=O)[C@@H]2[C@@H]3[C@H]4C[C@@H]5[C@@H]6[C@@H]4C[C@@H]3[C@@H]6[C@@H]52)cccc1-n1cn[nH]c1=O
vNsp10-ppi2-192	Z2465304492	-9.0	0.321	386.41	REAL	Cc1cc(C(=O)N2CCC[C@H](N3CCNCC3=O)C2)nc2nc(O)[nH]c(=O)c12
vNsp10-ppi2-193	Z2608168791	-9.0	0.360	335.33	REAL	c1cc(-c2noc([C@H]3CCCc4[nH]nnc43)n2)cc(-n2cnnn2)c1
vNsp10-ppi2-194	Z2622123402	-9.0	0.321	384.44	REAL	C[C@@]1(c2cccc(NC(=O)[C@@H]3CC(=O)N[C@@H]4CCCC[C@H]43)c2)NC(=O)NC1=O
vNsp10-ppi2-195	Z2626761178	-9.0	0.321	398.38	REAL	Cc1ccc(C(F)(F)F)c(NC(=O)N2CCC([C@]3(C)NC(=O)NC3=O)CC2)c1
vNsp10-ppi2-196	Z2638093741	-9.0	0.321	383.49	REAL	Cc1nnnn1-c1ccc(C(=O)N2CCCC[C@H]2[C@H]2C[C@H](C)CC[C@H]2O)cc1
vNsp10-ppi2-197	Z2904536008	-9.0	0.321	377.40	REAL	C[C@]1(c2cccc(N3C(=O)[C@@H]4c5ccccc5CCN4C3=O)c2)COC(=O)N1
vNsp10-ppi2-198	Z3095587690	-9.0	0.310	394.45	REAL	C[C@H]1CN(c2nnc(-c3c[nH]c(C4CC4)nc3=O)n2N)CCc2ccc(F)cc21
vNsp10-ppi2-199	Z3095663455	-9.0	0.310	387.49	REAL	Cc1ccc2[nH]ncc2c1-c1nnc(N2CCCN(c3ccccc3)CC2)n1C
vNsp10-ppi2-200	ZINC000253536483	-9.0	0.321	375.43	ZINC	Cc1nc(O)c2c(n1)CCN(Cc1ccc3c4c1cccc4C(=O)OC3)CC2

Supplementary Table 48. Virtual screening hits 101 to 200 of the screen against the nsp14/nsp16 binding site on nsp10 (Screen ID: 26). Compounds were filtered so that hits had MW < 600 dalton, cLogP < 6, number of hydrogen bond acceptors < 11, and no reactive functional groups. The name of each compound consists of the initial letter 'v' for virtual hit, followed by the target protein name and the target site ('ppi' for protein-protein interface, 2 for docking scenario 2). The score is the docking score given by QuickVina 2 in kcal/mol. The ligand efficiency (LE) is computed as LE = -score/#NonH, where #NonH is the number of heavy (i.e. non hydrogen) atoms.

Name	Catalog ID	Score	LE	MW	Library	SMILES
vNsp10-nsp14.1-1	ZINC000002859412	-9.6	0.267	472.50	ZINC	Cc1ccc(-c2nc3ccccc3o2)cc1NC(=O)c1cccc(-c2cc3ccccc3oc2=O)c1
vNsp10-nsp14.1-2	Z1024047020	-9.5	0.271	466.54	REAL	O=C1O[C@H](c2ccccc2)Cc2cc(C(=O)N3CCC([C@H]4C(=O)Nc5ccccc54)CC3)ccc21
vNsp10-nsp14.1-3	ZINC000008427408	-9.5	0.279	448.48	ZINC	Cc1ccc(/C=C2/N=C(c3cccc(C4=N/C(=C\c5ccc(C)cc5)C(=O)O4)c3)OC2=O)cc1
vNsp10-nsp14.1-4	Z2002423492	-9.4	0.294	425.48	REAL	O=C1[C@@H]2[C@@H]3C[C@H]4[C@@H]2[C@]2(C(=O)Oc5cccc(C(=O)N6CCc7ccccc7C6)c5)[C@H]1[C@@H]3[C@@H]42
vNsp10-nsp14.1-5	Z2524819091	-9.4	0.276	477.67	REAL	CC(C)NC(=O)CSc1ccccc1C(=O)N1C[C@H]2CC[C@H]1[C@H]1CN(Cc3ccccc3)C[C@H]21
vNsp10-nsp14.1-6	Z298644866	-9.4	0.276	449.51	REAL	O=C1O[C@H](c2ccccc2)Cc2cc(C(=O)N3CC=C(c4c[nH]c5ncccc45)CC3)ccc21
vNsp10-nsp14.1-7	ZINC000888090785	-9.4	0.261	482.56	ZINC	CN1c2ccccc2C(=O)N2CCc3c4ccccc4n(CCC(=O)NCc4ccccc4F)c3[C@@H]12
vNsp10-nsp14.1-8	Z113628018	-9.3	0.266	470.48	REAL	C[C@H](OC(=O)c1ccc2c(c1)C[C@@H](c1ccccc1)OC2=O)C(=O)N1CC(=O)Nc2ccccc21
vNsp10-nsp14.1-9	Z225722736	-9.3	0.258	482.58	REAL	O=C1NC(=O)C2(CCN(C(=O)c3cc(-c4cccc(C5CCCCC5)cc4)nc4ccccc34)CC2)N1
vNsp10-nsp14.1-10	ZINC000001588362	-9.3	0.274	440.51	ZINC	Nc1nc(-c2ccc3ccccc3c2)cc(-c2cc(-c3ccc4ccccc4c3)nc(N)n2)n1
vNsp10-nsp14.1-11	Z1103001100	-9.2	0.271	446.51	REAL	O=C(Cc1ccc(Nc2ccc3nnc(-c4ccccc4)n3n2)cc1)N1CCc2ccccc21
vNsp10-nsp14.1-12	Z1549426862	-9.2	0.287	424.46	REAL	O=C(Nc1c[nH]nc1-c1ccccc1)c1cccc(NC(=O)[C@H]2Cc3ccccc3O2)c1
vNsp10-nsp14.1-13	Z1943429978	-9.2	0.287	424.46	REAL	O=C(Nc1nccn1-c1ccccc1)c1cccc(NC(=O)[C@H]2Cc3ccccc3O2)c1
vNsp10-nsp14.1-14	Z401414116	-9.2	0.279	460.60	REAL	CN1CCC2(CC1)C[C@H](NS(=O)(=O)c1ccc3c(c1)Cc1ccccc1-3)c1ccccc1O2
vNsp10-nsp14.1-15	Z607062516	-9.2	0.279	437.50	REAL	O=C(Nc1cccc(C(=O)N2CCc3[nH]c4ccccc4c3C2)c1)[C@H]1Cc2ccccc2O1
vNsp10-nsp14.1-16	Z95872423	-9.2	0.271	452.51	REAL	O=C1O[C@H](c2ccccc2)Cc2cc(C(=O)N3CCC(c4nnc5ccccn45)CC3)ccc21
vNsp10-nsp14.1-17	ZINC000002908937	-9.2	0.249	494.45	ZINC	O=c1oc(-c2cccc(F)c2)nc2cc(Cc3ccc4nc(-c5cccc(F)c5)oc(=O)c4c3)ccc12
vNsp10-nsp14.1-18	ZINC000002933884	-9.2	0.249	494.45	ZINC	O=c1oc(-c2cccc(F)c2)nc2cc(Cc3ccc4c(=O)oc(-c5cccc(F)c5)nc4c3)ccc12
vNsp10-nsp14.1-19	ZINC000033284240	-9.2	0.249	491.55	ZINC	Cc1cccc(-c2noc(-c3cn(CC(=O)N[C@H]4CCc5ccccc54)c4nc(C)ccc4c3=O)n2)c1
vNsp10-nsp14.1-20	ZINC000033770468	-9.2	0.271	448.48	ZINC	Cc1ccc(/C=C2\N=C(c3cccc(C4=N/C(=C\c5ccc(C)cc5)C(=O)O4)c3)OC2=O)cc1
vNsp10-nsp14.1-21	ZINC000408718372	-9.2	0.271	456.40	ZINC	O=C1OC(c2ccc(F)cc2)=N/C1=C\c1ccc(/C=C2\N=C(c3ccc(F)cc3)OC2=O)cc1
vNsp10-nsp14.1-22	Z1023496434	-9.1	0.260	475.52	REAL	O=C(C1CCN(c2nc3ccccc3o2)CC1)N1CCC[C@@H](c2nc(-c3ccc(F)cc3)no2)C1
vNsp10-nsp14.1-23	Z1023508440	-9.1	0.284	434.47	REAL	O=C1CCCc2cc(C(=O)N3CCC[C@@H](c4nc(-c5cccc(F)c5)no4)C3)ccc2N1
vNsp10-nsp14.1-24	Z1069484738	-9.1	0.253	485.58	REAL	C[C@@H]1CCc2[nH]c3ccc(C(=O)N4CCC(C(=O)c5ccc6c(c5)NC(=O)[C@H](C)O6)CC4)cc3c2C1
vNsp10-nsp14.1-25	Z1128906577	-9.1	0.253	482.54	REAL	O=C(Nc1cccc(-c2noc(=O)[nH]2)c1)[C@H]1C[C@H]2CCCC[C@H]2N1C(=O)c1ccc2ccccc2c1
vNsp10-nsp14.1-26	Z1451907667	-9.1	0.276	445.47	REAL	O=C(Nc1cccc(-c2cn(Cc3ccccc3)nn2)c1)N1CCc2ccc(F)c(F)c2C1
vNsp10-nsp14.1-27	Z1452691933	-9.1	0.276	445.49	REAL	O=C(NC[C@H]1[C@@H]2Cc3ccccc3[C@H]12)NNC(=O)c1ccccc1OCc1ccc(F)cc1
vNsp10-nsp14.1-28	Z1453804507	-9.1	0.268	449.55	REAL	O=C(NC[C@@H]1[C@H]2Cc3ccccc3[C@@H]12)c1ccnc(C(=O)NC[C@@H]2[C@H]3Cc4ccccc4[C@@H]23)c1
vNsp10-nsp14.1-29	Z1466232523	-9.1	0.284	427.48	REAL	O=C(Nc1cccc(-c2cn(Cc3ccccc3)nn2)c1)N1CCc2ccc(F)cc2C1
vNsp10-nsp14.1-30	Z1664063609	-9.1	0.276	439.41	REAL	Cn1nc(-c2nnc(-c3ccc4noc(-c5ccc(F)cc5)c4c3)o2)c2ccccc2c1=O
vNsp10-nsp14.1-31	Z1684606061	-9.1	0.268	449.47	REAL	O=C1O[C@H](c2ccccc2)Cc2cc(-c3nc(Cc4nc(-c5cccc5)n[nH]4)no3)ccc21
vNsp10-nsp14.1-32	Z1723433445	-9.1	0.260	464.53	REAL	Cn1c(=O)[nH]c2ncc(-c3cccc(C(=O)N4CCN(c5ccc6ccccc6n5)CC4)c3)cc21
vNsp10-nsp14.1-33	Z1744199641	-9.1	0.276	438.48	REAL	O=C1O[C@@H](c2ccccc2)Cc2cc(C(=O)N3CC[C@@]4(C3)C(=O)Nc3ccccc34)ccc21
vNsp10-nsp14.1-34	Z1907680588	-9.1	0.294	421.58	REAL	CC(C)COc1ccc(C2(C(=O)NC[C@@]3(O)[C@@H]4[C@H]5C[C@H]6[C@H]7[C@H]5C[C@@H]4[C@H]7[C@H]63)CCC2)cc1
vNsp10-nsp14.1-35	Z2187203011	-9.1	0.284	422.48	REAL	O=C1O[C@H](c2ccccc2)Cc2cc(C(=O)N3CCn4c(cc5ccccc54)C3)ccc21
vNsp10-nsp14.1-36	Z278037106	-9.1	0.276	432.48	REAL	O=C(Nc1cc(-c2ccccc2)nc2ccccc12)c1ccc(=O)n(Cc2ccccc2)n1
vNsp10-nsp14.1-37	Z2940772808	-9.1	0.253	477.56	REAL	O=C1O[C@H](c2ccccc2)Cc2cc(C(=O)N3CCc4c(ncn4CCc4ccccc4)C3)ccc21
vNsp10-nsp14.1-38	Z66691732	-9.1	0.268	455.51	REAL	C[C@@H](OC(=O)c1ccc2c(c1)C[C@@H](c1ccccc1)OC2=O)C(=O)N1CCc2ccccc2C1
vNsp10-nsp14.1-39	Z979605650	-9.1	0.276	436.51	REAL	O=C(NNC(=O)c1cc(-c2ccccc2)nc2ccccc12)N[C@@H]1CCc2ccccc2C1
vNsp10-nsp14.1-40	ZINC000008312480	-9.1	0.294	409.48	ZINC	O=C(c1ccc2c(c1)C[C@@H](c1ccccc1)OC2=O)N1CC=C(c2ccccc2)CC1
vNsp10-nsp14.1-41	ZINC000035350936	-9.1	0.268	448.48	ZINC	Cc1ccccc1C1=N/C(=C\c2ccc(/C=C3\N=C(c4ccccc4C)OC3=O)cc2)C(=O)O1
vNsp10-nsp14.1-42	PV-001837093254	-9.0	0.290	444.87	REAL	O=C(Nc1cc(-c2cc(F)cc(F)c2)[nH]n1)[C@@H]1CCCN(C(=O)c2ccc(Cl)cc2)C1
vNsp10-nsp14.1-43	PV-001953983640	-9.0	0.333	358.44	REAL	CC(=O)c1ccc2c(c1)CN(C(=O)N[C@@H](C)c1cccc3ccccc13)C2
vNsp10-nsp14.1-44	Z1000672516	-9.0	0.265	453.54	REAL	Cc1nn(C)c2nc(-c3ccccc3)cc(C(=O)N[C@@H]3CCCN(C(=O)c4ccccc4)C3)c12
vNsp10-nsp14.1-45	Z1014397762	-9.0	0.257	469.58	REAL	O=C(N[C@@H]1CCCc2[nH]c(=O)ncc21)[C@@H]1C[C@@H]2CCCC[C@@H]2N1C(=O)c1ccc2ccccc2c1
vNsp10-nsp14.1-46	Z1014757394	-9.0	0.257	464.52	REAL	Cc1ccc2nc(-c3ccccc3)cc(C(=O)NCc3ccc([C@@]4(C)NC(=O)NC4=O)cc3)c2c1
vNsp10-nsp14.1-47	Z1023504216	-9.0	0.265	462.52	REAL	Cc1ccc(CN2C[C@H](C(=O)N3CCC[C@@H](c4nc(-c5ccc(F)c5)no4)C3)CC2=O)cc1
vNsp10-nsp14.1-48	Z1143878084	-9.0	0.290	420.49	REAL	Cc1ccc2c(c1)[C@@H](NC(=O)N1CCC[C@@H](c3nc(-c4ccc(F)c4)no3)C1)CC2
vNsp10-nsp14.1-49	Z1147984550	-9.0	0.250	475.56	REAL	O=C(Nc1ccccc1-c1ccc(-c2ccccc2)cc1)C1CCN(c2ccc3nnnn3n2)CC1
vNsp10-nsp14.1-50	Z1217404884	-9.0	0.281	424.54	REAL	O=C(c1cccc(C(=O)N2CCc3ccccc3CC2)c1)N1CCc2ccccc2CC1
vNsp10-nsp14.1-51	Z1217405483	-9.0	0.346	339.44	REAL	O=C(c1ccc2c(c1)Cc1ccccc1-2)N1CCc2ccccc2CC1
vNsp10-nsp14.1-52	Z153971464	-9.0	0.250	485.47	REAL	Nc1nc(COC(=O)c2ccc3c(c2)C[C@@H](c2ccccc2)OC3=O)nc(Nc2ccc(F)cc2)n1
vNsp10-nsp14.1-53	Z153971484	-9.0	0.250	494.42	REAL	O=C(OCc1nc2cc(C(F)(F)F)ccc2c(=O)[nH]1)c1ccc2c(c1)C[C@@H](c1ccccc1)OC2=O
vNsp10-nsp14.1-54	Z1614095491	-9.0	0.273	440.49	REAL	Fc1ccccc1-c1nnc2ccc(N3CCC[C@H](c4n[nH]c(-c5ccccc5)n4)C3)nn12
vNsp10-nsp14.1-55	Z1671298637	-9.0	0.281	434.53	REAL	O=C(Nc1cccc(C(=O)N2CCO[C@H](C3CCCCC3)C2)c1)[C@@H]1Cc2ccccc2O1
vNsp10-nsp14.1-56	Z1684581724	-9.0	0.290	412.45	REAL	C[C@@H](c1ccc2ccccc2c1)c1nc(-c2cccc([C@]3(C)NC(=O)NC3=O)c2)no1
vNsp10-nsp14.1-57	Z1685085222	-9.0	0.265	449.47	REAL	O=C1C[C@H](c2nc(-c3ccc4[nH]c(=O)[nH]c4c3)no2)CN1c1ccc2c(c1)Cc1ccccc1-2
vNsp10-nsp14.1-58	Z1723444755	-9.0	0.273	438.53	REAL	Cc1cc(C)cc(C2=CCN(C(=O)c3cccc(-c4cnc5[nH]c(=O)n(C)c5c4)c3)CC2)c1
vNsp10-nsp14.1-59	Z2001020385	-9.0	0.300	396.53	REAL	O=C([C@@H]1C[C@H]1c1ccc2ccccc2c1)N1CCC(N2CCc3ccccc32)CC1
vNsp10-nsp14.1-60	Z2128906469	-9.0	0.265	449.55	REAL	O=C(c1cncc(C(=O)N2CCC=C(c3ccccc3)C2)c1)N1CCC=C(c2ccccc2)C1
vNsp10-nsp14.1-61	Z2193901914	-9.0	0.273	434.46	REAL	O=C1C[C@H](c2nc(-c3ccc4[nH]nnc4c3)no2)CN1c1ccc2c(c1)Cc1ccccc1-2
vNsp10-nsp14.1-62	Z2524828119	-9.0	0.257	478.64	REAL	CC1(C)CCC[C@@]2(C1)NC(=O)N(CC(=O)N1C[C@H]3CC[C@H]1[C@@H]1CN(Cc4ccccc4)C[C@@H]31)C2=O
vNsp10-nsp14.1-63	Z372560378	-9.0	0.265	492.99	REAL	O=C(Nc1cccc(-c2ccn[nH]2)c1)c1cc(S(=O)(=O)N2CCc3ccccc3C2)ccc1Cl
vNsp10-nsp14.1-64	Z647030414	-9.0	0.273	440.47	REAL	O=C1O[C@@H](c2ccccc2)Cc2cc(C(=O)N3CCc4[nH]c5ccc(F)cc5c4C3)ccc21
vNsp10-nsp14.1-65	Z648314932	-9.0	0.265	454.57	REAL	O=C(NC1CCN(CCc2ccccc2)CC1)c1ccc2c(c1)C[C@@H](c1ccccc1)OC2=O
vNsp10-nsp14.1-66	Z804390806	-9.0	0.243	495.63	REAL	O=C([C@H]1CC(=O)N(c2ccc3c(c2)Cc2ccccc2-3)C1)N1CCC[C@@H](c2nnc3n2CCCCC3)C1
vNsp10-nsp14.1-67	Z952521270	-9.0	0.250	474.52	REAL	O=C(NCc1ccc(-n2cnc3ccccc32)nc1)c1ccc2c(c1)C[C@@H](c1ccccc1)OC2=O
vNsp10-nsp14.1-68	ZINC000001862466	-9.0	0.257	455.47	ZINC	Cc1nc(-c2cc3c(ccc4ccccc43)oc2=O)cc2c1c(=O)oc1ccc3ccccc3c12
vNsp10-nsp14.1-69	ZINC000002767615	-9.0	0.310	380.49	ZINC	Cc1ccc([C@H](C)NC(=O)c2cc(-c3cccc(C)c3)nc3ccccc32)cc1
vNsp10-nsp14.1-70	ZINC000016449460	-9.0	0.265	456.40	ZINC	O=C1OC(c2ccccc2F)=N/C1=C\c1ccc(/C=C2\N=C(c3ccccc3F)OC2=O)cc1
vNsp10-nsp14.1-71	ZINC000019497136	-9.0	0.273	443.55	ZINC	C[C@H]1CCc2onc(C(=O)N3CCNC(=O)[C@@H](Cc4ccc(-c5ccccc5)cc4)C3)c2C1
vNsp10-nsp14.1-72	ZINC000033284113	-9.0	0.243	491.55	ZINC	Cc1ccc2c(=O)c(-c3nc(-c4ccccc4C)no3)cn(CC(=O)N[C@H]3CCc4ccccc43)c2n1
vNsp10-nsp14.1-73	ZINC000043214914	-9.0	0.265	444.49	ZINC	O=C1c2cc3ccccc3cc2C(=O)[C@H]2C[C@H]3C(=O)c4cc5ccccc5cc4C(=O)[C@H]3C[C@@H]12
vNsp10-nsp14.1-74	ZINC000080346354	-9.0	0.265	463.61	ZINC	c1ccc(-c2cc(-c3nn4c(nnc4C45CC6CC(CC(C6)C4)C5)s3)c3ccccc3n2)cc1
vNsp10-nsp14.1-75	ZINC000408718023	-9.0	0.265	456.40	ZINC	O=C1OC(c2ccc(F)c2)=N/C1=C\c1ccc(/C=C2\N=C(c3cccc(F)c3)OC2=O)cc1
vNsp10-nsp14.1-76	PV-001791724704	-8.9	0.287	442.58	REAL	CO[C@@H](C(=O)Nc1ccc(S(=O)(=O)N[C@@H](C)[C@H]2C[C@H]3CC[C@H]2C3)cc1)c1ccccc1
vNsp10-nsp14.1-77	PV-001842008977	-8.9	0.270	442.56	REAL	Cc1ccc(N2C[C@H](C(=O)NC[C@@H](O)c3ccc(-c4ccccc4)cc3)CCC2=O)cc1C
vNsp10-nsp14.1-78	PV-001876713854	-8.9	0.278	454.46	REAL	O=C(Nc1[nH]ncc1-c1ccccc1)c1cccc(NS(=O)(=O)c2ccc(F)c(F)c2)c1
vNsp10-nsp14.1-79	PV-001940740368	-8.9	0.278	456.61	REAL	C[C@H](CNC(=O)Nc1ccc(S(=O)(=O)N[C@H](C)[C@@H]2C[C@H]3CC[C@H]2C3)cc1)c1ccncc1
vNsp10-nsp14.1-80	PV-001947212465	-8.9	0.270	449.50	REAL	O=C(Nc1cccc(-c2ccc(F)c(F)c2)c1)N[C@@H]1CCN(C(=O)CCc2ccccc2)C1
vNsp10-nsp14.1-81	PV-001955800795	-8.9	0.287	420.51	REAL	CC1(C)CN(C(=O)NCc2ccc([C@]3(C)NC(=O)NC3=O)cc2)CCc2ccccc21
vNsp10-nsp14.1-82	PV-001955813252	-8.9	0.297	425.96	REAL	O=C(NCC(=O)N1CCc2ccccc2C1)N[C@@H]1CCC[C@H](c2ccccc(Cl)c2)C1
vNsp10-nsp14.1-83	PV-001963308882	-8.9	0.318	376.43	REAL	CC(=O)c1ccc2c(c1)CN(C(=O)N[C@@H](C)c1ccc(F)c3ccccc13)C2
vNsp10-nsp14.1-84	Z1014751964	-8.9	0.287	411.46	REAL	C[C@@]1(c2ccc(CNC(=O)c3ccc4c(c3)Cc3ccccc3-4)cc2)NC(=O)NC1=O
vNsp10-nsp14.1-85	Z1023504610	-8.9	0.247	485.51	REAL	O=C(c1ccccc1)c1ccc(OCC(=O)N2CCC[C@@H](c3nc(-c4cccc(F)c4)no3)C2)cc1
vNsp10-nsp14.1-86	Z1024049916	-8.9	0.278	430.51	REAL	Cc1cccc(N2N=C(C(=O)N3CCC([C@H]4C(=O)Nc5ccccc54)CC3)CCC2=O)c1
vNsp10-nsp14.1-87	Z1024054450	-8.9	0.254	471.53	REAL	Cc1ccc(C(=O)N2CCC([C@@H]3C(=O)Nc4ccccc43)CC2)cc1NC(=O)c1ccccc1F
vNsp10-nsp14.1-88	Z1028177866	-8.9	0.270	449.53	REAL	O=C(NCCN1CCc2ccccc2C1)N1CCC[C@@H](c2nc(-c3cccc(F)c3)no2)C1
vNsp10-nsp14.1-89	Z1038860852	-8.9	0.262	449.51	REAL	O=C(NCc1ccncc1)Nc1cccc(CNC(=O)c2cc3c(ccc4ccccc43)[nH]2)c1
vNsp10-nsp14.1-90	Z1100526430	-8.9	0.297	397.48	REAL	C[C@@H](NC(=O)Nc1ccc2c(c1)Cc1ccccc1-2)c1ccc2c(c1)CC(=O)N2C
vNsp10-nsp14.1-91	Z1100930920	-8.9	0.247	482.54	REAL	COc1cccc2c1OC[C@@H](NC(=O)NNC(=O)c1cc(-c3ccc(C)cc3)nc3ccccc13)C2
vNsp10-nsp14.1-92	Z1275065382	-8.9	0.270	440.54	REAL	CN(Cc1ccccc1)[C@@H]1CCN(C(=O)c2ccc3c(c2)C[C@@H](c2ccccc2)OC3=O)C1
vNsp10-nsp14.1-93	Z1382492844	-8.9	0.278	433.45	REAL	O=C1O[C@H](c2ccccc2)Cc2cc(C(=O)N3CC(Cc4ccc(F)c(F)c4)C3)ccc21
vNsp10-nsp14.1-94	Z1407896910	-8.9	0.307	381.39	REAL	O=C1Nc2ccc(-c3ccccc3)cc2/C1=N\Nc1nc2ccccc2c(=O)[nH]1
vNsp10-nsp14.1-95	Z1417728717	-8.9	0.262	449.51	REAL	C[C@@H](c1ccccc1)n1ccc(NC(=O)c2nn(Cc3ccccc3)c(=O)c3ccccc23)n1
vNsp10-nsp14.1-96	Z14196786	-8.9	0.254	468.51	REAL	COc1ccc2cc([C@@]3(C)NC(=O)N(Cc4cc(=O)oc5cc6c(cc45)CCC6)C3=O)ccc2c1
vNsp10-nsp14.1-97	Z1420801145	-8.9	0.270	446.55	REAL	O=C(N[C@H]1CCN(C(=O)C2CCCCC2)C1)c1ccc2c(c1)C[C@@H](c1ccccc1)OC2=O
vNsp10-nsp14.1-98	Z1421713648	-8.9	0.270	438.49	REAL	C[C@H](NC(=O)c1ccc2c(c1)C[C@@H](c1ccccc1)OC2=O)c1cn(-c2ccccc2)nn1
vNsp10-nsp14.1-99	Z1423689618	-8.9	0.287	425.44	REAL	O=C(CCNC(=O)N1CCc2ccccc2C1)Nc1cc(-c2ccccc(F)c2F)n[nH]1
vNsp10-nsp14.1-100	Z1449094967	-8.9	0.287	409.48	REAL	O=C(NC[C@@H]1[C@H]2Cc3ccccc3[C@@H]12)c1ccc2c(c1)C[C@@H](c1ccccc1)OC2=O

Supplementary Table 49. Top 100 virtual hits of the screen against the nsp14 binding site on nsp10 (Screen ID: 27). The name of each compound consists of the initial letter 'v' for virtual hit, followed by the target protein name and the target site ('nasp14' for nsp14 binding site, 1 for docking scenario 1). The score is the docking score given by QuickVina 2 in kcal/mol. The ligand efficiency (LE) is computed as LE = -score/#NonH, where #NonH is the number of heavy (i.e. non hydrogen) atoms.

Name	Catalog ID	Score	LE	MW	Library	SMILES
vNsp10-nsp14.1-101	Z1507811378	-8.9	0.287	410.48	REAL	Cc1nc(-c2ccc3ccccc3c2)n(CC(=O)c2ccc3c(c2)CCC(=O)N3C)n1
vNsp10-nsp14.1-102	Z1552768547	-8.9	0.270	440.46	REAL	O=C(Nc1ccc2[nH]nc(NC(=O)[C@@H]3Cc4ccccc4O3)c2c1)[C@H]1Cc2ccccc2O1
vNsp10-nsp14.1-103	Z1612383025	-8.9	0.287	410.47	REAL	O=C1NC2(Cc3ccccc3C2)C(=O)N1Cc1ccc(-c2ccc3c(c2)CCO3)cc1
vNsp10-nsp14.1-104	Z1614094330	-8.9	0.270	446.53	REAL	Fc1ccccc1-c1nnc2ccc(N3CCC[C@H](c4n[nH]c(C5CCCCC5)n4)C3)nn12
vNsp10-nsp14.1-105	Z1614248236	-8.9	0.270	441.49	REAL	O=C(c1cc(-c2ccc3c(c2)CCO3)no1)N1CCC[C@@H](c2n[nH]c(-c3ccccc3)n2)C1
vNsp10-nsp14.1-106	Z1663160732	-8.9	0.270	434.45	REAL	O=C1Nc2ccccc2O[C@H]1Cc1nnc(-c2cc(-c3ccccc3)nc3ccccc23)o1
vNsp10-nsp14.1-107	Z1663794006	-8.9	0.262	445.49	REAL	Cc1ccc(-c2cc(-c3nnc(Cc4ccc(-n5cnnn5)cc4)o3)c3ccccc3n2)cc1
vNsp10-nsp14.1-108	Z1663797830	-8.9	0.262	449.45	REAL	Fc1ccc(-c2cc(-c3nnc(Cc4ccc(-n5cnnn5)cc4)o3)c3ccccc3n2)cc1
vNsp10-nsp14.1-109	Z1682390492	-8.9	0.278	424.46	REAL	C[C@@]1(c2ccc(-c3noc([C@H]4C[C@@H]4c4ccccc5ccccc45)n3)cc2)NC(=O)NC1=O
vNsp10-nsp14.1-110	Z1684079466	-8.9	0.262	449.47	REAL	Nc1nc(Cc2noc(-c3ccc4c(c3)C[C@@H](c3ccccc3)OC4=O)n2)nc2ccccc12
vNsp10-nsp14.1-111	Z1685320635	-8.9	0.278	428.50	REAL	Cc1ccc(C(=O)N2CCC[C@@H](c3nc(-c4cccc(-c5nnc(C)[nH]5)c4)no3)C2)cc1
vNsp10-nsp14.1-112	Z1723432844	-8.9	0.254	468.56	REAL	Cc1ccc(C(=O)C2CCN(C(=O)c3cccc(-c4cnc5[nH]c(=O)n(C)c5c4)c3)CC2)c(C)c1
vNsp10-nsp14.1-113	Z1723442803	-8.9	0.254	472.48	REAL	Cc1cc(-c2noc([C@@H](C)NC(=O)c3cccc(-c4cnc5[nH]c(=O)n(C)c5c4)c3)n2)ccc1F
vNsp10-nsp14.1-114	Z1723444909	-8.9	0.254	480.49	REAL	Cn1c(=O)[nH]c2ncc(-c3cccc(C(=O)N4CCC(c5ccc(C(F)(F)F)cc5)CC4)c3)cc21
vNsp10-nsp14.1-115	Z2006757649	-8.9	0.270	443.52	REAL	O=C(N[C@H]1CCc2nnc(-c3ccc(F)cc3)n2C1)N1[C@@H]2C=C(c3ccccc3)C[C@@H]1CC2
vNsp10-nsp14.1-116	Z2089242375	-8.9	0.270	441.57	REAL	O=C(C1CCN(c2ccc3cccc(O)c3n2)CC1)N1C[C@H](c2ccccc2)[C@H]2CCC[C@@H]21
vNsp10-nsp14.1-117	Z2160281880	-8.9	0.278	421.42	REAL	Cc1noc2nc(-c3ccccc3)cc(-c3nc(-c4cc(=O)[nH]c5ccccc45)no3)c12
vNsp10-nsp14.1-118	Z2167429497	-8.9	0.262	448.53	REAL	Cn1c(-c2nn(C)c(=O)c3ccccc23)nnc1N1CC=C(c2ccccc3ccccc23)CC1
vNsp10-nsp14.1-119	Z2181678801	-8.9	0.270	446.55	REAL	O=C(N[C@H]1c2ccccc2CC12CCOCC2)N1CC=C(c2ccc3c(c2)OCCO3)CC1
vNsp10-nsp14.1-120	Z228625892	-8.9	0.234	498.54	REAL	O=C(Cn1c2ccccc2c(=O)c2ccccc21)NNC(=O)c1cc(-c2ccccc2)nc2ccccc12
vNsp10-nsp14.1-121	Z2518802220	-8.9	0.278	509.49	REAL	Br.Cc1ccc(N/C(N)=N\Cc2ccccc(C/N=C(/N)Nc3ccc(C)c(C)c3)c2)cc1C
vNsp10-nsp14.1-122	Z2518802288	-8.9	0.278	509.49	REAL	Br.Cc1cc(C)cc(N/C(N)=N\Cc2ccccc(C/N=C(/N)Nc3cc(C)ccc(C)c3)c2)c1
vNsp10-nsp14.1-123	Z296289064	-8.9	0.254	464.53	REAL	Cc1ccc(-c2cc(NC(=O)CCc3nc4c(cnn4C)c(=O)[nH]3)nc(-c3ccccc3)c2)cc1
vNsp10-nsp14.1-124	Z394510666	-8.9	0.247	490.60	REAL	C[C@H]1CCCN(C(=O)C2CCN(C(=O)CN3C(=O)N[C@@](C)(c4ccc5ccccc5c4)C3=O)CC2)C1
vNsp10-nsp14.1-125	Z436118982	-8.9	0.247	484.56	REAL	Cc1cccc(C(=O)N2CCCN(C(=O)Nc3cccc(Cn4nc5ccccn5c4=O)c3)CC2)c1
vNsp10-nsp14.1-126	Z70913644	-8.9	0.247	482.58	REAL	CN1CCC2(CC1)C[C@H](NC(=O)c1ccc3c(c1)C[C@@H](c1ccccc1)OC3=O)c1ccccc1O2
vNsp10-nsp14.1-127	Z803944916	-8.9	0.247	479.50	REAL	O=C(NNC(=O)[C@@H]1CC(=O)N(c2ccc3c(c2)Cc2ccccc2-3)C1)c1n[nH]c(=O)c2ccccc12
vNsp10-nsp14.1-128	Z806445912	-8.9	0.247	485.63	REAL	CC1CCN(C(=O)C2CCN(C(=O)[C@H]3CC(=O)N(c4ccc5c(c4)Cc4ccccc4-5)C3)CC2)CC1
vNsp10-nsp14.1-129	Z941397708	-8.9	0.297	397.47	REAL	O=C1OC[C@H](c2ccccc2)Cc2cc(C(=O)N3CC[C@H](c4ccccc4)C3)ccc21
vNsp10-nsp14.1-130	Z941403984	-8.9	0.254	492.64	REAL	C[C@@H]1CN(S(=O)(=O)c2cccc(C(=O)N3CCC(c4cccc5ccccc45)CC3)c2)C[C@@H](C)O1
vNsp10-nsp14.1-131	Z998231366	-8.9	0.241	490.61	REAL	O=C(NC[C@@H]1CC2c3ccccc3C1c1ccccc12)[C@@H]1CCCN(C(=O)c2ccc3[nH]ncc3c2)C1
vNsp10-nsp14.1-132	ZINC000000637643	-8.9	0.234	546.67	ZINC	Cc1ccc(NS(=O)(=O)c2ccc3c(c2)C(=O)c2cc(S(=O)(=O)Nc4ccc(C)cc4C)ccc2-3)c(C)c1
vNsp10-nsp14.1-133	ZINC000002862195	-8.9	0.278	417.46	ZINC	O=C(Nc1ccc2c3c(cccc31)CC2)c1ccc(-c2cc3ccccc3oc2=O)cc1
vNsp10-nsp14.1-134	ZINC000002880802	-8.9	0.247	469.50	ZINC	O=C(Nc1cccc(-c2cnc3ccccc3n2)c1)c1ccnc(-c2nnc(-c3ccccc3)o2)c1
vNsp10-nsp14.1-135	ZINC000011665555	-8.9	0.262	442.48	ZINC	O=C(Nc1cccc(-c2ccc3nnc(-c4cccnc4)n3n2)c1)c1ccc2ccccc2c1
vNsp10-nsp14.1-136	ZINC000014114786	-8.9	0.254	467.52	ZINC	O=C(c1ccc2c(c1)C[C@@H](c1ccccc1)OC2=O)N1CCC(n2c(=O)[nH]c3ccccc32)CC1
vNsp10-nsp14.1-137	ZINC000014272514	-8.9	0.254	458.47	ZINC	O=C(Nc1ccc2oc(-c3ccccc3)nc2c1)c1ccc(-c2cc3ccccc3oc2=O)cc1
vNsp10-nsp14.1-138	ZINC000016292162	-8.9	0.262	448.48	ZINC	Cc1ccc(C2=N/C(=C\c3ccc(/C=C4\N=C(c5ccc(C)cc5)OC4=O)cc3)C(=O)O2)cc1
vNsp10-nsp14.1-139	ZINC000020494886	-8.9	0.262	489.31	ZINC	O=C1OC(c2ccccc2Cl)=N/C1=C\c1ccc(/C=C2\N=C(c3ccccc3Cl)OC2=O)cc1
vNsp10-nsp14.1-140	ZINC000033284195	-8.9	0.241	495.51	ZINC	Cc1ccc2c(=O)c(-c3nc(-c4ccc(F)cc4)no3)cn(CC(=O)Nc3ccc4c(c3)CCC4)c2n1
vNsp10-nsp14.1-141	ZINC000033284238	-8.9	0.241	491.55	ZINC	Cc1cccc(-c2noc(-c3cn(CC(=O)N[C@@H]4CCc5ccccc54)c4nc(C)ccc4c3=O)n2)c1
vNsp10-nsp14.1-142	ZINC000039754055	-8.9	0.270	434.45	ZINC	O=C(Nc1nnc(-c2ccccc2)o1)c1ccccc1NC(=O)c1cccc2ccccc21
vNsp10-nsp14.1-143	ZINC000072356259	-8.9	0.278	424.54	ZINC	O=C(c1cccc(-c2ccc(C[C@H]3CCCNC3=O)cc2)c1)N1CCc2ccccc2C1
vNsp10-nsp14.1-144	ZINC000095945823	-8.9	0.254	460.50	ZINC	Cn1c2cc(-c3cccc(C(=O)Nc4cccc(-c5nc6ccccc6[nH]5)c4)c3)cnc2[nH]c1=O
vNsp10-nsp14.1-145	ZINC000253589970	-8.9	0.262	468.68	ZINC	CC(=O)O[C@@H]1CC[C@]2(C)[C@H](CC[C@]3(C)[C@@H]4C(O)=CC5=C([C@H](C)[C@H](C)CC5)[C@H]4C(=O)C[C@H]32)C1(C)C
vNsp10-nsp14.1-146	ZINC000254350217	-8.9	0.254	455.51	ZINC	O=C1c2ccccc2C(=O)c2cc(N=C3C=C(c4ccccc4)[C@](O)(c4ccccc4)C3)ccc21
vNsp10-nsp14.1-147	PV-001800289904	-8.8	0.275	439.51	REAL	CC(C)(CC(=O)NCCN1C(=O)[C@@H]2[C@@H]3C=C[C@@H](C3)[C@@H]2C1=O)NC(=O)OCc1ccccc1
vNsp10-nsp14.1-148	PV-001802620784	-8.8	0.275	441.45	REAL	Cc1cc(=O)c(C(=O)N[C@H](C)c2ccc3c(c2)CCC3)nn1-c1ccccC(F)(F)F)c1
vNsp10-nsp14.1-149	PV-001906752868	-8.8	0.326	409.36	REAL	CC(C)C[C@@H](NC(=O)c1ccc(Cl)cc1Cl)C(=O)N[C@H]1C[C@@H]2C[C@@H]1[C@H]1C[C@@H]21
vNsp10-nsp14.1-150	PV-001941316222	-8.8	0.284	427.43	REAL	O=C(Nc1ccc(C(=O)NCCC(F)(F)F)cc1)N[C@H]1CCc2cccc3ccec1c23
vNsp10-nsp14.1-151	PV-001961776162	-8.8	0.326	366.48	REAL	C[C@@H]1CN(C(=O)N[C@H]2CC[C@@H](c3ccc(F)cc3)C2)CCc2ccccc21
vNsp10-nsp14.1-152	PV-001970280572	-8.8	0.338	344.46	REAL	Cc1ccc2c(c1)CCN(C(=O)N[C@H](C)c1ccccc3ccccc13)C2
vNsp10-nsp14.1-153	Z1014421792	-8.8	0.238	496.61	REAL	O=C(c1ccccn1)N1CCN(C(=O)[C@@H]2C[C@@H]3CCCC[C@@H]3N2C(=O)c2ccc3ccccc3c2)CC1
vNsp10-nsp14.1-154	Z1014754282	-8.8	0.284	411.46	REAL	C[C@@]1(c2ccc(CNC(=O)c3ccc4c(c3)-c3ccccc3C4)cc2)NC(=O)NC1=O
vNsp10-nsp14.1-155	Z1014756702	-8.8	0.251	468.49	REAL	C[C@@]1(c2ccc(CNC(=O)c3cc(-c4ccc(F)cc4)nc4ccccc34)cc2)NC(=O)NC1=O
vNsp10-nsp14.1-156	Z1014758188	-8.8	0.238	494.55	REAL	C[C@]1(c2ccc(CNC(=O)[C@@H]3CC(=O)N(c4ccc5c(c4)Cc4ccccc4-5)C3)cc2)NC(=O)NC1=O
vNsp10-nsp14.1-157	Z1016577424	-8.8	0.244	480.57	REAL	C[C@@]1(c2ccc(CNC(=O)NC[C@@H]3CC4c5ccccc5C3c3ccccc34)cc2)NC(=O)NC1=O
vNsp10-nsp14.1-158	Z1016606194	-8.8	0.244	485.54	REAL	C[C@@H](NC(=O)NCc1ccc([C@]2(C)NC(=O)NC2=O)cc1)c1cccc(NC(=O)c2ccccc2)c1
vNsp10-nsp14.1-159	Z1018159978	-8.8	0.275	430.55	REAL	O=C(N[C@H]1CCCN(C(=O)c2ccccc2)C1)N1CCC[C@H](c2cc3ccccc3[nH]2)C1
vNsp10-nsp14.1-160	Z1028332518	-8.8	0.284	420.49	REAL	Cc1ccc2c(c1)CC[C@@H]2NC(=O)N1CCC[C@@H](c2nc(-c3cccc(F)c3)no2)C1
vNsp10-nsp14.1-161	Z1040787142	-8.8	0.251	471.56	REAL	O=C(NCc1ccncc1)Nc1cccc(CNC(=O)N2CCC(C(=O)c3ccccc3)CC2)c1
vNsp10-nsp14.1-162	Z1070217284	-8.8	0.284	437.93	REAL	O=C1Nc2cc(Cl)ccc2[C@H]1C1CCN(C(=O)[C@@H]2CC(=O)N(c3ccccc3)C2)CC1
vNsp10-nsp14.1-163	Z1099342414	-8.8	0.259	455.56	REAL	C[C@@H](NC(=O)NCc1ccc(-c2ccc3c(c2)CCCO3)cc1)c1ccc2c(c1)CC(=O)N2C
vNsp10-nsp14.1-164	Z1116410942	-8.8	0.251	468.56	REAL	Cc1nn(-c2ccccc2)c2nc(C(=O)N3CCCC[C@@H]3CNC(=O)Nc3ccccc3)ccc12
vNsp10-nsp14.1-165	Z1119220455	-8.8	0.238	492.53	REAL	O=C1c2ccccc2C(=O)N1Cc1cccc(C(=O)N2CCCC[C@H]2c2nc(-c3ccccc3)no2)c1
vNsp10-nsp14.1-166	Z1129472770	-8.8	0.293	397.47	REAL	C[C@H]1Cc2ccccc2N(C(=O)c2ccc3c(c2)C[C@H](c2ccccc2)OC3=O)C1
vNsp10-nsp14.1-167	Z1177867116	-8.8	0.275	431.54	REAL	Cc1ccc2[nH]c([C@@H]3CCCN(C(=O)CNC(=O)N4CCc5ccccc5C4)C3)nc2c1
vNsp10-nsp14.1-168	Z1177886068	-8.8	0.284	417.51	REAL	Cc1cc(C)cc(-c2cc(NC(=O)CCNC(=O)N3CCc4ccccc4C3)[nH]n2)c1
vNsp10-nsp14.1-169	Z119603538	-8.8	0.275	489.33	REAL	O=C(Nc1nnc(-c2ccccc2Br)[nH]1)c1ccc2c(c1)C[C@H](c1ccccc1)OC2=O
vNsp10-nsp14.1-170	Z1212623669	-8.8	0.267	442.52	REAL	Cn1nc(-c2ccccc2)c2c(NC(=O)c3cccc(NC(=O)C4CCCCC4)c3)n[nH]c21
vNsp10-nsp14.1-171	Z1222602847	-8.8	0.284	412.49	REAL	O=C(NCC1Cc2ccccc2C1)c1cccc(NC(=O)[C@H]2Cc3ccccc3O2)c1
vNsp10-nsp14.1-172	Z1230899864	-8.8	0.284	418.54	REAL	O=C(Nc1cc([C@@H]2[C@@H]3CC[C@H]2C3)[nH]n1)C1CCN(C(=O)/C=C/c2ccccc2)CC1
vNsp10-nsp14.1-173	Z1246315268	-8.8	0.314	377.42	REAL	Cc1ccc(-c2noc(CCC(=O)N3[C@@H]4CC[C@@H]3c3ccccc34)n2)cc1F
vNsp10-nsp14.1-174	Z1278117339	-8.8	0.293	397.48	REAL	O=C1CCc2ccc(NC(=O)N3Cc4ccccc4[C@@H](c4ccccc4)C3)cc2N1
vNsp10-nsp14.1-175	Z137249674	-8.8	0.267	439.45	REAL	Cn1c(NNC(=O)c2cc(-c3ccc(F)cc3)nc3ccccc23)nc2ccccc2c1=O
vNsp10-nsp14.1-176	Z1449091094	-8.8	0.259	449.55	REAL	O=C(NC[C@@H]1[C@H]2Cc3ccccc3[C@@H]12)c1cccc(C(=O)NC[C@H]2[C@@H]3Cc4ccccc4[C@H]23)n1
vNsp10-nsp14.1-177	Z1449095738	-8.8	0.267	439.51	REAL	C[C@@]1(c2ccc3ccccc3c2)NC(=O)N(CC(=O)NC[C@@H]2[C@@H]3Cc4ccccc4[C@@H]23)C1=O
vNsp10-nsp14.1-178	Z1469587803	-8.8	0.267	434.50	REAL	Cc1nn(C)c2nc(-c3ccccc3)cc(C(=O)Nc3ccnc(Cc4ccccc4)n3)c12
vNsp10-nsp14.1-179	Z1473414653	-8.8	0.275	432.50	REAL	O=C(N[C@H]1[C@@H]2CCc3ccccc3[C@H]21)N1CCC[C@@H](c2nc(-c3cccc(F)c3)no2)C1
vNsp10-nsp14.1-180	Z1506264311	-8.8	0.293	402.45	REAL	O=C(c1cc(-c2ccc3c(c2)CCO3)no1)N1CCO[C@]2(CCc3ccccc32)C1
vNsp10-nsp14.1-181	Z1571947236	-8.8	0.275	428.57	REAL	Cc1cc(C)cc(C2=CCN(C(=O)C3CCN(C(=O)/C=C/c4ccccc4)CC3)CC2)c1
vNsp10-nsp14.1-182	Z1585515015	-8.8	0.267	443.55	REAL	Cc1cccc(C(=O)N2CCCN(C(=O)Nc3ccc(COc4ccccc4)cc3)CC2)c1
vNsp10-nsp14.1-183	Z1610591796	-8.8	0.267	438.49	REAL	Cc1cc2ccccc2nc1NNC(=O)c1cccc(NC(=O)[C@@H]2Cc3ccccc3O2)c1
vNsp10-nsp14.1-184	Z1614250929	-8.8	0.275	429.52	REAL	O=C1C[C@@H](C(=O)N2CCC[C@@H](c3n[nH]c(-c4ccccc4)n3)C2)CN1Cc1ccccc1
vNsp10-nsp14.1-185	Z1632200012	-8.8	0.267	448.50	REAL	O=C(NCC(=O)N1CCc2ccccc2C1)N[C@H]1CCc2nnc(-c3ccc(F)cc3)n2C1
vNsp10-nsp14.1-186	Z1632967229	-8.8	0.267	448.48	REAL	O=C(N[C@H]1CCc2nnc(-c3ccc(F)cc3)n2C1)N1CCc2[nH]c3ccc(F)cc3c2C1
vNsp10-nsp14.1-187	Z1653410339	-8.8	0.275	427.51	REAL	Cc1cccc([C@H]2CCN(C(=O)CCc3nc4c(cnn4-c4ccccc4)c(=O)[nH]3)C2)c1
vNsp10-nsp14.1-188	Z1658317637	-8.8	0.267	448.54	REAL	CN1CC[C@@H](NC(=O)N2CCC[C@@H](c3n[nH]c(-c4ccccc4)n3)C2)[C@@H]1c1ccc(F)cc1
vNsp10-nsp14.1-189	Z1662367801	-8.8	0.275	422.49	REAL	O=c1c2ccc(-c3nnc(Cc4ccc5ccccc5c4)o3)cc2nc2n1CCCCC2
vNsp10-nsp14.1-190	Z1682390906	-8.8	0.275	424.46	REAL	C[C@@]1(c2ccc(-c3noc([C@H]4C[C@@H]4c4ccc5ccccc5c4)n3)cc2)NC(=O)NC1=O
vNsp10-nsp14.1-191	Z1682391906	-8.8	0.284	412.45	REAL	C[C@@H](c1ccc2ccccc2c1)c1nc(-c2ccc([C@]3(C)NC(=O)NC3=O)cc2)no1
vNsp10-nsp14.1-192	Z1683536670	-8.8	0.259	448.48	REAL	O=C(Nc1cccc(-c2nc(Cc3ccc4ccccc4n3)no2)c1)[C@H]1Cc2ccccc2O1
vNsp10-nsp14.1-193	Z1683753884	-8.8	0.267	439.47	REAL	Cc1ccc(CNC(=O)c2ccc(-c3noc([C@@H]4Cc5ccccc5C(=O)O4)n3)c2)cc1
vNsp10-nsp14.1-194	Z1684581165	-8.8	0.275	442.40	REAL	C[C@@]1(c2cccc(-c3noc(C4(c5cccc(C(F)(F)F)c5)CC4)n3)c2)NC(=O)NC1=O
vNsp10-nsp14.1-195	Z1684581444	-8.8	0.293	398.42	REAL	C[C@@]1(c2cccc(-c3noc(Cc4ccc5ccccc5c4)n3)c2)NC(=O)NC1=O
vNsp10-nsp14.1-196	Z1684607334	-8.8	0.259	448.49	REAL	Cc1nn(C)c2nc(-c3ccccc3)cc(-c3nc(Cc4nc(-c5ccccc5)n[nH]4)no3)c12
vNsp10-nsp14.1-197	Z1685321662	-8.8	0.314	369.38	REAL	Cc1nnc(-c2cccc(-c3noc(-c4ccc5ccccc5c4O)n3)c2)[nH]1
vNsp10-nsp14.1-198	Z1718585125	-8.8	0.275	431.49	REAL	CC(C)(C(=O)N1CCC([C@H]2C(=O)Nc3ccccc32)CC1)N1C(=O)c2ccccc2C1=O
vNsp10-nsp14.1-199	Z1723430363	-8.8	0.251	469.54	REAL	Cn1c(=O)[nH]c2ncc(-c3cccc(C(=O)NCc4ccc(C(=O)N5CCCCC5)cc4)c3)cc21
vNsp10-nsp14.1-200	Z1723437303	-8.8	0.244	499.96	REAL	Cn1c(=O)[nH]c2ncc(-c3cccc(C(=O)N4CCC(=C5C(=O)Nc6cc(Cl)ccc65)CC4)c3)cc21

Supplementary Table 50. Virtual screening hits 101 to 200 of the screen against the nsp14 binding site on nsp10 (Screen ID: 27). Compounds were filtered so that hits had MW < 600 dalton, cLogP < 6, number of hydrogen bond acceptors < 11, and no reactive functional groups. The name of each compound consists of the initial letter 'v' for virtual hit, followed by the target protein name and the target site ('nsp14' for the nsp14 binding site, 1 for docking scenario 1). The score is the docking score given by QuickVina 2 in kcal/mol. The ligand efficiency (LE) is computed as LE = -score/#NonH, where #NonH is the number of heavy (i.e. non hydrogen) atoms.

Name	Catalog ID	Score	LE	MW	Library	SMILES
vNsp12-nsp8.1-1	Z1958362444	-11.5	0.397	438.567	REAL	CNS(=O)(=O)c1ccc(S(=O)(=O)NC[C@]2(O)[C@H]3[C@H]4C[C@@H]5[C@@H]6[C@H]4C[C@@H]3[C@H]6[C@H]52)cc1C
vNsp12-nsp8.1-2	Z2785110607	-11.5	0.426	365.428	REAL	CCCOc1ccccc1C(=O)CNC(=O)[C@]12[C@@H]3C(=O)[C@@H]4[C@H]5C[C@@H](C[C@@H](C[C@@H]41)[C@@H]2[C@H]53
vNsp12-nsp8.1-3	Z812396088	-11.5	0.397	386.41	REAL	O=C(c1cnc2[nH]c(=O)[nH]c(=O)c2c1)N1CCC[C@H]1c1cccc2ccccc12
vNsp12-nsp8.1-4	Z109821744	-11.4	0.335	458.512	REAL	CC(=O)c1ccc(-c2ccc(C(=O)N3C[C@@H](C(=O)N4CCCCC4)Oc4ccccc43)o2)cc1
vNsp12-nsp8.1-5	Z1769363381	-11.4	0.38	405.413	REAL	Cc1cccc2nc(C3CCN(C(=O)c4cnc5[nH]c(=O)[nH]c(=O)c5c4)CC3)oc12
vNsp12-nsp8.1-6	Z2002795192	-11.4	0.422	387.862	REAL	CCOCCOc1c(Cl)cccc1NC(=O)[C@@]12[C@@H]3C(=O)[C@H]4[C@@H]5C[C@H]([C@H]41)[C@H]2[C@H]53
vNsp12-nsp8.1-7	ZINC000253487590	-11.4	0.3	497.553	ZINC	O=C(c1ccccc1)[C@@H]1[C@H](c2ccccc2)[C@@]2(N=C(c3ccccc3)OC2=O)[C@@H]2c3ccccc3C=NN12
vNsp12-nsp8.1-8	Z2094108472	-11.3	0.353	432.498	REAL	O=C(NNc1cccc(F)n1)[C@@H]1C[C@@H]2CCCC[C@@H]2N1C(=O)c1ccc2ccccc2c1
vNsp12-nsp8.1-9	Z288957206	-11.3	0.314	492.549	REAL	CC(=O)c1ccc(N2CCN(C(=O)CN3C(=O)N[C@@](C)(c4ccc5c(c4)CCC5)C3=O)CC2)cF)c1
vNsp12-nsp8.1-10	Z31937411	-11.3	0.314	482.538	REAL	C[C@@]1(c2ccc3ccccc3c2)NC(=O)N(CC(=O)N2CCC(c3nc4ccccc4o3)CC2)C1=O
vNsp12-nsp8.1-11	Z667548890	-11.3	0.377	425.831	REAL	O=C(c1cnc2[nH]c(=O)[nH]c(=O)c2c1)N1CCC(c2nc3cc(Cl)ccc3o2)CC1
vNsp12-nsp8.1-12	Z951981746	-11.3	0.314	481.554	REAL	Cc1ccc2[nH]c([C@H]3CCCN3C(=O)CN3C(=O)N[C@@](C)(c4ccc5cccc5c4)C3=O)nc2c1
vNsp12-nsp8.1-13	ZINC000013828504	-11.3	0.353	437.881	ZINC	O=c1c2ccccc2occ1-c1cc(-c2ccc(Cl)cc2)nc2c1COc1ccccc1-2
vNsp12-nsp8.1-14	ZINC000408731626	-11.3	0.297	499.565	ZINC	Cc1ccc(N2C(=O)[C@H]3[C@H](C2=O)[C@@H]2C(=O)Oc4c5ccccc5ccc4C2=C[C@H]3c2ccccc2)cc1C
vNsp12-nsp8.1-15	Z1022496460	-11.2	0.303	495.621	REAL	O=C(NCC(=O)N1CCc2ccccc2C1)[C@@H]1C[C@@H]2CCCC[C@@H]2N1C(=O)c1ccc2ccccc2c1
vNsp12-nsp8.1-16	Z1697479114	-11.2	0.373	413.354	REAL	O=C1CC[C@H]2CN(C(=O)c3ccc(-c4noc(C(F)(F)F)n4)cc3)c3cccc1c32
vNsp12-nsp8.1-17	Z2126254694	-11.2	0.386	399.356	REAL	NC(=O)N1CCc2ccc(NC(=O)c3ccc(-c4noc(C(F)F)n4)cc3)cc21
vNsp12-nsp8.1-18	Z2483547003	-11.2	0.386	390.442	REAL	O=C(c1cnc2[nH]c(=O)[nH]c(=O)c2c1)N1CCC2(CCc3ccccc3C2)CC1
vNsp12-nsp8.1-19	Z383541426	-11.2	0.311	482.538	REAL	C[C@@]1(c2ccc3ccccc3c2)NC(=O)N(CC(=O)N2CCC[C@H](c3nc4ccccc4o3)C2)C1=O
vNsp12-nsp8.1-20	Z431891148	-11.2	0.35	424.459	REAL	O=C(NC[C@@H]1CC2c3ccccc3C1c1ccccc12)c1cnc2[nH]c(=O)[nH]c(=O)c2c1
vNsp12-nsp8.1-21	Z822272382	-11.2	0.311	482.626	REAL	Cc1ccc(C23C[C@@H]4C[C@H](CC(C(=O)N5CCN(C(=O)c6ccc7[nH]cnc7c6)CC5)(C4)C2)C3)cc1
vNsp12-nsp8.1-22	PV-001839585818	-11.1	0.396	371.443	REAL	CCc1n[nH]c(NC(=O)c2cc(-c3ccccc3)nc3cc(C)c(C)cc23)n1
vNsp12-nsp8.1-23	Z1014421792	-11.1	0.3	496.609	REAL	O=C(c1ccccn1)N1CCN(C(=O)[C@@H]2C[C@@H]3CCCC[C@@H]3N2C(=O)c2ccc3ccccc3c2)CC1
vNsp12-nsp8.1-24	Z1037873510	-11.1	0.317	465.508	REAL	C=CCN1C(=O)c2ccc(C(=O)N3c4ccccc4CC[C@@H]3C(=O)Nc3ccccc3)cc2C1=O
vNsp12-nsp8.1-25	Z1119604128	-11.1	0.308	489.524	REAL	C[C@@H](c1ccc(F)cc1F)N1CCN(C(=O)c2cccc(NC(=O)c3ccc4[nH]cnc4c3)c2)CC1
vNsp12-nsp8.1-26	Z1156361600	-11.1	0.317	472.5	REAL	Cc1nc(COc2ccc(NC(=O)[C@H]3CCCN3C(=O)c3ccc4ccccc4c3O)cc2)no1
vNsp12-nsp8.1-27	Z1540671946	-11.1	0.358	412.448	REAL	O=C(c1cnc2[nH]c(=O)[nH]c(=O)c2c1)N1CCc2ccccc2[C@@H]1Cc1ccccc1
vNsp12-nsp8.1-28	Z1724592382	-11.1	0.347	420.519	REAL	c1ccc2c3c([nH]c2c1)CN(c1cc(N2CCc4c([nH]c5ccccc45)C2)ncn1)CC3
vNsp12-nsp8.1-29	Z1752022802	-11.1	0.326	449.552	REAL	O=C(NC[C@@H]1CC2c3ccccc3C1c1ccccc12)N1CC[C@@]2(C1)C(=O)Nc1ccccc12
vNsp12-nsp8.1-30	Z1907680588	-11.1	0.358	421.579	REAL	CC(C)COc1ccc(C2(C(=O)NC[C@@]3(O)[C@@H]4[C@H]5C[C@H]6[C@H]7[C@H]5C[C@@H]4[C@H]7[C@H]63)CCC2)cc1
vNsp12-nsp8.1-31	Z1911615689	-11.1	0.396	379.415	REAL	O=C(NC[C@@]1(O)[C@H]2[C@@H]3C[C@H]4[C@@H]5[C@@H]3C[C@@H]2[C@@H]5[C@H]41)c1ccc(-c2noc(=O)[nH]2)cc1
vNsp12-nsp8.1-32	Z2117570313	-11.1	0.347	438.433	REAL	O=C(N[C@@H]1CC(=O)N(c1ccccc1)[C@H]2C[C@@H]2c2ccccc2)C1)c1ccc(-c2noc(C(F)F)n2)cc1
vNsp12-nsp8.1-33	Z226444914	-11.1	0.308	481.554	REAL	C[C@@]1(c2ccc3ccccc3c2)NC(=O)N(CC(=O)N2CCC[C@H](c3nc4ccccc4[nH]3)C2)C1=O
vNsp12-nsp8.1-34	Z2524819091	-11.1	0.326	477.671	REAL	CC(C)NC(=O)CSc1ccccc1C(=O)N1C[C@H]2CC[C@H]1[C@H]1CN(Cc3cccc3)C[C@H]21
vNsp12-nsp8.1-35	Z607064230	-11.1	0.347	437.498	REAL	O=C(c1cnc2[nH]c(=O)[nH]c(=O)c2c1)N1CCN(C(=O)C23CC4CC(CC(C4)C2)C3)CC1
vNsp12-nsp8.1-36	Z899288814	-11.1	0.37	402.457	REAL	O=C(Nc1n[nH]c2ccccc12)[C@@H]1CCC[C@@H](C(=O)Nc2n[nH]c3ccccc23)C1
vNsp12-nsp8.1-37	Z996019966	-11.1	0.308	483.61	REAL	CN(C)C(=O)c1cccc(CNC(=O)[C@@H]2C[C@@H]3CCCC[C@@H]3N2C(=O)c2ccc3ccccc3c2)c1
vNsp12-nsp8.1-38	Z996489826	-11.1	0.308	482.582	REAL	Cn1c(=O)n(C)c2cc(NC(=O)[C@@H]3C[C@@H]4CCCC[C@@H]4N3C(=O)c3ccc4ccccc4c3)ccc21
vNsp12-nsp8.1-39	Z998375970	-11.1	0.3	495.581	REAL	O=C(c1ccc2[nH]ncc2c1)N1CCC[C@H](C(=O)N2CCN(C(=O)c3ccc4ccccc34)CC2)C1
vNsp12-nsp8.1-40	ZINC000002401785	-11.1	0.3	489.505	ZINC	O=C(c1ccc(F)cc1)[C@@H]1[C@@H]2C(=O)N(c3ccc4ccccc4c3)C(=O)[C@@H]2[C@@H]2c3ccccc3C=NN21
vNsp12-nsp8.1-41	ZINC000071785267	-11.1	0.3	505.912	ZINC	O=c1oc2ccccc2cc1-c1cc(-c2coc3ccccc3c2=O)c2c(n1)-c1cc(Cl)ccc1OC2
vNsp12-nsp8.1-42	ZINC000408731630	-11.1	0.292	499.565	ZINC	Cc1ccc(N2C(=O)[C@@H]3[C@H](C2=O)[C@@H]2C(=O)Oc4c5ccccc5ccc4C2=C[C@H]3c2ccccc2)cc1C
vNsp12-nsp8.1-43	PV-001793228987	-11	0.393	380.353	REAL	Cc1cc(NC(=O)c2ccc(-c3noc(C(F)F)n3)cc2)c2ccccc2n1
vNsp12-nsp8.1-44	PV-001805359881	-11	0.367	410.379	REAL	Cc1c(C(=O)Nc2ccc(-c3noc(C(F)F)n3)cc2)c2ccccc2n(C)c1=O
vNsp12-nsp8.1-45	PV-001809070380	-11	0.393	387.345	REAL	O=C(Nc1nc(O)c2c(n1)CCCC2)c1ccc(-c2noc(C(F)F)n2)cc1
vNsp12-nsp8.1-46	PV-001817266632	-11	0.344	448.375	REAL	CN1C(=O)C[C@H](NC(=O)c2ccc(-c3noc(C(F)F)n3)cc2)[C@H]1c1ccc(F)c(F)c1
vNsp12-nsp8.1-47	PV-001841358464	-11	0.344	426.518	REAL	Cc1ccc(C)c(-c2cc(C(=O)NNC(=O)C(C)(C)c3ccc4ccccc4c3)[nH]n2)c1
vNsp12-nsp8.1-48	Z1014269000	-11	0.306	481.594	REAL	O=C(NCC(=O)N1CCc2ccccc21)[C@@H]1C[C@@H]2CCCC[C@@H]2N1C(=O)c1ccc2ccccc2c1
vNsp12-nsp8.1-49	Z1029986498	-11	0.344	427.511	REAL	Cc1ccccc(-c2cccc(CNC(=O)C3CCN(c4ccc5nnnn5n4)CC3)c2)c1
vNsp12-nsp8.1-50	Z1131590910	-11	0.314	477.51	REAL	C[C@@]1(c2ccc3ccccc3c2)NC(=O)N(CC(=O)N2CCC(c3ccc(F)c(F)c3)CC2)C1=O
vNsp12-nsp8.1-51	Z1143593378	-11	0.324	449.513	REAL	O=C(NC[C@H](c1ccccc1)c1c[nH]c2ccccc12)NNC(=O)c1ccc2ncccc12
vNsp12-nsp8.1-52	Z1225339781	-11	0.333	449.509	REAL	Cc1ccc([C@]2(C)NC(=O)N(CC(=O)N3CCN(c4ccc(C(N)=O)cc4)CC3)C2=O)cc1
vNsp12-nsp8.1-53	Z1231979179	-11	0.355	415.452	REAL	COC(=O)Cc1nnc(NC(=O)c2cc(-c3ccccc3)nc3cc(C)c(C)cc23)[nH]1
vNsp12-nsp8.1-54	Z14137765	-11	0.314	472.543	REAL	COc1ccc(N2CCN(C(=O)CN3C(=O)N[C@@](C)(c4ccc5ccccc5c4)C3=O)CC2)cc1
vNsp12-nsp8.1-55	Z1472909756	-11	0.344	426.475	REAL	C[C@H]1[C@H](c2ccccc2)c2cccc2CCN1C(=O)c1cnc2[nH]c(=O)[nH]c(=O)c2c1
vNsp12-nsp8.1-56	Z1596321856	-11	0.344	430.55	REAL	O=C(NC[C@H]1CN(C(=O)c2ccccc2)[C@@H]2CCN1C2)N[C@@H]1[C@@H]2CCc3ccccc3[C@@H]21
vNsp12-nsp8.1-57	Z1616661299	-11	0.344	431.495	REAL	NC(=O)c1cc(NC(=O)[C@@H]2C[C@H]3CCC[C@H]3N2C(=O)c2cc3ccccc3c2)[nH]n1
vNsp12-nsp8.1-58	Z1752541538	-11	0.355	411.504	REAL	Cc1ccc(-c2cccc(CNC(=O)N3CC[C@@]4(C3)C(=O)Nc3ccccc34)c2)cc1
vNsp12-nsp8.1-59	Z1953423174	-11	0.355	418.495	REAL	CCOC(=O)c1nc(-c2cccc(CNC(=O)[C@H]3[C@H]4[C@H]5C[C@@H]6[C@H]7[C@@H](C[C@@H](C[C@@H]41)[C@@H]2[C@H]53)[C@@H]67)c2)n[nH]1
vNsp12-nsp8.1-60	Z1979144291	-11	0.393	403.775	REAL	Cn1c(NC(=O)c2ccc(-c3noc(C(F)F)n3)cc2)nc2ccc(Cl)ccc21
vNsp12-nsp8.1-61	Z1982328665	-11	0.393	387.32	REAL	Cn1c(NC(=O)c2ccc(-c3noc(C(F)F)n3)cc2)nc2ccc(F)ccc21
vNsp12-nsp8.1-62	Z2180030189	-11	0.344	432.454	REAL	O=C(NNC(=O)N1CCC(c2noc3cc(F)ccc23)CC1)c1ccc2ccccc2c1
vNsp12-nsp8.1-63	Z2192886851	-11	0.333	442.561	REAL	Cn1nc(NC(=O)[C@@H]2C[C@H]3CCCC[C@@H]3N2C(=O)c2ccc3ccccc3c2)cc1C1CC1
vNsp12-nsp8.1-64	Z2218873114	-11	0.379	413.457	REAL	O=c1[nH]c(=O)c2cc(S(=O)(=O)N3C[C@H]4CCCCN4c4ccccc43)cnc2[nH]1
vNsp12-nsp8.1-65	Z228235430	-11	0.344	432.518	REAL	C[C@@H]1c2cc3c(cc2C2(CCCC2)CN1C(=O)c1ccc2c(c1)CCC(=O)N2)OCCO3
vNsp12-nsp8.1-66	Z2524821252	-11	0.306	486.614	REAL	Cc1ccc([C@]2(C)NC(=O)N(CC(=O)N3C[C@@H]4CC[C@H]3[C@H]3CN(Cc5ccccc5)C[C@H]43)C2=O)cc1
vNsp12-nsp8.1-67	Z286954404	-11	0.297	490.569	REAL	Cc1ccc(-c2cc(NC(=O)C3CCN(c4ccc5nnnn5n4)CC3)nc(-c3ccccc3)c2)cc1
vNsp12-nsp8.1-68	Z397589852	-11	0.344	425.487	REAL	CC(=O)c1ccc(-c2ccc(C(=O)N3CCN(c4ccc5ccccc5n4)CC3)o2)cc1
vNsp12-nsp8.1-69	Z751237258	-11	0.333	467.549	REAL	Cc1noc(-c2ccc(C(=O)Nc3ccc(S(=O)(=O)/N=C4/CCCCCN4C)c3)cc2)n1
vNsp12-nsp8.1-70	Z804640398	-11	0.344	425.443	REAL	O=C(Nc1ccc2oc(=O)[nH]c2c1)[C@@H]1CC(=O)N(c2ccc3c(c2)Cc2ccccc2-3)C1
vNsp12-nsp8.1-71	Z995722280	-11	0.306	481.55	REAL	CN1C(=O)c2ccc(NC(=O)[C@@H]3C[C@@H]4CCCC[C@@H]4N3C(=O)c3ccc4ccccc4c3)cc2C1=O
vNsp12-nsp8.1-72	Z996126134	-11	0.306	483.614	REAL	O=C(N[C@@H]1CCCN(c2nccn2)C1)[C@@H]1C[C@H]2CCCC[C@@H]2N1C(=O)c1ccc2ccccc2c1
vNsp12-nsp8.1-73	ZINC000004333670	-11	0.344	422.526	ZINC	O=C1O[C@@]2(C[C@@H](c3ccccc3)[C@H]3CCCC[C@]34Nc3ccccc3N42)c2ccccc21
vNsp12-nsp8.1-74	ZINC000008845603	-11	0.314	469.471	ZINC	Cc1ccc(O)c(-c2cc(C(=O)Nc3c4ccccc4oc3C(=O)c3ccc(C)c(F)c3)n[nH]2)c1
vNsp12-nsp8.1-75	ZINC000043716692	-11	0.324	489.357	ZINC	O=C(c1ccc(Cl)cc1)[C@@H]1[C@@H]2C(=O)N(c3ccc(Cl)cc3)C(=O)[C@@H]2[C@@H]2c3ccccc3C=CN21
vNsp12-nsp8.1-76	PV-000774892507	-10.9	0.436	342.481	REAL	C=CCOCCN[C@H]1C[C@@H](NC(=O)[C@H]2[C@@H]3[C@@H]4C[C@H]5[C@H]6[C@@H]4C[C@@H]3[C@H]6[C@H]52)C1
vNsp12-nsp8.1-77	PV-001817948899	-10.9	0.341	442.421	REAL	CN1C(=O)C(C)(C)COc2ccc(NC(=O)c3ccc(-c4noc(C(F)F)n4)cc3)cc21
vNsp12-nsp8.1-78	PV-001861006758	-10.9	0.341	453.42	REAL	O=C(c1cnc2[nH]c(=O)[nH]c(=O)c2c1)N1CCC([C@H]2CCCN(C(=O)C(F)(F)F)C2)CC1
vNsp12-nsp8.1-79	PV-001892526568	-10.9	0.33	455.507	REAL	Cc1cc(NC(=O)c2ccc(-c3noc(C(F)F)n3)cc2)cc(N2CCN(C(C)C)C2)c1
vNsp12-nsp8.1-80	PV-001966454376	-10.9	0.376	393.485	REAL	C[C@H](NC(=O)N[C@H]1CCC[C@H](c2ccccc2)CC1)c1ccc2[nH]c(=O)oc2c1
vNsp12-nsp8.1-81	Z1014420158	-10.9	0.303	482.626	REAL	O=C(NCc1ccc(N2CCCC2)nc1)[C@@H]1C[C@@H]2CCCC[C@@H]2N1C(=O)c1ccc2ccccc2c1
vNsp12-nsp8.1-82	Z1014477988	-10.9	0.303	482.582	REAL	C[C@@H](NC(=O)[C@H]1C[C@H]2CCCC[C@H]2N1C(=O)c1ccc2ccccc2c1)c1ccc2[nH]c(=O)[nH]c2c1
vNsp12-nsp8.1-83	Z1021007696	-10.9	0.321	453.497	REAL	Cc1ccccc1NC(=O)[C@H]1CCc2ccccc2N1C(=O)c1ccc2c(c1)C(=O)N(C)C2=O
vNsp12-nsp8.1-84	Z1024051824	-10.9	0.295	491.589	REAL	O=C1Nc2ccccc2[C@H]1C1CCN(C(=O)[C@@H]2CC(=O)N(c3cc4c(c3)Cc3ccccc3-4)C2)CC1
vNsp12-nsp8.1-85	Z102667784	-10.9	0.295	498.581	REAL	C[C@]1(c2ccc3ccccc3c2)NC(=O)N(CC(=O)N2CCN(Cc3ccc4c(c3)CCO4)CC2)C1=O
vNsp12-nsp8.1-86	Z1127325239	-10.9	0.33	436.47	REAL	CN(Cc1cn(-c2ccccc2)nc1-c1ccccc1)C(=O)c1ccc2c(c1)C(=O)NC2=O
vNsp12-nsp8.1-87	Z114856234	-10.9	0.341	427.438	REAL	Cc1ccc(-n2c(N/N=C3\C(=O)Nc4cc(F)ccc43)nc3ccccc3c2=O)c(C)c1
vNsp12-nsp8.1-88	Z1161663417	-10.9	0.33	436.474	REAL	Cc1c(C(=O)NNC(=O)Cc2ccc3ccccc3c2)nnn1-c1ccc2ncccc2c1
vNsp12-nsp8.1-89	Z1170266410	-10.9	0.352	417.443	REAL	Cc1cc(C)c(-c2cc(NC(=O)c3nn(-c4ccc(F)cc4)ccc3=O)[nH]n2)cc1C
vNsp12-nsp8.1-90	Z1171670002	-10.9	0.341	423.471	REAL	O=C(N[C@@H]1CC2c3ccccc3C1c1ccccc12)c1ccc(-c2noc(=O)[nH]2)cc1
vNsp12-nsp8.1-91	Z131515672	-10.9	0.321	472.559	REAL	CC(=O)c1ccc(N2CCN(C(=O)CN3C(=O)N[C@@]4(C[C@H](C)CC(C)(C)C4)C3=O)CC2)c(F)c1
vNsp12-nsp8.1-92	Z1326713822	-10.9	0.352	422.396	REAL	C[C@@H]1CN(C(=O)c2ccc3[nH]c(=O)oc3c2)CCN1C(=O)c1ccc2[nH]c(=O)oc2c1
vNsp12-nsp8.1-93	Z1370905559	-10.9	0.33	442.493	REAL	O=C(Nc1cccc(C(=O)N2CCC(c3ccc(F)cc3)CC2)c1)c1ccc2[nH]cnc2c1
vNsp12-nsp8.1-94	Z1454222685	-10.9	0.33	446.589	REAL	O=C(N[C@H]1CCOC2(CCC2)C1)[C@@H]1C[C@@H]2CCCC[C@@H]2N1C(=O)c1ccc2ccccc2c1
vNsp12-nsp8.1-95	Z1544993775	-10.9	0.341	449.49	REAL	O=c1[nH]c(=O)c2cc(S(=O)(=O)N3CCN(Cc4ccccc4)c4ccccc43)cnc2[nH]1
vNsp12-nsp8.1-96	Z1550591099	-10.9	0.352	413.436	REAL	O=C(c1cnc2[nH]c(=O)[nH]c(=O)c2c1)N1CCN(Cc2ccccc2)c2ccccc21
vNsp12-nsp8.1-97	Z1560998777	-10.9	0.341	434.578	REAL	C[C@H]1CC(NC(=O)[C@@H]2C[C@H]3CCCC[C@@H]3N2C(=O)c2ccc3ccccc3c2)C[C@H](C)O1
vNsp12-nsp8.1-98	Z1580037208	-10.9	0.352	414.507	REAL	Cc1cnc(NC(=O)[C@@H]2C[C@@H]3CCCC[C@@H]3N2C(=O)c2ccc3ccccc3c2)nc1
vNsp12-nsp8.1-99	Z1636272019	-10.9	0.341	432.498	REAL	O=C(NNc1ccnc(F)c1)[C@@H]1C[C@@H]2CCCC[C@@H]2N1C(=O)c1ccc2ccccc2c1
vNsp12-nsp8.1-100	Z1703876970	-10.9	0.33	443.51	REAL	O=C(NC[C@@H](O)c1ccc(-c2ccccc2)cc1)C1CCN(c2ccc3nnnn3n2)CC1

Supplementary Table 51. Top 100 virtual hits of the screen against the nsp8 binding site on nsp12 (Screen ID: 31). The name of each compound consists of the initial letter 'v' for virtual hit, followed by the target protein name and the target site ('nsp8' for nps8 binding site, 1 for docking scenario 1). The score is the docking score given by QuickVina 2 in kcal/mol. The ligand efficiency (LE) is computed as LE = -score/#NonH, where #NonH is the number of heavy (i.e. non hydrogen) atoms.

Name	Catalog ID	Score	LE	MW	Library	SMILES
vNsp12-nsp8.1-101	Z1850324232	-10.9	0.330	442.56	REAL	N#Cc1ccc(CN2CC[C@H](NC(=O)N3CCC[C@]4(CCCc5ccccc54)C3)C2=O)cc1
vNsp12-nsp8.1-102	Z1904820670	-10.9	0.389	380.53	REAL	CC(C)(C)[C@H](NC(=O)NC[C@@]1(O)[C@@H]2[C@@H]3C[C@@H]4[C@H]5[C@@H]3C[C@H]2[C@H]5[C@H]41)c1ccccc1
vNsp12-nsp8.1-103	Z1905200482	-10.9	0.376	404.46	REAL	O=C(NCc1cccc(OCC(F)F)c1)NC[C@]1(O)[C@H]2[C@H]3C[C@@H]4[C@@H]5[C@@H]3C[C@@H]2[C@@H]5[C@@H]41
vNsp12-nsp8.1-104	Z2079994423	-10.9	0.376	396.35	REAL	Cn1ccc2ccc(NC(=O)c3ccc(-c4noc(C(F)F)n4)cc3)cc2c1=O
vNsp12-nsp8.1-105	Z2090076229	-10.9	0.363	419.43	REAL	O=C(N[C@@H]1CCCN(C(=O)N2CCCC2)C1)c1ccc(-c2noc(C(F)F)n2)cc1
vNsp12-nsp8.1-106	Z2099681231	-10.9	0.352	420.45	REAL	Cc1c(C(=O)N2CCC(c3c[nH]c4ccc(F)cc34)CC2)cnn1-c1ccc(=O)[nH]n1
vNsp12-nsp8.1-107	Z2110633418	-10.9	0.352	427.37	REAL	CN1CC(=O)N(c2cccc(NC(=O)c3ccc(-c4noc(C(F)F)n4)cc3)c2)C1=O
vNsp12-nsp8.1-108	Z2159536862	-10.9	0.363	424.89	REAL	O=C(c1ccc(Cl)cc1)N1[C@H](c2nc(-c3ccc(=O)[nH]c3)no2)C[C@H]2CCCC[C@H]21
vNsp12-nsp8.1-109	Z2163445082	-10.9	0.330	442.48	REAL	Cc1ccc(NC(=O)Nc2cccc3c2CCN(C(=O)c2cnc4[nH]c(=O)[nH]c4c2)C3)cc1
vNsp12-nsp8.1-110	Z220348464	-10.9	0.303	499.63	REAL	O=C(c1ccccc(S(=O)(=O)N2CCc3ccccc3C2)c1)N1CCC(c2c[nH]c3ccccc23)CC1
vNsp12-nsp8.1-111	Z2232121002	-10.9	0.363	398.42	REAL	O=C(c1cnc2[nH]c(=O)[nH]c(=O)c2c1)N1CCc2ccccc2[C@@H]1c1ccccc1
vNsp12-nsp8.1-112	Z2524826924	-10.9	0.341	427.55	REAL	Cc1nnc(-c2ccc(C(=O)N3C[C@@H]4CC[C@H]3[C@@H]3CN(Cc5ccccc5)C[C@@H]43)cc2)[nH]1
vNsp12-nsp8.1-113	Z2647483480	-10.9	0.376	392.41	REAL	O=C(c1cnc2[nH]c(=O)[nH]c(=O)c2c1)N1CCC2(CCc3ccccc3O2)CC1
vNsp12-nsp8.1-114	Z2712304679	-10.9	0.389	378.52	REAL	Cc1ccc2[nH]c3c(c2c1)C[C@@H](NC(=O)N1C[C@H]2[C@H]4CC[C@H](NC4)[C@@H]2C1)CC3
vNsp12-nsp8.1-115	Z2804160621	-10.9	0.376	387.44	REAL	O=C(c1ccc2c(c1)-c1ccccc1C2)N1CCO[C@H](c2noc(C3CC3)n2)C1
vNsp12-nsp8.1-116	Z286720458	-10.9	0.303	477.53	REAL	Cc1nc2ccccc2c2c(NC(=O)C3CCN(c4ccc5nnnn5n4)CC3)c3ccccc3n12
vNsp12-nsp8.1-117	Z2940789653	-10.9	0.295	490.57	REAL	O=C(Nc1cccc(C(=O)N2CCc3c(ncn3CCc3ccccc3)C2)c1)c1ccc2[nH]cnc2c1
vNsp12-nsp8.1-118	Z3046824964	-10.9	0.376	397.48	REAL	Cc1noc(C2CCN(C(=O)N[C@@H]3C[C@@]4(CCNC4)Oc4ccccc43)CC2)n1
vNsp12-nsp8.1-119	Z3214699286	-10.9	0.311	461.52	REAL	O=C(c1cc(-c2cnc3[nH]ccc3c2)ccn1)N1CCN(C(=O)c2ccc3ccccc23)CC1
vNsp12-nsp8.1-120	Z730742308	-10.9	0.295	493.57	REAL	C[C@@]1(c2ccc3ccccc3c2)NC(=O)N(CC(=O)Nc2cccc(-c3cn4c(n3)CCCC4)c2)C1=O
vNsp12-nsp8.1-121	Z744865042	-10.9	0.341	434.47	REAL	CC(=O)c1ccc(N2CCN(C(=O)NNC(=O)c3ccc4ccccc4c3)CC2)c(F)c1
vNsp12-nsp8.1-122	Z822271558	-10.9	0.295	498.63	REAL	COc1ccc(C23C[C@@H]4C[C@H](CC(C(=O)N5CCN(C(=O)c6ccc7[nH]cnc7c6)CC5)(C4)C2)C3)cc1
vNsp12-nsp8.1-123	Z828253492	-10.9	0.311	467.53	REAL	Cc1ccc(C(=O)N2CCN(C(=O)c3cccc(NC(=O)c4ccc5[nH]cnc5c4)c3)CC2)cc1
vNsp12-nsp8.1-124	Z898628556	-10.9	0.311	488.97	REAL	Cc1cc(=O)oc2cc(NC(=O)c3cccnc3N3CCN(Cc4cccc(Cl)c4)CC3)ccc12
vNsp12-nsp8.1-125	Z905709720	-10.9	0.303	481.55	REAL	Cn1c([C@H]2CCCN2C(=O)CN2C(=O)N[C@@](C)(c3ccc4ccccc4c3)C2=O)nc2ccccc21
vNsp12-nsp8.1-126	Z911074390	-10.9	0.303	489.53	REAL	Cc1cc(C(=O)NC2CCN(C(=O)CN3C(=O)N[C@@](C)(c4ccc5ccccc5c4)C3=O)CC2)no1
vNsp12-nsp8.1-127	Z971662570	-10.9	0.295	496.61	REAL	COc1ccc(/C=C2/CCCc3c2nc2ccccc2c3C(=O)N2CCC[C@H](N3CCNC3=O)C2)cc1
vNsp12-nsp8.1-128	Z971663576	-10.9	0.303	482.58	REAL	COc1ccc(/C=C2\CCc3c2nc2ccccc2c3C(=O)N2CCC[C@H](N3CCNC3=O)C2)cc1
vNsp12-nsp8.1-129	Z980158210	-10.9	0.295	497.55	REAL	O=C(Nc1ccc(CC(=O)N2CCc3ccccc32)cc1)[C@H]1CCCN1C(=O)c1ccc2c(c1)OCO2
vNsp12-nsp8.1-130	Z995754372	-10.9	0.303	481.59	REAL	O=C1Nc2ccccc2[C@@H]1CCNC(=O)[C@@H]1C[C@@H]2CCCC[C@@H]2N1C(=O)c1ccc2ccccc2c1
vNsp12-nsp8.1-131	Z995845128	-10.9	0.303	483.61	REAL	CN(C)C(=O)c1ccc(CNC(=O)[C@@H]2C[C@@H]3CCCC[C@@H]3N2C(=O)c2ccc3ccccc3c2)cc1
vNsp12-nsp8.1-132	ZINC000004107418	-10.9	0.295	478.56	ZINC	C(=c1/c(-c2ccccc2)nn2c3ccccc3nc12)\[C@@H]1C(c2ccccc2)=NN2c3ccccc3N[C@@H]12
vNsp12-nsp8.1-133	ZINC000008845649	-10.9	0.311	465.51	ZINC	Cc1ccc(C(=O)c2oc3ccccc3c2NC(=O)c2cc(-c3ccc(C)c(C)c3O)[nH]n2)cc1
vNsp12-nsp8.1-134	ZINC000013396078	-10.9	0.321	448.48	ZINC	O=C1O/C(=C\N2CCc3c4ccccc4[nH]c3[C@@H]2[C@@H]2OC(=O)c3ccccc32)c2ccccc21
vNsp12-nsp8.1-135	ZINC000020478179	-10.9	0.389	373.45	ZINC	O=c1oc2c(ccc3c2CN([C@H]2CCCc4ccccc42)CO3)c2c1CCC2
vNsp12-nsp8.1-136	ZINC000253398505	-10.9	0.295	496.45	ZINC	O=C(O)c1ccc(-c2ccc([C@@H]3CC(=O)Oc4ccc5c(=O)c(-c6ccc(F)cc6)coc5c43)o2)cc1
vNsp12-nsp8.1-137	ZINC000575413821	-10.9	0.330	441.53	ZINC	CC(=O)c1ccc(N2CCN(C(=O)C3CN(c4cc(-c5ccccc5)ncn4)C3)CC2)cc1
vNsp12-nsp8.1-138	PV-00012680065	-10.8	0.400	369.51	REAL	CNC(=O)CN1[C@H]2CC[C@H]1CC(NC(=O)[C@@H]1C[C@H]1c1ccc(C)c(C)c1)C2
vNsp12-nsp8.1-139	PV-001795542815	-10.8	0.338	440.45	REAL	CC1CCN(C(=O)c2ccc(NC(=O)c3ccc(-c4noc(C(F)F)n4)cc3)cc2)CC1
vNsp12-nsp8.1-140	PV-001798580960	-10.8	0.327	453.47	REAL	C[C@@]1(c2ccc(F)cc2)NC(=O)N(CC(=O)N2CCN(c3ccc(C(N)=O)cc3)CC2)C1=O
vNsp12-nsp8.1-141	PV-001800120608	-10.8	0.327	455.46	REAL	CN1CCN(C(=O)Cc2cccc(NC(=O)c3ccc(-c4noc(C(F)F)n4)cc3)c2)CC1
vNsp12-nsp8.1-142	PV-001805359078	-10.8	0.372	396.35	REAL	Cn1c(=O)cc(C(=O)Nc2ccc(-c3noc(C(F)F)n3)cc2)c2ccccc21
vNsp12-nsp8.1-143	PV-001807356442	-10.8	0.360	409.40	REAL	CN(C)c1nccc2cc(NC(=O)c3ccc(-c4noc(C(F)F)n4)cc3)ccc12
vNsp12-nsp8.1-144	PV-001815699474	-10.8	0.386	387.36	REAL	O=C(N[C@@H]1c2ccccc2CC[C@@H]1F)c1ccc(-c2noc(C(F)F)n2)cc1
vNsp12-nsp8.1-145	PV-001817661654	-10.8	0.386	380.35	REAL	Cc1nccc2c(NC(=O)c3ccc(-c4noc(C(F)F)n4)cc3)cccc12
vNsp12-nsp8.1-146	PV-001818620440	-10.8	0.348	455.30	REAL	Cc1nnc(-c2ccc(C(=O)N3C[C@@H]4[C@H](C3)C(F)(F)C(F)(F)C(F)(F)F)C4(F)F)cc2)o1
vNsp12-nsp8.1-147	PV-001821634903	-10.8	0.327	458.53	REAL	CC(=O)c1ccc(N2CCN(C(=O)CN3C(=O)NC4(C[C@@H](C)C[C@H](C)C4)C3=O)CC2)c(F)c1
vNsp12-nsp8.1-148	PV-001828796856	-10.8	0.327	455.46	REAL	CC(=O)N1CCN(c2ccccc2CNC(=O)c2ccc(-c3noc(C(F)F)n3)cc2)CC1
vNsp12-nsp8.1-149	PV-001835968441	-10.8	0.360	410.38	REAL	Cc1nc(-c2ccc(C)c(NC(=O)c3ccc(-c4noc(C(F)F)n4)cc3)c2)n[nH]1
vNsp12-nsp8.1-150	PV-001846375405	-10.8	0.327	459.43	REAL	O=C(Nc1ccc(-c2noc(C(F)F)n2)cc1)[C@H]1CCCN(C(=O)Nc2ccccc2F)C1
vNsp12-nsp8.1-151	PV-001850793151	-10.8	0.372	404.46	REAL	CN1CCC2(CCC(NC(=O)c3ccc(-c4noc(C(F)F)n4)cc3)CC2)CC1
vNsp12-nsp8.1-152	PV-001861469668	-10.8	0.372	396.35	REAL	Cc1cc(O)nc2ccc(NC(=O)c3ccc(-c4noc(C(F)F)n4)cc3)ccc12
vNsp12-nsp8.1-153	PV-001873720918	-10.8	0.348	430.41	REAL	Cc1cc(=O)[nH]c(N2CCC(NC(=O)c3ccc(-c4noc(C(F)F)n4)cc3)CC2)n1
vNsp12-nsp8.1-154	PV-001874623161	-10.8	0.338	431.45	REAL	COC(=O)c1ccc2c(c1)CC[C@@H](NC(=O)c1cc(C(=O)c3ccccc3)c[nH]1)C(=O)N2
vNsp12-nsp8.1-155	PV-001946482860	-10.8	0.338	430.51	REAL	CC1(C)NC(=O)N(c2cccc(NC(=O)NC(C)(C)c3ccc4ccccc4c3)c2)C1=O
vNsp12-nsp8.1-156	PV-001947650545	-10.8	0.372	392.41	REAL	Cc1cc2cc(NC(=O)N[C@@H](C)c3ccc4[nH]c(=O)oc4c3)ccc2n(C)c1=O
vNsp12-nsp8.1-157	PV-001958713010	-10.8	0.360	404.51	REAL	Cc1noc(-c2ccc(CNC(=O)NC3CCC(C)(c4ccccc4)CC3)cc2)n1
vNsp12-nsp8.1-158	PV-001960858984	-10.8	0.338	444.44	REAL	C[C@H](NC(=O)N[C@H]1CCCN(Cc2ccc(F)cc2F)C1=O)c1ccc2[nH]c(=O)oc2c1
vNsp12-nsp8.1-159	Z1014395262	-10.8	0.309	471.60	REAL	O=C(NCc1nnc2n1CCCCC2)[C@@H]1C[C@H]2CCCC[C@@H]2N1C(=O)c1ccc2ccccc2c1
vNsp12-nsp8.1-160	Z1014402700	-10.8	0.338	431.51	REAL	O=C(NNc1ccc(F)cc1)[C@@H]1C[C@H]2CCCC[C@@H]2N1C(=O)c1ccc2ccccc2c1
vNsp12-nsp8.1-161	Z1014420816	-10.8	0.309	468.60	REAL	Cc1ncc2c(n1)CC[C@H](NC(=O)[C@@H]1C[C@H]3CCCC[C@@H]3N1C(=O)c1ccc3ccccc3c1)C2
vNsp12-nsp8.1-162	Z1020971052	-10.8	0.309	468.51	REAL	Cc1nc(COc2ccc(C(=O)N3c4ccccc4CC[C@@H]3C(=O)Nc3ccccc3)cc2)no1
vNsp12-nsp8.1-163	Z1033218934	-10.8	0.327	445.48	REAL	Cc1nc(COc2ccc(C(=O)N3CCCC[C@@H]3c3nc(-c4ccccc4)no3)cc2)no1
vNsp12-nsp8.1-164	Z1040555168	-10.8	0.300	495.46	REAL	O=C(Nc1ccc(-c2noc(C(F)(F)F)n2)cc1)N1CCN(C(=O)c2cccc3ccccc23)CC1
vNsp12-nsp8.1-165	Z1048781154	-10.8	0.318	457.58	REAL	Cc1nc2n(n1)C[C@H](NC(=O)[C@@H]1C[C@@H]3CCCC[C@@H]3N1C(=O)c1ccc3ccccc3c1)CC2
vNsp12-nsp8.1-166	Z1096470764	-10.8	0.318	481.55	REAL	O=C1N[C@H](C(=O)N2CCN(C(=O)c3ccc4[nH]cnc4c3)CC2)CS[C@H]1Cc1ccccc1F
vNsp12-nsp8.1-167	Z109822322	-10.8	0.318	459.50	REAL	C=CCN1C(=O)c2ccc(C(=O)N3C[C@@H](C(=O)N4CCCCC4)Oc4ccccc43)cc2C1=O
vNsp12-nsp8.1-168	Z109822566	-10.8	0.338	433.46	REAL	CN1C(=O)c2ccc(C(=O)N3C[C@H](C(=O)N4CCCC4)Oc4ccccc43)cc2C1=O
vNsp12-nsp8.1-169	Z1099420412	-10.8	0.300	490.56	REAL	C[C@H]1Oc2ccc(C(=O)C3CCN(C(=O)N[C@H](C)c4ccc5c(c4)CC(=O)N5C)CC3)cc2NC1=O
vNsp12-nsp8.1-170	Z1117089194	-10.8	0.360	400.49	REAL	Cc1nc(-c2cccc(NC(=O)N3CCC[C@@H](c4cc5ccccc5[nH]4)C3)c2)n[nH]1
vNsp12-nsp8.1-171	Z1119604442	-10.8	0.309	481.55	REAL	C[C@@H](c1ccc(F)cc1F)N1CCN(C(=O)[C@H]2CCCN(C(=O)c3ccc4[nH]ncc4c3)C2)CC1
vNsp12-nsp8.1-172	Z1128837152	-10.8	0.318	450.51	REAL	O=C(Nc1cccc(-c2ccc3ccccc3c2)n1)C1CCN(c2ccc3nnnn3n2)CC1
vNsp12-nsp8.1-173	Z1148211116	-10.8	0.318	472.47	REAL	CN1CCC2(CC1)C[C@H](NC(=O)c1ccc(-c3noc(C(F)(F)F)n3)cc1)c1ccccc1O2
vNsp12-nsp8.1-174	Z1151723422	-10.8	0.309	468.55	REAL	C[C@@H]1Oc2ccc(C(=O)C3CCN(C(=O)[C@@H]4C[C@@H]4c4cccc5ccccc45)CC3)cc2NC1=O
vNsp12-nsp8.1-175	Z1151988862	-10.8	0.318	475.57	REAL	NC(=O)[C@@H]1c2ccccc2CCN1C(=O)c1cccc(S(=O)(=O)N2CCc3ccccc3C2)c1
vNsp12-nsp8.1-176	Z1157951588	-10.8	0.338	421.46	REAL	O=C(Nc1ccccc1-n1ncc2c(=O)[nH]cnc21)[C@H]1C[C@H]1c1ccc2ccccc2c1
vNsp12-nsp8.1-177	Z1227861645	-10.8	0.348	418.50	REAL	CC(=O)NCC(=O)N1CCc2cc(C(=O)N3C[C@@H]4CCCN4c4ccccc43)ccc21
vNsp12-nsp8.1-178	Z1240738442	-10.8	0.327	447.58	REAL	NC(=O)[C@@H]1CCC[C@H](NC(=O)[C@@H]2C[C@@H]3CCCC[C@@H]3N2C(=O)c2ccc3ccccc3c2)C1
vNsp12-nsp8.1-179	Z1277626781	-10.8	0.348	433.50	REAL	C[C@H]1CCCCN1C[C@@H]1CCCN(C(=O)Nc2ccc(-c3noc(C(F)F)n3)cc2)C1
vNsp12-nsp8.1-180	Z1286397827	-10.8	0.360	404.43	REAL	O=C(N[C@@H]1CC(=O)N([C@H]2C[C@@H]2c2ccccc2)C1)c1ccc(-c2noc(=O)[nH]2)cc1
vNsp12-nsp8.1-181	Z131514570	-10.8	0.300	487.57	REAL	CC(=O)c1ccc(N2CCN(C(=O)[C@H]3CCN(C(=O)c4ccc5ccccc45)C3)CC2)c(F)c1
vNsp12-nsp8.1-182	Z1342134940	-10.8	0.348	416.44	REAL	Cc1ccc(-c2cnc(-c3ccccc3C(=O)N3CCN4C(=O)NC(=O)[C@H]4C3)o2)cc1
vNsp12-nsp8.1-183	Z1378091563	-10.8	0.338	427.44	REAL	Cc1ccc(-n2c(N/N=C3\C(=O)Nc4c(F)cccc43)nc3ccccc3c2=O)c(C)c1
vNsp12-nsp8.1-184	Z1393207770	-10.8	0.348	432.87	REAL	O=C(c1cnc2[nH]c(=O)[nH]c(=O)c2c1)N1Cc2cc(Cl)ccc2C[C@H]1c1ccccc1
vNsp12-nsp8.1-185	Z145983734	-10.8	0.300	482.58	REAL	O=C(c1ccccc2ccccc12)N1CCC[C@@H](C(=O)N2CCC(n3c(=O)[nH]c4ccccc43)CC2)C1
vNsp12-nsp8.1-186	Z1466194741	-10.8	0.338	431.51	REAL	CN(C(=O)[C@@H]1C[C@@H]2CCCC[C@@H]2N1C(=O)c1ccc2ccccc2c1)c1nccc1F
vNsp12-nsp8.1-187	Z1488144475	-10.8	0.348	416.52	REAL	Cc1cc(NC(=O)[C@@H]2C[C@@H]3CCCC[C@@H]3N2C(=O)c2ccc3ccccc3c2)nn1C
vNsp12-nsp8.1-188	Z1527371540	-10.8	0.386	397.41	REAL	O=c1[nH]c(=O)c2cc(S(=O)(=O)N3CCc4c([nH]c5ccccc45)C3)cnc2[nH]1
vNsp12-nsp8.1-189	Z1581469914	-10.8	0.327	442.56	REAL	O=C(N[C@@H]1CCc2[nH]cnc2C1)[C@@H]1C[C@H]2CCCC[C@H]2N1C(=O)c1ccc2ccccc2c1
vNsp12-nsp8.1-190	Z1626781991	-10.8	0.338	425.50	REAL	O=C(C1CCN(c2ccc3nnnn3n2)CC1)N1CC=C(c2ccc3ccccc23)C1
vNsp12-nsp8.1-191	Z1643374763	-10.8	0.327	443.50	REAL	C[C@H]1COc2ccccc2CN1C(=O)CN1C(=O)N[C@@](C)(c2ccc3ccccc3c2)C1=O
vNsp12-nsp8.1-192	Z1697484458	-10.8	0.400	359.38	REAL	Cc1noc(-c2ccc(C(=O)N3C[C@@H]4CCC(=O)c5cccc3c54)cc2)n1
vNsp12-nsp8.1-193	Z1720535475	-10.8	0.327	438.49	REAL	O=C(Nc1ccccc(C(=O)N2CC[C@@]3(C2)OCc2ccccc23)c1)c1ccc2[nH]cnc2c1
vNsp12-nsp8.1-194	Z1723432082	-10.8	0.292	491.55	REAL	Cn1c(=O)[nH]c2ncc(-c3cccc(C(=O)N4CCN(C(=O)c5cccc6ccccc56)CC4)c3)cc21
vNsp12-nsp8.1-195	Z1766711899	-10.8	0.327	445.53	REAL	Cc1ccc(-c2cc(C(=O)N3CCCCC[C@H]3c3noc(-c4cnn(C)c4)n3)[nH]n2)cc1C
vNsp12-nsp8.1-196	Z1815745615	-10.8	0.348	425.48	REAL	O=C(N[C@@H]1CCCN(Cc2ccc(F)cc2F)C1=O)N[C@@H]1[C@@H]2CCc3ccccc3[C@H]21
vNsp12-nsp8.1-197	Z1870059965	-10.8	0.348	414.55	REAL	O=C(C1Cc2ccccc2C1)N1C[C@@H]2CCCN(C(=O)C3Cc4ccccc4C3)[C@@H]2C1
vNsp12-nsp8.1-198	Z1940939703	-10.8	0.360	403.44	REAL	CNC(=O)c1cc2cc(NC(=O)N3CC[C@@]4(C3)C(=O)Nc3ccccc34)ccc2[nH]1
vNsp12-nsp8.1-199	Z1979181661	-10.8	0.372	398.37	REAL	CN1C(=O)CCc2cc(NC(=O)c3ccc(-c4noc(C(F)F)n4)cc3)ccc21
vNsp12-nsp8.1-200	Z2010193676	-10.8	0.327	448.50	REAL	Cc1cn(-c2ccc(F)cc2)nc1C(=O)N1C[C@@H](C(=O)N2CCCCC2)Oc2ccccc21

Supplementary Table 52. Virtual screening hits 101 to 200 of the screen against the nsp8 binding site on nsp12 (Screen ID: 31). Compounds were filtered so that hits had MW < 600 dalton, cLogP < 6, number of hydrogen bond acceptors < 11, and no reactive functional groups. The name of each compound consists of the initial letter 'v' for virtual hit, followed by the target protein name and the target site ('nsp8' for nsp8 binding site, 1 for docking scenario 1). The score is the docking score given by QuickVina 2 in kcal/mol. The ligand efficiency (LE) is computed as LE = -score/#NonH, where #NonH is the number of heavy (i.e. non hydrogen) atoms.

Name	Catalog ID	Score	LE	MW	Library	SMILES
vNsp12-as1-1	ZINC000019832272	-10.5	0.292	476.578	ZINC	Cc1ccc(NC(=O)C2=C(C)NC3=C(C(=O)CCC3)[C@@H]2c2ccc3c(c2)c2ccccc2n3C)nc1
vNsp12-as1-2	PV-001864857183	-10.2	0.329	434.417	REAL	O=C([C@@H]1CCCCN1C(=O)c1ccc(=O)[nH]n1)N1CCc2cccc(C(F)(F)F)c2C1
vNsp12-as1-3	Z1014963906	-10.2	0.34	397.437	REAL	Cc1c(C(=O)N2Cc3ccccc3-c3ccccc3C2)cnn1-c1ccc(=O)[nH]n1
vNsp12-as1-4	Z2108604502	-10.1	0.326	420.464	REAL	C[C@@H]1c2cc3c(cc2C(CCCC2)CN1C(=O)c1ccc2oc(=O)[nH]c2c1)OCCO3
vNsp12-as1-5	Z287938074	-10.1	0.281	489.578	REAL	C[C@@H]1c2cc3c(cc2C(CCCC2)CN1C(=O)C1CCN(c2ccc4nnnn4n2)CC1)OCCO3
vNsp12-as1-6	ZINC000079190060	-10.1	0.273	499.561	ZINC	C[C@H]1CCCC(=O)CCC/C=C/c2cc3c(c(O)c2C(=O)O1)[C@H](c1ccc2ncccc2c1)CC(=O)O3
vNsp12-as1-7	ZINC000100366101	-10.1	0.281	468.467	ZINC	O=C1c2ccccc2C(=O)C1c1ccc2cc3ccc(C4C(=O)c5ccccc5C4=O)nc3cc2n1
vNsp12-as1-8	Z1185259574	-10	0.333	402.496	REAL	C[C@H]1Cc2ccccc2N1C(=O)[C@@H]1CCCC[C@@H]1C(=O)Nc1nc2ccccc2[nH]1
vNsp12-as1-9	Z1185517110	-10	0.345	396.45	REAL	C[C@H]1Cc2ccccc2N1C(=O)[C@@H]1CCCC[C@@H]1C(=O)NNC(=O)c1c[nH]nn1
vNsp12-as1-10	Z1383816512	-10	0.294	453.461	REAL	O=C1c2ccccc2C(=O)c2cc(NC(=O)C3CCN(c4ccc5nnnn5n4)CC3)ccc21
vNsp12-as1-11	Z2229022794	-10	0.333	401.421	REAL	O=C(N[C@H](c1ccccc1)c1ccc2c(c1)CCCO2)c1ccc2oc(=O)[nH]c2n1
vNsp12-as1-12	Z295766342	-10	0.357	392.34	REAL	O=C(Nc1nnc(C(F)(F)F)[nH]1)c1ccc2c(=O)n3c(nc2c1)CCCCC3
vNsp12-as1-13	ZINC000001099260	-10	0.278	474.427	ZINC	O=C1NC(=O)c2cc(N3C(=O)c4ec5oc6ccccc6c6ccccc6oc5cc4C3=O)ccc21
vNsp12-as1-14	ZINC000002935991	-10	0.278	480.425	ZINC	O=c1oc(-c2ccccc(F)c2)nc2ccc(-c3ccc4nc(-c5cccc(F)c5)oc(=O)c4c3)cc21
vNsp12-as1-15	ZINC000009614215	-10	0.27	491.546	ZINC	C[C@@]1(c2ccc3ccccc3c2)NC(=O)N(CC(=O)N2c3ccccc3OC[C@H]2c2ccccc2)C1=O
vNsp12-as1-16	ZINC000013770904	-10	0.278	480.479	ZINC	O=C(Nc1ccccc1)[C@H]1[C@H]2C(=O)N(c3ccc4c(c3)OCO4)C(=O)[C@H]2[C@@H]2c3ccccc3C=NN12
vNsp12-as1-17	ZINC000020601960	-10	0.27	490.605	ZINC	CC1=C(C(=O)Nc2ccccn2)[C@@H](c2ccc3c(c2)c2ccccc2n3C)C2=C(CC(C)(C)CC2=O)N1
vNsp12-as1-18	PV-001952050882	-9.9	0.309	433.554	REAL	CC1(C)CCC[C@@H](c2cccc(NC(=O)N[C@@H](Cc3ccccc3)c3n[nH]c(=O)[nH]3)c2)C1
vNsp12-as1-19	Z2176722244	-9.9	0.33	412.532	REAL	CC(C)CC(=O)N[C@@H](Cc1c[nH]cn1)C(=O)NC[C@@]1(O)[C@@H]2[C@H]3C[C@H]4[C@H]5[C@H]3C[C@@H]2[C@H]5[C@H]41
vNsp12-as1-20	Z2228579691	-9.9	0.33	397.433	REAL	O=C(NC[C@H]1CC2c3ccccc3C1c1ccccc12)c1ccc2oc(=O)[nH]c2n1
vNsp12-as1-21	ZINC000000659879	-9.9	0.261	496.565	ZINC	O=C(c1ccccc1)c1ccc2c(c1)NC1=C(C(=O)C[C@H](c3ccccc3)C1)[C@@H]1c3ccccc3C(=O)N21
vNsp12-as1-22	ZINC000001588368	-9.9	0.291	446.517	ZINC	Cc1[nH]c2ccccc2c1-c1cc(-c2cc(-c3c(C)[nH]c4ccccc43)nc(N)n2)nc(N)n1
vNsp12-as1-23	ZINC000002831958	-9.9	0.275	470.531	ZINC	Cc1cc(-c2ccc(/N=C3/c4ccccc4NC3=O)c(C)c2)ccc1/N=C1/c2ccccc2NC1=O
vNsp12-as1-24	ZINC000004552165	-9.9	0.291	442.429	ZINC	O=c1c2ccccc2[nH]c2c1ccc1c2C(=O)c2ccc3c(=O)c4ccccc4[nH]c3c2C1=O
vNsp12-as1-25	ZINC000025783866	-9.9	0.268	490.605	ZINC	CC1=C(C(=O)Nc2ccccn2)[C@@H](c2ccc3c4ccccc4n(C)c3c2)C2=C(CC(C)(C)CC2=O)N1
vNsp12-as1-26	ZINC000027532688	-9.9	0.3	455.479	ZINC	CC1=C(C(=O)Nc2ccccn2)[C@H](c2ccccc2C(F)(F)F)C2=C(CC(C)(C)CC2=O)N1
vNsp12-as1-27	ZINC000038703736	-9.9	0.291	498.95	ZINC	Cc1cc(C)nc(NS(=O)(=O)c2ccc(NC(=O)c3cc(-c4cc(Cl)ccc4O)n[nH]3)cc2)n1
vNsp12-as1-28	ZINC000048523764	-9.9	0.275	464.475	ZINC	O=C1c2ccccc2C(=O)C2=C3C=CC4=CC5=C(C(=O)c6ccccc6C5=O)C5=CC=C(C=C12)[C@@H]3[C@@H]45
vNsp12-as1-29	ZINC000096280916	-9.9	0.275	487.515	ZINC	Cc1ccccc(C(=O)N2CCC(NC(=O)c3nccnc3NC(=O)c3cce4c(c3)OCO4)CC2)c1
vNsp12-as1-30	ZINC000100005067	-9.9	0.291	442.429	ZINC	O=c1c2ccccc2c(=O)c2c1ccc1[nH]c3c(cce4c(=O)c5ccccc5c(=O)c43)[nH]c12
vNsp12-as1-31	ZINC000100504092	-9.9	0.319	404.512	ZINC	O=c1ccc2n1C[C@H]1C[C@H]2CN(Cc2ccc3cce4ccc5ccc2c3c45)C1
vNsp12-as1-32	ZINC000247703671	-9.9	0.275	479.47	ZINC	O=C([C@@H]1[C@H]2C(=O)N(c3ccc(F)cc3)C(=O)[C@H]2[C@@H]2C=Cc3ccccc3N21)n1nnc2ccccc21
vNsp12-as1-33	PV-001796958833	-9.8	0.338	401.351	REAL	Cn1nnc(C(=O)Nc2nc3ccccc3n2Cc2ccccc2)c1
vNsp12-as1-34	PV-001848261411	-9.8	0.327	421.374	REAL	O=C(N[C@@H](c1ccccc(C(F)(F)F)c1)C1COCOC1)c1ccc2oc(=O)[nH]c2n1
vNsp12-as1-35	Z1183485147	-9.8	0.327	426.304	REAL	Cc1cc(NC(=O)[C@@H]2CC(c3cc(F)ccc3F)=NO2)nc2nc(C(F)(F)F)nn12
vNsp12-as1-36	Z1452691933	-9.8	0.297	445.493	REAL	O=C(NC[C@H]1[C@@H]2Cc3ccccc3[C@H]12)NNC(=O)c1ccccc1OCc1ccc(F)cc1
vNsp12-as1-37	Z1663781896	-9.8	0.316	413.444	REAL	Cc1cc(-c2nnc(C3CCN(c4ccc5nnnn5n4)CC3)o2)c2ccccc2n1
vNsp12-as1-38	Z1740627961	-9.8	0.363	362.428	REAL	O=C(c1ccccc2[nH]c(=O)oc12)N1C[C@@H](c2ccccc2)[C@H]2CCCC[C@H]21
vNsp12-as1-39	Z1896776640	-9.8	0.35	389.513	REAL	COCCN(C(=O)NC[C@@H]1CCN(c2ccc(F)cc2)C1)[C@@H]1C[C@@H]2CC[C@@H]1C2
vNsp12-as1-40	Z2193902132	-9.8	0.316	414.468	REAL	O=C(c1ccccc1)N1[C@H](c2nc(-c3ccc4[nH]nnc4c3)no2)C[C@H]2CCCC[C@H]21
vNsp12-as1-41	Z2228011250	-9.8	0.327	425.425	REAL	C[C@@]12CCN(C(=O)c3ccnc(C(=O)N4CC[C@@]5(C)[C@H](C4)C5(F)F)c3)C[C@@H]1C2(F)F
vNsp12-as1-42	Z2691526245	-9.8	0.363	365.388	REAL	C[C@@H]1Oc2c(ccc2C(=O)N2Cc3ccccc3NC(=O)[C@H]2C)NC1=O
vNsp12-as1-43	Z2801388274	-9.8	0.338	390.446	REAL	Nc1nnnn1-c1cccc(C(=O)N2C[C@H](c3ccccc3)[C@H]3COCC[C@H]32)c1
vNsp12-as1-44	Z3059702039	-9.8	0.377	355.437	REAL	CN1C[C@]23CCCC[C@]2(C1)CN(C(=O)c1cccc2c1oc(=O)n2C)C3
vNsp12-as1-45	Z743656142	-9.8	0.35	389.446	REAL	COC(=O)COc1cccc(C(=O)OCC(=O)N[C@@H](C)[C@H]2C[C@@H]3CC[C@@H]2C3)c1
vNsp12-as1-46	Z86765742	-9.8	0.327	424.382	REAL	Cc1cc(NC(=O)[C@H](C)N2C(=O)[C@H]3CCCC[C@@H]3C2=O)nc2nc(C(F)(F)F)nn12
vNsp12-as1-47	ZINC000009389022	-9.8	0.288	448.477	ZINC	C[C@@]1(c2ccc3ccccc3c2)NC(=O)N(Cc2cc(=O)oc3cce4ccccc4c23)C1=O
vNsp12-as1-48	ZINC000014361443	-9.8	0.35	390.408	ZINC	O=C(Nc1nnc(C(F)(F)F)[nH]1)C12C[C@@H]3C[C@H](C1)CC(c1ccccc1)(C3)C2
vNsp12-as1-49	ZINC000015972854	-9.8	0.265	494.525	ZINC	Cc1ccc2c(c1)[C@]1(N[C@H](Cc3c[nH]c4ccccc34)[C@H]3C(=O)N(c4ccc(F)cc4)C(=O)[C@H]31)C(=O)N2
vNsp12-as1-50	ZINC000015990071	-9.8	0.245	527.626	ZINC	Cc1cccc(Nc2nnc(-c3ccc(C(=O)N4C[C@H]5C[C@@H](C4)c4ccccc4)o4C5)cc3)c3ccccc32)c1
vNsp12-as1-51	ZINC000017967458	-9.8	0.272	479.47	ZINC	O=C([C@H]1[C@H]2C(=O)N(c3ccc(F)cc3)C(=O)[C@H]2[C@@H]2C=Cc3cccc3N12)n1nnc2ccccc21
vNsp12-as1-52	ZINC000033939916	-9.8	0.272	491.546	ZINC	Cc1cc(NC(=O)[C@H]2[C@H]3C(=O)N(c4cccnc4)[C@H](C(=O)NC4CCCCC4)[C@@]34C=C[C@]2(C)O4)no1
vNsp12-as1-53	ZINC000035807134	-9.8	0.265	491.589	ZINC	Cc1ccc(C(=O)[C@@H]2[C@@H]3CCCN3[C@]3(c4ccc(C)cc(C)c4NC3=O)[C@@]23c2ccccc2NC3=O)cc1
vNsp12-as1-54	ZINC000100243014	-9.8	0.306	441.48	ZINC	CC(=O)N1CCc2nc3cc([C@H]4CCCCN4Cc4ccc(F)c(F)c4)nn3c(O)c2C1
vNsp12-as1-55	ZINC000100517951	-9.8	0.272	476.531	ZINC	O=C1[C@@H]2[C@H]3C=C[C@@H](C3)[C@@H]2C(=O)N1c1ccc(-c2ccc(N3C(=O)[C@@H]4[C@@H]5C=C[C@@H](C5)[C@@H]4C3=O)cc2)cc1
vNsp12-as1-56	ZINC000223914240	-9.8	0.28	508.665	ZINC	Cc1cccc(C(=O)Nc2nnc(S(=O)(=O)Nc3ccc(C45CC6CC(CC(C6)C4)C5)cc3)s2)c1
vNsp12-as1-57	ZINC000230038145	-9.8	0.265	494.525	ZINC	Cc1ccc2c(c1)[C@]1(N[C@H](Cc3c[nH]c4ccccc34)[C@H]3C(=O)N(c4ccc(F)cc4)C(=O)[C@@H]31)C(=O)N2
vNsp12-as1-58	ZINC000239426032	-9.8	0.258	504.541	ZINC	O=C(c1cccc(N2C(=O)[C@@H]3[C@H]4C=C[C@@H](C4)[C@H]3C2=O)c1)c1cccc(N2C(=O)[C@@H]3[C@H]4C=C[C@@H](C4)[C@@H]3C2=O)c1
vNsp12-as1-59	ZINC000952857405	-9.8	0.265	499.569	ZINC	Cc1ncc(C(=O)N2CC[C@@]34c5ccccc5N(CC(=O)N(C)CCCOc5ccccc5)[C@H]23)C4=O)[nH]1
vNsp12-as1-60	PV-000011187859	-9.7	0.359	370.343	REAL	O=C(N[C@@H]1C[C@H]2CC[C@@H]1N2c1nccnc1F)c1ccc2oc(=O)[nH]c2n1
vNsp12-as1-61	PV-000011609717	-9.7	0.359	371.375	REAL	Cc1noc2ncnc(N3C[C@@H]4CCC[C@]4(NC(=O)c4n[nH]cc4F)C3)c12
vNsp12-as1-62	PV-000340015533	-9.7	0.334	403.481	REAL	C[C@@H]1CCN(C(=O)[C@@H]2C[C@@H]3CCCC[C@@H]32)[C@H](CNC(=O)c2n[nH]c(=O)[nH]c2=O)C1
vNsp12-as1-63	PV-001859060022	-9.7	0.323	419.358	REAL	Cn1c(=O)oc2c(C(=O)N[C@H]3Cc4ccccc4N(C(=O)C(F)(F)F)C3)cccc21
vNsp12-as1-64	PV-001869253053	-9.7	0.346	385.427	REAL	Cn1cnnc1[C@@H]1CCN(C(=O)[C@H]2CCCCN2C(=O)c2ccc(=O)[nH]n2)C1
vNsp12-as1-65	PV-001878640291	-9.7	0.334	394.473	REAL	Cc1cc(C)c2c(c1)CCN(C(=O)[C@@H]1CCCCN1C(=O)c1ccc(=O)[nH]n1)C2
vNsp12-as1-66	PV-001916844879	-9.7	0.334	411.437	REAL	Cc1cc2oc(=O)cc(Cn3cnc4ccc(S(N)(=O)=O)cc4c3=O)c2cc1C
vNsp12-as1-67	PV-002002772225	-9.7	0.303	442.566	REAL	CC(=O)N1CCN(c2nnc(C(C)C)n2CCNC(=O)c2ccn[nH]2)CC12CCCCC2
vNsp12-as1-68	Z1024051824	-9.7	0.262	491.589	REAL	O=C1Nc2ccccc2[C@@H]1C1CCN(C(=O)[C@H]2CC(=O)N(c3ccc4c(c3)Cc3ccccc3-4)C2)CC1
vNsp12-as1-69	Z1070422660	-9.7	0.285	455.517	REAL	Cc1cc2nc(N3CCC(C(=O)c4ccc5c(c4)NC(=O)[C@@H](C)O5)CC3)c3ccccc3n2n1
vNsp12-as1-70	Z1158072308	-9.7	0.285	457.493	REAL	C[C@@]12CCC(=O)N1c1ccccc1C(=O)N2CC(=O)Nc1cc(C2CC2)nn1-c1nccn1
vNsp12-as1-71	Z1325132780	-9.7	0.313	435.384	REAL	Cc1nc(C(=O)N2CC3(CCCC3)c3c(F)ccc32)nn1-c1nnc(C(F)(F)F)[nH]1
vNsp12-as1-72	Z1614059000	-9.7	0.334	390.489	REAL	O=C(c1cnc2[nH]nnc2c1)N1CCN(Cc2ccccc2)C2(CCCCC2)C1
vNsp12-as1-73	Z1685087832	-9.7	0.346	374.359	REAL	Cc1noc2nc(C3CC3)cc(-c3nc(-c4ccc5[nH]c(=O)[nH]c5c4)no3)c12
vNsp12-as1-74	Z1685385235	-9.7	0.334	388.386	REAL	Cc1cnc(-c2noc(-c3cc(-c4cc(C)oc4C)nc4onc(C)c34)n2)nc1
vNsp12-as1-75	Z1689103670	-9.7	0.334	391.361	REAL	Cc1cc(-c2cc(-c3nc(-c4ccc(F)cn4)no3)c3c(C)noc3n2)c(C)o1
vNsp12-as1-76	Z1870846324	-9.7	0.313	435.384	REAL	Cc1nc(C(=O)N2CC3(CCCC3)c3cccc(F)c32)nn1-c1nnc(C(F)(F)F)[nH]1
vNsp12-as1-77	Z2004573921	-9.7	0.346	373.415	REAL	NC(=O)c1cnn2c(C(=O)N3[C@H]4C=C(c5ccccc5)C[C@@H]3CC4)ccnc12
vNsp12-as1-78	Z2007491092	-9.7	0.294	444.498	REAL	Cc1cccc(NC(=O)[C@@H]2CCCN(c3nnc(-c4n[nH]c(=O)c5ccccc45)n3C)C2)n1
vNsp12-as1-79	Z2015849991	-9.7	0.334	396.446	REAL	CC1=C(c2ccco2)CN(C(=O)[C@@H]2CCCCN2C(=O)c2ccc(=O)[nH]n2)CC1
vNsp12-as1-80	Z2027286273	-9.7	0.346	373.415	REAL	O=C(c1cc2ccccc2c2ccnc12)N1CCC[C@H](c2nc(=O)[nH][nH]2)C1
vNsp12-as1-81	Z2090578246	-9.7	0.359	364.404	REAL	O=C(c1ccc2[nH]c(=O)[nH]c2n1)N1C[C@@H](c2ccccc2)[C@@H]2COCC[C@@H]21
vNsp12-as1-82	Z2227159726	-9.7	0.323	399.413	REAL	O=C(Nc1nnc2[nH]cnn12)[C@H]1CC(=O)N(c2ccc3c(c2)Cc2ccccc2-3)C1
vNsp12-as1-83	Z230800324	-9.7	0.323	404.469	REAL	C[C@@H]1c2cc3c(cc2C(CCCC2)CN1C(=O)c1ccc2[nH]nnc2c1)OCCO3
vNsp12-as1-84	Z2635689986	-9.7	0.359	363.416	REAL	CC1(C)CC[C@H]2C[C@@H](NC(=O)c3ccc4oc(=O)[nH]c4n3)c3cccc1c32
vNsp12-as1-85	Z2641552240	-9.7	0.359	365.344	REAL	O=C1C[C@]2(CCN(C(=O)c3ccc4oc(=O)[nH]c4n3)C2)Oc2ccccc21
vNsp12-as1-86	Z2830784081	-9.7	0.262	495.534	REAL	O=C1c2ccccc2C(=O)N1[C@H]1CCC[C@@]2(C1)Nc1ccccc1C(=O)N2c1ccc2e(c1)OCCO2
vNsp12-as1-87	Z3094948425	-9.7	0.373	354.369	REAL	Cn1c(C2=NNC(=O)C2)nnc1N1CCC[C@H]1c1ccc2c(c1)OCO2
vNsp12-as1-88	Z3201320175	-9.7	0.346	392.38	REAL	C[C@H](NC(=O)N1[C@H]2C=C(c3ccccc3)C[C@@H]1CC2)c1nc(C(F)(F)F)no1
vNsp12-as1-89	Z728620964	-9.7	0.323	398.381	REAL	O=C(Nc1nc2ccccc2n1-c1ccccc1)c1cnc2[nH]c(=O)[nH]c(=O)c2c1
vNsp12-as1-90	Z806435698	-9.7	0.269	481.554	REAL	C[C@@]1(c2ccc3ccccc3c2)NC(=O)N(CC(=O)N2CCC(c3c[nH]c4ncccc34)CC2)C1=O
vNsp12-as1-91	Z809882774	-9.7	0.313	420.464	REAL	C[C@@H]1c2cc3c(cc2C(CCCC2)CN1C(=O)c1ccc2[nH]c(=O)oc2c1)OCCO3
vNsp12-as1-92	Z996704074	-9.7	0.269	486.502	REAL	O=C(Nc1cccc(F)c1)C1CCN(C(=O)c2ccc3c(=O)n(-c4ccccc4)c(=O)[nH]c3c2)CC1
vNsp12-as1-93	ZINC000008614742	-9.7	0.277	476.515	ZINC	Cc1nc2c3ccccc3nc(NNC(=O)CCC(=O)N3CCN(c4ccccc4F)CC3)n2n1
vNsp12-as1-94	ZINC000019795177	-9.7	0.285	437.453	ZINC	O=C1c2ccccc2C2=C1C1(c3ccccc4ccccc34)C1=O)C1=C(N2)c2ccccc2C1=O
vNsp12-as1-95	ZINC000059785693	-9.7	0.243	527.622	ZINC	CCc1ccc2c(c1)[C@]1(C(=O)N2)N2CCC[C@@H]2[C@@H](C(=O)c2ccc3ccccc3c2)[C@@]12c1ccccc1NC2=O
vNsp12-as1-96	ZINC000059932652	-9.7	0.243	527.622	ZINC	Cc1ccc2c(c1C)NC(=O)[C@@]21N2CCC[C@@H]2[C@@H](C(=O)c2ccc3ccccc3c2)[C@@]12c1ccccc1NC2=O
vNsp12-as1-97	ZINC000096335973	-9.7	0.303	432.387	ZINC	Cc1cc(NC(=O)[C@H]2Oc3c(c(=O)oc4ccccc34)[C@H]2c2ccc3c(c2)OCO3)no1
vNsp12-as1-98	ZINC000102658513	-9.7	0.285	452.56	ZINC	C[C@@]12C[C@H](CC(C)(C)C1)N(C(=O)c1cc(-c3cccc4ccenc43)cc(-n3cnnn3)c1)C2
vNsp12-as1-99	ZINC000103193285	-9.7	0.269	480.562	ZINC	CC1=CC[C@H]2C(=O)N(c3ccc(-c4ccc(N5C(=O)[C@H]6CC=C(C)C[C@@H]6C5=O)cc4)cc3)C(=O)[C@@H]2C1
vNsp12-as1-100	ZINC000239426033	-9.7	0.255	504.541	ZINC	O=C(c1cccc(N2C(=O)[C@@H]3[C@H]4C=C[C@@H](C4)[C@H]3C2=O)c1)c1cccc(N2C(=O)[C@@H]3[C@H]4C=C[C@@H](C4)[C@@H]3C2=O)c1

Supplementary Table 53. Top 100 virtual hits of the screen against the active site of nsp12 (Screen ID: 30). The name of each compound consists of the initial letter 'v' for virtual hit, followed by the target protein name and the target site ('as' for active site, 1 for docking scenario 1). The score is the docking score given by QuickVina 2 in kcal/mol. The ligand efficiency (LE) is computed as LE = -score/#NonH, where #NonH is the number of heavy (i.e. non hydrogen) atoms.

Name	Catalog ID	Score	LE	MW	Library	SMILES
vNsp12-as1-101	ZINC000240824835	-9.7	0.249	516.56	ZINC	O=C1[C@@H]2[C@H]3C=C[C@@H](C3)[C@H]2C(=O)N1c1ccc2nc(-c3ccc(N4C(=O)[C@@H]5[C@H]6C=C[C@@H](C6)[C@@H]5C4=O)cc3)[nH]c2c1
vNsp12-as1-102	ZINC000253414129	-9.7	0.262	494.45	ZINC	O=C1c2ccc3c(c2O/C1=C\c1ccc2c(c1)OCCO2)[C@H](c1coc2ccccc2c1=O)CC(=O)O3
vNsp12-as1-103	ZINC000263585879	-9.7	0.303	429.48	ZINC	CC(=O)N1CC2=C(C1=O)[C@H](c1ccc3c(c1)OCO3)c1cn(C(C)C)c3cccc(c13)N2
vNsp12-as1-104	ZINC000409334997	-9.7	0.269	466.50	ZINC	O=C(Nc1ccc2ccccc2c1)Nc1ccc2nc3c4ccnc4c4nccc4c3nc2c1
vNsp12-as1-105	ZINC000952856461	-9.7	0.277	475.55	ZINC	COc1ccc2cc1Oc1cccc(c1)CO[C@@H]1CCN(c3cc(N)ncn3)C[C@@H]1NC(=O)CC2
vNsp12-as1-106	ZINC000952863770	-9.7	0.243	549.67	ZINC	Cc1ccc2cc1Oc1cccc(c1)CO[C@H]1CN(C(=O)CN3CCCN(C)CC3)C[C@@H]1NC(=O)CN(C)C2=O
vNsp12-as1-107	ZINC000952867975	-9.7	0.262	499.57	ZINC	Cn1cnc(C(=O)N2CC[C@@]34c5ccccc5N(CC(=O)N(C)CCCOc5ccccc5)C[C@H]23)C4=O)c1
vNsp12-as1-108	PV-000383253954	-9.6	0.310	423.47	REAL	O=C(N[C@]12CCC[C@H]1CN(C(=O)c1cccc3[nH]c(=O)oc13)C2)[C@@H]1C[C@@H]2O[C@H]1[C@H]1C[C@@H]21
vNsp12-as1-109	PV-000558363837	-9.6	0.331	398.42	REAL	C[C@@]1(NC(=O)c2ccc3oc(=O)[nH]c3n2)CCN(C(=O)[C@@H]2C[C@@H]3O[C@H]2[C@H]2C[C@@H]32)C1
vNsp12-as1-110	PV-001794524029	-9.6	0.343	383.40	REAL	Cc1cc(NC(=O)CN(C)C(=O)[C@H]2c3ccccc3C(=O)OC23CCC3)no1
vNsp12-as1-111	PV-001808153294	-9.6	0.331	412.80	REAL	O=C(Cc1cccc(F)c1)c1cc(Cl)cnc1NC(=O)c1cccc2c1OCO2
vNsp12-as1-112	PV-001824854882	-9.6	0.356	366.42	REAL	Cc1cc2c(o1)CC(C)(C)C[C@@H]2NC(=O)c1cccc(-n2nnnc2N)c1
vNsp12-as1-113	PV-001838716679	-9.6	0.356	377.30	REAL	O=C(NNc1ncc(F)cn1)c1cc(-c2cccc(C(F)(F)F)c2)ccn1
vNsp12-as1-114	PV-001841565214	-9.6	0.331	407.35	REAL	C[C@H]1C=C[C@H]2C(=O)N(CC(F)(F)F)C(=O)[C@H]2[C@H]1C(=O)Nc1nc2cnccc2[nH]1
vNsp12-as1-115	PV-001842275288	-9.6	0.343	399.78	REAL	O=C(N[C@@H](c1ccc(Cl)c(F)c1)c1nnn[nH]1)c1cccc(-n2cncn2)n1
vNsp12-as1-116	PV-001844691233	-9.6	0.331	402.38	REAL	O=C(c1ccc(-c2nnn[nH]2)cn1)N1CCCC[C@H]1c1cccc(C(F)(F)F)c1
vNsp12-as1-117	PV-001856487959	-9.6	0.320	411.37	REAL	Cc1cc(CC(=O)NNC(=O)c2cc(F)cc3c(=O)c4cc(F)ccc4[nH]c23)[nH]n1
vNsp12-as1-118	PV-001858405996	-9.6	0.343	382.40	REAL	CC1(C)C[C@@H](NC(=O)c2cccc(-n3nnnc3N)c2)c2cc(F)ccc2O1
vNsp12-as1-119	PV-001859361323	-9.6	0.320	426.39	REAL	O=C(c1ccc2oc(=O)[nH]c2n1)N1CCCC[C@@H]1[C@H]1CCCN(C(=O)C(F)(F)F)C1
vNsp12-as1-120	PV-001866261699	-9.6	0.356	369.40	REAL	O=C(N[C@@H](c1ccc(F)cc1)C1CCCC1)c1ccc2oc(=O)[nH]c2n1
vNsp12-as1-121	PV-001868517623	-9.6	0.331	402.40	REAL	O=C([C@@H]1CCCCN1C(=O)c1ccc(=O)[nH]n1)N1CCc2cc(F)c(F)cc2C1
vNsp12-as1-122	PV-001961261613	-9.6	0.343	393.41	REAL	O=C(NNc1ccnn1)N[C@@H](c1cccc(C(F)(F)F)c1)C1CCCCC1
vNsp12-as1-123	PV-002002944746	-9.6	0.282	461.57	REAL	CC(=O)Nc1cccc(Cn2c(C(=O)Nc3cccn3)nnc2N2C[C@@H](C)CC(C)(C)C2)c1
vNsp12-as1-124	PV-002015220305	-9.6	0.291	462.45	REAL	C[C@@H]1CN(c2nnc(C(=O)Nc3cccn3)n2Cc2ccc(F)cc2C(F)(F)F)C[C@H]1C
vNsp12-as1-125	Z1229878139	-9.6	0.320	408.50	REAL	COC(=O)Cc1nnc(NC(=O)C23C[C@@H]4C[C@@H](C2)CC(c2cccc(C)cc2)(C4)C3)[nH]1
vNsp12-as1-126	Z1251080561	-9.6	0.310	419.42	REAL	Cc1cc(C(=O)N2CC=C(c3c[nH]c4cc(F)ccc34)CC2)nc2nc(O)[nH]c(=O)c12
vNsp12-as1-127	Z1252294667	-9.6	0.331	390.40	REAL	O=C(Nc1nc2ccccc2n1C1CCCC1)c1cnc2[nH]c(=O)[nH]c(=O)c2c1
vNsp12-as1-128	Z1284917076	-9.6	0.331	419.50	REAL	Cc1cc(NS(=O)(=O)c2cccc(C(=O)N3CCOC4(CCCCC4)C3)c2)no1
vNsp12-as1-129	Z1314813159	-9.6	0.310	421.43	REAL	Cc1cc(C(=O)N2CCC(c3c[nH]c4cc(F)ccc34)CC2)nc2nc(O)[nH]c(=O)c12
vNsp12-as1-130	Z1325425603	-9.6	0.291	444.50	REAL	O=C(c1cnn2cccnc12)N1CCN(C(=O)c2cnn3ccnc23)C2(CCCCC2)C1
vNsp12-as1-131	Z1521768115	-9.6	0.369	354.41	REAL	Cc1cc2c(o1)CC(C)(C)C[C@@H]2NC(=O)c1cccc2c1oc(=O)n2C
vNsp12-as1-132	Z1663629127	-9.6	0.310	415.45	REAL	COc1cc2c(cc1OC)[C@@H](c1cccc1)N(C(=O)c1ccc3[nH]nnc3n1)CC2
vNsp12-as1-133	Z1733269868	-9.6	0.320	430.48	REAL	O=C([C@@H]1CCCCN1C(=O)c1ccc(=O)[nH]n1)N1CCS(=O)(=O)c2ccccc2C1
vNsp12-as1-134	Z1832442925	-9.6	0.343	372.43	REAL	O=C1C[C@@H](C(=O)Nc2nc3ccccc3nc2N2CCCC2)c2ccccc21
vNsp12-as1-135	Z1902112177	-9.6	0.331	397.52	REAL	CC(C)(C)OC(=O)Nc1ccc(CNC[C@]2(O)[C@H]3[C@H]4C[C@H]5[C@H]6[C@H]4C[C@H]3[C@@H]6[C@H]52)cn1
vNsp12-as1-136	Z1902956226	-9.6	0.310	413.41	REAL	Cc1cccc(-c2nnc(-c3ccc(C(=O)Nc4ne5ccc(F)cc5[nH]4)cc3)o2)c1
vNsp12-as1-137	Z2001434317	-9.6	0.356	360.41	REAL	Cn1c(=O)oc2c(C(=O)N3[C@H]4C=C(c5ccccc5)C[C@@H]3CC4)ccc21
vNsp12-as1-138	Z2002894507	-9.6	0.291	446.50	REAL	C[C@@H]1Oc2ccc(C(=O)C3CCN(C(=O)[C@]45[C@@H]6C(=O)[C@H]7[C@H]8C[C@H]([C@H]74)[C@H]5[C@@H]86)CC3)cc2NC1=O
vNsp12-as1-139	Z2014978883	-9.6	0.331	400.41	REAL	O=C([C@@H]1CCCCN1C(=O)c1ccc(=O)[nH]n1)N1CCOc2ccccc2C1
vNsp12-as1-140	Z2068418498	-9.6	0.320	405.46	REAL	O=C(c1ccc(=O)[nH]n1)N1CCCC[C@H]1c1nc([C@@H]2CCCc3ccccc32)no1
vNsp12-as1-141	Z212459564	-9.6	0.274	497.50	REAL	O=C(Nc1nc2c(ccc3ccccc32)s1)C1CCN(c2ccc3nnc(C(F)(F)F)n3n2)CC1
vNsp12-as1-142	Z2158676837	-9.6	0.320	414.30	REAL	O=c1[nH]c2cc(-c3nc(-c4ccc(C(F)(F)F)ccc4-n4cncn4)no3)ccc2o1
vNsp12-as1-143	Z2160285927	-9.6	0.369	346.30	REAL	O=c1cc(-c2noc(-c3ccc4oc(=O)[nH]c4c3)n2)c2ccccc2[nH]1
vNsp12-as1-144	Z2193901792	-9.6	0.343	370.33	REAL	O=c1nc2c(-c3nc(-c4ccc5[nH]nnc5c4)no3)c[nH]n2c2ccccc12
vNsp12-as1-145	Z2193903049	-9.6	0.356	361.36	REAL	Cc1noc2nc(C(C)C)cc(-c3nc(-c4ccc5[nH]nnc5c4)no3)c12
vNsp12-as1-146	Z2204154118	-9.6	0.310	423.40	REAL	Cc1cc(C(=O)N2CCC(c3noc4cc(F)ccc34)CC2)nc2nc(O)[nH]c(=O)c12
vNsp12-as1-147	Z2204271597	-9.6	0.310	421.50	REAL	O=C([C@@H]1CCCCN1C(=O)c1ccc(=O)[nH]n1)N1CCCN2c3ccccc3C[C@H]2C1
vNsp12-as1-148	Z2633866149	-9.6	0.331	392.46	REAL	O=C(c1ccc2oc(=O)[nH]c2n1)N1CC[C@@H]2[C@@H](CCCN2Cc2ccccc2)C1
vNsp12-as1-149	Z2633948756	-9.6	0.356	367.38	REAL	CC1(C)C[C@@H](NC(=O)c2cccc(-n3cncn3)n2)c2ccc(F)cc2O1
vNsp12-as1-150	Z2638349066	-9.6	0.384	345.40	REAL	C[C@H]1CC[C@@H](O)[C@@H]([C@@H]2CCCN2C(=O)c2ccc3oc(=O)[nH]c3n2)C1
vNsp12-as1-151	Z2638588641	-9.6	0.369	347.37	REAL	O=C(c1ccc2oc(=O)[nH]c2n1)N1[C@@H]2C=C(c3ccccc3)C[C@@H]1CC2
vNsp12-as1-152	Z2639145402	-9.6	0.356	365.39	REAL	O=C(c1ccc2oc(=O)[nH]c2n1)N1C[C@@H](c2ccccc2)[C@@H]2COCC[C@@H]21
vNsp12-as1-153	Z2642266661	-9.6	0.356	367.38	REAL	CC1(C)C[C@@H](NC(=O)c2cccc(-n3cncn3)n2)c2cc(F)ccc2O1
vNsp12-as1-154	Z2825218363	-9.6	0.343	387.43	REAL	O=C(c1nnn[C@H]2CCNC2)c1C(F)FN1CC2(CCCC2)c2ccccc21
vNsp12-as1-155	Z2854649114	-9.6	0.384	380.23	REAL	C[C@H]1c2cc(Cl)cc(Cl)c2CCN1C(=O)NNC(=O)c1cccnn1
vNsp12-as1-156	Z2879112092	-9.6	0.369	348.36	REAL	Cc1ccc(-c2noc([C@H]3c4ccccc4C(=O)OC34CCC4)n2)nn1
vNsp12-as1-157	Z2892550859	-9.6	0.343	374.40	REAL	Cc1cnc2c(C(=O)N3Cc4ccccc4C[C@H]3c3nnc(C)o3)cnn2c1
vNsp12-as1-158	Z2902586549	-9.6	0.369	348.33	REAL	Cc1cc(C)n2ncc(-c3noc(-c4ccc5[nH]c(=O)[nH]c5n4)n3)c2n1
vNsp12-as1-159	Z296906178	-9.6	0.356	365.39	REAL	CC(=O)N1CCc2ccccc2[C@H]1CC(=O)Nc1nnc(-c2ccco2)[nH]1
vNsp12-as1-160	Z3059715268	-9.6	0.356	395.50	REAL	Cc1c(F)cc(S(N)(=O)=O)cc1C(=O)N1C[C@@]23CCCC[C@]2(CN(C)C3)C1
vNsp12-as1-161	Z3171449662	-9.6	0.343	394.43	REAL	C[C@H]1CCC(F)(F)CN1c1nnc(-c2ccc(=O)[nH]n2)n1C[C@H]1CCCCO1
vNsp12-as1-162	Z3197763782	-9.6	0.331	398.47	REAL	Cc1cc(Cn2c([C@@H]3CC=NO3)nnc2N2C[C@]34CCCC[C@@]3(COC4)C2)no1
vNsp12-as1-163	Z352456216	-9.6	0.331	406.32	REAL	Cc1cc(-c2cc(C(=O)Nc3nnc(C(F)(F)F)[nH]3)c3c(C)noc3n2)c(C)o1
vNsp12-as1-164	Z510365222	-9.6	0.267	482.50	REAL	Cc1ccc2c(c1)C(=O)N([C@@H](C)C(=O)Nc1ccc(C(=O)N3CC(=O)Nc4ccccc43)cc1)C2=O
vNsp12-as1-165	ZINC000009345276	-9.6	0.274	468.49	ZINC	COC(=O)c1ccc([C@H]2Oc3ccc(C)cc3C3=C2[C@@H](c2ccccc2F)N2N=CNC2=N3)cc1
vNsp12-as1-166	ZINC000009487803	-9.6	0.274	466.49	ZINC	Cc1cc(N2C(=O)c3oc4c5ccccc5ccc4c(=O)c3[C@@H]2c2cccc(OC(C)C)c2)no1
vNsp12-as1-167	ZINC000011663444	-9.6	0.356	362.48	ZINC	Cc1c[nH]c(C(=O)N2CCc3c4ccccc4[nH]c3[C@H]2C2CCCC2)n1
vNsp12-as1-168	ZINC000014249193	-9.6	0.274	466.50	ZINC	O=C(c1ccc2c(c1)[nH]c(=O)n(-c1ccccc1)c2=O)N1CCC(c2nc3ccccc3o2)CC1
vNsp12-as1-169	ZINC000015306585	-9.6	0.259	487.56	ZINC	C[C@@H]1N[C@@]2(c3ccccc3N(Cc3ccccc3)C2=O)[C@@H]2C(=O)N(c3cccc4ccccc43)C(=O)[C@H]21
vNsp12-as1-170	ZINC000015728014	-9.6	0.282	490.55	ZINC	O=C([C@H]1CCCN(c2nnc(-n3cccc3)s2)C1)N1CCN(c2cccc(C(F)(F)F)c2)CC1
vNsp12-as1-171	ZINC000016919178	-9.6	0.282	448.52	ZINC	O=C1c2ccccc2C(=O)[C@H]2CC3=C(CC4=C(C3)C[C@@H]3C(=O)c5ccccc5C(=O)[C@@H]3C4)C[C@@H]12
vNsp12-as1-172	ZINC000018067143	-9.6	0.253	501.58	ZINC	Cc1ccc(NC(=O)c2ccccc2N/C=C2/c3ccccc3C(=O)N(c3ccc(C)c(C)c3)C2=O)cc1
vNsp12-as1-173	ZINC000029747459	-9.6	0.234	545.64	ZINC	O=C(NCCN1CCN(C(=O)C2c3ccccc3Oc3ccccc32)CC1)C1c2ccccc2Oc2ccccc21
vNsp12-as1-174	ZINC000049027007	-9.6	0.310	417.46	ZINC	Cc1cc(NC(=O)C2CCN(C(=O)C3c4ccccc4Oc4ccccc43)CC2)no1
vNsp12-as1-175	ZINC000059796310	-9.6	0.246	513.60	ZINC	Cc1ccc2c1NC(=O)[C@@]21N2CCC[C@@H]2[C@@H](C(=O)c2ccc3ccccc3c2)[C@@]12c1ccccc1NC2=O
vNsp12-as1-176	ZINC000072327270	-9.6	0.291	444.53	ZINC	O=C(c1noc2c1CCCC2)N1CCC2(C[C@]3(CO2)Nc2ccccc2-n2ccc23)CC1
vNsp12-as1-177	ZINC000079188706	-9.6	0.267	492.52	ZINC	C[C@H]1CCCC(=O)CCC/C=C/c2cc3c(c(O)c2C(=O)O1)[C@H](c1ccc2c(c1)OCO2)CC(=O)O3
vNsp12-as1-178	ZINC000085392555	-9.6	0.246	520.61	ZINC	O=C([C@H]1CC(=O)N(c2ccc(F)cc2)C1)N1CCC(c2c[nH]c3ccccc32)(c2c[nH]c3ccccc32)CC1
vNsp12-as1-179	ZINC000085878560	-9.6	0.274	465.46	ZINC	COc1ccc(-c2coc3c(c(O)cc4c3[C@H](c3cccc5ccccc53)CC(=O)O4)c2=O)cc1
vNsp12-as1-180	ZINC000101064562	-9.6	0.240	597.42	ZINC	O=C(c1ccccc1)C1=C[C@@H]2[C@H]3C(=O)N(c4ccc5c(c4)OCO5)C(=O)[C@@H]3[C@H](C(=O)c3ccc(Br)cc3)N2C=C1
vNsp12-as1-181	ZINC000101835937	-9.6	0.291	435.53	ZINC	Cc1ccc(C2=C[C@H](c3ccc(C)cc3)n3nc(NC(=O)c4cccc(C)c4)nc3N2)cc1
vNsp12-as1-182	ZINC000102553907	-9.6	0.267	480.56	ZINC	CC1=CC[C@@H]2C(=O)N(c3ccc(-c4ccc(N5C(=O)[C@@H]6CC=C(C)C[C@@H]6C5=O)cc4)cc3)C(=O)[C@@H]2C1
vNsp12-as1-183	ZINC000222273484	-9.6	0.274	465.59	ZINC	O=C1c2ccccc2C(=O)c2cc3c(cc21)N[C@@H]1CC[C@@H]2[C@@H]4CCCC[C@@H]4C(=O)[C@@H]4CC[C@@H]3[C@@H]1[C@@H]42
vNsp12-as1-184	ZINC000226074035	-9.6	0.300	426.56	ZINC	C[C@@H]1CC(C)(C)N(C)c2ccc([C@@H]3C4=C(CCCC4=O)Nc4nc5ccccc5n43)cc21
vNsp12-as1-185	ZINC000229895971	-9.6	0.267	480.48	ZINC	O=C(Nc1ccccc1)[C@@H]1[C@@H]2C(=O)N(c3ccc4c(c3)OCO4)C(=O)[C@@H]2[C@@H]2c3ccccc3C=NN21
vNsp12-as1-186	ZINC000229930169	-9.6	0.223	589.05	ZINC	CC1=C[C@@H]2N(c3ccccc31)[C@H](C(=O)c1ccc(Cl)cc1)[C@@H](C(=O)c1ccc3c(c1)OCO3)[C@@]21C(=O)Nc2ccccc21
vNsp12-as1-187	ZINC000229940133	-9.6	0.234	563.03	ZINC	CC1=C[C@@H]2N(c3ccccc31)[C@H](C(=O)c1ccc(Cl)cc1)[C@@H](C(=O)c1ccc(F)cc1)[C@@]21C(=O)Nc2ccccc21
vNsp12-as1-188	ZINC000261361844	-9.6	0.300	449.49	ZINC	CSc1nc(O)c2[n+](n1)[C@@H](c1ccc(-c3ccc(F)cc3)o1)N(C(C)=O)c1ccccc1-2
vNsp12-as1-189	ZINC000952865435	-9.6	0.259	500.56	ZINC	CC(=O)NCC(=O)N1CC[C@]23c4ccccc4N(Cc4cn(nn4)CCCOc4ccccc4)[C@H]12)C3=O
vNsp12-as1-190	PV-000346470495	-9.5	0.306	424.46	REAL	O=C(c1ccc2oc(=O)[nH]c2n1)N1CC[C@@H]2CN(C(=O)[C@@H]3C[C@@H]4O[C@H]3[C@H]3C[C@@H]43)C[C@@H]2C1
vNsp12-as1-191	PV-001793215016	-9.5	0.306	432.41	REAL	Cc1cccc(C(=O)N2CCC[C@@H]2C(=O)Nc2cc(C)n3nc(C(F)(F)F)nc3n2)c1
vNsp12-as1-192	PV-001806015390	-9.5	0.288	447.43	REAL	Cc1c(C(=O)Nc2ncccc2C(=O)c2ccc(F)cc2)cnc2c1c(=O)n(C)c(=O)n2C
vNsp12-as1-193	PV-001833827111	-9.5	0.297	457.55	REAL	Cc1cc(S(N)(=O)=O)cc(C(=O)N2CCCC[C@@H]2C(=O)Nc2ccc3c(c2)CCO3)c1C
vNsp12-as1-194	PV-001870537223	-9.5	0.306	418.50	REAL	CCc1ccc2ccccc2c1CNC(=O)[C@@H]1CCCCN1C(=O)c1ccc(=O)[nH]n1
vNsp12-as1-195	PV-001947181995	-9.5	0.306	430.39	REAL	O=C(Nc1ccccc2c(=O)[nH]ccc12)N1c2ccccc2C[C@H]1CNC(=O)C(F)(F)F
vNsp12-as1-196	PV-001948334219	-9.5	0.306	432.40	REAL	O=C1NCCc2c(NC(=O)N3c4ccccc4C[C@H]3CNC(=O)C(F)(F)F)cccc21
vNsp12-as1-197	PV-001949221877	-9.5	0.306	430.39	REAL	O=C(Nc1ccc2c(=O)[nH]ccc2c1)N1c2ccccc2C[C@H]1CNC(=O)C(F)(F)F
vNsp12-as1-198	Z1102449576	-9.5	0.306	411.42	REAL	Cc1c(C(=O)Nc2nc3ccccc3n2-c2ccccc2)cnn1-c1ccc(=O)[nH]n1
vNsp12-as1-199	Z119683478	-9.5	0.297	436.46	REAL	C[C@]1(C(=O)N2C[C@H](C(=O)N3CCOCC3)Oc3ccccc32)Cc2ccccc2C(=O)O1
vNsp12-as1-200	Z1273949691	-9.5	0.306	421.47	REAL	Cc1cc2c(cc1C)O[C@H](C(=O)N1CCC[C@@H](c3nc(-c4cccc(F)c4)no3)C1)C2

Supplementary Table 54. Virtual screening hits 101 to 200 of the screen against the active site of nsp12 (Screen ID: 30). Compounds were filtered so that hits had MW < 600 dalton, cLogP < 6, number of hydrogen bond acceptors < 11, and no reactive functional groups. The name of each compound consists of the initial letter 'v' for virtual hit, followed by the target protein name and the target site ('as' for active site, 1 for docking scenario 1). The score is the docking score given by QuickVina 2 in kcal/mol. The ligand efficiency (LE) is computed as LE = -score/#NonH, where #NonH is the number of heavy (i.e. non hydrogen) atoms.

Name	Catalog ID	Score	LE	MW	Library	SMILES
vNsp12-rna1-1	Z1948615421	-10.3	0.381	361.444	REAL	O=C(Cc1c[nH]c2ccccc12)NNC(=O)[C@@H]1[C@@H]2[C@H]3C[C@@H]4[C@@H]5[C@H]3C[C@H]2[C@@H]5[C@H]41
vNsp12-rna1-2	Z1552768547	-10.2	0.309	440.458	REAL	O=C(Nc1ccc2[nH]nc(NC(=O)[C@@H]3Cc4ccccc4O3)c2c1)[C@@H]1Cc2ccccc2O1
vNsp12-rna1-3	Z1964946249	-10.2	0.309	436.47	REAL	O=C(Nc1ncc(-c2ccccc2)cn1)c1cccc(NC(=O)[C@H]2Cc3ccccc3O2)c1
vNsp12-rna1-4	Z2107144412	-10.2	0.34	439.398	REAL	O=C(Nc1nc2cc3c(cc2s1)OC(F)(F)O3)NC1CCC2(CC1)NC(=O)NC2=O
vNsp12-rna1-5	Z2902833602	-10.2	0.283	474.519	REAL	O=C1[C@@H]2[C@@H]3C=C[C@H]([C@@H]2C(=O)N1Cc1ccccc1)[C@@H]1C(c2nc(-c4nccc5ccccc45)no2)[C@H]31
vNsp12-rna1-6	Z771659438	-10.2	0.309	435.438	REAL	O=C(NNC(=O)c1ccc2ccccc2c1)c1cccc(N2C(=O)c3ccccc3C2=O)c1
vNsp12-rna1-7	Z808823656	-10.2	0.3	451.485	REAL	Cc1ccc(-c2nnc(NC(=O)Cc3ccc(NC(=O)c4cc5ccccc5o4)cc3)[nH]2)cc1
vNsp12-rna1-8	Z1155349940	-10.1	0.306	454.509	REAL	Cc1ccc(Cc2nnc(NC(=O)c3cccc(N4C(=O)c5ccccc5C4=O)c3)s2)cc1
vNsp12-rna1-9	Z1846564942	-10.1	0.316	429.479	REAL	C[C@@]1(C(=O)Nc2nnc(-c3cc4ccccc4o3)[nH]2)CCCN(C(=O)c2ccccc2)C1
vNsp12-rna1-10	Z1951855995	-10.1	0.374	361.444	REAL	O=C(Cn1ccc2ccccc21)NNC(=O)[C@@H]1[C@@H]2[C@@H]3C[C@H]4[C@H]5[C@@H]3C[C@H]2[C@H]5[C@H]41
vNsp12-rna1-11	Z1983283234	-10.1	0.316	446.428	REAL	O=C1N[C@@]2(C[C@@H]3C[C@H]2[C@@H]2CCC[C@@H]32)C(=O)N1Cc1nc(-c2ccc(C(F)(F)F)cc2)no1
vNsp12-rna1-12	Z1983290694	-10.1	0.348	392.458	REAL	O=C1N[C@]2(C[C@H]3C[C@H]2[C@H]2CCC[C@H]32)C(=O)N1Cc1nc(Cc2ccccc2)no1
vNsp12-rna1-13	Z424333662	-10.1	0.326	413.432	REAL	Cc1c(C(=O)Nc2cccc([C@@]3(C)NC(=O)NC3=O)c2)oc2c1ccc1ccccc12
vNsp12-rna1-14	Z606310524	-10.1	0.297	452.469	REAL	O=C(NNC(=O)c1ccc2ccccc2n1)c1cccc(NC(=O)[C@H]2Cc3ccccc3O2)c1
vNsp12-rna1-15	ZINC000146057035	-10.1	0.24	566.639	ZINC	CCc1cc(O)c(F)cc1-c1ccc2c(c1)[nH]nc2-c1nc2c([nH]1)CCN(C(=O)c1cnc(N3CCCCC3)cn1)C2
vNsp12-rna1-16	PV-001940740368	-10	0.313	456.609	REAL	C[C@H](CNC(=O)Nc1ccc(S(=O)(=O)N[C@H](C)[C@@H]2C[C@H]3CC[C@H]2C3)cc1)c1ccncc1
vNsp12-rna1-17	Z1092442234	-10	0.286	468.468	REAL	Cc1cc(=O)oc2cc(OCc3ccc(C(=O)NNc4nc(-c5ccccc5)no4)cc3)ccc12
vNsp12-rna1-18	Z1147973033	-10	0.303	458.472	REAL	O=C(Nc1nnc(Cc2cccc(F)c2)s1)c1cccc(N2C(=O)c3ccccc3C2=O)c1
vNsp12-rna1-19	Z1155287541	-10	0.303	458.472	REAL	O=C(Nc1nnc(Cc2ccccc2F)s1)c1cccc(N2C(=O)c3ccccc3C2=O)c1
vNsp12-rna1-20	Z1846550710	-10	0.313	421.415	REAL	O=C(Nc1nnc(-c2cc3ccccc3o2)[nH]1)c1ccc2[nH]c3ccccc3c(=O)c2c1
vNsp12-rna1-21	Z2003415070	-10	0.313	422.526	REAL	O=C1[C@@H]2[C@@H]3C[C@@H]4[C@H]2[C@]2(C(=O)N5CCN(C6c7ccccc7-c7ccccc76)CC5)[C@H]1[C@H]3[C@H]42
vNsp12-rna1-22	Z2168988264	-10	0.294	449.509	REAL	O=C(Nc1ccc2ccccc2n1)C1[C@H]2[C@@H]3C=C[C@@H]([C@H]4C(=O)N(Cc5ccccc5)C(=O)[C@H]34)[C@H]12
vNsp12-rna1-23	Z2233592032	-10	0.303	443.441	REAL	Cc1cc(-c2noc(CCC(=O)Nc3nc(-c4ccc5ccccc5n4)n[nH]3)n2)ccc1F
vNsp12-rna1-24	Z2902416169	-10	0.278	477.523	REAL	Cc1c(NC(=O)Cc2noc(-c3ccc4c(c3)-c3ccccc3C4)n2)c(=O)n(-c2ccccc2)n1C
vNsp12-rna1-25	Z2902490588	-10	0.278	491.468	REAL	O=C1[C@@H]2[C@@H]3C=C[C@H]([C@H]2C(=O)N1Cc1ccccc1)[C@H]1C(c2nc(-c4cccc(C(F)(F)F)c4)no2)[C@@H]31
vNsp12-rna1-26	Z2902892451	-10	0.27	498.56	REAL	CC(=O)N1Cc2ccccc2C[C@@H]1c1nc(-c2ccc(N3CCN(c4ccc(F)cc4)CC3)nc2)no1
vNsp12-rna1-27	Z899977586	-10	0.278	498.46	REAL	O=C(NCc1cccc(C(F)(F)F)c1)NNC(=O)c1cccc(NC(=O)[C@H]2Cc3ccccc3O2)c1
vNsp12-rna1-28	ZINC000005209194	-10	0.37	351.364	ZINC	Cc1nc2oc3c4ccccc4ccc3c(=O)c2c2nc3ccccc3n21
vNsp12-rna1-29	ZINC000009062320	-10	0.294	470.508	ZINC	COc1ccc(-c2nnc(NC(=O)c3cccc(NC(=O)c4cc5ccccc5o4)c3)s2)cc1
vNsp12-rna1-30	ZINC000198754475	-10	0.278	464.475	ZINC	O=C1c2ccccc2C(=O)C2=C3C=CC4=CC5=C(C(=O)c6ccccc6C5=O)C5=CC=C(C=C12)[C@@H]3[C@H]45
vNsp12-rna1-31	Z1024053506	-9.9	0.275	481.55	REAL	O=C(Nc1cccc(C(=O)N2CCC([C@H]3C(=O)Nc4ccccc43)CC2)c1)[C@@H]1Cc2ccccc2O1
vNsp12-rna1-32	Z1102797879	-9.9	0.309	422.443	REAL	Cc1ccc(-c2cc(C(=O)Nc3cccc(N4C(=O)c5ccccc5C4=O)c3)[nH]n2)cc1
vNsp12-rna1-33	Z1160993935	-9.9	0.275	474.479	REAL	Cc1c(C(=O)Nc2cccc(N3C(=O)c4ccccc4C3=O)c2)nnn1-c1ccc2ncccc2c1
vNsp12-rna1-34	Z1479030117	-9.9	0.3	444.469	REAL	O=C(Nc1ccc(-c2ccccc2)nn1)N1CCC[C@H](c2nc(-c3cccc(F)c3)no2)C1
vNsp12-rna1-35	Z1685321062	-9.9	0.291	449.469	REAL	Cc1nnc(-c2cccc(-c3noc(-c4ccc5c(c4)C[C@@H](c4ccccc4)OC5=O)n3)c2)[nH]1
vNsp12-rna1-36	Z1891122752	-9.9	0.3	433.47	REAL	O=C1C[C@@H](c2nc(-c3cccn4ccnc34)no2)CN1c1ccc2c(c1)Cc1ccccc1-2
vNsp12-rna1-37	Z2159455398	-9.9	0.3	438.49	REAL	O=C(Cc1noc(-c2cccc3c4c([nH]c23)CCCC4)n1)N1CCn2c1nc1ccccc12
vNsp12-rna1-38	Z2201098239	-9.9	0.354	385.506	REAL	C[C@H]1[C@H](NC(=O)NCC[C@@]2(O)C[C@H]3CC[C@H]2C3)CC(=O)N1Cc1ccccc1
vNsp12-rna1-39	Z2311242839	-9.9	0.341	398.461	REAL	CCOC(=O)c1ccn(-c2cccc(NC(=O)NCC[C@H]3C[C@H]4CC[C@H]3O4)c2)n1
vNsp12-rna1-40	Z2524825833	-9.9	0.275	478.598	REAL	Cc1c(C(=O)N2C[C@H]3CC[C@@H]2[C@@H]2CN(Cc4ccccc4)C[C@@H]32)nnn1-c1ccc2ncccc2c1
vNsp12-rna1-41	Z2524825842	-9.9	0.275	478.598	REAL	Cc1c(C(=O)N2C[C@H]3CC[C@@H]2[C@@H]2CN(Cc4ccccc4)C[C@@H]32)nnn1-c1ccc2ccncc12
vNsp12-rna1-42	Z29556762	-9.9	0.275	484.598	REAL	Cc1ccc(C23C[C@H]4C[C@@H](CC(C(=O)NNC(=O)c5nn(C)c(=O)c6ccccc56)(C4)C2)C3)cc1C
vNsp12-rna1-43	Z808757820	-9.9	0.275	479.491	REAL	O=C(Cc1ccc(NC(=O)c2cc3ccccc3o2)cc1)NNC(=O)c1cc2ccccc2cc1O
vNsp12-rna1-44	Z829079690	-9.9	0.268	488.55	REAL	O=C(Nc1cccc(C(=O)N[C@H]2CCc3nc(-c4ccccc4)ncc3C2)c1)c1ccc2[nH]cnc2c1
vNsp12-rna1-45	ZINC000072442535	-9.9	0.291	448.529	ZINC	Cc1nn(-c2ccc(Nc3ccc(NC(=O)c4cccc5ccccc54)cc3)nn2)c(C)c1C
vNsp12-rna1-46	ZINC000101094108	-9.9	0.291	444.485	ZINC	O=C1c2cc3ccccc3cc2C(=O)[C@@H]2C[C@@H]3C(=O)c4cc5ccccc5cc4C(=O)[C@H]3C[C@@H]12
vNsp12-rna1-47	PV-001850233873	-9.8	0.306	450.522	REAL	C[C@@H](C(=O)Nc1nc(-c2ccc3ccccc3n2)n[nH]1)c1ccc(S(=O)(=O)N(C)C)cc1
vNsp12-rna1-48	Z1005784192	-9.8	0.272	480.57	REAL	O=C(N[C@H]1CCc2nc(-c3ccccc3)ncc2C1)[C@H]1CCCN(C(=O)c2ccc3[nH]ncc3c2)C1
vNsp12-rna1-49	Z1021880870	-9.8	0.28	464.524	REAL	CC(=O)N1c2ccccc2C[C@H]1C(=O)NNC(=O)c1cc(-c2ccc(C)cc2)nc2ccccc12
vNsp12-rna1-50	Z1069485232	-9.8	0.272	489.57	REAL	CCc1ccc(N2C[C@H](C(=O)N3CCC(C(=O)c4ccc5c(c4)NC(=O)[C@@H](C)O5)CC3)CC2=O)cc1
vNsp12-rna1-51	Z1072129990	-9.8	0.265	495.581	REAL	Cc1ccc2[nH]c([C@@H]3CCCN(C(=O)CN4C(=O)N[C@@](C)(c5cc6ccccc6c5)C4=O)C3)nc2c1
vNsp12-rna1-52	Z1095049540	-9.8	0.288	491.599	REAL	Cc1sc2nc(CS[C@@H](C)C(=O)Nc3nc(-c4ccc5ccccc5n4)n[nH]3)[nH]c(=O)c2c1C
vNsp12-rna1-53	Z1095049674	-9.8	0.306	423.475	REAL	COc1ccc2cc([C@H](C)C(=O)Nc3nc(-c4ccc5ccccc5n4)n[nH]3)ccc2c1
vNsp12-rna1-54	Z1101833000	-9.8	0.272	483.479	REAL	O=C(Nc1ccc(N2C(=O)c3ccccc3C2=O)cc1)[C@H]1CCCN1C(=O)c1ccc2c(c1)OCO2
vNsp12-rna1-55	Z1101833812	-9.8	0.28	465.508	REAL	O=C(Nc1ccc(N2C(=O)c3ccccc3C2=O)cc1)[C@H]1CC(=O)N(c2ccc3c(c2)CCC3)C1
vNsp12-rna1-56	Z1101835374	-9.8	0.272	475.503	REAL	O=C(Nc1ccc(N2C(=O)c3ccccc3C2=O)cc1)[C@H]1CC(=O)N(c2ccc3ccccc23)C1
vNsp12-rna1-57	Z1103944103	-9.8	0.272	493.444	REAL	O=C(Nc1nc(-c2ccccc(C(F)(F)F)c2)n[nH]1)c1cccc(NC(=O)[C@H]2Cc3ccccc3O2)c1
vNsp12-rna1-58	Z1155077407	-9.8	0.297	443.506	REAL	Cc1ccc(-n2nc(C(=O)Nc3cccc([C@@]4(C)NC(=O)NC4=O)c3)c3c2CCCC3)cc1
vNsp12-rna1-59	Z1160968427	-9.8	0.272	495.508	REAL	Cc1c(C(=O)Nc2ccc(N3CCN(C)CC3)cc2C(F)(F)F)nnn1-c1ccc2ncccc2c1
vNsp12-rna1-60	Z1210296918	-9.8	0.306	445.546	REAL	Cc1cc(C)cc(-c2nnc(NC(=O)c3ccc4c(=O)n5c(nc4c3)CCCCC5)s2)c1
vNsp12-rna1-61	Z1452196960	-9.8	0.316	446.389	REAL	C[C@]1(c2cccc(C(=O)Nc3nc4cc5c(cc4s3)OC(F)(F)O5)c2)NC(=O)NC1=O
vNsp12-rna1-62	Z1479031925	-9.8	0.297	444.469	REAL	O=C(Nc1ccc(-c2ccccc2)nn1)N1CCC[C@H](c2nc(-c3ccc(F)cc3)no2)C1
vNsp12-rna1-63	Z1661123317	-9.8	0.297	434.454	REAL	O=C(Nc1cccc(-c2nnc(-c3ccc4ccccc4n3)o2)c1)[C@H]1Cc2ccccc2O1
vNsp12-rna1-64	Z1674158613	-9.8	0.297	449.485	REAL	O=C1NCCc2ccc(CNC(=O)N3CCC[C@H](c4nc(-c5cccc(F)c5)no4)C3)cc21
vNsp12-rna1-65	Z1674182675	-9.8	0.297	449.485	REAL	O=C1NCCc2ccc(CNC(=O)N3CCC[C@H](c4nc(-c5ccc(F)cc5)no4)C3)cc21
vNsp12-rna1-66	Z1686303679	-9.8	0.288	448.445	REAL	Cc1c(-c2nc(-c3cnc(Oc4ccccc4)cn3)no2)nnn1-c1ccc2ncccc2c1
vNsp12-rna1-67	Z1723433958	-9.8	0.297	437.458	REAL	Cn1c(=O)[nH]c2ncc(-c3cccc(C(=O)NNC(=O)c4ccc5ccccc5c4)c3)cc21
vNsp12-rna1-68	Z1767223512	-9.8	0.316	417.374	REAL	O=C(NNc1cnc2ccccc2n1)c1cc(F)cc2c(=O)c3cc(F)ccc3[nH]c12
vNsp12-rna1-69	Z1903488524	-9.8	0.327	405.457	REAL	Cc1ccc(NC(=O)NNc2ccc3ccccc3n2)cc1C(=O)N1CCOCC1
vNsp12-rna1-70	Z1983283446	-9.8	0.327	406.484	REAL	CCc1ccc(-c2noc(CN3C(=O)N[C@@]4(C[C@@H]5C[C@H]4[C@@H]4CCC[C@@H]54)C3=O)n2)cc1
vNsp12-rna1-71	Z2008413435	-9.8	0.297	446.485	REAL	Cn1c([C@H]2Cc3ccccc3O2)nnc1N1CCC[C@@H](c2nc(-c3ccc(F)cc3)no2)C1
vNsp12-rna1-72	Z2008646069	-9.8	0.297	446.485	REAL	Cn1c([C@H]2Cc3ccccc3O2)nnc1N1CCC[C@@H](c2nc(-c3cccc(F)c3)no2)C1
vNsp12-rna1-73	Z2233254539	-9.8	0.316	420.378	REAL	Cc1nnc2[nH]nc(NC(=O)c3cc(F)cc4c(=O)c5cc(F)ccc5[nH]c34)c2c1C
vNsp12-rna1-74	Z2233591130	-9.8	0.316	415.452	REAL	CC(C)(C(=O)Nc1nc(-c2ccc3ccccc3n2)n[nH]1)c1ccc2c(c1)OCCO2
vNsp12-rna1-75	Z2233591344	-9.8	0.297	443.441	REAL	Cc1ccc(-c2noc(CCC(=O)Nc3nc(-c4ccc5ccccc5n4)n[nH]3)n2)cc1F
vNsp12-rna1-76	Z2902893618	-9.8	0.272	491.525	REAL	O=C1NC(=O)C2(CCC(c3nc(-c4ccc(N5CCN(c6ccc(F)cc6)CC5)nc4)no3)CC2)N1
vNsp12-rna1-77	Z2902950838	-9.8	0.28	465.508	REAL	O=C1[C@@H]2[C@@H]3C=C[C@H]([C@@H]2C(=O)N1Cc1ccccc1)[C@@H]1C(c2nc(-c4ccc5c(c4)CCO5)no2)[C@H]31
vNsp12-rna1-78	Z51772012	-9.8	0.28	499.586	REAL	O=C(NNC(=O)[C@H]1COc2ccccc2O1)C1CCN(S(=O)(=O)c2ccc3c(c2)CCCC3)CC1
vNsp12-rna1-79	Z764667660	-9.8	0.28	463.496	REAL	O=C(Nc1nc2ccccc2nc1N1CCCC1)c1cccc(N2C(=O)c3ccccc3C2=O)c1
vNsp12-rna1-80	Z767056986	-9.8	0.288	450.497	REAL	Cc1ccc(-c2cc(C(=O)Nc3cccc([C@@]4(C)NC(=O)NC4=O)c3)c3ccccc3n2)cc1
vNsp12-rna1-81	Z787555460	-9.8	0.28	464.528	REAL	O=C(Nc1cccc(C(=O)N2CCC[C@H](c3nc4ccccc4[nH]3)C2)c1)c1ccc2[nH]cnc2c1
vNsp12-rna1-82	Z808665656	-9.8	0.265	495.494	REAL	Cn1nc(C(=O)NNC(=O)Cc2ccc(NC(=O)c3cc4ccccc4o3)cc2)c2ccccc2c1=O
vNsp12-rna1-83	Z809048190	-9.8	0.28	463.492	REAL	O=C(Cc1ccc(NC(=O)c2cc3ccccc3o2)cc1)NNC(=O)c1ccc2ccccc2c1
vNsp12-rna1-84	Z854877598	-9.8	0.306	445.546	REAL	Cc1ccc(-c2nnc(NC(=O)c3ccc4c(=O)n5c(nc4c3)CCCCC5)s2)c(C)c1
vNsp12-rna1-85	Z980425624	-9.8	0.265	498.494	REAL	O=C(NNC(=O)[C@@H]1CCCN1C(=O)c1ccc2c(c1)OCO2)c1cc(-c2ccco2)nc2ccccc12
vNsp12-rna1-86	ZINC000008792183	-9.8	0.265	486.573	ZINC	Cc1cccc(N2CCN(C(=O)c3cc4c5ccccc5n5c4c(n3)c3ccccc3c5=O)CC2)c1C
vNsp12-rna1-87	ZINC000008901175	-9.8	0.306	486.32	ZINC	O=C(Nc1cccc(-c2cc3ccccc3oc2=O)c1)c1ccc(-c2ccc(Br)cc2)o1
vNsp12-rna1-88	ZINC000009747932	-9.8	0.297	467.596	ZINC	Cc1ccc2[nH]c(CCNC(=O)C3CCN(c4nnc(N5CCCCC5=O)s4)CC3)nc2c1
vNsp12-rna1-89	ZINC000013000660	-9.8	0.288	453.409	ZINC	O=C(Nc1cccc(NC(=O)c2cc(=O)c3ccccc3o2)n1)c1cc(=O)c2ccccc2o1
vNsp12-rna1-90	ZINC000039930672	-9.8	0.272	469.455	ZINC	O=C1c2ccccc2C(=O)N1c1ccc2cc3ccc(N4C(=O)c5ccccc5C4=O)cc3nc2c1
vNsp12-rna1-91	ZINC000048523764	-9.8	0.272	464.475	ZINC	O=C1c2ccccc2C(=O)C2=C3C=CC4=CC5=C(C(=O)c6ccccc6C5=O)C5=CC=C(C=C12)[C@@H]3[C@@H]45
vNsp12-rna1-92	ZINC000101094105	-9.8	0.288	444.485	ZINC	O=C1c2cc3ccccc3cc2C(=O)[C@@H]2C[C@@H]3C(=O)c4cc5ccccc5cc4C(=O)[C@@H]3C[C@@H]12
vNsp12-rna1-93	PV-001793137839	-9.7	0.334	422.382	REAL	CC1(C)OC(=O)c2c(C(=O)Nc3nc4ccc(OC(F)(F)F)cc4s3)cccc21
vNsp12-rna1-94	PV-001850232656	-9.7	0.323	421.48	REAL	C[C@@H](C(=O)Nc1nc(-c2ccc3ccccc3n2)n[nH]1)c1ccc(S(C)(=O)=O)cc1
vNsp12-rna1-95	PV-001874566486	-9.7	0.303	452.494	REAL	CCc1ccc(-c2ccc(C(=O)Nc3cccc(S(=O)(=O)Nc4nnn(C)n4)c3)o2)cc1
vNsp12-rna1-96	PV-001943072779	-9.7	0.359	405.371	REAL	CC1(NC(=O)Nc2nc3cc4c(cc3s2)OC(F)(F)O4)CCC(F)(F)CC1
vNsp12-rna1-97	PV-001943073079	-9.7	0.359	399.373	REAL	CC1(C)C[C@@](C)(NC(=O)Nc2nc3cc4c(cc3s2)OC(F)(F)O4)CC(=O)O1
vNsp12-rna1-98	Z1001377822	-9.7	0.269	481.554	REAL	Cc1ccc(CC(=O)N2CCN(C(=O)c3cccc(NC(=O)c4ccc5[nH]cnc5c4)c3)CC2)cc1
vNsp12-rna1-99	Z1023593500	-9.7	0.277	489.918	REAL	O=C(Cn1cnc2c(oc3ccccc32)c1=O)N1CCC[C@H](c2nc(-c3ccc(Cl)cc3)no2)C1
vNsp12-rna1-100	Z1070905940	-9.7	0.285	473.959	REAL	O=C1Nc2cc(Cl)ccc2[C@@H]1C1CCN([C@H]2CC(=O)N(c3cccc4ccccc34)C2=O)CC1

Supplementary Table 55. Excluded. Top 100 virtual hits of the screen against the RNA binding site of nsp12 (Screen ID: 28). Compounds were filtered so that hits had MW < 600 dalton, cLogP < 6, number of hydrogen bond acceptors < 11, and no reactive functional groups. A few compounds unsuitable for drug discovery were removed by visual inspection. The name of each compound consists of the initial letter 'v' for virtual hit, followed by the target protein name and the target site ('rna' for RNA binding site, 1 for docking scenario 1). The score is the docking score given by QuickVina 2 in kcal/mol. The ligand efficiency (LE) is computed as LE = -score/#NonH, where #NonH is the number of heavy (i.e. non hydrogen) atoms.

Name	Catalog ID	Score	LE	MW	Library	SMILES
vNsp12-rna1-101	Z1082330228	-9.7	0.313	410.41	REAL	O=C(Nc1nc2ccccc2c(=O)[nH]1)c1cc(-c2ccc(F)cc2)nc2ccccc12
vNsp12-rna1-102	Z1095049034	-9.7	0.285	452.45	REAL	O=C(Nc1cccc(C(=O)Nc2nc(-c3ccc4ccccc4n3)n[nH]2)c1)c1ccc(F)cc1
vNsp12-rna1-103	Z1095050608	-9.7	0.303	444.47	REAL	Cc1cc(NC(=O)c2ccco2)sc1C(=O)Nc1nc(-c2ccc3ccccc3n2)n[nH]1
vNsp12-rna1-104	Z1101912380	-9.7	0.277	487.94	REAL	O=C(Nc1cccc(N2C(=O)c3ccccc3C2=O)c1)[C@@H]1CCCN(C(=O)c2ccc(Cl)cc2)C1
vNsp12-rna1-105	Z1102048790	-9.7	0.277	481.53	REAL	Cn1c2ccccc2c2cc(S(=O)(=O)Nc3cccc(N4C(=O)c5ccccc5C4=O)c3)ccc21
vNsp12-rna1-106	Z1116830710	-9.7	0.285	452.47	REAL	O=C(Nc1cnc(-c2cccc(O)c2)nc1)c1cccc(NC(=O)[C@H]2Cc3ccccc3O2)c1
vNsp12-rna1-107	Z1119218242	-9.7	0.269	484.56	REAL	O=C(c1ccc2[nH]ncc2c1)N1CCC[C@@H](C(=O)N2CCCC[C@H]2c2nc(-c3ccccc3)no2)C1
vNsp12-rna1-108	Z1147775494	-9.7	0.294	447.47	REAL	Cc1ccc(-n2nc(C(=O)Nc3cccc([C@@]4(C)NC(=O)NC4=O)c3)c3c2CCC3)c(F)c1
vNsp12-rna1-109	Z1158428684	-9.7	0.269	498.46	REAL	Cc1c(C(=O)N2CCC[C@@H](c3nc(-c4cccc(F)c4)no3)C2)nnn1-c1ccc(OC(F)F)cc1
vNsp12-rna1-110	Z1160944167	-9.7	0.285	445.49	REAL	Cc1c(C(=O)Nc2cccc(-c3nc4ccccc4[nH]3)c2)nnn1-c1ccc2ncccc2c1
vNsp12-rna1-111	Z1167944866	-9.7	0.323	423.47	REAL	O=C(Nc1ccc(F)c(N2CCCS2(=O)=O)c1)c1cc2c(ccc3ccccc32)[nH]1
vNsp12-rna1-112	Z137252906	-9.7	0.277	470.49	REAL	Cn1c(NNC(=O)CN2C(=O)N[C@](C)(c3ccc4ccccc4c3)C2=O)nc2ccccc2c1=O
vNsp12-rna1-113	Z1421543340	-9.7	0.294	449.49	REAL	Cc1cc(-c2noc([C@H](C)NC(=O)N3CCC[C@H](c4nc5ccccc5o4)C3)n2)ccc1F
vNsp12-rna1-114	Z15882232	-9.7	0.262	496.47	REAL	C[C@H](OC(=O)c1ccc(N2C(=O)CCC2=O)cc1)C(=O)Nc1ccc2c(c1)C(=O)c1ccccc1C2=O
vNsp12-rna1-115	Z1610505890	-9.7	0.323	398.40	REAL	O=C(NNc1ccc2ccccc2n1)c1ccc2noc(-c3ccc(F)cc3)c2c1
vNsp12-rna1-116	Z1614243453	-9.7	0.294	447.54	REAL	O=C(c1cc(-c2ccc3c(c2)CCO3)no1)N1CCC[C@H](c2n[nH]c(C3CCCCC3)n2)C1
vNsp12-rna1-117	Z1614248236	-9.7	0.294	441.49	REAL	O=C(c1cc(-c2ccc3c(c2)CCO3)no1)N1CCC[C@H](c2n[nH]c(-c3ccccc3)n2)C1
vNsp12-rna1-118	Z1670614279	-9.7	0.303	442.36	REAL	O=C(NNC(=O)c1ccc2ccccc2n1)Nc1ccc(-c2noc(C(F)(F)F)n2)cc1
vNsp12-rna1-119	Z1685085222	-9.7	0.285	449.47	REAL	O=C1C[C@@H](c2nc(-c3ccc4[nH]c(=O)[nH]c4c3)no2)CN1c1ccc2c(c1)Cc1ccccc1-2
vNsp12-rna1-120	Z1685497038	-9.7	0.294	448.53	REAL	CN1CCN(C(=O)c2ccc(-c3noc(-c4cc5c([nH]c4=O)CCC(C)(C)C5)n3)cn2)CC1
vNsp12-rna1-121	Z1686349530	-9.7	0.294	438.45	REAL	Cc1c(-c2nc(-c3ccc4oc(N(C)C)nc4c3)no2)nnn1-c1ccc2ncccc2c1
vNsp12-rna1-122	Z1723430482	-9.7	0.294	438.45	REAL	Cn1c(=O)[nH]c2ncc(-c3cccc(C(=O)NNC(=O)c4ccc5ccccc5n4)c3)cc21
vNsp12-rna1-123	Z1723430646	-9.7	0.285	453.46	REAL	Cn1c(=O)[nH]c2ncc(-c3cccc(C(=O)NNC(=O)c4cc5ccccc5cc4O)c3)cc21
vNsp12-rna1-124	Z1770924222	-9.7	0.313	423.42	REAL	CC(C)(C)c1ccc(NNC(=O)c2cc(F)cc3c(=O)c4cc(F)ccc4[nH]c23)nn1
vNsp12-rna1-125	Z1846566417	-9.7	0.303	444.52	REAL	O=C(Nc1nnc(-c2cc3ccccc3o2)[nH]1)C1CCN(c2nc3ccccc3s2)CC1
vNsp12-rna1-126	Z1903106471	-9.7	0.313	434.53	REAL	Cc1cc(C)cc(-c2nnc(NC(=O)N[C@@H](C)C3nc(-c4cc(C)ccn4)n[nH]3)s2)c1
vNsp12-rna1-127	Z1983291903	-9.7	0.334	388.47	REAL	O=C(CN1C(=O)N[C@@]2(C[C@H]3C[C@H]2[C@H]2CCC[C@H]32)C1=O)c1ccc2ccccc2c1
vNsp12-rna1-128	Z1983293833	-9.7	0.313	436.54	REAL	NC(=O)c1ccc(-c2nc(CN3C(=O)N[C@@]4(C[C@@H]5C[C@H]4[C@@H]5C[C@H]4[C@@H]4CCC[C@H]54)C3=O)cs2)cc1
vNsp12-rna1-129	Z2002423492	-9.7	0.303	425.48	REAL	O=C1[C@@H]2[C@@H]3C[C@H]4[C@@H]2[C@]2(C(=O)Oc5cccc(C(=O)N6CCc7ccccc7C6)c5)[C@H]1[C@@H]3[C@@H]42
vNsp12-rna1-130	Z2008323258	-9.7	0.294	444.54	REAL	Cc1ccc(C2=NO[C@H](CNC(=O)N3CCC(c4nc(-c5ccccc5)n[nH]4)CC3)C2)cc1
vNsp12-rna1-131	Z2095293271	-9.7	0.303	429.41	REAL	O=C(Nc1ccc(F)c(N2C(=O)CCC2=O)c1)c1cccc2c(=O)c3ccccc3[nH]c12
vNsp12-rna1-132	Z2166789118	-9.7	0.294	443.47	REAL	Cn1c(-c2n[nH]c(=O)c3ccccc23)nnc1N1CCc2c(cccc2N2CCOC2=O)C1
vNsp12-rna1-133	Z2171963536	-9.7	0.294	443.55	REAL	CC1CCC(c2noc(C3[C@H]4[C@@H]5C=C[C@@H]([C@H]6C(=O)N(Cc7ccccc7)C(=O)[C@H]56)[C@H]34)n2)CC1
vNsp12-rna1-134	Z2225797920	-9.7	0.303	426.48	REAL	CC(=O)N1CCN(c2cccc(NC(=O)c3cc4c(ccc5ccccc54)[nH]3)c2C)C1=O
vNsp12-rna1-135	Z2233592864	-9.7	0.334	385.38	REAL	O=C1O[C@@H](C(=O)Nc2nc(-c3ccc4ccccc4n3)n[nH]2)Cc2ccccc21
vNsp12-rna1-136	Z2640094831	-9.7	0.346	375.40	REAL	O=C(Nc1nc(-c2ccc3ccccc3n2)n[nH]1)[C@@H]1CCc2nnnn2CC1
vNsp12-rna1-137	Z2694215218	-9.7	0.269	483.57	REAL	Cc1ccc(O[C@H]2CCN(C(=O)C3[C@H]4[C@H]5C=C[C@@H]([C@H]6C(=O)N(Cc7ccccc7)C(=O)[C@@H]56)[C@@H]34)C2)nc1
vNsp12-rna1-138	Z27231053	-9.7	0.269	484.49	REAL	COc1cccc([C@@]2(C)NC(=O)N(NC(=O)c3cc(-c4ccc(F)cc4)nc4ccccc34)C2=O)c1
vNsp12-rna1-139	Z31435674	-9.7	0.277	490.50	REAL	O=C(NNC(=O)c1ccc2ccccc2n1)c1cccc(S(=O)(=O)Nc2ccc3c(c2)OCO3)c1
vNsp12-rna1-140	Z370760050	-9.7	0.285	478.66	REAL	O=C(Nc1nnc(C23CC4CC(CC(C4)C2)C3)s1)C1CCN(C(=O)CCc2ccccc2)CC1
vNsp12-rna1-141	Z442416066	-9.7	0.285	452.43	REAL	O=C(Nn1cnc2ccccc2c1=O)c1cccc(C(=O)Nn2cnc3ccccc3c2=O)c1
vNsp12-rna1-142	Z685930356	-9.7	0.313	405.42	REAL	Cn1nc(-c2nnc(-c3cc4ccccc4c4cccnc34)o2)c2ccccc2c1=O
vNsp12-rna1-143	Z735279506	-9.7	0.269	493.49	REAL	O=C1/C(=C/N[C@@H]2CCCN(c3ncccn3)C2)c2ccccc2C(=O)N1c1cccc(C(F)(F)F)c1
vNsp12-rna1-144	Z735827844	-9.7	0.269	499.49	REAL	Cc1ccc(-c2noc(CN3CCN([C@@H]4CC(=O)N(c5cccc(C(F)(F)F)c5)C4=O)CC3)n2)cc1
vNsp12-rna1-145	Z735833794	-9.7	0.262	495.58	REAL	Cc1ccc(-c2noc([C@H](C)N3CCN([C@@H]4CC(=O)N(c5ccc6ccccc56)C4=O)CC3)n2)cc1
vNsp12-rna1-146	Z770086334	-9.7	0.269	497.48	REAL	C[C@H](c1nc(-c2cccc(C(F)(F)F)c2)no1)N1CCN(C(=O)c2cc(-c3ccccc3)on2)CC1
vNsp12-rna1-147	Z774431874	-9.7	0.285	455.52	REAL	Cc1ccc(C(=O)Nc2cccc(CNC(=O)C3=NN(c4ccccc4)C(=O)[C@@H](C)N3)c2)cc1
vNsp12-rna1-148	Z787547112	-9.7	0.285	450.46	REAL	O=C(NNC(=O)c1ccc2ccccc2n1)c1cccc(NC(=O)c2ccc3[nH]cnc3c2)c1
vNsp12-rna1-149	Z790177448	-9.7	0.277	467.48	REAL	O=C(NNC(=O)c1cc2ccccc2cc1O)c1cccc(NC(=O)[C@H]2Cc3ccccc3O2)c1
vNsp12-rna1-150	Z828218840	-9.7	0.262	495.58	REAL	CN1CCC2(CC1)C[C@H](NC(=O)c1cccc(NC(=O)c3ccc4[nH]cnc4c3)c1)c1ccccc1O2
vNsp12-rna1-151	Z838610796	-9.7	0.285	475.55	REAL	O=C(C(=O)N1CCN(c2nn3cc(-c4ccc(F)cc4)nc3s2)CC1)c1ccc2c(c1)CCC2
vNsp12-rna1-152	Z988056782	-9.7	0.269	486.55	REAL	CC(=O)c1ccc(N2CCN(C(=O)Nc3cccc(C(=O)N4CCc5ccccc54)c3)CC2)c(F)c1
vNsp12-rna1-153	ZINC000004277692	-9.7	0.262	493.56	ZINC	O=C(COc1cccc1)Nc1ccc2n(c1=O)C[C@H]1C[C@@H]2CN(C(=O)c2ccc3ccccc3c2)C1
vNsp12-rna1-154	ZINC000008599007	-9.7	0.277	476.52	ZINC	Cc1nc2c3ccccc3nc(NNC(=O)CCC(=O)N3CCN(c4ccc(F)cc4)CC3)n2n1
vNsp12-rna1-155	ZINC000011880626	-9.7	0.294	447.51	ZINC	O=C(c1cn(C2CCN(C(=O)c3cccc(-c4ccc(F)cc4)c3)CC2)nn1)N1CCCC1
vNsp12-rna1-156	ZINC000012353311	-9.7	0.303	441.87	ZINC	O=C(Nc1cccc(-c2cc3ccccc3oc2=O)c1)c1ccc(-c2ccc(Cl)cc2)o1
vNsp12-rna1-157	ZINC000015863645	-9.7	0.294	433.51	ZINC	O=C(Nc1cccc(CCc2nc3ccccc3[nH]2)c1)c1n[nH]c2c1CCc1ccccc1-2
vNsp12-rna1-158	ZINC000017988176	-9.7	0.243	521.57	ZINC	O=C(Oc1ccc2ccccc2c1)c1cccc(N2C(=O)[C@H]3[C@@H](C2=O)C2c4ccccc4C3c3ccccc32)c1
vNsp12-rna1-159	ZINC000034856480	-9.7	0.285	451.53	ZINC	Cc1cc2c(c(C)c1)NC(=O)[C@@]21[C@@H]2C(=O)N(c3ccc4ccccc4c3)C(=O)[C@@H]2[C@H]2CCCN21
vNsp12-rna1-160	ZINC000035944105	-9.7	0.249	528.65	ZINC	C[C@@H]1CC[C@H](C)[C@H](N2C(=O)c3ccc(Oc4ccc5c(c4)C(=O)N([C@@H]4C[C@H](C)CC[C@@H]4C)C5=O)cc3C2=O)C1
vNsp12-rna1-161	ZINC000096324344	-9.7	0.294	447.42	ZINC	Cc1ccc(-n2cc(-c3nc(-c4ccc(C(F)(F)F)cc4)no3)c3ccccc3c2=O)cc1
vNsp12-rna1-162	ZINC000096324389	-9.7	0.294	467.83	ZINC	O=c1c2ccccc2c(-c2nc(-c3ccc(C(F)(F)F)cc3)no2)cn1-c1ccc(Cl)cc1
vNsp12-rna1-163	ZINC000096602166	-9.7	0.303	411.47	ZINC	c1ccc2cc3[nH]c(-c4cccc(-c5nc6cc7ccccc7cc6[nH]5)n4)nc3cc2c1
vNsp12-rna1-164	ZINC000108104867	-9.7	0.269	485.59	ZINC	O=C(Nc1cccc(C(=O)N2CCC[C@@H](c3nnc4n3CCCCC4)C2)c1)[C@H]1Cc2ccccc2O1
vNsp12-rna1-165	ZINC000254598298	-9.7	0.285	465.53	ZINC	Cc1c2ccccc2oc1-c1nc2sc(=Cc3ccc(OCc4ccccc4)cc3)c(=O)n2n1
vNsp12-rna1-166	PV-001811968521	-9.6	0.320	414.38	REAL	C[C@@H]1C(=O)Nc2ccccc2CN1C(=O)c1ccc(-c2ccc(C(F)(F)F)cc2)o1
vNsp12-rna1-167	PV-001817025364	-9.6	0.320	435.34	REAL	Cc1c(C(=O)N2CC[C@]3(C2)CC(F)(F)C3(F)F)cnn1-c1ccc(C(F)(F)F)cc1
vNsp12-rna1-168	PV-001847889192	-9.6	0.331	401.35	REAL	Cc1nnc2[nH]nc(NC(=O)c3ccc(-c4ccc(C(F)(F)F)cc4)o3)c2c1C
vNsp12-rna1-169	PV-001850781837	-9.6	0.291	442.43	REAL	O=C(NNC(=O)[C@@H]1C(=O)Nc2ccccc2C1=O)c1cccc(C(=O)Nc2ccccc2)c1
vNsp12-rna1-170	PV-001878080383	-9.6	0.300	452.44	REAL	C[C@@H]1CC(C)(C)C[C@]2(C1)NC(=O)N(CC(=O)Nc1n[nH]c3nc(C(F)(F)F)ccc13)C2=O
vNsp12-rna1-171	PV-001943068378	-9.6	0.310	456.83	REAL	O=C(Nc1ccc(Cl)cn1)c1cccc(NC(=O)N2CCC3(CC2)C(F)(F)C3(F)F)c1
vNsp12-rna1-172	PV-001943070473	-9.6	0.369	383.42	REAL	CC1CCC(C)(NC(=O)Nc2nc3cc4c(cc3s2)OC(F)(F)O4)CC1
vNsp12-rna1-173	PV-001946689956	-9.6	0.331	433.85	REAL	C[C@H](NC(=O)Nc1nnc(-c2ccc(Cl)cc2F)s1)c1ccc2[nH]c(=O)oc2c1
vNsp12-rna1-174	PV-001950167475	-9.6	0.369	392.35	REAL	O=C(Nc1nnc(-c2ccc(C(F)(F)F)cc2)s1)N[C@H]1CCC(F)(F)C1
vNsp12-rna1-175	PV-001950169455	-9.6	0.310	449.41	REAL	C[C@H](NC(=O)Nc1nnc(-c2ccc(C(F)(F)F)cc2)s1)c1ccc2[nH]c(=O)oc2c1
vNsp12-rna1-176	PV-001950170094	-9.6	0.310	453.49	REAL	CC(=O)N1C[C@H]2CCC[C@H](NC(=O)Nc3nnc(-c4ccc(C(F)(F)F)cc4)s3)[C@H]2C1
vNsp12-rna1-177	PV-001954399966	-9.6	0.291	453.44	REAL	Cc1ccc(C(=O)Nc2cccc(CNC(=O)NCc3ccc4c(c3)OC(F)(F)O4)c2)cc1
vNsp12-rna1-178	PV-001954766777	-9.6	0.310	438.42	REAL	O=C(N[C@H]1CCCOc2ccc(F)cc21)N1CCO[C@@H](c2cccc(C(F)(F)F)cc2)C1
vNsp12-rna1-179	PV-001958593376	-9.6	0.320	444.93	REAL	C[C@@H]1CCC[C@@H](C2CN(C(=O)N[C@H]3CCN(c4ncc(C(F)(F)F)cc4Cl)C3)CC2)C1
vNsp12-rna1-180	PV-002017929246	-9.6	0.300	446.59	REAL	CCC(CC)NC(=O)c1nnc(N2CCC(OCC(N)=O)CC2)n1C[C@@H]1C[C@@H]2CC[C@@H]1C2
vNsp12-rna1-181	Z1095049134	-9.6	0.310	430.47	REAL	Cc1nc(-c2ccc(F)cc2)sc1C(=O)Nc1nc(-c2ccc3ccccc3n2)n[nH]1
vNsp12-rna1-182	Z1095050500	-9.6	0.291	446.42	REAL	O=C(CCc1ncc(-c2ccc(F)cc2F)o1)Nc1nc(-c2ccc3ccccc3n2)n[nH]1
vNsp12-rna1-183	Z1095050822	-9.6	0.310	410.44	REAL	Cc1ccc(-n2nnc(C(=O)Nc3nc(-c4ccc5ccccc5n4)n[nH]3)c2C)cc1
vNsp12-rna1-184	Z1144975103	-9.6	0.310	439.51	REAL	O=C(Nc1nnc(Cc2ccc(F)cc2)s1)C1CCN(C(=O)Nc2ccccc2)CC1
vNsp12-rna1-185	Z1161138586	-9.6	0.291	438.49	REAL	Cc1c(C(=O)N2CCC(c3nc4ccccc4o3)CC2)nnn1-c1ccc2ncccc2c1
vNsp12-rna1-186	Z1162535345	-9.6	0.310	410.41	REAL	O=C(Nc1nc2ccccc2c(=O)[nH]1)c1cc(-c2ccccc2)nc2cc(F)ccc12
vNsp12-rna1-187	Z1165484524	-9.6	0.300	447.89	REAL	Cc1ccc(-c2nnn(CC(=O)Nc3cccc(C(=O)Nc4ccc(Cl)cn4)c3)n2)cc1
vNsp12-rna1-188	Z1180432091	-9.6	0.291	444.47	REAL	O=C(NCC(=O)N1CCc2ccccc2C1)Nc1ccc2nc(-c3ccc(F)cc3)oc2c1
vNsp12-rna1-189	Z1197674150	-9.6	0.300	425.44	REAL	O=C(Cc1noc(-c2ccc3c(c2)-c2ccccc2C3)n1)Nc1ccc2c(c1)OCCO2
vNsp12-rna1-190	Z1217450237	-9.6	0.291	443.48	REAL	O=C(N[C@@H]1CCCN(c2cccc(F)c2)C1)c1cccc(N2C(=O)c3ccccc3C2=O)c1
vNsp12-rna1-191	Z1323785248	-9.6	0.300	423.44	REAL	O=C(NCc1nc(NC(=O)c2ccc3ccccc3n2)n[nH]1)c1ccc2ccccc2n1
vNsp12-rna1-192	Z1408170318	-9.6	0.310	412.42	REAL	O=C(Nc1cccc(C(=O)Nc2ccc(-c3ccccc3)nn2)c1)c1ccc(F)cc1
vNsp12-rna1-193	Z1408175781	-9.6	0.291	436.47	REAL	O=C(Nc1ccc(-c2ccccc2)nn1)c1cccc(NC(=O)[C@H]2Cc3ccccc3O2)c1
vNsp12-rna1-194	Z1409795507	-9.6	0.300	423.52	REAL	Cc1ccc(-c2cncc(C(=O)N3CCC(c4nc(-c5ccccc5)n[nH]4)CC3)c2)cc1
vNsp12-rna1-195	Z14228733	-9.6	0.291	450.45	REAL	O=C(CN1C(=O)N[C@]2(CCc3ccccc3C2)C1=O)NC(=O)Nc1ccc2c(c1)OCCO2
vNsp12-rna1-196	Z1610525321	-9.6	0.300	424.46	REAL	O=C(NNc1ccc2ccccc2n1)c1cccc(NC(=O)[C@H]2Cc3ccccc3O2)c1
vNsp12-rna1-197	Z1610574755	-9.6	0.310	421.48	REAL	Cc1cc2ccccc2nc1NNC(=O)[C@@H]1CCCN(C(=O)Nc2ccccc2F)C1
vNsp12-rna1-198	Z1610590237	-9.6	0.320	403.49	REAL	Cc1cc2ccccc2nc1NNC(=O)[C@@H]1CCCN(C(=O)Nc2ccccc2)C1
vNsp12-rna1-199	Z1610591796	-9.6	0.291	438.49	REAL	Cc1cc2ccccc2nc1NNC(=O)c1cccc(NC(=O)[C@H]2Cc3ccccc3O2)c1
vNsp12-rna1-200	Z1633909384	-9.6	0.291	443.55	REAL	O=C(Nc1nnc2n1CCCC2)[C@@H]1C[C@H]2CCCC[C@@H]2N1C(=O)c1ccc2ccccc2c1

Supplementary Table 56. Excluded. Virtual screening hits 101 to 200 of the screen against the RNA binding site of nsp12 (Screen ID: 28). Compounds were filtered so that hits had MW < 600 dalton, cLogP < 6, number of hydrogen bond acceptors < 11, and no reactive functional groups. A few compounds unsuitable for drug discovery were removed by visual inspection. The name of each compound consists of the initial letter 'v' for virtual hit, followed by the target protein name and the target site ('rna' for RNA binding site, 1 for docking scenario 1). The score is the docking score given by QuickVina 2 in kcal/mol. The ligand efficiency (LE) is computed as LE = -score/#NonH, where #NonH is the number of heavy (i.e. non hydrogen) atoms.

Name	Catalog ID	Score	LE	MW	Library	SMILES
vNsp12-rna2-1	ZINC000253623869	-9.8	0.265	488.498	ZINC	Cn1cc(/C=C2/Oc3c(ccc4c3[C@H](c3cc5ccccc5nc3O)CC(=O)O4)C2=O)c2ccccc21
vNsp12-rna2-2	ZINC000263586232	-9.8	0.265	488.498	ZINC	Cn1cc(/C=C2\Oc3c(ccc4c3[C@H](c3cc5ccccc5nc3O)CC(=O)O4)C2=O)c2ccccc21
vNsp12-rna2-3	Z1907681182	-9.7	0.346	382.434	REAL	O=C1CCc2cc(C(=O)NC[C@]3(O)[C@H]4[C@H]5C[C@@H]6[C@@H]7[C@H]5C[C@@H]4[C@@H]7[C@H]63)c(F)cc2N1
vNsp12-rna2-4	Z1907687348	-9.5	0.339	412.577	REAL	C[C@H](Sc1nc2ccccc2s1)C(=O)NC[C@]1(O)[C@H]2[C@H]3C[C@H]4[C@H]5[C@H]3C[C@H]2[C@@H]5[C@@H]41
vNsp12-rna2-5	Z2484322075	-9.5	0.339	386.386	REAL	Cc1nnnn1/C(=C\c1ccc(F)cc1)C(=O)NNC(=O)[C@H]1C[C@H]2CC[C@H]1O2
vNsp12-rna2-6	Z1071593910	-9.4	0.303	414.503	REAL	O=C(NCc1ccc2c(c1)OCCCO2)N1Cc2ccccc2[C@@H](c2ccccc2)C1
vNsp12-rna2-7	Z1587898765	-9.4	0.303	417.551	REAL	C[C@@]1(CNC(=O)N2CCC([C@H]3C(=O)Nc4ccccc43)CC2)CCCc2ccccc21
vNsp12-rna2-8	Z2176722244	-9.4	0.313	412.532	REAL	CC(C)CC(=O)N[C@@H](Cc1c[nH]cn1)C(=O)NC[C@@]1(O)[C@@H]2[C@H]3C[C@H]4[C@H]5[C@@H]3C[C@@H]2[C@H]5[C@H]41
vNsp12-rna2-9	Z2201098239	-9.4	0.336	385.506	REAL	C[C@H]1[C@H](NC(=O)NCC[C@@]2(O)C[C@H]3CC[C@H]2C3)CC(=O)N1Cc1ccccc1
vNsp12-rna2-10	ZINC000009075722	-9.4	0.269	462.547	ZINC	Cc1cc(C)c(N2C(=O)[C@H]3ON(c4ccccc4)[C@H](c4ccc5ccccc54)[C@@H]3C2=O)c(C)c1
vNsp12-rna2-11	ZINC000012548776	-9.4	0.235	523.595	ZINC	Cc1ccc(N2C(=O)c3ccccc3/C(=C\Nc3nnc(-c4ccccc4)c(-c4ccccc4)n3)C2=O)c(C)c1
vNsp12-rna2-12	ZINC000072356258	-9.4	0.294	424.542	ZINC	O=C(c1ccccc(-c2ccc(C[C@@H]3CCCNC3=O)cc2)c1)N1CCc2ccccc2C1
vNsp12-rna2-13	ZINC000085392618	-9.4	0.254	493.569	ZINC	O=C([C@@H]1CC(=O)N(c2nc[nH]n2)C1)N1CCC(c2c[nH]c3ccccc32)(c2c[nH]c3ccccc32)CC1
vNsp12-rna2-14	ZINC000085392752	-9.4	0.235	530.67	ZINC	Cc1ccc(N2C[C@H](C(=O)N3CCC(c4c[nH]c5ccccc54)(c4c[nH]c5ccccc54)CC3)CC2=O)c(C)c1
vNsp12-rna2-15	ZINC000100505726	-9.4	0.254	488.542	ZINC	O=C1[C@@H]2[C@H]3C=C[C@@H](C3)[C@@H]2C(=O)N1c1ccc2c(c1)-c1cc(N3C(=O)[C@@H]4[C@H]5C=C[C@@H](C5)[C@@H]4C3=O)ccc1C2
vNsp12-rna2-16	ZINC000102753798	-9.4	0.254	488.517	ZINC	O=C1[C@H]2ON(c3ccccc3)[C@@H](c3c4ccccc4cc4ccccc43)[C@@H]2C(=O)N1c1ccc(F)cc1
vNsp12-rna2-17	ZINC000102753800	-9.4	0.254	488.517	ZINC	O=C1[C@@H]2ON(c3ccccc3)[C@@H](c3c4ccccc4cc4ccccc43)[C@@H]2C(=O)N1c1ccc(F)cc1
vNsp12-rna2-18	ZINC000229955902	-9.4	0.269	462.547	ZINC	Cc1cc(C)c(N2C(=O)[C@@H]3ON(c4ccccc4)[C@H](c4ccc5ccccc54)[C@@H]3C2=O)c(C)c1
vNsp12-rna2-19	ZINC000247756661	-9.4	0.269	465.591	ZINC	O=C1c2ccccc2C(=O)c2cc3c(cc21)N[C@@H]1CC[C@H]2[C@H]4[C@@H](CC[C@@H]3[C@@H]14)C(=O)[C@H]1CCCC[C@@H]21
vNsp12-rna2-20	Z1505440085	-9.3	0.321	390.446	REAL	O=C([C@@H]1CC(=O)N(c2cccc3ccccc23)C1)N1CCC[C@@H](c2nnn[nH]2)C1
vNsp12-rna2-21	Z1785158108	-9.3	0.291	421.459	REAL	O=C(c1ccc(-c2cccc3ccccc23)nc2ccccc12)N1CCn2c(n[nH]c2=O)C1
vNsp12-rna2-22	Z2002402837	-9.3	0.31	399.445	REAL	O=C(NCc1ccccc1)c1cccc(OC(=O)[C@]23[C@@H]4C(=O)[C@H]5[C@@H]6C[C@@H]([C@H]52)[C@@H]3[C@H]64)c1
vNsp12-rna2-23	ZINC000001266504	-9.3	0.266	456.456	ZINC	O=C1c2cc3oc4ccccc4c4ccccc4oc3cc2C(=O)N1c1ccccc2ccncc21
vNsp12-rna2-24	ZINC000013759321	-9.3	0.251	484.554	ZINC	Cc1ccc(N2C(=O)[C@H]3ON(c4ccccc4)[C@@H](c4c5ccccc5cc5ccccc54)[C@@H]3C2=O)cc1
vNsp12-rna2-25	ZINC000019589408	-9.3	0.282	448.521	ZINC	CN1CCN(C(=O)[C@H]2CCC(=O)NC(=O)N2)C[C@@H](Cc2ccc(-c3ccccc3)cc2)C1=O
vNsp12-rna2-26	ZINC000100694082	-9.3	0.291	416.606	ZINC	C1=CC2C3C=CC(C4C5C6C7C=CC(C=CC76)C5C43)C2C2C1C1C2C2C3C=CC1C=CC32
vNsp12-rna2-27	ZINC000101483291	-9.3	0.251	487.51	ZINC	Cc1ccc(N2C(=O)[C@H]3[C@@H](c4cccc5ccccc54)OC4(C(=O)c5ccccc5C4=O)[C@H]3C2=O)cc1
vNsp12-rna2-28	ZINC000102740839	-9.3	0.251	484.554	ZINC	Cc1ccc(N2C(=O)[C@@H]3ON(c4ccccc4)[C@@H](c4c5ccccc5cc5ccccc54)[C@@H]3C2=O)cc1
vNsp12-rna2-29	ZINC000408978119	-9.3	0.245	495.493	ZINC	O=C(Oc1ccc2nc3c4ccccc4c4ccccc4c3nc2c1)c1ccc(N2C(=O)C=CC2=O)cc1
vNsp12-rna2-30	Z1037875254	-9.2	0.249	496.573	REAL	Cc1ccccc1NC(=O)[C@@H]1CCc2ccccc2N1C(=O)C1CCN(c2ccc3nnnn3n2)CC1
vNsp12-rna2-31	Z1127921797	-9.2	0.307	398.461	REAL	C[C@@H]1Oc2c(cccc2C(=O)N2Cc3ccccc3[C@H](c3ccccc3)C2)NC1=O
vNsp12-rna2-32	Z131407602	-9.2	0.287	424.542	REAL	CN1CCC2(CC1)C[C@H](NC(=O)c1ccc3c(c1)-c1ccccc1C3)c1ccccc1O2
vNsp12-rna2-33	Z1626783611	-9.2	0.329	366.419	REAL	O=C(c1ccc2ccccc2c(=O)[nH]1)N1CC=C(c2ccccc3ccccc23)C1
vNsp12-rna2-34	Z1653427607	-9.2	0.287	445.448	REAL	O=C(C1CCN(c2ccc3nnnn3n2)CC1)N1CC[C@@H](c2cccc(C(F)(F)F)c2)C1
vNsp12-rna2-35	Z2108986966	-9.2	0.297	420.468	REAL	O=C(Nc1cccc(-c2ccc3c(c2)CCO3)c1)NC1CCC2(CC1)NC(=O)NC2=O
vNsp12-rna2-36	Z2590314585	-9.2	0.341	371.44	REAL	Cc1cnc2nc(C(=O)O[C@@H](C)C(=O)N[C@H](C)[C@@H]3C[C@H]4CC[C@H]3C4)nn2c1
vNsp12-rna2-37	Z31298221	-9.2	0.256	480.523	REAL	Cc1ccc(N2C(=O)/C(=C/NN3C(=O)N[C@](C)(c4ccccc4)C3=O)c3ccccc3C2=O)cc1C
vNsp12-rna2-38	ZINC000000692392	-9.2	0.287	418.407	ZINC	O=C1c2ccc(-c3nc4ccccc4c(=O)o3)cc2C(=O)N1c1ccccc2ccccc21
vNsp12-rna2-39	ZINC000003672765	-9.2	0.249	486.621	ZINC	Cc1cc(N2CCN(c3nc(N4CCc5ccccc5C4)nc4ccccc43)CC2)c2ccccc2n1
vNsp12-rna2-40	ZINC000006161729	-9.2	0.219	588.613	ZINC	Cc1ccc(-c2nnc(Nc3cccc(C(F)(F)F)c3)c3ccccc32)cc1S(=O)(=O)NCc1nc2ccccc2[nH]1
vNsp12-rna2-41	ZINC000013564332	-9.2	0.249	504.972	ZINC	O=C(c1ccc(Cl)cc1)[C@@H]1[C@@H]2C(=O)N(c3ccc4ccccc4c3)C(=O)[C@@H]2[C@@H]2c3ccccc3C=CN21
vNsp12-rna2-42	ZINC000017123578	-9.2	0.242	523.659	ZINC	Cc1ccc(-c2nnc(Nc3cccc4ccccc43)c3ccccc32)cc1S(=O)(=O)N1CCN(C)CC1
vNsp12-rna2-43	ZINC000020110122	-9.2	0.256	472.59	ZINC	Oc1ccccc1-c1nc2ccccc2c(N2CCN(C(c3ccccc3)c3ccccc3)CC2)n1
vNsp12-rna2-44	ZINC000021867174	-9.2	0.249	492.581	ZINC	Cc1cccc(-c2nnn3c2nc(O)c2ccc(C(=O)N4CCN(c5cc(C)ccc5C)CC4)cc23)c1
vNsp12-rna2-45	ZINC000034707359	-9.2	0.242	522.573	ZINC	C[C@@H]1CN(c2nc3ccccc3c3nnc(C4CCCC4)n32)CCN1C(=O)c1ccccC(F)(F)F)c1
vNsp12-rna2-46	ZINC000058133137	-9.2	0.263	459.552	ZINC	Cc1[nH]c2ccccc2c1C1=CCN(C(=O)c2nc(-c3ccccc3)n(-c3ccccc3)n2)CC1
vNsp12-rna2-47	ZINC000097111857	-9.2	0.249	492.538	ZINC	COc1ccc2c(c1)CCc1c(C(=O)N3CCc4c(nc5cc(-c6ccccc6)[nH]n5c4=O)C3)n[nH]c1-2
vNsp12-rna2-48	ZINC000229937939	-9.2	0.219	554.6	ZINC	CC1=C[C@@H]2N(c3ccccc31)[C@H](C(=O)c1ccccc1)[C@@H](C(=O)c1ccc3c(c1)OCO3)[C@]21c2ccccc2NC1=O
vNsp12-rna2-49	ZINC000254350209	-9.2	0.263	455.512	ZINC	O=C1c2ccccc2C(=O)c2cc(N=C3C=C(c4ccccc4)[C@@](O)(c4ccccc4)C3)ccc21
vNsp12-rna2-50	PV-001832260727	-9.1	0.303	407.473	REAL	CN1C[C@H](C(=O)Nc2ccccc(NC(=O)Nc3ccccc4c3CCCC4)c2)NC1=O
vNsp12-rna2-51	Z1229932710	-9.1	0.303	396.453	REAL	C[C@@H]1C/C(=C\c2ccccc2)c2nc3ccccc3c(C(=O)Nc3nnn[nH]3)c2C1
vNsp12-rna2-52	Z1315661211	-9.1	0.303	394.477	REAL	Cc1nnc(-c2ccc(C(=O)N3Cc4ccccc4C[C@H]3c3ccccc3)cc2)[nH]1
vNsp12-rna2-53	Z1576366492	-9.1	0.276	440.502	REAL	Cc1ccccc1Cn1c(NC(=O)CN2C(=O)[C@@H]3[C@H]4C=C[C@@H](C4)[C@H]3C2=O)nc2ccccc21
vNsp12-rna2-54	Z1626781463	-9.1	0.284	424.459	REAL	O=C(c1cnc2c(c1)c(=O)[nH]c(=O)n2C1CC1)N1CC=C(c2cccc3ccccc23)C1
vNsp12-rna2-55	Z1626783643	-9.1	0.303	398.421	REAL	Cn1c(=O)[nH]c(=O)c2cc(C(=O)N3CC=C(c4ccccc5ccccc45)C3)cnc21
vNsp12-rna2-56	Z1626785072	-9.1	0.294	411.46	REAL	C[C@]1(c2ccccc(C(=O)N3CC=C(c4ccccc5ccccc45)C3)c2)NC(=O)NC1=O
vNsp12-rna2-57	Z1740682282	-9.1	0.284	449.534	REAL	O=C(c1ccc2c(c1)S(=O)(=O)Nc1ncnn1-2)N1C[C@@H](c2ccccc2)[C@@H]2CCCC[C@H]21
vNsp12-rna2-58	Z1873332964	-9.1	0.284	436.486	REAL	C[C@]1(c2ccccc(CNC(=O)N3CC4(CCCC4)c4ccccc4)c2)NC(=O)NC1=O
vNsp12-rna2-59	Z1888975699	-9.1	0.276	440.502	REAL	C[C@]1(c2ccccc(CNC(=O)N3C[C@H](c4ccccc4)c4ccccc43)c2)NC(=O)NC1=O
vNsp12-rna2-60	Z1891087259	-9.1	0.294	431.475	REAL	Cc1ccc(NS(=O)(=O)c2cccc(-c3nc(-c4ccc5cc[nH]c5n4)no3)c2)cc1
vNsp12-rna2-61	Z1907685565	-9.1	0.284	448.419	REAL	O=C(NC[C@]1(O)[C@H]2[C@@H]3C[C@@H]4[C@@H]5[C@@H]3C[C@@H]2[C@@H]5[C@@H]41)c1nnn(-c2ccccc2F)c1C(F)(F)F
vNsp12-rna2-62	Z1991454930	-9.1	0.284	437.538	REAL	Cc1cc(O[C@@H]2CCN(C)C2=O)ccc1NC(=O)NC[C@@]1(O)[C@@H]2[C@@H]3C[C@H]4[C@H]5[C@@H]3C[C@@H]2[C@@H]5[C@@H]41
vNsp12-rna2-63	Z1991746043	-9.1	0.276	439.514	REAL	CN1C(=O)COc2cc(NC(=O)NC[C@@H]3CC4c5ccccc5C3c3ccccc34)ccc21
vNsp12-rna2-64	Z2093727904	-9.1	0.284	435.566	REAL	Cc1ccc(C23C[C@@H]4C[C@H](CC(C(=O)NC5CCC6(CC5)NC(=O)NC6=O)(C4)C2)C3)cc1
vNsp12-rna2-65	Z2112412450	-9.1	0.284	433.55	REAL	CC1(C)CC[C@@H](NC(=O)N2C[C@@H](C[C@H]3COCC(=O)N3)c3ccccc32)c2ccccc21
vNsp12-rna2-66	Z2119577473	-9.1	0.325	384.478	REAL	C[C@H]1CCCc2ccccc2[C@H]1NC(=O)NC1CCC2(CC1)NC(=O)NC2=O
vNsp12-rna2-67	Z2155695547	-9.1	0.303	402.453	REAL	C[C@@]1(c2ccc(-c3noc([C@H]4[C@H]5[C@@H]6C[C@H]7[C@H]8[C@@H]6C[C@H]5[C@@H]8[C@@H]74)n3)cc2)NC(=O)NC1=O
vNsp12-rna2-68	Z2157920189	-9.1	0.303	402.453	REAL	C[C@@]1(c2ccccc(-c3noc([C@H]4[C@H]5[C@H]6C[C@H]7[C@H]8[C@H]6C[C@H]5[C@H]8[C@H]74)n3)c2)NC(=O)NC1=O
vNsp12-rna2-69	Z225733110	-9.1	0.294	419.436	REAL	O=C1NC(=O)C2(CCN(C(=O)c3ccc4c(c3)C[C@H](c3ccccc3)OC4=O)CC2)N1
vNsp12-rna2-70	Z318479656	-9.1	0.294	411.46	REAL	O=C(c1cc2ccccc2c(=O)[nH]1)N1CCN(C(=O)c2cccc3ccccc23)CC1
vNsp12-rna2-71	Z363627986	-9.1	0.26	465.551	REAL	C[C@]12CCC(=O)N1c1ccccc1C(=O)N2CC(=O)N1Cc2ccccc2[C@H](c2ccccc2)C1
vNsp12-rna2-72	Z432524218	-9.1	0.284	447.558	REAL	NS(=O)(=O)c1ccc(CNC(=O)NC[C@@H]2CC3c4ccccc4C2c2ccccc23)cc1
vNsp12-rna2-73	Z992454150	-9.1	0.314	388.426	REAL	C[C@]1(c2ccccc(CNC(=O)Nc3cccc4ccccc34)c2)NC(=O)NC1=O
vNsp12-rna2-74	ZINC000000970621	-9.1	0.314	375.47	ZINC	O=C1CCCC2=C1c1c(ccc3ccccc31)N[C@@H]2c1cccc2ccccc21
vNsp12-rna2-75	ZINC000001789604	-9.1	0.233	532.666	ZINC	O=c1[nH]c(CSc2nc3ccccc3c(=O)n2-c2ccccc2)nc2c1C1(CCCCC1)Cc1ccccc1-2
vNsp12-rna2-76	ZINC000002751243	-9.1	0.26	455.468	ZINC	O=C1c2cc3oc4ccccc4c4ccccc4oc3cc2C(=O)N1c1ccccc2ccccc21
vNsp12-rna2-77	ZINC000003205568	-9.1	0.253	558.411	ZINC	O=C(/N=C1\N=C2C=CC(Br)=CN2Cc2ccccc21)c1ccc2c(c1)S(=O)(=O)c1ccccc1C2=O
vNsp12-rna2-78	ZINC000003371319	-9.1	0.217	563.538	ZINC	O=C1c2ccccc2/C(=C/Nc2nnc(-c3ccccc3)c(-c3ccccc3)n2)C(=O)N1c1ccccC(F)(F)F)c1
vNsp12-rna2-79	ZINC000012526505	-9.1	0.268	444.533	ZINC	O=C(Cn1c2ccccc2c(=O)c2ccccc21)N1CCc2ccccc2[C@@H](c2ccccc2)C1
vNsp12-rna2-80	ZINC000017862766	-9.1	0.228	520.587	ZINC	O=C(Nc1ccc2ccccc2c1)c1cccc(N2C(=O)[C@H]3[C@@H](C2=O)C2c4ccccc4C3c3ccccc32)c1
vNsp12-rna2-81	ZINC000038830264	-9.1	0.253	479.535	ZINC	O=C1C[C@@H](N2Cc3[nH]c4ccccc4c3[C@H](c3ccccc3)C2)C(=O)N1c1ccc2c(c1)OCCO2
vNsp12-rna2-82	ZINC000038830266	-9.1	0.253	479.535	ZINC	O=C1C[C@@H](N2Cc3[nH]c4ccccc4c3[C@H](c3ccccc3)C2)C(=O)N1c1ccc2c(c1)OCCO2
vNsp12-rna2-83	ZINC000039929440	-9.1	0.268	449.596	ZINC	O=c1[nH]c2ccccc2n1C1CCN(CCC=C2c3ccccc3CCc3ccccc32)CC1
vNsp12-rna2-84	ZINC000100504092	-9.1	0.294	404.512	ZINC	O=c1ccc2n1C[C@H]1C[C@H]2CN(Cc2cccc3ccc4ccc5ccc2c3c45)C1
vNsp12-rna2-85	ZINC000100505724	-9.1	0.246	488.542	ZINC	O=C1[C@@H]2[C@H]3C=C[C@@H](C3)[C@@H]2C(=O)N1c1ccc2c(c1)-c1cc(N3C(=O)[C@@H]4[C@H]5C=C[C@@H](C5)[C@@H]4C3=O)ccc1C2
vNsp12-rna2-86	ZINC000100505727	-9.1	0.246	488.542	ZINC	O=C1[C@@H]2[C@H]3C=C[C@@H](C3)[C@@H]2C(=O)N1c1ccc2c(c1)-c1cc(N3C(=O)[C@H]4[C@H]5C=C[C@H](C5)[C@@H]4C3=O)ccc1C2
vNsp12-rna2-87	ZINC000102648603	-9.1	0.246	495.665	ZINC	CC1(C)CC(O)=C2C(=Nc3cccc3N(C(=O)NC34CC5CC(CC(C5)C3)C4)[C@@H]2c2ccccc2)C1
vNsp12-rna2-88	ZINC000104480052	-9.1	0.253	490.945	ZINC	O=C(NC1=CC=C[C@@H]2C(=O)c3ccccc3C(=O)[C@H]12)c1cc(-c2ccccc2Cl)nc2ccccc21
vNsp12-rna2-89	ZINC000137060050	-9.1	0.222	561.562	ZINC	O=C(Nc1cccc(-c2ccnc(N3CCN(Cc4ccc5c(c4)OCO5)CC3)n2)c1)c1ccccC(F)(F)F)c1
vNsp12-rna2-90	ZINC000226919882	-9.1	0.26	484.981	ZINC	Cc1ccc(Cl)cc1NC(=O)c1ccccc1N1C(=O)[C@@H]2[C@H]3C[C@@H](c4ccccc4)[C@@H](C3)[C@@H]2C1=O
vNsp12-rna2-91	ZINC000229905129	-9.1	0.212	589.046	ZINC	CC1=C[C@@H]2N(c3ccccc31)[C@H](C(=O)c1ccccc1Cl)[C@@H](C(=O)c1ccc3c(c1)OCO3)[C@@]21C(=O)Nc2ccccc21
vNsp12-rna2-92	ZINC000230076522	-9.1	0.268	489.357	ZINC	O=C1[C@@H]2ON(c3ccccc3)[C@H](c3ccc4ccccc43)[C@@H]2C(=O)N1c1c(Cl)cccc1Cl
vNsp12-rna2-93	ZINC000245377192	-9.1	0.246	488.542	ZINC	O=C1[C@@H]2[C@H]3C=C[C@@H](C3)[C@H]2C(=O)N1c1ccc2c(c1)-c1cc(N3C(=O)[C@@H]4[C@H]5C=C[C@@H](C5)[C@@H]4C3=O)ccc1C2
vNsp12-rna2-94	ZINC000247756664	-9.1	0.26	465.591	ZINC	O=C1c2ccccc2C(=O)c2cc3c(cc21)N[C@@H]1CC[C@H]2[C@H]4[C@@H](CC[C@@H]3[C@H]14)C(=O)[C@H]1CCCC[C@@H]21
vNsp12-rna2-95	ZINC000247889806	-9.1	0.239	498.58	ZINC	Cc1ccc(N2C(=O)[C@H]3[C@H]4C=Cc5c6ccccc6ccc5N4[C@@H](C(=O)c4ccccc4)[C@H]3C2=O)c(C)c1
vNsp12-rna2-96	ZINC000254722125	-9.1	0.253	558.411	ZINC	O=C(N=C1N=C2C=CC(Br)=CN2Cc2ccccc21)c1ccc2c(c1)S(=O)(=O)c1ccccc1C2=O
vNsp12-rna2-97	ZINC000409044394	-9.1	0.246	481.593	ZINC	Cc1ccc(C(=C2[C@H]3C=C[C@H]2[C@@H]2C(=O)N(c4ccccc5ccccc54)C(=O)[C@@H]32)c2ccc(C)cc2)cc1
vNsp12-rna2-98	ZINC000409334997	-9.1	0.253	466.503	ZINC	O=C(Nc1ccc2ccccc2c1)Nc1ccc2nc3c4ccccn4c4ncccc4c3nc2c1
vNsp12-rna2-99	PV-001824490387	-9	0.321	380.378	REAL	Cc1ccc(F)c2[nH]c(C(=O)Nc3cccc([C@@]4(C)NC(=O)NC4=O)c3)cc12
vNsp12-rna2-100	PV-001961987050	-9	0.31	418.923	REAL	O=C(NC1CCC2(CC1)NC(=O)NC2=O)N[C@H]1CCC[C@@H](c2ccc(Cl)cc2)C1

Supplementary Table 57. Top 100 virtual hits of the screen against the RNA binding site of nsp12 (Screen ID: 29). The name of each compound consists of the initial letter 'v' for virtual hit, followed by the target protein name and the target site ('rna' for RNA binding site, 2 for docking scenario 2). The score is the docking score given by QuickVina 2 in kcal/mol. The ligand efficiency (LE) is computed as LE = -score/#NonH, where #NonH is the number of heavy (i.e. non hydrogen) atoms.

Name	Catalog ID	Score	LE	MW	Library	SMILES
vNsp12-rna2-101	Z1007506116	-9.0	0.257	493.58	REAL	Cc1ccc(C)c(S(=O)(=O)Nc2cccc(C(=O)N3CCN(C(=O)c4cccc(O)c4)CC3)c2)c1
vNsp12-rna2-102	Z1082329362	-9.0	0.281	423.43	REAL	O=C(Nc1nc2ccccc2c(=O)[nH]1)c1nn(Cc2ccccc2)c(=O)c2ccccc12
vNsp12-rna2-103	Z1082706532	-9.0	0.281	429.52	REAL	O=C1NC(=O)C2(CCC(C(=O)NC[C@H]3CC4c5ccccc5C3c3ccccc34)CC2)N1
vNsp12-rna2-104	Z1278579190	-9.0	0.273	439.51	REAL	CN1C(=O)COc2ccc(NC(=O)NC[C@@H]3CC4c5ccccc5C3c3ccccc34)cc21
vNsp12-rna2-105	Z1312817852	-9.0	0.290	412.45	REAL	Cc1cc(C(=O)N2Cc3ccccc3[C@H](c3ccccc3)C2)nc2nc(O)[nH]c(=O)c12
vNsp12-rna2-106	Z1334317478	-9.0	0.300	395.42	REAL	O=C(NCc1n[nH]c(=O)[nH]1)c1cc(-c2cccc3ccccc23)nc2ccccc12
vNsp12-rna2-107	Z1374247342	-9.0	0.290	414.51	REAL	NC(=O)c1cc(C(=O)N2CCC[C@]3(CCCc4ccccc43)C2)nn1-c1ccccc1
vNsp12-rna2-108	Z1451196645	-9.0	0.300	410.47	REAL	C[C@]1(c2cccc(C(=O)NNC(=O)C34CC5CC(CC(C5)C3)C4)c2)NC(=O)NC1=O
vNsp12-rna2-109	Z1460558960	-9.0	0.310	384.48	REAL	O=C(NCc1ccc2c(c1)COC2)N1Cc2ccccc2[C@@H](c2ccccc2)C1
vNsp12-rna2-110	Z1507814109	-9.0	0.300	402.45	REAL	NC(=O)c1cc(C(=O)N2CCO[C@]3(CCc4ccccc43)C2)nn1-c1ccccc1
vNsp12-rna2-111	Z1545339320	-9.0	0.281	430.55	REAL	C[C@H](Cn1ncc2ccccc2c1=O)NC(=O)N1CCC[C@]2(CCCc3ccccc32)C1
vNsp12-rna2-112	Z1608113516	-9.0	0.321	367.41	REAL	O=C(c1nc2ccccc2c(=O)[nH]1)N1CC=C(c2ccccc3ccccc23)C1
vNsp12-rna2-113	Z1626784984	-9.0	0.281	426.48	REAL	Cc1cc(C(=O)N2CC=C(c3cccc4ccccc34)C2)nc2c1c(=O)n(C)c(=O)n2C
vNsp12-rna2-114	Z1682390413	-9.0	0.273	440.46	REAL	C[C@@]1(c2ccc(-c3noc(-c4cc(Cc5ccccc5)ccc4O)n3)cc2)NC(=O)NC1=O
vNsp12-rna2-115	Z1684580231	-9.0	0.273	440.46	REAL	C[C@]1(c2cccc(-c3noc(-c4cc(Cc5ccccc5)ccc4O)n3)c2)NC(=O)NC1=O
vNsp12-rna2-116	Z1684581857	-9.0	0.310	390.40	REAL	C[C@]1(c2cccc(-c3noc([C@H]4OCCc5ccccc54)n3)c2)NC(=O)NC1=O
vNsp12-rna2-117	Z1888993359	-9.0	0.273	440.50	REAL	C[C@]1(c2ccc(CNC(=O)N3C[C@H](c4ccccc4)c4ccccc43)cc2)NC(=O)NC1=O
vNsp12-rna2-118	Z1907681376	-9.0	0.273	442.52	REAL	Cn1c(=O)[nH]c2ncc(-c3cccc(C(=O)NC[C@]4(O)[C@@H]5[C@H]6C[C@@H]7[C@H]8[C@H]6C[C@H]5[C@@H]8[C@H]74)c3)cc21
vNsp12-rna2-119	Z1921555484	-9.0	0.290	418.50	REAL	O=C1NC(=O)[C@@]2(CCCN(CC(=O)N3Cc4ccccc4[C@@H](c4ccccc4)C3)C2)N1
vNsp12-rna2-120	Z1987511564	-9.0	0.290	417.42	REAL	Cc1cc(C(=O)NNC(=O)c2ccccc[C@@]3(C)NC(=O)NC3=O)c2)c2ccccc2n1
vNsp12-rna2-121	Z2012462622	-9.0	0.290	436.36	REAL	Cc1cc(C(=O)N2CC[C@@](F)(c3cccc(C(F)(F)F)c3)C2)nc2nc(O)[nH]c(=O)c12
vNsp12-rna2-122	Z2071432641	-9.0	0.310	390.49	REAL	Cc1ccc(-n2cnnn2)cc1NC(=O)N1CCC[C@@](C)(c2ccccc2)CC1
vNsp12-rna2-123	Z2104800155	-9.0	0.281	429.56	REAL	O=C1Nc2ccccc2[C@@H]1C1CCN(C(=O)NC2[C@H]3CC[C@H]2Cc2ccccc2C3)CC1
vNsp12-rna2-124	Z2157919734	-9.0	0.290	424.48	REAL	C[C@]1(c2cccc(-c3noc(CC45C[C@H]6C[C@@H](CC(F)(C6)C4)C5)n3)c2)NC(=O)NC1=O
vNsp12-rna2-125	Z2171979207	-9.0	0.300	402.41	REAL	C[C@]1(c2cccc(-c3noc(-c4cccc5c4CC(=O)CC5)n3)c2)NC(=O)NC1=O
vNsp12-rna2-126	Z2212550647	-9.0	0.273	437.50	REAL	O=C1CNC(=O)c2ccc(C(=O)NC[C@H]3CC4c5ccccc5C3c3ccccc34)cc2N1
vNsp12-rna2-127	Z228329578	-9.0	0.310	394.56	REAL	Cc1ccc(C23C[C@H]4C[C@@H](CC(C(=O)NCC(=O)N5CCCC5)(C4)C2)C3)cc1C
vNsp12-rna2-128	Z2299371305	-9.0	0.300	395.50	REAL	O=C(c1ccc2c(c1)-c1ccccc1C2)N1CCC2(CC1)OCCc1ccccc12
vNsp12-rna2-129	Z2781387438	-9.0	0.333	370.45	REAL	NC(=O)CCN(Cc1ccccc1)C(=O)COC(=O)[C@@H]1C[C@@H]2C[C@@H]1[C@H]1C[C@H]21
vNsp12-rna2-130	Z2785110607	-9.0	0.333	365.43	REAL	CCCOc1ccccc1C(=O)CNC(=O)[C@]12[C@@H]3C(=O)[C@@H]4[C@H]5C[C@@H]([C@@H]41)[C@@H]2[C@H]53
vNsp12-rna2-131	Z289554710	-9.0	0.290	412.45	REAL	Cn1c(=O)[nH]c(=O)c2cc(C(=O)N3Cc4ccccc4[C@@H](c4ccccc4)C3)cnc21
vNsp12-rna2-132	Z2903471154	-9.0	0.243	499.53	REAL	Cn1cc(-c2noc([C@H]3CCCN(C(=O)OCC4c5ccccc5-c5ccccc54)C3)n2)c(=O)[nH]c1=O
vNsp12-rna2-133	Z2972035205	-9.0	0.310	393.42	REAL	O=C1Nc2ccc(F)cc2C2(CN(C(=O)NC[C@H]3[C@@H]4Cc5ccccc5[C@@H]34)C2)O1
vNsp12-rna2-134	Z411714436	-9.0	0.243	499.61	REAL	Cc1c(NC(=O)c2cccc(NC(=O)N[C@H]3C[C@@H]4C[C@H]3[C@H]3CCC[C@H]43)c2)c(=O)n(-c2ccccc2)n1C
vNsp12-rna2-135	Z493139922	-9.0	0.290	415.54	REAL	O=C(NCCc1nnc2n1CCCCC2)N1Cc2ccccc2[C@@H](c2ccccc2)C1
vNsp12-rna2-136	Z56990041	-9.0	0.281	422.49	REAL	O=C(c1n[nH]c(=O)c2ccccc12)N1CCN(C2c3ccccc3-c3ccccc32)CC1
vNsp12-rna2-137	Z743656142	-9.0	0.321	389.45	REAL	COC(=O)COc1cccc(C(=O)OCC(=O)N[C@@H](C)[C@H]2C[C@@H]3CC[C@@H]2C3)c1
vNsp12-rna2-138	Z855944666	-9.0	0.250	498.51	REAL	Cc1ccc(NC(=O)c2cccc(C(F)(F)F)c2)cc1NC(=O)N[C@@H]1CCCN(c2nccn2)C1
vNsp12-rna2-139	Z975213858	-9.0	0.265	471.62	REAL	O=C(Cc1ccc(NC(=O)N2Cc3ccccc3[C@H](c3ccccc3)C2)cc1)N1CCSCC1
vNsp12-rna2-140	ZINC000000659879	-9.0	0.237	496.57	ZINC	O=C(c1ccccc1)c1ccc2c(c1)NC1=C(C(=O)C[C@H](c3ccccc3)C1)[C@@H]1c3ccccc3C(=O)N21
vNsp12-rna2-141	ZINC000000828306	-9.0	0.250	469.46	ZINC	O=C1c2cccc3cccc(c32)C(=O)N1c1cccc(N2C(=O)c3ccc4cccc(c43)C2=O)n1
vNsp12-rna2-142	ZINC000001076771	-9.0	0.290	414.44	ZINC	O=C(Nc1nc2n(n1)[C@@H](c1ccc(F)cc1)C[C@@H](c1ccccc1)N2)c1ccccnc1
vNsp12-rna2-143	ZINC000001263231	-9.0	0.257	456.46	ZINC	O=C1c2cc3oc4ccccc4c4ccccc4oc3cc2C(=O)N1c1cccc2ncccc21
vNsp12-rna2-144	ZINC000001588368	-9.0	0.265	446.52	ZINC	Cc1[nH]c2ccccc2c1-c1cc(-c2cc(-c3c(C)[nH]c4ccccc43)nc(N)n2)nc(N)n1
vNsp12-rna2-145	ZINC000002412360	-9.0	0.243	485.49	ZINC	O=C(Nc1ccc(-c2cc3ccccc3oc2=O)cc1)c1cccc(-c2cc3ccccc3oc2=O)c1
vNsp12-rna2-146	ZINC000002939976	-9.0	0.250	472.50	ZINC	Cc1ccc2nc(-c3cccc(NC(=O)c4oc(=O)c5ccccc5c4-c4ccccc4)c3)oc2c1
vNsp12-rna2-147	ZINC000008454451	-9.0	0.257	468.60	ZINC	Cc1ccc(-c2cc(C(=O)NNC(=O)NC34CC5CC(CC(C5)C3)C4)c3ccccc3n2)c(C)c1
vNsp12-rna2-148	ZINC000009714961	-9.0	0.257	492.53	ZINC	O=C(Nc1nnc(-c2ccc3c(c2)CCCC3)o1)c1ccc(NS(=O)(=O)c2ccc(F)cc2)cc1
vNsp12-rna2-149	ZINC000009971314	-9.0	0.257	462.56	ZINC	Cc1cc(C)nc(N/C(=N/C(=O)c2ccccc3ccccc32)NCCc2c[nH]c3ccccc23)n1
vNsp12-rna2-150	ZINC000012742035	-9.0	0.257	490.62	ZINC	C[C@@H]1CN(S(=O)(=O)c2ccccC(C(=O)N3Cc4ccccc4[C@H](c4ccccc4)C3)c2)C[C@H](C)O1
vNsp12-rna2-151	ZINC000012812871	-9.0	0.257	461.53	ZINC	CN1CCCN(C(=O)c2nc(-c3ccccc3)n(-c3ccccc3)n2)c2nc3ccccc3nc21
vNsp12-rna2-152	ZINC000016695652	-9.0	0.265	485.65	ZINC	C[C@H]1C[C@@]2(CC(C)(C)C1)NC(=O)N(CC(=O)Nc1nnc(C34CC5CC(CC(C5)C3)C4)s1)C2=O
vNsp12-rna2-153	ZINC000017159461	-9.0	0.237	524.64	ZINC	Cc1ccc(-c2nnc(Nc3ccc4ccccc43)c3ccccc32)cc1S(=O)(=O)NC[C@H]1CCCO1
vNsp12-rna2-154	ZINC000019782240	-9.0	0.265	461.65	ZINC	CC1(C)C[C@]2(CCCN(Cc3nc4c(c(=O)[nH]3)C(CCCCC3)Cc3ccccc3-4)C2)CCO1
vNsp12-rna2-155	ZINC000034703510	-9.0	0.265	441.49	ZINC	C[C@H]1Cc2ccccc2N1C(=O)c1ccc2nc3c4nccc4c4ccenc4c3nc2c1
vNsp12-rna2-156	ZINC000085392802	-9.0	0.237	502.62	ZINC	O=C([C@H]1CC(=O)N(c2ccccc2)C1)N1CCC(c2c[nH]c3ccccc32)(c2c[nH]c3ccccc32)CC1
vNsp12-rna2-157	ZINC000100505725	-9.0	0.243	488.54	ZINC	O=C1[C@@H]2[C@H]3C=C[C@@H](C3)[C@@H]2C(=O)N1c1ccc2c(c1)-c1cc(N3C(=O)[C@H]4[C@H]5C=C[C@@H](C5)[C@@H]4C3=O)ccc1C2
vNsp12-rna2-158	ZINC000101360494	-9.0	0.257	453.54	ZINC	O=C1[C@H]2[C@H]3C=C[C@@H](C3=C(c3ccccc3)c3ccccc3)[C@@H]2C(=O)N1c1ccccc2ccccc21
vNsp12-rna2-159	ZINC000169314210	-9.0	0.205	575.64	ZINC	O=C1[C@@H]2[C@@H](C(=O)N1c1ccc(F)cc1)[C@@]1(c3ccccc3)C(=O)[C@@]2(c2ccccc2)C(c2ccccc2)=C1c1ccccc1
vNsp12-rna2-160	ZINC000169314212	-9.0	0.205	575.64	ZINC	O=C1[C@@H]2[C@H](C(=O)N1c1ccc(F)cc1)[C@@]1(c3ccccc3)C(=O)[C@@]2(c2ccccc2)C(c2ccccc2)=C1c1ccccc1
vNsp12-rna2-161	ZINC000169314214	-9.0	0.205	575.64	ZINC	O=C1[C@H]2[C@H](C(=O)N1c1ccc(F)cc1)[C@@]1(c3ccccc3)C(=O)[C@@]2(c2ccccc2)C(c2ccccc2)=C1c1ccccc1
vNsp12-rna2-162	ZINC000229954725	-9.0	0.265	472.90	ZINC	O=C1[C@@H]2ON(c3ccccc3)[C@H](c3ccc4ccccc43)[C@@H]2C(=O)N1c1ccc(Cl)c(F)c1
vNsp12-rna2-163	ZINC000229956291	-9.0	0.250	488.46	ZINC	O=C1[C@@H]2ON(c3ccccc3)[C@H](c3ccc4ccccc43)[C@@H]2C(=O)N1c1cccc(C(F)(F)F)c1
vNsp12-rna2-164	ZINC000245377193	-9.0	0.243	488.54	ZINC	O=C1[C@@H]2[C@H]3C=C[C@@H](C3)[C@H]2C(=O)N1c1ccc2c(c1)-c1cc(N3C(=O)[C@@H]4[C@H]5C=C[C@@H](C5)[C@H]4C3=O)ccc1C2
vNsp12-rna2-165	ZINC000247756658	-9.0	0.257	465.59	ZINC	O=C1c2ccccc2C(=O)c2ec3c(cc21)N[C@@H]1CC[C@@H]2[C@@H]4CCCC[C@@H]4C(=O)[C@@H]4CC[C@@H]3[C@H]1[C@@H]42
vNsp12-rna2-166	ZINC000253407012	-9.0	0.250	475.50	ZINC	Cn1cc/C=C2\Oc3c(ccc4c3[C@H](C3=Cc5ccccc5OC3)CC(=O)O4)C2=O)c2ccccc21
vNsp12-rna2-167	ZINC000257196115	-9.0	0.265	463.60	ZINC	O=C([C@@H]1C[C@@H]2[C@H](C1)C(=O)NCCCCCN2Cc1ccccc(F)c1)N1CCc2ccccc2C1
vNsp12-rna2-168	ZINC000257309042	-9.0	0.273	444.58	ZINC	Cc1ccccc1Cc1ccccc([C@H]2CN(C(=O)c3n[nH]c4c3CCCCC4)CCO2)n1
vNsp12-rna2-169	ZINC000524733410	-9.0	0.281	450.93	ZINC	O=C(CC[C@@H]1NC(=O)c2ccccc2NC1=O)N[C@@H]1CCCc2c3ccccc(Cl)c3[nH]c21
vNsp12-rna2-170	PV-001798863491	-8.9	0.307	388.42	REAL	Cc1ccc2c(c1)C(=O)O[C@@](C)(C(=O)NNC(=O)c1cccc3ccccc13)C2
vNsp12-rna2-171	PV-001808365005	-8.9	0.297	407.42	REAL	O=C(/C=C/c1ccc(F)c2ccccc12)Nc1ccc(F)c(N2CCCNC2=O)c1
vNsp12-rna2-172	PV-001833854348	-8.9	0.318	374.36	REAL	O=C(NNC(=O)c1cccc2ccccc12)c1cccc(-c2noc(O)n2)c1
vNsp12-rna2-173	PV-001844913027	-8.9	0.318	376.46	REAL	CC1(C)CCc2ccccc2[C@@H](NC(=O)c2cccc(Nc3nnn[nH]3)c2)C1
vNsp12-rna2-174	PV-001850122044	-8.9	0.287	420.42	REAL	C[C@]1(c2cccc(C(=O)Nc3cccc(C4CC(=O)NC(=O)C4)c3)c2)NC(=O)NC1=O
vNsp12-rna2-175	PV-001850122491	-8.9	0.287	420.42	REAL	C[C@@]1(c2cccc(C(=O)Nc3cccc(C4CC(=O)NC(=O)C4)c3)cc2)NC(=O)NC1=O
vNsp12-rna2-176	PV-001857842639	-8.9	0.297	419.41	REAL	Cc1n[nH]c(N2CCN(C(=O)c3nc(-c4ccccc(C(F)(F)F)c4)[nH]c3C)CC2)n1
vNsp12-rna2-177	PV-001948140128	-8.9	0.287	420.44	REAL	Cc1c(NC(=O)N[C@@H](C)c2ccc(F)c3ccccc23)cccc1N1C(=O)CNC1=O
vNsp12-rna2-178	PV-001948844490	-8.9	0.371	346.39	REAL	O=C(NC[C@H]1C[C@H]2[C@H]1[C@H]1C[C@H]21)N[C@H](C[C@H]1CCCO1)C(F)(F)F
vNsp12-rna2-179	PV-001950144951	-8.9	0.307	390.49	REAL	CC1(C)CCc2ccccc2[C@@H](NC(=O)Nc2ccc3[nH]c(C(N)=O)cc3c2)C1
vNsp12-rna2-180	PV-001958247051	-8.9	0.297	405.50	REAL	Cc1cccc(C(NC(=O)N2CCC[C@@H](c3nc(=O)[nH][nH]3)C2)c2ccccc2C)c1
vNsp12-rna2-181	PV-001961986936	-8.9	0.307	418.92	REAL	O=C(NC1CCC2(CC1)NC(=O)NC2=O)N[C@H]1CCC[C@@H](c2cccc(Cl)c2)C1
vNsp12-rna2-182	PV-001965881797	-8.9	0.318	382.48	REAL	CC1(C)CCc2ccccc2[C@@H](NC(=O)N[C@H]2COc3cc(F)ccc3C2)C1
vNsp12-rna2-183	PV-001969236179	-8.9	0.307	389.50	REAL	CC1(C)CCc2ccccc2[C@@H](NC(=O)NCc2c[nH]c(=O)c3ccccc23)C1
vNsp12-rna2-184	Z1000934670	-8.9	0.278	424.46	REAL	C[C@@]1(c2cccc(CNC(=O)c3cc4ccccc4c4cccnc34)c2)NC(=O)NC1=O
vNsp12-rna2-185	Z1014750122	-8.9	0.278	424.46	REAL	C[C@@]1(c2ccc(CNC(=O)c3cc4ccccc4c4cccnc34)cc2)NC(=O)NC1=O
vNsp12-rna2-186	Z1126828423	-8.9	0.278	424.50	REAL	C[C@@H]1Oc2c(cccc2C(=O)NC[C@@H]2CC3c4ccccc4C2c2ccccc23)NC1=O
vNsp12-rna2-187	Z1180570708	-8.9	0.278	423.52	REAL	O=C(N[C@@H]1CCCc2[nH]c(=O)ccc21)N[C@H](c1ccccc1)c1cccc2ccccc12
vNsp12-rna2-188	Z1311812314	-8.9	0.307	392.50	REAL	CCNC(=O)N1CCc2ccc(NC(=O)N[C@]3(C)CCCc4ccccc43)cc21
vNsp12-rna2-189	Z1313212974	-8.9	0.307	384.39	REAL	Cc1cc(C(=O)N2Cc3ccccc3-c3ccccc32)nc2nc(O)[nH]c(=O)c12
vNsp12-rna2-190	Z1331865194	-8.9	0.307	395.50	REAL	C[C@H](NC(=O)c1ccc([C@@]2(C)NC(=O)NC2=O)cc1)C12CC3CC(CC(C3)C1)C2
vNsp12-rna2-191	Z1371499539	-8.9	0.287	419.52	REAL	O=C1CC2(CCN(C(=O)[C@H]3CCCN(C(=O)c4cccc5ccccc45)C3)CC2)CN1
vNsp12-rna2-192	Z1374246953	-8.9	0.287	421.50	REAL	Cn1c(=O)[nH]c(=O)c2[nH]c(CCC(=O)N3CCC[C@]4(CCCc5ccccc54)C3)nc21
vNsp12-rna2-193	Z1374247013	-8.9	0.278	445.45	REAL	Cc1nc(C(=O)N2CCC[C@]3(CCCc4ccccc43)C2)nn1-c1nnc(C(F)(F)F)[nH]1
vNsp12-rna2-194	Z1382170248	-8.9	0.278	434.54	REAL	Cc1cccc(C(NC(=O)N2CCC([C@@]3(C)NC(=O)NC3=O)CC2)c2ccccc2)c1
vNsp12-rna2-195	Z1413608816	-8.9	0.287	419.52	REAL	O=C1CN(C(=O)[C@H]2CCCN(C(=O)c3ccc4ccccc34)C2)[C@H]2CCCC[C@H]2N1
vNsp12-rna2-196	Z1554953321	-8.9	0.287	415.54	REAL	CCc1c(C)nn(-c2cccc(C(=O)N3CCO[C@]4(CCc5ccccc54)C3)c2)c1C
vNsp12-rna2-197	Z1578292081	-8.9	0.278	425.49	REAL	Cn1cnn(-c2ccc(NC(=O)N3Cc4ccccc4[C@H](c4ccccc4)C3)cc2)c1=O
vNsp12-rna2-198	Z1593680269	-8.9	0.278	430.51	REAL	CN(C(=O)c1n[nH]c2ccccc12)[C@@H]1CCCC[C@@H]1N(C)C(=O)c1n[nH]c2ccccc12
vNsp12-rna2-199	Z1626784946	-8.9	0.307	384.43	REAL	C[C@H]1Oc2c(cccc2C(=O)N2CC=C(c3cccc4ccccc34)C2)NC1=O
vNsp12-rna2-200	Z1684580509	-8.9	0.307	384.39	REAL	C[C@]1(c2cccc(-c3noc(-c4cccc5ccccc45)n3)c2)NC(=O)NC1=O

Supplementary Table 58. Virtual screening hits 101 to 200 of the screen against the RNA binding site of nsp12 (Screen ID: 29). Compounds were filtered so that hits had MW < 600 dalton, cLogP < 6, number of hydrogen bond acceptors < 11, and no reactive functional groups. The name of each compound consists of the initial letter 'v' for virtual hit, followed by the target protein name and the target site ('rna' for RNA binding site, 2 for docking scenario 2). The score is the docking score given by QuickVina 2 in kcal/mol. The ligand efficiency (LE) is computed as LE = -score/#NonH, where #NonH is the number of heavy (i.e. non hydrogen) atoms.

Name	Catalog ID	Score	LE	MW	Library	SMILES
vNsp12-nsp7.1-1	ZINC000001862466	-11.2	0.32	455.468	ZINC	Cc1nc(-c2cc3c(ccc4ccccc43)oc2=O)cc2c1c(=O)oc1ccc3ccccc3c12
vNsp12-nsp7.1-2	Z355404454	-10.8	0.348	409.488	REAL	Cc1ccc2[nH]c3c(c2c1)CN([C@@H]1CC(=O)N(c2ccc4ccccc4c2)C1=O)CC3
vNsp12-nsp7.1-3	ZINC000002212711	-10.8	0.327	429.474	ZINC	O=C(Nc1ccc2c(c1)Cc1ccccc1-2)c1ccnc(-c2cc3ccccc3oc2=O)c1
vNsp12-nsp7.1-4	ZINC000408765156	-10.7	0.289	479.578	ZINC	O=C1[C@H]2[C@H]3C=C[C@@H](C3=C(c3ccccc3)c3ccccc3)[C@@H]2C(=O)N1c1ccccc1-c1ccccc1
vNsp12-nsp7.1-5	ZINC000408765164	-10.7	0.289	479.578	ZINC	O=C1[C@@H]2[C@H]3C=C[C@@H](C3=C(c3ccccc3)c3ccccc3)[C@@H]2C(=O)N1c1ccccc1-c1ccccc1
vNsp12-nsp7.1-6	ZINC000001099260	-10.6	0.294	474.427	ZINC	O=C1NC(=O)c2cc(N3C(=O)c4cc5oc6ccccc6c6ccccc6oc5cc4C3=O)ccc21
vNsp12-nsp7.1-7	ZINC000012847889	-10.6	0.321	436.51	ZINC	O=C(CN1C(=O)N[C@@]2(CCCCc3ccccc32)C1=O)c1ccc2c(c1)-c1ccccc1C2
vNsp12-nsp7.1-8	ZINC000014120765	-10.6	0.342	413.476	ZINC	O=C(CN1C(=O)N[C@@]2(CCCCc3ccccc32)C1=O)Nc1ccc2ccccc2c1
vNsp12-nsp7.1-9	ZINC000247756664	-10.6	0.303	465.591	ZINC	O=C1c2ccccc2C(=O)c2cc3c(cc21)N[C@@H]1CC[C@H]2[C@H]4[C@@H](CC[C@@H]3[C@H]14)C(=O)[C@H]1CCCC[C@@H]21
vNsp12-nsp7.1-10	ZINC000408765161	-10.6	0.286	479.578	ZINC	O=C1[C@@H]2[C@H]3C=C[C@@H](C3=C(c3ccccc3)c3ccccc3)[C@H]2C(=O)N1c1ccccc1-c1ccccc1
vNsp12-nsp7.1-11	Z1101973473	-10.5	0.339	413.476	REAL	O=C1CCCc2cc(NC(=O)[C@H]3CC(=O)N(c4ccccc5ccccc45)C3)ccc2N1
vNsp12-nsp7.1-12	Z1897861395	-10.5	0.328	446.486	REAL	O=C1Cc2cc(S(=O)(=O)Nc3nnc(-c4cccc5ccccc45)o3)cc3c2N1CCC3
vNsp12-nsp7.1-13	Z2207980234	-10.5	0.328	425.487	REAL	Cc1cc2cc(NC(=O)[C@H]3CC(=O)N(c4cccc5ccccc45)C3)ccc2n(C)c1=O
vNsp12-nsp7.1-14	ZINC000004713898	-10.5	0.339	399.448	ZINC	O=C1Nc2ccccc2[C@]12c1ccc3ccccc3c1Oc1ccc3ccccc3c12
vNsp12-nsp7.1-15	ZINC000008901217	-10.5	0.276	499.521	ZINC	Cc1cc(NC(=O)c2cccc(-c3cc4ccccc4oc3=O)c2)ccc1-c1cc2ccccc2oc1=O
vNsp12-nsp7.1-16	ZINC000198754475	-10.5	0.292	464.475	ZINC	O=C1c2ccccc2C(=O)C2=C3C=CC4=CC5=C(C(=O)c6ccccc6C5=O)C5=CC=C(C=C12)[C@@H]3[C@H]45
vNsp12-nsp7.1-17	ZINC000245377192	-10.5	0.284	488.542	ZINC	O=C1[C@@H]2[C@H]3C=C[C@@H](C3)[C@H]2C(=O)N1c1ccc2c(c1)-c1cc(N3C(=O)[C@@H]4[C@H]5C=C[C@@H](C5)[C@@H]4C3=O)ccc1C2
vNsp12-nsp7.1-18	ZINC000409337249	-10.5	0.276	499.565	ZINC	Cc1ccc(N2C(=O)[C@H]3[C@H](C2=O)[C@@H]2C(=O)Oc4ccc5ccccc5c4C2=C[C@@H]3c2ccccc2)c(C)c1
vNsp12-nsp7.1-19	ZINC000409337254	-10.5	0.276	499.565	ZINC	Cc1ccc(N2C(=O)[C@H]3[C@H](C2=O)[C@@H]2C(=O)Oc4ccc5ccccc5c4C2=C[C@@H]3c2ccccc2)c(C)c1
vNsp12-nsp7.1-20	Z1102111626	-10.4	0.335	411.504	REAL	C[C@H]1Cc2ccccc2N1Cc1ccoc1C(=O)N1CCc2[nH]c3ccccc3c2C1
vNsp12-nsp7.1-21	Z1431635582	-10.4	0.325	431.49	REAL	CC1(C)C(=O)Nc2ccc(C(=O)CN3C(=O)N[C@@]4(CCCCc5ccccc54)C3=O)cc21
vNsp12-nsp7.1-22	ZINC000001588362	-10.4	0.306	440.509	ZINC	Nc1nc(-c2ccc3ccccc3c2)cc(-c2cc(-c3ccc4ccccc4c3)nc(N)n2)n1
vNsp12-nsp7.1-23	ZINC000100119951	-10.4	0.306	461.544	ZINC	O=C1C[C@H](Sc2nc3ccccc3c(-c3ccccc3)n2)C(=O)N1c1ccc2ccccc2c1
vNsp12-nsp7.1-24	ZINC000245377193	-10.4	0.281	488.542	ZINC	O=C1[C@@H]2[C@H]3C=C[C@@H](C3)[C@H]2C(=O)N1c1ccc2c(c1)-c1cc(N3C(=O)[C@@H]4[C@H]5C=C[C@@H](C5)[C@H]4C3=O)ccc1C2
vNsp12-nsp7.1-25	ZINC000408731315	-10.4	0.274	499.565	ZINC	Cc1ccc(C)c(N2C(=O)[C@H]3[C@H](C2=O)[C@@H]2C(=O)Oc4c5ccccc5ccc4C2=C[C@H]3c2ccccc2)c1
vNsp12-nsp7.1-26	ZINC000408732825	-10.4	0.281	485.538	ZINC	Cc1ccccc1N1C(=O)[C@H]2[C@H](C1=O)[C@@H]1C(=O)Oc3ccc4ccccc4c3C1=C[C@@H]2c1ccccc1
vNsp12-nsp7.1-27	ZINC000408732832	-10.4	0.281	485.538	ZINC	Cc1ccccc1N1C(=O)[C@@H]2[C@H](C1=O)[C@@H]1C(=O)Oc3ccc4ccccc4c3C1=C[C@@H]2c1ccccc1
vNsp12-nsp7.1-28	Z1446836160	-10.3	0.322	435.454	REAL	O=C1CCc2cc(C(=O)CN3C(=O)N[C@@]4(CCCCc5ccccc54)C3=O)c(F)cc2N1
vNsp12-nsp7.1-29	Z1662212871	-10.3	0.332	409.488	REAL	O=C1C[C@@H](c2nnc(Cc3cccc4ccccc34)o2)CN1c1ccc2c(c1)CCC2
vNsp12-nsp7.1-30	Z1663792332	-10.3	0.332	410.476	REAL	Cc1cc(-c2nnc([C@@H]3CC(=O)N(c4ccc5c(c4)CCC5)C3)o2)c2ccccc2n1
vNsp12-nsp7.1-31	Z1890920427	-10.3	0.312	438.486	REAL	Cc1ccc(-c2noc([C@@H]3CC(=O)N(c4ccc5c(c4)Cc4ccccc4-5)C3)n2)c(=O)n1C
vNsp12-nsp7.1-32	Z924788612	-10.3	0.343	397.433	REAL	O=C1NC(=O)c2cc(NC(=O)N3CC=C(c4ccccc5ccccc45)CC3)ccc21
vNsp12-nsp7.1-33	Z988053876	-10.3	0.278	494.593	REAL	O=C(Nc1ccccc1N1C(=O)N2CCc3ccccc32)c1)N1CCC(C(=O)N2CCc3ccccc32)CC1
vNsp12-nsp7.1-34	ZINC000003192991	-10.3	0.332	408.456	ZINC	Cc1ccc(-c2nnc(Oc3ccc4c(C)cc(=O)oc4c3)c3ccccc32)cc1C
vNsp12-nsp7.1-35	ZINC000004713899	-10.3	0.332	399.448	ZINC	O=C1Nc2ccccc2[C@]12c1ccc3ccccc3c1Oc1ccc3ccccc3c12
vNsp12-nsp7.1-36	ZINC000009389051	-10.3	0.303	448.477	ZINC	C[C@]1(c2ccc3ccccc3c2)NC(=O)N(Cc2cc(=O)oc3ccc4ccccc4c23)C1=O
vNsp12-nsp7.1-37	ZINC000018117591	-10.3	0.312	431.446	ZINC	O=C(Nc1cccc2c1C(=O)[C@H]1C=CC=C[C@@H]1C2=O)c1cccc2c1C(=O)c1ccccc1-2
vNsp12-nsp7.1-38	ZINC000059785691	-10.3	0.257	527.622	ZINC	CCc1ccc2c(c1)[C@]1(C(=O)N2)N2CCC[C@@H]2[C@@H](C(=O)c2ccc3ccccc3c2)[C@]12c1ccccc1NC2=O
vNsp12-nsp7.1-39	ZINC000059932650	-10.3	0.257	527.622	ZINC	Cc1ccc2c(c1C)NC(=O)[C@@]21N2CCC[C@@H]2[C@@H](C(=O)c2ccc3ccccc3c2)[C@]12c1ccccc1NC2=O
vNsp12-nsp7.1-40	ZINC000100485501	-10.3	0.322	410.431	ZINC	O=C1c2ccc3c4c(ccc(c24)C2=Nc4ccccc4[C@H]21)C1=Nc2ccccc2[C@@H]1C3=O
vNsp12-nsp7.1-41	ZINC000408687237	-10.3	0.322	420.467	ZINC	O=C(Nc1ccc2c(c1)oc1ccccc12)[C@H]1CC(=O)N(c2cccc3ccccc32)C1
vNsp12-nsp7.1-42	ZINC000408731626	-10.3	0.271	499.565	ZINC	Cc1ccc(N2C(=O)[C@H]3[C@H](C2=O)[C@@H]2C(=O)Oc4c5ccccc5ccc4C2=C[C@H]3c2ccccc2)cc1C
vNsp12-nsp7.1-43	ZINC000585656590	-10.3	0.294	454.528	ZINC	O=C(Cn1ccc(=NC(=O)c2ccccc2)c2ccccc21)c1ccc2c(c1)Cc1ccccc1-2
vNsp12-nsp7.1-44	Z14010305	-10.2	0.34	403.481	REAL	O=C(CN1C(=O)N[C@@]2(CCCCc3ccccc32)C1=O)Nc1ccc2c(c1)CCC2
vNsp12-nsp7.1-45	Z1664065587	-10.2	0.319	427.463	REAL	Cn1nc(-c2nnc([C@@H]3CC(=O)N(c4ccc5c(c4)CCC5)C3)o2)c2ccccc2c1=O
vNsp12-nsp7.1-46	Z2003012929	-10.2	0.329	405.496	REAL	O=C1[C@@H]2[C@H]3C[C@H]4[C@@H]2[C@@]2(C(=O)N[C@H](c5ccccc5)c5ccccc6ccccc56)[C@@H]1[C@@H]3[C@@H]42
vNsp12-nsp7.1-47	Z2032865632	-10.2	0.352	381.434	REAL	O=C1CC[C@H](C(=O)Nc2nc3ccccc3n2-c2ccccc2)c2ccccc21
vNsp12-nsp7.1-48	Z2090600440	-10.2	0.34	395.501	REAL	O=C(c1ccc2c(c1)-c1ccccc1C2)N1C[C@@H](c2ccccc2)[C@H]2COCC[C@H]21
vNsp12-nsp7.1-49	Z232376928	-10.2	0.34	395.461	REAL	O=C1C[C@@H](N2CCc3[nH]c4ccccc4c3C2)C(=O)N1c1ccc2ccccc2c1
vNsp12-nsp7.1-50	Z2524818266	-10.2	0.34	396.532	REAL	O=C(c1ccc2ccccc2c1)N1C[C@H]2CC[C@@H]1[C@H]1CN(Cc3ccccc3)C[C@H]21
vNsp12-nsp7.1-51	Z999683352	-10.2	0.291	464.567	REAL	O=C(c1ccc2[nH]ncc2c1)N1CCC[C@H](C(=O)N2CC=C(c3cccc4ccccc34)CC2)C1
vNsp12-nsp7.1-52	ZINC000001570225	-10.2	0.364	358.439	ZINC	O=C1c2ccccc2C(=C(c2ccccc2)c2ccccc21
vNsp12-nsp7.1-53	ZINC000002137741	-10.2	0.3	459.572	ZINC	O=c1/c(=C/c2c[nH]c3ccccc23)sc2n1[C@H](c1ccccc1)C1=C(N=2)c2ccccc2CC1
vNsp12-nsp7.1-54	ZINC000002416286	-10.2	0.309	431.446	ZINC	O=C(Nc1ccc2c(c1)oc1ccccc12)c1cccc(-c2cc3ccccc3oc2=O)c1
vNsp12-nsp7.1-55	ZINC000003873988	-10.2	0.309	429.43	ZINC	O=C1c2ccccc2C(=O)c2c(Nc3cccc4c3C(=O)c3ccccc3C4=O)cccc21
vNsp12-nsp7.1-56	ZINC000008772454	-10.2	0.34	403.481	ZINC	O=C(CN1C(=O)N[C@@]2(CCCCc3ccccc32)C1=O)Nc1ccc2c(c1)CCC2
vNsp12-nsp7.1-57	ZINC000017988176	-10.2	0.255	521.571	ZINC	O=C(Oc1ccc2ccccc2c1)c1cccc(N2C(=O)[C@H]3[C@@H](C2=O)C2c4ccccc4C3c3ccccc32)c1
vNsp12-nsp7.1-58	ZINC000059474345	-10.2	0.364	364.399	ZINC	O=C(Cc1cc2cc3ccccc3cc2oc1=O)c1ccc2ccccc2c1
vNsp12-nsp7.1-59	ZINC000100505727	-10.2	0.276	488.542	ZINC	O=C1[C@@H]2[C@H]3C=C[C@@H](C3)[C@@H]2C(=O)N1c1ccc2c(c1)-c1cc(N3C(=O)[C@H]4[C@H]5C=C[C@H](C5)[C@@H]4C3=O)ccc1C2
vNsp12-nsp7.1-60	ZINC000100737710	-10.2	0.309	431.446	ZINC	O=C(Nc1cccc2c1C(=O)[C@H]1C=CC=C[C@H]1C2=O)c1cccc2c1C(=O)c1ccccc1-2
vNsp12-nsp7.1-61	ZINC000196247496	-10.2	0.319	434.881	ZINC	O=c1oc2ccc3ccccc3c2cc1-c1nc2ccc(Cl)cc2c(-c2ccccc2)n1
vNsp12-nsp7.1-62	ZINC000226759430	-10.2	0.329	399.448	ZINC	O=C1Nc2ccccc2C12c1ccc3ccccc3c1Oc1c3ccccc3cc12
vNsp12-nsp7.1-63	ZINC000247747572	-10.2	0.276	486.53	ZINC	O=C(Nc1ccccc1)[C@@H]1[C@@H]2C(=O)N(c3ccc4ccccc4c3)C(=O)[C@H]2[C@@H]2c3ccccc3C=NN21
vNsp12-nsp7.1-64	ZINC000252677479	-10.2	0.3	459.572	ZINC	O=c1c(=Cc2c[nH]c3ccccc23)sc2n1[C@H](c1ccccc1)C1=C(N=2)c2ccccc2CC1
vNsp12-nsp7.1-65	ZINC000408730080	-10.2	0.268	499.565	ZINC	Cc1ccc(N2C(=O)[C@H]3[C@H](C2=O)[C@@H]2C(=O)Oc4c5ccccc5ccc4C2=C[C@H]3c2ccccc2)c(C)c1
vNsp12-nsp7.1-66	ZINC000408735138	-10.2	0.319	420.515	ZINC	O=C(Nc1ccc2nc3c4ccccc4c4ccccc4c3nc2c1)NC1CCCC1
vNsp12-nsp7.1-67	PV-001832900237	-10.1	0.361	370.451	REAL	Cc1cccc(-c2cccc(C(=O)N3CCc4ccccc4[C@H]3C(N)=O)c2)c1
vNsp12-nsp7.1-68	PV-001935001732	-10.1	0.337	455.952	REAL	Cc1cc(Cl)cc(C)c1S(=O)(=O)N1[C@@H]2CC[C@@H]1CC(O)(Cc1ccc(F)cc1F)C2
vNsp12-nsp7.1-69	PV-001961631429	-10.1	0.326	435.42	REAL	O=C(N[C@@H]1Cc2ccccc2N(C(=O)C(F)(F)F)C1)N[C@H]1CCCc2ccc(F)cc21
vNsp12-nsp7.1-70	Z1101971423	-10.1	0.337	403.481	REAL	O=C1CCCc2cc(NC(=O)[C@H]3CC(=O)N(c4ccc5c(c4)CCC5)C3)ccc2N1
vNsp12-nsp7.1-71	Z1143408070	-10.1	0.326	411.504	REAL	C[C@H]1Cc2ccccc2N1Cc1occc1C(=O)N1CCc2[nH]c3ccccc3c2C1
vNsp12-nsp7.1-72	Z1417280760	-10.1	0.348	383.49	REAL	O=C([C@H]1C[C@H]1c1ccc2ccccc2c1)N1CCC2(CC1)OCc1ccccc12
vNsp12-nsp7.1-73	Z1473414235	-10.1	0.337	398.508	REAL	O=C(N[C@H]1c2ccccc2CC[C@H]1n1ccnc1)N[C@@H]1[C@H]2CCc3ccccc3[C@H]21
vNsp12-nsp7.1-74	Z1507787650	-10.1	0.306	441.486	REAL	CN1C(=O)CCc2cc(C(=O)CN3C(=O)N[C@]3(C)c4ccc5ccccc5c4)C3=Occc21
vNsp12-nsp7.1-75	Z1626782479	-10.1	0.306	435.526	REAL	O=C(c1ccc2c(=O)n3c(nc2c1)CCCCC3)N1CC=C(c2cccc3ccccc23)C1
vNsp12-nsp7.1-76	Z1626783352	-10.1	0.337	395.461	REAL	Cc1ccc(-n2[nH]c(C(=O)N3CC=C(c4ccccc5ccccc45)C3)cc2=O)cc1
vNsp12-nsp7.1-77	Z1685539148	-10.1	0.348	387.482	REAL	Cc1cccc(N2C[C@H](c3nc([C@@H]4CCc5ccccc5C4)no3)CC2=O)c1C
vNsp12-nsp7.1-78	Z1891796430	-10.1	0.374	352.392	REAL	O=C1N[C@@H](c2ccc3ccccc3c2)C(=O)N1c1ccc2ccccc2c1
vNsp12-nsp7.1-79	Z1897863177	-10.1	0.316	442.454	REAL	O=C1Nc2ccc(S(=O)(=O)Nc3nnc(-c4cccc5ccccc45)o3)c3cccc1c23
vNsp12-nsp7.1-80	Z1897864431	-10.1	0.316	446.486	REAL	O=C1Cc2cc(S(=O)(=O)Nc3nnc(-c4ccc5ccccc5c4)o3)cc3c2N1CCC3
vNsp12-nsp7.1-81	Z2003425446	-10.1	0.374	364.487	REAL	CN(Cc1ccccc1)CC(C)(C)NC(=O)[C@]12[C@H]3C(=O)[C@H]4[C@@H]5C[C@H]([C@@H]4[C@H]41)[C@H]2[C@H]53
vNsp12-nsp7.1-82	Z2087157351	-10.1	0.348	383.406	REAL	Cn1c(=O)cc2ccc(N3C(=O)N[C@@H](c4ccc5ccccc5c4)C3=O)cc21
vNsp12-nsp7.1-83	Z2087406868	-10.1	0.348	383.406	REAL	Cn1ccc2ccc(N3C(=O)N[C@@H](c4ccc5ccccc5c4)C3=O)cc2c1=O
vNsp12-nsp7.1-84	Z2089214770	-10.1	0.337	403.481	REAL	C[C@@]1(c2cccc(C(=O)N3C[C@@H](c4ccccc4)[C@H]4CCC[C@H]43)c2)NC(=O)NC1=O
vNsp12-nsp7.1-85	Z2090584330	-10.1	0.337	395.501	REAL	O=C(c1ccc2c(c1)Cc1ccccc1-2)N1C[C@@H](c2ccccc2)[C@H]2COCC[C@H]21
vNsp12-nsp7.1-86	Z2172193547	-10.1	0.361	373.455	REAL	Cc1cccc(N2C[C@H](c3nc(-c4ccc5c(c4)CCC5)no3)CC2=O)c1C
vNsp12-nsp7.1-87	Z2178344073	-10.1	0.337	393.489	REAL	O=C(c1ccc2ccccc2c2cccnc12)N1CCCN2c3ccccc3C[C@@H]2C1
vNsp12-nsp7.1-88	Z2202175821	-10.1	0.326	411.504	REAL	Cn1c(=O)c(CNC(=O)N2CCC[C@@H]2c2cccc3ccccc23)cc2ccccc21
vNsp12-nsp7.1-89	Z225654962	-10.1	0.297	471.58	REAL	C[C@H]1Cc2ccccc2N1S(=O)(=O)c1cccc(C(=O)N2CCc3[nH]c4ccccc4c3C2)c1
vNsp12-nsp7.1-90	Z3135338791	-10.1	0.361	370.455	REAL	O=C(c1ccc2c(c1)-c1ccccc1C2)N1CCc2nc[nH]c2[C@@]12CCNC2
vNsp12-nsp7.1-91	Z805423474	-10.1	0.281	497.561	REAL	Fc1ccc(-c2cn3nc(N4CCN(c5ccc6nnc(-c7ccccc7)n6n5)CC4)sc3n2)cc1
vNsp12-nsp7.1-92	ZINC000000992877	-10.1	0.337	392.409	ZINC	O=C(COC(=O)c1ccc2c(c1)-c1ccccc1C2=O)c1ccc2ccccc21
vNsp12-nsp7.1-93	ZINC000001066554	-10.1	0.361	365.391	ZINC	O=C(O)c1cc(-c2c[nH]nc2-c2ccccc2)nc2ccc3ccccc3c21
vNsp12-nsp7.1-94	ZINC000002213809	-10.1	0.374	352.388	ZINC	O=c1oc2cc3ccc(-c4ccc5ccccc5c4)c3cc2c2c1CCC2
vNsp12-nsp7.1-95	ZINC000002230184	-10.1	0.361	366.415	ZINC	O=c1oc2cc3ccc(-c4ccc5ccccc5c4)c3cc2c2c1CCCC2
vNsp12-nsp7.1-96	ZINC000002386999	-10.1	0.306	437.494	ZINC	O=C(O)C[C@@H](NC(=O)OCC1c2ccccc2-c2ccccc21)c1ccc2ccccc2c1
vNsp12-nsp7.1-97	ZINC000002592693	-10.1	0.289	473.405	ZINC	O=C1c2cc3oc4ccccc4c4ccccc4oc3cc2C(=O)N1c1ccccc(C(F)(F)F)c1
vNsp12-nsp7.1-98	ZINC000003286995	-10.1	0.337	412.516	ZINC	Cc1ccc(C)c(-n2nnnc2SCC(=O)c2ccc3c(c2)-c2ccccc2C3)c1
vNsp12-nsp7.1-99	ZINC000004081198	-10.1	0.289	463.623	ZINC	CCn1c2ccccc2c2cc([C@@H]3Nc4cc(C)c(C)cc4NC4=C3C(=O)CC(C)(C)C4)ccc21
vNsp12-nsp7.1-100	ZINC000004972046	-10.1	0.337	395.457	ZINC	O=C(N[C@@H]1CCCc2ccccc21)c1oc(=O)c2ccccc2c1-c1ccccc1

Supplementary Table 59. Top 100 virtual hits of the screen against the nsp7 binding site of nsp12 (Screen ID: 32). Compounds were filtered so that hits had MW < 600 dalton, cLogP < 6, number of hydrogen bond acceptors < 11, and no reactive functional groups. A few compounds unsuitable for drug discovery were removed by visual inspection. The name of each compound consists of the initial letter 'v' for virtual hit, followed by the target protein name and the target site ('nsp7' for nsp7 binding site, 1 for docking scenario 1). The score is the docking score given by QuickVina 2 in kcal/mol. The ligand efficiency (LE) is computed as LE = -score/#NonH, where #NonH is the number of heavy (i.e. non hydrogen) atoms.

Name	Catalog ID	Score	LE	MW	Library	SMILES
vNsp12-nsp7.1-101	ZINC000006079580	-10.1	0.289	478.58	ZINC	Cc1ccc(-c2nn3c4ccc(NS(=O)(=O)c5ccc(C)cc5)cc4nc3c3ccccc32)cc1
vNsp12-nsp7.1-102	ZINC000009408653	-10.1	0.306	474.60	ZINC	Cc1ccc(N2C(=O)[C@H]3[C@@H]4C[C@H]([C@@H]3C2=O)[C@@H]2[C@@H]4Sc3[nH]c(=O)sc3[C@H]2c2ccccc2)cc1
vNsp12-nsp7.1-103	ZINC000012241328	-10.1	0.273	494.60	ZINC	O=C(c1cccc(N2CCNC2=O)c1)N1CCC(n2c(CCC3ccccc3)nc3ccenc32)CC1
vNsp12-nsp7.1-104	ZINC000014122643	-10.1	0.273	496.57	ZINC	Cc1ccc(C2=NN(C(=O)CN3C(=O)N[C@@]4(CCCCc5ccccc54)C3=O)[C@@H](c3ccco3)C2)cc1
vNsp12-nsp7.1-105	ZINC000019782240	-10.1	0.297	461.65	ZINC	CC1(C)C[C@]2(CCCN(Cc3nc4c(c(=O)[nH]3)C3(CCCCC3)Cc3ccccc3-4)C2)CCO1
vNsp12-nsp7.1-106	ZINC000101025558	-10.1	0.281	479.49	ZINC	O=C1C[C@@H](N(O)[C@H]2CC(=O)N(c3ccc4ccccc4c3)C2=O)C(=O)N1c1ccc2ccccc2c1
vNsp12-nsp7.1-107	ZINC000101407765	-10.1	0.326	409.44	ZINC	CC(=O)[C@H]1[C@H]2C(=O)N(c3ccc4ccccc4c3)C(=O)[C@@H]2[C@H]2c3ccccc3C=NN12
vNsp12-nsp7.1-108	ZINC000101407769	-10.1	0.326	409.44	ZINC	CC(=O)[C@H]1[C@@H]2C(=O)N(c3ccc4ccccc4c3)C(=O)[C@@H]2[C@H]2c3ccccc3C=NN12
vNsp12-nsp7.1-109	ZINC000118913478	-10.1	0.316	446.55	ZINC	C[C@]12CC[C@H]3[C@@H](CC=C4C[C@@H](O)CC[C@@]43C)[C@@H]1C/C(=C\c1ccc(C(F)(F)F)cc1)[C@@H]2O
vNsp12-nsp7.1-110	ZINC000118913479	-10.1	0.316	446.55	ZINC	C[C@]12CC[C@H]3[C@@H](CC=C4C[C@H](O)CC[C@@]43C)[C@@H]1C/C(=C\c1ccc(C(F)(F)F)cc1)[C@@H]2O
vNsp12-nsp7.1-111	ZINC000399733022	-10.1	0.306	449.45	ZINC	O=C(O)[C@@H]1CN(C(=O)OCC2c3ccccc3-c3ccccc32)C[C@H]1c1ccc(F)cc1F
vNsp12-nsp7.1-112	ZINC000408719153	-10.1	0.273	483.57	ZINC	C[C@]12C(=O)[C@](C)(C(c3ccccc3)=C1c1ccccc1)[C@H]1C(=O)N(c3ccc4ccccc4c3)C(=O)[C@H]12
vNsp12-nsp7.1-113	ZINC000408719155	-10.1	0.273	483.57	ZINC	C[C@]12C(=O)[C@](C)(C(c3ccccc3)=C1c1ccccc1)[C@@H]1C(=O)N(c3ccc4ccccc4c3)C(=O)[C@H]12
vNsp12-nsp7.1-114	ZINC000408730040	-10.1	0.273	485.54	ZINC	Cc1ccc(N2C(=O)[C@H]3[C@H](C2=O)[C@@H]2C(=O)Oc4cccccc5ccc4C2=C[C@@H]3c2ccccc2)cc1
vNsp12-nsp7.1-115	ZINC000408730070	-10.1	0.273	485.54	ZINC	Cc1ccc(N2C(=O)[C@@H]3[C@H](C2=O)[C@@H]2C(=O)Oc4cccccc5ccc4C2=C[C@@H]3c2ccccc2)cc1
vNsp12-nsp7.1-116	ZINC000408730073	-10.1	0.273	485.54	ZINC	Cc1ccc(N2C(=O)[C@H]3[C@H](C2=O)[C@@H]2C(=O)Oc4ccc5ccccc5c4C2=C[C@@H]3c2ccccc2)cc1
vNsp12-nsp7.1-117	ZINC000408732458	-10.1	0.266	499.57	ZINC	Cc1ccc(C)c(N2C(=O)[C@@H]3[C@H](C2=O)[C@@H]2C(=O)Oc4ccc5ccccc5c4C2=C[C@@H]3c2ccccc2)c1
vNsp12-nsp7.1-118	ZINC000408732459	-10.1	0.266	499.57	ZINC	Cc1ccc(C)c(N2C(=O)[C@H]3[C@H](C2=O)[C@@H]2C(=O)Oc4ccc5ccccc5c4C2=C[C@@H]3c2ccccc2)c1
vNsp12-nsp7.1-119	ZINC000409334997	-10.1	0.281	466.50	ZINC	O=C(Nc1ccc2ccccc2c1)Nc1ccc2nc3c4ccenc4c4nccc4c3nc2c1
vNsp12-nsp7.1-120	ZINC000409336215	-10.1	0.266	499.57	ZINC	Cc1ccc(N2C(=O)[C@@H]3[C@H](C2=O)[C@@H]2C(=O)Oc4ccc5ccccc5c4C2=C[C@@H]3c2ccccc2)cc1C
vNsp12-nsp7.1-121	ZINC000409336222	-10.1	0.266	499.57	ZINC	Cc1ccc(N2C(=O)[C@H]3[C@H](C2=O)[C@@H]2C(=O)Oc4ccc5ccccc5c4C2=C[C@@H]3c2ccccc2)cc1C
vNsp12-nsp7.1-122	ZINC000409336236	-10.1	0.266	499.57	ZINC	Cc1ccc(N2C(=O)[C@@H]3[C@H](C2=O)[C@@H]2C(=O)Oc4ccc5ccccc5c4C2=C[C@H]3c2ccccc2)cc1C
vNsp12-nsp7.1-123	PV-001796740426	-10.0	0.333	399.49	REAL	Cc1cccc(-c2cccc(CNC(=O)[C@]3(C)Cc4ccc(C)cc4C(=O)O3)c2)c1
vNsp12-nsp7.1-124	PV-001797183967	-10.0	0.370	368.38	REAL	Cc1cc(F)c2nc(O)cc(C(=O)N3CCCc4c(C)ccc(F)c43)c2c1
vNsp12-nsp7.1-125	PV-001806014065	-10.0	0.345	384.41	REAL	O=C(Cc1ccc2ccccc2c1)Nc1nccc1C(=O)c1ccc(F)cc1
vNsp12-nsp7.1-126	PV-001806071433	-10.0	0.345	391.51	REAL	CCc1ccc([C@H]2CCCN(C(=O)[C@]3(C)Cc4ccc(C)cc4C(=O)O3)C2)cc1
vNsp12-nsp7.1-127	PV-001807671417	-10.0	0.357	376.50	REAL	Cc1ccc2c(c1)CN(C(=O)c1ccc3c(c1)C(C)(C)C(=O)N3C)C(C)(C)C2
vNsp12-nsp7.1-128	PV-001808104117	-10.0	0.357	376.50	REAL	Cc1ccc2c1CC(C)(C)N(C(=O)c1ccc3c(c1)C(C)(C)C(=O)N3C)C2
vNsp12-nsp7.1-129	PV-001808104396	-10.0	0.385	344.46	REAL	Cc1ccc2nc(C(=O)N3Cc4cccc(C)c4CC3(C)C)ccc2c1
vNsp12-nsp7.1-130	PV-001814106712	-10.0	0.345	386.49	REAL	CC(C)(CNC(=O)[C@]1(c2ccccc2)CNC(=O)C1)c1ccc2ccccc2c1
vNsp12-nsp7.1-131	PV-001840349532	-10.0	0.345	388.47	REAL	Cc1ccc(N2C[C@H](C(=O)Nc3cc(-c4ccccc4C)n[nH]3)CC2=O)cc1C
vNsp12-nsp7.1-132	Z1260002546	-10.0	0.333	401.47	REAL	Cc1cccc(N2C[C@H](C(=O)NNC(=O)c3cccc4ccccc34)CC2=O)c1C
vNsp12-nsp7.1-133	Z1265415510	-10.0	0.345	386.49	REAL	Cc1ccc(C)c([C@@H]2CN(C(=O)/C=C\c3ccnc4ccccc34)[C@H](C)CO2)c1
vNsp12-nsp7.1-134	Z1661121208	-10.0	0.345	384.44	REAL	Cc1cccc(N2C[C@H](c3nnc(-c4ccc5ccccc5n4)o3)CC2=O)c1C
vNsp12-nsp7.1-135	Z1662836347	-10.0	0.333	395.46	REAL	O=C1C[C@H](c2nnc(-c3cccc4ccccc34)o2)CN1c1ccc2c(c1)CCC2
vNsp12-nsp7.1-136	Z1683496358	-10.0	0.345	384.44	REAL	Cc1cccc(N2C[C@H](c3nc(-c4cnc5ccccc5c4)no3)CC2=O)c1C
vNsp12-nsp7.1-137	Z1684154378	-10.0	0.345	384.44	REAL	Cc1cccc(N2C[C@H](c3nc(-c4ccc5nccccc5c4)no3)CC2=O)c1C
vNsp12-nsp7.1-138	Z1685426665	-10.0	0.345	388.47	REAL	Cc1cccc(N2C[C@H](c3nc(-c4ccc5c(n4)CCCC5)no3)CC2=O)c1C
vNsp12-nsp7.1-139	Z1715344018	-10.0	0.333	398.46	REAL	O=C1C[C@@H](N2CC[C@@]3(C2)OCc2ccccc23)C(=O)N1c1ccc2ccccc2c1
vNsp12-nsp7.1-140	Z1739137680	-10.0	0.370	381.45	REAL	O=C(O)C[C@@H]1c2ccccc2CCN1S(=O)(=O)c1ccc2ccccc2c1
vNsp12-nsp7.1-141	Z1767257525	-10.0	0.345	382.46	REAL	CC[C@H]1Cc2ccccc2CN1C(=O)c1ccc2[nH]c3ccccc3c(=O)c2c1
vNsp12-nsp7.1-142	Z1890369782	-10.0	0.333	395.42	REAL	O=C(Cc1noc(-c2ccc3ccccc3cc2O)n1)Nc1ccccc2ccccc12
vNsp12-nsp7.1-143	Z1890371032	-10.0	0.333	399.45	REAL	O=C(Cc1noc(-c2cc3c(cc2O)CCCC3)n1)Nc1ccccc2ccccc12
vNsp12-nsp7.1-144	Z1890760540	-10.0	0.345	384.44	REAL	O=C1C[C@@H](c2nc(-c3c[nH]c4ccccc34)no2)CN1c1ccc2c(c1)CCC2
vNsp12-nsp7.1-145	Z1890913355	-10.0	0.333	402.43	REAL	Cc1ccc(N2C[C@H](c3nc(-c4cc(C)c5ccccc5n4)no3)CC2=O)cc1F
vNsp12-nsp7.1-146	Z1891194093	-10.0	0.345	395.41	REAL	O=C1C[C@@H](c2nc(-c3cccc(C(F)F)c3)no2)CN1c1ccc2c(c1)CCC2
vNsp12-nsp7.1-147	Z1892011706	-10.0	0.345	385.42	REAL	CN1CCc2ccc(N3C(=O)N[C@@H](c4ccc5ccccc5c4)C3=O)cc2C1=O
vNsp12-nsp7.1-148	Z1897862098	-10.0	0.323	434.48	REAL	CC(=O)N1CCc2cc(S(=O)(=O)Nc3nnc(-c4ccccc5ccccc45)o3)ccc21
vNsp12-nsp7.1-149	Z2087376571	-10.0	0.345	382.42	REAL	COc1ccc2cc(N3C(=O)N[C@@H](c4ccc5ccccc5c4)C3=O)ccc2c1
vNsp12-nsp7.1-150	Z2089212661	-10.0	0.370	360.46	REAL	O=C1CCc2cc(C(=O)N3C[C@@H](c4ccccc4)[C@H]4CCC[C@H]43)ccc2N1
vNsp12-nsp7.1-151	Z2099332460	-10.0	0.303	443.55	REAL	O=C([C@H]1CCN(C(=O)[C@@H]2CC(=O)N(c3ccc4c(c3)Cc3ccccc3-4)C2)C1)N1CCCC1
vNsp12-nsp7.1-152	Z2099605296	-10.0	0.357	376.43	REAL	O=C(NC1[C@H]2CC[C@H]1Cc1ccccc1C2)c1cc(=O)[nH]c2ccc(F)cc12
vNsp12-nsp7.1-153	Z2178344971	-10.0	0.345	385.51	REAL	O=C(c1ccc2[nH]c3c(c2c1)CCCC3)N1CCCN2c3ccccc3C[C@@H]2C1
vNsp12-nsp7.1-154	Z426653990	-10.0	0.323	417.46	REAL	O=CN1CCc2cc(C(=O)CN3C(=O)N[C@@]4(CCCCc5ccccc54)C3=O)ccc21
vNsp12-nsp7.1-155	Z509399372	-10.0	0.345	382.46	REAL	C[C@@H](NC(=O)c1ccc2c(c1)-c1ccccc1C2)c1ccc2c(c1)CCC(=O)N2
vNsp12-nsp7.1-156	Z804787624	-10.0	0.303	437.50	REAL	O=C1CCc2cc(NC(=O)[C@H]3CC(=O)N(c4ccc5c(c4)Cc4ccccc4-5)C3)ccc2N1
vNsp12-nsp7.1-157	Z941458154	-10.0	0.313	423.47	REAL	O=C1NCc2ccc(NC(=O)[C@@H]3CC(=O)N(c4ccc5c(c4)Cc4ccccc4-5)C3)cc21
vNsp12-nsp7.1-158	Z998162622	-10.0	0.313	424.50	REAL	O=C(Nc1ccc2c3c(cccc13)CC2)[C@H]1CCCN(C(=O)c2ccc3[nH]ncc3c2)C1
vNsp12-nsp7.1-159	ZINC000000126553	-10.0	0.370	348.40	ZINC	c1ccc(-c2nnc(Oc3ccc4ccccc4c3)c3ccccc32)cc1
vNsp12-nsp7.1-160	ZINC000001465879	-10.0	0.333	394.43	ZINC	Cc1ccc(-c2nnc(Oc3ccc4c(C)cc(=O)oc4c3)c3ccccc32)cc1
vNsp12-nsp7.1-161	ZINC000001588368	-10.0	0.294	446.52	ZINC	Cc1[nH]c2ccccc2c1-c1cc(-c2cc(-c3c(C)[nH]c4ccccc43)nc(N)n2)nc(N)n1
vNsp12-nsp7.1-162	ZINC000002060689	-10.0	0.333	501.32	ZINC	O=c1oc2ccccc2c2c1[C@@H](c1ccccc1I)Nc1ccc3ccccc3c1-2
vNsp12-nsp7.1-163	ZINC000002117176	-10.0	0.333	399.49	ZINC	Cc1cccc(C(C)C)c1N1COc2c(C)c3oc(=O)c4ccccc4c3cc2C1
vNsp12-nsp7.1-164	ZINC000002294237	-10.0	0.357	366.42	ZINC	Cc1c2occ(-c3ccc4ccccc4c3)c2cc2c3c(c(=O)oc12)CCC3
vNsp12-nsp7.1-165	ZINC000002366044	-10.0	0.278	471.52	ZINC	O=C(c1ccccc1)[C@H]1[C@H]2C(=O)N(c3ccc4ccccc4c3)C(=O)[C@@H]2[C@H]2c3ccccc3C=NN12
vNsp12-nsp7.1-166	ZINC000006301202	-10.0	0.270	496.66	ZINC	Cc1cc(C)c2[nH]c(=O)c([C@H](c3nnnn3Cc3ccccc3)N3CCCC4(CCCCC4)C3)cc2c1
vNsp12-nsp7.1-167	ZINC000008475488	-10.0	0.333	398.46	ZINC	Cc1ccc(N2C[C@@H](C(=O)Nc3ccc4c(c3)oc3ccccc34)CC2=O)c(C)c1
vNsp12-nsp7.1-168	ZINC000008699170	-10.0	0.313	423.47	ZINC	O=C(O)[C@@H](NC(=O)OCC1c2ccccc2-c2ccccc21)c1ccccc2ccccc21
vNsp12-nsp7.1-169	ZINC000009356565	-10.0	0.294	442.48	ZINC	Oc1ccccc1-c1nc2c3c(ncn2n1)Oc1c2ccccc2ccc1[C@@H]3c1ccccc1
vNsp12-nsp7.1-170	ZINC000011665532	-10.0	0.294	442.48	ZINC	O=C(Nc1ccc(-c2ccc3nnc(-c4ccncc4)n3n2)cc1)c1ccc2ccccc2c1
vNsp12-nsp7.1-171	ZINC000012274563	-10.0	0.333	393.44	ZINC	O=C(Nc1ccc2ccccc2c1)c1ccc2c(c1)C[C@@H](c1ccccc1)OC2=O
vNsp12-nsp7.1-172	ZINC000012360361	-10.0	0.286	458.52	ZINC	O=C(Cc1ccc2ccccc21)NN1C(=O)[C@H]2[C@@H](C1=O)C1c3ccccc3C2c2ccccc21
vNsp12-nsp7.1-173	ZINC000013513993	-10.0	0.263	515.57	ZINC	O=c1/c(=C/c2cn(-c3ccccc3)nc2-c2ccc3ccccc3c2)sc2nc(-c3ccc(F)cc3)nn12
vNsp12-nsp7.1-174	ZINC000013757548	-10.0	0.263	511.61	ZINC	Cc1cccc(-c2nc3s/c(=C\c4cn(-c5ccccc5)nc4-c4ccc5ccccc5c4)c(=O)n3n2)c1
vNsp12-nsp7.1-175	ZINC000014272522	-10.0	0.278	472.50	ZINC	Cc1cccc(-c2nc3cc(NC(=O)c4cccc(-c5cc6ccccc6oc5=O)c4)ccc3o2)cc1
vNsp12-nsp7.1-176	ZINC000016037585	-10.0	0.263	500.55	ZINC	COc1ccc(C(=O)[C@@H]2[C@@H]3C(=O)N(c4ccccc5ccccc54)C(=O)[C@@H]3[C@H]3c4ccccc4C=CN23)cc1
vNsp12-nsp7.1-177	ZINC000016525610	-10.0	0.303	429.47	ZINC	O=C(Nc1ccc2c(c1)Cc1ccccc1-2)c1ccc(-c2cc3ccccc3oc2=O)cc1
vNsp12-nsp7.1-178	ZINC000017862766	-10.0	0.250	520.59	ZINC	O=C(Nc1ccc2ccccc2c1)c1cccc(N2C(=O)[C@H]3[C@@H](C2=O)C2c4ccccc4C3c3ccccc32)c1
vNsp12-nsp7.1-179	ZINC000020100563	-10.0	0.270	504.97	ZINC	O=C(c1ccc(Cl)cc1)[C@@H]1[C@@H]2C(=O)N(c3cccc4ccccc43)C(=O)[C@@H]2[C@@H]2c3ccccc3C=CN21
vNsp12-nsp7.1-180	ZINC000020633960	-10.0	0.357	371.44	ZINC	Cc1ccc(-c2cc(=O)[nH]c(Nc3nc(C)c4cc(C)c(C)cc4n3)n2)cc1
vNsp12-nsp7.1-181	ZINC000020634926	-10.0	0.313	460.32	ZINC	O=c1cc(-c2ccc(Cl)cc2)[nH]c(Nc2nc3ccc(Cl)cc3c(-c3ccccc3)n2)n1
vNsp12-nsp7.1-182	ZINC000059796308	-10.0	0.256	513.60	ZINC	Cc1ccccc2c1NC(=O)[C@@]21N2CCC[C@@H]2[C@@H](C(=O)c2ccc3ccccc3c2)[C@]12c1ccccc1NC2=O
vNsp12-nsp7.1-183	ZINC000095918523	-10.0	0.278	464.56	ZINC	O=C1[C@@H]2C(c3ccccc3)=C(c3ccccc3)[C@@H]2C(=O)[C@H]2C3c4ccccc4C(c4ccccc43)[C@@H]12
vNsp12-nsp7.1-184	ZINC000096343569	-10.0	0.270	498.62	ZINC	Cc1c2occ(-c3ccccc3)c2cc2c(C)c(CC(=O)NC[C@H]3CCCN4CCCC[C@H]34)c(=O)oc12
vNsp12-nsp7.1-185	ZINC000100688954	-10.0	0.256	511.58	ZINC	Cc1ccc(N2C(=O)[C@@H]3[C@H](C2=O)[C@H]2c4ccccc4C=NN2[C@@H]3C(=O)c2ccc(-c3ccccc3)cc2)cc1
vNsp12-nsp7.1-186	ZINC000101025561	-10.0	0.278	479.49	ZINC	O=C1C[C@@H](N(O)[C@H]2CC(=O)N(c3ccc4ccccc4c3)C2=O)C(=O)N1c1ccc2ccccc2c1
vNsp12-nsp7.1-187	ZINC000104529567	-10.0	0.286	468.55	ZINC	Cc1ccc(N2C(=O)C3=C(C2=O)C(C)=C[C@@H](C)C[C@@H]3C)cc1N(c4ccc(C)c(C)c4)C2=O)C3)cc1C
vNsp12-nsp7.1-188	ZINC000118916170	-10.0	0.345	457.45	ZINC	C[C@]12CC[C@H]3[C@@H](CC=C4C[C@@H](O)CC[C@@]43C)[C@@H]1C/C(=C\c1ccc(Br)cc1)[C@@H]2O
vNsp12-nsp7.1-189	ZINC000118916423	-10.0	0.345	413.00	ZINC	C[C@]12CC[C@H]3[C@@H](CC=C4C[C@@H](O)CC[C@@]43C)[C@@H]1C/C(=C\c1ccc(Cl)cc1)[C@@H]2O
vNsp12-nsp7.1-190	ZINC000118916424	-10.0	0.345	413.00	ZINC	C[C@]12CC[C@H]3[C@@H](CC=C4C[C@H](O)CC[C@@]43C)[C@@H]1C/C(=C\c1ccc(Cl)cc1)[C@@H]2O
vNsp12-nsp7.1-191	ZINC000240824838	-10.0	0.256	516.56	ZINC	O=C1[C@@H]2[C@H]3C=C[C@@H](C3)[C@H]2C(=O)N1c1ccc(-c2nc3ccc(N4C(=O)[C@@H]5[C@H]6C=C[C@@H](C6)[C@@H]5C4=O)cc3[nH]2)cc1
vNsp12-nsp7.1-192	ZINC000257349355	-10.0	0.250	554.70	ZINC	C[C@H]1C[C@@H]2[C@H]3CCC4=CC(=O)C=C[C@]4(C)[C@]3(F)[C@@H](O)C[C@@]2(C)[C@]1(O)C(=O)COC(=O)C12CC3CC(CC(C3)C1)C2
vNsp12-nsp7.1-193	ZINC000408731726	-10.0	0.286	463.53	ZINC	Cc1ccc2c(c1)OC(=O)[C@@H]1C2=C[C@H](c2ccccc2)[C@H]2C(=O)N(c3ccc(C)c(C)c3)C(=O)[C@@H]21
vNsp12-nsp7.1-194	ZINC000408977131	-10.0	0.270	480.53	ZINC	CN(C(=O)Nc1ccc2nc3c4ccenc4c4nccc4c3nc2c1)c1ccc2ccccc2c1
vNsp12-nsp7.1-195	ZINC000409337264	-10.0	0.263	499.57	ZINC	Cc1ccc(N2C(=O)[C@@H]3[C@H](C2=O)[C@@H]2C(=O)Oc4ccc5ccccc5c4C2=C[C@H]3c2ccccc2)c(C)c1
vNsp12-nsp7.1-196	PV-000383251384	-9.9	0.319	418.54	REAL	O=C(N[C@]12CCC[C@H]1CN(C(=O)c1ccc3c(c1)CCC=C3)C2)[C@@H]1C[C@@H]2O[C@H]1[C@H]1C[C@@H]21
vNsp12-nsp7.1-197	PV-001791931931	-9.9	0.367	358.44	REAL	Cc1ccc(N2C[C@H](C(=O)Nc3ccc4ccccc4c3)CC2=O)cc1C
vNsp12-nsp7.1-198	PV-001796342011	-9.9	0.341	388.51	REAL	Cc1ccc(C2=CCN(C(=O)[C@@H]3CC(=O)N(c4cccc(C)c4C)C3)CC2)cc1
vNsp12-nsp7.1-199	PV-001804879061	-9.9	0.354	387.40	REAL	C[C@@]1(C(F)(F)F)c2ccccc2CCN1C(=O)c1ccc2c(c1)CCCC2=O
vNsp12-nsp7.1-200	PV-001805425926	-9.9	0.341	387.48	REAL	Cc1ccc(C2(C(=O)Nc3ccc(C)nc(-c4ccccc4)n3)CCOCC2)cc1

Supplementary Table 60. Virtual screening hits 101 to 200 of the screen against the nsp7 binding site of nsp12 (Screen ID: 32). Compounds were filtered so that hits had MW < 600 dalton, cLogP < 6, number of hydrogen bond acceptors < 11, and no reactive functional groups. A few compounds unsuitable for drug discovery were removed by visual inspection. The name of each compound consists of the initial letter 'v' for virtual hit, followed by the target protein name and the target site ('nsp7' for nps7 binding site, 1 for docking scenario 1). The score is the docking score given by QuickVina 2 in kcal/mol. The ligand efficiency (LE) is computed as LE = -score/#NonH, where #NonH is the number of heavy (i.e. non hydrogen) atoms.

Name	Catalog ID	Score	LE	MW	Library	SMILES
vNsp13-as1-1	ZINC000037226178	-10.8	0.309	476.413	ZINC	O=C1Nc2ccccc2/C1=N/N/C=C1/C(=O)N(c2ccccc2C(F)(F)F)C(=O)c2ccccc21
vNsp13-as1-2	ZINC000604405315	-10.6	0.303	467.48	ZINC	CC(=O)N1CC2=C(C1=O)[C@H](c1ccc(-c3ccccc3C(=O)O)o1)c1cn(C)c3cccc(c13)N2
vNsp13-as1-3	Z1213022199	-10.5	0.328	433.442	REAL	Cc1c(F)cccc1-c1ccc([C@H]2NC(N)=Nc3nc4cc5c(cc4n32)OCCCO5)o1
vNsp13-as1-4	Z1766348377	-10.5	0.339	426.368	REAL	O=C(c1cc(F)cc2c(=O)c3cc(F)ccc3[nH]c12)N1CCc2c(F)cc(F)cc2C1
vNsp13-as1-5	Z1766360984	-10.5	0.339	426.368	REAL	O=C(c1cc(F)cc2c(=O)c3cc(F)ccc3[nH]c12)N1CCc2ccc(F)c(F)c2C1
vNsp13-as1-6	Z1870462980	-10.5	0.339	417.443	REAL	O=C1NC2(Cc3ccccc3C2)C(=O)N1[C@@H]1CCc2nnc(-c3ccc(F)cc3)n2C1
vNsp13-as1-7	Z2118684028	-10.5	0.375	383.313	REAL	O=C(NNc1nc2ccccc2c(=O)[nH]1)c1cnc2c(F)cc(F)cc2c1O
vNsp13-as1-8	Z1177635971	-10.4	0.385	371.386	REAL	O=C(NCC(=O)N1CCc2cc(F)c(F)cc21)N1CCc2ccccc2C1
vNsp13-as1-9	ZINC000001139247	-10.4	0.325	443.482	ZINC	Cc1cc(C(=O)Oc2cccc(NC3=NS(=O)(=O)c4ccccc43)c2)c2ccccc2n1
vNsp13-as1-10	Z1098711166	-10.3	0.322	438.437	REAL	O=C(Nc1n[nH]c2ccc(F)cc12)[C@@H]1CCC[C@@H](C(=O)Nc2n[nH]c3ccc(F)cc23)C1
vNsp13-as1-11	Z1863314277	-10.3	0.322	431.451	REAL	O=C(c1cccc(C(=O)N2CCc3ccnc(O)c3C2)n1)N1CCc2ccnc(O)c2C1
vNsp13-as1-12	Z226201106	-10.3	0.322	449.857	REAL	C[C@@]1(c2ccc3ccccc3c2)NC(=O)N(CC(=O)Nc2nnc3ccc(Cl)nn23)C1=O
vNsp13-as1-13	ZINC000013785711	-10.3	0.322	446.864	ZINC	O=c1c2cc(F)ccc2occ1[C@H]1Oc2ccccc2[C@@H]2CC(c3ccc(Cl)cc3)=NN21
vNsp13-as1-14	ZINC000016037828	-10.3	0.278	504.972	ZINC	O=C(c1ccc(Cl)cc1)[C@@H]1[C@@H]2C(=O)N(c3cccc4ccccc43)C(=O)[C@@H]2[C@H]2c3ccccc3C=CN12
vNsp13-as1-15	ZINC000096319667	-10.3	0.286	476.543	ZINC	Cc1ccc(C2=C[C@H](c3ccc(C)cc3)n3nnnc3N2CC(=O)N=c2[nH]c3ccccc3[nH]2)cc1
vNsp13-as1-16	ZINC000101344117	-10.3	0.278	489.505	ZINC	O=C(c1ccc(F)cc1)[C@@H]1[C@@H]2C(=O)N(c3ccc4ccccc4c3)C(=O)[C@@H]2[C@H]2c3ccccc3C=NN12
vNsp13-as1-17	ZINC000101344120	-10.3	0.278	489.505	ZINC	O=C(c1ccc(F)cc1)[C@@H]1[C@@H]2C(=O)N(c3ccc4ccccc4c3)C(=O)[C@H]2[C@H]2c3ccccc3C=NN12
vNsp13-as1-18	ZINC000247747569	-10.3	0.278	486.53	ZINC	O=C(Nc1ccccc1)[C@@H]1[C@@H]2C(=O)N(c3ccc4ccccc4c3)C(=O)[C@H]2[C@H]2c3ccccc3C=NN12
vNsp13-as1-19	ZINC000408732461	-10.3	0.271	499.565	ZINC	Cc1ccc(C)c(N2C(=O)[C@@H]3[C@H](C2=O)[C@@H]2C(=O)Oc4ccc5ccccc5c4C2=C[C@H]3c2ccccc2)c1
vNsp13-as1-20	ZINC000524729443	-10.3	0.278	494.454	ZINC	O=C(O)c1ccc(-c2ccc([C@@H]3CC(=O)Oc4cc(O)c5c(=O)c(-c6ccccc6)coc5c43)o2)cc1
vNsp13-as1-21	PV-001857843067	-10.2	0.34	420.394	REAL	Cc1n[nH]c(N2CCN(C(=O)c3nc(-c4cccc(C(F)(F)F)c4)oc3C)CC2)n1
vNsp13-as1-22	PV-001868519018	-10.2	0.352	400.384	REAL	Cc1c(C(=O)N2CCCc3cc(F)c(F)cc3C2)cnc2c1c(=O)n(C)c(=O)n2C
vNsp13-as1-23	PV-001952127672	-10.2	0.378	370.402	REAL	Cn1nc(NC(=O)N2CCC[C@H]2Cc2cc(F)ccc2F)c2ccccc21
vNsp13-as1-24	Z2004704195	-10.2	0.329	422.405	REAL	Cc1cc(F)cc2c1CN(C(=O)c1cc(F)cc3c(=O)c4cc(F)ccc4[nH]c13)CC2
vNsp13-as1-25	Z2227156625	-10.2	0.329	413.396	REAL	O=C(Nc1nnc2[nH]cnn12)c1cc(-c2ccc3c(c2)OCCO3)nc2ccccc12
vNsp13-as1-26	ZINC000003953839	-10.2	0.3	437.525	ZINC	Nc1cc2c(nc3c4ccccc4c(N)cc3[n+]2-c2cccc3ccccc32)c2ccccc12
vNsp13-as1-27	ZINC000004844433	-10.2	0.329	412.419	ZINC	O=c1c2cc(F)ccc2occ1[C@H]1Oc2ccccc2[C@@H]2CC(c3ccccc3)=NN21
vNsp13-as1-28	ZINC000008768708	-10.2	0.3	492.002	ZINC	Cc1ccc(Nc2nc3c(S(=O)(=O)c4ccc(C)c(C)c4)nnn3c3ccc(Cl)cc32)cc1C
vNsp13-as1-29	ZINC000016037199	-10.2	0.276	504.972	ZINC	O=C(c1ccc(Cl)cc1)[C@@H]1[C@@H]2C(=O)N(c3cccc4ccccc4c3)C(=O)[C@@H]2[C@H]2c3ccccc3C=CN12
vNsp13-as1-30	ZINC000016038169	-10.2	0.276	505.96	ZINC	O=C(c1ccc(Cl)cc1)[C@@H]1[C@@H]2C(=O)N(c3cccc4ccccc43)C(=O)[C@@H]2[C@H]2c3ccccc3C=NN12
vNsp13-as1-31	ZINC000016038238	-10.2	0.276	505.96	ZINC	O=C(c1ccc(Cl)cc1)[C@@H]1[C@@H]2C(=O)N(c3cccc4ccccc4c3)C(=O)[C@@H]2[C@H]2c3ccccc3C=NN12
vNsp13-as1-32	ZINC000064986838	-10.2	0.291	492.594	ZINC	Cc1ccc(Oc2cc3c(cc2S(=O)(=O)N2CCC(C)CC2)C(=O)Nc2ccc(C)cc2O3)cc1
vNsp13-as1-33	ZINC000096025270	-10.2	0.309	440.437	ZINC	O=C(Nc1cc(-n2ccc3ccccc32)ncn1)c1ccc(=O)n(Cc2cccc(F)c2)n1
vNsp13-as1-34	ZINC000101983999	-10.2	0.329	417.424	ZINC	COc1cccc(N2C(=O)C[C@@H](c3c(C)nn(-c4nc5ccccc5[nH]4)c3O)C2=O)c1
vNsp13-as1-35	ZINC000229889742	-10.2	0.262	555.914	ZINC	O=C(Nc1cccc(C(F)(F)F)c1)[C@@H]1[C@@H]2C(=O)N(c3ccc(F)c(Cl)c3)C(=O)[C@@H]2[C@H]2c3ccccc3C=CN12
vNsp13-as1-36	PV-001815889801	-10.1	0.348	397.424	REAL	CC(C)(C)c1noc(-c2ccccc2C(=O)N2CCc3cc(F)c(F)cc3C2)n1
vNsp13-as1-37	PV-001878579886	-10.1	0.348	400.384	REAL	Cc1c(C(=O)N2CCCc3cc(F)cc(F)c3C2)cnc2c1c(=O)n(C)c(=O)n2C
vNsp13-as1-38	PV-001885289189	-10.1	0.348	459.234	REAL	O=C1CNC(=O)c2ccc(C(=O)Nc3nc(-c4ccc(Br)cc4F)n[nH]3)cc2N1
vNsp13-as1-39	Z1162535183	-10.1	0.326	407.432	REAL	O=C(Nc1nc2ccccc2c(=O)[nH]1)c1cc(-c2ccccc2)nn1-c1ccccc1
vNsp13-as1-40	Z1213022201	-10.1	0.316	433.442	REAL	Cc1cc(F)ccc1-c1ccc([C@H]2NC(N)=Nc3nc4cc5c(cc4n32)OCCCO5)o1
vNsp13-as1-41	Z1232080016	-10.1	0.348	390.446	REAL	O=C(Nc1nnn[nH]1)[C@H]1C[C@@H]2CCCC[C@H]2N1C(=O)c1ccc2ccccc2c1
vNsp13-as1-42	Z1265197408	-10.1	0.306	438.529	REAL	O=C(Nc1cccc2nccn12)[C@H]1C[C@@H]2CCCC[C@H]2N1C(=O)c1ccc2ccccc2c1
vNsp13-as1-43	Z1368708937	-10.1	0.348	397.424	REAL	CC(C)(C)c1noc(-c2ccccc2C(=O)N2CCc3c(F)ccc(F)c3C2)n1
vNsp13-as1-44	Z1454113026	-10.1	0.348	397.424	REAL	CC(C)(C)c1noc(-c2ccccc2C(=O)N2CCc3ccc(F)c(F)c3C2)n1
vNsp13-as1-45	Z1486793397	-10.1	0.348	400.384	REAL	Cc1c(C(=O)N2CCc3c(F)ccc(F)c3C2)cnc2c1c(=O)n(C)c(=O)n2C
vNsp13-as1-46	Z1610504963	-10.1	0.326	429.455	REAL	O=C(NNc1ccc2ccccc2n1)c1ccc2c(c1)S(=O)(=O)c1ccccc1C2=O
vNsp13-as1-47	Z17072220	-10.1	0.316	457.437	REAL	O=C1N[C@@]2(CCS(=O)(=O)c3ccc(F)cc32)C(=O)N1CCN1C(=O)c2ccccc2C1=O
vNsp13-as1-48	Z1766157856	-10.1	0.326	426.368	REAL	O=C(c1cc(F)cc2c(=O)c3cc(F)ccc3[nH]c12)N1CCc2c(F)ccc(F)c2C1
vNsp13-as1-49	Z1767338577	-10.1	0.337	408.363	REAL	O=C(c1cc(F)cc2c(=O)c3cc(F)ccc3[nH]c12)N1CCc2n[nH]c(=O)cc2C1
vNsp13-as1-50	Z1863308744	-10.1	0.316	431.451	REAL	O=C(c1cncc(C(=O)N2CCc3ccnc(O)c3C2)c1)N1CCc2ccnc(O)c2C1
vNsp13-as1-51	Z1934181248	-10.1	0.306	449.466	REAL	C[C@]1(c2ccc3ccccc3c2)NC(=O)N(CC(=O)N2CCC[C@]3(C2)NC(=O)NC3=O)C1=O
vNsp13-as1-52	Z1983290694	-10.1	0.348	392.458	REAL	O=C1N[C@]2(C[C@H]3C[C@H]2[C@H]2CCC[C@H]32)C(=O)N1Cc1nc(Cc2ccccc2)no1
vNsp13-as1-53	Z1985096585	-10.1	0.306	445.474	REAL	O=C1N[C@H]2CCN(C(=O)c3cc(-c4ccc5c(c4)OCCO5)nc4ccccc34)C[C@@H]2CO1
vNsp13-as1-54	Z2040486166	-10.1	0.374	376.341	REAL	O=c1[nH]c(N/N=C2/CCC[C@H]2c2ccccc(C(F)(F)F)c2)nc2[nH]ncc12
vNsp13-as1-55	Z2111595058	-10.1	0.326	416.444	REAL	Cc1ccccc1-n1cc([C@H]2NC(N)=Nc3nc4cc5c(cc4n32)OCCCO5)nn1
vNsp13-as1-56	Z2115933270	-10.1	0.361	387.305	REAL	Cn1ncc2c(=O)[nH]c(NNC(=O)c3cnc4c(F)cc(F)cc4c3O)nc21
vNsp13-as1-57	Z219422760	-10.1	0.326	419.419	REAL	NC1=Nc2nc3cc4c(cc3n2[C@H](c2c[nH]nc2-c2ccc(F)cc2)N1)OCCCO4
vNsp13-as1-58	Z2198323213	-10.1	0.306	446.466	REAL	Cc1ccC(=O)N2CCc3n[nH]c(=O)cc3C2)cc(C(=O)N2CCc3n[nH]c(=O)cc3C2)c1
vNsp13-as1-59	Z2830825681	-10.1	0.326	415.456	REAL	Cc1ccccc1-n1cc([C@H]2NC(N)=Nc3nc4cc5c(cc4n32)OCCCO5)cn1
vNsp13-as1-60	Z384982934	-10.1	0.281	494.582	REAL	Cc1ccc(-n2c(=O)c3ccccc3n3c(S[C@@H](C)c4nnnn4-c4ccccc4)nnc23)c(C)c1
vNsp13-as1-61	Z384987856	-10.1	0.281	494.582	REAL	Cc1ccc(-n2c(=O)c3ccccc3n3c(S[C@@H](C)c4nnnn4-c4ccccc4)nnc23)c1C
vNsp13-as1-62	Z980023660	-10.1	0.281	492.524	REAL	O=C(Nc1ccc2nc3n(c(=O)c2c1)CCC3)[C@@H]1C[C@@H]2CCCC[C@H]2N1C(=O)c1ccc(F)cc1F
vNsp13-as1-63	ZINC000000990146	-10.1	0.259	581.421	ZINC	CCN1C(=O)COc2ccc(C(=O)c3oc4ccc(Br)cc4c3-c3cnc4c(c3)COc3ccccc3-4)cc21
vNsp13-as1-64	ZINC000002152735	-10.1	0.316	421.499	ZINC	Cc1cccc([C@@H]2c3[nH]c4ccccc4c3C[C@H]3C(=O)N(c4cccc(C)c4)C(=O)N32)c1
vNsp13-as1-65	ZINC000003399091	-10.1	0.348	400.505	ZINC	Cc1sc2nc3c4ccccc4c(Nc4ccc(C)c(C)c4)nn3c(=O)c2c1C
vNsp13-as1-66	ZINC000006149677	-10.1	0.246	549.559	ZINC	Cc1nn(-c2cccn2)c2c1[C@@H](c1cccc1)N1c3ccccc3N=C(Nc3cccc(C(F)(F)F)c3)C1=N2
vNsp13-as1-67	ZINC000006149935	-10.1	0.24	567.549	ZINC	Cc1nn(-c2cccn2)c2c1[C@@H](c1ccc(F)cc1)N1c3ccccc3N=C(Nc3cccc(C(F)(F)F)c3)C1=N2
vNsp13-as1-68	ZINC000009829909	-10.1	0.316	443.53	ZINC	Cc1ccc(S(=O)(=O)c2nnn3c2nc(Nc2ccccc2C)c2ccccc23)cc1C
vNsp13-as1-69	ZINC000012760686	-10.1	0.348	444.287	ZINC	O=C1Nc2ccccc2[C@]12Oc1ccc(Br)cc1-c1cc(-c3ccccc3)nn12
vNsp13-as1-70	ZINC000016037585	-10.1	0.266	500.553	ZINC	COc1ccc(C(=O)[C@@H]2[C@@H]3C(=O)N(c4cccc5ccccc54)C(=O)[C@@H]3[C@H]3c4ccccc4C=CN23)cc1
vNsp13-as1-71	ZINC000016038256	-10.1	0.281	499.909	ZINC	O=C(c1ccc(Cl)cc1)[C@@H]1[C@@H]2C(=O)N(c3ccc4c(c3)OCO4)C(=O)[C@@H]2[C@H]2c3ccccc3C=NN12
vNsp13-as1-72	ZINC000019323388	-10.1	0.337	400.485	ZINC	Cc1cc2c3c(c1)C(=CC(C)(C)N3C(=O)[C@]21N=C(N)N/C(=N/c2ccccc2)N1
vNsp13-as1-73	ZINC000059488049	-10.1	0.326	428.467	ZINC	O=C(Oc1cccc(NC2=NS(=O)(=O)c3ccccc32)c1)c1cccc2ccccc21
vNsp13-as1-74	ZINC000065011053	-10.1	0.297	478.571	ZINC	Cc1nn2c(c1-c1ccc(C)c(S(=O)(=O)N[C@H]3CCCc4ccccc43)c1)NC(=O)CCC2=O
vNsp13-as1-75	ZINC000096310043	-10.1	0.326	442.925	ZINC	O=C(Nc1ccc(Cl)cc1F)N1CC[C@]2(C1)Nc1ccccnc1N/C2=N\C1CCCC1
vNsp13-as1-76	ZINC000097993226	-10.1	0.297	487.345	ZINC	Oc1nc(/C(Cl)=C\c2ccccc(/C=C(/Cl)c3nc(O)c4ccccc4n3)c2)nc2ccccc12
vNsp13-as1-77	ZINC000253413600	-10.1	0.281	478.455	ZINC	O=C(O)c1ccc(-c2ccc([C@@H]3CC(=O)Oc4ccc5c(=O)c(-c6ccccc6)coc5c43)o2)cc1
vNsp13-as1-78	ZINC000408729324	-10.1	0.289	463.531	ZINC	Cc1ccc2c(c1)OC(=O)[C@@H]1C2=C[C@H](c2ccccc2)[C@H]2C(=O)N(c3cc(C)ccc3C)C(=O)[C@H]21
vNsp13-as1-79	PV-001817572093	-10	0.323	427.45	REAL	Cc1cc(C)cc(C(=O)N2CCC[C@H](C(=O)N3CC(=O)Nc4cc(F)c(F)cc43)C2)c1
vNsp13-as1-80	PV-001819877884	-10	0.345	397.424	REAL	CC(C)(C)c1noc(-c2ccccc2C(=O)N2CCc3cc(F)cc(F)c3C2)n1
vNsp13-as1-81	PV-001860195452	-10	0.345	412.375	REAL	Cc1nc(C(=O)N2NC(=O)C[C@@]23CCCC[C@@H]3C)nn1-c1nnc(C(F)(F)F)[nH]1
vNsp13-as1-82	PV-001947029801	-10	0.323	429.445	REAL	Cc1c(NC(=O)N2CCC[C@H]2Cc2cc(F)ccc2F)nnn1Cc1ccccc1F
vNsp13-as1-83	Z1024047410	-10	0.323	438.507	REAL	O=C1Nc2ccccc2[C@@H]1C1CCN(C(=O)CNC2=NS(=O)(=O)c3ccccc32)CC1
vNsp13-as1-84	Z1027823858	-10	0.303	448.461	REAL	Cc1nnnn1-c1cccc(NC(=O)N2CCC[C@@H](c3nc(-c4cccc(F)c4)no3)C2)c1
vNsp13-as1-85	Z1081937624	-10	0.303	444.577	REAL	Cc1nn(C)cc1[C@@H](C)NC(=O)[C@H]1C[C@@H]2CCCC[C@H]2N1C(=O)c1ccc2ccccc2c1
vNsp13-as1-86	Z1149406131	-10	0.333	395.461	REAL	Cc1ccc2nc(-c3cccnc3)cc(C(=O)N3CCc4ccc(O)cc4C3)c2c1
vNsp13-as1-87	Z1167294927	-10	0.313	430.478	REAL	Cc1ccc(F)c2c1CCCN2C(=O)c1cccc(NC(=O)[C@@H]2Cc3ccccc3O2)c1
vNsp13-as1-88	Z1212625159	-10	0.303	442.521	REAL	Cc1ccc(C(=O)N2CCC[C@@H](C(=O)Nc3n[nH]c4c3c(-c3ccccc3)nn4C)C2)cc1
vNsp13-as1-89	Z1391612746	-10	0.303	439.518	REAL	O=C(N[C@H]1CCCN(C(=O)c2ccccc2Cn2cncn2)C1)c1ccc2ccccc2c1
vNsp13-as1-90	Z1423984401	-10	0.333	410.448	REAL	O=C1CN(C(=O)Nc2cccc(C(=O)Nc3ccc(F)c3)c2)[C@@H]2CCCC[C@@H]2N1
vNsp13-as1-91	Z1442967637	-10	0.37	372.33	REAL	Cc1cc(C(=O)N2CCc3c(F)cc(F)c3C2)nc2nc(O)[nH]c(=O)c12
vNsp13-as1-92	Z1468566166	-10	0.313	433.457	REAL	O=C(c1ccnc(C(=O)N2CCc3ccc(F)cc3C2)c1)N1CCc2ccc(F)cc2C1
vNsp13-as1-93	Z1472017866	-10	0.303	441.529	REAL	O=C1C[C@H](c2cccc(NC(=O)[C@H]3CCCN(C(=O)c4cccc5ccccc45)C3)c2)CN1
vNsp13-as1-94	Z1544520525	-10	0.333	403.485	REAL	Cc1ccc(C)cc(C(=O)NCC(=O)N2CCC[C@@H]2c2nc(-c3ccccc3)n[nH]2)c1
vNsp13-as1-95	Z1613078057	-10	0.303	445.529	REAL	Cc1ccc(C)cc(-n2nc(NC(=O)N3CCN(c4nccn5cnnc45)[C@H](C)C3)cc2C)c1
vNsp13-as1-96	Z1625864097	-10	0.303	444.49	REAL	O=C(Nc1c[nH]nc1[C@H]1CCCN(C(=O)[C@@H]2Cc3ccccc3C(=O)O2)C1)c1ccccc1
vNsp13-as1-97	Z1646973092	-10	0.323	436.393	REAL	O=C(NC[C@@H]1CCC[C@@]12NC(=O)NC2=O)Nc1ccn(-c2cccc(C(F)(F)F)c2)n1
vNsp13-as1-98	Z1647944762	-10	0.313	428.418	REAL	Cc1c(-c2ccccc2)oc2c(C(=O)N3CC(=O)Nc4c(F)cccc43)cccc2c1=O
vNsp13-as1-99	Z1650755988	-10	0.323	419.386	REAL	O=C1/C(=C/N[C@H]2COc3cc(F)cc(F)c32)c2ccccc2C(=O)N1c1ccccn1
vNsp13-as1-100	Z1664065086	-10	0.323	423.378	REAL	Cn1nc(-c2nnc([C@@H]3CC(=O)N(c4ccc(F)cc4F)C3)o2)c2ccccc2c1=O

Supplementary Table 61. Top 100 virtual hits of the screen against the nsp7 binding site of nsp12 (Screen ID: 32). Compounds were filtered so that hits had MW < 600 dalton, cLogP < 6, number of hydrogen bond acceptors < 11, and no reactive functional groups. A few compounds unsuitable for drug discovery were removed by visual inspection. The name of each compound consists of the initial letter 'v' for virtual hit, followed by the target protein name and the target site ('nsp7' for nsp7 binding site, 1 for docking scenario 1). The score is the docking score given by QuickVina 2 in kcal/mol. The ligand efficiency (LE) is computed as LE = -score/#NonH, where #NonH is the number of heavy (i.e. non hydrogen) atoms.

Name	Catalog ID	Score	LE	MW	Library	SMILES
vNsp13-as1-101	Z1702694070	-10.0	0.333	405.45	REAL	O=C(Nc1cccc2c1OCC[C@H]2O)c1ccc2c(=O)n3c(nc2c1)CCCCC3
vNsp13-as1-102	Z1730123371	-10.0	0.345	399.43	REAL	O=C(Nc1ccccc1F)N1CCC[C@H](C(=O)N2CCc3n[nH]c(=O)cc3C2)C1
vNsp13-as1-103	Z1862853911	-10.0	0.333	407.38	REAL	O=C(c1cc(F)cc2c(=O)c3cc(F)ccc3[nH]c12)N1CCc2ccnc(O)c2C1
vNsp13-as1-104	Z1869958902	-10.0	0.323	421.40	REAL	O=C1[C@H](N2C(=O)N[C@H](c3cccc4ccccc34)C2=O)CCN1c1c(F)cccc1F
vNsp13-as1-105	Z1907737385	-10.0	0.313	438.44	REAL	O=C(Nc1nc2ccc(F)cc2[nH]1)[C@@H]1CCCC[C@H]1C(=O)Nc1nc2ccc(F)cc2[nH]1
vNsp13-as1-106	Z1915931158	-10.0	0.333	407.49	REAL	O=C(N[C@@H]1CCc2[nH]c(C3CCCCC3)nc2C1)c1c[nH]nc1-c1ccc(F)cc1
vNsp13-as1-107	Z1964890237	-10.0	0.345	399.45	REAL	CNC(=O)C[C@H](NC(=O)CCN1C(=O)[C@@H]2[C@@H]3CC[C@@H](O3)[C@H]2C1=O)c1ccccc1
vNsp13-as1-108	Z1985082805	-10.0	0.303	437.50	REAL	O=C1N[C@H]2CCN(C(=O)c3cc(-c4cccc5ccccc45)nc4ccccc34)C[C@@H]2CO1
vNsp13-as1-109	Z2003764017	-10.0	0.323	417.48	REAL	O=C1[C@@H]2[C@@H]3C[C@H]4[C@H]2[C@]2(C(=O)N5CCCC[C@H]5c5nc(-c6cccc(F)c6)c[nH]5)[C@H]1[C@H]3[C@H]42
vNsp13-as1-110	Z2021078221	-10.0	0.303	440.51	REAL	Cn1nccc1C1=C[C@H]2CC[C@@H](C1)N2C(=O)c1cccc(-c2cnc3[nH]c(=O)n(C)c3c2)c1
vNsp13-as1-111	Z2069734623	-10.0	0.323	417.36	REAL	O=C(Nc1ccccc1-n1nce2c(=O)[nH]cnc21)c1cc(=O)c2ccc(F)cc2o1
vNsp13-as1-112	Z2099942397	-10.0	0.303	446.41	REAL	Cc1cc(=O)oc2cc(N(C)C(=O)c3cc(F)cc4c(=O)c5cc(F)ccc5[nH]c34)ccc12
vNsp13-as1-113	Z2143205380	-10.0	0.323	410.44	REAL	Cc1nnc2[nH]nc(NC(=O)c3cccc3-c3ncc(-c4ccccc4)o3)c2c1C
vNsp13-as1-114	Z2169620116	-10.0	0.333	410.38	REAL	O=C1O[C@]2(CCCc3ccccc32)C(=O)N1Cc1coc(-c2c(F)cccc2F)n1
vNsp13-as1-115	Z2169620740	-10.0	0.333	444.27	REAL	O=C1O[C@]2(CCCc3ccccc32)C(=O)N1Cc1nnc(-c2c(Cl)cccc2Cl)o1
vNsp13-as1-116	Z2227159809	-10.0	0.370	364.37	REAL	O=C(Nc1nnc2[nH]cnn12)c1ccc2c(=O)n3c(nc2c1)CCCCC3
vNsp13-as1-117	Z2227338798	-10.0	0.333	396.41	REAL	O=C(Nc1[nH]nc2nc(O)ccc12)c1cn(-c2ccccc2)nc1-c1ccccc1
vNsp13-as1-118	Z2233663908	-10.0	0.323	442.54	REAL	Cc1cc(C)c(S(=O)(=O)N2CCC(C(=O)Nc3n[nH]c4cc(O)ccc34)CC2)c(C)c1
vNsp13-as1-119	Z238449986	-10.0	0.323	410.39	REAL	O=C1NC(=O)c2c(N/C=C3\C(=O)N(c4ccccn4)C(=O)c4ccccc43)cccc21
vNsp13-as1-120	Z2524822472	-10.0	0.303	439.56	REAL	O=C(c1cccc(Nc2ncccn2)c1)N1C[C@H]2CC[C@H]1[C@H]1CN(Cc3ccccc3)C[C@H]21
vNsp13-as1-121	Z264966332	-10.0	0.303	442.52	REAL	C[C@@]1(c2ccc3c(c2)CCC3)NC(=O)N(CC(=O)N2CCc3[nH]c4ccccc4c3C2)C1=O
vNsp13-as1-122	Z2830927910	-10.0	0.303	454.56	REAL	Cc1nn2c(nc(N3CCCC3)c3ccccc32)c1[C@H]1NC(=O)c2sc3ccccc3c2N1
vNsp13-as1-123	Z2938602373	-10.0	0.345	390.49	REAL	c1ccc2c(c1)CC[C@H](n1nnnc1N1CCC[C@H](c3nnc4n3CCC4)C1)C2
vNsp13-as1-124	Z29637948	-10.0	0.313	437.49	REAL	C[C@@H](C(=O)Oc1ccc2c3c(c(=O)oc2c1)CCCCC3)N1C(=O)[C@@H]2CCCC[C@H]2C1=O
vNsp13-as1-125	Z365647828	-10.0	0.323	417.47	REAL	Cn1c(=O)c2cc(NC(=O)c3ccc4[nH]c5c(c4c3)CCCCC5)cnc2n(C)c1=O
vNsp13-as1-126	Z370782400	-10.0	0.303	446.43	REAL	O=C(Oc1ccc2c3c(c(=O)oc2c1)CCCC3)c1ccc(=O)n(-c2ccc(F)cc2)n1
vNsp13-as1-127	Z450597722	-10.0	0.303	448.52	REAL	Cc1ccc2c(c1)[C@@H]1CN(C)CC[C@H]1N2C(=O)c1nn(-c2ccc(F)c(F)c2)c2c1CCC2
vNsp13-as1-128	Z650339558	-10.0	0.333	428.52	REAL	O=C(CCCNC1=NS(=O)(=O)c2ccccc21)NC1CCN(c2nccn2)CC1
vNsp13-as1-129	Z913105970	-10.0	0.313	449.55	REAL	O=C(NC1CCN(c2nc3ccccc3s2)CC1)N1CCc2[nH]c3ccc(F)cc3c2C1
vNsp13-as1-130	ZINC000001733741	-10.0	0.278	468.42	ZINC	O=c1c2ccccc2c(=O)c2c1c1c(=O)c3ccccc3c(=O)c1c1c(=O)c3ccccc3c(=O)c21
vNsp13-as1-131	ZINC000002148919	-10.0	0.286	465.51	ZINC	Cc1ccc([C@H]2c3[nH]c4ccccc4c3C[C@H]3C(=O)N(c4ccc5c(c4)OCCO5)C(=O)N32)cc1
vNsp13-as1-132	ZINC000002693121	-10.0	0.313	447.49	ZINC	Cc1ccc(S(=O)(=O)c2nnn3c2nc(Nc2ccc(F)cc2)c2ccccc23)cc1C
vNsp13-as1-133	ZINC000003741768	-10.0	0.286	467.52	ZINC	C[C@H]1CCCCN1c1cc(Nc2ccc3c(c2)OCCO3)c2c3c1noc3-c1ccccc1C2=O
vNsp13-as1-134	ZINC000003741904	-10.0	0.278	481.55	ZINC	C[C@@H]1C[C@@H](C)CN(c2cc(Nc3ccc4c(c3)OCCO4)c3c4c2noc4-c2ccccc2C3=O)C1
vNsp13-as1-135	ZINC000003741905	-10.0	0.278	481.55	ZINC	C[C@H]1C[C@H](C)CN(c2cc(Nc3ccc4c(c3)OCCO4)c3c4c2noc4-c2ccccc2C3=O)C1
vNsp13-as1-136	ZINC000006149762	-10.0	0.233	579.59	ZINC	COc1ccccc1[C@@H]1c2c(C)nn(-c3cccn3)c2N=C2C(Nc3ccc(C(F)(F)F)c3)=Nc3ccccc3N21
vNsp13-as1-137	ZINC000008436441	-10.0	0.357	396.40	ZINC	O=C(Oc1cccc(NC2=NS(=O)(=O)c3ccccc32)c1)c1ccccc1F
vNsp13-as1-138	ZINC000008767718	-10.0	0.278	489.45	ZINC	O=C(c1ccccc1)[C@H]1[C@@H]2C(=O)N(c3ccccc3C(F)(F)F)C(=O)[C@@H]2[C@H]2c3ccccc3C=NN12
vNsp13-as1-139	ZINC000008768694	-10.0	0.294	492.00	ZINC	Cc1ccc(C)c(Nc2nc3c(S(=O)(=O)c4ccc(C)c(C)c4)nnn3c3ccc(Cl)cc32)c1
vNsp13-as1-140	ZINC000008768715	-10.0	0.294	492.00	ZINC	CCc1cccc(Nc2nc3c(S(=O)(=O)c4ccc(C)c(C)c4)nnn3c3ccc(Cl)cc32)c1
vNsp13-as1-141	ZINC000009830020	-10.0	0.303	481.94	ZINC	Cc1ccc(S(=O)(=O)c2nnn3c2nc(Nc2ccc(F)cc2)c2cc(Cl)ccc23)cc1C
vNsp13-as1-142	ZINC000009849146	-10.0	0.313	443.53	ZINC	Cc1ccc(S(=O)(=O)c2nnn3c2nc(Nc2ccc(C)cc2C)c2ccccc23)cc1
vNsp13-as1-143	ZINC000015305595	-10.0	0.256	521.71	ZINC	O=C(c1cc2n(n1)[C@H](c1ccccc1)C[C@@H](c1ccccc1)N2)N1CCN(C23CC4CC(CC(C4)C2)C3)CC1
vNsp13-as1-144	ZINC000015989674	-10.0	0.278	482.47	ZINC	O=C(c1ccc2c(c1)OCO2)[C@@H]1[C@@H]2C(=O)N(c3ccc(F)cc3)C(=O)[C@@H]2[C@H]2c3ccccc3C=CN12
vNsp13-as1-145	ZINC000016671813	-10.0	0.385	347.31	ZINC	O=C1Nc2ccc(F)cc2/C1=N/Nc1nnc2c3ccccc3[nH]c2n1
vNsp13-as1-146	ZINC000049916776	-10.0	0.278	482.47	ZINC	O=C(c1ccc2c(c1)OCO2)[C@H]1[C@H]2C(=O)N(c3ccc(F)cc3)C(=O)[C@@H]2[C@H]2c3ccccc3C=CN12
vNsp13-as1-147	ZINC000101343766	-10.0	0.270	486.53	ZINC	O=C(Nc1ccccc1)[C@@H]1[C@@H]2C(=O)N(c3ccc4ccccc4c3)C(=O)[C@@H]2[C@H]2c3ccccc3C=NN12
vNsp13-as1-148	ZINC000102658513	-10.0	0.294	452.56	ZINC	C[C@@]12C[C@H](CC(C)(C)C1)N(C(=O)c1cc(-c3cccc4ccccc43)cc(-n3cnnn3)c1)C2
vNsp13-as1-149	ZINC000103540565	-10.0	0.263	571.40	ZINC	O=C(c1ccccc1)C1=C[C@H]2[C@@H]3C(=O)N(c4cccc(F)c4)C(=O)[C@@H]3[C@H](C(=O)c3ccc(Br)cc3)N2C=C1
vNsp13-as1-150	ZINC000104192899	-10.0	0.278	489.45	ZINC	O=C(c1ccccc1)[C@@H]1[C@H]2C(=O)N(c3ccccc3C(F)(F)F)C(=O)[C@@H]2[C@H]2c3ccccc3C=NN12
vNsp13-as1-151	ZINC000104192903	-10.0	0.278	489.45	ZINC	O=C(c1ccccc1)[C@H]1[C@H]2C(=O)N(c3ccccc3C(F)(F)F)C(=O)[C@@H]2[C@H]2c3ccccc3C=NN12
vNsp13-as1-152	ZINC000106536310	-10.0	0.278	482.47	ZINC	O=C(c1ccc2c(c1)OCO2)[C@@H]1[C@@H]2C(=O)N(c3ccc(F)cc3)C(=O)[C@H]2[C@H]2c3ccccc3C=CN12
vNsp13-as1-153	ZINC000229799013	-10.0	0.278	489.45	ZINC	O=C(c1ccccc1)[C@@H]1[C@@H]2C(=O)N(c3ccccc3C(F)(F)F)C(=O)[C@H]2[C@H]2c3ccccc3C=NN12
vNsp13-as1-154	ZINC000247703669	-10.0	0.278	479.47	ZINC	O=C([C@H]1[C@H]2C(=O)N(c3ccc(F)cc3)C(=O)[C@H]2[C@H]2C=Cc3ccccc3N21)n1nnc2ccccc21
vNsp13-as1-155	ZINC000247748586	-10.0	0.278	495.93	ZINC	O=C([C@H]1[C@H]2C(=O)N(c3cccc(Cl)c3)C(=O)[C@H]2[C@H]2C=Cc3ccccc3N21)n1nnc2ccccc21
vNsp13-as1-156	ZINC000253623741	-10.0	0.270	493.47	ZINC	O=C1c2ccc3c(c2O/C1=C\c1ccc2c(c1)OCCO2)[C@@H](c1cc2ccccc2nc1O)CC(=O)O3
vNsp13-as1-157	ZINC000263585014	-10.0	0.270	495.53	ZINC	CC(=O)N1CC2=C(C1=O)[C@H](c1ccc(-c3ccccc3C(=O)O)o1)c1cn(C(C)C)c3ccnc(c13)N2
vNsp13-as1-158	ZINC000408679811	-10.0	0.263	498.58	ZINC	Cc1cc(C)cc(NC(=O)c2cccc(N3C(=O)[C@H]4[C@@H](C3=O)C3c5ccccc5C4c4ccccc43)c2)c1
vNsp13-as1-159	ZINC000408679814	-10.0	0.263	498.58	ZINC	Cc1cc(C)cc(NC(=O)c2cccc(N3C(=O)[C@H]4[C@@H](C3=O)C3c5ccccc5C4c4ccccc43)c2)c1
vNsp13-as1-160	ZINC000409336230	-10.0	0.263	499.57	ZINC	Cc1ccc(N2C(=O)[C@H]3[C@H](C2=O)[C@@H]2C(=O)Oc4ccc5ccccc5c4C2=C[C@H]3c2ccccc2)cc1C
vNsp13-as1-161	ZINC000409336236	-10.0	0.263	499.57	ZINC	Cc1ccc(N2C(=O)[C@@H]3[C@H](C2=O)[C@@H]2C(=O)Oc4ccc5ccccc5c4C2=C[C@H]3c2ccccc2)cc1C
vNsp13-as1-162	PV-001794841361	-9.9	0.319	417.46	REAL	CCc1cc(=O)[nH]c(-c2cccc(NC(=O)[C@]3(C)Cc4ccc(C)cc4C(=O)O3)c2)n1
vNsp13-as1-163	PV-001838225253	-9.9	0.381	354.36	REAL	Cc1c(C(=O)N2CCc3ccc(F)c(F)c3C2)[nH]c(=O)c2ccccc12
vNsp13-as1-164	PV-001844277319	-9.9	0.300	455.39	REAL	O=C1CNC(=O)c2ccc(C(=O)Nc3cccc(Oc4cccc(C(F)(F)F)c4)c3)cc2N1
vNsp13-as1-165	PV-001856994778	-9.9	0.341	412.38	REAL	Cc1nc(C(=O)N2NC(=O)CC23CCCCC3)nn1-c1nnc(C(F)(F)F)[nH]1
vNsp13-as1-166	PV-001858159135	-9.9	0.319	446.45	REAL	Cc1cc(NC(=O)c2ccc3c(c2)NC(=O)CCS3)nn1-c1cccc(C(F)(F)F)c1
vNsp13-as1-167	PV-001868518091	-9.9	0.367	372.33	REAL	Cc1cc(C(=O)N2CCc3cc(F)c(F)cc3C2)nc2nc(O)[nH]c(=O)c12
vNsp13-as1-168	PV-001868520353	-9.9	0.381	354.36	REAL	Cc1c(C(=O)N2CCc3cc(F)c(F)cc3C2)[nH]c(=O)c2ccccc12
vNsp13-as1-169	PV-001878584691	-9.9	0.381	356.34	REAL	Nc1nnnn1-c1cccc(C(=O)N2CCc3cc(F)cc(F)c3C2)c1
vNsp13-as1-170	PV-001944204698	-9.9	0.319	420.51	REAL	C[C@H]1C(=O)Nc2ccccc2CN1C(=O)Nc1cccc(NC(=O)C2CCCCC2)c1
vNsp13-as1-171	PV-001946483686	-9.9	0.319	421.46	REAL	C[C@H]1C(=O)Nc2ccccc2CN1C(=O)Nc1cccc(N2C(=O)NC(C)(C)C2=O)c1
vNsp13-as1-172	Z1004161780	-9.9	0.300	448.46	REAL	Cc1ccc(-n2cnnn2)cc1NC(=O)N1CCC[C@@H](c2nc(-c3cccc(F)c3)no2)C1
vNsp13-as1-173	Z1014422078	-9.9	0.319	413.52	REAL	Cc1ccc(NC(=O)[C@H]2C[C@H]3CCCC[C@@H]3N2C(=O)c2ccc3ccccc3c2)nc1
vNsp13-as1-174	Z1268311220	-9.9	0.309	446.53	REAL	Cc1nsc(N2CCN(C(=O)c3cccc4c(=O)c(C)c(-c5ccccc5)oc34)CC2)n1
vNsp13-as1-175	Z1274012075	-9.9	0.300	448.52	REAL	Cc1cc2c(cc1C)O[C@H](C(=O)N1CCC(C(=O)c3ccc4c(c3)NC(=O)[C@H](C)O4)CC1)C2
vNsp13-as1-176	Z1275445431	-9.9	0.319	445.42	REAL	O=C(Nc1ccccc(CC(F)(F)F)c1)c1ccc2c(c1)S(=O)(=O)c1ccccc1C2=O
vNsp13-as1-177	Z1308103546	-9.9	0.367	367.45	REAL	C[C@@H]1Cc2ccccc2CN1C(=O)N[C@@H]1CCCN(c2ccn(C)n2)C1=O
vNsp13-as1-178	Z1372572249	-9.9	0.330	414.41	REAL	C[C@@]1(c2cccc(CNC(=O)N3CCc4c(F)ccc(F)c4C3)c2)NC(=O)NC1=O
vNsp13-as1-179	Z1413611356	-9.9	0.309	439.51	REAL	O=C1CN(C(=O)c2ccccc(C(=O)N3CC(=O)N[C@@H]4CCCC[C@@H]43)n2)[C@@H]2CCCC[C@H]2N1
vNsp13-as1-180	Z1469588115	-9.9	0.309	445.55	REAL	Cc1c(C(=O)Nc2ccnc(Cc3ccccc3)n2)sc2nc3n(c(=O)c12)CCCCC3
vNsp13-as1-181	Z1523029856	-9.9	0.309	433.46	REAL	O=C(c1ccnc(C(=O)N2CCc3c(F)cccc3C2)c1)N1CCc2c(F)cccc2C1
vNsp13-as1-182	Z1533640221	-9.9	0.319	416.44	REAL	NC(=O)c1n[nH]c2ccc(NC(=O)c3ccc4c(=O)n5c(nc4c3)CCCCC5)cc12
vNsp13-as1-183	Z1552325299	-9.9	0.309	425.46	REAL	O=C(c1ccc(=O)n(-c2ccccc2F)n1)N1CC=C(c2ccnc3ccccc23)CC1
vNsp13-as1-184	Z1611860606	-9.9	0.367	359.43	REAL	O=C(N1CCc2ccccc21)N1CCC[C@@H]1c1nc(-c2ccccc2)n[nH]1
vNsp13-as1-185	Z1724785040	-9.9	0.341	407.54	REAL	O=c1cc2c(n[nH]1)CCN(c1nc(C3CCCC3)nc3sc4c(c13)CCC4)C2
vNsp13-as1-186	Z1752044691	-9.9	0.309	434.47	REAL	O=C(NCc1cn(-c2ccccc2)nc1-c1ccc(F)cc1)N1CCC[C@@]12CCOC2=O
vNsp13-as1-187	Z1763488509	-9.9	0.354	372.42	REAL	O=C1/C(=C/c2cc3ccccc3nc2N2CCOCC2)Cc2cc(O)ccc21
vNsp13-as1-188	Z1766449470	-9.9	0.330	408.36	REAL	O=C(c1cc(F)cc2c(=O)c3cc(F)ccc3[nH]c12)N1CCc2nc[nH]c(=O)c2C1
vNsp13-as1-189	Z1798328739	-9.9	0.319	437.45	REAL	O=C(N[C@H]1CCOc2c(F)cccc21)c1ccc2c(c1)S(=O)(=O)c1ccccc1C2=O
vNsp13-as1-190	Z1849645035	-9.9	0.309	440.50	REAL	Cc1cc(N[C@@H]2CCCN(c3cc(N4CCOCC4)ncn3)C2)c2ccc(F)c(F)c2n1
vNsp13-as1-191	Z1869633995	-9.9	0.319	417.47	REAL	Cn1ccc(N2CCC[C@@H](N3C(=O)N[C@@H](Cc4cccc5ccccc45)C3=O)C2=O)n1
vNsp13-as1-192	Z1870709033	-9.9	0.309	447.49	REAL	O=C(Nc1nnc([C@H]2CCCc3ccccc32)s1)c1ccc(=O)n(-c2ccc(F)cc2)n1
vNsp13-as1-193	Z1876301910	-9.9	0.330	406.44	REAL	Cc1noc(C2CN(C(=O)[C@H]3CCCN3C(=O)c3ccc4ccccc4c3O)C2)n1
vNsp13-as1-194	Z2003705318	-9.9	0.309	430.49	REAL	O=C(Nc1ccc(F)c(-n2nnnc2C2CC2)c1)N1[C@@H]2C=C(c3ccccc3)C[C@@H]1CC2
vNsp13-as1-195	Z2008407080	-9.9	0.300	437.55	REAL	Cn1c(Cc2ccc3ccccc3c2)nnc1N1CCC([C@H]2C(=O)Nc3ccccc32)CC1
vNsp13-as1-196	Z2019957223	-9.9	0.341	395.46	REAL	O=C(NCc1cc2c([nH]c1=O)CCC2)N[C@@H]1CCN(C(=O)Nc2ccccc2)C1
vNsp13-as1-197	Z2041559218	-9.9	0.319	411.42	REAL	O=C1N[C@]2(CCc3ccccc32)C(=O)N1Cc1nc(-c2cccc3ncccc23)no1
vNsp13-as1-198	Z2067513613	-9.9	0.309	438.55	REAL	CN(C)C(=O)CN1[C@H]2CC[C@H]1CC(N[C@@H](C(=O)Nc1ccc(F)cc1)c1ccccc1)C2
vNsp13-as1-199	Z2080217884	-9.9	0.319	432.91	REAL	Cc1ccc(-c2nn(-c3ccccc3Cl)cc2C(=O)Nc2nnc(C)n2C2CC2)cc1
vNsp13-as1-200	Z2093965154	-9.9	0.300	442.56	REAL	O=C(Nc1cc2n(n1)CCCC2)[C@H]1C[C@H]2CCCC[C@H]2N1C(=O)c1ccc2ccccc2c1

Supplementary Table 62. Virtual screening hits 101 to 200 of the screen against the active site of the helicase (Screen ID: 33). Compounds were filtered so that hits had MW < 600 dalton, cLogP < 6, number of hydrogen bond acceptors < 11, and no reactive functional groups. A few compounds unsuitable for drug discovery were removed by visual inspection. The name of each compound consists of the initial letter 'v' for virtual hit, followed by the target protein name and the target site ('as' for active site, 1 for docking scenario 1). The score is the docking score given by QuickVina 2 in kcal/mol. The ligand efficiency (LE) is computed as LE = -score/#NonH, where #NonH is the number of heavy (i.e. non hydrogen) atoms.

Name	Catalog ID	Score	LE	MW	Library	SMILES
vNsp13-rna1-1	Z1070215962	-11.1	0.326	479.97	REAL	O=C1Nc2cc(Cl)ccc2[C@H]1C1CCN(C(=O)C2CCN(c3ccc4nncn4n3)CC2)CC1
vNsp13-rna1-2	ZINC000095474115	-11	0.314	468.52	ZINC	Cc1nn(-c2ncnc3[nH]cnc32)c2c1[C@@]1(CC(O)=N2)c2cccc3c2N(C1=O)C(C)(C)C[C@@H]3C
vNsp13-rna1-3	ZINC000008921457	-10.9	0.287	498.537	ZINC	O=C(NN1C(=O)[C@H]2[C@H](C1=O)C1c3ccccc3C2c2ccccc21)C1(O)c2ccccc2-c2ccccc21
vNsp13-rna1-4	ZINC000009635898	-10.9	0.295	488.56	ZINC	O=C(c1ccccc1)c1ccc2c(c1)NC1=C(C(=O)C[C@@H](c3ccccc3)C1)[C@H](c1ccc(F)cc1)N2
vNsp13-rna1-5	ZINC000018180685	-10.9	0.295	487.51	ZINC	Cc1ccc(N2C(=O)[C@@H]3[C@H](C2=O)[C@H](c2ccce4ccccc42)OC32C(=O)c3ccccc3C2=O)cc1
vNsp13-rna1-6	ZINC000226838254	-10.9	0.295	484.554	ZINC	CC(=O)[C@@H]1[C@H](C(=O)c2ccccc2)[C@@]2(C(=O)Nc3ccccc32)[C@@H]2C=Cc3c4ccccc4ccc3N21
vNsp13-rna1-7	ZINC000247703670	-10.9	0.303	479.47	ZINC	O=C([C@@H]1[C@H]2C(=O)N(c3ccc(F)cc3)C(=O)[C@H]2[C@H]2C=Cc3ccccc3N21)n1nnc2ccccc21
vNsp13-rna1-8	Z1374246659	-10.8	0.338	431.542	REAL	O=C(C1CCN(c2ccc3nnnn3n2)CC1)N1CCC[C@@]2(CCCc3ccccc32)C1
vNsp13-rna1-9	ZINC000000629962	-10.8	0.386	365.431	ZINC	C[C@@]12C(=O)N(c3ccccc3)C(=O)[C@H]1C1c3ccccc3C2c2ccccc21
vNsp13-rna1-10	ZINC000000842017	-10.8	0.386	369.394	ZINC	O=C1[C@@H]2[C@@H](C(=O)N1c1ccc(F)cc1)C1c3ccccc3C2c2ccccc21
vNsp13-rna1-11	ZINC000009782937	-10.8	0.292	486.569	ZINC	O=C(c1ccccc1)c1ccc2c(c1)NC1=C(C(=O)C[C@@H](c3ccccc3)C1)[C@H](c1cccc(O)c1)N2
vNsp13-rna1-12	ZINC000085392620	-10.8	0.292	493.569	ZINC	O=C([C@H]1CCC(=O)N(c2nc[nH]n2)C1)N1CCC(c2c[nH]c3ccccc32)(c2c[nH]c3ccccc32)CC1
vNsp13-rna1-13	ZINC000095477514	-10.8	0.292	494.489	ZINC	Cc1nn(-c2ncnc3[nH]cnc32)c2c1[C@]1(CC(O)=N2)C(=O)N(Cc2ccc(F)cc2)c2ccccc21
vNsp13-rna1-14	ZINC000239439106	-10.8	0.338	434.397	ZINC	O=C1[C@H]2[C@H](C(=O)N1c1ccc(F)cc1)[C@H]1C=C[C@@H]2[C@H]2C(=O)N(c3ccc(F)cc3)C(=O)[C@H]21
vNsp13-rna1-15	ZINC000247802733	-10.8	0.3	470.527	ZINC	O=C(c1ccccc1)[C@@H]1[C@@H]2C(=O)N(c3ccccc3)C(=O)[C@H]2[C@H]2C=Cc3c4ccccc4ccc3N21
vNsp13-rna1-16	ZINC000408669443	-10.8	0.292	484.554	ZINC	O=C(CN1C(=O)[C@H]2[C@@H](C1=O)C1c3ccccc3C2c2ccccc21)N(c1ccccc1)c1ccccc1
vNsp13-rna1-17	ZINC000409131371	-10.8	0.318	464.504	ZINC	O=C(Nc1ccc2nc(N3C(=O)c4ccccc4C3=O)sc2c1)Nc1ccnc2ccccc21
vNsp13-rna1-18	ZINC000409337264	-10.8	0.284	499.565	ZINC	Cc1ccc(N2C(=O)[C@@H]3[C@H](C2=O)[C@@H]2C(=O)Oc4ccc5ccccc5c4C2=C[C@H]3c2ccccc2)c(C)c1
vNsp13-rna1-19	Z1026191534	-10.7	0.324	482.584	REAL	O=C1Nc2ccccc2[C@@H]1C1CCN(C(=O)c2ccc3c(c2)SC2=NS(=O)(=O)CCN23)CC1
vNsp13-rna1-20	Z1240385996	-10.7	0.357	404.385	REAL	Cc1nnc([C@H]2Cc3ccccc3CN2C(=O)c2cnc3[nH]c(=O)[nH]c(=O)c3c2)o1
vNsp13-rna1-21	Z1374246450	-10.7	0.334	432.522	REAL	Cc1cc(C(=O)N2CCC[C@]3(CCCc4ccccc43)C2)nc2c1c(=O)n(C)c(=O)n2C
vNsp13-rna1-22	ZINC000001181715	-10.7	0.357	415.875	ZINC	C[C@@]12C(=O)N(c3ccc(Cl)cc3O)C(=O)[C@H]1C1c3ccccc3C2c2ccccc21
vNsp13-rna1-23	ZINC000002896234	-10.7	0.297	472.499	ZINC	Cc1ccccc1-c1nc2ccc(-c3ccc4nc(-c5ccccc5C)oc(=O)c4c3)cc2c(=O)o1
vNsp13-rna1-24	ZINC000002933672	-10.7	0.297	513.335	ZINC	O=c1oc(-c2ccccc2Cl)nc2ccc(-c3ccc4nc(-c5ccccc5Cl)oc(=O)c4c3)cc21
vNsp13-rna1-25	ZINC000016346787	-10.7	0.315	452.488	ZINC	O=C1C[C@@H](c2ccc(F)cc2)CC2=C1[C@@H](c1cccc1)N=C(Nc1nc3ccccc3o1)N2
vNsp13-rna1-26	ZINC000017027490	-10.7	0.315	452.513	ZINC	O=C1N=C(O)[C@@]2(Cc3ccccc3N3CCN(c4ccccc4)C[C@@H]32)C(=O)N1c1ccccc1
vNsp13-rna1-27	ZINC000021171152	-10.7	0.297	486.53	ZINC	Cc1ccc(Cn2nnc3c2nc(C2CCN(C(=O)c4ccc5c(c4)OCCO5)CC2)[nH]c3=O)cc1
vNsp13-rna1-28	ZINC000085392752	-10.7	0.268	530.67	ZINC	Cc1ccc(N2C[C@@H](C(=O)N3CCC(c4c[nH]c5ccccc54)(c4c[nH]c5ccccc54)CC3)CC2=O)c(C)c1
vNsp13-rna1-29	ZINC000085392756	-10.7	0.268	530.67	ZINC	Cc1ccc(N2C[C@@H](C(=O)N3CCC(c4c[nH]c5ccccc54)(c4c[nH]c5ccccc54)CC3)CC2=O)c(C)c1
vNsp13-rna1-30	ZINC000085392784	-10.7	0.274	516.643	ZINC	Cc1ccc(N2C[C@@H](C(=O)N3CCC(c4cc5ccccc5[nH]4)(c4cc5ccccc5[nH]4)CC3)CC2=O)c1
vNsp13-rna1-31	ZINC000100366101	-10.7	0.297	468.467	ZINC	O=C1c2ccccc2C(=O)C1c1ccc2cc3ccc(C4C(=O)c5ccccc5C4=O)nc3cc2n1
vNsp13-rna1-32	ZINC000408730040	-10.7	0.289	485.538	ZINC	Cc1ccc(N2C(=O)[C@H]3[C@H](C2=O)[C@@H]2C(=O)Oc4c5ccccc5ccc4C2=C[C@H]3c2ccccc2)cc1
vNsp13-rna1-33	ZINC000409178837	-10.7	0.274	521.659	ZINC	O=C(c1ccc2c(c1)[C@H]1[C@@H]([C@H]3CC[C@H]1C3)[C@H](c1ccccc1)N2)N1CCN(Cc2ccc3c(c2)OCO3)CC1
vNsp13-rna1-34	PV-001842599069	-10.6	0.342	435.376	REAL	O=C1Nc2ccc(F)cc2C[C@@H]1C(=O)N1CCNC(=O)[C@@H]1c1ccccc1C(F)(F)F
vNsp13-rna1-35	PV-002017929246	-10.6	0.331	446.594	REAL	CCC(CC)NC(=O)c1nnc(N2CCC(OCC(N)=O)CC2)n1C[C@@H]1C[C@@H]2C[C@@H]1C2
vNsp13-rna1-36	Z1151470309	-10.6	0.303	471.491	REAL	Cc1ccc([C@]2(C)NC(=O)N(CC(=O)Nc3ccc(-c4nc5c(F)cccc5[nH]4)cc3)C2=O)cc1
vNsp13-rna1-37	Z1461552102	-10.6	0.321	441.494	REAL	Cn1ncc2c(=O)[nH]c(NNC(=O)NC[C@@H]3CC4c5ccccc5C3c3ccccc34)nc21
vNsp13-rna1-38	Z1929436403	-10.6	0.321	443.506	REAL	Cc1ccc(-c2nn(Cc3ccccc3)cc2C(=O)N2CCC[C@@]3(C2)NC(=O)NC3=O)cc1
vNsp13-rna1-39	Z2178302485	-10.6	0.321	446.452	REAL	O=C(c1cc(F)cc2c(=O)c3cc(F)ccc3[nH]c12)N1CC[C@@]2(CCc3ccccc3O2)C1
vNsp13-rna1-40	ZINC000000704991	-10.6	0.312	451.393	ZINC	Cc1ccc2nc(-c3ccc4c(c3)C(=O)N(N3C(=O)c5ccccc5C3=O)C4=O)oc(=O)c2c1
vNsp13-rna1-41	ZINC000001187048	-10.6	0.379	366.419	ZINC	O=C1NN(c2ccccc2)C(=O)[C@H]2C3c4ccccc4C(c4ccccc43)[C@H]12
vNsp13-rna1-42	ZINC000015971748	-10.6	0.294	480.498	ZINC	O=C1Nc2ccccc2[C@@]12N[C@@H](Cc1c[nH]c3ccccc13)[C@H]1C(=O)N(c3ccc(F)cc3)C(=O)[C@H]12
vNsp13-rna1-43	ZINC000018948605	-10.6	0.286	496.518	ZINC	O=C(Nc1c2ccccc2oc1C(=O)N1CCOCC1)c1ccc2c(c1)C[C@H](c1ccccc1)OC2=O
vNsp13-rna1-44	ZINC000020572382	-10.6	0.286	494.525	ZINC	Cc1ccc(N2C(=O)[C@@H]3[C@H](C2=O)[C@@H](Cc2c[nH]c4ccccc24)N[C@@]32C(=O)Nc3ccc(F)cc32)cc1
vNsp13-rna1-45	ZINC000025783766	-10.6	0.286	490.605	ZINC	CC1=C(C(=O)Nc2ccccn2)[C@@H](c2ccc3c4ccccc4n(C)c3c2)C2=C(CC(C)(C)CC2=O)N1
vNsp13-rna1-46	ZINC000064198085	-10.6	0.294	477.562	ZINC	Cc1ccc(C(=O)[C@H]2[C@H]3CCCN3[C@]3(c4ccccc4)c4NC3=O)[C@@]23c2ccccc2NC3=O)cc1
vNsp13-rna1-47	ZINC000095474117	-10.6	0.303	468.52	ZINC	Cc1nn(-c2ncnc3[nH]cnc32)c2c1[C@@]1(CC(O)=N2)c2cccc3c2N(C1=O)C(C)(C)C[C@H]3C
vNsp13-rna1-48	ZINC000095474734	-10.6	0.342	455.264	ZINC	Cc1nn(-c2ncnc3[nH]cnc32)c2c1[C@]1(CC(O)=N2)C(=O)Nc2c1cc(Cl)cc2Cl
vNsp13-rna1-49	ZINC000095478335	-10.6	0.342	499.715	ZINC	Cc1nn(-c2ncnc3[nH]cnc32)c2c1[C@]1(CC(O)=N2)C(=O)Nc2c1cc(Cl)cc2Br
vNsp13-rna1-50	ZINC000097945320	-10.6	0.265	522.559	ZINC	O=C(Oc1cccc2ccccn21)c1cccc(N2C(=O)[C@H]3[C@H](C2=O)C2c4ccccc4C3c3ccccc32)c1
vNsp13-rna1-51	ZINC000097945321	-10.6	0.265	522.559	ZINC	O=C(Oc1cccc2ccccn21)c1cccc(N2C(=O)[C@H]3[C@@H](C2=O)C2c4ccccc4C3c3ccccc32)c1
vNsp13-rna1-52	ZINC000101481991	-10.6	0.303	493.848	ZINC	O=C1c2ccccc2C(=O)C12O[C@H](c1ccc(Cl)cc1)[C@H]1C(=O)N(c3ccc(F)cc3F)C(=O)[C@H]12
vNsp13-rna1-53	ZINC000102615204	-10.6	0.342	407.472	ZINC	Oc1c2c(nn1-c1ccccc1)N=C1CCCC(O)=C1[C@@H]2c1ccc2ccccc21
vNsp13-rna1-54	ZINC000229969564	-10.6	0.252	554.6	ZINC	Cc1ccc(C(=O)[C@@H]2[C@H](C(=O)c3ccc4c(c3)OCO4)N3C=Cc4ccccc4[C@@H]3[C@]23c2ccccc2NC3=O)cc1
vNsp13-rna1-55	ZINC000239433430	-10.6	0.265	534.527	ZINC	O=C1[C@H]2[C@@H](C(=O)N1c1ccccc1)[C@H](c1ccco1)N1[C@@H]3C(=O)N(c4ccccc4)C(=O)[C@H]3[C@@H](c3ccco3)N21
vNsp13-rna1-56	ZINC000239439294	-10.6	0.286	487.51	ZINC	Cc1ccc(N2C(=O)[C@@H]3[C@H](c4ccc5ccccc54)OC4(C(=O)c5ccccc5C4=O)[C@H]3C2=O)cc1
vNsp13-rna1-57	ZINC000408682268	-10.6	0.279	498.58	ZINC	Cc1cc(C)cc(NC(=O)c2ccccc2N2C(=O)[C@H]3[C@@H](C2=O)C2c4ccccc4C3c3ccccc32)c1
vNsp13-rna1-58	PV-001832648004	-10.5	0.362	386.414	REAL	Cc1ccc(-n2c(NNC(=O)c3ccnn3)nc3ccccc3c2=O)c(C)c1
vNsp13-rna1-59	PV-001832648075	-10.5	0.339	417.443	REAL	Cc1ccc(-n2c(NNC(=O)c3cccc(F)c3N)nc3ccccc3c2=O)c(C)c1
vNsp13-rna1-60	Z1024049144	-10.5	0.3	465.508	REAL	O=C1Nc2ccccc2[C@@H]1C1CCN(C(=O)c2cccc(N3C(=O)c4ccccc4C3=O)c2)CC1
vNsp13-rna1-61	Z2021232015	-10.5	0.375	399.92	REAL	CN1[C@@H]2CC[C@@H]1CC([C@@H](NC(=O)[C@H](O)c1ccccn1)c1ccc(Cl)cc1)C2
vNsp13-rna1-62	ZINC000000659879	-10.5	0.276	496.565	ZINC	O=C(c1ccccc1)c1ccc2c(c1)NC1=C(C(=O)C[C@H](c3ccccc3)C1)[C@@H]1c3ccccc3C(=O)N21
vNsp13-rna1-63	ZINC000001856939	-10.5	0.25	576.719	ZINC	Cc1ccc(-n2c(=O)c3cc4c(nc3nc2SCC(=O)NC(c2ccccc2)c2ccccc2)CC(C)(C)OC4)cc1
vNsp13-rna1-64	ZINC000004107444	-10.5	0.284	478.558	ZINC	C(=c1/c(-c2ccccc2)nn2c3ccccc3nc12)\[C@H]1C(c2ccccc2)=NN2c3ccccc3N[C@H]12
vNsp13-rna1-65	ZINC000004620409	-10.5	0.3	468.52	ZINC	Cc1ccc(Cn2nnc3c2nc(C2CCN(C(=O)Nc4ccc(C\#N)cc4)CC2)[nH]c3=O)cc1
vNsp13-rna1-66	ZINC000009192115	-10.5	0.284	489.505	ZINC	O=C(c1ccc(F)cc1)[C@H]1[C@H]2C(=O)N(c3ccc4ccccc4c3)C(=O)[C@H]2[C@@H]2c3ccccc3C=NN12
vNsp13-rna1-67	ZINC000012444335	-10.5	0.284	493.501	ZINC	Cc1cc(NC(=O)Cc2cccc3ccccc32)n(-c2nc3c(cnn3-c3ccc(F)cc3)c(=O)[nH]2)n1
vNsp13-rna1-68	ZINC000013757548	-10.5	0.276	511.608	ZINC	Cc1ccc(-c2nc3s/c(=C\c4cn(-c5ccccc5)nc4-c4ccc5ccccc5c4)c(=O)n3n2)c1
vNsp13-rna1-69	ZINC000015969174	-10.5	0.292	496.953	ZINC	O=C1Nc2c(cccc2Cl)[C@@]12N[C@@H](Cc1c[nH]c3ccccc13)[C@H]1C(=O)N(c3ccccc3)C(=O)[C@H]12
vNsp13-rna1-70	ZINC000015996653	-10.5	0.309	457.435	ZINC	O=C(c1ccc(F)cc1)[C@@H]1[C@@H]2C(=O)N(c3ccc(F)cc3)C(=O)[C@H]2[C@H]2c3ccccc3C=NN12
vNsp13-rna1-71	ZINC000016193632	-10.5	0.328	439.494	ZINC	C[C@H]1Cc2ccccc2N1C(=O)c1ccc2nc(N3C(=O)c4ccccc4C3=O)sc2c1
vNsp13-rna1-72	ZINC000017862766	-10.5	0.262	520.587	ZINC	O=C(Nc1ccc2ccccc2c1)c1cccc(N2C(=O)[C@H]3[C@@H](C2=O)C2c4ccccc4C3c3ccccc32)c1
vNsp13-rna1-73	ZINC000020410562	-10.5	0.292	496.949	ZINC	O=C(c1ccc(Cl)cc1)[C@@H]1C2(C(=O)c3ccccc3C2=O)N2CCC[C@H]2[C@@]12C(=O)Nc1ccccc12
vNsp13-rna1-74	ZINC000022595782	-10.5	0.292	480.698	ZINC	C[C@@H]1C[C@@H](c2ccc3ccccc3c2)NCCN[C@H](c2ccc3ccccc3c2)C[C@H](C)NCCN1
vNsp13-rna1-75	ZINC000034792844	-10.5	0.3	497.957	ZINC	CN1C2=C(C(=O)N(CC(=O)N3CCN(c4ccccc4F)CC3)C2)[C@H](c2ccccc2Cl)NC1=O
vNsp13-rna1-76	ZINC000034792866	-10.5	0.3	493.993	ZINC	CN1C2=C(C(=O)N(CC(=O)N3CCN(Cc4ccccc4)CC3)C2)[C@H](c2ccccc2Cl)NC1=O
vNsp13-rna1-77	ZINC000035806741	-10.5	0.292	477.562	ZINC	Cc1ccc(C(=O)[C@H]2[C@H]3CCCN3[C@]3(c4cc(C)ccc4NC3=O)[C@@]23c2ccccc2NC3=O)cc1
vNsp13-rna1-78	ZINC000064819307	-10.5	0.292	483.57	ZINC	Cc1ccc(-n2c(=O)c3ccc(C(=O)N[C@@H](C)c4ccenc4)cc3nc2N2CCOCC2)cc1C
vNsp13-rna1-79	ZINC000085392731	-10.5	0.269	516.643	ZINC	Cc1ccc(N2C[C@H](C(=O)N3CCC(c4c[nH]c5ccccc54)(c4c[nH]c5ccccc54)CC3)CC2=O)cc1
vNsp13-rna1-80	ZINC000085601772	-10.5	0.318	440.414	ZINC	Cc1ccc(-n2c(=O)[nH]c3cc(-c4nc(-c5ccc6c(c5)OCO6)no4)ccc3c2=O)cc1
vNsp13-rna1-81	ZINC000103508650	-10.5	0.284	488.546	ZINC	Cc1ccccc1N1C(=O)[C@@H]2[C@H](C1=O)[C@H]1CCCN1[C@]21c2ccccc2-n2c1nc1ccccc1c2=O
vNsp13-rna1-82	ZINC000106536310	-10.5	0.292	482.466	ZINC	O=C(c1ccc2c(c1)OCO2)[C@@H]1[C@@H]2C(=O)N(c3ccc(F)cc3)C(=O)[C@H]2[C@H]2c3ccccc3C=CN12
vNsp13-rna1-83	ZINC000169684223	-10.5	0.284	487.51	ZINC	Cc1ccccc([C@@H]2OC3(C(=O)c4ccccc4C3=O)[C@H]3C(=O)N(c4ccccc5ccccc54)C(=O)[C@@H]23)c1
vNsp13-rna1-84	ZINC000226630502	-10.5	0.3	459.587	ZINC	Cc1ccc(C(=C2[C@H]3C=C[C@H]2[C@@H]2C(=O)N(c4ccc(C)cc4C)C(=O)[C@@H]32)c2ccc(C)cc2)cc1
vNsp13-rna1-85	ZINC000229869935	-10.5	0.233	598.609	ZINC	CC(=O)Oc1ccc(C(=O)[C@@H]2[C@H](C(=O)c3ccc4c(c3)OCO4)[C@@]3(C(=O)Nc4ccccc43)[C@@H]3C=Cc4ccccc4N32)cc1
vNsp13-rna1-86	ZINC000229934566	-10.5	0.25	556.635	ZINC	Cc1ccc(C(=O)[C@@H]2[C@H](C(=O)c3ccc(F)cc3)[C@]3(C(=O)Nc4ccccc43)[C@@H]3C=C(C)c4cc(C)ccc4N32)cc1
vNsp13-rna1-87	ZINC000245226938	-10.5	0.3	459.587	ZINC	Cc1ccc(C(=C2[C@H]3C=C[C@H]2[C@@H]2C(=O)N(c4ccc(C)cc4C)C(=O)[C@H]32)c2ccc(C)cc2)cc1
vNsp13-rna1-88	ZINC000247889799	-10.5	0.276	498.58	ZINC	Cc1ccc(N2C(=O)[C@H]3[C@@H]4C=Cc5c6ccccc6ccc5N4[C@@H](C(=O)c4ccccc4)[C@H]3C2=O)c(C)c1
vNsp13-rna1-89	ZINC000257269797	-10.5	0.318	444.573	ZINC	O=C(c1ccc2c(c1)CCC2)N1CCC2(CC1)C/C=C/Cc1ccccc1OCC(=O)NC2
vNsp13-rna1-90	ZINC000263615320	-10.5	0.309	467.475	ZINC	Cc1ccc(C(=O)N2CCN(C(=O)c3nnn4c3CO[C@H](c3ccc(F)cc3)C4)CC2)cc1F
vNsp13-rna1-91	ZINC000408731626	-10.5	0.276	499.565	ZINC	Cc1ccc(N2C(=O)[C@H]3[C@H](C2=O)[C@@H]2C(=O)Oc4c5ccccc5ccc4C2=C[C@H]3c2ccccc2)cc1C
vNsp13-rna1-92	ZINC000409178840	-10.5	0.269	521.659	ZINC	O=C(c1ccc2c(c1)[C@H]1[C@@H]([C@H]3CC[C@H]1C3)[C@@H](c1ccccc1)N2)N1CCN(Cc2ccc3c(c2)OCO3)CC1
vNsp13-rna1-93	ZINC000409331930	-10.5	0.284	493.557	ZINC	COc1ccc([C@@H]2C=C3c4ccc(C)cc4OC(=O)[C@@H]3[C@H]3C(=O)N(c4ccc(C)cc4C)C(=O)[C@H]32)cc1
vNsp13-rna1-94	ZINC000409331933	-10.5	0.284	493.557	ZINC	COc1ccc([C@@H]2C=C3c4ccc(C)cc4OC(=O)[C@@H]3[C@@H]3C(=O)N(c4ccc(C)cc4C)C(=O)[C@H]32)cc1
vNsp13-rna1-95	ZINC000409331936	-10.5	0.284	493.557	ZINC	COc1ccc([C@@H]2C=C3c4ccc(C)cc4OC(=O)[C@@H]3[C@H]3C(=O)N(c4ccc(C)cc4C)C(=O)[C@@H]32)cc1
vNsp13-rna1-96	ZINC000409331938	-10.5	0.284	493.557	ZINC	COc1ccc([C@@H]2C=C3c4ccc(C)cc4OC(=O)[C@@H]3[C@@H]3C(=O)N(c4ccc(C)cc4C)C(=O)[C@@H]32)cc1
vNsp13-rna1-97	ZINC000524733314	-10.5	0.292	482.478	ZINC	Cc1nn(-c2ncnc3[nH]cnc32)c2c1[C@H](c1ccc(C(=O)Nc3ccc(F)cc3)cc1)CC(=O)N2
vNsp13-rna1-98	ZINC000952857582	-10.5	0.25	581.687	ZINC	CC(C)C[C@@H]1NC(=O)CN(C(=O)Cc2ccc(F)cc2)CCNC(=O)[C@H](Cc2ccccc2)NC(=O)[C@H](C)N(C)C1=O
vNsp13-rna1-99	PV-001822794313	-10.4	0.325	444.486	REAL	CC(C)(C)OC(=O)N1CCOc2ccccc2[C@@H]1C(=O)N1CCC2(CC1)NC(=O)NC2=O
vNsp13-rna1-100	Z1005577984	-10.4	0.325	449.901	REAL	O=C(Nc1nnc(-c2ccccc2Cl)[nH]1)[C@@H]1CCCN(C(=O)c2ccc3[nH]ncc3c2)C1

Supplementary Table 63. Top 100 virtual hits of the screen against the RNA binding site of nsp13 (Screen ID: 34). Compounds were filtered so that hits had MW < 600 dalton, cLogP < 6, number of hydrogen bond acceptors < 11, and no reactive functional groups. A few compounds unsuitable for drug discovery were removed by visual inspection. The name of each compound consists of the initial letter 'v' for virtual hit, followed by the target protein name and the target site ('rna' for RNA binding site, 1 for docking scenario 1). The score is the docking score given by QuickVina 2 in kcal/mol. The ligand efficiency (LE) is computed as LE = -score/#NonH, where #NonH is the number of heavy (i.e. non hydrogen) atoms.

Name	Catalog ID	Score	LE	MW	Library	SMILES
vNsp13-rna1-101	Z1024051690	-10.4	0.306	451.53	REAL	Cc1nn(-c2ccccc2)c2nc(C(=O)N3CCC([C@@H]4C(=O)Nc5ccccc54)CC3)ccc12
vNsp13-rna1-102	Z1226938500	-10.4	0.315	445.46	REAL	O=C(Nc1ccc(F)cc1)Nc1cccc2c1CCN(C(=O)Nc1nnc3ccccn13)C2
vNsp13-rna1-103	Z1374244896	-10.4	0.347	403.52	REAL	C[C@@H]1C(=O)Nc2cc(C(=O)N3CCC[C@]4(CCCc5ccccc54)C3)ccc2N1C
vNsp13-rna1-104	Z1374246633	-10.4	0.335	418.50	REAL	Cn1c(=O)c2ccc(C(=O)N3CCC[C@]4(CCCc5ccccc54)C3)nc2n(C)c1=O
vNsp13-rna1-105	Z1462726711	-10.4	0.315	438.49	REAL	Cc1nnc([C@H]2Cc3ccccc3CN2C(=O)c2cncc(-c3ccc4c(c3)CCO4)c2)o1
vNsp13-rna1-106	Z1656138401	-10.4	0.347	403.42	REAL	Cc1ccc(-n2c(NNC(=O)c3ccc(F)cn3)nc3ccccc3c2=O)c(C)c1
vNsp13-rna1-107	Z1902851335	-10.4	0.315	449.59	REAL	C[C@@H]1CN(C2CCOCC2)CCN1C(=O)[C@H]1CCCN(C(=O)c2ccccc3ccccc23)C1
vNsp13-rna1-108	Z2007472672	-10.4	0.306	448.53	REAL	Cn1c(-c2ccc3ccccc3n2)nnc1N1CCN(C(=O)c2ccc3ccccc23)CC1
vNsp13-rna1-109	Z2014714478	-10.4	0.325	446.93	REAL	O=C1O[C@@H](c2ccccc2)Cc2cc(C(=O)N3CCN[C@H](c4ccccc4Cl)C3)ccc21
vNsp13-rna1-110	Z2167006687	-10.4	0.315	441.47	REAL	Cn1c(-c2n[nH]c(=O)c3ccccc23)nnc1N1CC=C(c2c[nH]c3cc(F)ccc23)CC1
vNsp13-rna1-111	Z2174926886	-10.4	0.315	438.53	REAL	O=C1O[C@@H](c2ccccc2)Cc2cc(C(=O)N3CCCN4c5ccccc5C[C@@H]4C3)ccc21
vNsp13-rna1-112	Z2232118042	-10.4	0.371	368.44	REAL	Cc1nc2c(C(=O)N3CCc4ccccc4[C@@H]3c3ccccc3)ccnc2[nH]1
vNsp13-rna1-113	Z237330932	-10.4	0.325	427.50	REAL	O=C1O[C@@H](c2ccccc2)Cc2cc(C(=O)N3CCC(c4ccc(O)cc4)CC3)ccc21
vNsp13-rna1-114	Z2990647800	-10.4	0.347	399.46	REAL	CC1(C)CN(c2nnnn2Cc2ccc(-c3nncnn3)cc2)Cc2ccccc21
vNsp13-rna1-115	Z3214701994	-10.4	0.297	484.95	REAL	O=C(c1ccc2[nH]cnc2c1)N1CCN(C(=O)c2ccc(-n3ncc4ccccc43)cc2Cl)CC1
vNsp13-rna1-116	Z357612154	-10.4	0.306	455.47	REAL	O=C(c1ccc2c(=O)n(-c3ccccc3)c(=O)[nH]c2c1)N1CCN(C(=O)c2ccccn2)CC1
vNsp13-rna1-117	Z645681002	-10.4	0.297	484.62	REAL	O=C(c1cccc2ccccc12)N1CCN(C(=O)[C@H]2CCCN(c3nc4ccccc4s3)C2)CC1
vNsp13-rna1-118	Z645681528	-10.4	0.325	429.44	REAL	O=C(c1cnc2[nH]c(=O)[nH]c(=O)c2c1)N1CCN(C(=O)c2cccc3ccccc23)CC1
vNsp13-rna1-119	Z749768724	-10.4	0.315	442.52	REAL	O=C1O[C@@H](c2ccccc2)Cc2cc(C(=O)N3CCC(c4nnc5n4CCC5)CC3)ccc21
vNsp13-rna1-120	Z859061644	-10.4	0.315	442.50	REAL	O=C(Nc1cccc(-c2nnc3n2CCC3)c1)N1CC=C(c2c[nH]c3cc(F)ccc23)CC1
vNsp13-rna1-121	ZINC000001225262	-10.4	0.267	553.36	ZINC	O=C1c2cccc(Cl)c2C(=O)N1c1ccc(-c2nc3ccc(N4C(=O)c5cccc(Cl)c5C4=O)cc3[nH]2)cc1
vNsp13-rna1-122	ZINC000001238226	-10.4	0.281	497.53	ZINC	O=C(Nc1cccc2ccccc21)N1CCC(c2nc(=O)c3nnn(Cc4ccc(F)cc4)c3[nH]2)CC1
vNsp13-rna1-123	ZINC000002417585	-10.4	0.335	432.48	ZINC	Cc1ccc(S(=O)(=O)c2c(N)n(-c3ccc(F)cc3)c3nc4ccccc4nc32)cc1
vNsp13-rna1-124	ZINC000002446885	-10.4	0.274	499.54	ZINC	O=C(c1ccccc1F)[C@@H]1[C@@H](c2ccccc2)C2(C(=O)c3ccccc3C2=O)[C@@H]2C=Cc3ccccc3N21
vNsp13-rna1-125	ZINC000003146966	-10.4	0.315	424.46	ZINC	c1ccc2nc(-c3ccc4c(c3)oc3cc(-c5cnc6ccccc6n5)ccc34)cnc2c1
vNsp13-rna1-126	ZINC000004236421	-10.4	0.289	494.47	ZINC	O=C(Nc1ccccc1)N1CCN2C(=O)c3cc(-c4cccc(C(F)(F)F)c4)ccc3NC(=O)[C@@H]2C1
vNsp13-rna1-127	ZINC000008654667	-10.4	0.306	471.99	ZINC	Cc1nn(-c2nc(C)cc(C)n2)c2c1[C@H](c1ccc(Cl)cc1)CC(=O)N2Cc1ccc(C)cc1
vNsp13-rna1-128	ZINC000008694925	-10.4	0.297	452.47	ZINC	O=C1c2ccccc2C(=O)c2c3[nH]nc(-c4nc5ccccc5nc4-c4ccccc4)c3ccc21
vNsp13-rna1-129	ZINC000009015957	-10.4	0.289	495.93	ZINC	O=C([C@@H]1[C@H]2C(=O)N(c3ccc(Cl)c3)C(=O)[C@@H]2[C@@H]2C=Cc3ccccc3N21)n1nnc2ccccc21
vNsp13-rna1-130	ZINC000009015958	-10.4	0.289	495.93	ZINC	O=C([C@@H]1[C@H]2C(=O)N(c3ccc(Cl)c3)C(=O)[C@@H]2[C@H]2C=Cc3ccccc3N21)n1nnc2ccccc21
vNsp13-rna1-131	ZINC000009158129	-10.4	0.306	457.44	ZINC	O=C(c1ccc(F)cc1)[C@H]1[C@H]2C(=O)N(c3ccc(F)cc3)C(=O)[C@H]2[C@H]2c3ccccc3C=NN12
vNsp13-rna1-132	ZINC000009202275	-10.4	0.297	476.47	ZINC	O=C(c1ccc2c(c1)OCO2)N1CCC(c2nc3c(nnn3Cc3ccccc3F)c(O)n2)CC1
vNsp13-rna1-133	ZINC000009202307	-10.4	0.289	490.49	ZINC	O=C(c1ccc2c(c1)OCCO2)N1CCC(c2nc3c(nnn3Cc3ccccc3F)c(O)n2)CC1
vNsp13-rna1-134	ZINC000009291128	-10.4	0.297	457.50	ZINC	O=C1Nc2ccccc2[C@]12N=C(N1CCCc3ccccc31)N=c1nc3c(n12)=Nc1ccccc1-3
vNsp13-rna1-135	ZINC000009969421	-10.4	0.297	469.52	ZINC	O=C(c1ccccc1)c1cnc2cc3c(cc2c1N1CCN(c2ccc(F)cc2)CC1)OCCO3
vNsp13-rna1-136	ZINC000011171958	-10.4	0.281	496.48	ZINC	CC(=O)Nc1ccc(N2C(=O)c3ccc(C(=O)O[C@H](C)c4nc5ccccc5c(=O)[nH]4)cc3C2=O)cc1
vNsp13-rna1-137	ZINC000012360361	-10.4	0.297	458.52	ZINC	O=C(Cc1cccc2ccccc21)NN1C(=O)[C@H]2[C@@H](C1=O)C1c3ccccc3C2c2ccccc21
vNsp13-rna1-138	ZINC000012548776	-10.4	0.260	523.60	ZINC	Cc1ccc(N2C(=O)c3ccccc3/C(=C\Nc3nnc(-c4ccccc4)c(-c4ccccc4)n3)C2=O)c(C)c1
vNsp13-rna1-139	ZINC000013382161	-10.4	0.274	519.00	ZINC	O=C(Cc1ccccc1)Nc1ccc(N2C(=O)[C@H]3[C@@H](C2=O)C2c4ccccc4C3c3ccccc32)cc1Cl
vNsp13-rna1-140	ZINC000013770246	-10.4	0.281	486.53	ZINC	O=C(Nc1ccccc1)[C@H]1[C@H]2C(=O)N(c3ccc4ccccc4c3)C(=O)[C@H]2[C@@H]2c3ccccc3C=NN12
vNsp13-rna1-141	ZINC000015972032	-10.4	0.281	494.53	ZINC	Cc1cccc(N2C(=O)[C@@H]3[C@H](C2=O)[C@@H](Cc2c[nH]c4ccccc24)N[C@]32C(=O)Nc3ccc(F)cc32)c1
vNsp13-rna1-142	ZINC000015972376	-10.4	0.281	494.53	ZINC	Cc1ccc(N2C(=O)[C@@H]3[C@H](C2=O)[C@H](Cc2c[nH]c4ccccc24)N[C@]32C(=O)Nc3ccc(F)cc32)cc1
vNsp13-rna1-143	ZINC000015997026	-10.4	0.281	482.54	ZINC	O=C(c1ccccc1)[C@@H]1[C@@H](c2cccnc2)C2(C(=O)c3ccccc3C2=O)[C@@H]2C=Cc3ccccc3N21
vNsp13-rna1-144	ZINC000017988475	-10.4	0.260	533.67	ZINC	Cc1ccc(C(C)C)c(OC(=O)C2CCC(N3C(=O)[C@H]4[C@@H](C3=O)C3c5ccccc5C4c4ccccc43)CC2)c1
vNsp13-rna1-145	ZINC000018044861	-10.4	0.289	481.46	ZINC	O=C1c2ccccc2C(=O)C12O[C@@H](c1ccccc1)[C@H]1C(=O)N(c3ccc4c(c3)OCO4)C(=O)[C@H]12
vNsp13-rna1-146	ZINC000019973870	-10.4	0.335	416.48	ZINC	Cc1ccc([C@@H]2CC(=O)c3cnc(N4CCN(C(=O)c5ccco5)CC4)nc3C2)cc1
vNsp13-rna1-147	ZINC000021171157	-10.4	0.297	472.50	ZINC	Cc1ccc(Cn2nnc3c2nc(C2CCN(C(=O)c4ccc5c(c4)OCO5)CC2)[nH]c3=O)cc1
vNsp13-rna1-148	ZINC000021171169	-10.4	0.289	490.49	ZINC	O=C(Cc1ccc2c(c1)OCO2)N1CCC(c2nc(=O)c3nnn(Cc4ccccc4F)c3[nH]2)CC1
vNsp13-rna1-149	ZINC000021867174	-10.4	0.281	492.58	ZINC	Cc1ccc(-c2nnn3c2nc(O)c2ccc(C(=O)N4CCN(c5cc(C)ccc5C)CC4)cc23)c1
vNsp13-rna1-150	ZINC000033855704	-10.4	0.281	482.54	ZINC	O=C(c1ccccc1)[C@@H]1[C@@H](c2cccnc2)C2(C(=O)c3ccccc3C2=O)[C@@H]2C=Cc3ccccc3N21
vNsp13-rna1-151	ZINC000034792034	-10.4	0.289	487.60	ZINC	Cc1ccc([C@@H]2NC(=O)N(C)C3=C2C(=O)N(CC(=O)N2CCN(c4c(C)cccc4C)CC2)C3)cc1
vNsp13-rna1-152	ZINC000035848329	-10.4	0.274	499.54	ZINC	O=C(c1ccc(F)cc1)[C@@H]1[C@@H](c2ccccc2)C2(C(=O)c3ccccc3C2=O)[C@@H]2C=Cc3ccccc3N21
vNsp13-rna1-153	ZINC000048272370	-10.4	0.306	458.51	ZINC	O=C(Nc1cccc2ccccc21)N1CC=C(c2c[nH]c3cc(F)ccc32)CC1
vNsp13-rna1-154	ZINC000057099770	-10.4	0.289	497.98	ZINC	Cc1cccc2c1NC(=O)[C@]21N2CCC[C@H]2[C@@H](C(=O)c2ccccc2Cl)[C@]12C(=O)Nc1ccccc12
vNsp13-rna1-155	ZINC000067262781	-10.4	0.297	472.50	ZINC	Cc1ccc(N2CCN(c3ncc4c(=O)n(-c5ccc6c(c5)OCO6)c(O)nc4n3)CC2)c(C)c1
vNsp13-rna1-156	ZINC000072405137	-10.4	0.306	457.47	ZINC	Cc1nn(-c2ccc(F)cc2)c(C)c1[C@@H]1CC(O)=Nc2c1c(C)nn2-c1ncnc2[nH]cnc21
vNsp13-rna1-157	ZINC000085392553	-10.4	0.267	520.61	ZINC	O=C([C@@H]1CC(=O)N(c2ccc(F)cc2)C1)N1CCC(c2c[nH]c3ccccc32)c2c[nH]c3ccccc32)CC1
vNsp13-rna1-158	ZINC000085392641	-10.4	0.267	517.63	ZINC	O=C([C@@H]1CC(=O)N(Cc2ccccn2)C1)N1CCC(c2c[nH]c3ccccc32)c2c[nH]c3ccccc32)CC1
vNsp13-rna1-159	ZINC000100505724	-10.4	0.281	488.54	ZINC	O=C1[C@@H]2[C@H]3C=C[C@@H](C3)[C@@H]2C(=O)N1c1ccc2c(c1)-c1cc(N3C(=O)[C@@H]4[C@H]5C=C[C@@H](C5)[C@@H]4C3=O)ccc1C2
vNsp13-rna1-160	ZINC000102485937	-10.4	0.297	470.46	ZINC	Cc1cc(N2C(=O)C(=O)/C(=C(/O)c3ccc(F)cc3)[C@@H]2c2ccccc(Oc3cccc3)c2)no1
vNsp13-rna1-161	ZINC000102608292	-10.4	0.297	482.52	ZINC	Cc1cccc(N2C(=O)c3ccccc3/C(=C/Nc3ccccc3-c3nnc(S)nc3O)C2=O)n1
vNsp13-rna1-162	ZINC000102983156	-10.4	0.248	591.61	ZINC	Cc1ccc(N2C(=O)c3ccccc3/C(=C/Nc3cccc(S(=O)(=O)Nc4cccc(C(F)(F)F)c4)c3)C2=O)cc1C
vNsp13-rna1-163	ZINC000103518122	-10.4	0.281	494.53	ZINC	Cc1ccc2c(c1)[C@]1(N[C@@H](Cc3c[nH]c4ccccc34)[C@H]3C(=O)N(c4ccc(F)cc4)C(=O)[C@@H]31)C(=O)N2
vNsp13-rna1-164	ZINC000229890704	-10.4	0.248	552.67	ZINC	Cc1ccc(C(=O)[C@H]2[C@@H](C(=O)c3ccc(C)cc3)N3c4ccc(C)cc4C(C)=C[C@H]3[C@@]23C(=O)Nc2ccccc23)cc1
vNsp13-rna1-165	ZINC000229905129	-10.4	0.242	589.05	ZINC	CC1=C[C@@H]2N(c3ccccc31)[C@H](C(=O)c1ccccc1Cl)[C@@H](C(=O)c1ccc3c(c1)OCO3)[C@@]21C(=O)Nc2ccccc21
vNsp13-rna1-166	ZINC000229978903	-10.4	0.260	546.03	ZINC	O=C(Nc1ccccc1)[C@@H]1[C@H](C(=O)c2ccc(Cl)cc2)[C@]2(C(=O)Nc3ccccc32)[C@@H]2C=Cc3ccccc3N21
vNsp13-rna1-167	ZINC000247748619	-10.4	0.335	427.38	ZINC	NC(=O)[C@@H]1[C@@H]2C(=O)N(c3ccccc(C(F)(F)F)c3)C(=O)[C@H]2[C@@H]2c3ccccc3C=CN21
vNsp13-rna1-168	ZINC000247797224	-10.4	0.274	497.55	ZINC	O=C(c1ccc(-c2ccccc2)cc1)[C@@H]1[C@@H]2C(=O)N(c3ccccc3)C(=O)[C@H]2[C@H]2c3ccccc3C=NN12
vNsp13-rna1-169	ZINC000247850321	-10.4	0.281	489.53	ZINC	Cc1ccc(N2C(=O)[C@H]3[C@@H]4C=Cc5ccccc5N4[C@H](C(=O)n4nnc5ccccc54)[C@H]3C2=O)c(C)c1
vNsp13-rna1-170	ZINC000247850343	-10.4	0.281	489.53	ZINC	Cc1ccc(N2C(=O)[C@H]3[C@@H]4C=Cc5ccccc5N4[C@H](C(=O)n4nnc5ccccc54)[C@H]3C2=O)c(C)c1
vNsp13-rna1-171	ZINC000257263399	-10.4	0.315	439.52	ZINC	Cc1cc(Nc2ncccc2C)cc([C@@H]2CN(C(=O)c3cccc4ncccc43)CCO2)n1
vNsp13-rna1-172	ZINC000408675226	-10.4	0.274	498.58	ZINC	Cc1cccc(NC(=O)c2cccc(N3C(=O)[C@H]4[C@@H](C3=O)C3c5ccccc5C4c4ccccc43)c2)c1C
vNsp13-rna1-173	ZINC000408680522	-10.4	0.289	476.57	ZINC	O=C(c1ccc(N2C(=O)[C@H]3[C@@H](C2=O)C2c4ccccc4C3c3ccccc32)cc1)N1CCCCC1
vNsp13-rna1-174	ZINC000408686158	-10.4	0.274	498.58	ZINC	Cc1cc(C)cc(NC(=O)c2ccc(N3C(=O)[C@H]4[C@@H](C3=O)C3c5ccccc5C4c4ccccc43)cc2)c1
vNsp13-rna1-175	ZINC000604405464	-10.4	0.289	480.43	ZINC	O=c1oc2ccccc2c2oc(-c3ccc4c(c3)OCCO4)c(-c3c(=O)oc4ccccc4c3O)c21
vNsp13-rna1-176	ZINC000604419204	-10.4	0.297	462.51	ZINC	O=C(CN1C(=O)c2ccccc2N2C(=O)c3ccccc3[C@@H]21)N1CCc2c3ccccc3[nH]c2C1
vNsp13-rna1-177	Z1069484790	-10.3	0.312	445.47	REAL	C[C@H]1Oc2ccc(C(=O)C3CCN(C(=O)c4cc(O)nc5ccccc45)CC3)cc2NC1=O
vNsp13-rna1-178	Z1071337020	-10.3	0.312	443.50	REAL	C[C@H]1Oc2ccc(C(=O)C3CCN(C(=O)Nc4cccc5ccccc45)CC3)cc2NC1=O
vNsp13-rna1-179	Z1144492947	-10.3	0.312	440.55	REAL	Cc1ccc(-n2nc(C(=O)N3CCC[C@@H](c4nnc5ccccn45)C3)c3c2CCC3)c(C)c1
vNsp13-rna1-180	Z1161173996	-10.3	0.312	436.52	REAL	Cc1c(C(=O)N2CCC[C@H](c3cc4ccccc4[nH]3)C2)nnn1-c1ccc2ncccc2c1
vNsp13-rna1-181	Z1250586272	-10.3	0.312	438.49	REAL	Cc1cc(C(=O)NC[C@H]2CC3c4ccccc4C2c2ccccc23)nc2nc(O)[nH]c(=O)c12
vNsp13-rna1-182	Z1280799883	-10.3	0.312	444.53	REAL	C[C@@H]1Oc2ccc(C(=O)C3CCN(C(=O)[C@H]4C[C@]45CCc4ccccc45)CC3)c2NC1=O
vNsp13-rna1-183	Z1374246802	-10.3	0.343	404.47	REAL	Cc1cc(C(=O)N2CCC[C@]3(CCCc4ccccc43)C2)nc2nc(O)[nH]c(=O)c12
vNsp13-rna1-184	Z1383812253	-10.3	0.303	452.51	REAL	Cc1ccc(C(=O)N2CCC[C@@H](C(=O)Nc3ccc4c(c3)C(=O)c3ccccc3C4=O)C2)cc1
vNsp13-rna1-185	Z14014220	-10.3	0.312	446.51	REAL	Cc1cc(-n2c(C)cc(C(=O)CN3C(=O)N[C@@]4(CCCCc5ccccc54)C3=O)c2C)no1
vNsp13-rna1-186	Z1423391170	-10.3	0.322	423.47	REAL	O=C1O[C@@H](c2ccccc2)Cc2cc(C(=O)N3CCc4nc5ccccc5[nH]4)C3)ccc21
vNsp13-rna1-187	Z1472556068	-10.3	0.312	442.52	REAL	O=C1C[C@H](c2ccc(NC(=O)N3CCN(C(=O)c4ccc5ccccc45)CC3)c2)CN1
vNsp13-rna1-188	Z1510260836	-10.3	0.312	446.55	REAL	CCc1c(C(=O)N2CCC[C@]3(CCCc4ccccc43)C2)cnc2c1c(=O)n(C)c(=O)n2C
vNsp13-rna1-189	Z1531754985	-10.3	0.332	420.45	REAL	O=C1Nc2ccccc2[C@@H]1C1CCN(C(=O)Nc2ccn(-c3nccc3F)n2)CC1
vNsp13-rna1-190	Z1578876633	-10.3	0.332	417.48	REAL	Cc1ccc([C@]2(C)CC(=O)N(Cc3nn(-c4ccc(F)cc4)c4c3CCC4)C2=O)cc1
vNsp13-rna1-191	Z1632951313	-10.3	0.312	447.51	REAL	O=C(N[C@@H]1CCc2nnc(-c3ccc(F)cc3)n2C1)N1CCO[C@]2(CCc3ccccc32)C1
vNsp13-rna1-192	Z1723443920	-10.3	0.312	440.50	REAL	Cn1c(=O)[nH]c2ncc(-c3cccc(C(=O)N4CCO[C@]5(CCc6ccccc65)C4)c3)cc21
vNsp13-rna1-193	Z1728614571	-10.3	0.312	442.47	REAL	C[C@@H]1CN(C(=O)c2cc(=O)c3ccccc3[nH]2)CCN1C(=O)c1cc(=O)c2ccccc2[nH]1
vNsp13-rna1-194	Z2003406991	-10.3	0.322	440.41	REAL	C[C@H]1CN(C(=O)c2cc(F)cc3[nH]nnc23)[C@H](C)CN1C(=O)c1cc(F)cc2[nH]nnc12
vNsp13-rna1-195	Z2007851949	-10.3	0.312	442.48	REAL	Cn1c(-c2cccc3ccncc23)nnc1N1CCN(C(=O)c2ccc3c(c2)OCO3)CC1
vNsp13-rna1-196	Z2008701854	-10.3	0.322	431.50	REAL	Cn1c(-c2ccc3c(c2)OCCO3)nnc1N1CCC([C@@H]2C(=O)Nc3ccccc32)CC1
vNsp13-rna1-197	Z2008716005	-10.3	0.332	414.47	REAL	Cn1c(-c2n[nH]c(=O)c3ccccc23)nnc1N1CCC2(CC1)OCc1ccccc12
vNsp13-rna1-198	Z2014784669	-10.3	0.312	441.51	REAL	O=C(c1ccc2[nH]c3ccccc3c(=O)c2c1)N1CCC(N2CCc3cc(F)ccc32)CC1
vNsp13-rna1-199	Z2085931218	-10.3	0.332	417.51	REAL	Cc1ccc([C@]2(C)NC(=O)N(CC(=O)N3Cc4ccccc4C4(CCC4)C3)C2=O)cc1
vNsp13-rna1-200	Z2157852663	-10.3	0.312	442.51	REAL	O=C(c1cccc2ccccc12)N1CCC[C@H](C(=O)N2CCC3(C2)Oc2ccccc2O3)C1

Supplementary Table 64. Virtual screening hits 101 to 200 of the screen against the RNA binding site of nsp13 (Screen ID: 34). Compounds were filtered so that hits had MW < 600 dalton, cLogP < 6, number of hydrogen bond acceptors < 11, and no reactive functional groups. A few compounds unsuitable for drug discovery were removed by visual inspection. The name of each compound consists of the initial letter 'v' for virtual hit, followed by the target protein name and the target site ('rna' for RNA binding site, 1 for docking scenario 1). The score is the docking score given by QuickVina 2 in kcal/mol. The ligand efficiency (LE) is computed as LE = -score/#NonH, where #NonH is the number of heavy (i.e. non hydrogen) atoms.

Name	Catalog ID	Score	LE	MW	Library	SMILES
vNsp13-rna2-1	ZINC000004015296	-10.6	0.279	493.477	ZINC	O=c1nc2c3cccc4cccc(c(=O)n2c2cc(N5C(=O)c6cccc7cccc(c76)C5=O)ccc12)c43
vNsp13-rna2-2	ZINC000254722125	-10.4	0.289	558.411	ZINC	O=C(N=C1N=C2C=CC(Br)=CN2Cc2ccccc21)c1ccc2c(c1)S(=O)(=O)c1ccccc1C2=O
vNsp13-rna2-3	ZINC000015990071	-10.3	0.257	527.626	ZINC	Cc1cccc(Nc2nnc(-c3ccc(C(=O)N4C[C@H]5C[C@@H](C4)c4cccc(=O)n4C5)cc3)c3ccccc32)c1
vNsp13-rna2-4	ZINC000409330841	-10.3	0.271	494.509	ZINC	O=C(Nc1ccc2nc3c4ccccc4c4ccccc4c3nc2c1)c1ccc(N2C(=O)C=CC2=O)cc1
vNsp13-rna2-5	ZINC000409336236	-10.3	0.271	499.565	ZINC	Cc1ccc(N2C(=O)[C@@H]3[C@H](C2=O)[C@@H]2C(=O)Oc4ccc5ccccc5c4C2=C[C@H]3c2ccccc2)cc1C
vNsp13-rna2-6	ZINC000409337264	-10.3	0.271	499.565	ZINC	Cc1ccc(N2C(=O)[C@@H]3[C@H](C2=O)[C@@H]2C(=O)Oc4ccc5ccccc5c4C2=C[C@H]3c2ccccc2)c(C)c1
vNsp13-rna2-7	ZINC000019375342	-10.2	0.276	498.585	ZINC	O=c1[nH]c2cc3c(cc2cc1[C@H](c1nnnn1C1CCCCC1)N1CCc2ccccc2C1)OCCO3
vNsp13-rna2-8	Z1024048888	-10.1	0.316	427.546	REAL	C[C@@H]1CCc2[nH]c3ccc(C(=O)N4CCC([C@H]5C(=O)Nc6ccccc65)CC4)cc3c2C1
vNsp13-rna2-9	Z1451423747	-10.1	0.316	425.487	REAL	C[C@@]1(c2cccc(C(=O)N3Cc4ccccc4[C@H](c4ccccc4)C3)c2)NC(=O)NC1=O
vNsp13-rna2-10	Z2008317854	-10.1	0.297	449.513	REAL	Cn1c(-c2cc(-c3ccco3)nc3ccccc23)nnc1N1CC[C@]2(C1)OCc1ccccc12
vNsp13-rna2-11	ZINC000001225262	-10.1	0.259	553.36	ZINC	O=C1c2cccc(Cl)c2C(=O)N1c1ccc(-c2nc3ccc(N4C(=O)c5cccc(Cl)c5C4=O)ccc3[nH]2)cc1
vNsp13-rna2-12	ZINC000001862466	-10.1	0.289	455.468	ZINC	Cc1nc(-c2cc3c(ccc4ccccc43)oc2=O)cc2c1c(=O)oc1ccc3ccccc3c12
vNsp13-rna2-13	ZINC000008921457	-10.1	0.266	498.537	ZINC	O=C(NN1C(=O)[C@H]2[C@H](C1=O)C1c3ccccc3C2c2ccccc21)C1(O)c2ccccc2-c2ccccc21
vNsp13-rna2-14	ZINC000079188711	-10.1	0.281	492.522	ZINC	C[C@@H]1CCCC(=O)CCC/C=C/c2cc3c(c(O)c2C(=O)O1)[C@@H](c1ccc2c(c1)OCO2)CC(=O)O3
vNsp13-rna2-15	ZINC000100485505	-10.1	0.316	410.431	ZINC	O=C1c2ccc3c4c(ccc(c24)C2=Nc4ccccc4[C@@H]21)C1=Nc2ccccc2[C@@H]1C3=O
vNsp13-rna2-16	ZINC000101076130	-10.1	0.266	499.521	ZINC	O=C1c2ccccc2C(=O)C12O[C@@H](c1ccccc1)[C@@H]1C(=O)N(c3ccc(-c4ccccc4)cc3)C(=O)[C@@H]12
vNsp13-rna2-17	ZINC000245311382	-10.1	0.281	478.503	ZINC	Cc1ccc(N2C(=O)[C@H]3[C@H](C(=O)c4ccc5c(c4)OCO5)N4C=Cc5ccccc5[C@H]4[C@H]3C2=O)cc1
vNsp13-rna2-18	ZINC000245377193	-10.1	0.273	488.542	ZINC	O=C1[C@@H]2[C@H]3C=C[C@@H](C3)[C@H]2C(=O)N1c1ccc2c(c1)-c1cc(N3C(=O)[C@@H]4[C@H]5C=C[C@@H](C5)[C@H]4C3=O)ccc1C2
vNsp13-rna2-19	ZINC000247778287	-10.1	0.281	479.491	ZINC	O=C(Nc1ccccc1)[C@@H]1[C@@H]2C(=O)N(c3ccc4c(c3)OCO4)C(=O)[C@H]2[C@@H]2c3ccccc3C=CN21
vNsp13-rna2-20	ZINC000408730080	-10.1	0.266	499.565	ZINC	Cc1ccc(N2C(=O)[C@H]3[C@H](C2=O)[C@@H]2C(=O)Oc4c5ccccc5ccc4C2=C[C@H]3c2ccccc2)c(C)c1
vNsp13-rna2-21	ZINC000408732827	-10.1	0.273	485.538	ZINC	Cc1ccccc1N1C(=O)[C@@H]2[C@H](C1=O)[C@@H]1C(=O)Oc3ccc4ccccc4c3C1=C[C@H]2c1ccccc1
vNsp13-rna2-22	Z1766668118	-10	0.313	421.499	REAL	Cc1ccc2[nH]c3c(c2c1)C[C@H](NC(=O)c1ccc2[nH]c4ccccc4c(=O)c2c1)CC3
vNsp13-rna2-23	ZINC000001099260	-10	0.278	474.427	ZINC	O=C1NC(=O)c2cc(N3C(=O)c4cc5oc6ccccc6c6ccccc6oc5cc4C3=O)ccc21
vNsp13-rna2-24	ZINC000001789604	-10	0.256	532.666	ZINC	O=c1[nH]c(CSc2nc3ccccc3c(=O)n2-c2ccccc2)nc2c1C1(CCCCC1)Cc1ccccc1-2
vNsp13-rna2-25	ZINC000002420588	-10	0.27	488.546	ZINC	CC1(C)CC(=O)C2=C(C1)Oc1ncn3nc(-c4ccc5ccccc5cc4O)nc3c1[C@H]2c1ccccc1
vNsp13-rna2-26	ZINC000002439806	-10	0.278	472.547	ZINC	CC1(C)CC(=O)C2=C(C1)Oc1ncn3nc(-c4ccc5ccccc54)nc3c1[C@@H]2c1ccccc1
vNsp13-rna2-27	ZINC000003371634	-10	0.286	480.591	ZINC	Cc1ccc(N2C(=O)c3ccccc3/C(=C/Nc3ncnc4sc5c(c43)CCCC5)C2=O)c(C)c1
vNsp13-rna2-28	ZINC000008792183	-10	0.27	486.573	ZINC	Cc1ccccc(N2CCN(C(=O)c3cc4c5ccccc5n5c4c(n3)c3ccccc3c5=O)CC2)c1C
vNsp13-rna2-29	ZINC000008921453	-10	0.263	498.537	ZINC	O=C(NN1C(=O)[C@@H]2[C@@H](C1=O)C1c3ccccc3C2c2ccccc21)C1(O)c2ccccc2-c2ccccc21
vNsp13-rna2-30	ZINC000009320043	-10	0.278	479.491	ZINC	O=C(Nc1ccc2c(c1)OCO2)[C@@H]1[C@@H]2C(=O)N(c3ccccc3)C(=O)[C@H]2[C@@H]2c3ccccc3C=CN21
vNsp13-rna2-31	ZINC000018045008	-10	0.278	479.578	ZINC	Cc1ccc(C(=O)/C=C2/Nc3c4ccccc4oc(=O)c3N/C2=N\C23CC4CC(CC(C4)C2)C3)cc1
vNsp13-rna2-32	ZINC000059932652	-10	0.25	527.622	ZINC	Cc1ccc2c(c1C)NC(=O)[C@@]21N2CCC[C@@H]2[C@@H](C(=O)c2ccc3ccccc3c2)[C@@]12c1ccccc1NC2=O
vNsp13-rna2-33	ZINC000095475858	-10	0.27	496.478	ZINC	O=c1[nH]c2cc3c(cc2cc1-c1c2oc4cc(O)ccc4c2nc2c1c(O)nn2C1CCCC1)OCO3
vNsp13-rna2-34	ZINC000102908582	-10	0.294	473.552	ZINC	CN1c2ccccc2C(C)(C)[C@]12CC(c1ccc3c(c1)S(=O)(=O)c1ccccc1/C3=N\O)=NO2
vNsp13-rna2-35	ZINC000102952252	-10	0.278	479.578	ZINC	Cc1ccc(C(=O)/C=C2\Nc3c4ccccc4oc(=O)c3N=C2NC23CC4CC(CC(C4)C2)C3)cc1
vNsp13-rna2-36	ZINC000253623625	-10	0.286	465.46	ZINC	COc1ccc2nc(O)c([C@H]3CC(=O)Oc4ccc5c(c43)O/C(=C/c3ccccc3)C5=O)cc2c1
vNsp13-rna2-37	ZINC000408675225	-10	0.263	498.58	ZINC	Cc1cccc(NC(=O)c2cccc(N3C(=O)[C@@H]4[C@@H](C3=O)C3c5ccccc5C4c4ccccc43)c2)c1C
vNsp13-rna2-38	ZINC000408731315	-10	0.263	499.565	ZINC	Cc1ccc(C)c(N2C(=O)[C@H]3[C@H](C2=O)[C@@H]2C(=O)Oc4c5ccccc5ccc4C2=C[C@H]3c2ccccc2)c1
vNsp13-rna2-39	ZINC000408731626	-10	0.263	499.565	ZINC	Cc1ccc(N2C(=O)[C@H]3[C@H](C2=O)[C@@H]2C(=O)Oc4c5ccccc5ccc4C2=C[C@H]3c2ccccc2)cc1C
vNsp13-rna2-40	ZINC000408732460	-10	0.263	499.565	ZINC	Cc1ccc(C)c(N2C(=O)[C@H]3[C@H](C2=O)[C@@H]2C(=O)Oc4ccc5ccccc5c4C2=C[C@H]3c2ccccc2)c1
vNsp13-rna2-41	ZINC000408978419	-10	0.286	456.508	ZINC	C[C@@H]1Cc2ccccc2N1C(=O)Nc1ccc2nc3c4ccncc4cnccc4c3nc2c1
vNsp13-rna2-42	ZINC000409336222	-10	0.263	499.565	ZINC	Cc1ccc(N2C(=O)[C@H]3[C@H](C2=O)[C@@H]2C(=O)Oc4ccc5ccccc5c4C2=C[C@@H]3c2ccccc2)cc1C
vNsp13-rna2-43	ZINC000409336230	-10	0.263	499.565	ZINC	Cc1ccc(N2C(=O)[C@H]3[C@H](C2=O)[C@@H]2C(=O)Oc4ccc5ccccc5c4C2=C[C@H]3c2ccccc2)cc1C
vNsp13-rna2-44	ZINC000409336691	-10	0.27	483.486	ZINC	O=C(Nc1ccc2nc3[nH]c4ccccc4c3nc2c1)c1ccc(N2C(=O)c3ccccc3C2=O)cc1
vNsp13-rna2-45	ZINC000409337159	-10	0.263	494.509	ZINC	O=C(Nc1ccc2nc3ccc4ccccc4c3nc2c1)c1ccc(N2C(=O)c3ccccc3C2=O)cc1
vNsp13-rna2-46	PV-001860453824	-9.9	0.319	441.914	REAL	CC1(C)CO[C@H](c2ccccc(Cl)c2)CN1C(=O)c1ccccc1[C@]2(C)NC(=O)NC2=O)c1
vNsp13-rna2-47	Z1504177441	-9.9	0.33	405.417	REAL	O=C1c2ccccc2C(=O)N1[C@@H]1CCCC/C(=N/Nc2nc3[nH]ncc3c(=O)[nH]2)C1
vNsp13-rna2-48	Z571164164	-9.9	0.283	467.48	REAL	Cc1c(-c2ccccc2)oc2c(C(=O)Nc3cccc([C@]4(C)NC(=O)NC4=O)c3)cccc2c1=O
vNsp13-rna2-49	Z979198394	-9.9	0.3	457.509	REAL	O=C(Nc1ccc2[nH]c(C3CCC3)nc2c1)c1ccc2c(c1)S(=O)(=O)c1ccccc1C2=O
vNsp13-rna2-50	ZINC000002908937	-9.9	0.268	494.452	ZINC	O=c1oc(-c2cccc(F)c2)nc2cc(Cc3ccc4nc(-c5cccc(F)c5)oc(=O)c4c3)ccc12
vNsp13-rna2-51	ZINC000002940126	-9.9	0.261	518.999	ZINC	Cc1ccc(NC(=O)c2cccc(N3C(=O)[C@@H]4[C@@H](C3=O)C3c5ccccc5C4c4ccccc43)c2)cc1Cl
vNsp13-rna2-52	ZINC000003017722	-9.9	0.268	496.501	ZINC	O=C(CN1C(=O)c2ccccc2C1=O)Nc1nc2n(n1)[C@H](c1ccc(F)cc1)C[C@@H](c1ccccc1)N2
vNsp13-rna2-53	ZINC000008792389	-9.9	0.275	476.51	ZINC	O=C(c1cc2c3ccccc3n3c2c(n1)c1ccccc1c3=O)N1CCN(c2ccccc2F)CC1
vNsp13-rna2-54	ZINC000009012096	-9.9	0.309	423.471	ZINC	O=C1Nc2ccccc2[C@@]12[C@@H]1C(=O)N(c3ccc4ccccc4c3)C(=O)[C@H]1[C@@H]1CCCN12
vNsp13-rna2-55	ZINC000009057162	-9.9	0.319	422.372	ZINC	O=c1c2ccc3c4ccc5c(=O)c(=O)c6cc7c(c8c(cc(c1=O)c2c83)S7(=O)=O)c4c56
vNsp13-rna2-56	ZINC000009291126	-9.9	0.283	457.496	ZINC	O=C1Nc2ccccc2[C@@]12N=C(N1CCCc3ccccc31)N=c1nc3c(n12)=Nc1ccccc1-3
vNsp13-rna2-57	ZINC000013304712	-9.9	0.291	472.564	ZINC	Cc1ccc2c(c1)[C@@H]1CN(C)CC[C@H]1N2C(=O)c1ccc2c(c1)S(=O)(=O)c1ccccc1C2=O
vNsp13-rna2-58	ZINC000015996247	-9.9	0.3	465.892	ZINC	O=C1Nc2ccc(Cl)cc2[C@@]12[C@@H]1C(=O)N(c3ccc4c(c3)OCCO4)C(=O)[C@H]1[C@@H]1CCCN12
vNsp13-rna2-59	ZINC000022130509	-9.9	0.268	484.562	ZINC	O=C(Nc1ccc2nc3c4ccccc4c4ccccc4c3nc2c1)N1CCN(c2ccccn2)CC1
vNsp13-rna2-60	ZINC000059796310	-9.9	0.254	513.595	ZINC	Cc1ccccc2c1NC(=O)[C@@]21N2CCC[C@@H]2[C@@H](C(=O)c2ccc3ccccc3c2)[C@@]12c1ccccc1NC2=O
vNsp13-rna2-61	ZINC000100505726	-9.9	0.268	488.542	ZINC	O=C1[C@@H]2[C@H]3C=C[C@@H](C3)[C@@H]2C(=O)N1c1ccc2c(c1)-c1cc(N3C(=O)[C@@H]4[C@@H]5C=C[C@@H](C5)[C@@H]4C3=O)ccc1C2
vNsp13-rna2-62	ZINC000100640729	-9.9	0.275	480.519	ZINC	O=C(c1ccc(N2C(=O)[C@@H]3CC=CC[C@@H]3C2=O)cc1)c1ccc(N2C(=O)[C@@H]3CC=CC[C@@H]3C2=O)cc1
vNsp13-rna2-63	ZINC000100908670	-9.9	0.291	492.365	ZINC	O=C1[C@@H]2CC=CC[C@@H]2C(=O)N1c1nc2n(n1)[C@H](c1ccc(Cl)cc1)C=C(c1ccc(Cl)cc1)N2
vNsp13-rna2-64	ZINC000104480060	-9.9	0.275	490.945	ZINC	O=C(NC1=CC=C[C@@H]2C(=O)c3ccccc3C(=O)[C@@H]12)c1cc(-c2ccccc2Cl)nc2ccccc21
vNsp13-rna2-65	ZINC000226073803	-9.9	0.291	452.6	ZINC	CC1=CC(C)(C)N(C)c2ccc([C@H]3C4=C(CC(C)(C)CC4=O)Nc4nc5ccccc5n43)cc21
vNsp13-rna2-66	ZINC000240824838	-9.9	0.254	516.556	ZINC	O=C1[C@@H]2[C@H]3C=C[C@@H](C3)[C@H]2C(=O)N1c1ccc(-c2nc3ccc(N4C(=O)[C@@H]5[C@H]6C=C[C@@H](C6)[C@@H]5C4=O)cc3[nH]2)cc1
vNsp13-rna2-67	ZINC000252518059	-9.9	0.3	437.498	ZINC	Cc1ccc2c(c1)[C@]1(C(=O)N2)[C@@H]2C(=O)N(c3ccc4ccccc4c3)C(=O)[C@H]2[C@@H]2CCCN21
vNsp13-rna2-68	ZINC000263584889	-9.9	0.283	465.46	ZINC	COc1ccc2nc(O)c([C@H]3CC(=O)Oc4ccc5c(c43)O/C(=C\c3ccccc3)C5=O)cc2c1
vNsp13-rna2-69	ZINC000263586502	-9.9	0.3	435.434	ZINC	O=C1c2ccc3c(c2O/C1=C\c1ccccc1)[C@@H](c1cc2ccccc2nc1O)CC(=O)O3
vNsp13-rna2-70	ZINC000408679806	-9.9	0.261	498.58	ZINC	Cc1cc(C)cc(NC(=O)c2cccc(N3C(=O)[C@@H]4[C@@H](C3=O)C3c5ccccc5C4c4ccccc43)c2)c1
vNsp13-rna2-71	ZINC000408680275	-9.9	0.261	498.58	ZINC	Cc1cccc(NC(=O)c2cccc(N3C(=O)[C@@H]4[C@@H](C3=O)C3c5ccccc5C4c4ccccc43)c2)c1C
vNsp13-rna2-72	ZINC000408730070	-9.9	0.268	485.538	ZINC	Cc1ccc(N2C(=O)[C@@H]3[C@H](C2=O)[C@@H]2C(=O)Oc4ccc5ccccc5c4C2=C[C@@H]3c2ccccc2)cc1
vNsp13-rna2-73	ZINC000408732461	-9.9	0.261	499.565	ZINC	Cc1ccc(C)c(N2C(=O)[C@@H]3[C@H](C2=O)[C@@H]2C(=O)Oc4ccc5ccccc5c4C2=C[C@H]3c2ccccc2)c1
vNsp13-rna2-74	ZINC000408975892	-9.9	0.275	466.503	ZINC	O=C(Nc1ccc2nc3c4cccnc4c4ncccc4c3nc2c1)Nc1ccccc2ccccc21
vNsp13-rna2-75	ZINC000408977745	-9.9	0.283	455.52	ZINC	O=C(c1ccc2nc3c4cccnc4c4ncccc4c3nc2c1)N1CC[C@H](c2ccccc2)C1
vNsp13-rna2-76	ZINC000408978119	-9.9	0.261	495.493	ZINC	O=C(Oc1ccc2nc3c4ccccc4c4ccccc4c3nc2c1)c1ccc(N2C(=O)C=CC2=O)cc1
vNsp13-rna2-77	ZINC000409334839	-9.9	0.268	493.514	ZINC	Cc1ccc(N2C(=O)[C@H]3[C@H](C2=O)[C@@H]2C(=O)Oc4cc(C)ccc4C2=C[C@H]3c2ccc3c(c2)OCO3)cc1
vNsp13-rna2-78	ZINC000409337249	-9.9	0.261	499.565	ZINC	Cc1ccc(N2C(=O)[C@@H]3[C@H](C2=O)[C@@H]2C(=O)Oc4ccc5ccccc5c4C2=C[C@@H]3c2ccccc2)c(C)c1
vNsp13-rna2-79	ZINC000604404118	-9.9	0.291	451.441	ZINC	O=C(CN1C(=O)c2ccccc2N2C(=O)c3ccccc3[C@H]21)Nc1ccc2ncnc(O)c2c1
vNsp13-rna2-80	Z1162537090	-9.8	0.297	436.47	REAL	O=C(Nc1nc2ccccc2c(=O)[nH]1)[C@@H]1CC(=O)N(c2ccc3c(c2)Cc2ccccc2-3)C1
vNsp13-rna2-81	Z1260482413	-9.8	0.306	430.59	REAL	C[C@@H]1Cc2ccccc2CN1C(=O)[C@H]1CCC[C@H](C(=O)N2Cc3ccccc3C[C@H]2C)C1
vNsp13-rna2-82	Z1547433285	-9.8	0.306	429.483	REAL	Cc1cc(C)nc(-n2nc(C(=O)N3Cc4ccccc4C[C@H]3c3nnc(C)o3)cc2C)n1
vNsp13-rna2-83	Z1663815549	-9.8	0.288	447.497	REAL	Cc1nc2ccccn2c1-c1nnc([C@@H]2CC(=O)N(c3ccc4c(c3)Cc3ccccc3-4)C2)o1
vNsp13-rna2-84	Z1723441401	-9.8	0.297	448.482	REAL	Cn1c(=O)[nH]c2ncc(-c3cccc(C(=O)N4CCC([C@]5(C)NC(=O)NC5=O)CC4)c3)cc21
vNsp13-rna2-85	Z1764004735	-9.8	0.297	443.452	REAL	Cc1ccc2[nH]c3c(c2c1)CN(C(=O)c1cc(F)cc2c(=O)c4cc(F)ccc4[nH]c12)CC3
vNsp13-rna2-86	Z1921545983	-9.8	0.297	446.462	REAL	C[C@H](C(=O)Nc1ccc2c(c1)C(=O)c1ccccc1C2=O)N1CCC[C@]2(C1)NC(=O)NC2=O
vNsp13-rna2-87	Z2004578506	-9.8	0.327	401.465	REAL	C[C@@]1(c2ccccc(C(=O)N3[C@H]4C=C(c5ccccc5)C[C@H]3CC4)c2)NC(=O)NC1=O
vNsp13-rna2-88	Z2198323213	-9.8	0.297	446.466	REAL	Cc1cc(C(=O)N2CCc3n[nH]c(=O)cc3C2)cc(C(=O)N2CCc3n[nH]c(=O)cc3C2)c1
vNsp13-rna2-89	Z225733282	-9.8	0.316	423.428	REAL	Cc1cc(-c2cc(C(=O)N3CCC4(CC3)NC(=O)NC4=O)c3c(C)noc3n2)c(C)o1
vNsp13-rna2-90	Z237105182	-9.8	0.306	431.582	REAL	C[C@@H]1CCc2[nH]c3ccc(C(=O)N4CCC[C@H](c5nnc6n5CCCCC6)C4)cc3c2C1
vNsp13-rna2-91	Z33398350	-9.8	0.327	393.445	REAL	Cc1ccc(-c2cc(C(=O)N3CC(=O)Nc4ccccc43)c3ccccc3n2)cc1
vNsp13-rna2-92	ZINC000001116293	-9.8	0.272	478.546	ZINC	C[C@]12C(=O)N(c3ccc(C(=O)N4CCOCC4)cc3)C(=O)[C@@H]1C1c3ccccc3C2c2ccccc21
vNsp13-rna2-93	ZINC000001714466	-9.8	0.239	560.585	ZINC	O=C1C=C(Nc2ccc(S(=O)(=O)c3ccc(NC4=CC(=O)C(=O)c5ccccc54)cc3)cc2)c2ccccc2C1=O
vNsp13-rna2-94	ZINC000001801020	-9.8	0.239	562.692	ZINC	COc1ccc(-n2c(=O)c3ccccc3nc2SCc2nc3c(c(=O)[nH]2)C2(CCCCC2)Cc2ccccc2-3)cc1
vNsp13-rna2-95	ZINC000003772019	-9.8	0.306	414.463	ZINC	O=c1oc2ccccc2c2c1[C@H](c1c[nH]c3ccccc31)Nc1ccc3ccccc3c1-2
vNsp13-rna2-96	ZINC000003845263	-9.8	0.297	444.465	ZINC	O=C1c2cccc3cccc(c23)/C1=C1\Sc2ccc3c(c2C1=O)C(=O)c1ccccc1C3=O
vNsp13-rna2-97	ZINC000003954537	-9.8	0.265	481.466	ZINC	O=C(Nc1cccc2c1C(=O)c1ccccc1C2=O)c1ccc2c3c1ncnc3-c1ccccc1C2=O
vNsp13-rna2-98	ZINC000012654825	-9.8	0.251	518.567	ZINC	C[C@H]1Cc2ccccc2N1C(=O)COC(=O)c1c2c(nc3ccccc31)/C(=C/c1ccc3c(c1)OCO3)CC2
vNsp13-rna2-99	ZINC000014534467	-9.8	0.265	493.565	ZINC	COc1ccc(-c2cc3c(n(C)c2=O)CCN(C(=O)c2cn4c(cccc4C)n2)C3)c2ccc(C)nc12
vNsp13-rna2-100	ZINC000014540764	-9.8	0.265	498.56	ZINC	Cc1cc(C(=O)N2CCc3c(c(C(=O)N4CCCC4)nn3Cc3ccncc3)C2)c2ccc(F)cc2n1

Supplementary Table 65. Top 100 virtual hits of the screen against the RNA binding site of nsp13 (Screen ID: 35). Compounds were filtered so that hits had MW < 600 dalton, cLogP < 6, number of hydrogen bond acceptors < 11, and no reactive functional groups. A few compounds unsuitable for drug discovery were removed by visual inspection. The name of each compound consists of the initial letter 'v' for virtual hit, followed by the target protein name and the target site ('rna' for RNA binding site, 2 for docking scenario 2). The score is the docking score given by QuickVina 2 in kcal/mol. The ligand efficiency (LE) is computed as LE = -score/#NonH, where #NonH is the number of heavy (i.e. non hydrogen) atoms.

Name	Catalog ID	Score	LE	MW	Library	SMILES
vNsp13-rna2-101	ZINC000014953292	-9.8	0.265	496.59	ZINC	Cc1c(C(=O)N2CCN([C@H]3CCc4ccccc4C3)CC2)cnn1-c1nccc(-c2ccccc2F)n1
vNsp13-rna2-102	ZINC000015305602	-9.8	0.251	521.71	ZINC	O=C(c1cc2n(n1)[C@@H](c1ccccc1)C[C@@H](c1ccccc1)N2)N1CCN(C23CC4CC(CC(C4)C2)C3)CC1
vNsp13-rna2-103	ZINC000015502321	-9.8	0.265	496.52	ZINC	Cn1cc([C@H]2Nc3ccccc3C(=O)N2c2ccc3c(c2)OCO3)c(-c2ccc3c(c2)OCCCO3)n1
vNsp13-rna2-104	ZINC000016757167	-9.8	0.258	498.54	ZINC	Cc1ccc(N2C(=O)c3ccccc3/C(=C/Nc3ccc4c(c3)C(=O)c3ccccc3C4=O)C2=O)c(C)c1
vNsp13-rna2-105	ZINC000019354041	-9.8	0.265	494.55	ZINC	O=C1c2ccccc2N[C@@H](c2cc3ccccc3nc2N2CCOC2)N1c1ccc2c(c1)OCCO2
vNsp13-rna2-106	ZINC000034703509	-9.8	0.288	441.49	ZINC	C[C@@H]1Cc2ccccc2N1C(=O)c1ccc2nc3c4ncccc4c4ccnc4c3nc2c1
vNsp13-rna2-107	ZINC000035241256	-9.8	0.272	470.53	ZINC	O=C(c1ccccc1)[C@H]1[C@@H]2C(=O)N(c3cccc4ccccc43)C(=O)[C@@H]2[C@@H]2c3ccccc3C=CN12
vNsp13-rna2-108	ZINC000035375706	-9.8	0.265	490.56	ZINC	Cc1cc(C)cc(N2C(=O)[C@@H]3[C@H](C2=O)[C@H](Cc2c[nH]c4ccccc24)N[C@@]32C(=O)Nc3ccccc32)c1
vNsp13-rna2-109	ZINC000100485501	-9.8	0.306	410.43	ZINC	O=C1c2ccc3c4c(ccc(c24)C2=Nc4ccccc4[C@H]21)C1=Nc2ccccc2[C@@H]1C3=O
vNsp13-rna2-110	ZINC000101026429	-9.8	0.233	550.67	ZINC	c1ccc(N2CN(c3ccccc3)NC(c3cccc(C4=NN(c5ccccc5)CN(c5ccccc5)N4)c3)=N2)cc1
vNsp13-rna2-111	ZINC000101064566	-9.8	0.245	597.42	ZINC	O=C(c1ccccc1)C1=C[C@@H]2[C@@H]3C(=O)N(c4ccc5c(c4)OCO5)C(=O)[C@@H]3[C@H](C(=O)c3ccc(Br)cc3)N2C=C1
vNsp13-rna2-112	ZINC000101997481	-9.8	0.272	499.55	ZINC	O=C(C[C@@H]1SC(=O)NC1=O)Oc1ccc([C@H]2Oc3ccccc3[C@H]3CC(c4ccccc4)=NN32)cc1
vNsp13-rna2-113	ZINC000226404692	-9.8	0.223	586.64	ZINC	O=C(Oc1ccc(N2C(=O)[C@@H]3[C@H]4C=C[C@@H](C4)[C@@H]3C2=O)cc1)c1cccc(N2C(=O)[C@@H]3CC[C@@H](c4ccccc4)C[C@@H]3C2=O)c1
vNsp13-rna2-114	ZINC000229867083	-9.8	0.218	598.65	ZINC	COc1cccc(C(=O)[C@@H]2[C@H](C(=O)c3ccc4c(c3)OCO4)[C@@]3(C(=O)Nc4ccccc43)[C@@H]3C=C(c3ccc(Br)cc3)N2C=O)c1
vNsp13-rna2-115	ZINC000245377192	-9.8	0.265	488.54	ZINC	O=C1[C@@H]2[C@H]3C=C[C@@H](C3)[C@H]2C(=O)N1c1ccc2c(c1)-c1cc(N3C(=O)[C@@H]4[C@H]5C=C[C@@H](C5)[C@@H]4C3=O)ccc1C2
vNsp13-rna2-116	ZINC000247714414	-9.8	0.306	423.47	ZINC	O=C1Nc2ccccc2[C@@]12[C@H]1C(=O)N(c3ccc4ccccc4c3)C(=O)[C@@H]1[C@@H]1CCCN12
vNsp13-rna2-117	ZINC000247747572	-9.8	0.265	486.53	ZINC	O=C(Nc1ccccc1)[C@@H]1[C@@H]2C(=O)N(c3ccc4ccccc4c3)C(=O)[C@H]2[C@@H]2c3ccccc3C=NN21
vNsp13-rna2-118	ZINC000253388500	-9.8	0.265	488.55	ZINC	Cc1ccccc1N1C(=O)[C@H]2[C@@H]3CCCN3[C@@]3(c4ccccc4-n4c3nc3ccccc3c4=O)[C@H]2C1=O
vNsp13-rna2-119	ZINC000253623944	-9.8	0.297	435.43	ZINC	O=C1c2ccc3c(c2O/C1=C/c1ccccc1)[C@@H](c1cc2ccccc2nc1O)CC(=O)O3
vNsp13-rna2-120	ZINC000263585784	-9.8	0.280	466.45	ZINC	COc1ccc2cc([C@H]3CC(=O)Oc4ccc5c(c43)O/C(=C/c3ccnc3)C5=O)c(O)nc2c1
vNsp13-rna2-121	ZINC000408730040	-9.8	0.265	485.54	ZINC	Cc1ccc(N2C(=O)[C@H]3[C@H](C2=O)[C@@H]2C(=O)Oc4c5ccccc5ccc4C2=C[C@H]3c2ccccc2)cc1
vNsp13-rna2-122	ZINC000408730041	-9.8	0.265	485.54	ZINC	Cc1ccc(N2C(=O)[C@@H]3[C@H](C2=O)[C@@H]2C(=O)Oc4c5ccccc5ccc4C2=C[C@H]3c2ccccc2)cc1
vNsp13-rna2-123	ZINC000408731627	-9.8	0.258	499.57	ZINC	Cc1ccc(N2C(=O)[C@@H]3[C@H](C2=O)[C@@H]2C(=O)Oc4c5ccccc5ccc4C2=C[C@@H]3c2ccccc2)cc1C
vNsp13-rna2-124	ZINC000408731630	-9.8	0.258	499.57	ZINC	Cc1ccc(N2C(=O)[C@@H]3[C@H](C2=O)[C@@H]2C(=O)Oc4c5ccccc5ccc4C2=C[C@H]3c2ccccc2)cc1C
vNsp13-rna2-125	ZINC000408976154	-9.8	0.280	461.57	ZINC	C[C@@]12C[C@H](CC(C)(C)C1)N(C(=O)c1ccc3nc4c5ccenc5c5ncccc5c4nc3c1)C2
vNsp13-rna2-126	ZINC000408976897	-9.8	0.280	461.57	ZINC	C[C@@]12C[C@H](CC(C)(C)C1)N(C(=O)c1ccc3nc4c5neccc5c5ccnc5c4nc3c1)C2
vNsp13-rna2-127	ZINC000409331191	-9.8	0.272	470.54	ZINC	O=C(Nc1ccc2nc3c4ccenc4c4ncccc4c3nc2c1)N1CC[C@@H](c2ccccc2)C1
vNsp13-rna2-128	ZINC000409337259	-9.8	0.258	499.57	ZINC	Cc1ccc(N2C(=O)[C@H]3[C@H](C2=O)[C@@H]2C(=O)Oc4ccc5ccccc5c4C2=C[C@H]3c2ccccc2)c(C)c1
vNsp13-rna2-129	ZINC000409337466	-9.8	0.272	465.52	ZINC	CN(C(=O)c1ccc2nc3c4ncccc4c4ccnc4c3nc2c1)c1ccc2ccccc2c1
vNsp13-rna2-130	Z1014962592	-9.7	0.294	435.53	REAL	O=C(c1ccc2c(=O)n3c(nc2c1)CCCCC3)N1Cc2ccccc2-c2ccccc2C1
vNsp13-rna2-131	Z1174754345	-9.7	0.303	430.47	REAL	O=C([C@@H]1CC(=O)N(c2ccc3c(c2)Cc2ccccc2-3)C1)N1CCO[C@@H](c2nnn[nH]2)C1
vNsp13-rna2-132	Z1314453644	-9.7	0.303	425.53	REAL	Cc1ccnc2c1CCN(C(=O)c1ccnc(C(=O)N3CCc4c(C)cccc4C3)c1)C2
vNsp13-rna2-133	Z1391150635	-9.7	0.323	437.86	REAL	O=C(Nc1nc2c(Cl)cccc2[nH]1)c1ccc2c(c1)S(=O)(=O)c1ccccc1C2=O
vNsp13-rna2-134	Z1451694715	-9.7	0.323	422.87	REAL	C[C@@]1(c2cccc(C(=O)N3CCc4[nH]c5ccc(Cl)cc5c4C3)c2)NC(=O)NC1=O
vNsp13-rna2-135	Z1474666707	-9.7	0.303	425.44	REAL	Cc1conc1NC(=O)c1c2c(nc3ccccc13)/C(=C/c1ccc3c(c1)OCO3)CC2
vNsp13-rna2-136	Z1487641111	-9.7	0.313	417.51	REAL	O=C(NNc1cccc2c1CCCC2)[C@H]1CCCN(C(=O)c2ccc3[nH]ncc3c2)C1
vNsp13-rna2-137	Z1507101364	-9.7	0.303	425.44	REAL	Cc1ccc(N2C(=O)/C(=C/Nc3cccc4c3oc(=O)n4C)c3ccccc3C2=O)cc1
vNsp13-rna2-138	Z1533341546	-9.7	0.303	434.49	REAL	Cc1ccc(N2C[C@@H](C(=O)Nc3cccc([C@@]4(C)NC(=O)NC4=O)c3)CCC2=O)cc1C
vNsp13-rna2-139	Z1591176249	-9.7	0.303	432.39	REAL	O=C(Nc1n[nH]c2ccc(F)cc12)c1cccc(C(=O)Nc2n[nH]c3ccc(F)cc23)c1
vNsp13-rna2-140	Z1684582119	-9.7	0.313	434.84	REAL	C[C@@]1(c2cccc(-c3noc(-c4cc(Cl)c5ccccc5c4O)n3)c2)NC(=O)NC1=O
vNsp13-rna2-141	Z1684582482	-9.7	0.313	421.39	REAL	C[C@]1(c2cccc(-c3noc([C@H]4CC(=O)Nc5cc(F)ccc54)n3)c2)NC(=O)NC1=O
vNsp13-rna2-142	Z1685085222	-9.7	0.285	449.47	REAL	O=C1C[C@@H](c2nc(-c3ccc4[nH]c(=O)[nH]c4c3)no2)CN1c1ccc2c(c1)Cc1ccccc1-2
vNsp13-rna2-143	Z1705238973	-9.7	0.285	448.49	REAL	NC(=O)c1cn(C2CN(C(=O)c3cc(-c4cccc5ccccc45)nc4ccccc34)C2)nn1
vNsp13-rna2-144	Z1744192444	-9.7	0.303	428.49	REAL	O=C(c1ccc2c(=O)n3c(nc2c1)CCCCC3)N1CC[C@]2(C1)C(=O)Nc1ccccc12
vNsp13-rna2-145	Z1752322128	-9.7	0.303	433.47	REAL	C[C@]1(c2cccc(CNC(=O)N3CC[C@]4(C3)C(=O)Nc3ccccc34)c2)NC(=O)NC1=O
vNsp13-rna2-146	Z1891089789	-9.7	0.294	433.47	REAL	O=C1C[C@@H](c2nc(-c3ccc4cc[nH]c4n3)no2)CN1c1ccc2c(c1)Cc1ccccc1-2
vNsp13-rna2-147	Z1907683314	-9.7	0.303	427.50	REAL	Cc1noc2nc(-c3ccccc3)cc(C(=O)NC[C@@]3(O)[C@H]4[C@@H]5C[C@@H]6[C@@H]7[C@@H]5C[C@H]4[C@@H]7[C@H]63)c12
vNsp13-rna2-148	Z1983282382	-9.7	0.294	446.51	REAL	Cc1ccc2c(c1)c(=O)n(C)c1nnc(CN3C(=O)N[C@@]4(C[C@@H]5C[C@H]4[C@H]4CCC[C@@H]54)C3=O)n21
vNsp13-rna2-149	Z2001253163	-9.7	0.334	427.92	REAL	O=S(=O)(c1ccc(Cl)c(-c2nnn[nH]2)c1)N1[C@H]2C=C(c3ccccc3)C[C@H]1CC2
vNsp13-rna2-150	Z2008259530	-9.7	0.303	424.51	REAL	Cn1c(-c2cc(-c3ccccc3)nc3ccccc23)nnc1N1CC[C@@]2(CNC(=O)C2)C1
vNsp13-rna2-151	Z211287752	-9.7	0.285	468.53	REAL	O=C1c2ccccc2S(=O)(=O)c2cc(C(=O)N3CC=C(c4c[nH]c5ccccc45)CC3)ccc21
vNsp13-rna2-152	Z2157917798	-9.7	0.294	444.43	REAL	C[C@@]1(c2cccc(-c3noc(-c4cccnc4Nc4ccccc4F)n3)c2)NC(=O)NC1=O
vNsp13-rna2-153	Z2158428702	-9.7	0.313	420.51	REAL	O=C1C[C@@H](c2noc([C@@H]3C[C@H]4CCCC[C@@H]4N3C(=O)c3ccccc3)n2)CN1C1CC1
vNsp13-rna2-154	Z2178302485	-9.7	0.294	446.45	REAL	O=C(c1ccc(F)cc2c(=O)c3cc(F)ccc3[nH]c12)N1CC[C@@]2(CCc3ccccc3O2)C1
vNsp13-rna2-155	Z2232179512	-9.7	0.294	446.55	REAL	Cc1ccc2c(c1)CN(C(=O)[C@H]1CN(Cc3nc4ccccc4c(=O)[nH]3)CCO1)C(C)(C)C2
vNsp13-rna2-156	Z282688162	-9.7	0.277	485.57	REAL	O=C(c1ccc(NC2=NS(=O)(=O)c3ccccc32)cc1)N1CCC(c2nc3ccccc3[nH]2)CC1
vNsp13-rna2-157	Z284417902	-9.7	0.277	471.50	REAL	Cn1c(C(=O)Nc2cc(-c3nnc4n3CCCC4)ccc2F)cc2c(=O)n3ccccc3nc21
vNsp13-rna2-158	Z286720458	-9.7	0.269	477.53	REAL	Cc1nc2ccccc2c2c(NC(=O)C3CCN(c4ccc5nnnn5n4)CC3)c3ccccc3n12
vNsp13-rna2-159	Z2903525748	-9.7	0.285	455.47	REAL	Cc1c(-c2noc([C@@H]3CC(=O)N(c4ccc5c(c4)Cc4ccccc4-5)C3)n2)c(=O)[nH]c(=O)n1C
vNsp13-rna2-160	Z735966588	-9.7	0.277	493.52	REAL	CC(=O)N(c1ccc(F)cc1)c1nc([C@@H]2NC(N)=Nc3nc4cc5c(cc4n32)OCCCO5)cs1
vNsp13-rna2-161	Z804355952	-9.7	0.294	439.51	REAL	O=C(N[C@@H]1CCCc2[nH]c(=O)ccc21)[C@@H]1CC(=O)N(c2ccc3c(c2)Cc2ccccc2-3)C1
vNsp13-rna2-162	Z971663580	-9.7	0.262	496.57	REAL	O=C(c1c2c(nc3ccccc13)/C(=C/c1ccc3c(c1)OCO3)CC2)N1CCC[C@@H](N2CCNC2=O)C1
vNsp13-rna2-163	ZINC000000990902	-9.7	0.277	462.55	ZINC	O=C(c1ccc(N2C(=O)[C@@H]3[C@@H](C2=O)C2c4ccccc4C3c3ccccc32)cc1)N1CCCCC1
vNsp13-rna2-164	ZINC000001269423	-9.7	0.249	554.65	ZINC	Cc1nc2ccccc2n1S(=O)(=O)c1ccc2c(c1)Cc1cc(S(=O)(=O)n3c(C)nc4ccccc43)ccc1-2
vNsp13-rna2-165	ZINC000001333976	-9.7	0.262	498.63	ZINC	Cc1ccc(C)c(Cn2nnc3c2nc([C@@H]2CCCN(C(=O)c4ccc(C(C)(C)C)cc4)C2)[nH]c3=O)c1
vNsp13-rna2-166	ZINC000002105833	-9.7	0.285	440.46	ZINC	O=c1c2ccccc2nc2c3ccccc3n3c(=O)c4ccccc4nc3c3ccccc3n12
vNsp13-rna2-167	ZINC000002426493	-9.7	0.262	498.54	ZINC	COc1ccc([C@H]2c3c4nc(-c5ccccc5O)nn4cnc3OC3=C2C(=O)CC(C)(C)C3)cc1OC
vNsp13-rna2-168	ZINC000002939310	-9.7	0.249	573.86	ZINC	O=C(Nc1ccc(N2C(=O)[C@@H]3[C@@H](C2=O)C2c4ccccc4C3c3ccccc32)cc1Cl)c1ccc(Cl)cc1Cl
vNsp13-rna2-169	ZINC000003637488	-9.7	0.285	468.51	ZINC	Cc1ccccc1-c1nc2s/c(=C3/c4ccccc4N(Cc4ccccc4F)C3=O)c(=O)n2n1
vNsp13-rna2-170	ZINC000003741814	-9.7	0.277	467.52	ZINC	CC1CCN(c2cc(Nc3ccc4c(c3)OCCO4)c3c4c2noc4-c2ccccc2C3=O)CC1
vNsp13-rna2-171	ZINC000004522764	-9.7	0.269	472.46	ZINC	Nc1c(C(=O)Nc2ccc3c(c2)C(=O)c2ccccc2C3=O)ccc2c1C(=O)c1ccccc1C2=O
vNsp13-rna2-172	ZINC000004542488	-9.7	0.255	497.55	ZINC	O=C(c1ccc(-c2ccccc2)cc1)[C@H]1[C@@H]2C(=O)N(c3ccccc3)C(=O)[C@@H]2[C@H]2c3ccccc3C=NN12
vNsp13-rna2-173	ZINC000006229106	-9.7	0.269	498.65	ZINC	Cc1ccc(S(=O)(=O)Nc2cc3c(c4ccccc24)O[C@@]2(C3)N(C)c3ccccc3C2(C)C)c(C)c1
vNsp13-rna2-174	ZINC000008694925	-9.7	0.277	452.47	ZINC	O=C1c2ccccc2C(=O)c2c3[nH]nc(-c4nc5ccccc5nc4-c4ccccc4)c3ccc21
vNsp13-rna2-175	ZINC000008792187	-9.7	0.277	458.52	ZINC	O=C(c1cc2c3ccccc3n3c2c(n1)c1ccccc1c3=O)N1CCN(c2ccccc2)CC1
vNsp13-rna2-176	ZINC000008792352	-9.7	0.269	492.97	ZINC	O=C(c1cc2c3ccccc3n3c2c(n1)c1ccccc1c3=O)N1CCN(c2cccc(Cl)c2)CC1
vNsp13-rna2-177	ZINC000008792406	-9.7	0.269	476.51	ZINC	O=C(c1cc2c3ccccc3n3c2c(n1)c1ccccc1c3=O)N1CCN(c2ccc(F)cc2)CC1
vNsp13-rna2-178	ZINC000008836513	-9.7	0.255	495.59	ZINC	Cc1nn(-c2ccc(C)cc2)c2c1[C@H](c1ccccc1)N1c3ccccc3N=C(Nc3ccccc3)C1=N2
vNsp13-rna2-179	ZINC000009076324	-9.7	0.262	495.49	ZINC	COc1ccc(C(=O)[C@H]2[C@H]3C(=O)N(c4ccc5c(c4)OCO5)C(=O)[C@H]3[C@@H]3c4ccccc4C=NN23)cc1
vNsp13-rna2-180	ZINC000009282059	-9.7	0.294	457.92	ZINC	O=C1Nc2ccc(Cl)cc2[C@@]12[C@@H]1C(=O)N(c3ccc4ccccc43)C(=O)[C@@H]1[C@@H]1CCCN12
vNsp13-rna2-181	ZINC000009953701	-9.7	0.277	470.57	ZINC	Cc1cc(N2CCN(C(=O)c3ccc4c(c3)C[C@@H](c3ccccc3)OC4=O)CC2)nc(C(C)C)n1
vNsp13-rna2-182	ZINC000009970195	-9.7	0.303	441.51	ZINC	Cc1ccc(S(=O)(=O)c2nnn3c2nc(N2CCc4ccccc42)c2ccccc23)cc1
vNsp13-rna2-183	ZINC000014114786	-9.7	0.277	467.52	ZINC	O=C(c1ccc2c(c1)C[C@@H](c1ccccc1)OC2=O)N1CCC(n2c(=O)[nH]c3ccccc32)CC1
vNsp13-rna2-184	ZINC000015785742	-9.7	0.255	501.54	ZINC	CC(=O)Oc1ccc2ccccc2c1C1=NN(C(C)=O)[C@H](c2cc(-c3ccccc3)nc3ccccc32)O1
vNsp13-rna2-185	ZINC000015858946	-9.7	0.262	489.53	ZINC	Cc1ccc(-c2c3c(c4n2-c2ccccc2O[C@H]4c2nc4ccccc4[nH]2)n(C)c(=O)n(C)c3=O)cc1
vNsp13-rna2-186	ZINC000016037585	-9.7	0.255	500.55	ZINC	COc1ccc(C(=O)[C@@H]2[C@@H]3C(=O)N(c4ccc5ccccc54)C(=O)[C@@H]3[C@H]3c4ccccc4C=CN23)cc1
vNsp13-rna2-187	ZINC000017862766	-9.7	0.243	520.59	ZINC	O=C(Nc1ccc2ccccc2c1)c1cccc(N2C(=O)[C@H]3[C@@H](C2=O)C2c4ccccc4C3c3ccccc32)c1
vNsp13-rna2-188	ZINC000020760240	-9.7	0.269	476.54	ZINC	CC(C)[C@@H]1N[C@@]2(c3ccccc3-n3c2nc2ccccc2c3=O)[C@H]2C(=O)N(c3ccccc3)C(=O)[C@@H]12
vNsp13-rna2-189	ZINC000030903358	-9.7	0.303	451.91	ZINC	NC(=O)C1CCN(c2nc3ncc4c(c3c(=O)[nH]2)C[C@@H](c2ccccc(Cl)c2)CC4=O)CC1
vNsp13-rna2-190	ZINC000033297583	-9.7	0.285	455.51	ZINC	Cc1ccc(N2C[C@H](C(=O)Nc3ccc4c(c3)N(C)C(=O)c3ccccc3O4)CC2=O)cc1C
vNsp13-rna2-191	ZINC000034703510	-9.7	0.285	441.49	ZINC	C[C@H]1Cc2ccccc2N1C(=O)c1ccc2nc3c4ncccc4c4ccnc4c3nc2c1
vNsp13-rna2-192	ZINC000034837664	-9.7	0.262	494.50	ZINC	COc1ccc(N2C(=O)[C@@H]3[C@H](C2=O)[C@@H]2c4ccccc4C=CN2[C@@H]3C(=O)c2ccc3c(c2)OCO3)cc1
vNsp13-rna2-193	ZINC000052955754	-9.7	0.226	581.67	ZINC	CN1C[C@H](C(=O)N[C@]2(C)O[C@@]3(O)[C@@H]4CCCN4C(=O)[C@H](Cc4ccccc4)N3C2=O)C=C2c3cccc4[nH]cc(c43)C[C@H]21
vNsp13-rna2-194	ZINC000084668186	-9.7	0.323	422.87	ZINC	C[C@@]1(c2cccc(C(=O)N3CCc4[nH]c5ccc(Cl)cc5c4C3)c2)NC(=O)NC1=O
vNsp13-rna2-195	ZINC000095092808	-9.7	0.277	466.50	ZINC	CC1=NN(c2ccc(C)c(C)c2)C(=O)/C1=N/Nc1cccc(-c2cccc(-c3nnn[nH]3)c2)c1O
vNsp13-rna2-196	ZINC000100485510	-9.7	0.303	410.43	ZINC	O=C1c2ccc3c4c(ccc(c24)C2=Nc4ccccc4[C@H]21)C1=Nc2ccccc2[C@H]1C3=O
vNsp13-rna2-197	ZINC000100493001	-9.7	0.269	481.55	ZINC	O=C(c1ccccc1)N1CCc2nc3cc([C@H]4CCCN(C(=O)c5ccccc5)C4)nn3c(O)c2C1
vNsp13-rna2-198	ZINC000101064563	-9.7	0.243	597.42	ZINC	O=C(c1ccccc1)C1=C[C@H]2[C@H]3C(=O)N(c4ccc5c(c4)OCO5)C(=O)[C@@H]3[C@H](C(=O)c3ccc(Br)cc3)N2C=C1
vNsp13-rna2-199	ZINC000101344117	-9.7	0.262	489.51	ZINC	O=C(c1ccc(F)cc1)[C@@H]1[C@@H]2C(=O)N(c3ccc4ccccc4c3)C(=O)[C@@H]2[C@H]2c3ccccc3C=NN12
vNsp13-rna2-200	ZINC000101500434	-9.7	0.262	492.51	ZINC	O=C1[C@H]2[C@H]3CCCN3[C@@]3(c4ccccc4-n4c3nc3ccccc3c4=O)[C@H]2C(=O)N1c1ccccc1F

Supplementary Table 66. Virtual screening hits 101 to 200 of the screen against the RNA binding site of nsp13 (Screen ID: 35). Compounds were filtered so that hits had MW < 600 dalton, cLogP < 6, number of hydrogen bond acceptors < 11, and no reactive functional groups. A few compounds unsuitable for drug discovery were removed by visual inspection. The name of each compound consists of the initial letter 'v' for virtual hit, followed by the target protein name and the target site ('rna' for RNA binding site, 2 for docking scenario 2). The score is the docking score given by QuickVina 2 in kcal/mol. The ligand efficiency (LE) is computed as LE = -score/#NonH, where #NonH is the number of heavy (i.e. non hydrogen) atoms.

Name	Catalog ID	Score	LE	MW	Library	SMILES
vNsp14-nsp10.1-1	Z1744518572	-11	0.344	423.471	REAL	O=C(Cn1c2ccccc2c(=O)c2ccccc21)N1CC[C@@]2(C1)C(=O)Nc1ccccc12
vNsp14-nsp10.1-2	Z1280745057	-10.8	0.36	400.52	REAL	O=C1Nc2ccccc2[C@@H]1C1CCN(C(=O)[C@H]2C[C@@]23CCCc2ccccc23)CC1
vNsp14-nsp10.1-3	Z1752022802	-10.8	0.318	449.552	REAL	O=C(NC[C@@H]1CC2c3ccccc3C1c1ccccc12)N1CC[C@@]2(C1)C(=O)Nc1ccccc12
vNsp14-nsp10.1-4	ZINC000002212711	-10.7	0.324	429.474	ZINC	O=C(Nc1ccc2c(c1)Cc1ccccc1-2)c1ccnc(-c2cc3ccccc3oc2=O)c1
vNsp14-nsp10.1-5	ZINC000003174011	-10.7	0.345	443.521	ZINC	O=C(c1ccc(F)cc1)N1C(=O)/C(=C/c2c3ccccc3sc3ccccc32)SC1=S
vNsp14-nsp10.1-6	Z1024053346	-10.6	0.312	459.588	REAL	Cc1cc(C)cc(C(=O)N2CCC[C@H](C(=O)N3CCC([C@@H]4C(=O)Nc5ccccc54)CC3)C2)c1
vNsp14-nsp10.1-7	Z1070217002	-10.6	0.303	485.97	REAL	O=C1Nc2cc(Cl)ccc2[C@@H]1C1CCN(C(=O)Cn2c3ccccc3c(=O)c3ccccc32)CC1
vNsp14-nsp10.1-8	ZINC000016525756	-10.6	0.342	443.521	ZINC	O=C(c1ccccc1F)N1C(=O)/C(=C/c2c3ccccc3cc3ccccc32)SC1=S
vNsp14-nsp10.1-9	ZINC000409330857	-10.6	0.342	459.976	ZINC	O=C(c1ccccc1Cl)N1C(=O)/C(=C/c2c3ccccc3cc3ccccc32)SC1=S
vNsp14-nsp10.1-10	PV-001818621876	-10.5	0.35	441.361	REAL	O=C(C1CCc2ccccc2CC1)N1C[C@H]2[C@H](C1)C(F)(F)C(F)(F)C(F)(F)C2(F)F
vNsp14-nsp10.1-11	PV-001953052764	-10.5	0.339	456.376	REAL	O=C(NC[C@@H]1CCCc2ccccc21)N1C[C@@H]2[C@@H](C1)C(F)(F)C(F)(F)C(F)(F)C2(F)F
vNsp14-nsp10.1-12	PV-001969885760	-10.5	0.339	456.376	REAL	O=C(N[C@H]1CCCc2ccccc2C1)N1C[C@H]2[C@H](C1)C(F)(F)C(F)(F)C(F)(F)C2(F)F
vNsp14-nsp10.1-13	Z126939246	-10.5	0.284	497.553	REAL	C[C@]1(c2ccc3ccccc3c2)NC(=O)N(CC(=O)N2CCC(n3c(=O)[nH]c4ccccc43)CC2)C1=O
vNsp14-nsp10.1-14	Z1500120620	-10.5	0.318	437.541	REAL	CC(=O)N/C(=C/c1ccccc1)C(=O)N1CCN(C2c3ccccc3-c3ccccc32)CC1
vNsp14-nsp10.1-15	Z2233376534	-10.5	0.318	444.529	REAL	C[C@@]1(NC(=O)[C@@H]2CCC(=O)c3ccccc32)CCN(C(=O)[C@H]2CC(=O)c3ccccc32)C1
vNsp14-nsp10.1-16	Z995656030	-10.5	0.284	499.565	REAL	O=C(NNC(=O)[C@@H]1C[C@H]2CCCC[C@@H]2N1C(=O)c1ccc2ccccc2c1)[C@@H]1COc2ccccc2O1
vNsp14-nsp10.1-17	Z995754372	-10.5	0.292	481.594	REAL	O=C1Nc2ccccc2[C@@H]1CCNC(=O)[C@@H]1C[C@H]2CCCC[C@@H]2N1C(=O)c1ccc2ccccc2c1
vNsp14-nsp10.1-18	ZINC000524731813	-10.5	0.292	477.515	ZINC	CC(C)c1ccc(/C=C2\Oc3c(ccc4c3[C@H](c3cc5ccccc5nc3O)CC(=O)O4)C2=O)cc1
vNsp14-nsp10.1-19	Z1020943126	-10.4	0.315	465.979	REAL	O=C1Nc2ccccc2[C@@H]1C1CCN(C(=O)[C@H]2CCCN(C(=O)c3ccc(Cl)cc3)C2)CC1
vNsp14-nsp10.1-20	Z1147907130	-10.4	0.289	480.57	REAL	O=C(NCc1nnnn1-c1ccccc1)[C@@H]1C[C@H]2CCCC[C@@H]2N1C(=O)c1ccc2ccccc2c1
vNsp14-nsp10.1-21	Z1204918363	-10.4	0.315	442.561	REAL	O=C(N[C@@H]1CCc2[nH]ncc2C1)[C@@H]1C[C@H]2CCCC[C@@H]2N1C(=O)c1ccc2ccccc2c1
vNsp14-nsp10.1-22	Z1499463174	-10.4	0.315	437.498	REAL	O=C(Nc1ccc2oc(=O)ccc2c1)N1CCN(C2c3ccccc3-c3ccccc32)CC1
vNsp14-nsp10.1-23	Z1507808000	-10.4	0.315	439.514	REAL	Cc1ccc(-c2cc(C(=O)N3CCO[C@]4(CCc5ccccc54)C3)c3c(C)noc3n2)cc1
vNsp14-nsp10.1-24	Z1658286589	-10.4	0.335	413.523	REAL	O=C(N[C@H]1[C@@H]2CCc3ccccc3[C@@H]21)N1CCC[C@@H](c2n[nH]c(-c3ccccc3)n2)C1
vNsp14-nsp10.1-25	Z1716063227	-10.4	0.315	440.541	REAL	O=C(c1cccc2ccccc12)N1CCC[C@@H](C(=O)N2CC[C@@]3(C2)OCc2ccccc23)C1
vNsp14-nsp10.1-26	Z1720538465	-10.4	0.315	444.573	REAL	C[C@H]1Cc2ccccc2N1C(=O)[C@H]1CCCC[C@@H]1C(=O)N1CC[C@@]2(C1)OCc1ccccc12
vNsp14-nsp10.1-27	Z1734853615	-10.4	0.371	374.482	REAL	O=C(N[C@@H]1[C@H]2CCc3ccccc3[C@H]21)N1CCC[C@@]2(C1)OCc1ccccc12
vNsp14-nsp10.1-28	Z1743907853	-10.4	0.347	392.461	REAL	O=C1Nc2ccccc2[C@@]12CCN(c1nc(-c3ccccc3)nc3ccccc13)C2
vNsp14-nsp10.1-29	Z2183256228	-10.4	0.371	373.498	REAL	O=C(N[C@@H]1[C@H]2CCc3ccccc3[C@H]21)N1CCCN2c3ccccc3C[C@@H]2C1
vNsp14-nsp10.1-30	Z225653128	-10.4	0.335	409.488	REAL	O=C([C@H]1CC(=O)N(c2ccc3ccccc23)C1)N1CCc2[nH]c3ccccc3c2C1
vNsp14-nsp10.1-31	Z228329578	-10.4	0.359	394.557	REAL	Cc1ccc(C23C[C@H]4C[C@@H](CC(C(=O)NCC(=O)N5CCCC5)(C4)C2)C3)cc1C
vNsp14-nsp10.1-32	Z2495882389	-10.4	0.385	361.444	REAL	O=C(N[C@H]1CCc2ccccc2NC1=O)N[C@@H]1[C@H]2CCc3ccccc3[C@H]21
vNsp14-nsp10.1-33	Z2767460673	-10.4	0.359	394.513	REAL	O=C1[C@H]2CCCC[C@H]1CC(C(=O)N1CCC([C@@H]3C(=O)Nc4ccccc43)CC1)C2
vNsp14-nsp10.1-34	ZINC000019835162	-10.4	0.315	435.526	ZINC	Cc1onc(-c2ccccc2)c1C(=O)N1CCN(C2c3ccccc3-c3ccccc32)CC1
vNsp14-nsp10.1-35	Z1024053902	-10.3	0.294	485.504	REAL	O=C1Nc2ccccc2[C@@H]1C1CCN(C(=O)[C@H]2CC(=O)N(Cc3ccc(C(F)(F)F)c3)C2)CC1
vNsp14-nsp10.1-36	Z1033343054	-10.3	0.322	420.471	REAL	Cn1nc(CC(=O)Nc2ccccc(-c3ccc4ccccc4c3)n2)c2ccccc2c1=O
vNsp14-nsp10.1-37	Z1068314458	-10.3	0.286	487.642	REAL	CN1CCC2(CC1)C[C@@H](NC(=O)[C@@H]1C[C@H]3CCCC[C@@H]3N1C(=O)c1ccccc1)c1ccccc1O2
vNsp14-nsp10.1-38	Z1128836954	-10.3	0.278	486.534	REAL	O=C(CCc1nc2c(cnn2-c2ccccc2)c(=O)[nH]1)Nc1cccc(-c2ccc3ccccc3c2)n1
vNsp14-nsp10.1-39	Z1241281994	-10.3	0.368	366.467	REAL	c1ccc2c(c1)-c1ccccc1C2N1CCC[C@H](c2nnc3ccccn23)C1
vNsp14-nsp10.1-40	Z1280816751	-10.3	0.332	434.965	REAL	O=C1Nc2cc(Cl)ccc2[C@H]1C1CCN(C(=O)[C@H]2C[C@@]23CCCc2ccccc23)CC1
vNsp14-nsp10.1-41	Z1344200657	-10.3	0.312	444.617	REAL	O=C(C[C@@H]1CCc2ccccc2C1)N1CCCN(C(=O)C[C@@H]2CCc3ccccc3C2)CC1
vNsp14-nsp10.1-42	Z1374245126	-10.3	0.343	402.536	REAL	CC(=O)N1Cc2ccccc2C[C@H]1C(=O)N1CCC[C@]2(CCCc3ccccc32)C1
vNsp14-nsp10.1-43	Z1374245614	-10.3	0.312	443.545	REAL	O=C(CN1C(=O)N[C@]2(CCc3ccccc32)C1=O)N1CCC[C@]2(CCCc3ccccc32)C1
vNsp14-nsp10.1-44	Z1411947320	-10.3	0.312	442.561	REAL	O=C(N[C@@H]1CCc2cn[nH]c2C1)[C@@H]1C[C@H]2CCCC[C@@H]2N1C(=O)c1ccc2ccccc2c1
vNsp14-nsp10.1-45	Z1417276490	-10.3	0.312	439.51	REAL	O=C1O[C@H](c2ccccc2)Cc2cc(C(=O)N3CCC4(CC3)OCc3ccccc34)ccc21
vNsp14-nsp10.1-46	Z1473414653	-10.3	0.322	432.498	REAL	O=C(N[C@H]1[C@@H]2CCc3ccccc3[C@@H]21)N1CCC[C@@H](c2nc(-c3cccc(F)c3)no2)C1
vNsp14-nsp10.1-47	Z1473416266	-10.3	0.412	332.446	REAL	C[C@H]1Cc2ccccc2CN1C(=O)N[C@@H]1[C@H]2CCc3ccccc3[C@H]21
vNsp14-nsp10.1-48	Z1476713258	-10.3	0.332	412.488	REAL	O=C(N[C@@H]1CCCN(C(=O)c2ccccc2)C1)C1c2ccccc2Oc2ccccc21
vNsp14-nsp10.1-49	Z1507806300	-10.3	0.312	438.529	REAL	Cc1nn(C)c2nc(-c3ccccc3)cc(C(=O)N3CCO[C@]4(CCc5ccccc54)C3)c12
vNsp14-nsp10.1-50	Z1507808003	-10.3	0.355	390.481	REAL	CC(=O)N1Cc2ccccc2C[C@H]1C(=O)N1CCO[C@]2(CCc3ccccc32)C1
vNsp14-nsp10.1-51	Z1581473271	-10.3	0.312	440.585	REAL	O=C(NC[C@H]1CCCN1C(=O)[C@@H]1C[C@@]12CCCc1ccccc12)[C@H]1C[C@]12CCCc1ccccc12
vNsp14-nsp10.1-52	Z1631989495	-10.3	0.312	437.477	REAL	O=C(N[C@@H]1CCc2nnc(-c3ccc(F)cc3)n2C1)c1cc2ccccc2c2ccnc12
vNsp14-nsp10.1-53	Z1662361768	-10.3	0.322	424.459	REAL	O=C1N[C@]2(CCc3ccccc32)C(=O)N1Cc1nnc(Cc2ccc3ccccc3c2)o1
vNsp14-nsp10.1-54	Z1748294717	-10.3	0.355	385.466	REAL	O=C(c1cccc2c3c([nH]c12)CCCC3)N1CC[C@@]2(C1)C(=O)Nc1ccccc12
vNsp14-nsp10.1-55	Z1750667161	-10.3	0.312	446.549	REAL	C[C@@H]1C[C@H](C)CN(C(=O)c2ccccc2NC(=O)N2CC[C@@]3(C2)C(=O)Nc2ccccc23)C1
vNsp14-nsp10.1-56	Z792115066	-10.3	0.294	466.492	REAL	O=C(CN1C(=O)N[C@]2(CCc3ccccc32)C1=O)OCC(=O)c1ccc2c(c1)Cc1ccccc1-2
vNsp14-nsp10.1-57	ZINC000015730186	-10.3	0.278	494.597	ZINC	Cc1ccc(-n2nc(N3CCCN(C(=O)c4n[nH]c5c4CCc4ccccc4-5)CC3)ccc2=O)cc1C
vNsp14-nsp10.1-58	ZINC000033038242	-10.3	0.312	461.584	ZINC	Cc1cc(C)c(S(=O)(=O)N2CCN(C3=Nc4ccccc4Oc4ccccc43)CC2)c(C)c1
vNsp14-nsp10.1-59	PV-001964069954	-10.2	0.378	359.428	REAL	Cc1ccc(CNC(=O)N[C@H]2Cc3ccccc3NC2=O)c2ccccc12
vNsp14-nsp10.1-60	Z1010365610	-10.2	0.276	495.581	REAL	O=C(OCc1nnnn1Cc1ccccc1)[C@@H]1C[C@H]2CCCC[C@@H]2N1C(=O)c1ccc2ccccc2c1
vNsp14-nsp10.1-61	Z1014370920	-10.2	0.276	495.581	REAL	Cc1nc2ccccn2c1C(=O)NNC(=O)[C@@H]1C[C@H]2CCCC[C@@H]2N1C(=O)c1ccc2ccccc2c1
vNsp14-nsp10.1-62	Z1014641074	-10.2	0.276	492.577	REAL	O=C(NNC(=O)[C@@H]1C[C@@H]2CCCC[C@@H]2N1C(=O)c1ccc2ccccc2c1)c1cccc2ccccn12
vNsp14-nsp10.1-63	Z1022078740	-10.2	0.319	430.506	REAL	CC(=O)N1c2ccccc2C[C@H]1C(=O)N1CCN(C(=O)Cc2c[nH]c3ccccc23)CC1
vNsp14-nsp10.1-64	Z1026191060	-10.2	0.309	441.529	REAL	O=C(Cc1cccc2ccccc12)NCC(=O)N1CCC([C@@H]2C(=O)Nc3ccccc32)CC1
vNsp14-nsp10.1-65	Z1101911840	-10.2	0.3	453.497	REAL	CC(=O)N1CCc2ccccc2[C@@H]1CC(=O)Nc1cccc(N2C(=O)c3ccccc3C2=O)c1
vNsp14-nsp10.1-66	Z1128837724	-10.2	0.329	405.456	REAL	O=C(Cn1ccc(=O)c2ccccc21)Nc1cccc(-c2ccc3ccccc3c2)n1
vNsp14-nsp10.1-67	Z1131324305	-10.2	0.319	422.443	REAL	O=C(Cn1c(=O)[nH]c(=O)c2ccccc21)Nc1cccc(-c2ccc3ccccc3c2)n1
vNsp14-nsp10.1-68	Z1265332074	-10.2	0.309	440.498	REAL	Cc1ccccc1[C@H]1CN(C(=O)c2ccc(N3C(=O)c4ccccc4C3=O)cc2)[C@@H](C)CO1
vNsp14-nsp10.1-69	Z1391618497	-10.2	0.309	441.529	REAL	CC(=O)N1CCc2cc(C(=O)N3CCC[C@@H](NC(=O)c4ccc5ccccc5c4)C3)ccc21
vNsp14-nsp10.1-70	Z1500299528	-10.2	0.319	425.534	REAL	O=C([C@@H]1CCCN1c1nccn1)N1CCN(C2c3ccccc3-c3ccccc32)CC1
vNsp14-nsp10.1-71	Z1560236188	-10.2	0.3	449.552	REAL	O=C(CCc1cc2ccccc2[nH]c1=O)N1CCN(C2c3ccccc3-c3ccccc32)CC1
vNsp14-nsp10.1-72	Z1627784622	-10.2	0.319	429.562	REAL	Cc1ccc(-c2nn(CC(=O)N3CCC[C@H]4CCCC[C@@H]43)c(=O)c3ccccc23)cc1C
vNsp14-nsp10.1-73	Z1672654827	-10.2	0.309	442.565	REAL	O=C(Nc1ncn(C2CCCCC2)n1)N1CCN(C2c3ccccc3-c3ccccc32)CC1
vNsp14-nsp10.1-74	Z1744197666	-10.2	0.378	356.424	REAL	O=C(Cc1cccc2ccccc12)N1CC[C@@]2(C1)C(=O)Nc1ccccc12
vNsp14-nsp10.1-75	Z1744514502	-10.2	0.309	440.585	REAL	Cc1ccc(C23C[C@@H]4C[C@@H](CC(C(=O)N5CC[C@@]6(C5)C(=O)Nc5ccccc56)(C4)C2)C3)cc1
vNsp14-nsp10.1-76	Z1752594572	-10.2	0.319	443.468	REAL	O=C(N[C@@H]1CCC[C@@H]1c1ccccc1C(F)(F)F)N1CC[C@@]2(C1)C(=O)Nc1ccccc12
vNsp14-nsp10.1-77	Z1869179036	-10.2	0.34	403.481	REAL	Cc1ccc(C(=O)N2CCC(N3C(=O)N[C@]4(CCc5ccccc54)C3=O)CC2)cc1
vNsp14-nsp10.1-78	Z18857670	-10.2	0.3	452.421	REAL	O=C(COC(=O)c1cc(O)nc2ccccc12)Nc1ccnc2c1C(=O)c1ccccc1C2=O
vNsp14-nsp10.1-79	Z1983287764	-10.2	0.352	395.433	REAL	O=C1N[C@@]2(C[C@H]3C[C@H]2[C@H]2CCC[C@H]32)C(=O)N1Cc1ncc(-c2ccc(F)cc2)o1
vNsp14-nsp10.1-80	Z2001020385	-10.2	0.34	396.532	REAL	O=C([C@@H]1C[C@H]1c1ccc2ccccc2c1)N1CCC(N2CCc3ccccc32)CC1
vNsp14-nsp10.1-81	Z2091496215	-10.2	0.319	428.53	REAL	Cc1ccc2c(c1)CN(C(=O)C1CCN(C(=O)c3cccc4ccccc34)CC1)CCO2
vNsp14-nsp10.1-82	Z2168800571	-10.2	0.3	448.521	REAL	O=C(Nc1ccc2ccccc2c1)C1[C@H]2[C@@H]3C=C[C@@H]([C@@H]4C(=O)N(Cc5ccccc5)C(=O)[C@@H]34)[C@@H]12
vNsp14-nsp10.1-83	Z2174372362	-10.2	0.309	432.526	REAL	O=C(c1cnnc(-c2ccccc2)c1)N1CCN(C2c3ccccc3-c3ccccc32)CC1
vNsp14-nsp10.1-84	Z226970162	-10.2	0.291	465.551	REAL	O=C(Cc1cccc2ccccc12)NNC(=O)[C@@H]1CCCN(C(=O)c2cccc3ccccc23)C1
vNsp14-nsp10.1-85	Z227925854	-10.2	0.283	499.593	REAL	O=C(c1cc(S(=O)(=O)N2CCc3[nH]c4ccccc4c3C2)c[nH]1)N1CCc2[nH]c3ccccc3c2C1
vNsp14-nsp10.1-86	Z2347890120	-10.2	0.352	388.466	REAL	O=C1C[C@@]2(CCN(C(=O)N[C@@H]3[C@H]4CCc5ccccc5[C@@H]43)C2)Oc2ccccc21
vNsp14-nsp10.1-87	Z2701653577	-10.2	0.364	372.51	REAL	C[C@H]1Cc2ccccc2N1C1CCN(C(=O)[C@@H]2[C@H]3Cc4ccccc4[C@H]32)CC1
vNsp14-nsp10.1-88	Z448674688	-10.2	0.291	463.583	REAL	O=C(NC[C@@H]1CC2c3ccccc3C1c1ccccc12)N1CCC(c2nnc3ccccn23)CC1
vNsp14-nsp10.1-89	Z790846854	-10.2	0.291	465.547	REAL	O=C(COC(=O)C1CCN(C(=O)/C=C/c2ccccc2)CC1)c1ccc2c(c1)Cc1ccccc1-2
vNsp14-nsp10.1-90	Z996276962	-10.2	0.283	481.594	REAL	C[C@@H](NC(=O)[C@H]1C[C@H]2CCCC[C@@H]2N1C(=O)c1ccc2ccccc2c1)c1ccc2c(c1)CC(=O)N2
vNsp14-nsp10.1-91	Z996744910	-10.2	0.276	494.593	REAL	O=C(c1cc2ccccc2[nH]1)N1CCN(C(=O)C2CCN(C(=O)c3cccc4ccccc34)CC2)CC1
vNsp14-nsp10.1-92	Z997048282	-10.2	0.291	465.551	REAL	O=C(CNC(=O)C1CCN(C(=O)c2cccc3ccccc23)CC1)Nc1ccccc2ccccc12
vNsp14-nsp10.1-93	Z997324866	-10.2	0.283	481.594	REAL	O=C(NCCN1C(=O)Cc2ccccc21)[C@@H]1C[C@H]2CCCC[C@@H]2N1C(=O)c1ccc2ccccc2c1
vNsp14-nsp10.1-94	ZINC000001015329	-10.2	0.34	389.497	ZINC	C[C@H]1C2c3ccccc3C(c3ccccc32)[C@@H]1C(=O)Nc1ccccc2ccccc21
vNsp14-nsp10.1-95	ZINC000002416286	-10.2	0.309	431.446	ZINC	O=C(Nc1ccc2c(c1)oc1ccccc12)c1cccc(-c2cc3ccccc3oc2=O)c1
vNsp14-nsp10.1-96	ZINC000002768028	-10.2	0.276	490.557	ZINC	C[C@@H](CNC(=O)C1c2ccccc2Oc2ccccc21)NC(=O)C1c2ccccc2Oc2ccccc21
vNsp14-nsp10.1-97	ZINC000014747991	-10.2	0.276	496.613	ZINC	O=C(c1nn(CCc2ccccc2)c2c1CN(Cc1cc3ccccc3[nH]1)CC2)N1CCNC(=O)CC1
vNsp14-nsp10.1-98	ZINC000039929440	-10.2	0.3	449.596	ZINC	O=c1[nH]c2ccccc2n1C1CCN(CCC=C2c3ccccc3CCc3ccccc32)CC1
vNsp14-nsp10.1-99	ZINC000257212118	-10.2	0.309	450.503	ZINC	O=C1CCC[C@]2(CN(Cc3cccc(-c4ccccc4F)c3)C[C@H]2c2ccc(F)c(F)c2)N1
vNsp14-nsp10.1-100	ZINC000604404773	-10.2	0.276	490.561	ZINC	O=C(CCCN1C(=O)c2ccccc2N2C(=O)c3ccccc3[C@H]21)N1CCc2c3ccccc3[nH]c2C1

Supplementary Table 67. Top 100 virtual hits of the screen against the nsp10 binding site of nsp14 (Screen ID: 36). Compounds were filtered so that hits had MW < 600 dalton, cLogP < 6, number of hydrogen bond acceptors < 11, and no reactive functional groups. A few compounds unsuitable for drug discovery were removed by visual inspection. The name of each compound consists of the initial letter 'v' for virtual hit, followed by the target protein name and the target site ('nsp10' for nsp10 binding site, 1 for docking scenario 1). The score is the docking score given by QuickVina 2 in kcal/mol. The ligand efficiency (LE) is computed as LE = -score/#NonH, where #NonH is the number of heavy (i.e. non hydrogen) atoms.

Name	Catalog ID	Score	LE	MW	Library	SMILES
vNsp14-nsp10.1-101	PV-001817117457	-10.1	0.348	396.35	REAL	C[C@]1(C(=O)Nc2ncc(-c3ccc(F)c(F)c3)n2)Oc2ccccc2NC1=O
vNsp14-nsp10.1-102	PV-001818621362	-10.1	0.337	441.27	REAL	O=C(c1cc2ccccc2c(=O)o1)N1C[C@@H]2[C@@H](C1)C(F)(F)C(F)(F)(F)C2(F)F
vNsp14-nsp10.1-103	Z1005676246	-10.1	0.281	483.61	REAL	C[C@H]1Cc2ccccc2N1C1CCN(C(=O)[C@@H]2CCCN2C(=O)c2ccc3ccccc3c2O)CC1
vNsp14-nsp10.1-104	Z1014397762	-10.1	0.289	469.58	REAL	O=C(N[C@@H]1CCCc2[nH]c(=O)ccc21)[C@H]1C[C@H]2CCCC[C@H]2N1C(=O)c1ccc2ccccc2c1
vNsp14-nsp10.1-105	Z1014963130	-10.1	0.289	461.52	REAL	O=C(CCc1nc2c(cnn2-c2ccccc2)c(=O)[nH]1)N1Cc2ccccc2-c2ccccc2C1
vNsp14-nsp10.1-106	Z1070216992	-10.1	0.297	480.01	REAL	Cc1ccc(C(=O)N2CCC[C@H](C(=O)N3CCC([C@@H]4C(=O)Nc5cc(Cl)ccc54)CC3)C2)cc1
vNsp14-nsp10.1-107	Z1082362686	-10.1	0.306	441.53	REAL	NC(=O)[C@@H]1Cc2ccccc2N(C(=O)C2CCN(C(=O)c3cccc4ccccc34)CC2)C1
vNsp14-nsp10.1-108	Z1101911838	-10.1	0.297	451.48	REAL	CC(=O)N1C=Cc2ccccc2[C@@H]1CC(=O)Nc1cccc(N2C(=O)c3ccccc3C2=O)c1
vNsp14-nsp10.1-109	Z1103340954	-10.1	0.289	461.48	REAL	O=C1c2ccccc2C(=O)N1c1cccc(N[C@H]2CC(=O)N(c3cccc4ccccc34)C2=O)c1
vNsp14-nsp10.1-110	Z1155124260	-10.1	0.273	498.56	REAL	Cc1nnnn1-c1ccc(F)c(NC(=O)[C@H]2C[C@H]3CCCC[C@H]3N2C(=O)c2ccc3ccccc3c2)c1
vNsp14-nsp10.1-111	Z1155566976	-10.1	0.306	442.52	REAL	O=C1N[C@]2(CCc3ccccc32)C(=O)N1CC(=O)N1CCCC[C@H]1c1cc2ccccc2[nH]1
vNsp14-nsp10.1-112	Z1222665744	-10.1	0.316	427.50	REAL	O=C1NCCc2ccc(NC(=O)C3CCN(C(=O)c4cccc5ccccc45)CC3)cc21
vNsp14-nsp10.1-113	Z1304356347	-10.1	0.306	439.51	REAL	O=C(COC(=O)C1CCN(C(=O)c2ccccc2)CC1)c1ccc2c(c1)Cc1ccccc1-2
vNsp14-nsp10.1-114	Z1337172781	-10.1	0.316	430.52	REAL	O=C(Cc1ccccc(F)c1)N1CCCN(C(=O)[C@H]2C[C@H]2c2ccc3ccccc3c2)CC1
vNsp14-nsp10.1-115	Z1382048204	-10.1	0.306	435.53	REAL	O=C(NCc1cc(=O)[nH]c2ccccc12)NC[C@@H]1CC2c3ccccc3C1c1ccccc12
vNsp14-nsp10.1-116	Z1390133133	-10.1	0.348	406.38	REAL	O=C1Nc2ccccc2[C@@H]1C1CCN(C(=O)c2cc(F)cc(C(F)(F)F)c2)CC1
vNsp14-nsp10.1-117	Z1447721298	-10.1	0.337	410.46	REAL	O=C(c1cc(F)ccc1F)C1CCN(C(=O)NC[C@@H]2[C@@H]3Cc4ccccc4[C@H]23)CC1
vNsp14-nsp10.1-118	Z1449090626	-10.1	0.316	424.54	REAL	O=C(NC[C@H]1[C@@H]2Cc3ccccc3[C@H]12)[C@@H]1CCCN(C(=O)c2cccc3ccccc23)C1
vNsp14-nsp10.1-119	Z1468496400	-10.1	0.306	445.61	REAL	C[C@H](NC(=O)[C@@H](C)N1CCC[C@@H](c2nnc3n2CCCCC3)C1)c1ccc2ccccc2c1
vNsp14-nsp10.1-120	Z1473415556	-10.1	0.326	435.95	REAL	O=C1Nc2cc(Cl)ccc2[C@@H]1C1CCN(C(=O)N[C@@H]2[C@H]3CCc4ccccc4[C@H]32)CC1
vNsp14-nsp10.1-121	Z1474429871	-10.1	0.316	426.56	REAL	O=C(N[C@@H]1[C@H]2CCc3ccccc3[C@H]21)C1(C(=O)N[C@H]2[C@@H]3CCc4ccccc4[C@@H]32)CCC1
vNsp14-nsp10.1-122	Z1499273555	-10.1	0.306	438.53	REAL	O=C1CCc2cc(NC(=O)N3CCN(C4c5ccccc5-c5ccccc54)CC3)ccc2N1
vNsp14-nsp10.1-123	Z1500120469	-10.1	0.306	436.51	REAL	O=C(Cc1n[nH]c(=O)c2ccccc12)N1CCN(C2c3ccccc3-c3ccccc32)CC1
vNsp14-nsp10.1-124	Z1500303976	-10.1	0.306	439.49	REAL	O=C(c1cc(=O)[nH]c2cc(F)ccc12)N1CCN(C2c3ccccc3-c3ccccc32)CC1
vNsp14-nsp10.1-125	Z1500304046	-10.1	0.316	423.52	REAL	O=C1Nc2ccccc2[C@@H]1CC(=O)N1CCN(C2c3ccccc3-c3ccccc32)CC1
vNsp14-nsp10.1-126	Z1506260528	-10.1	0.374	357.45	REAL	O=C(Cc1ccccc2ccccc12)N1CCO[C@]2(CCc3ccccc32)C1
vNsp14-nsp10.1-127	Z1556149152	-10.1	0.326	435.91	REAL	Cc1cn(-c2ccccc2Cl)nc1C(=O)N1CCC(n2c(=O)[nH]c3ccccc32)CC1
vNsp14-nsp10.1-128	Z1627786342	-10.1	0.316	423.52	REAL	Cc1ccc(-c2nn(CC(=O)N3CCCc4ccccc43)c(=O)c3ccccc23)cc1C
vNsp14-nsp10.1-129	Z1657308572	-10.1	0.306	439.56	REAL	CO[C@H]1Cc2ccc(NC(=O)N3CCN(C4c5ccccc5-c5ccccc54)CC3)cc2C1
vNsp14-nsp10.1-130	Z1733383345	-10.1	0.306	438.53	REAL	Cc1nn(C)c2nc(-c3ccccc3)cc(C(=O)N3CCC[C@@]4(C3)OCc3ccccc34)c12
vNsp14-nsp10.1-131	Z1748297916	-10.1	0.316	420.47	REAL	O=C(c1cc(-c2ccccn2)nc2ccccc12)N1CC[C@@]2(C1)C(=O)Nc1ccccc12
vNsp14-nsp10.1-132	Z1832420013	-10.1	0.337	393.49	REAL	O=C1C[C@H](C(=O)NC[C@@H]2CC3c4ccccc4C2c2ccccc23)c2ccccc21
vNsp14-nsp10.1-133	Z1969055830	-10.1	0.361	374.48	REAL	C[C@@H]1[C@H](C(=O)N2CCC([C@@H]3C(=O)Nc4ccccc43)CC2)[C@H]1c1ccccc1
vNsp14-nsp10.1-134	Z1983291903	-10.1	0.348	388.47	REAL	O=C(CN1C(=O)N[C@@]2(C[C@H]3C[C@H]2[C@H]2CCC[C@H]32)C1=O)c1ccc2ccccc2c1
vNsp14-nsp10.1-135	Z1985082805	-10.1	0.306	437.50	REAL	O=C1N[C@H]2CCN(C(=O)c3cc(-c4cccc5ccccc45)nc4ccccc34)C[C@H]2CO1
vNsp14-nsp10.1-136	Z1997967534	-10.1	0.326	437.49	REAL	O=C(c1cccc2ccccc12)N1CCN(S(=O)(=O)c2c[nH]c3ccccc23)CC1
vNsp14-nsp10.1-137	Z2002724890	-10.1	0.326	414.55	REAL	O=C1[C@@H]2[C@@H]3C[C@@H]4[C@H]2[C@@]2(C(=O)Nc5ccccc5NC56CC7CC(CC(C7)C5)C6)[C@@H]1[C@@H]3[C@H]42
vNsp14-nsp10.1-138	Z2003685433	-10.1	0.348	381.47	REAL	O=C1[C@@H]2[C@@H]3C[C@@H]4[C@H]2[C@]2(C(=O)N[C@@H]5CCc6ccc(-c7ccccc7)cc65)[C@H]1[C@H]3[C@H]42
vNsp14-nsp10.1-139	Z2012854857	-10.1	0.326	410.48	REAL	O=C(N[C@@H]1CCN(C(=O)Nc2ccccc2)C1)c1cc2ccccc2c2ccnc12
vNsp14-nsp10.1-140	Z2073258156	-10.1	0.306	436.51	REAL	Cc1onc(-c2ccccc2)c1C(=O)N1CCN(C2c3ccccc3-c3ccccc32)CC1
vNsp14-nsp10.1-141	Z2141014680	-10.1	0.337	400.48	REAL	O=C(c1cccc2ccccc12)N1CCC(C(=O)N2Cc3ccccc3CO2)CC1
vNsp14-nsp10.1-142	Z225320126	-10.1	0.289	488.91	REAL	O=C1C[C@@H](C(=O)NNC(=O)c2cc(-c3ccccc3Cl)nc3ccccc23)c2ccc(F)cc2N1
vNsp14-nsp10.1-143	Z228625892	-10.1	0.266	498.54	REAL	O=C(Cn1c2ccccc2c(=O)c2ccccc21)NNC(=O)c1cc(-c2ccccc2)nc2ccccc12
vNsp14-nsp10.1-144	Z229282058	-10.1	0.281	481.60	REAL	Cc1nn(C)c2nc(-c3ccccc3)cc(C(=O)N[C@@H]3CC4(CCN(C)CC4)Oc4ccccc43)c12
vNsp14-nsp10.1-145	Z2480240456	-10.1	0.388	347.46	REAL	O=C([C@H]1CCc2ccccc2C1)N1CCO[C@]2(CCc3ccccc32)C1
vNsp14-nsp10.1-146	Z2811527670	-10.1	0.388	347.42	REAL	O=C(N[C@H]1Cc2ccccc2NC1=O)N[C@@H]1[C@H]2CCc3ccccc3[C@H]21
vNsp14-nsp10.1-147	Z289543000	-10.1	0.281	475.55	REAL	O=C(CCc1nc2c(cnn2-c2ccccc2)c(=O)[nH]1)N1Cc2ccccc2[C@@H](c2ccccc2)C1
vNsp14-nsp10.1-148	Z595378952	-10.1	0.289	466.54	REAL	O=C(Nc1cccc(Cn2nc3ccccn3c2=O)c1)N1CCC[C@@H](c2cc3ccccc3[nH]2)C1
vNsp14-nsp10.1-149	Z738062724	-10.1	0.297	468.54	REAL	O=c1n(Cc2cccc(NS(=O)(=O)c3ccc4c(c3)Cc3ccccc3-4)c2)nc2ccccn12
vNsp14-nsp10.1-150	Z758345294	-10.1	0.281	483.57	REAL	Cc1ccc(C(=O)C2CCN(C(=O)CN3C(=O)N[C@](C)(c4ccc5ccccc5c4)C3=O)CC2)cc1
vNsp14-nsp10.1-151	Z995740106	-10.1	0.289	469.54	REAL	O=C1COc2ccc(NC(=O)[C@H]3C[C@H]4CCCC[C@H]4N3C(=O)c3ccc4ccccc4c3)cc2N1
vNsp14-nsp10.1-152	Z998231366	-10.1	0.273	490.61	REAL	O=C(NC[C@@H]1CC2c3ccccc3C1c1ccccc12)[C@@H]1CCCN(C(=O)c2ccc3[nH]ncc3c2)C1
vNsp14-nsp10.1-153	ZINC000002221818	-10.1	0.316	417.46	ZINC	O=C(Nc1ccc2c3c(cccc31)CC2)c1cccc(-c2cc3ccccc3oc2=O)c1
vNsp14-nsp10.1-154	ZINC000002651867	-10.1	0.297	444.49	ZINC	O=C(OC1c2ccccc2-c2ccccc21)c1nn(Cc2ccccc2)c(=O)c2ccccc21
vNsp14-nsp10.1-155	ZINC000003277189	-10.1	0.289	464.56	ZINC	O=C(OCc1cc(=O)oc2ccc3ccccc3c12)C12C[C@@H]3C[C@H](C1)CC(c1ccccc1)(C3)C2
vNsp14-nsp10.1-156	ZINC000014120768	-10.1	0.326	413.48	ZINC	O=C(CN1C(=O)N[C@]2(CCCCc3ccccc32)C1=O)Nc1ccc2ccccc2c1
vNsp14-nsp10.1-157	ZINC000015080442	-10.1	0.306	437.49	ZINC	O=C(c1ccc2c3c(cccc31)CC2)[C@@H]1CCCN(C(=O)c2cc(=O)c3ccccc3o2)C1
vNsp14-nsp10.1-158	ZINC000072356486	-10.1	0.326	411.48	ZINC	O=C(c1cnc2ccccc2c1)N1CCC[C@@H](c2cccc(-c3ccc(F)cc3)n2)C1
vNsp14-nsp10.1-159	ZINC000253623869	-10.1	0.273	488.50	ZINC	Cn1cc(/C=C2/Oc3c(ccc4c3[C@H](c3cc5ccccc5nc3O)CC(=O)O4)C2=O)c2ccccc21
vNsp14-nsp10.1-160	ZINC000257325671	-10.1	0.306	442.49	ZINC	Cc1cc(-c2ccc(F)cc2)cc([C@@H]2CCCN(C(=O)c3n[nH]c(=O)c4ccccc43)C2)n1
vNsp14-nsp10.1-161	ZINC000263586232	-10.1	0.273	488.50	ZINC	Cn1cc(/C=C2\Oc3c(ccc4c3[C@H](c3cc5ccccc5nc3O)CC(=O)O4)C2=O)c2ccccc21
vNsp14-nsp10.1-162	PV-001809915608	-10.0	0.323	426.40	REAL	Cc1c(C(=O)Nc2ccn(-c3ccccc3C(F)(F)F)n2)c2ccccc2n(C)c1=O
vNsp14-nsp10.1-163	PV-001811178589	-10.0	0.333	414.39	REAL	Cc1cc(NC(=O)[C@@H]2CC(=O)Nc3ccccc32)nn1-c1ccccc(C(F)(F)F)c1
vNsp14-nsp10.1-164	PV-001817114612	-10.0	0.345	398.34	REAL	O=C1C[C@@H](C(=O)Nc2nccc(-c3ccc(F)c(F)c3)n2)c2ccc(F)cc2N1
vNsp14-nsp10.1-165	PV-001818619223	-10.0	0.323	453.33	REAL	O=C(COc1cccc2ccccc12)N1C[C@H]2[C@H](C1)C(F)(F)C(F)(F)C(F)(F)C2(F)F
vNsp14-nsp10.1-166	PV-001818622197	-10.0	0.323	450.33	REAL	O=C(c1cc(-c2ccccc2)ccn1)N1C[C@@H]2[C@H](C1)C(F)(F)C(F)(F)C(F)(F)C2(F)F
vNsp14-nsp10.1-167	PV-001862346596	-10.0	0.313	441.52	REAL	Cc1cccc(NC(=O)N2CCC[C@H](C(=O)N3CCC[C@@H](c4ccc(F)c(F)c4)C3)C2)c1
vNsp14-nsp10.1-168	PV-001869196828	-10.0	0.313	440.42	REAL	O=C(NCC[C@]1(O)C(=O)Nc2ccccc21)c1cccc1-c1ccc(C(F)(F)F)cc1
vNsp14-nsp10.1-169	PV-001875532070	-10.0	0.323	458.28	REAL	O=C(c1cc2cc(F)ccc2nc1O)N1C[C@@H]2[C@@H](C1)C(F)(F)C(F)(F)C(F)(F)C2(F)F
vNsp14-nsp10.1-170	PV-001949043422	-10.0	0.345	445.33	REAL	O=C(Nc1nsc2ccccc12)N1C[C@H]2[C@H](C1)C(F)(F)C(F)(F)C(F)(F)C2(F)F
vNsp14-nsp10.1-171	PV-001949094299	-10.0	0.370	363.46	REAL	O=C(Nc1ccc2c(c1)CCCCC2)N[C@H]1CCc2ccccc2NC1=O
vNsp14-nsp10.1-172	PV-001956824407	-10.0	0.333	442.35	REAL	O=C(NCC1Cc2ccccc2C1)N1C[C@H]2[C@H](C1)C(F)(F)C(F)(F)C(F)(F)C2(F)F
vNsp14-nsp10.1-173	PV-001964841916	-10.0	0.357	377.49	REAL	C[C@H]1CN(C(=O)N[C@@H]2CCc3ccccc3NC2=O)CC[C@@H]1c1ccccc1
vNsp14-nsp10.1-174	PV-001965456420	-10.0	0.345	442.30	REAL	O=C(N[C@H]1CC[C@@H]2[C@H](C1)C2(F)F)N1C[C@H]2[C@H](C1)C(F)(F)C(F)(F)C(F)(F)C2(F)F
vNsp14-nsp10.1-175	Z1004755640	-10.0	0.323	411.50	REAL	O=C(NCCN1C(=O)Cc2ccccc21)N1Cc2ccccc2[C@H](c2ccccc2)C1
vNsp14-nsp10.1-176	Z1024049916	-10.0	0.313	430.51	REAL	Cc1cccc(N2N=C(C(=O)N3CCC([C@@H]4C(=O)Nc5ccccc54)CC3)CCC2=O)c1
vNsp14-nsp10.1-177	Z1024050894	-10.0	0.333	404.47	REAL	C[C@@]1(C(=O)N2CCC([C@@H]3C(=O)Nc4ccccc43)CC2)Cc2ccccc2C(=O)O1
vNsp14-nsp10.1-178	Z1024052512	-10.0	0.345	387.48	REAL	Cc1ccc2c(CC(=O)N3CCC([C@@H]4C(=O)Nc5ccccc54)CC3)c[nH]c2c1
vNsp14-nsp10.1-179	Z1024537352	-10.0	0.323	410.48	REAL	O=C1Nc2ccccc2[C@@H]1C1CCN(c2cc(-c3ccccc3)nc3ncnn23)CC1
vNsp14-nsp10.1-180	Z1128821654	-10.0	0.323	417.51	REAL	CC(=O)N1Cc2ccccc2C[C@H]1C(=O)N1CCC([C@@H]2C(=O)Nc3ccccc32)CC1
vNsp14-nsp10.1-181	Z1128836885	-10.0	0.313	423.47	REAL	O=C(CN1C(=O)CCOc2ccccc21)Nc1cccc(-c2ccc3ccccc3c2)n1
vNsp14-nsp10.1-182	Z1128837701	-10.0	0.345	378.43	REAL	O=C(Cc1n[nH]c2ccccc12)Nc1cccc(-c2ccc3ccccc3c2)n1
vNsp14-nsp10.1-183	Z1151317440	-10.0	0.303	437.54	REAL	O=C(Cc1c[nH]c2ccccc12)N1CCN(C(=O)[C@@H]2C[C@H]2c2cccc3ccccc23)CC1
vNsp14-nsp10.1-184	Z1158232229	-10.0	0.323	411.50	REAL	O=C([C@@H]1C[C@H]1c1ccc2ccccc2c1)N1CCC(n2c(=O)[nH]c3ccccc32)CC1
vNsp14-nsp10.1-185	Z1171415559	-10.0	0.323	408.51	REAL	c1ccc(-n2nnnc2CN2CCN(C3c4ccccc4-c4ccccc43)CC2)cc1
vNsp14-nsp10.1-186	Z1211972707	-10.0	0.345	391.45	REAL	O=C1Nc2ccccc2[C@@H]1C1CCN(C(=O)Cc2c[nH]c3ccc(F)cc23)CC1
vNsp14-nsp10.1-187	Z1217629463	-10.0	0.345	396.48	REAL	C[C@H]1Cc2ccccc2N1C1CCN(C(=O)[C@H]2C[C@@H]2c2c(F)cccc2F)CC1
vNsp14-nsp10.1-188	Z1240384639	-10.0	0.323	408.46	REAL	Cc1nnc([C@H]2Cc3ccccc3CN2C(=O)c2cc3c(ccc4ccccc43)[nH]2)o1
vNsp14-nsp10.1-189	Z1255978584	-10.0	0.303	446.59	REAL	CC1(C)[C@H](NC(=O)[C@@H]2[C@H]3CCCC[C@@H]3N2C(=O)c2ccc3ccccc3c2)[C@H]2CCO[C@H]21
vNsp14-nsp10.1-190	Z1260002709	-10.0	0.303	441.53	REAL	O=C(NNC(=O)[C@H]1C[C@H]2CCCC[C@@H]2N1C(=O)c1ccccc1)c1ccc2ccccc12
vNsp14-nsp10.1-191	Z1260120205	-10.0	0.313	446.57	REAL	O=C(c1cccc(S(=O)(=O)N2CCc3ccccc32)c1)N1CC[C@@H](Cc2ccccc2)C1
vNsp14-nsp10.1-192	Z1260481792	-10.0	0.313	448.59	REAL	C[C@H]1Cc2ccccc2CN1C(=O)C1CCN(S(=O)(=O)c2ccc3ccccc3c2)CC1
vNsp14-nsp10.1-193	Z1261014278	-10.0	0.345	396.48	REAL	C[C@H]1Cc2ccccc2N1C1CCN(C(=O)[C@H]2C[C@@H]2c2cccc(F)c2F)CC1
vNsp14-nsp10.1-194	Z1265333541	-10.0	0.303	446.55	REAL	Cc1ccccc1[C@H]1CN(C(=O)c2ccc3c(c2)C(=O)N(C2CCCCC2)C3=O)[C@@H](C)CO1
vNsp14-nsp10.1-195	Z1318939585	-10.0	0.333	394.43	REAL	O=C(Cc1cn2ccccc2n1)NNC(=O)c1c2ccccc2cc2ccccc12
vNsp14-nsp10.1-196	Z1374247454	-10.0	0.333	404.51	REAL	O=C(CN1C(=O)[C@H]2[C@H]3C=C[C@@H](C3)[C@H]2C1=O)N1CCC[C@]2(CCCc3ccccc32)C1
vNsp14-nsp10.1-197	Z1382205886	-10.0	0.323	409.49	REAL	O=C(NCc1cc(=O)[nH]c2ccccc12)N1Cc2ccccc2[C@H](c2ccccc2)C1
vNsp14-nsp10.1-198	Z1410524149	-10.0	0.345	384.39	REAL	O=C(NNc1nc2ccccc2c(=O)[nH]1)C1c2ccccc2Oc2ccccc21
vNsp14-nsp10.1-199	Z1440831445	-10.0	0.313	437.51	REAL	CC1(C)C[C@H](NC(=O)N2CCC([C@H]3C(=O)Nc4ccccc43)CC2)c2ccc(F)cc2O1
vNsp14-nsp10.1-200	Z1452696527	-10.0	0.313	432.50	REAL	O=C(NC[C@@H]1[C@@H]2Cc3ccccc3[C@H]12)N1CCC[C@@H](c2nc(-c3cccc(F)c3)no2)C1

Supplementary Table 68. Virtual screening hits 101 to 200 of the screen against the nsp10 binding site of nsp14 (Screen ID: 36). Compounds were filtered so that hits had MW < 600 dalton, cLogP < 6, number of hydrogen bond acceptors < 11, and no reactive functional groups. A few compounds unsuitable for drug discovery were removed by visual inspection. The name of each compound consists of the initial letter 'v' for virtual hit, followed by the target protein name and the target site ('nsp10' for nsp10 binding site, 1 for docking scenario 1). The score is the docking score given by QuickVina 2 in kcal/mol. The ligand efficiency (LE) is computed as LE = -score/#NonH, where #NonH is the number of heavy (i.e. non hydrogen) atoms.

Name	Catalog ID	Score	LE	MW	Library	SMILES
vNsp14-as2-1	Z1375388198	-10.4	0.347	405.496	REAL	C[C@H]1Oc2ccc(NC(=O)N3CCC[C@]4(CCCc5ccccc54)C3)cc2NC1=O
vNsp14-as2-2	Z1024047020	-10.3	0.294	466.535	REAL	O=C1O[C@@H](c2ccccc2)Cc2cc(C(=O)N3CCC([C@H]4C(=O)Nc5ccccc54)CC3)ccc21
vNsp14-as2-3	Z2524819091	-10.3	0.303	477.671	REAL	CC(C)NC(=O)CSc1ccccc1C(=O)N1C[C@H]2CC[C@H]1[C@H]1CN(Cc3ccccc3)C[C@H]21
vNsp14-as2-4	Z3095177725	-10.3	0.355	394.434	REAL	Cn1nc(-c2nnc(N3CCC[C@]4(CC(=O)c5ccccc5O4)C3)n2C)cc1O
vNsp14-as2-5	ZINC000408731628	-10.3	0.271	499.565	ZINC	Cc1ccc(N2C(=O)[C@H]3[C@H](C2=O)[C@@H]2C(=O)Oc4c5ccccc5ccc4C2=C[C@@H]3c2ccccc2)cc1C
vNsp14-as2-6	Z1128906577	-10.1	0.281	482.538	REAL	O=C(Nc1cccc(-c2noc(=O)[nH]2)c1)[C@@H]1C[C@H]2CCCC[C@H]2N1C(=O)c1ccc2ccccc2c1
vNsp14-as2-7	Z804319726	-10.1	0.306	448.478	REAL	C[C@@H]1c2ec3c(ce2C2(CCCC2)CN1C(=O)c1cnc2[nH]c(=O)[nH]c(=O)c2c1)OCCO3
vNsp14-as2-8	Z980048004	-10.1	0.297	465.503	REAL	Cc1nc(-c2cccc(NC(=O)[C@@H]3C[C@@H]4CCCC[C@H]4N3C(=O)c3ccc(F)cc3F)c2)n[nH]1
vNsp14-as2-9	Z1375407436	-10	0.323	420.491	REAL	Cc1nnnn1-c1cc(NC(=O)N2CCC[C@]3(CCCc4ccccc43)C2)ccc1F
vNsp14-as2-10	Z2002724890	-10	0.323	414.547	REAL	O=C1[C@@H]2[C@@H]3C[C@@H]4[C@H]2[C@@]2(C(=O)Nc5ccccc5NC56CC7CC(CC(C7)C5)C6)[C@@H]1[C@@H]3[C@H]42
vNsp14-as2-11	Z363564868	-10	0.323	419.48	REAL	C[C@@H]1c2cc3c(cc2C2(CCCC2)CN1C(=O)c1ccc2[nH]c(=O)[nH]c2c1)OCCO3
vNsp14-as2-12	ZINC000015972852	-10	0.27	494.525	ZINC	Cc1ccc2c(c1)[C@]1(N[C@@H](Cc3c[nH]c4ccccc34)[C@H]3C(=O)N(c4ccc(F)cc4)C(=O)[C@H]31)C(=O)N2
vNsp14-as2-13	ZINC000029748614	-10	0.256	560.65	ZINC	C[C@H]1CN(S(=O)(=O)c2ccc3oc4ccccc4c3c2)CCN1S(=O)(=O)c1ccc2oc3ccccc3c2c1
vNsp14-as2-14	ZINC000408731317	-10	0.263	499.565	ZINC	Cc1ccc(C)c(N2C(=O)[C@H]3[C@H](C2=O)[C@@H]2C(=O)Oc4c5ccccc5ccc4C2=C[C@@H]3c2ccccc2)c1
vNsp14-as2-15	Z1069479500	-9.9	0.3	448.478	REAL	CCc1noc2ncc(C(=O)N3CCC(C(=O)c4ccc5c(c4)NC(=O)[C@H](C)O5)CC3)cc12
vNsp14-as2-16	Z1286742852	-9.9	0.33	402.417	REAL	Cc1c(C(=O)N2CCn3c(nnc3-c3ccccc3)C2)cnn1-c1ccc(=O)[nH]n1
vNsp14-as2-17	Z1375407921	-9.9	0.341	391.47	REAL	Cn1c(=O)oc2cc(NC(=O)N3CCC[C@]4(CCCc5ccccc54)C3)ccc21
vNsp14-as2-18	Z1375416574	-9.9	0.33	405.496	REAL	CN1C(=O)COc2ccc(NC(=O)N3CCC[C@]4(CCCc5ccccc54)C3)ccc21
vNsp14-as2-19	ZINC000008921453	-9.9	0.261	498.537	ZINC	O=C(NN1C(=O)[C@@H]2[C@@H](C1=O)C1c3ccccc3C2c2ccccc21)C1(O)c2ccccc2-c2ccccc21
vNsp14-as2-20	ZINC000018021374	-9.9	0.261	498.537	ZINC	O=C(NN1C(=O)[C@H]2[C@@H](C1=O)C1c3ccccc3C2c2ccccc21)C1(O)c2ccccc2-c2ccccc21
vNsp14-as2-21	Z1014500564	-9.8	0.297	463.967	REAL	Cc1nc(-c2cccc(NC(=O)[C@@H]3C[C@@H]4CCCC[C@H]4N3C(=O)c3ccc(Cl)c3)c2)n[nH]1
vNsp14-as2-22	Z1375393010	-9.8	0.327	402.5	REAL	Cc1nnnn1-c1cccc(NC(=O)N2CCC[C@]3(CCCc4ccccc43)C2)c1
vNsp14-as2-23	Z1730914635	-9.8	0.338	393.442	REAL	C[C@H]1Oc2ccc(NC(=O)N3CCC[C@@]4(C3)OCc3ccccc34)cc2NC1=O
vNsp14-as2-24	Z1907684399	-9.8	0.338	416.54	REAL	CCS(=O)(=O)NCc1ccc(C(=O)NC[C@@]2(O)[C@H]3[C@@H]4C[C@H]5[C@H]6[C@H]4C[C@@H]3[C@H]6[C@@H]52)cc1
vNsp14-as2-25	Z2167520785	-9.8	0.306	433.49	REAL	O=C(Nc1ccc(F)c(-n2nnnc2C2CC2)c1)N1CCCN2c3ccccc3C[C@H]2C1
vNsp14-as2-26	Z816768986	-9.8	0.265	498.581	REAL	O=C1CN(C(=O)CC23C[C@H]4C[C@@H](C2)CC(C(=O)N2CC(=O)Nc5ccccc52)(C4)C3)c2ccccc2N1
vNsp14-as2-27	ZINC000004015296	-9.8	0.258	493.477	ZINC	O=c1nc2c3cccc4cccc(c(=O)n2c2cc(N5C(=O)c6cccc7cccc(c76)C5=O)ccc12)c43
vNsp14-as2-28	ZINC000015967689	-9.8	0.272	476.535	ZINC	Cc1ccc2c(c1)[C@]1(N[C@@H](Cc3c[nH]c4ccccc34)[C@H]3C(=O)N(c4ccccc4)C(=O)[C@H]31)C(=O)N2
vNsp14-as2-29	ZINC000035375696	-9.8	0.265	490.561	ZINC	Cc1ccc2c(c1)[C@]1(N[C@@H](Cc3c[nH]c4ccccc34)[C@H]3C(=O)N(c4cccc(C)c4)C(=O)[C@H]31)C(=O)N2
vNsp14-as2-30	ZINC000085392620	-9.8	0.265	493.569	ZINC	O=C([C@H]1CC(=O)N(c2nc[nH]n2)C1)N1CCC(c2c[nH]c3ccccc32)(c2c[nH]c3ccccc32)CC1
vNsp14-as2-31	ZINC000085392737	-9.8	0.251	516.643	ZINC	Cc1ccc(N2C[C@@H](C(=O)N3CCC(c4c[nH]c5ccccc54)(c4c[nH]c5ccccc54)CC3)CC2=O)cc1
vNsp14-as2-32	ZINC000085392752	-9.8	0.245	530.67	ZINC	Cc1ccc(N2C[C@H](C(=O)N3CCC(c4c[nH]c5ccccc54)(c4c[nH]c5ccccc54)CC3)CC2=O)c(C)c1
vNsp14-as2-33	ZINC000408675934	-9.8	0.258	498.58	ZINC	Cc1ccc(NC(=O)c2ccccc2N2C(=O)[C@H]3[C@@H](C2=O)C2c4ccccc4C3c3ccccc32)cc1C
vNsp14-as2-34	ZINC000408675939	-9.8	0.258	498.58	ZINC	Cc1ccc(NC(=O)c2ccccc2N2C(=O)[C@H]3[C@H](C2=O)C2c4ccccc4C3c3ccccc32)cc1C
vNsp14-as2-35	ZINC000408730039	-9.8	0.265	485.538	ZINC	Cc1ccc(N2C(=O)[C@H]3[C@H](C2=O)[C@@H]2C(=O)Oc4c5ccccc5ccc4C2=C[C@@H]3c2ccccc2)cc1
vNsp14-as2-36	PV-001820484397	-9.7	0.313	442.495	REAL	Cc1ccc(C)c(S(=O)(=O)N2CCN(C(=O)c3cccc(-c4noc(O)n4)c3)CC2)c1
vNsp14-as2-37	PV-001822944745	-9.7	0.313	442.495	REAL	Cc1ccc(S(=O)(=O)N2CCN(C(=O)c3cccc(-c4noc(O)n4)c3)CC2)cc1C
vNsp14-as2-38	PV-001845558042	-9.7	0.303	450.391	REAL	Cc1cc(C(=O)N2CCC(F)(c3ccccc3C(F)(F)F)CC2)nc2nc(O)[nH]c(=O)c12
vNsp14-as2-39	PV-001947445820	-9.7	0.323	404.444	REAL	NC(=O)Nc1cc(NC(=O)N2CC=C(c3cccc4ccccc34)CC2)ccc1F
vNsp14-as2-40	Z1082317300	-9.7	0.285	457.445	REAL	C[C@@]1(c2ccc3ccccc3c2)NC(=O)N(CC(=O)Nc2cccc(-c3noc(=O)[nH]3)c2)C1=O
vNsp14-as2-41	Z1117086514	-9.7	0.313	412.496	REAL	Cc1nc(-c2cccc(NC(=O)N3CC=C(c4c(C)[nH]c5ccccc45)CC3)c2)n[nH]1
vNsp14-as2-42	Z1161373478	-9.7	0.277	494.57	REAL	O=C1COc2ccc(S(=O)(=O)N3CCN(C(=O)c4cccc5c6c([nH]c45)CCCC6)CC3)cc2N1
vNsp14-as2-43	Z1174758925	-9.7	0.323	405.413	REAL	O=C1O[C@@H](c2ccccc2)Cc2cc(C(=O)N3CCO[C@@H](c4nnn[nH]4)C3)ccc21
vNsp14-as2-44	Z1273409220	-9.7	0.303	431.474	REAL	Cc1cc(N2CCN(C(=O)c3cc(C4CC4)nc4ccc(F)cc34)CC2)n2ncnc2n1
vNsp14-as2-45	Z1375391167	-9.7	0.323	402.5	REAL	Cc1ccc(NC(=O)N2CCC[C@]3(CCCc4ccccc43)C2)cc1-n1cnnn1
vNsp14-as2-46	Z1375394593	-9.7	0.303	433.51	REAL	Cn1c(=O)c2cc(NC(=O)N3CCC[C@]4(CCCc5ccccc54)C3)cnc2n(C)c1=O
vNsp14-as2-47	Z1422310123	-9.7	0.303	446.432	REAL	Cc1nc([C@H]2CCCN(C(=O)c3nn(-c4ccccc4C(F)(F)F)c(C)cc3=O)C2)n[nH]1
vNsp14-as2-48	Z1629839702	-9.7	0.294	448.501	REAL	O=C(Nc1ccccc(CN2CCCC2=O)c1)N[C@H]1CCc2nnc(-c3cccc(F)cc3)n2C1
vNsp14-as2-49	Z1631039202	-9.7	0.313	415.514	REAL	Cc1ccc2[nH]c3c(c2c1)C[C@H](N[C@H]1CCc2nnc(-c4ccc(F)cc4)n2C1)CC3
vNsp14-as2-50	Z1656867584	-9.7	0.313	440.93	REAL	O=C([C@H]1C[C@@H]2CCCC[C@H]2N1C(=O)c1cccc(Cl)c1)N1CCc2c(nc[nH]c2=O)C1
vNsp14-as2-51	Z1883396970	-9.7	0.323	437.333	REAL	Clc1cc(Cl)cc(-c2nnc3ccc(N4CC[C@]5(CNc6ccccc65)C4)nn23)c1
vNsp14-as2-52	Z2077125337	-9.7	0.313	413.436	REAL	O=C(Nc1cccc(-c2n[nH]c(=O)[nH]2)c1)[C@@H]1CC(=O)N(c2cccc3ccccc23)C1
vNsp14-as2-53	Z2233383359	-9.7	0.323	404.473	REAL	Nc1nnc(C2CCN(C(=O)[C@@H]3CC(=O)N(c4cccc5ccccc45)C3)CC2)[nH]1
vNsp14-as2-54	Z226646320	-9.7	0.285	454.576	REAL	C[C@@H]1CCc2[nH]c3ccc(C(=O)N4CCN(Cc5nc(N)c6ccccc6n5)CC4)cc3c2C1
vNsp14-as2-55	Z230801774	-9.7	0.303	430.502	REAL	C[C@@H]1c2cc3c(cc2C2(CCCC2)CN1C(=O)c1cc2ccccc2c(=O)[nH]1)OCCO3
vNsp14-as2-56	Z245796024	-9.7	0.303	430.502	REAL	C[C@@H]1c2cc3c(cc2C2(CCCC2)CN1C(=O)c1cc(=O)c2ccccc2[nH]1)OCCO3
vNsp14-as2-57	Z2718650933	-9.7	0.334	390.438	REAL	O=C1Cc2ccc(CC(=O)N3CCC[C@]4(CC(=O)c5ccccc5O4)C3)cc2N1
vNsp14-as2-58	Z3094210447	-9.7	0.359	378.361	REAL	Cn1c(-c2nnn[nH]2)nnc1N1CCC(c2ccc(C(F)(F)F)cc2)CC1
vNsp14-as2-59	Z332388888	-9.7	0.303	431.49	REAL	C[C@@H]1c2cc3c(cc2C2(CCCC2)CN1C(=O)c1nc2ccccc2c(=O)[nH]1)OCCO3
vNsp14-as2-60	Z358334242	-9.7	0.277	495.538	REAL	Cc1cc(N2CCN(C(=O)c3ccccc3NS(=O)(=O)c3ccc(F)cc3)CC2)n2ncnc2n1
vNsp14-as2-61	Z412184662	-9.7	0.269	488.59	REAL	Cc1cc(C)nc(-n2nc(C)cc2NC(=O)N2CC3(CCCC3)c3cc4c(cc3[C@H]2C)OCCO4)n1
vNsp14-as2-62	Z509610482	-9.7	0.262	495.534	REAL	O=C(Nc1cccc(C(=O)N2CCOCC2)c1)c1cc(-c2ccc3c(c2)OCCO3)nc2ccccc12
vNsp14-as2-63	Z744863034	-9.7	0.285	459.505	REAL	C[C@@H]1CC(=O)Nc2ccccc2N1C(=O)CN(C)C(=O)NNC(=O)c1ccc2ccccc2c1
vNsp14-as2-64	ZINC000003425158	-9.7	0.255	518.494	ZINC	COc1ccc2c(C)cc(NN/C=C3/c4ccccc4C(=O)N(c4cccc(C(F)(F)F)c4)C3=O)nc2c1
vNsp14-as2-65	ZINC000012375021	-9.7	0.277	485.417	ZINC	O=C1Nc2c(cccc2C(F)(F)F)[C@@]12[C@H]1C(=O)N(c3ccc4c(c3)OCO4)C(=O)[C@@H]1[C@H]1CCCN12
vNsp14-as2-66	ZINC000016000214	-9.7	0.285	451.525	ZINC	Cc1cc2c(c(C)c1)NC(=O)[C@]21[C@@H]2C(=O)N(c3ccc4ccccc4c3)C(=O)[C@@H]2[C@@H]2CCCN21
vNsp14-as2-67	ZINC000016013265	-9.7	0.285	471.943	ZINC	Cc1cc2c(c(Cl)c1)NC(=O)[C@]21[C@@H]2C(=O)N(c3ccc4ccccc4c3)C(=O)[C@@H]2[C@@H]2CCCN21
vNsp14-as2-68	ZINC000035375706	-9.7	0.262	490.561	ZINC	Cc1ccc(C)cc(N2C(=O)[C@@H]3[C@H](C2=O)[C@H](Cc2c[nH]c4ccccc24)N[C@@]32C(=O)Nc3ccccc32)c1
vNsp14-as2-69	ZINC000100999609	-9.7	0.285	471.492	ZINC	Cc1ccc(S(=O)(=O)/N=C2/C=C(O/N=C3\c4ccccc4NC3=O)C(=O)c3ccccc32)cc1
vNsp14-as2-70	ZINC000195529726	-9.7	0.237	562.024	ZINC	O=C1c2ccccc2[C@H]([C@@H]2NC[C@@H](c3ccccc3Cl)c3c4ccccc4[nH]c32)C(=O)N1c1ccc2c(c1)OCO2
vNsp14-as2-71	ZINC000218084222	-9.7	0.313	417.372	ZINC	O=C(COc1ccc2c(c1)O/C(=C/c1ccco1)C2=O)c1ccc2c(c1)NC(=O)CO2
vNsp14-as2-72	PV-001946446294	-9.6	0.31	420.511	REAL	Cc1ccc(NC(=O)N[C@@H]2CCc3ccccc3NC2=O)cc1C(=O)N1CCCCC1
vNsp14-as2-73	Z1014383874	-9.6	0.274	466.543	REAL	O=C(Nc1cccc(-c2nnn[nH]2)c1)[C@@H]1C[C@@H]2CCCC[C@H]2N1C(=O)c1ccc2ccccc2c1
vNsp14-as2-74	Z1027965800	-9.6	0.267	490.562	REAL	COc1ccc(NC(=O)N2CC3(CCCC3)c3cc4c(cc3[C@H]2C)OCCO4)cc1-n1nnnc1C
vNsp14-as2-75	Z1039083142	-9.6	0.282	493.397	REAL	O=C(C1CCN(c2ccc3nnc(-c4cc(Cl)cc(Cl)c4)n3n2)CC1)N1CCc2ccccc21
vNsp14-as2-76	Z1069338314	-9.6	0.274	468.559	REAL	O=C(Nc1ccnn1[C@@H]1CCCc2ccccc21)[C@@H]1CCCN(C(=O)c2ccc3[nH]ncc3c2)C1
vNsp14-as2-77	Z1096333257	-9.6	0.291	455.46	REAL	Cn1c(=O)oc2cc(NC(=O)[C@@H]3C[C@@H]4CCCC[C@H]4N3C(=O)c3ccc(F)cc3F)ccc21
vNsp14-as2-78	Z1117086940	-9.6	0.3	450.929	REAL	Cc1nc(-c2cccc(NC(=O)N3CCC([C@@H]4C(=O)Nc5cc(Cl)ccc54)CC3)c2)n[nH]1
vNsp14-as2-79	Z1128759055	-9.6	0.282	474.544	REAL	Cc1ccc(S(=O)(=O)N2Cc3ccccc3C[C@@H]2C(=O)Nc2ccc(-c3nnn[nH]3)cc2)cc1
vNsp14-as2-80	Z1250977085	-9.6	0.31	430.349	REAL	Cc1cc(=O)c(C(=O)NNc2ncnc3nc[nH]c23)nn1-c1ccccc1C(F)(F)F
vNsp14-as2-81	Z1322673694	-9.6	0.3	427.511	REAL	Cc1ccc2nc(C3CC3)cc(C(=O)N3CCN(c4cc(C)nc5ncnn45)CC3)c2c1
vNsp14-as2-82	Z1360171218	-9.6	0.3	447.929	REAL	Cc1ccc(N2CCN(C(=O)c3cc(C4CC4)nc4ccc(Cl)cc34)CC2)n2ncnc2n1
vNsp14-as2-83	Z1460161310	-9.6	0.291	441.45	REAL	Cc1ccc(N2C(=O)/C(=C/NNc3nc4c(cnn4C)c(=O)[nH]3)c3ccccc3C2=O)cc1
vNsp14-as2-84	Z1463877810	-9.6	0.3	430.423	REAL	Cn1ncc2c(=O)[nH]c(NNC(=O)c3ccc4c(c3)C[C@@H](c3ccccc3)OC4=O)nc21
vNsp14-as2-85	Z1505440080	-9.6	0.31	433.393	REAL	Cc1cc(=O)c(C(=O)N2CCC[C@H](c3nnn[nH]3)C2)nn1-c1ccccc1C(F)(F)F
vNsp14-as2-86	Z1505813425	-9.6	0.291	442.47	REAL	O=C(Cc1cc2c(ccc3ccccc32)o1)N1CCN(C(=O)c2ccc3c(c2)OCO3)CC1
vNsp14-as2-87	Z1575432086	-9.6	0.3	435.479	REAL	C[C@@H]1c2cc3c(cc2C2(CCCC2)CN1C(=O)c1cnc2c(c1)NC(=O)CO2)OCCO3
vNsp14-as2-88	Z1643822107	-9.6	0.32	395.465	REAL	Cc1nc(-c2cccc(NC(=O)N3CC=C(c4cccc5ccccc45)C3)c2)n[nH]1
vNsp14-as2-89	Z1653931427	-9.6	0.343	374.482	REAL	O=C1Cc2ccc(CC(=O)N3CCC[C@]4(CCCc5ccccc54)C3)cc2N1
vNsp14-as2-90	Z1891910653	-9.6	0.331	384.394	REAL	Cc1nc(-c2cccc(N3C(=O)N[C@H](c4cccc5ccccc5c4)C3=O)c2)no1
vNsp14-as2-91	Z1903663225	-9.6	0.31	427.503	REAL	Cc1ccc(NC(=O)NC[C@@H]2CCC[C@@]23NC(=O)NC3=O)cc1C(=O)N1CCCCC1
vNsp14-as2-92	Z1974161210	-9.6	0.31	409.492	REAL	Cc1nc2c(C(=O)N3CCN(C4c5ccccc5-c5ccccc54)CC3)ccnc2[nH]1
vNsp14-as2-93	Z2179830391	-9.6	0.291	444.49	REAL	O=C1[C@H]2Cc3ccccc3CN2C(=O)N1Cc1cccc(N2C(=O)NC3(CCCC3)C2=O)c1
vNsp14-as2-94	Z230788436	-9.6	0.274	477.559	REAL	CC(=O)Nc1cc(NC(C)=O)cc(C(=O)N2CC3(CCCC3)c3cc4c(cc3[C@H]2C)OCCO4)c1
vNsp14-as2-95	Z325118426	-9.6	0.331	395.497	REAL	Cc1ccc(C23C[C@H]4C[C@@H](CC(C(=O)OCCN5C(=O)CCC5=O)(C4)C2)C3)cc1
vNsp14-as2-96	Z412147130	-9.6	0.31	421.495	REAL	C[C@@H]1c2cc3c(cc2C2(CCCC2)CN1C(=O)Nc1ccc(C(N)=O)cc1)OCCO3
vNsp14-as2-97	Z413363388	-9.6	0.31	410.48	REAL	Cc1ccc(NC(=O)N2Cc3ccccc3[C@@H](c3cccc3)C2)cc1-n1cnnn1
vNsp14-as2-98	Z413812746	-9.6	0.274	492.602	REAL	CSc1nnnn1-c1ccc(NC(=O)N2CC3(CCCC3)c3cc4c(cc3[C@H]2C)OCCO4)c1
vNsp14-as2-99	Z753644774	-9.6	0.31	418.495	REAL	Cc1[nH]nc2ncc(C(=O)N3CC4(CCCC4)c4cc5c(cc4[C@H]3C)OCCO5)cc12
vNsp14-as2-100	Z785662624	-9.6	0.274	489.555	REAL	O=C1C[C@H](N2CCN(S(=O)(=O)c3c[nH]c4nccc34)CC2)C(=O)N1c1ccc2ccccc2c1

Supplementary Table 69. Top 100 virtual hits of the screen against the active site of the ExoN domain of nsp14 (Screen ID: 37). Compounds were filtered so that hits had MW < 600 dalton, cLogP < 6, number of hydrogen bond acceptors < 11, and no reactive functional groups. A few compounds unsuitable for drug discovery were removed by visual inspection. The name of each compound consists of the initial letter 'v' for virtual hit, followed by the target protein name and the target site ('as' for active site, 2 for docking scenario 2). The score is the docking score given by QuickVina 2 in kcal/mol. The ligand efficiency (LE) is computed as LE = -score/#NonH, where #NonH is the number of heavy (i.e. non hydrogen) atoms.

Name	Catalog ID	Score	LE	MW	Library	SMILES
vNsp14-as2-101	Z827033132	-9.6	0.291	463.51	REAL	O=C(Nc1ccc2oc(=O)ccc2c1)N1CCN(S(=O)(=O)c2ccc3ccccc3c2)CC1
vNsp14-as2-102	ZINC000002619944	-9.6	0.320	405.41	ZINC	O=C(CN1C(=O)N[C@@]2(CCCc3ccccc32)C1=O)Nc1ccc2[nH]c(=O)[nH]c2c1
vNsp14-as2-103	ZINC000003770978	-9.6	0.291	432.48	ZINC	CC(=O)Nc1ccc([C@@H]2Nc3ccc4ccccc4c3-c3c4ccccc4oc(=O)c32)cc1
vNsp14-as2-104	ZINC000009129478	-9.6	0.300	451.50	ZINC	Cc1cc(=O)oc2cc(NC(=O)c3ccc4c(c3)S(=O)(=O)N=C3CCCCN43)ccc12
vNsp14-as2-105	ZINC000014752022	-9.6	0.300	451.50	ZINC	Cc1cc(=O)oc2cc(NC(=O)[C@H]3CCCN(C4=NS(=O)(=O)c5ccccc54)C3)ccc12
vNsp14-as2-106	ZINC000015971909	-9.6	0.259	490.56	ZINC	Cc1ccc(N2C(=O)[C@@H]3[C@H](C2=O)[C@@H](Cc2c[nH]c4ccccc24)N[C@]32C(=O)Nc3c2cccc3C)cc1
vNsp14-as2-107	ZINC000015972403	-9.6	0.259	494.53	ZINC	Cc1cccc2c1NC(=O)[C@@]21N[C@@H](Cc2c[nH]c3ccccc23)[C@H]2C(=O)N(c3ccc(F)cc3)C(=O)[C@H]21
vNsp14-as2-108	ZINC000015972854	-9.6	0.259	494.53	ZINC	Cc1ccc2c(c1)[C@]1(N[C@H](Cc3c[nH]c4ccccc34)[C@H]3C(=O)N(c4ccc(F)cc4)C(=O)[C@H]31)C(=O)N2
vNsp14-as2-109	ZINC000016001399	-9.6	0.282	489.88	ZINC	Cc1c2c(ccc1Cl)[C@]1(C(=O)N2)[C@@H]2C(=O)N(c3ccccc3C(F)(F)F)C(=O)[C@@H]2[C@@H]2CCCN21
vNsp14-as2-110	ZINC000017862766	-9.6	0.240	520.59	ZINC	O=C(Nc1ccc2ccccc2c1)c1cccc(N2C(=O)[C@H]3[C@@H](C2=O)C2c4ccccc4C3c3ccccc32)c1
vNsp14-as2-111	ZINC000019795177	-9.6	0.282	437.45	ZINC	O=C1c2ccccc2C2=C1C1(c3cccc4cccc(c34)C1=O)C1=C(N2)c2ccccc2C1=O
vNsp14-as2-112	ZINC000239338631	-9.6	0.282	454.52	ZINC	Cc1ccc(N2C(=O)[C@H]3[C@@H](C2=O)[C@@H]2C=C[C@H]3[C@@H]3C(=O)N(c4ccc(C)c(C)c4)C(=O)[C@H]32)cc1C
vNsp14-as2-113	ZINC000408674312	-9.6	0.267	476.57	ZINC	CC1CCN(C(=O)c2cccc(N3C(=O)[C@@H]4[C@@H](C3=O)C3c5ccccc5C4c4ccccc43)c2)CC1
vNsp14-as2-114	ZINC000408682268	-9.6	0.253	498.58	ZINC	Cc1cc(C)cc(NC(=O)c2ccccc2N2C(=O)[C@H]3[C@@H](C2=O)C2c4ccccc4C3c3ccccc32)c1
vNsp14-as2-115	ZINC000408682271	-9.6	0.253	498.58	ZINC	Cc1cc(C)cc(NC(=O)c2ccccc2N2C(=O)[C@H]3[C@@H](C2=O)C2c4ccccc4C3c3ccccc32)c1
vNsp14-as2-116	ZINC000408730082	-9.6	0.253	499.57	ZINC	Cc1ccc(N2C(=O)[C@H]3[C@H](C2=O)[C@@H]2C(=O)Oc4c5ccccc5ccc4C2=C[C@@H]3c2ccccc2)c(C)c1
vNsp14-as2-117	PV-001810158400	-9.5	0.306	440.33	REAL	Cc1nc(-c2cc(NC(=O)Cc3ccc4c(c3)OC(F)(F)O4)cc(C(F)(F)F)c2)n[nH]1
vNsp14-as2-118	PV-001843054767	-9.5	0.297	450.41	REAL	O=C1NCCOc2ccc(C(=O)N3CCC(O)(c4cccc(OC(F)(F)F)c4)CC3)cc21
vNsp14-as2-119	PV-001847242545	-9.5	0.306	436.40	REAL	O=C1Nc2c(F)cccc2[C@@H]1CC(=O)N1CCC(O)(c2ccccc2C(F)(F)F)CC1
vNsp14-as2-120	PV-001847826710	-9.5	0.352	374.30	REAL	O=C(Cc1ccc2c(c1)OC(F)(F)O2)Nc1cccc(-c2n[nH]c(=O)[nH]2)c1
vNsp14-as2-121	PV-001850638389	-9.5	0.317	430.31	REAL	Cc1nc2cc(C(=O)NNc3cc(C(F)(F)F)cc(C(F)(F)F)c3)ccc2c(=O)[nH]1
vNsp14-as2-122	PV-001869309257	-9.5	0.306	432.41	REAL	Cc1cc(=O)c(C(=O)N2CCC[C@H](c3nnc[nH]3)C2)nn1-c1ccccc1C(F)(F)F
vNsp14-as2-123	PV-001873296147	-9.5	0.297	454.55	REAL	Cc1ccc(S(=O)(=O)Nc2ccccc2C(=O)N2CCC(Cc3noc(C)n3)CC2)cc1
vNsp14-as2-124	PV-001935614880	-9.5	0.306	455.44	REAL	O=S(=O)(c1ccc(-n2cnnn2)cc1)N1CCC(F)(c2ccccc2C(F)(F)F)CC1
vNsp14-as2-125	PV-001935866190	-9.5	0.306	453.44	REAL	O=S(=O)(c1ccc(-n2cnnn2)cc1)N1CCC(O)(c2ccccc2C(F)(F)F)CC1
vNsp14-as2-126	PV-001942627617	-9.5	0.317	413.42	REAL	CC(=O)Nc1cc(NC(=O)N2CCC3(C=Cc4ccccc4O3)CC2)c(F)cc1F
vNsp14-as2-127	PV-001943086176	-9.5	0.352	367.50	REAL	Cc1nc(-c2cccc(NC(=O)N3CCCC4(CCCCC4)CC3)c2)n[nH]1
vNsp14-as2-128	PV-001947436141	-9.5	0.306	447.60	REAL	CC(=O)N1C[C@@H]2CCC[C@H](NC(=O)Nc3ccc(C)c(S(=O)(=O)C4CCCC4)c3)[C@H]2C1
vNsp14-as2-129	PV-001947992877	-9.5	0.297	450.44	REAL	O=C(Nc1ccc(F)c(N2CCCNC2=O)c1)NC1(c2ccc(C(F)(F)F)cc2)CCC1
vNsp14-as2-130	PV-001948673750	-9.5	0.297	456.33	REAL	Cc1nc(-c2cc(NC(=O)NNc3cccc4c3OC(F)(F)O4)cc(C(F)(F)F)c2)n[nH]1
vNsp14-as2-131	PV-001958246873	-9.5	0.297	432.53	REAL	Cc1cccc(C(NC(=O)N2CCC(n3cc(C(N)=O)nn3)CC2)c2cccc(C)c2)c1
vNsp14-as2-132	Z1000939152	-9.5	0.257	492.53	REAL	C[C@@]1(c2cccc(CNC(=O)c3c4c(nc5ccccc35)/C(=C/c3ccco3)CC4)c2)NC(=O)NC1=O
vNsp14-as2-133	Z1014376968	-9.5	0.279	454.53	REAL	O=C(Nc1ccc2[nH]c(=O)[nH]c2c1)[C@@H]1C[C@@H]2CCC[C@H]2N1C(=O)c1ccc2ccccc2c1
vNsp14-as2-134	Z1014397590	-9.5	0.271	474.56	REAL	O=C1NC(=O)C2(CCN(C(=O)[C@H]3C[C@H]4CCCC[C@H]4N3C(=O)c3ccc4ccccc4c3)CC2)N1
vNsp14-as2-135	Z1014464368	-9.5	0.271	494.98	REAL	C[C@@]1(c2cccc(NC(=O)[C@@H]3C[C@H]4CCCC[C@H]4N3C(=O)c3cccc(Cl)c3)c2)NC(=O)NC1=O
vNsp14-as2-136	Z1014465300	-9.5	0.271	494.98	REAL	C[C@@]1(c2ccc(NC(=O)[C@@H]3C[C@@H]4CCCC[C@H]4N3C(=O)c3cccc(Cl)c3)cc2)NC(=O)NC1=O
vNsp14-as2-137	Z1014534434	-9.5	0.271	498.60	REAL	O=C(NNC(=O)[C@H]1C[C@H]2CCCC[C@H]2N1C(=O)c1ccc2ccccc2c1)N[C@H]1CCS(=O)(=O)C1
vNsp14-as2-138	Z1018165564	-9.5	0.257	493.57	REAL	O=C(NNC(=O)c1cc(-c2ccccc2)nc2ccccc12)N[C@@H]1CCCN(C(=O)c2ccccc2)C1
vNsp14-as2-139	Z1022405136	-9.5	0.288	455.46	REAL	Cn1c(=O)oc2ccc(NC(=O)[C@@H]3C[C@@H]4CCCC[C@H]4N3C(=O)c3ccc(F)cc3F)cc21
vNsp14-as2-140	Z1023035970	-9.5	0.317	424.48	REAL	Cc1cc(C(=O)N2CCN(S(=O)(=O)c3c[nH]c4ncccc34)CC2)c2n[nH]cc2c1
vNsp14-as2-141	Z1027963874	-9.5	0.288	440.51	REAL	COc1ccc(NC(=O)N2Cc3ccccc3[C@@H](c3ccccc3)C2)cc1-n1nnnc1C
vNsp14-as2-142	Z1066862178	-9.5	0.297	429.52	REAL	Cc1nc(-c2cccc(NC(=O)[C@@H]3C[C@@H]4CCCC[C@H]4N3C(=O)c3ccccc3)c2)n[nH]1
vNsp14-as2-143	Z1083438676	-9.5	0.271	484.48	REAL	Cc1nnnn1-c1cc(NC(=O)[C@@H]2C[C@@H]3CCCC[C@H]3N2C(=O)c2ccc(F)cc2F)ccc1F
vNsp14-as2-144	Z1088492438	-9.5	0.271	479.56	REAL	Cc1nnnn1-c1cc(NC(=O)N2CCC[C@H](CN3CCN(c4ccccn4)CC3)C2)ccc1F
vNsp14-as2-145	Z1099516715	-9.5	0.352	367.37	REAL	Cc1nc(C(=O)N2CCC[C@H]2c2ccc3c(c2)OCO3)nn1-c1nnc[nH]1
vNsp14-as2-146	Z1158013629	-9.5	0.279	480.56	REAL	O=C(Nc1cccc(F)c1)C1CCN(C(=O)c2ccccc2CS(=O)(=O)c2ccccc2)CC1
vNsp14-as2-147	Z1158268108	-9.5	0.279	481.55	REAL	O=C(Nc1ccc(F)cc1)N1CCN(C(=O)c2ccccc2CS(=O)(=O)c2ccccc2)CC1
vNsp14-as2-148	Z1161372234	-9.5	0.271	494.57	REAL	O=C1COc2ccc(S(=O)(=O)N3CCN(C(=O)c4ccc5[nH]c6c(c5c4)CCCC6)CC3)cc2N1
vNsp14-as2-149	Z1171597456	-9.5	0.297	428.45	REAL	Cc1nnc2[nH]nc(NC(=O)CCCN3C(=O)c4ccec5cccc(c45)C3=O)c2c1C
vNsp14-as2-150	Z1335192709	-9.5	0.279	449.51	REAL	C[C@@]1(c2ccc(C(=O)N[C@@H](c3ccccc3)c3cccc4ccccc34)cc2)NC(=O)NC1=O
vNsp14-as2-151	Z1369051796	-9.5	0.288	441.54	REAL	Cc1cc(C)c2nc(C3CC3)cc(C(=O)N3CCN(c4cc(C)nc5ncnn45)CC3)c2c1
vNsp14-as2-152	Z1372080549	-9.5	0.317	399.45	REAL	Cc1cccc(C(NC(=O)c2ccc(-c3noc(=O)[nH]3)cc2)c2cccc(C)c2)c1
vNsp14-as2-153	Z1375391148	-9.5	0.317	402.50	REAL	Cc1cc(NC(=O)N2CCC[C@]3(CCCc4ccccc43)C2)ccc1-n1cnnn1
vNsp14-as2-154	Z1375407468	-9.5	0.317	406.46	REAL	O=C(Nc1cc(-n2cnnn2)ccc1F)N1CCC[C@]2(CCCc3ccccc32)C1
vNsp14-as2-155	Z1463880202	-9.5	0.288	446.55	REAL	Cc1ccc(C23C[C@@H]4C[C@@H](CC(C(=O)NNc5nc6c(cnn6C)c(=O)[nH]5)(C4)C2)C3)cc1C
vNsp14-as2-156	Z1463884357	-9.5	0.328	420.27	REAL	Cn1ncc2c(=O)[nH]c(NNC(=O)c3cc(C(F)(F)F)cc(C(F)(F)F)c3)nc21
vNsp14-as2-157	Z1559726405	-9.5	0.352	383.83	REAL	NC(=O)[C@H](NC(=O)CCc1cc2ccccc2[nH]c1=O)c1ccc(Cl)cc1
vNsp14-as2-158	Z1566175289	-9.5	0.306	414.55	REAL	CC(=O)Nc1cccc2c1CCN(Cc1cc3ccccc3nc1N1CCCCC1)C2
vNsp14-as2-159	Z1630064458	-9.5	0.297	432.46	REAL	Cc1nc(-c2cccc(NC(=O)N[C@H]3CCc4nnc(-c5ccc(F)cc5)n4C3)c2)n[nH]1
vNsp14-as2-160	Z1637424128	-9.5	0.288	446.55	REAL	Cc1noc(C2(C)CCN(C(=O)[C@H]3CCCN(C(=O)c4cccc5ccccc45)C3)CC2)n1
vNsp14-as2-161	Z1659783764	-9.5	0.297	431.45	REAL	C[C@]1(c2ccc3ccccc3c2)NC(=O)N(CC(=O)N2CCc3c(nc[nH]c3=O)C2)C1=O
vNsp14-as2-162	Z1670730219	-9.5	0.288	448.50	REAL	O=C(NCc1ccc2c(c1)C(=O)NCC2)Nc1cc(-c2nnc3n2CCCCC3)ccc1F
vNsp14-as2-163	Z1723437303	-9.5	0.264	499.96	REAL	Cn1c(=O)[nH]c2ncc(-c3cccc(C(=O)N4CCC(=C5C(=O)Nc6cc(Cl)ccc65)CC4)c3)cc21
vNsp14-as2-164	Z1736169293	-9.5	0.297	431.45	REAL	C[C@]1(c2ccc3ccccc3c2)NC(=O)N(CC(=O)N2CCc3n[nH]c(=O)cc3C2)C1=O
vNsp14-as2-165	Z1842764322	-9.5	0.288	438.45	REAL	O=C(NNc1nc2ccccn2n1)c1cc(-c2ccc3c(c2)OCCO3)nc2ccccc12
vNsp14-as2-166	Z1903679135	-9.5	0.297	438.53	REAL	Cc1ccc(NC(=O)N[C@H]2CCCN(c3ccn(C)n3)C2=O)cc1C(=O)N1CCCCC1
vNsp14-as2-167	Z1927716069	-9.5	0.297	430.50	REAL	C[C@H]1CN(C(=O)[C@H]2CC(=O)c3ccccc32)C[C@@H](C)N1C(=O)[C@@H]1CC(=O)c2ccccc21
vNsp14-as2-168	Z198296716	-9.5	0.306	412.41	REAL	O=C(NN1C(=O)NC(c2ccccc2)(c2ccccc2)C1=O)c1ccc2[nH]nnc2c1
vNsp14-as2-169	Z1984185460	-9.5	0.317	443.42	REAL	O=c1[nH]c2ccc(S(=O)(=O)N3CCC(F)(c4ccccc4C(F)(F)F)CC3)cc2[nH]1
vNsp14-as2-170	Z2004712129	-9.5	0.297	428.47	REAL	Cc1cc(F)cc2c1CN(C(=O)c1cccc(NC(=O)c3ccc4[nH]cnc4c3)c1)CC2
vNsp14-as2-171	Z203507364	-9.5	0.297	421.46	REAL	O=C(Nc1nccc(-c2ccccc2)n1)c1ccc2c(c1)C[C@H](c1ccccc1)OC2=O
vNsp14-as2-172	Z212568674	-9.5	0.271	474.52	REAL	Cc1cc(NC(=O)CN2CCN(C(=O)c3ccc4c(c3)C[C@H](c3ccccc3)OC4=O)CC2)no1
vNsp14-as2-173	Z2158538331	-9.5	0.319	370.38	REAL	Cc1nnc(-c2cccc(-c3noc(-c4nn[nH]c4-c4ccccc4)n3)c2)[nH]1
vNsp14-as2-174	Z2167355607	-9.5	0.288	446.49	REAL	O=C(Nc1cccc(-c2nnc3n2CCC3)c1)N1CCC(c2noc3cc(F)ccc23)CC1
vNsp14-as2-175	Z2167786968	-9.5	0.297	433.51	REAL	Cc1nc2ccc(NC(=O)N3CC4(CCCC4)c4cc5c(cc4[C@H]3C)OCCO5)cn2n1
vNsp14-as2-176	Z2232649657	-9.5	0.317	417.43	REAL	O=C1[C@@H]2[C@@H]3C[C@@H]4[C@H]2[C@@]2(C(=O)N5CCC(c6ccc(OC(F)(F)F)cc6)CC5)[C@@H]1[C@H]3[C@@H]42
vNsp14-as2-177	Z2233591493	-9.5	0.279	443.47	REAL	O=C(Nc1nc(-c2ccc3ccccc3n2)n[nH]1)c1cc(-c2cccnc2)nc2ccccc12
vNsp14-as2-178	Z2698983905	-9.5	0.328	385.47	REAL	O=C(CNc1nccc(N2Cc3ccccc3C2)n1)N1CCc2ccccc2C1
vNsp14-as2-179	Z27935410	-9.5	0.271	490.58	REAL	C[C@@]1(c2ccc3ccccc3c2)NC(=O)N(CC(=O)Nc2sc3c(c2C(N)=O)CCCCC3)C1=O
vNsp14-as2-180	Z2890523424	-9.5	0.264	478.55	REAL	O=C(C1[C@H]2[C@@H]3C=C[C@@H]([C@H]4C(=O)N(Cc5ccccc5)C(=O)[C@H]34)[C@H]12)N(O)Cc1cccc2ccccc12
vNsp14-as2-181	Z3094947607	-9.5	0.365	364.33	REAL	Cn1c(C2=NNC(=O)C2)nnc1N1CCc2ccc(C(F)(F)F)cc2C1
vNsp14-as2-182	Z31308110	-9.5	0.271	497.46	REAL	Cc1cc(=O)n2nc(N/C=C3/C(=O)N(c4cccc(C(F)(F)F)c4)C(=O)c4ccccc43)sc2n1
vNsp14-as2-183	Z3172360162	-9.5	0.328	393.45	REAL	Cn1nc(-c2nnc(N3CCC([C@H]4C(=O)Nc5ccccc54)CC3)n2C)c1O
vNsp14-as2-184	Z356684316	-9.5	0.279	486.52	REAL	Cc1c(C(=O)N2CCN(Cc3nc(N)c4ccccc4n3)CC2)sc2nc(C(F)(F)F)ccc12
vNsp14-as2-185	Z411014288	-9.5	0.306	410.48	REAL	Cc1c(NC(=O)N2Cc3ccccc3[C@@H](c3ccccc3)C2)cccc1-n1cnnn1
vNsp14-as2-186	Z433472214	-9.5	0.306	412.49	REAL	O=C(Nc1cccc(N2CCNC2=O)c1)N1Cc2ccccc2[C@@H](c2ccccc2)C1
vNsp14-as2-187	Z558578872	-9.5	0.279	463.58	REAL	C[C@@H]1c2cc3c(cc2C2(CCCC2)CN1C(=O)N[C@@H]1CCCN(c2nccn2)C1)OCCO3
vNsp14-as2-188	Z645863750	-9.5	0.306	421.46	REAL	CN1CCC2(CC1)C[C@@H](NC(=O)c1cnc3[nH]c(=O)[nH]c(=O)c3c1)c1ccccc1O2
vNsp14-as2-189	Z647258828	-9.5	0.288	459.39	REAL	O=C(c1cnc2[nH]c(=O)[nH]c(=O)c2c1)N1CCC[C@H](c2nnc3ccc(C(F)(F)F)cn23)C1
vNsp14-as2-190	Z730733422	-9.5	0.297	447.42	REAL	Cc1noc([C@H]2CCCN(C(=O)c3nn(-c4ccccc4C(F)(F)F)c(C)cc3=O)C2)n1
vNsp14-as2-191	Z759182976	-9.5	0.264	498.57	REAL	O=C(c1cc(-c2cccnc2)nc2ccccc12)N1CCN(S(=O)(=O)c2c[nH]c3ncccc23)CC1
vNsp14-as2-192	Z775747980	-9.5	0.328	387.48	REAL	CC(=O)Nc1cccc2c1CCN(C(=O)c1cc(C(C)C)nc3ccccc13)C2
vNsp14-as2-193	Z785210480	-9.5	0.279	470.56	REAL	O=S(=O)(c1c[nH]c2ncccc12)N1CCN(c2nc(-c3ccccc3)c3ccccc3n2)CC1
vNsp14-as2-194	Z813643410	-9.5	0.297	453.54	REAL	O=C(Nc1cc(N2CCCS2(=O)=O)ccc1F)N1CCC[C@H]1c1cccc2ccccc12
vNsp14-as2-195	Z822272382	-9.5	0.264	482.63	REAL	Cc1ccc(C23C[C@@H]4C[C@H](CC(C(=O)N5CCN(C(=O)c6ccc7[nH]cnc7c6)CC5)(C4)C2)C3)cc1
vNsp14-as2-196	Z979958324	-9.5	0.279	467.47	REAL	CN1C(=O)c2ccc(NC(=O)[C@@H]3C[C@@H]4CCCC[C@H]4N3C(=O)c3ccc(F)cc3F)cc2C1=O
vNsp14-as2-197	Z980035768	-9.5	0.264	496.51	REAL	CN1CC(=O)N(c2cccc(NC(=O)[C@@H]3C[C@@H]4CCCC[C@H]4N3C(=O)c3ccc(F)cc3F)c2)C1=O
vNsp14-as2-198	Z994279464	-9.5	0.288	474.55	REAL	C[C@@H]1c2cc3c(cc2C2(CCCC2)CN1C(=O)c1ccc(F)c(NS(C)(=O)=O)c1)OCCO3
vNsp14-as2-199	Z998027406	-9.5	0.328	392.41	REAL	O=C1COc2ccc(NC(=O)c3ccc4c(c3)[nH]c(=O)n4C3CCCC3)cc2N1
vNsp14-as2-200	ZINC000002191669	-9.5	0.279	449.52	ZINC	O=C1CCCC2=C1[C@H](c1ccc(OCc3ccccc3F)cc1)Nc1ccc3ccccc3c12

Supplementary Table 70. Virtual screening hits 101 to 200 of the screen against the active site of the ExoN domain of nsp14 (Screen ID: 37). Compounds were filtered so that hits had MW < 600 dalton, cLogP < 6, number of hydrogen bond acceptors < 11, and no reactive functional groups. A few compounds unsuitable for drug discovery were removed by visual inspection. The name of each compound consists of the initial letter 'v' for virtual hit, followed by the target protein name and the target site ('as' for active site, 2 for docking scenario 2). The score is the docking score given by QuickVina 2 in kcal/mol. The ligand efficiency (LE) is computed as LE = -score/#NonH, where #NonH is the number of heavy (i.e. non hydrogen) atoms.

Name	Catalog ID	Score	LE	MW	Library	SMILES
vNsp14-as1-1	ZINC000001862466	-14.2	0.406	455.468	ZINC	Cc1nc(-c2cc3c(ccc4ccccc43)oc2=O)cc2c1c(=O)oc1ccc3ccccc3c12
vNsp14-as1-2	ZINC000409336230	-14.2	0.374	499.565	ZINC	Cc1ccc(N2C(=O)[C@H]3[C@H](C2=O)[C@@H]2C(=O)Oc4ccc5ccccc5c4C2=C[C@H]3c2ccccc2)cc1C
vNsp14-as1-3	ZINC000409337259	-14.2	0.374	499.565	ZINC	Cc1ccc(N2C(=O)[C@H]3[C@H](C2=O)[C@@H]2C(=O)Oc4ccc5ccccc5c4C2=C[C@H]3c2ccccc2)c(C)c1
vNsp14-as1-4	ZINC000002832254	-14.1	0.403	473.507	ZINC	O=c1oc2ccc3ccccc3c2cc1-c1ccsc(-c2cc3c(ccc4ccccc43)oc2=O)n1
vNsp14-as1-5	ZINC000008792389	-14.1	0.392	476.51	ZINC	O=C(c1cc2c3ccccc3n3c2c(n1)c1ccccc1c3=O)N1CCN(c2ccccc2F)CC1
vNsp14-as1-6	ZINC000408732829	-14.1	0.381	485.538	ZINC	Cc1ccccc1N1C(=O)[C@H]2[C@H](C1=O)[C@@H]1C(=O)Oc3ccc4ccccc4c3C1=C[C@H]2c1ccccc1
vNsp14-as1-7	ZINC000008792352	-13.9	0.386	492.965	ZINC	O=C(c1cc2c3ccccc3n3c2c(n1)c1ccccc1c3=O)N1CCN(c2ccc(Cl)c2)CC1
vNsp14-as1-8	Z1452691933	-13.8	0.418	445.493	REAL	O=C(NC[C@H]1[C@@H]2Cc3ccccc3[C@H]12)NNC(=O)c1ccccc1OCc1ccc(F)cc1
vNsp14-as1-9	Z318134014	-13.8	0.394	470.499	REAL	Cc1c(-c2ccccc2)oc2c(C(=O)N3CCN(C(=O)c4ccc(F)cc4)CC3)cccc2c1=O
vNsp14-as1-10	Z46127396	-13.8	0.406	448.477	REAL	CN1C(=O)/C(=C\c2cccc(/C=C3\C(=O)N(C)C(=O)c4ccccc43)c2)ccccc2C1=O
vNsp14-as1-11	ZINC000408978119	-13.8	0.363	495.493	ZINC	O=C(Oc1ccc2nc3c4ccccc4c4ccccc4c3nc2c1)c1ccc(N2C(=O)C=CC2=O)cc1
vNsp14-as1-12	ZINC000001641985	-13.7	0.381	495.929	ZINC	O=C1C(/C=C/c2ccc(Cl)cc2)=NN[C@@H]2N1N=C1N=C(O)C3(NN12)c1ccccc1-c1ccccc13
vNsp14-as1-13	ZINC000005955034	-13.7	0.381	495.929	ZINC	O=C1NC2=NN3C(=O)C(/C=C\c4ccc(Cl)cc4)=NN[C@H]3N2NC12c1ccccc1-c1ccccc12
vNsp14-as1-14	Z1022496460	-13.6	0.368	495.621	REAL	O=C(NCC(=O)N1CCc2ccccc2C1)[C@@H]1C[C@@H]2CCC[C@@H]2N1C(=O)c1ccc2ccccc2c1
vNsp14-as1-15	Z804195986	-13.6	0.389	493.435	REAL	O=C([C@H]1CC(=O)N(c2cc(F)cc(F)c2)C1)N1CCC[C@@H](c2nnc3ccc(C(F)(F)F)cn23)C1
vNsp14-as1-16	ZINC000002154274	-13.6	0.4	444.445	ZINC	O=c1oc(-c2cccc(-n3c(=O)c4ccccc4c4ccccc4c3=O)c2)nc2ccccc21
vNsp14-as1-17	ZINC000008792406	-13.6	0.378	476.51	ZINC	O=C(c1cc2c3ccccc3n3c2c(n1)c1ccccc1c3=O)N1CCN(c2ccc(F)cc2)CC1
vNsp14-as1-18	ZINC000012847889	-13.6	0.412	436.51	ZINC	O=C(CN1C(=O)N[C@@]2(CCCCc3ccccc32)C1=O)c1ccc2c(c1)-c1ccccc1C2
vNsp14-as1-19	ZINC000100505727	-13.6	0.368	488.542	ZINC	O=C1[C@@H]2[C@H]3C=C[C@@H](C3)[C@@H]2C(=O)N1c1ccc2c(c1)-c1cc(N3C(=O)[C@H]4[C@H]5C=C[C@H](C5)[C@@H]4C3=O)ccc1C2
vNsp14-as1-20	ZINC000104480048	-13.6	0.378	490.945	ZINC	O=C(NC1=CC=C[C@H]2C(=O)c3ccccc3C(=O)[C@H]12)c1cc(-c2ccccc2Cl)nc2ccccc21
vNsp14-as1-21	Z1081123722	-13.5	0.466	380.406	REAL	Cc1nonc1NC(=O)c1cc(-c2cccc3ccccc23)nc2ccccc12
vNsp14-as1-22	Z25741554	-13.5	0.386	465.464	REAL	O=C(CN1C(=O)N[C@]2(CCc3ccccc32)C1=O)Nc1ccc2c(c1)C(=O)c1ccccc1C2=O
vNsp14-as1-23	Z26978198	-13.5	0.397	452.509	REAL	Cc1c(-c2ccccc2)oc2c(C(=O)N3CCN(C(=O)c4ccccc4)CC3)cccc2c1=O
vNsp14-as1-24	Z787516708	-13.5	0.365	495.581	REAL	O=C(c1ccc2[nH]cnc2c1)N1CCN(C(=O)[C@@H]2CCCN(C(=O)c3cccc4ccccc34)C2)CC1
vNsp14-as1-25	Z996489826	-13.5	0.375	482.582	REAL	Cn1c(=O)n(C)c2cc(NC(=O)[C@@H]3C[C@@H]4CCCC[C@@H]4N3C(=O)c3cc4ccccc4c3)ccc21
vNsp14-as1-26	ZINC000003206809	-13.5	0.409	428.446	ZINC	O=C(c1ccccc1)c1ccc(C(=O)n2nc3c4c2cccc4C(=O)c2ccccc2-3)cc1
vNsp14-as1-27	ZINC000008445573	-13.5	0.375	473.483	ZINC	O=C1c2ccccc2C(=O)C12O[C@@H](c1ccccc1)[C@H]1C(=O)N(c3cccc4ccccc43)C(=O)[C@H]12
vNsp14-as1-28	ZINC000014540821	-13.5	0.375	479.578	ZINC	CC(=O)c1cccc(-c2cc3c(n(C)c2=O)CCN(C(=O)c2ccc4[nH]c5c(c4c2)CCCC5)C3)c1
vNsp14-as1-29	Z1014397762	-13.4	0.383	469.583	REAL	O=C(N[C@H]1CCCc2[nH]c(=O)ccc21)[C@H]1C[C@@H]2CCCC[C@@H]2N1C(=O)c1ccc2ccccc2c1
vNsp14-as1-30	Z1014421792	-13.4	0.362	496.609	REAL	O=C(c1ccccn1)N1CCN(C(=O)[C@H]2C[C@@H]3CCCC[C@H]3N2C(=O)c2cc3ccccc3c2)CC1
vNsp14-as1-31	Z1014525870	-13.4	0.362	493.609	REAL	Cc1nccn1-c1ncccc1CNC(=O)[C@@H]1C[C@@H]2CCCC[C@@H]2N1C(=O)c1ccc2ccccc2c1
vNsp14-as1-32	Z119679586	-13.4	0.372	479.535	REAL	O=C([C@@H]1CN(C(=O)c2cc(-c3cccc3)nc3ccccc23)c2ccccc2O1)N1CCOCC1
vNsp14-as1-33	Z1544359640	-13.4	0.432	410.476	REAL	NC(=O)N[C@@H]1CCN(C(=O)c2cc(-c3cccc4ccccc34)nc3ccccc23)C1
vNsp14-as1-34	Z1643756379	-13.4	0.406	441.529	REAL	Cc1c(NC(=O)N2CC=C(c3cccc4ccccc34)C2)cccc1C(=O)N1CCOCC1
vNsp14-as1-35	Z50157029	-13.4	0.406	453.477	REAL	Cc1cc(-c2nnc(-c3ccc4c(c3)S(=O)(=O)c3ccccc3C4=O)o2)c2ccccc2n1
vNsp14-as1-36	Z973902086	-13.4	0.406	457.513	REAL	Cc1n[nH]c(NC(=O)c2ccc(NC3=NS(=O)(=O)c4ccccc43)cc2)c1-c1ccccc1
vNsp14-as1-37	Z996016390	-13.4	0.372	480.57	REAL	Cc1ccc(NC(=O)[C@@H]2C[C@H]3CCCC[C@@H]3N2C(=O)c2ccc3ccccc3c2)cc1-n1cnnn1
vNsp14-as1-38	ZINC000002776613	-13.4	0.394	458.442	ZINC	O=C(c1cnn2c1nc(-c1cccc3ccccc31)cc2C(F)(F)F)N1CCc2ccccc21
vNsp14-as1-39	ZINC000004551929	-13.4	0.312	556.632	ZINC	c1ccc(-c2cc(-c3cccc3)n3nc(Cc4nc5nc(-c6ccccc6)cc(-c6ccccc6)n5n4)nc3n2)cc1
vNsp14-as1-40	ZINC000014814843	-13.4	0.383	462.508	ZINC	Cc1c(=O)c2cccc(C(=O)N3CCN(C)c4nc5ccccc5nc43)c2oc1-c1ccccc1
vNsp14-as1-41	ZINC000247726752	-13.4	0.372	478.569	ZINC	O=C(Nc1cccc2ccccc21)[C@@H]1CCCN(Cc2nc3ccccc3n2-c2ccc(F)cc2)C1
vNsp14-as1-42	Z1014668582	-13.3	0.369	483.566	REAL	O=C(NNC(=O)[C@H]1C[C@H]2CCCC[C@H]2N1C(=O)c1ccc2ccccc2c1)[C@@H]1Cc2ccccc2O1
vNsp14-as1-43	Z1312691764	-13.3	0.403	441.49	REAL	CCn1c2ccccc2c2cc(CN(C)C(=O)c3cc(C)c4c(=O)[nH]c(O)nc4n3)ccc21
vNsp14-as1-44	Z146971088	-13.3	0.38	459.504	REAL	O=C(NN1C(=O)NC(c2ccccc2)(c2ccccc2)C1=O)c1ccc2c(c1)-c1ccccc1C2
vNsp14-as1-45	Z1538962334	-13.3	0.429	408.504	REAL	O=C(c1ccc2c(c1)-c1ccccc1C2)N1CCN(Cc2nc3ccccc3[nH]2)CC1
vNsp14-as1-46	Z1552767584	-13.3	0.429	420.418	REAL	Cc1ccccC(=O)Nc2ccc3[nH]nc(NC(=O)c4ccccC(C)c4F)c3c2)c1F
vNsp14-as1-47	Z2154388204	-13.3	0.429	418.402	REAL	Cc1ccc(N2C(=O)N[C@H](c3ccc4ccccc4c3)C2=O)nn1-c1ccc(F)cc1F
vNsp14-as1-48	Z364958852	-13.3	0.38	483.591	REAL	Cc1cnc2c(S(=O)(=O)N3CCN(C(=O)c4ccc5c(c4)-c4ccccc4C5)CC3)ccccc2c1
vNsp14-as1-49	Z415220808	-13.3	0.38	481.575	REAL	O=C(c1ccc2ccccc2c2cccnc12)N1CCN(S(=O)(=O)c2ccc3ccccc3c2)CC1
vNsp14-as1-50	Z920794266	-13.3	0.391	475.568	REAL	O=C1CN(S(=O)(=O)c2cccc(C(=O)N3CC=C(c4cccc5ccccc45)CC3)c2)CCN1
vNsp14-as1-51	Z973899924	-13.3	0.391	472.568	REAL	Cc1n[nH]c(NC(=O)c2cccc(S(=O)(=O)N3CCCc4ccccc43)c2)c1-c1ccccc1
vNsp14-as1-52	Z995695182	-13.3	0.359	494.593	REAL	CN(Cc1nc2ccccc2c(=O)[nH]1)C(=O)[C@H]1C[C@@H]2CCCC[C@H]2N1C(=O)c1ccc2ccccc2c1
vNsp14-as1-53	Z996175024	-13.3	0.369	479.582	REAL	O=C(Nc1ncn(Cc2ccccc2)n1)[C@@H]1C[C@@H]2CCCC[C@@H]2N1C(=O)c1ccc2ccccc2c1
vNsp14-as1-54	ZINC000017194074	-13.3	0.38	466.452	ZINC	Cc1c(=O)c2cccc(C(=O)NNC(=O)c3n[nH]c(=O)c4ccccc43)c2oc1-c1ccccc1
vNsp14-as1-55	ZINC000027496395	-13.3	0.403	429.43	ZINC	O=C(Nc1ccnc2c1C(=O)c1ccccc1C2=O)c1ccnc2c1C(=O)c1ccccc1-2
vNsp14-as1-56	ZINC000239125204	-13.3	0.38	464.563	ZINC	Cc1cc(C)cc(NC(=O)c2cccc(N3C(=O)[C@@H]4[C@@H]5C[C@@H]([C@H]4C3=O)[C@@H](c3ccccc3)C5)c2)c1
vNsp14-as1-57	PV-001962762214	-13.2	0.4	448.497	REAL	C[C@@H](c1ccccc1F)N1CCC[C@H](NC(=O)NNC(=O)c2cccc3ccccc23)C1=O
vNsp14-as1-58	Z1000676060	-13.2	0.388	480.587	REAL	O=C(N[C@@H]1CCCN(C(=O)c2ccccc2)C1)C1CCN(C2=NS(=O)(=O)c3ccccc32)CC1
vNsp14-as1-59	Z1003487644	-13.2	0.388	472.568	REAL	Cn1c2ccccc2c2cc(S(=O)(=O)N3CCN(C(=O)c4cc5ccccc5[nH]4)CC3)ccc21
vNsp14-as1-60	Z1015592432	-13.2	0.357	487.561	REAL	NC(=O)c1cccnc1N1CCN(C(=O)c2cc(-c3cccc4ccccc34)nc3ccccc23)CC1
vNsp14-as1-61	Z1083439990	-13.2	0.357	498.56	REAL	Cc1nnnn1-c1cc(NC(=O)[C@@H]2C[C@@H]3CCCC[C@@H]3N2C(=O)c2ccc3ccccc3c2)ccc1F
vNsp14-as1-62	Z112684214	-13.2	0.367	482.491	REAL	Cc1c(-c2ccccc2)oc2c(C(=O)O[C@@H](C)C(=O)N3CC(=O)Nc4ccccc43)cccc2c1=O
vNsp14-as1-63	Z1174754345	-13.2	0.412	430.467	REAL	O=C([C@@H]1CC(=O)N(c2ccc3c(c2)Cc2ccccc2-3)C1)N1CCO[C@H](c2nnn[nH]2)C1
vNsp14-as1-64	Z1175750411	-13.2	0.388	446.513	REAL	O=C(NNc1nnc(-c2ccccc2)n1-c1ccccc1)c1c2c(nc3ccccc13)CCC2
vNsp14-as1-65	Z119680042	-13.2	0.357	497.525	REAL	O=C([C@@H]1CN(C(=O)c2ccc(-c3ccc(F)cc3)nc3ccccc23)c2ccccc2O1)N1CCOCC1
vNsp14-as1-66	Z1264832329	-13.2	0.4	441.529	REAL	C[C@H]1CN(C(=O)[C@H]2CCCN(C(=O)c3cccc4ccccc34)C2)c2ccccc2NC1=O
vNsp14-as1-67	Z1371503597	-13.2	0.4	435.526	REAL	O=C1CC2(CCN(C(=O)c3ccc(-c4cccc5ccccc45)nc4ccccc34)CC2)CN1
vNsp14-as1-68	Z1371931188	-13.2	0.412	422.487	REAL	O=C(c1cc(-c2cccc3ccccc23)nc2ccccc12)N1CCN2C(=O)NC[C@H]2C1
vNsp14-as1-69	Z1435566693	-13.2	0.412	423.471	REAL	O=C(c1cc(-c2cccc3ccccc23)nc2ccccc12)N1CCN2C(=O)OC[C@@H]2C1
vNsp14-as1-70	Z1524008212	-13.2	0.426	407.432	REAL	NC(=O)c1cc(NC(=O)c2cc(-c3cccc4ccccc34)nc3ccccc23)[nH]n1
vNsp14-as1-71	Z1663786498	-13.2	0.426	412.456	REAL	Cc1cc(-c2nnc(C3CCN(c4ccc5nncn5n4)CC3)o2)c2ccccc2n1
vNsp14-as1-72	Z2006751433	-13.2	0.412	431.582	REAL	Cc1ccc2[nH]c3c(c2c1)C[C@@H](NC(=O)N1CCC[C@H](c2nc4n2CCCC4)C1)CC3
vNsp14-as1-73	Z225725692	-13.2	0.388	450.497	REAL	O=C1NC(=O)C2(CCN(C(=O)c3cc(-c4cccc5ccccc45)nc4ccccc34)CC2)N1
vNsp14-as1-74	Z260722184	-13.2	0.357	492.53	REAL	Cc1c(-c2ccccc2)oc2c(C(=O)OCC(=O)N3CCc4[nH]c5ccccc5c4C3)cccc2c1=O
vNsp14-as1-75	Z286720458	-13.2	0.367	477.531	REAL	Cc1nc2ccccc2c2c(NC(=O)C3CCN(c4ccc5nnnn5n4)CC3)c3ccccc3n12
vNsp14-as1-76	Z29578336	-13.2	0.357	485.502	REAL	O=C(NNC(=O)c1n[nH]c(=O)c2ccccc12)c1cc(-c2cccc3ccccc23)nc2ccccc12
vNsp14-as1-77	Z324699944	-13.2	0.357	499.54	REAL	C[C@@H](C(=O)Nc1ccnc2c1C(=O)c1ccccc1C2=O)N1CCCN(C(=O)c2cccc(F)c2)CC1
vNsp14-as1-78	Z335395752	-13.2	0.388	453.497	REAL	Cc1c(-c2ccccc2)oc2c(C(=O)N3CCN(C(=O)c4ccccn4)CC3)cccc2c1=O
vNsp14-as1-79	Z357611466	-13.2	0.357	492.577	REAL	C[C@@H]1C/C(=C\c2ccco2)c2nc3ccccc3c(C(=O)N3CCN(C(=O)c4ccccn4)CC3)c2C1
vNsp14-as1-80	Z407583046	-13.2	0.367	498.483	REAL	O=C(c1nn(-c2ccccc2F)c2c1CCC2)N1CCC[C@@H](c2nnc3ccc(C(F)(F)F)cn23)C1
vNsp14-as1-81	Z62211931	-13.2	0.4	476.58	REAL	O=C(Nc1ncc2c(ccc3ccccc32)s1)C1CCN(C2=NS(=O)(=O)c3ccccc32)CC1
vNsp14-as1-82	Z70913492	-13.2	0.357	494.593	REAL	Cc1nc2ccccc2c(=O)n1-c1ccc(C(=O)N[C@@H]2CC3(CCN(C)CC3)Oc3ccccc32)cc1
vNsp14-as1-83	Z759183910	-13.2	0.4	458.541	REAL	O=C(c1ccc2c(c1)-c1ccccc1C2)N1CCN(S(=O)(=O)c2c[nH]c3ncccc23)CC1
vNsp14-as1-84	Z804767774	-13.2	0.377	467.524	REAL	CNC(=O)[C@@H]1CN(C(=O)[C@@H]2CC(=O)N(c3ccc4c(c3)Cc3ccccc3-4)C2)c2ccccc2O1
vNsp14-as1-85	Z810428734	-13.2	0.367	481.55	REAL	Cc1cccc(NC(=O)[C@@H]2CCCN(C(=O)c3cccc4c(=O)c(C)c(-c5ccccc5)oc34)C2)n1
vNsp14-as1-86	Z856250978	-13.2	0.367	494.52	REAL	Cc1cccc1-n1nc(C(=O)N2CCC[C@@H](c3nnc4ccc(C(F)(F)F)cn34)C2)c2c1CCC2
vNsp14-as1-87	Z976477790	-13.2	0.44	401.425	REAL	Cn1c(=O)[nH]c(=O)c2[nH]c(CCC(=O)N3Cc4ccccc4-c4ccccc43)nc21
vNsp14-as1-88	Z995722280	-13.2	0.367	481.55	REAL	CN1C(=O)c2ccc(NC(=O)[C@@H]3C[C@@H]4CCCC[C@@H]4N3C(=O)c3cc4ccccc4c3)cc2C1=O
vNsp14-as1-89	ZINC000001789604	-13.2	0.338	532.666	ZINC	O=c1[nH]c(CSc2nc3ccccc3c(=O)n2-c2ccccc2)nc2c1C1(CCCCC1)Cc1ccccc1-2
vNsp14-as1-90	ZINC000003037864	-13.2	0.347	512.393	ZINC	O=C1c2ccc(-c3ccc4c(c3)C(=O)N(c3c[nH]c(=O)[nH]c3=O)C4=O)cc2C(=O)N1c1c[nH]c(=O)[nH]c1=O
vNsp14-as1-91	ZINC000003878239	-13.2	0.367	499.542	ZINC	CC1(C)Cc2oc3ccc(NS(=O)(=O)c4ccccc5c4C(=O)c4ccccc4C5=O)cc3c2C(=O)C1
vNsp14-as1-92	ZINC000012436788	-13.2	0.4	431.446	ZINC	O=C(Nc1cccc2c1C(=O)[C@@H]1C=CC=C[C@H]1C2=O)c1cccc2c1C(=O)c1cccc1-2
vNsp14-as1-93	ZINC000018117591	-13.2	0.4	431.446	ZINC	O=C(Nc1cccc2c1C(=O)[C@H]1C=CC=C[C@@H]1C2=O)c1cccc2c1C(=O)c1cccc1-2
vNsp14-as1-94	ZINC000035375709	-13.2	0.357	490.561	ZINC	Cc1ccc(C)cc(N2C(=O)[C@@H]3[C@H](C2=O)[C@@H](Cc2c[nH]c4ccccc24)N[C@@]32C(=O)Nc3ccccc32)c1
vNsp14-as1-95	ZINC000100737710	-13.2	0.4	431.446	ZINC	O=C(Nc1cccc2c1C(=O)[C@H]1C=CC=C[C@H]1C2=O)c1cccc2c1C(=O)c1cccc1-2
vNsp14-as1-96	ZINC000408732827	-13.2	0.357	485.538	ZINC	Cc1ccccc1N1C(=O)[C@@H]2[C@H](C1=O)[C@@H]1C(=O)Oc3ccc4ccccc4c3C1=C[C@H]2c1ccccc1
vNsp14-as1-97	PV-001844864463	-13.1	0.409	430.506	REAL	Cc1cc(C(=O)NNC(=O)[C@H]2CCC(=O)N(c3ccc(C)c(C)c3)C2)c2ccccc2n1
vNsp14-as1-98	PV-001878938316	-13.1	0.423	412.496	REAL	Cc1cccc(-c2c(C)n[nH]c2NC(=O)c2ccc(CNc3ccnc(C)n3)c2)c1
vNsp14-as1-99	Z1010365850	-13.1	0.354	495.577	REAL	Cc1cccn2c(=O)cc(COC(=O)[C@@H]3C[C@@H]4CCCC[C@@H]4N3C(=O)c3cc4ccccc4c3)nc12
vNsp14-as1-100	Z1014376968	-13.1	0.385	454.528	REAL	O=C(Nc1ccc2[nH]c(=O)[nH]c2c1)[C@@H]1C[C@H]2CCCC[C@@H]2N1C(=O)c1ccc2ccccc2c1

Supplementary Table 71. Top 100 virtual hits of the screen against the active site of the N7-MTase domain of nsp14 (Screen ID: 38). Compounds were filtered so that hits had MW < 600 dalton, cLogP < 6, number of hydrogen bond acceptors < 11, and no reactive functional groups. A few compounds unsuitable for drug discovery were removed by visual inspection. The name of each compound consists of the initial letter 'v' for virtual hit, followed by the target protein name and the target site ('as' for active site, 1 for docking scenario 1). The score is the docking score given by QuickVina 2 in kcal/mol. The ligand efficiency (LE) is computed as LE = -score/#NonH, where #NonH is the number of heavy (i.e. non hydrogen) atoms.

Name	Catalog ID	Score	LE	MW	Library	SMILES
vNsp14-as1-101	Z1014392644	-13.1	0.385	456.54	REAL	NC(=O)Nc1cccc(NC(=O)[C@@H]2C[C@@H]3CCCC[C@@H]3N2C(=O)c2ccc3ccccc3c2)c1
vNsp14-as1-102	Z1024046328	-13.1	0.385	453.54	REAL	O=C1Nc2ccccc2[C@H]1C1CCN(C(=O)[C@H]2CC(=O)N(c3cccc4ccccc34)C2)CC1
vNsp14-as1-103	Z1088277222	-13.1	0.423	421.45	REAL	O=C(Nc1ccc2c3c(cccc13)CC2)N1CCN(C(=O)c2c(F)cccc2F)CC1
vNsp14-as1-104	Z1116941372	-13.1	0.354	495.58	REAL	Cc1cccc2c(=O)[nH]c(COC(=O)[C@@H]3C[C@@H]4CCCC[C@@H]4N3C(=O)c3ccc4ccccc4c3)nc12
vNsp14-as1-105	Z1137562871	-13.1	0.354	497.57	REAL	O=C(NCc1nc(-c2ccc(F)cc2)n[nH]1)[C@H]1C[C@@H]2CCCC[C@H]2N1C(=O)c1ccc2ccccc2c1
vNsp14-as1-106	Z1161372620	-13.1	0.374	491.57	REAL	O=C1COc2ccc(S(=O)(=O)N3CCN(C(=O)[C@H]4C[C@@H]4c4ccc5ccccc45)CC3)cc2N1
vNsp14-as1-107	Z1229898813	-13.1	0.409	445.54	REAL	Cc1cnc(N2CCN(C(=O)c3ccc4c(=O)c(C)c(-c5ccccc5)oc34)CC2)s1
vNsp14-as1-108	Z131309068	-13.1	0.397	459.57	REAL	O=C(Nc1ccc(S(=O)(=O)/N=C2/CCCCCN2)cc1)c1ccc2c(c1)-c1ccccc1C2
vNsp14-as1-109	Z131405014	-13.1	0.364	482.58	REAL	O=C(c1cccc2ccccc12)N1CCC(C(=O)N2CCC(n3c(=O)[nH]c4ccccc43)CC2)CC1
vNsp14-as1-110	Z1335516349	-13.1	0.423	438.51	REAL	CN1C(=O)CN(C(=O)C2CCN(C3=NS(=O)(=O)c4ccccc43)CC2)c2ccccc21
vNsp14-as1-111	Z1460191452	-13.1	0.468	370.42	REAL	C/C(=N\Nc1nc2c(cnn2C)c(=O)[nH]1)c1ccc2c(c1)Cc1ccccc1-2
vNsp14-as1-112	Z1548046997	-13.1	0.397	447.47	REAL	CN1C(=O)NC2(CCN(C(=O)c3ccc(-n4ncce4-c4ccc(F)cc4)cc3)CC2)C1=O
vNsp14-as1-113	Z1557772186	-13.1	0.397	439.56	REAL	O=C(NC[C@@H]1CN(C(=O)c2ccccc2)[C@@H]2CCN1C2)[C@H]1C[C@@H]1c1ccccc2ccccc12
vNsp14-as1-114	Z1744193725	-13.1	0.452	382.46	REAL	O=C([C@@H]1C[C@H]1c1ccc2ccccc12)N1CC[C@@]2(C1)C(=O)Nc1ccccc12
vNsp14-as1-115	Z1785158108	-13.1	0.409	421.46	REAL	O=C(c1cc(-c2cccc3ccccc23)nc2ccccc12)N1CCn2c(n[nH]c2=O)C1
vNsp14-as1-116	Z1888636115	-13.1	0.423	411.46	REAL	O=C(Nc1cccc(N2CCCCC2=O)c1)c1ccc2c(=O)c3ccccc3[nH]c12
vNsp14-as1-117	Z1891946723	-13.1	0.409	423.47	REAL	O=C(c1cccc(N2C(=O)N[C@]3(CCc4ccccc43)C2=O)c1)N1CCc2ccccc21
vNsp14-as1-118	Z2001438856	-13.1	0.397	434.49	REAL	O=C1c2ccccc2C(=O)N1c1cccc(C(=O)N2[C@H]3C=C(c4ccccc4)C[C@@H]2CC3)c1
vNsp14-as1-119	Z220541284	-13.1	0.397	438.53	REAL	O=C([C@@H]1CC(=O)N(c2ccc3ccccc23)C1)N1CCC[C@H](c2nc3ccccc3[nH]2)C1
vNsp14-as1-120	Z226646538	-13.1	0.385	451.53	REAL	Cc1c(C(=O)N2CCN(Cc3nc(N)c4ccccc4n3)CC2)oc2c1ccc1ccccc12
vNsp14-as1-121	Z272395518	-13.1	0.374	495.98	REAL	O=C(Nc1ccc(F)c(-c2nnc3n2CCCCC3)c1)[C@@H]1CCCN(C(=O)c2ccc(Cl)cc2)C1
vNsp14-as1-122	Z2902834428	-13.1	0.385	468.54	REAL	O=S(=O)(c1ccccc(-c2nc(-c3ncccc4ccccc34)no2)c1)N1CCc2ccccc2C1
vNsp14-as1-123	Z338860050	-13.1	0.364	497.52	REAL	O=C([C@@H]1CC(=O)N(c2ccc3c(c2)CCC3)C1)N1CCC[C@H](c2nnc3ccc(C(F)(F)F)cn23)C1
vNsp14-as1-124	Z393677666	-13.1	0.385	454.49	REAL	O=C(Nc1ccccc1-n1ncc2c(=O)[nH]cnc21)[C@@H]1CC(=O)N(c2ccc3c(c2)CCC3)C1
vNsp14-as1-125	Z730538216	-13.1	0.397	440.55	REAL	O=C(Cc1c[nH]c2ccccc12)N1CCN(C(=O)c2cccc3c4c([nH]c23)CCCC4)CC1
vNsp14-as1-126	Z804069372	-13.1	0.364	477.57	REAL	O=C([C@@H]1CC(=O)N(c2ccc3c(c2)Cc2ccccc2-3)C1)N1CCC(c2nnc3ccccn23)CC1
vNsp14-as1-127	Z806248884	-13.1	0.374	467.57	REAL	O=C([C@H]1CC(=O)N(c2ccc3c(c2)Cc2ccccc2-3)C1)N1CCC[C@H](c2nnc3n2CCC3)C1
vNsp14-as1-128	Z910836024	-13.1	0.385	450.54	REAL	O=C(c1cc(-c2cccc3ccccc23)nc2ccccc12)N1CCC[C@@H](N2CCNC2=O)C1
vNsp14-as1-129	Z941605640	-13.1	0.354	489.53	REAL	O=C(N[C@@H](Cc1c[nH]c2ccccc12)C(=O)Nc1ccc2[nH]c(=O)[nH]c2c1)c1ccc2ccccc2c1
vNsp14-as1-130	Z955272326	-13.1	0.374	461.52	REAL	O=C(CCCc1ccc2c(c1)-c1ccccc1C2)Nc1ccccc1-n1ncc2c(=O)[nH]cnc21
vNsp14-as1-131	Z973899764	-13.1	0.385	472.57	REAL	Cc1n[nH]c(NC(=O)c2cccc(S(=O)(=O)N3CCc4ccccc4C3)c2)c1-c1ccccc1
vNsp14-as1-132	Z995643820	-13.1	0.409	433.55	REAL	NC(=O)C1CCN(C(=O)[C@H]2C[C@@H]3CCCC[C@H]3N2C(=O)c2ccc3ccccc3c2)CC1
vNsp14-as1-133	Z995656030	-13.1	0.354	499.57	REAL	O=C(NNC(=O)[C@H]1C[C@@H]2CCCC[C@@H]2N1C(=O)c1ccc2ccccc2c1)[C@H]1COc2ccccc2O1
vNsp14-as1-134	Z995754372	-13.1	0.364	481.59	REAL	O=C1Nc2ccccc2[C@@H]1CCNC(=O)[C@@H]1C[C@@H]2CCCC[C@@H]2N1C(=O)c1ccc2ccccc2c1
vNsp14-as1-135	ZINC000001641983	-13.1	0.364	495.93	ZINC	O=C1C(/C=C/c2ccc(Cl)cc2)=NN[C@H]2N1N=C1N=C(O)C3(NN12)c1ccccc1-c1ccccc13
vNsp14-as1-136	ZINC000005955032	-13.1	0.364	495.93	ZINC	O=C1NC2=NN3C(=O)C(/C=C\c4ccc(Cl)cc4)=NN[C@@H]3N2NC12c1ccccc1-c1ccccc12
vNsp14-as1-137	ZINC000008832384	-13.1	0.423	470.32	ZINC	O=C(Nc1cccc(-c2cc3ccccc3oc2=O)c1)c1ccc2c(Br)cccc12
vNsp14-as1-138	ZINC000008877857	-13.1	0.385	447.45	ZINC	O=C(NCc1ccc2c(c1)OCO2)c1cc2c3ccccc3n3c2c(n1)c1ccccc1c3=O
vNsp14-as1-139	ZINC000009015957	-13.1	0.364	495.93	ZINC	O=C([C@@H]1[C@H]2C(=O)N(c3cccc(Cl)c3)C(=O)[C@@H]2[C@@H]2C=Cc3ccccc3N21)n1nnc2ccccc21
vNsp14-as1-140	ZINC000012360361	-13.1	0.374	458.52	ZINC	O=C(Cc1ccc2ccccc21)NN1C(=O)[C@H]2[C@@H](C1=O)C1c3ccccc3C2c2ccccc21
vNsp14-as1-141	ZINC000013164696	-13.1	0.354	496.52	ZINC	O=C(c1nn(-c2ccccc2)c(=O)c2ccccc21)N1CCN(C(=O)[C@@H]2COc3ccccc3O2)CC1
vNsp14-as1-142	ZINC000014981104	-13.1	0.385	446.55	ZINC	Cn1c2ccccc2c2cc(C(=O)N3CCC(c4ccnc(-c5ccccc5)n4)CC3)ccc21
vNsp14-as1-143	ZINC000016037261	-13.1	0.364	495.93	ZINC	O=C([C@H]1[C@H]2C(=O)N(c3cccc(Cl)c3)C(=O)[C@H]2[C@@H]2C=Cc3ccccc3N12)n1nnc2ccccc21
vNsp14-as1-144	ZINC000019376520	-13.1	0.397	441.47	ZINC	O=C(c1ccc2c(cccc2F)[nH]1)N1CCC(c2nnc(-c3ncccc4ccccc43)o2)CC1
vNsp14-as1-145	ZINC000026780145	-13.1	0.364	490.95	ZINC	O=C(NC1=CC=C[C@H]2C(=O)c3ccccc3C(=O)[C@@H]12)c1cc(-c2ccccc2Cl)nc2ccccc21
vNsp14-as1-146	ZINC000029748612	-13.1	0.336	560.65	ZINC	C[C@@H]1CN(S(=O)(=O)c2ccc3oc4ccccc4c3c2)CCN1S(=O)(=O)c1ccc2oc3ccccc3c2c1
vNsp14-as1-147	ZINC000100504092	-13.1	0.423	404.51	ZINC	O=c1cccc2n1C[C@H]1C[C@H]2CN(Cc2ccc3ccc4ccccc5ccc2c3c45)C1
vNsp14-as1-148	ZINC000100737708	-13.1	0.397	431.45	ZINC	O=C(Nc1cccc2c1C(=O)[C@@H]1C=CC=C[C@@H]1C2=O)c1cccc2c1C(=O)c1ccccc1-2
vNsp14-as1-149	ZINC000104480060	-13.1	0.364	490.95	ZINC	O=C(NC1=CC=C[C@@H]2C(=O)c3ccccc3C(=O)[C@@H]12)c1cc(-c2ccccc2Cl)nc2ccccc21
vNsp14-as1-150	ZINC000208180070	-13.1	0.354	498.58	ZINC	Cc1c2oc3c(c2cc2c(C)c(CC(=O)N4C[C@H]5C[C@@H](C4)Cn4c(=O)ccce45)c(=O)oc12)CCCC3
vNsp14-as1-151	ZINC000408975099	-13.1	0.374	451.49	ZINC	O=C(Nc1ccc2ccccc2c1)c1ccc2nc3c4cccnc4c4nccc4c3nc2c1
vNsp14-as1-152	PV-001798861712	-13.0	0.419	415.49	REAL	Cc1ccc(N2C[C@H](C(=O)NNC(=O)c3ccc4ccccc34)CCC2=O)cc1C
vNsp14-as1-153	Z100034794	-13.0	0.371	465.52	REAL	C/C(=N\Nc1nncc2ccccc12)c1ccc(NC(=O)C[C@@H]2Nc3ccccc3NC2=O)cc1
vNsp14-as1-154	Z1000673822	-13.0	0.371	469.58	REAL	O=C(N[C@@H]1CCCN(C(=O)c2ccccc2)C1)C1CCN(C(=O)c2ccccc3ccccc23)CC1
vNsp14-as1-155	Z1014389548	-13.0	0.382	474.63	REAL	O=C([C@H]1C[C@@H]2CCCC[C@H]2N1C(=O)c1ccc2ccccc2c1)N1CCN(c2nccs2)CC1
vNsp14-as1-156	Z1014448996	-13.0	0.351	496.57	REAL	O=C(Nc1cccc(N2C(=O)CNC2=O)c1)[C@@H]1C[C@@H]2CCCC[C@@H]2N1C(=O)c1ccc2ccccc2c1
vNsp14-as1-157	Z1030514170	-13.0	0.361	479.58	REAL	O=C(NCc1nc(-c2ccccc2)n[nH]1)[C@H]1C[C@@H]2CCCC[C@H]2N1C(=O)c1ccc2ccccc2c1
vNsp14-as1-158	Z1070904338	-13.0	0.351	497.55	REAL	C[C@@H]1Oc2ccc(C(=O)C3CCN([C@@H]4CC(=O)N(c5ccc6ccccc56)C4=O)CC3)cc2NC1=O
vNsp14-as1-159	Z1101912578	-13.0	0.361	475.50	REAL	O=C(Nc1cccc(N2C(=O)c3ccccc3C2=O)c1)[C@H]1CC(=O)N(c2ccc3ccccc23)C1
vNsp14-as1-160	Z1128906577	-13.0	0.361	482.54	REAL	O=C(Nc1cccc(-c2noc(=O)[nH]2)c1)[C@H]1C[C@@H]2CCCC[C@H]2N1C(=O)c1ccc2ccccc2c1
vNsp14-as1-161	Z1155124260	-13.0	0.351	498.56	REAL	Cc1nnnn1-c1ccc(F)c(NC(=O)[C@@H]2C[C@@H]3CCCC[C@@H]3N2C(=O)c2ccc3ccccc3c2)c1
vNsp14-as1-162	Z1161374423	-13.0	0.371	489.55	REAL	O=C1COc2ccc(S(=O)(=O)N3CCN(C(=O)c4ccc5c(c4)-c4ccccc4C5)CC3)cc2N1
vNsp14-as1-163	Z1225982700	-13.0	0.406	421.46	REAL	Cc1n[nH]cc1C(=O)NNC(=O)c1cc(-c2cccc3ccccc23)nc2ccccc12
vNsp14-as1-164	Z1239575359	-13.0	0.419	409.49	REAL	CN1C[C@H](NC(=O)c2cc(-c3cccc4ccccc34)nc3ccccc23)CCC1=O
vNsp14-as1-165	Z1246317385	-13.0	0.406	425.49	REAL	C[C@@]1(c2ccc3ccccc3c2)NC(=O)N(CC(=O)N2[C@H]3CC[C@@H]2c2ccccc23)C1=O
vNsp14-as1-166	Z1257205965	-13.0	0.448	379.42	REAL	Cc1nc(NC(=O)c2cc(-c3cccc4ccccc34)nc3ccccc23)n[nH]1
vNsp14-as1-167	Z1333927156	-13.0	0.419	405.46	REAL	O=C(c1cc(-c2cccc3ccccc23)nc2ccccc12)N1CCc2nn[nH]c2C1
vNsp14-as1-168	Z1391355653	-13.0	0.406	448.88	REAL	O=C(c1ccc2c(c1)C(=O)N(c1ccccc1Cl)C2=O)N1CC[C@@H](c2ccc(F)cc2)C1
vNsp14-as1-169	Z1544053298	-13.0	0.406	434.54	REAL	NC(=O)N[C@H]1CCN(C(=O)[C@H]2C[C@@H]3CCCC[C@H]3N2C(=O)c2ccc3ccccc3c2)C1
vNsp14-as1-170	Z1546762676	-13.0	0.406	426.52	REAL	O=C(c1cc2ccccc2[nH]1)N1CCN(c2nc3ccccc3nc2N2CCCC2)CC1
vNsp14-as1-171	Z1550852113	-13.0	0.394	443.55	REAL	O=C1C[C@H]([C@H]2CCCCN2C(=O)[C@@H]2CC(=O)N(c3ccc4c(c3)Cc3ccccc3-4)C2)CN1
vNsp14-as1-172	Z1610573037	-13.0	0.433	403.45	REAL	Cc1cc2ccccc2nc1NNC(=O)C1CCN(c2ccc3nnnn3n2)CC1
vNsp14-as1-173	Z1637941305	-13.0	0.394	447.49	REAL	Cc1cc2c(cc1NC(=O)N1CCC[C@H](c3n[nH]cc3NC(=O)c3ccccc3)C1)OCO2
vNsp14-as1-174	Z1646012510	-13.0	0.433	397.44	REAL	c1ccc2c(-c3nnc(C4CCN(c5ccc6nncn6n5)CC4)o3)cccc2c1
vNsp14-as1-175	Z1685323575	-13.0	0.394	436.47	REAL	Cc1nnc(-c2cccc(-c3noc([C@H]4CC(=O)N(c5cccc6ccccc56)C4)n3)c2)[nH]1
vNsp14-as1-176	Z1744183511	-13.0	0.406	425.49	REAL	O=C([C@H]1CC(=O)N(c2cccc3ccccc23)C1)N1CC[C@@]2(C1)C(=O)Nc1ccccc12
vNsp14-as1-177	Z1751213636	-13.0	0.406	418.50	REAL	O=C(N[C@H]1CCn2ccnc2C1)c1cc(-c2ccccc3ccccc23)nc2ccccc12
vNsp14-as1-178	Z1771463627	-13.0	0.394	449.39	REAL	O=C(Nc1n[nH]c(Cc2cccc(F)c2)n1)c1cc(F)cc2c(=O)c3cc(F)ccc3[nH]c12
vNsp14-as1-179	Z1847258694	-13.0	0.394	430.47	REAL	O=C(NNc1nc2ccccn2n1)c1cc(-c2ccccc3ccccc23)nc2ccccc12
vNsp14-as1-180	Z1888525474	-13.0	0.406	423.48	REAL	O=C(c1cccc2c(=O)c3ccccc3[nH]c12)N1CCC(c2nnc3ccccn23)CC1
vNsp14-as1-181	Z1888618764	-13.0	0.394	447.44	REAL	O=C(c1ccc(F)c(F)c1)N1CCN(C(=O)c2cccc3c(=O)c4ccccc4[nH]c23)CC1
vNsp14-as1-182	Z1889103014	-13.0	0.394	439.47	REAL	O=C(c1cccc2c(=O)c3ccccc3[nH]c12)N1CCc2c(cccc2N2CCOC2=O)C1
vNsp14-as1-183	Z1889182194	-13.0	0.419	416.39	REAL	O=C(Nc1cc(-c2cc(F)cc(F)c2)[nH]n1)c1cccc2c(=O)c3ccccc3[nH]c12
vNsp14-as1-184	Z1889264296	-13.0	0.419	411.46	REAL	CC(=O)N1CC[C@H](NC(=O)c2cccc3c(=O)c4ccccc4[nH]c23)c2ccccc21
vNsp14-as1-185	Z2087363682	-13.0	0.433	396.41	REAL	O=C1N[C@]2(CCc3ccccc32)C(=O)N1c1ccc(-c2ccc3nccc3c2)on1
vNsp14-as1-186	Z2160281124	-13.0	0.406	420.43	REAL	Cc1nn(-c2ccccc2)c2ncc(-c3nc(-c4cc(=O)[nH]c5ccccc45)no3)cc12
vNsp14-as1-187	Z225655128	-13.0	0.382	492.00	REAL	O=C(c1ccc(Cl)c(S(=O)(=O)N2CCc3ccccc32)c1)N1CCc2[nH]c3ccccc3c2C1
vNsp14-as1-188	Z2642635500	-13.0	0.433	397.48	REAL	Cc1cccc(-c2nnc3n2C[C@@H](C(=O)Nc2ncc4ccc(C)cc24)CC3)c1
vNsp14-as1-189	Z29404408	-13.0	0.382	471.58	REAL	O=C(c1c2c(nc3ccccc13)CCC2)N1CCN(S(=O)(=O)c2ccc3ccccc3c2)CC1
vNsp14-as1-190	Z362739648	-13.0	0.361	475.55	REAL	O=C(c1cccc(C(=O)N2CCc3[nH]c4ccccc4c3C2)n1)N1CCc2[nH]c3ccccc3c2C1
vNsp14-as1-191	Z367232120	-13.0	0.371	488.61	REAL	Cc1cnc2c(S(=O)(=O)N3CCN(C(=O)c4cccc5c6c([nH]c45)CCCC6)CC3)ccc2c1
vNsp14-as1-192	Z367596726	-13.0	0.406	445.54	REAL	Cc1csc(N2CCN(C(=O)c3cccc4c(=O)c(C)c(-c5ccccc5)oc34)CC2)n1
vNsp14-as1-193	Z367877800	-13.0	0.371	475.57	REAL	Cc1cccC(=O)N2CCC[C@H](C(=O)Nc3ccc(F)c(-c4nnc5n4CCCC5)c3)C2)cc1
vNsp14-as1-194	Z368268116	-13.0	0.371	476.58	REAL	Cc1ccc(C(=O)N2CCC[C@@H](C(=O)N(C)CC(=O)N3c4ccccc4NC(=O)C[C@@H]3C)C2)cc1
vNsp14-as1-195	Z394502078	-13.0	0.394	437.46	REAL	Cc1c(-c2ccccc2)oc2c(C(=O)Nc3cccc(-n4nnnc4C)c3)cccc2c1=O
vNsp14-as1-196	Z413316676	-13.0	0.351	498.63	REAL	C[C@@H]1C[C@H](C)CN(C(=O)c2ccccc2NC(=O)N2CCN(C(=O)c3cccc4ccccc34)CC2)C1
vNsp14-as1-197	Z462192646	-13.0	0.361	483.61	REAL	Cc1cc(C)cc(C(=O)N2CCC[C@H](C(=O)N3CCN(C(=O)c4ccccc5ccccc45)CC3)C2)c1
vNsp14-as1-198	Z552453834	-13.0	0.351	493.61	REAL	O=C(N[C@H]1CCCc2c1cnn2Cc1ccccc1)N1CCN(C(=O)c2cccc3ccccc23)CC1
vNsp14-as1-199	Z730537870	-13.0	0.382	451.53	REAL	Cc1c(C(=O)N2CCN(C(=O)Cc3c[nH]c4ccccc34)CC2)oc2c1ccc1ccccc12
vNsp14-as1-200	Z731278064	-13.0	0.351	495.51	REAL	Cn1ncc2c(=O)[nH]c(COC(=O)c3c4c(nc5ccccc35)/C(=C\c3ccc(F)cc3)CCC4)nc21

Supplementary Table 72. Virtual screening hits 101 to 200 of the screen against the active site of the N7-MTase domain of nsp14 (Screen ID: 38). Compounds were filtered so that hits had MW < 600 dalton, cLogP < 6, number of hydrogen bond acceptors < 11, and no reactive functional groups. A few compounds unsuitable for drug discovery were removed by visual inspection. The name of each compound consists of the initial letter 'v' for virtual hit, followed by the target protein name and the target site ('as' for active site, 1 for docking scenario 1). The score is the docking score given by QuickVina 2 in kcal/mol. The ligand efficiency (LE) is computed as LE = -score/#NonH, where #NonH is the number of heavy (i.e. non hydrogen) atoms.

Name	Catalog ID	Score	LE	MW	Library	SMILES
vNsp15-as1-1	Z2371500224	-11.3	0.39	390.481	REAL	O=C1CCCCc2ccc(NC(=O)N3CCC[C@]4(C3)OCc3ccccc34)cc21
vNsp15-as1-2	Z1171598144	-11.2	0.35	426.435	REAL	Cc1nnc2[nH]nc(NC(=O)c3ccc4c(c3)C(=O)N(Cc3ccccc3)C4=O)c2c1C
vNsp15-as1-3	ZINC000107765190	-11.2	0.303	480.585	ZINC	O=C(/C=C\c1cc[n+](CC(=O)c2ccc3cccc4c3c2CC4)cc1)c1ccc2cccc3c2c1CC3
vNsp15-as1-4	Z1101835374	-11.1	0.308	475.503	REAL	O=C(Nc1ccc(N2C(=O)c3ccccc3C2=O)cc1)[C@H]1CC(=O)N(c2cccc3ccccc23)C1
vNsp15-as1-5	Z1128651011	-11.1	0.347	426.514	REAL	CC(=O)N1Cc2ccccc2C[C@@H]1C(=O)NCc1ccc(-c2ccc3c(c2)CCO3)cc1
vNsp15-as1-6	Z1170162723	-11.1	0.326	446.429	REAL	O=c1nc2c(-c3nc(-c4ccc(-n5cnc6ccccc65)nc4)no3)c[nH]n2c2ccccc12
vNsp15-as1-7	Z2111575407	-11.1	0.37	406.48	REAL	CC1(C)CC(=O)c2cc(NC(=O)N3CCC[C@]4(C3)OCc3ccccc34)ccc2O1
vNsp15-as1-8	Z2371498431	-11.1	0.383	390.481	REAL	O=C1CCCCc2ccc(NC(=O)N3CCO[C@@]4(CCc5ccccc54)C3)cc21
vNsp15-as1-9	Z2902669716	-11.1	0.347	424.394	REAL	Oc1nc2ccc(F)cc2cc1-c1nc(-c2ccc(-n3cnc4ccccc43)nc2)no1
vNsp15-as1-10	ZINC000002267002	-11.1	0.358	406.396	ZINC	O=c1oc2ccc3ccccc3c2cc1-c1nnc(-c2cc3ccccc3cc2O)o1
vNsp15-as1-11	PV-001940740368	-11	0.344	456.609	REAL	C[C@H](CNC(=O)Nc1ccc(S(=O)(=O)N[C@H](C)[C@@H]2C[C@H]3CC[C@H]2C3)cc1)c1ccncc1
vNsp15-as1-12	Z1683114726	-11	0.344	436.373	REAL	NC(=O)c1ccc(-c2noc(-c3ccc(NC(=O)c4cc(F)cc(F)c4)cc3O)n2)cc1
vNsp15-as1-13	Z1766495345	-11	0.333	435.486	REAL	O=C(c1ccc2[nH]c3ccccc3c(=O)c2c1)N1CCC[C@H]1c1nc(-c2ccccc2)n[nH]1
vNsp15-as1-14	Z1891230343	-11	0.333	448.388	REAL	Cc1nnc2ccc(-c3noc(-c4ccc(NC(=O)c5cc(F)cc(F)c5)cc4O)n3)cn12
vNsp15-as1-15	Z2176007556	-11	0.344	446.482	REAL	O=C(NS(=O)(=O)c1ccc2c(c1)C(=O)CCC2)c1ccc2[nH]c3ccccc3c(=O)c2c1
vNsp15-as1-16	Z2902672984	-11	0.314	468.491	REAL	O=C(c1ccc(F)cc1)N1CCC[C@@H](c2nc(-c3ccc(-n4cnc5ccccc54)nc3)no2)C1
vNsp15-as1-17	Z2902673513	-11	0.314	464.528	REAL	Cc1ccc(C(=O)N2CCC[C@@H](c3nc(-c4ccc(-n5cnc6ccccc65)nc4)no3)C2)cc1
vNsp15-as1-18	ZINC000004015296	-11	0.289	493.477	ZINC	O=c1nc2c3cccc4cccc(c(=O)n2c2cc(N5C(=O)c6cccc7ccccc(c76)C5=O)ccc12)c43
vNsp15-as1-19	ZINC000022504887	-11	0.355	415.448	ZINC	O=C(Nc1ccc2c(c1)OCO2)Nc1ccc2c(c1)CCCN2C(=O)c1ccccc1
vNsp15-as1-20	ZINC000247889806	-11	0.289	498.58	ZINC	Cc1ccc(N2C(=O)[C@H]3[C@H]4C=Cc5c6ccccc6ccc5N4[C@@H](C(=O)c4ccccc4)[C@H]3C2=O)c(C)c1
vNsp15-as1-21	ZINC000247889819	-11	0.289	498.58	ZINC	Cc1ccc(N2C(=O)[C@H]3[C@H]4C=Cc5c6ccccc6ccc5N4[C@H](C(=O)c4ccccc4)[C@H]3C2=O)c(C)c1
vNsp15-as1-22	ZINC000408674328	-11	0.297	494.545	ZINC	CC1=CC[C@@H]2C(=O)N(c3cccc(OC(=O)[C@@H]4CC(=O)N(c5ccccc6ccccc65)C4)c3)C(=O)[C@H]2C1
vNsp15-as1-23	Z1472863826	-10.9	0.352	429.495	REAL	O=C(N[C@H]1[C@@H]2CCc3ccccc3[C@H]21)c1ccc2c(c1)S(=O)(=O)c1ccccc1C2=O
vNsp15-as1-24	Z1549987944	-10.9	0.363	423.452	REAL	O=C1c2ccccc2S(=O)(=O)c2cc(C(=O)N3CCC[C@@H](c4nnn[nH]4)C3)ccc21
vNsp15-as1-25	Z1684428213	-10.9	0.321	445.441	REAL	O=c1nc2c(-c3nc(-c4ccc(-n5cnc6ccccc65)cc4)no3)c[nH]n2c2ccccc12
vNsp15-as1-26	Z1685085222	-10.9	0.321	449.469	REAL	O=C1C[C@@H](c2nc(-c3ccc4[nH]c(=O)[nH]c4c3)no2)CN1c1ccc2c(c1)Cc1ccccc1-2
vNsp15-as1-27	Z1685180149	-10.9	0.33	447.4	REAL	Cn1ncc2ccc(-c3noc(-c4ccc(NC(=O)c5cc(F)cc(F)c5)cc4O)n3)cc21
vNsp15-as1-28	Z1764809309	-10.9	0.33	437.541	REAL	C[C@H]1Cc2ccccc2N1C1CCN(C(=O)c2ccc3[nH]c4ccccc4c(=O)c3c2)CC1
vNsp15-as1-29	Z1831525989	-10.9	0.376	388.418	REAL	O=C1C[C@H](C(=O)Oc2ccc3c4c(c(=O)oc3c2)CCCCC4)c2ccccc21
vNsp15-as1-30	Z1890698064	-10.9	0.352	434.475	REAL	O=c1ccc(-c2noc(-c3cccc(S(=O)(=O)N4CCc5ccccc5C4)c3)n2)c[nH]1
vNsp15-as1-31	Z1890947874	-10.9	0.352	423.374	REAL	Cc1cc(-c2noc(-c3ccc(NC(=O)c4cc(F)cc(F)c4)cc3O)n2)ccc1O
vNsp15-as1-32	Z2160715108	-10.9	0.33	447.4	REAL	Cc1ccc2ncc(-c3noc(-c4ccc(NC(=O)c5cc(F)cc(F)c5)cc4O)n3)n2c1
vNsp15-as1-33	Z2193901914	-10.9	0.33	434.458	REAL	O=C1C[C@@H](c2nc(-c3cc4[nH]nnc4c3)no2)CN1c1ccc2c(c1)Cc1ccccc1-2
vNsp15-as1-34	Z924351844	-10.9	0.341	446.569	REAL	CC(=O)N1CCCc2cc(S(=O)(=O)N3CC=C(c4ccccc5ccccc45)CC3)ccc21
vNsp15-as1-35	ZINC000033821753	-10.9	0.341	442.901	ZINC	O=C1[C@H]2[C@@H]3C[C@@H]([C@H]4C(c5ccccc5Cl)=NO[C@H]34)[C@@H]2C(=O)N1c1ccc2ccccc2c1
vNsp15-as1-36	ZINC000036569539	-10.9	0.33	477.346	ZINC	O=C1[C@@H]2[C@H]3C[C@H]([C@H]4ON=C(c5ccc(Cl)cc5Cl)[C@@H]43)[C@@H]2C(=O)N1c1ccc2ccccc2c1
vNsp15-as1-37	ZINC000036569540	-10.9	0.33	477.346	ZINC	O=C1[C@H]2[C@@H]3C[C@@H]([C@H]4C(c5ccc(Cl)cc5Cl)=NO[C@H]34)[C@@H]2C(=O)N1c1ccc2ccccc2c1
vNsp15-as1-38	ZINC000100504092	-10.9	0.352	404.512	ZINC	O=c1cccc2n1C[C@H]1C[C@H]2CN(Cc2ccc3ccc4cccc5ccc2c3c45)C1
vNsp15-as1-39	ZINC000104268210	-10.9	0.279	511.58	ZINC	Cc1ccc(N2C(=O)[C@@H]3[C@H](C2=O)[C@@H]2c4ccccc4C=NN2[C@@H]3C(=O)c2ccc(-c3ccccc3)cc2)cc1
vNsp15-as1-40	ZINC000408674321	-10.9	0.295	494.545	ZINC	CC1=CC[C@@H]2C(=O)N(c3cccc(OC(=O)[C@@H]4CC(=O)N(c5ccccc6ccccc65)C4)c3)C(=O)[C@@H]2C1
vNsp15-as1-41	PV-001809673564	-10.8	0.36	424.927	REAL	O=C1CCCCc2ccc(NC(=O)[C@H]3CCCN(C(=O)c4ccc(Cl)cc4)C3)cc21
vNsp15-as1-42	PV-001809673844	-10.8	0.36	408.472	REAL	O=C1CCCCc2ccc(NC(=O)[C@H]3CCCN(C(=O)c4ccc(F)cc4)C3)cc21
vNsp15-as1-43	Z1101911578	-10.8	0.292	485.502	REAL	O=C(Nc1ccc(N2C(=O)c3ccccc3C2=O)c1)c1cn(-c2ccccc2)nc1-c1ccncc1
vNsp15-as1-44	Z1101912984	-10.8	0.3	478.507	REAL	O=C(Nc1ccc(N2C(=O)c3ccccc3C2=O)c1)c1ccc2c(=O)n3c(nc2c1)CCCCC3
vNsp15-as1-45	Z1310411852	-10.8	0.327	439.47	REAL	CN1C(=O)CCN(CC(=O)Nc2ccc3c(c2)C(=O)c2ccccc2C3=O)c2ccccc21
vNsp15-as1-46	Z1672800391	-10.8	0.327	443.458	REAL	O=C(Cc1noc(-c2cc(Cc3ccccc3)ccc2O)n1)Nc1ccc2c(c1)OCCO2
vNsp15-as1-47	Z1685440054	-10.8	0.338	423.431	REAL	Cc1noc2nc(-c3ccccc3)cc(-c3nc(-c4ccc5c(c4)CCC(=O)N5)no3)c12
vNsp15-as1-48	Z1890694891	-10.8	0.36	420.448	REAL	O=c1ccc(-c2noc(-c3cccc(S(=O)(=O)N4CCc5ccccc54)c3)n2)c[nH]1
vNsp15-as1-49	Z1890696255	-10.8	0.36	440.503	REAL	O=c1ccc(-c2noc(-c3csc(S(=O)(=O)N4CCc5ccccc5C4)c3)n2)c[nH]1
vNsp15-as1-50	Z1891670569	-10.8	0.36	396.405	REAL	Oc1ccc(Cc2ccccc2)cc1-c1nc(-c2nnc(-c3ccccc3)o2)no1
vNsp15-as1-51	Z2087182409	-10.8	0.327	446.505	REAL	CC1(C)CC(=O)c2cc(NC(=O)[C@H]3CCCN(C(=O)c4ccc5[nH]ncc5c4)C3)ccc2O1
vNsp15-as1-52	Z2159553687	-10.8	0.327	443.462	REAL	O=C1NC2(CCCC2)C(=O)N1CCc1noc(-c2ccc3[nH]c4ccccc4c(=O)c3c2)n1
vNsp15-as1-53	Z2372630308	-10.8	0.372	390.481	REAL	O=C1CCCCc2ccc(NC(=O)[C@H]3CCCN(C(=O)c4ccccc4)C3)cc21
vNsp15-as1-54	Z2902834428	-10.8	0.318	468.536	REAL	O=S(=O)(c1cccc(-c2nc(-c3ncc4ccccc34)no2)c1)N1CCc2ccccc2C1
vNsp15-as1-55	Z2903526595	-10.8	0.309	497.506	REAL	Cc1c(-c2noc(-c3cc(S(=O)(=O)N4c5ccccc5C[C@H]4C)ccc3F)n2)c(=O)[nH]c(=O)n1C
vNsp15-as1-56	Z685555782	-10.8	0.327	474.564	REAL	O=S(=O)(c1cc(-c2nnc(-c3ccc4ccccc4n3)o2)cs1)N1CCc2ccccc2C1
vNsp15-as1-57	ZINC000004522763	-10.8	0.3	472.455	ZINC	Nc1c(C(=O)Nc2cccc3c2C(=O)c2ccccc2C3=O)ccc2c1C(=O)c1cccc1C2=O
vNsp15-as1-58	ZINC000008855796	-10.8	0.309	496.005	ZINC	O=C(c1ccc(Cl)cc1)N1CCC(C(=O)N2C[C@H](C(=O)N3CCCCC3)Oc3ccccc32)CC1
vNsp15-as1-59	ZINC000009410849	-10.8	0.338	427.459	ZINC	Cc1c2ccc3c(cc2oc(=O)c1CC(=O)N=c1[nH]c2ccccc2[nH]1)oc1c3CCCC1
vNsp15-as1-60	ZINC000198754475	-10.8	0.3	464.475	ZINC	O=C1c2ccccc2C(=O)C2=C3C=CC4=CC5=C(C(=O)c6ccccc6C5=O)C5=CC=C(C=C12)[C@@H]3[C@H]45
vNsp15-as1-61	ZINC000263585032	-10.8	0.318	459.592	ZINC	O=C([C@@H]1CC(=O)N(c2n[nH]c3ccccc32)C1)N1CCCC2=C[C@H]3C[C@@H](CN4CCCC[C@H]34)[C@@H]21
vNsp15-as1-62	ZINC000952862600	-10.8	0.27	542.638	ZINC	O=C([C@@H]1Cc2ccccc2C(=O)N1)N1CCC2(Cc3cn(nn3)CCOc3ccc(cc3)CCNC2=O)CC1
vNsp15-as1-63	PV-001838744249	-10.7	0.324	447.44	REAL	C[C@H](NC(=O)C1=NN(c2ccc(F)cc2)C(=O)CC1=O)c1ccc(-c2ccc(F)cc2)cc1
vNsp15-as1-64	Z109823584	-10.7	0.289	496.561	REAL	O=C1O[C@H](c2ccccc2)Cc2cc(C(=O)N3C[C@H](C(=O)N4CCCCC4)Oc4ccccc43)ccc21
vNsp15-as1-65	Z1098711057	-10.7	0.345	414.395	REAL	O=C(Nc1nn[nH]c2ccc(F)cc12)c1ccc2c(c1)C(=O)N(Cc1ccccc1)C2=O
vNsp15-as1-66	Z118359034	-10.7	0.324	443.502	REAL	C[C@H]1Oc2ccc(NC(=O)[C@H]3CCCN(C(=O)c4cccc5ccccc45)C3)cc2NC1=O
vNsp15-as1-67	Z1199918128	-10.7	0.345	430.443	REAL	O=C(NNc1cnnc2ccccc12)c1ccc2c(c1)S(=O)(=O)c1ccccc1C2=O
vNsp15-as1-68	Z1217404649	-10.7	0.334	446.569	REAL	O=C(c1cccc(S(=O)(=O)N2CCc3ccccc3C2)c1)N1CCc2ccccc2CC1
vNsp15-as1-69	Z1391747360	-10.7	0.357	414.44	REAL	O=C(Nc1ccc2ccncc12)c1ccc2c(c1)S(=O)(=O)c1ccccc1C2=O
vNsp15-as1-70	Z1392039560	-10.7	0.334	447.518	REAL	Cc1ccn2c(NC(=O)c3cccc(S(=O)(=O)N4CCc5ccccc5C4)c3)nnc2c1
vNsp15-as1-71	Z1420695816	-10.7	0.357	439.519	REAL	O=C(Nc1ccc2[nH]nnc2c1)c1csc(S(=O)(=O)N2CCc3ccccc3C2)c1
vNsp15-as1-72	Z1450512667	-10.7	0.345	436.506	REAL	C[C@@H]1Cc2ccccc2N1S(=O)(=O)c1cccc(C(=O)N2CCc3cccc(F)c32)c1
vNsp15-as1-73	Z1664491368	-10.7	0.345	415.452	REAL	Cc1ccc(C(=O)N2CCC[C@@H](c3nnc(-c4nnc(-c5ccccc5)o4)o3)C2)cc1
vNsp15-as1-74	Z1672832607	-10.7	0.345	405.416	REAL	Oc1cc2ccccc2cc1-c1nc(-c2ccc(-n3cnc4ccccc43)nc2)no1
vNsp15-as1-75	Z1672836099	-10.7	0.345	424.362	REAL	COc1ccc(-c2noc(-c3ccc(NC(=O)c4cc(F)cc(F)c4)cc3O)n2)cn1
vNsp15-as1-76	Z1697483552	-10.7	0.334	423.467	REAL	O=C1O[C@@H](c2ccccc2)Cc2cc(C(=O)N3C[C@@H]4CCC(=O)c5cccc3c54)ccc21
vNsp15-as1-77	Z1771001447	-10.7	0.315	448.485	REAL	O=C(NNc1nc(-c2ccccn2)nc2c1CCC2)c1ccc2[nH]c3ccccc3c(=O)c2c1
vNsp15-as1-78	Z1832393247	-10.7	0.334	448.542	REAL	CC(C)c1ccc(S(=O)(=O)c2ccc(NNC(=O)[C@H]3CC(=O)c4ccccc43)cc2)cc1
vNsp15-as1-79	Z1834344842	-10.7	0.345	414.395	REAL	O=C(Nc1n[nH]c2cc(F)ccc12)c1ccc2c(c1)C(=O)N(Cc1ccccc1)C2=O
vNsp15-as1-80	Z1890696519	-10.7	0.345	434.475	REAL	O=c1ccc(-c2noc(-c3cccc(S(=O)(=O)N4CCCc5ccccc54)c3)n2)c[nH]1
vNsp15-as1-81	Z1890836632	-10.7	0.334	448.506	REAL	Cc1ncc(-c2noc(-c3cccc(S(=O)(=O)N4CCc5ccccc5C4)c3)n2)c(N)n1
vNsp15-as1-82	Z1890863389	-10.7	0.345	427.337	REAL	O=C(Nc1ccc(-c2nc(-c3ccc(O)c(F)c3)no2)c(O)c1)c1cc(F)cc(F)c1
vNsp15-as1-83	Z1957565450	-10.7	0.382	396.848	REAL	O=C1Nc2cc(Cl)ccc2C1=C1CCN(C(=O)[C@H]2Cc3ccc(F)cc32)CC1
vNsp15-as1-84	Z1957565505	-10.7	0.357	420.939	REAL	O=C1Nc2cc(Cl)ccc2C1=C1CCN(C(=O)[C@@H]2[C@H]3[C@@H]4C[C@@H]5[C@@H]6[C@H]4C[C@H]3[C@@H]6[C@@H]52)CC1
vNsp15-as1-85	Z1983288167	-10.7	0.357	406.488	REAL	Cc1cccc(C)c1-n1nnnc1CN1C(=O)N[C@]2(C[C@@H]3C[C@H]2[C@@H]2CCC[C@@H]32)C1=O
vNsp15-as1-86	Z2032280889	-10.7	0.334	448.542	REAL	O=C1CC[C@H](C(=O)N2CCN(S(=O)(=O)c3ccc4ccccc4c3)CC2)c2ccccc21
vNsp15-as1-87	Z2072436656	-10.7	0.357	420.444	REAL	O=C(NS(=O)(=O)c1ccc2c(c1)C(=O)NCC2)c1ccc2c(c1)oc1ccccc12
vNsp15-as1-88	Z2073244436	-10.7	0.345	438.434	REAL	O=C1CCc2cc(S(=O)(=O)NC(=O)c3ccc4c(c3)oc3ccccc34)c(F)cc2N1
vNsp15-as1-89	Z2111557687	-10.7	0.357	406.48	REAL	CC1(C)CC(=O)c2cc(NC(=O)N3CCO[C@@]4(CCc5ccccc54)C3)ccc2O1
vNsp15-as1-90	Z2156594494	-10.7	0.324	435.482	REAL	O=C(c1ccc(N2C(=O)c3ccccc3C2=O)cc1)N1CCCn2cc(c3ccccc32)C1
vNsp15-as1-91	Z2172073698	-10.7	0.324	440.458	REAL	O=C1[C@@H]2[C@@H]3C=C[C@H]([C@@H]2C(=O)N1Cc1ccccc1)[C@H]1C(c2nc(-c4ccc(=O)[nH]c4)no2)[C@@H]31
vNsp15-as1-92	Z2172725179	-10.7	0.324	447.533	REAL	CNC(=O)[C@H]1CCCN(C(=O)C2[C@@H]3[C@@H]4C=C[C@@H]([C@H]5C(=O)N(Cc6ccccc6)C(=O)[C@@H]45)[C@H]23)C1
vNsp15-as1-93	Z2193900194	-10.7	0.345	438.511	REAL	C[C@H]1C[C@H](C)CN(S(=O)(=O)c2cccc(-c3nc(-c4ccc5[nH]nnc5c4)no3)c2)C1
vNsp15-as1-94	Z2233254101	-10.7	0.345	433.447	REAL	Cc1nnc2[nH]nc(NC(=O)c3ccc4c(c3)S(=O)(=O)c3ccccc3C4=O)c2c1C
vNsp15-as1-95	Z2902672344	-10.7	0.345	409.448	REAL	Oc1cc2c(cc1-c1nc(-c3ccc(-n4cnc5ccccc54)nc3)no1)CCCC2
vNsp15-as1-96	Z2902834278	-10.7	0.324	474.564	REAL	O=S(=O)(c1cc(-c2nc(-c3nccc4ccccc34)no2)cs1)N1CCc2ccccc2C1
vNsp15-as1-97	Z2903521928	-10.7	0.297	485.499	REAL	Cc1c(-c2noc(C3[C@@H]4[C@@H]5C=C[C@@H]([C@H]6C(=O)N(Cc7ccccc7)C(=O)[C@@H]56)[C@H]34)n2)c(=O)[nH]c(=O)n1C
vNsp15-as1-98	Z2903529871	-10.7	0.315	479.516	REAL	Cc1c(-c2noc(-c3cccc(S(=O)(=O)N4CCc5ccccc5C4)c3)n2)c(=O)[nH]c(=O)n1C
vNsp15-as1-99	Z2990969147	-10.7	0.382	371.443	REAL	c1ccc2c(c1)C[C@H]1[C@@H]2[C@@H]1n1nnnc1N1CC[C@]2(C1)OCc1ccccc12
vNsp15-as1-100	Z368084960	-10.7	0.315	455.556	REAL	O=C(Nc1ccc(N2CCCCC2=O)c1)[C@H]1CCCN(C(=O)c2cccc3ccccc23)C1

Supplementary Table 73. Top 100 virtual hits of the screen against the active site of nsp15 (Screen ID: 39). Compounds were filtered so that hits had MW < 600 dalton, cLogP < 6, number of hydrogen bond acceptors < 11, and no reactive functional groups. A few compounds unsuitable for drug discovery were removed by visual inspection. The name of each compound consists of the initial letter 'v' for virtual hit, followed by the target protein name and the target site ('as' for active site, 1 for docking scenario 1). The score is the docking score given by QuickVina 2 in kcal/mol. The ligand efficiency (LE) is computed as LE = -score/#NonH, where #NonH is the number of heavy (i.e. non hydrogen) atoms.

Name	Catalog ID	Score	LE	MW	Library	SMILES
vNsp15-as1-101	Z408842844	-10.7	0.297	485.58	REAL	COc1ccc(NC(=O)[C@H]2CCCN(C(=O)c3ccc4ccccc34)C2)cc1N1CCCCC1=O
vNsp15-as1-102	Z686120320	-10.7	0.315	470.55	REAL	Cn1cc(-c2nnc(-c3cccc(S(=O)(=O)N4CCc5ccccc5C4)c3)o2)c2ccccc21
vNsp15-as1-103	Z872896364	-10.7	0.334	424.50	REAL	O=C(Nc1cc(-c2ccccc2)n[nH]1)[C@H]1CCCN(C(=O)c2cccc3ccccc23)C1
vNsp15-as1-104	ZINC000001333979	-10.7	0.315	460.51	ZINC	Cc1ccc(C)c(Cn2nnc3c2nc([C@H]2CCCN(C(=O)c4ccccc4)C2)[nH]c3=O)c1
vNsp15-as1-105	ZINC000001641983	-10.7	0.297	495.93	ZINC	O=C1C(/C=C/c2ccc(Cl)cc2)=NN[C@H]2N1N=C1N=C(O)C3(NN12)c1ccccc1-c1ccccc13
vNsp15-as1-106	ZINC000001641985	-10.7	0.297	495.93	ZINC	O=C1C(/C=C/c2ccc(Cl)cc2)=NN[C@@H]2N1N=C1N=C(O)C3(NN12)c1ccccc1-c1ccccc13
vNsp15-as1-107	ZINC000005955034	-10.7	0.297	495.93	ZINC	O=C1NC2=NN3C(=O)C(/C=C\c4ccc(Cl)cc4)=NN[C@H]3N2NC12c1ccccc1-c1ccccc12
vNsp15-as1-108	ZINC000012863378	-10.7	0.274	525.64	ZINC	Cc1c2ccc(OCc3cccc4ccccc43)cc2oc(=O)c1CCC(=O)N1CC[C@@]2(O)CCCC[C@H]2C1
vNsp15-as1-109	ZINC000039742926	-10.7	0.324	434.45	ZINC	O=C(Nc1nnc(-c2ccccc2)o1)c1cccc(NC(=O)c2cccc3ccccc32)c1
vNsp15-as1-110	ZINC000408674180	-10.7	0.297	476.49	ZINC	O=C(Oc1ccc(N2C(=O)c3ccccc3C2=O)cc1)[C@H]1CC(=O)N(c2cccc3ccccc32)C1
vNsp15-as1-111	ZINC000408997472	-10.7	0.334	417.51	ZINC	O=C(O)c1ccccc2c1N[C@H](c1ccc3c4c(cccc41)CC3)[C@H]1Cc3ccccc3[C@@H]21
vNsp15-as1-112	PV-001804636098	-10.6	0.312	458.56	REAL	Cc1ccc(NC(=O)[C@H]2CCCN(C(=O)c3cccc4ccccc34)C2)cc1NC(=O)N(C)C
vNsp15-as1-113	PV-001948844490	-10.6	0.442	346.39	REAL	O=C(NC[C@H]1C[C@H]2[C@H]1[C@H]1C[C@H]21)N[C@H](C[C@H]1CCCO1)C(F)(F)F
vNsp15-as1-114	Z1014961746	-10.6	0.321	461.54	REAL	O=C1CN(S(=O)(=O)c2cccc(C(=O)N3Cc4ccccc4-c4ccccc4C3)c2)CCN1
vNsp15-as1-115	Z1024047402	-10.6	0.286	493.56	REAL	Cc1ccc(C)c(N2C(=O)c3ccc(C(=O)N4CCC([C@@H]5C(=O)Nc6ccccc65)CC4)cc3C2=O)c1
vNsp15-as1-116	Z1095050644	-10.6	0.321	440.51	REAL	Cc1ccc(C(=O)N2CCC[C@@H](C(=O)Nc3nc(-c4ccc5ccccc5n4)n[nH]3)C2)cc1
vNsp15-as1-117	Z1095050702	-10.6	0.312	454.53	REAL	Cc1cc(C)cc(C(=O)N2CCC[C@@H](C(=O)Nc3nc(-c4ccc5ccccc5n4)n[nH]3)C2)c1
vNsp15-as1-118	Z1102048968	-10.6	0.312	466.52	REAL	O=C1c2ccccc2C(=O)N1c1cccc(NS(=O)(=O)c2ccc3c(c2)Cc2ccccc2-3)c1
vNsp15-as1-119	Z1130669518	-10.6	0.312	481.57	REAL	O=C1NC(=O)c2cc(C(=O)N3CCN(S(=O)(=O)c4ccc(C5CCCCC5)cc4)CC3)ccc21
vNsp15-as1-120	Z1171597924	-10.6	0.321	440.46	REAL	Cc1nnc2[nH]nc(NC(=O)c3ccc4c(c3)C(=O)N(CCc3ccccc3)C4=O)c2c1C
vNsp15-as1-121	Z1171598595	-10.6	0.331	426.44	REAL	Cc1nnc2[nH]nc(NC(=O)c3cccc(CN4C(=O)c5ccccc5C4=O)c3)c2c1C
vNsp15-as1-122	Z118348250	-10.6	0.321	441.49	REAL	CN1C(=O)c2ccc(NC(=O)[C@H]3CCCN(C(=O)c4ccc5ccccc45)C3)cc2C1=O
vNsp15-as1-123	Z118358090	-10.6	0.321	441.53	REAL	O=C(Nc1cccc(N2CCCC2=O)c1)[C@H]1CCCN(C(=O)c2ccccc3ccccc23)C1
vNsp15-as1-124	Z1217455625	-10.6	0.331	428.53	REAL	Cc1ncc2c(n1)CCC[C@@H]2NC(=O)[C@H]1CCCN(C(=O)c3ccc3ccccc23)C1
vNsp15-as1-125	Z1391606023	-10.6	0.331	428.53	REAL	O=C(N[C@@H]1CCCN(C(=O)[C@@H]2C[C@]23CCCc2ccccc23)C1)c1cc2ccccc2o1
vNsp15-as1-126	Z1422677992	-10.6	0.331	431.50	REAL	CN1CCc2cccc(NC(=O)[C@H]3CCCN(C(=O)c4ccc5[nH]ncc5c4)C3)cc2C1=O
vNsp15-as1-127	Z1453804507	-10.6	0.312	449.55	REAL	O=C(NC[C@@H]1[C@@H]2Cc3ccccc3[C@H]12)c1ccnc(C(=O)N[C@@H]2[C@H]3Cc4ccccc4[C@H]23)c1
vNsp15-as1-128	Z1505440662	-10.6	0.408	346.39	REAL	O=C(c1cc2c(ccc3ccccc32)[nH]1)N1CCC[C@@H](c2nnn[nH]2)C1
vNsp15-as1-129	Z1539813606	-10.6	0.353	424.86	REAL	O=C1Nc2cc(Cl)ccc2C1=C1CCN(C(=O)C2=Cc3cc(F)ccc3OC2)CC1
vNsp15-as1-130	Z15458061	-10.6	0.286	489.49	REAL	C[C@@H](OC(=O)c1ccc(N2C(=O)c3cccc4cccc(c34)C2=O)cc1)c1nc2ccccc2c(=O)[nH]1
vNsp15-as1-131	Z1589243537	-10.6	0.331	447.52	REAL	CN1CCCc2ccc(S(=O)(=O)NC(=O)c3ccc(-n4cnc5ccccc54)nc3)cc21
vNsp15-as1-132	Z1601885412	-10.6	0.331	430.55	REAL	C[C@@H](Cn1ncc2ccccc2c1=O)NC(=O)N[C@H]1C[C@H]2CCC(C)(C)c3cccc1c32
vNsp15-as1-133	Z1672806606	-10.6	0.353	409.35	REAL	O=C(Nc1ccc(-c2nc(-c3ccc(O)cc3)no2)c(O)c1)c1cc(F)cc(F)c1
vNsp15-as1-134	Z1673836738	-10.6	0.342	432.54	REAL	CC(=O)N1CCCc2cc(S(=O)(=O)N3CC=C(c4ccccc5ccccc45)C3)ccc21
vNsp15-as1-135	Z1683390111	-10.6	0.353	438.53	REAL	Cc1cncc(-c2noc(-c3csc(S(=O)(=O)N4CCc5ccccc5C4)c3)n2)c1
vNsp15-as1-136	Z1684181625	-10.6	0.353	408.36	REAL	Cc1cccc(-c2noc(-c3ccc(NC(=O)c4cc(F)cc(F)c4)cc3O)n2)n1
vNsp15-as1-137	Z1685083408	-10.6	0.331	428.41	REAL	Cc1cc(-c2cc(-c3nc(-c4ccc5[nH]c(=O)[nH]c5c4)no3)c3c(C)noc3n2)c(C)o1
vNsp15-as1-138	Z1685200807	-10.6	0.321	447.40	REAL	Cn1cnc2cc(-c3noc(-c4ccc(NC(=O)c5cc(F)cc(F)c5)cc4O)n3)ccc21
vNsp15-as1-139	Z1723434322	-10.6	0.303	465.56	REAL	Cc1[nH]c2ccccc2c1C1CCN(C(=O)c2cccc(-c3cnc4[nH]c(=O)n(C)c4c3)c2)CC1
vNsp15-as1-140	Z1729458576	-10.6	0.366	412.51	REAL	CC(=O)N1CCc2ccc(S(=O)(=O)N3CCC[C@]4(C3)OCc3ccccc34)cc21
vNsp15-as1-141	Z1731900193	-10.6	0.366	391.47	REAL	CN1CCc2ccc(NC(=O)N3CCC[C@]4(C3)OCc3ccccc34)cc2C1=O
vNsp15-as1-142	Z1764208898	-10.6	0.353	390.40	REAL	O=c1c2ccccc2[nH]c2ccc(-c3nc(-c4nccc5ccccc45)no3)cc12
vNsp15-as1-143	Z1766739308	-10.6	0.342	412.49	REAL	COc1ccc2c(c1)C[C@@H](C)N(C(=O)c1ccc3[nH]c4ccccc4c(=O)c3c1)[C@H]2C
vNsp15-as1-144	Z1767360678	-10.6	0.342	409.44	REAL	O=C(c1ccc2[nH]c3ccccc3c(=O)c2c1)N1CC[C@]2(C1)C(=O)Nc1ccccc12
vNsp15-as1-145	Z1768177668	-10.6	0.331	447.47	REAL	O=C1CCc2cc(S(=O)(=O)NC(=O)c3ccc4[nH]c5ccccc5c(=O)c4c3)ccc2N1
vNsp15-as1-146	Z1768248164	-10.6	0.342	433.49	REAL	O=C(NS(=O)(=O)N1CCc2ccccc2C1)c1ccc2[nH]c3ccccc3c(=O)c2c1
vNsp15-as1-147	Z1799062522	-10.6	0.342	427.52	REAL	O=C(N[C@H]1CCOc2c(F)cccc21)N1CCC[C@@H](c2n[nH]c(C3CCCCC3)n2)C1
vNsp15-as1-148	Z1817113647	-10.6	0.331	419.44	REAL	O=c1[nH]cc(-c2nc(-c3cccc(Cn4cnc5ccccc54)c3)no2)c2ccccc12
vNsp15-as1-149	Z1832391778	-10.6	0.342	434.52	REAL	O=C1CC[C@H](C(=O)N2CCN(S(=O)(=O)c3ccc4ccccc4c3)CC2)c2ccccc21
vNsp15-as1-150	Z1834342185	-10.6	0.379	399.37	REAL	O=C(Nc1n[nH]c2cc(F)ccc12)c1ccc2c(c1)S(=O)(=O)Nc1ncnn1-2
vNsp15-as1-151	Z1890698017	-10.6	0.342	434.48	REAL	C[C@@H]1Cc2ccccc2N1S(=O)(=O)c1cccc(-c2nc(-c3ccc(=O)[nH]c3)no2)c1
vNsp15-as1-152	Z1891668333	-10.6	0.379	375.34	REAL	O=C1CCCc2[nH]c(=O)c(-c3nc(-c4nnc(-c5ccccc5)o4)no3)cc21
vNsp15-as1-153	Z1891828970	-10.6	0.331	427.51	REAL	O=C1N[C@]2(CCc3ccccc32)C(=O)N1c1ccc(-c2nnc3n2CCCCCC3)cc1
vNsp15-as1-154	Z1897921570	-10.6	0.342	442.45	REAL	O=C1CCCc2ccc(S(=O)(=O)Nc3nnc([C@@H]4COc5ccccc5O4)o3)ccc21
vNsp15-as1-155	Z1902654279	-10.6	0.353	432.95	REAL	CCOCCOc1c(Cl)cccc1NC(=O)NC[C@@]1(O)[C@H]2[C@H]3C[C@@H]4[C@@H]5[C@H]3C[C@@H]2[C@@H]5[C@@H]41
vNsp15-as1-156	Z1918061562	-10.6	0.353	408.36	REAL	Cc1ccc(-c2noc(-c3ccc(NC(=O)c4cc(F)cc(F)c4)cc3O)n2)ccn1
vNsp15-as1-157	Z1928420726	-10.6	0.331	449.50	REAL	O=C1c2ccccc2S(=O)(=O)c2cc(C(=O)N3CCC(F)(c4ccccc4)CC3)ccc21
vNsp15-as1-158	Z1953423174	-10.6	0.342	418.50	REAL	CCOC(=O)c1nc(-c2cccc(CNC(=O)[C@H]3[C@H]4[C@H]5C[C@@H]6[C@H]7[C@@H]5C[C@@H]4[C@@H]7[C@@H]63)c2)n[nH]1
vNsp15-as1-159	Z1972578890	-10.6	0.321	444.44	REAL	O=C(NC[C@H]1CCCN1C(=O)c1cc2ccccc2c(=O)o1)c1cc2ccccc2c(=O)o1
vNsp15-as1-160	Z2002848514	-10.6	0.321	438.53	REAL	O=C1[C@@H]2[C@@H]3C[C@H]4[C@@H]2[C@@]2(C(=O)Nc5ccc(CC(=O)N6CCCc7ccccc76)cc5)[C@H]1[C@@H]3[C@@H]42
vNsp15-as1-161	Z2114110381	-10.6	0.342	423.44	REAL	O=C(Nc1ccc(F)c(N2C(=O)CCC2=O)c1)N1CCC[C@]2(C1)OCc1ccccc12
vNsp15-as1-162	Z2157325819	-10.6	0.331	420.43	REAL	Nc1nc(Cc2noc(-c3ccc4[nH]c5ccccc5c(=O)c4c3)n2)nc2ccccc12
vNsp15-as1-163	Z2158485968	-10.6	0.353	393.41	REAL	Cc1cc(-c2noc(-c3ccc4[nH]c5ccccc5c(=O)c4c3)n2)cc2nc[nH]c12
vNsp15-as1-164	Z2159201557	-10.6	0.321	435.44	REAL	O=c1c2ccccc2[nH]c2ccc(-c3nc(CCn4cnc5ccccc5c4=O)no3)cc12
vNsp15-as1-165	Z2160048396	-10.6	0.353	402.45	REAL	O=c1c2ccccc2[nH]c2ccc(-c3nc([C@H]4CN5CCCC[C@@H]5CO4)no3)cc12
vNsp15-as1-166	Z2171929968	-10.6	0.321	438.49	REAL	Cc1cncc(-c2noc(C3[C@@H]4[C@@H]5C=C[C@@H]([C@H]6C(=O)N(Cc7ccccc7)C(=O)[C@@H]56)[C@H]34)n2)c1
vNsp15-as1-167	Z2192042062	-10.6	0.342	415.50	REAL	Cc1ccccc(-c2nnnn2[C@@H]2C[C@H]2C)c1NC(=O)c1ccc2c(c1)CCCCC2=O
vNsp15-as1-168	Z2224372704	-10.6	0.366	412.47	REAL	CC1(C)C(=O)Nc2cc(C(=O)NS(=O)(=O)c3ccc4c(c3)C(=O)CCC4)ccc21
vNsp15-as1-169	Z2233591332	-10.6	0.321	444.47	REAL	O=C(Nc1nc(-c2ccc3ccccc3n2)n[nH]1)[C@@H]1CCCN(C(=O)c2ccc(F)cc2)C1
vNsp15-as1-170	Z2282607591	-10.6	0.366	385.46	REAL	O=C1O[C@@H](c2ccccc2)Cc2cc(C(=O)N3C[C@H]4[C@H]5C=C[C@@H](C5)[C@H]4C3)ccc21
vNsp15-as1-171	Z2899224306	-10.6	0.366	390.44	REAL	Cc1ccccc1C1=NO[C@@H](c2nc(-c3cc4c([nH]c3=O)CC[C@H](C)C4)no2)C1
vNsp15-as1-172	Z2902488092	-10.6	0.312	492.36	REAL	O=C1[C@H]2[C@H]3C=C[C@H]([C@H]2C(=O)N1Cc1ccccc1)[C@H]1C(c2nc(-c4c(Cl)cccc4Cl)no2)[C@@H]31
vNsp15-as1-173	Z2902669726	-10.6	0.303	474.40	REAL	O=c1[nH]c2c(C(F)(F)F)cccc2cc1-c1nc(-c2ccc(-n3cnc4ccccc43)nc2)no1
vNsp15-as1-174	Z2902700788	-10.6	0.294	488.45	REAL	Cc1cc(C)n(-c2ccc(-c3noc(-c4ccc(NC(=O)c5cc(F)cc(F)c5)cc4O)n3)cn2)n1
vNsp15-as1-175	Z2903469909	-10.6	0.312	499.93	REAL	Cn1cc(-c2noc(-c3ccc(S(=O)(=O)N4CCc5ccccc5C4)ccc3Cl)n2)c(=O)[nH]c1=O
vNsp15-as1-176	Z2903470197	-10.6	0.303	471.47	REAL	Cn1cc(-c2noc(C3[C@@H]4[C@@H]5C=C[C@@H]([C@H]6C(=O)N(Cc7ccccc7)C(=O)[C@@H]56)[C@H]34)n2)c(=O)[nH]c1=O
vNsp15-as1-177	Z29402875	-10.6	0.303	488.57	REAL	O=C(c1ccc2c(=O)n3c(nc2c1)CCC3)N1CCN(S(=O)(=O)c2ccc3ccccc3c2)CC1
vNsp15-as1-178	Z2990209196	-10.6	0.353	399.46	REAL	O=C1Cc2ccccc2N1CCn1nnnc1N1CCc2c([nH]c3ccccc23)C1
vNsp15-as1-179	Z325118426	-10.6	0.366	395.50	REAL	Cc1ccc(C23C[C@H]4C[C@@H](CC(C(=O)OCCN5C(=O)CCC5=O)(C4)C2)C3)cc1
vNsp15-as1-180	Z394427738	-10.6	0.294	481.55	REAL	C[C@@H]1C[C@H](C)CN(C(=O)c2ccccc2NC(=O)c2ccc(N3C(=O)c4ccccc4C3=O)cc2)C1
vNsp15-as1-181	Z418091240	-10.6	0.303	484.89	REAL	C[C@H](OC(=O)c1cc2ccccc2c(Cl)n1)C(=O)Nc1ccc2c(c1)C(=O)c1ccccc1C2=O
vNsp15-as1-182	Z452223078	-10.6	0.342	432.54	REAL	C[C@@H]1CN(C(=O)c2cccc(S(=O)(=O)N3CCc4ccccc4C3)c2)ccccc21
vNsp15-as1-183	Z510448534	-10.6	0.331	456.56	REAL	O=C(NC1CCC2(CC1)OCCO2)c1cccc(S(=O)(=O)N2CCc3ccccc3C2)c1
vNsp15-as1-184	Z735301842	-10.6	0.342	411.46	REAL	Cc1ccc(C(=O)Nc2cccc(CN/C=C3\C(=O)NC(=O)c4ccccc43)c2)cc1
vNsp15-as1-185	Z767780038	-10.6	0.321	462.55	REAL	Cc1sc(=O)n(CC(=O)Nc2cccc(-c3n[nH]c4c3CCCC4)c2)c1-c1ccc(F)cc1
vNsp15-as1-186	Z804246722	-10.6	0.312	455.52	REAL	O=C(NNC(=O)[C@H]1CC(=O)N(c2ccc3c(c2)Cc2ccccc2-3)C1)c1n[nH]c2c1CCCC2
vNsp15-as1-187	Z899288814	-10.6	0.353	402.46	REAL	O=C(Nc1n[nH]c2ccccc12)[C@@H]1CCC[C@H](C(=O)Nc2n[nH]c3ccccc23)C1
vNsp15-as1-188	Z983988502	-10.6	0.331	427.51	REAL	C[C@H](NC(=O)NCc1ccc(-c2ccc3c(c2)CCCO3)cc1)c1nnc2ccccn12
vNsp15-as1-189	ZINC000001334041	-10.6	0.312	476.97	ZINC	Cc1ccc(C)c(Cn2nnc3c2nc([C@H]2CCCN(C(=O)c4ccc(Cl)cc4)C2)[nH]c3=O)c1
vNsp15-as1-190	ZINC000002212711	-10.6	0.321	429.47	ZINC	O=C(Nc1ccc2c(c1)Cc1ccccc1-2)c1cccc(-c2cc3ccccc3oc2=O)c1
vNsp15-as1-191	ZINC000002832254	-10.6	0.303	473.51	ZINC	O=c1oc2ccc3ccccc3c2cc1-c1ccc(-c2cc3c(ccc4ccccc43)oc2=O)n1
vNsp15-as1-192	ZINC000008862292	-10.6	0.303	478.60	ZINC	C[C@@H]1C[C@@]2(CC(C)(C)C1)NC(=O)N(CC(=O)Nc1cccc(-c3nnc4n3CCCCC4)c1)C2=O
vNsp15-as1-193	ZINC000013684184	-10.6	0.286	480.59	ZINC	O=C(/C=C/c1cc[n+](CC(=O)c2ccc3ccccc4c3c2CC4)cc1)c1ccc2ccccc3c2c1CC3
vNsp15-as1-194	ZINC000015002312	-10.6	0.321	457.51	ZINC	O=C(c1ccc(-c2cccc3c2Oc2ccccc2S3)cc(-n2cnnn2)c1)N1CCOCC1
vNsp15-as1-195	ZINC000016919178	-10.6	0.312	448.52	ZINC	O=C1c2ccccc2C(=O)[C@H]2CC3=C(CC4=C(C3)C[C@@H]3C(=O)c5ccccc5C(=O)[C@@H]3C4)C[C@@H]12
vNsp15-as1-196	ZINC000017988666	-10.6	0.272	516.55	ZINC	O=C(COC(=O)c1cc(-c2ccc(N3C(=O)[C@H]4CC=CC[C@@H]4C3=O)cc2)nc2ccccc21)c1ccccc1
vNsp15-as1-197	ZINC000037246228	-10.6	0.303	465.59	ZINC	O=C1c2ccccc2C(=O)c2cc3c(cc21)N[C@@H]1CC[C@H]2[C@@H]4CCCC[C@@H]4C(=O)[C@H]4CC[C@H]3[C@H]1[C@@H]42
vNsp15-as1-198	ZINC000100115224	-10.6	0.294	488.54	ZINC	C[C@]12CC(=O)[C@@](C)(C1)[C@@H]1C(=O)N(c3ccc(N4C(=O)[C@H]5[C@H](C4=O)[C@@]4(C)C[C@]5(C)CC4=O)cc3)C(=O)[C@H]12
vNsp15-as1-199	ZINC000100237625	-10.6	0.286	490.56	ZINC	O=C1[C@@H]2[C@H]3C=C[C@@H](C3)[C@@H]2C(=O)Nc1ccc(Cc2ccc(N3C(=O)[C@H]4[C@H]5C=C[C@H](C5)[C@@H]4C3=O)cc2)cc1
vNsp15-as1-200	ZINC000102077159	-10.6	0.321	435.48	ZINC	O=C(Oc1ccc2ccccc2c1)c1cccc(N2C(=O)[C@H]3[C@@H](C2=O)[C@@H]2C=C[C@@H]3[C@H]3C[C@@H]32)c1

Supplementary Table 74. Virtual screening hits 101 to 200 of the screen against the active site of nsp15 (Screen ID: 39). Compounds were filtered so that hits had MW < 600 dalton, cLogP < 6, number of hydrogen bond acceptors < 11, and no reactive functional groups. A few compounds unsuitable for drug discovery were removed by visual inspection. The name of each compound consists of the initial letter 'v' for virtual hit, followed by the target protein name and the target site ('as' for active site, 1 for docking scenario 1). The score is the docking score given by QuickVina 2 in kcal/mol. The ligand efficiency (LE) is computed as LE = -score/#NonH, where #NonH is the number of heavy (i.e. non hydrogen) atoms.

Name	Catalog ID	Score	LE	MW	Library	SMILES
vNsp16-as1-1	Z1902654279	-12.2	0.407	432.946	REAL	CCOCCOc1c(Cl)cccc1NC(=O)NC[C@@]1(O)[C@H]2[C@H]3C[C@@H]4[C@@H]5[C@H]3C[C@@H]2[C@@H]5[C@@H]4[C@H]3[C@H]6[C@H]52)cc1
vNsp16-as1-2	Z1907681358	-12.2	0.421	414.524	REAL	C=CCNS(=O)(=O)c1ccc(C(=O)NC[C@]2(O)[C@H]3[C@@H]4C[C@@H]5[C@@H]6[C@H]4[C@H]3[C@H]6[C@H]52)cc1
vNsp16-as1-3	Z2641366477	-12	0.414	391.426	REAL	O=C(c1ccccc(-c2noc(O)n2)c1)N1CCC2(CC1)OCCc1ccccc12
vNsp16-as1-4	Z1030834984	-11.9	0.34	484.539	REAL	O=C(Nc1cccc(-c2nc(C3CC3)n[nH]2)c1)c1ccc(NC2=NS(=O)(=O)c3ccccc32)cc1
vNsp16-as1-5	Z2910813077	-11.8	0.407	390.446	REAL	O=C(c1cccc(Nc2nnn[nH]2)c1)N1CCC2(CC1)OCCc1ccccc12
vNsp16-as1-6	ZINC000002027565	-11.8	0.295	528.563	ZINC15	Cc1ccc(C)c(N2C(=O)c3ccc(C(=O)c4ccc5c(c4)C(=O)N(c4cc(C)ccc4C)C5=O)cc3C2=O)c1
vNsp16-as1-7	Z2158539625	-11.7	0.418	370.371	REAL	Cc1nnc(-c2cccc(-c3noc(-c4c[nH]c(=O)c5ccccc45)n3)c2)[nH]1
vNsp16-as1-8	ZINC000109965938	-11.7	0.334	475.571	ZINC15	O=S1(=O)c2ccccc2-c2cc(-c3nc(C4=CN[C@H]5C=CC=C[C@H]45)[nH]c3-c3ccccc3)ccc21
vNsp16-as1-9	Z1155703713	-11.6	0.322	496.546	REAL	O=C(Nc1cccc(-c2ccc3c(c2)CCO3)n1)c1ccc(NC2=NS(=O)(=O)c3ccccc32)cc1
vNsp16-as1-10	Z2002724890	-11.6	0.374	414.547	REAL	O=C1[C@@H]2[C@@H]3C[C@@H]4[C@H]2[C@@]2(C(=O)Nc5ccccc5NC56CC7CC(CC(C7)C5)C6)[C@@H]1[C@@H]3[C@H]42
vNsp16-as1-11	Z2021034781	-11.6	0.4	390.442	REAL	C[C@@H]1CCc2[nH]c3ccc(C(=O)Nc4cccc(C(=O)NC(N)=O)c4)cc3c2C1
vNsp16-as1-12	Z2158539899	-11.6	0.4	384.398	REAL	Cc1nnc(-c2cccc(-c3noc(-c4cn(C)c(=O)c5ccccc45)n3)c2)[nH]1
vNsp16-as1-13	ZINC000002079077	-11.6	0.29	528.563	ZINC15	Cc1ccc(N2C(=O)c3ccc(C(=O)c4ccc5c(c4)C(=O)N(c4ccc(C)cc4C)C5=O)cc3C2=O)c(C)c1
vNsp16-as1-14	ZINC000100505727	-11.6	0.314	488.542	ZINC15	O=C1[C@@H]2[C@H]3C=C[C@@H](C3)[C@@H]2C(=O)N1c1ccc2c(c1)-c1cc(N3C(=O)[C@H]4[C@H]5C=C[C@H](C5)[C@@H]4C3=O)ccc1C2
vNsp16-as1-15	ZINC000101076136	-11.6	0.305	499.521	ZINC15	O=C1c2ccccc2C(=O)C12O[C@@H](c1ccccc1)[C@H]1C(=O)N(c3ccc(-c4ccccc4)cc3)C(=O)[C@@H]12
vNsp16-as1-16	PV-001948673125	-11.5	0.371	436.397	REAL	Cc1nc(-c2cc(NC(=O)N3CCC[C@@H](c4nc(=O)[nH][nH]4)C3)cc(C(F)(F)F)c2)n[nH]1
vNsp16-as1-17	Z1128906577	-11.5	0.319	482.538	REAL	O=C(Nc1cccc(-c2noc(=O)[nH]2)c1)[C@@H]1C[C@@H]2CCCC[C@@H]2N1C(=O)c1ccc2ccccc2c1
vNsp16-as1-18	Z1452691933	-11.5	0.348	445.493	REAL	O=C(NC[C@H]1[C@@H]2C3ccccc3[C@H]12)NNC(=O)c1ccccc1OCc1ccc(F)cc1
vNsp16-as1-19	Z1680770562	-11.5	0.348	446.505	REAL	C[C@H](C(=O)Nc1ccc2c(c1)C(=O)c1ccccc1C2=O)N1CC[C@@H](NC(=O)NC2CC2)C1
vNsp16-as1-20	Z1905191614	-11.5	0.359	436.51	REAL	C[C@@]1(c2ccc(CNC(=O)NC[C@@]3(O)[C@H]4[C@H]5C[C@@H]6[C@@H]7[C@@H]5[C@@H]4[C@H]7[C@@H]63)cc2)NC(=O)NC1=O
vNsp16-as1-21	Z1921545983	-11.5	0.348	446.462	REAL	C[C@@H](C(=O)Nc1ccc2c(c1)C(=O)c1ccccc1C2=O)N1CCC[C@]2(C1)NC(=O)NC2=O
vNsp16-as1-22	Z2299368576	-11.5	0.411	374.443	REAL	O=C(c1cccc(-c2ncn[nH]2)c1)N1CCC2(CC1)OCCc1ccccc12
vNsp16-as1-23	ZINC000009111513	-11.5	0.311	489.534	ZINC15	Cc1ccc(N2C(=O)[C@@H]3[C@H](C2=O)[C@@H]2C=Cc4ccccc4N2[C@@H]3C(=O)n2nnc3ccccc32)c(C)c1
vNsp16-as1-24	ZINC000104100953	-11.5	0.311	489.534	ZINC15	Cc1ccc(N2C(=O)[C@@H]3[C@@H](C2=O)[C@@H](C(=O)n2nnc4ccccc42)N2c4ccccc4C=C[C@@H]32)c(C)c1
vNsp16-as1-25	ZINC000247958480	-11.5	0.319	471.515	ZINC15	O=C(c1ccccc1)[C@@H]1[C@@H]2C(=O)N(c3ccc4ccccc4c3)C(=O)[C@H]2[C@@H]2c3ccccc3C=NN21
vNsp16-as1-26	ZINC000409334850	-11.5	0.311	493.514	ZINC15	Cc1ccc(N2C(=O)[C@H]3[C@H](C2=O)[C@@H]2C(=O)Oc4cc(C)ccc4C2=C[C@@H]3c2ccc3c(c2)OCO3)cc1
vNsp16-as1-27	PV-001846349167	-11.4	0.393	400.477	REAL	Cc1cc(C(=O)N2CCCC[C@@H]2[C@@H]2C[C@H](C)CC[C@@H]2O)nc2nc(O)[nH]c(=O)c12
vNsp16-as1-28	Z1103944103	-11.4	0.317	493.444	REAL	O=C(Nc1nc(-c2ccccc(C(F)(F)F)c2)n[nH]1)c1cccc(NC(=O)[C@@H]2Cc3ccccc3O2)c1
vNsp16-as1-29	Z1311423282	-11.4	0.356	430.467	REAL	Cc1cnn([C@H]2CCCc3ccccc32)c1NC(=O)c1cc(C)c2c(=O)[nH]c(O)nc2n1
vNsp16-as1-30	Z16225739	-11.4	0.335	467.508	REAL	C[C@@H](Sc1nnc2[nH]c3ccccc3n12)C(=O)Nc1ccc2c(c1)C(=O)c1ccccc1C2=O
vNsp16-as1-31	Z2021015830	-11.4	0.356	429.431	REAL	NC(=O)NC(=O)c1cccc(NC(=O)c2ccc3c(c2)C[C@H](c2ccccc2)OC3=O)c1
vNsp16-as1-32	Z2157917872	-11.4	0.38	401.385	REAL	C[C@]1(c2cccc(-c3noc(-c4nn[nH]c4-c4ccccc4)n3)c2)NC(=O)NC1=O
vNsp16-as1-33	Z2524830104	-11.4	0.326	463.579	REAL	O=C(c1ccc2[nH]c3ccccc3c(=O)c2c1)N1C[C@H]2CC[C@H]1[C@H]1CN(Cc3ccccc3)C[C@H]21
vNsp16-as1-34	Z30821612	-11.4	0.308	489.534	REAL	C[C@@]1(c2ccc3ccccc3c2)NC(=O)N(CC(=O)Nc2ccccc2-c2nc3ccccc3[nH]2)C1=O
vNsp16-as1-35	Z804767774	-11.4	0.326	467.524	REAL	CNC(=O)[C@@H]1CN(C(=O)[C@@H]2CC(=O)N(c3ccc4c(c3)Cc3ccccc3-4)C2)c2ccccc2O1
vNsp16-as1-36	ZINC000002366044	-11.4	0.317	471.515	ZINC15	O=C(c1ccccc1)[C@H]1[C@H]2C(=O)N(c3ccc4ccccc4c3)C(=O)[C@@H]2[C@H]2c3ccccc3C=NN12
vNsp16-as1-37	ZINC000002832254	-11.4	0.326	473.507	ZINC15	O=c1oc2ccc3ccccc3c2cc1-c1csc(-c2cc3c(ccc4ccccc43)oc2=O)n1
vNsp16-as1-38	ZINC000257195434	-11.4	0.317	492.578	ZINC15	O=C(NC1CCN(C(=O)N2C[C@@H]3[C@H](C2)[C@H]2CCCC(=O)N2C3)CC1)c1n[nH]c(=O)c2ccccc21
vNsp16-as1-39	PV-001819607375	-11.3	0.365	453.909	REAL	Cc1nn(-c2ccc(Cl)c2)c2sc(C(=O)Nc3cccc(C(=O)NC(N)=O)c3)cc12
vNsp16-as1-40	PV-001819607717	-11.3	0.365	453.909	REAL	Cc1nn(-c2ccc(Cl)cc2)c2sc(C(=O)Nc3cccc(C(=O)NC(N)=O)c3)cc12
vNsp16-as1-41	PV-001942502139	-11.3	0.332	476.454	REAL	Cc1ccc(NC(=O)c2cccc(C(F)(F)F)c2)cc1NC(=O)N1CC[C@H]2OCC(=O)N[C@@H]2C1
vNsp16-as1-42	PV-001948060730	-11.3	0.377	444.277	REAL	O=C1OCc2ccc(NC(=O)N3C[C@@H]4[C@H](C3)C(F)(F)C(F)(F)C(F)(F)C4(F)F)cc21
vNsp16-as1-43	Z1000267564	-11.3	0.314	497.534	REAL	O=C(Nc1cccc(C(=O)Nc2cccn2)c1)c1ccc(NC2=NS(=O)(=O)c3ccccc32)cc1
vNsp16-as1-44	Z1119589380	-11.3	0.342	481.6	REAL	O=C(Nc1nnc(CC2CCCCC2)s1)c1ccc(NC2=NS(=O)(=O)c3ccccc32)cc1
vNsp16-as1-45	Z1251065307	-11.3	0.365	423.476	REAL	Cc1cc(C(=O)N2CCC[C@@H](c3nnc4n3CCCCC4)C2)nc2nc(O)[nH]c(=O)c12
vNsp16-as1-46	Z1299132644	-11.3	0.342	439.47	REAL	NC(=O)[C@H]1c2ccccc2CCN1CC(=O)Nc1ccc2c(c1)C(=O)c1ccccc1C2=O
vNsp16-as1-47	Z1312796016	-11.3	0.377	405.417	REAL	Cc1cc(C(=O)N2CCC[C@@H](c3nnc4ccccn34)C2)nc2nc(O)[nH]c(=O)c12
vNsp16-as1-48	Z1313242018	-11.3	0.39	413.82	REAL	Cc1cc(C(=O)Nc2ccc(Cl)c(C(=O)NC3CC3)c2)nc2nc(O)[nH]c(=O)c12
vNsp16-as1-49	Z1314693539	-11.3	0.377	433.35	REAL	Cc1cc(C(=O)Nc2nc3cc4c(cc3s2)OC(F)(F)O4)nc2nc(O)[nH]c(=O)c12
vNsp16-as1-50	Z1383814912	-11.3	0.353	426.427	REAL	CC(=O)N1C[C@@H](C(=O)Nc2ccc3c(c2)C(=O)c2ccccc2C3=O)c2ccccc21
vNsp16-as1-51	Z1383816771	-11.3	0.332	451.481	REAL	CC(=O)N[C@@H](Cc1c[nH]c2ccccc12)C(=O)Nc1ccc2c(c1)C(=O)c1ccccc1C2=O
vNsp16-as1-52	Z1383818695	-11.3	0.365	410.428	REAL	CN1C(=O)C[C@@H](C(=O)Nc2ccc3c(c2)C(=O)c2ccccc2C3=O)c2ccccc21
vNsp16-as1-53	Z1421880357	-11.3	0.342	443.506	REAL	Cc1nc([C@H]2CCCN([C@@H](C)C(=O)Nc3ccc4c(c3)C(=O)c3ccccc3C4=O)C2)n[nH]1
vNsp16-as1-54	Z1576132713	-11.3	0.353	444.474	REAL	O=C(Nc1ccccc1-c1nnc[nH]1)c1ccc(NC2=NS(=O)(=O)c3ccccc32)cc1
vNsp16-as1-55	Z1602168895	-11.3	0.353	449.534	REAL	CC1(C)CC[C@H]2C[C@H](NC(=O)c3ccc4c(c3)S(=O)(=O)Nc3ncnn3-4)c3cccc1c32
vNsp16-as1-56	Z1603537098	-11.3	0.342	449.557	REAL	CC1(C)CC[C@H]2C[C@H](NC(=O)NNc3nc4c(cnn4C(C)(C)C)c(=O)[nH]3)c3cccc1c32
vNsp16-as1-57	Z1647941598	-11.3	0.365	416.407	REAL	O=C1CN(C(=O)c2ccc3c(c2)C[C@H](c2ccccc2)OC3=O)c2ccccc2N1
vNsp16-as1-58	Z1685319763	-11.3	0.353	422.447	REAL	Cc1nnc(-c2cccc(-c3noc(-c4cncc(-c5ccc6c(c5)CCO6)c4)n3)c2)[nH]1
vNsp16-as1-59	Z1685320660	-11.3	0.342	445.432	REAL	Cc1nnc(-c2cccc(-c3noc(-c4nn(-c5ccc(F)c(F)c5)c5c4CCC5)n3)c2)[nH]1
vNsp16-as1-60	Z1685321602	-11.3	0.377	394.437	REAL	Cc1cccc(-c2cncc(-c3nc(-c4cccc(-c5nnc(C)[nH]5)c4)no3)c2)c1
vNsp16-as1-61	Z1685324007	-11.3	0.404	370.375	REAL	Cc1nnc(-c2cccc(-c3noc(-c4cccc(-c5ncn[nH]5)c4)n3)c2)[nH]1
vNsp16-as1-62	Z1685380085	-11.3	0.404	371.355	REAL	COc1cc(-c2noc(-c3n[nH]c(=O)c4ccccc34)n2)c2ccccc2n1
vNsp16-as1-63	Z1765540692	-11.3	0.353	428.47	REAL	Cc1cccc2nc(C3CCN(c4ccc5nnc(-c6ccccc6F)n5n4)CC3)oc12
vNsp16-as1-64	Z1817778918	-11.3	0.353	431.49	REAL	C[C@H](C(=O)Nc1ccc2c(c1)C(=O)c1ccccc1C2=O)N1C[C@@H]2CCC[C@H]2[C@@H]1C(N)=O
vNsp16-as1-65	Z185066044	-11.3	0.332	468.536	REAL	O=C(Nc1ccc(Cc2cncc2)cc1)c1ccc(NC2=NS(=O)(=O)c3ccccc32)cc1
vNsp16-as1-66	Z1890371731	-11.3	0.377	397.393	REAL	O=C(Cc1noc(-c2n[nH]c(=O)c3ccccc23)n1)Nc1ccc2ccccc12
vNsp16-as1-67	Z1905519675	-11.3	0.39	394.557	REAL	CCC[C@@H](CCc1ccccc1)NC(=O)NC[C@@]1(O)[C@@H]2[C@@H]3C[C@@H]4[C@H]5[C@@H]3C[C@@H]2[C@H]5[C@@H]41
vNsp16-as1-68	Z1927716069	-11.3	0.353	430.502	REAL	C[C@H]1CN(C(=O)[C@@H]2CC(=O)c3ccccc32)C[C@@H](C)N1C(=O)[C@@H]1CC(=O)c2ccccc21
vNsp16-as1-69	Z1972675799	-11.3	0.365	418.456	REAL	Cc1cc(C(=O)N2CCC[C@@H](Cn3cnc4ccccc43)C2)nc2nc(O)[nH]c(=O)c12
vNsp16-as1-70	Z2021020620	-11.3	0.365	437.454	REAL	Cc1nn(-c2ccc(F)cc2)c2sc(C(=O)Nc3cccc(C(=O)NC(N)=O)c3)cc12
vNsp16-as1-71	Z2021023833	-11.3	0.377	419.464	REAL	Cc1nn(-c2ccccc2)c2sc(C(=O)Nc3cccc(C(=O)NC(N)=O)c3)cc12
vNsp16-as1-72	Z2021035950	-11.3	0.404	371.395	REAL	NC(=O)NC(=O)c1cccc(NC(=O)c2ccc3c(c2)-c2ccccc2C3)c1
vNsp16-as1-73	Z2166013088	-11.3	0.419	364.36	REAL	Cc1cc(=O)[nH]c2cc(C(=O)Nc3cccc(C(=O)NC(N)=O)c3)ccc12
vNsp16-as1-74	Z2167429497	-11.3	0.332	448.529	REAL	Cn1c(-c2nn(C)c(=O)c3ccccc23)nnc1N1CC=C(c2ccccc3ccccc23)CC1
vNsp16-as1-75	Z2477138047	-11.3	0.39	390.529	REAL	Cc1ncc2c(n1)CCC[C@@H]2NC(=O)N1CCC2(CCc3ccccc3C2)CC1
vNsp16-as1-76	Z358867962	-11.3	0.377	415.532	REAL	Cc1cccc([C@@H](CC(=O)O[C@@H](C)C(=O)N[C@@H](C)[C@H]2C[C@H]3CC[C@H]2C3)NC(N)=O)c1
vNsp16-as1-77	Z423679538	-11.3	0.323	485.523	REAL	O=C(Nc1cce2nc3n(c(=O)c2c1)CCC3)c1ccc(NC2=NS(=O)(=O)c3ccccc32)cc1
vNsp16-as1-78	Z809673240	-11.3	0.353	491.388	REAL	O=C(c1ccc2c(=O)n3c(nc2c1)CCCCC3)N1CCc2[nH]c3c(Br)cccc3c2C1
vNsp16-as1-79	ZINC000003848528	-11.3	0.323	459.46	ZINC15	Nc1cc(Nc2cc(N)c3c(c2)C(=O)c2cccc2C3=O)cc2c1C(=O)c1ccccc1C2=O
vNsp16-as1-80	ZINC000009331319	-11.3	0.342	441.461	ZINC15	O=C1Nc2ccc(F)cc2[C@@]12[C@@H]1C(=O)N(c3cccc4ccccc43)C(=O)[C@H]1[C@@H]1CCCN12
vNsp16-as1-81	ZINC000016038238	-11.3	0.305	505.96	ZINC15	O=C(c1ccc(Cl)cc1)[C@@H]1[C@@H]2C(=O)N(c3ccc4ccccc4c3)C(=O)[C@@H]2[C@H]2c3ccccc3C=NN12
vNsp16-as1-82	ZINC000018179759	-11.3	0.323	489.885	ZINC15	Cc1ccc(N2C(=O)[C@H]3[C@H](c4ccc(F)cc4)OC4(C(=O)c5ccccc5C4=O)[C@@H]3C2=O)cc1Cl
vNsp16-as1-83	ZINC000101343308	-11.3	0.342	457.916	ZINC15	O=C1Nc2c(cccc2Cl)[C@@]12[C@@H]1C(=O)N(c3cccc4ccccc43)C(=O)[C@H]1[C@@H]1CCCN12
vNsp16-as1-84	ZINC000102319789	-11.3	0.353	414.463	ZINC15	O=C1Nc2ccccc2/C1=C\c1ccc2ccc(/C=C3/C(=O)Nc4ccccc43)cc2c1
vNsp16-as1-85	ZINC000109965949	-11.3	0.323	475.571	ZINC15	O=S1(=O)c2ccccc2-c2cc(-c3nc(C4=CN[C@@H]5C=CC=C[C@@H]45)[nH]c3-c3ccccc3)ccc21
vNsp16-as1-86	PV-001825921630	-11.2	0.35	455.901	REAL	Cc1cc(C(=O)Nc2ccc(C(=O)N3CCCC[C@@H]3C)c(Cl)c2)nc2nc(O)[nH]c(=O)c12
vNsp16-as1-87	PV-001850783415	-11.2	0.373	404.381	REAL	COc1cc(C(=O)NNC(=O)[C@@H]2C(=O)Nc3ccccc3C2=O)c2ccccc2n1
vNsp16-as1-88	PV-001855726434	-11.2	0.361	429.365	REAL	Cc1nc(-c2cc(NC(=O)c3cccc(Nc4nnn[nH]4)c3)cc(C(F)(F)F)c2)n[nH]1
vNsp16-as1-89	PV-001856071464	-11.2	0.431	349.345	REAL	O=C(Nc1ccc2c(c1)CCCC2=O)c1cccc(-c2noc(O)n2)c1
vNsp16-as1-90	PV-001867570432	-11.2	0.386	398.545	REAL	CC(C)(C)OC(=O)N[C@H](c1ccccc1)C(C)(C)C(=O)N[C@@H]1C[C@H]2C[C@@H]1[C@H]1C[C@H]21
vNsp16-as1-91	PV-001919117310	-11.2	0.361	419.48	REAL	CNC(=O)[C@H]1CCC[C@@H]1N[C@@H](C)C(=O)Nc1ccc2c(c1)C(=O)c1ccccc1C2=O
vNsp16-as1-92	PV-001936962679	-11.2	0.415	412.573	REAL	CCCCS(=O)(=O)Nc1ccc(S(=O)(=O)NC[C@H]2C[C@H]3C=C[C@H]2CC3)cc1
vNsp16-as1-93	PV-001961487888	-11.2	0.361	458.348	REAL	O=C(N[C@H]1CCc2cc(O)ccc2C1)N1C[C@@H]2[C@@H](C1)C(F)(F)C(F)(F)C(F)(F)C2(F)F
vNsp16-as1-94	Z1023503068	-11.2	0.311	487.533	REAL	O=C(c1ccc2c(=O)n3c(nc2c1)CCCCC3)N1CCC[C@@H](c2nc(-c3cccc(F)c3)no2)C1
vNsp16-as1-95	Z1070098842	-11.2	0.329	455.509	REAL	O=C1O[C@H](c2ccccc2)Cc2cc(C(=O)N3CCC[C@@H]3c3ccc4c3OCCO4)ccc21
vNsp16-as1-96	Z1082317300	-11.2	0.329	457.445	REAL	C[C@@]1(c2ccc3ccccc3c2)NC(=O)N(CC(=O)Nc2ccccc(-c3noc(=O)[nH]3)c2)C1=O
vNsp16-as1-97	Z1097406844	-11.2	0.373	431.451	REAL	O=C(Nc1nnn[nH]1)c1cccc(S(=O)(=O)N2CCN(c3ccc(F)cc3)CC2)c1
vNsp16-as1-98	Z1099516426	-11.2	0.32	471.511	REAL	C[C@@]1(c2ccc3ccccc3c2)NC(=O)N(CC(=O)N2CCC[C@H]2c2ccc3c(c2)OCO3)C1=O
vNsp16-as1-99	Z1129122415	-11.2	0.311	484.554	REAL	NC(=O)C1CCN(c2nccc2CNC(=O)c2ccc3c(c2)C[C@H](c2ccccc2)OC3=O)CC1
vNsp16-as1-100	Z1250586272	-11.2	0.339	438.486	REAL	Cc1cc(C(=O)NC[C@H]2CC3c4ccccc4C2c2ccccc23)nc2nc(O)[nH]c(=O)c12

Supplementary Table 75. Top 100 virtual hits of the screen against the active site of nsp16 (Screen ID: 41). Compounds were filtered so that hits had MW < 600 dalton, cLogP < 6, number of hydrogen bond acceptors < 11, and no reactive functional groups. A few compounds unsuitable for drug discovery were removed by visual inspection. The name of each compound consists of the initial letter 'v' for virtual hit, followed by the target protein name and the target site ('as' for active site, 1 for docking scenario 1). The score is the docking score given by QuickVina 2 in kcal/mol. The ligand efficiency (LE) is computed as LE = -score/#NonH, where #NonH is the number of heavy (i.e. non hydrogen) atoms.

Name	Catalog ID	Score	LE	MW	Library	SMILES
vNsp16-as1-101	Z1250868715	-11.2	0.373	398.42	REAL	Cc1cc(C(=O)N2Cc3ccccc3-c3ccccc3C2)nc2nc(O)[nH]c(=O)c12
vNsp16-as1-102	Z1314146635	-11.2	0.350	430.47	REAL	Cc1cc(C(=O)Nc2cc(C3CCCC3)nn2-c2ccccc2)nc2nc(O)[nH]c(=O)c12
vNsp16-as1-103	Z1374246802	-11.2	0.373	404.47	REAL	Cc1cc(C(=O)N2CCC[C@@]3(CCCc4ccccc43)C2)nc2nc(O)[nH]c(=O)c12
vNsp16-as1-104	Z1518008193	-11.2	0.361	418.46	REAL	Cc1cc(C(=O)N2CCC[C@H]2Cn2c(C)nc3ccccc32)nc2nc(O)[nH]c(=O)c12
vNsp16-as1-105	Z1549996196	-11.2	0.350	433.47	REAL	C[C@@]1(c2ccc3ccccc3c2)NC(=O)N(CC(=O)N2CCC[C@H](c3nnn[nH]3)C2)C1=O
vNsp16-as1-106	Z1620488094	-11.2	0.373	402.50	REAL	Cc1ccc2[nH]c3c(c2c1)C[C@@H](NC(=O)Nc1ccc2c(c1)CCCC(=O)N2)CC3
vNsp16-as1-107	Z1685319746	-11.2	0.373	394.44	REAL	Cc1ccc(-c2cncc(-c3nc(-c4cccc(-c5nnc(C)[nH]5)c4)no3)c2)cc1
vNsp16-as1-108	Z1685322651	-11.2	0.415	422.25	REAL	Cc1nnc(-c2cccc(-c3noc(-c4n[nH]c5ccc(Br)cc45)n3)c2)[nH]1
vNsp16-as1-109	Z1902877949	-11.2	0.361	426.56	REAL	CCOCCOCc1cccc(NC(=O)NC[C@@]2(O)[C@@H]3[C@@H]4C[C@@H]5[C@@H]6[C@@H]4C[C@@H]3[C@@H]6[C@@H]52)c1C
vNsp16-as1-110	Z19986062	-11.2	0.311	495.52	REAL	C[C@H](Sc1nnc2c(=O)[nH]c3ccccc3n12)C(=O)Nc1ccc2c(c1)C(=O)c1ccccc1C2=O
vNsp16-as1-111	Z2001002581	-11.2	0.373	408.46	REAL	Cc1cc(C(=O)N2CCC[C@@H](c3ncc4n3CCCC4)C2)nc2nc(O)[nH]c(=O)c12
vNsp16-as1-112	Z2007490921	-11.2	0.350	445.91	REAL	Cn1c(-c2nn(C)c(=O)c3ccccc23)nnc1N1CCn2c(cc3cc(Cl)ccc32)C1
vNsp16-as1-113	Z2008042363	-11.2	0.350	434.54	REAL	Cn1c(-c2nn(C)c(=O)c3ccccc23)nnc1N1CC(C)(C)O[C@@]2(C[C@@H]3CC[C@H]2C3)C1
vNsp16-as1-114	Z2008605395	-11.2	0.350	445.91	REAL	Cn1c(-c2nn(C)c(=O)c3ccccc23)nnc1N1CCn2c(cc3c(Cl)ccc32)C1
vNsp16-as1-115	Z2021028408	-11.2	0.361	424.46	REAL	COc1ccc([C@H]2[C@H](C(=O)Nc3cccc(C(=O)NC(N)=O)c3)CCC(=O)N2C)cc1
vNsp16-as1-116	Z2021035964	-11.2	0.431	353.33	REAL	NC(=O)NC(=O)c1cccc(NC(=O)[C@H]2Cc3ccccc3C(=O)O2)c1
vNsp16-as1-117	Z2027285076	-11.2	0.373	404.43	REAL	Cc1c(C(=O)N2CCC[C@H](c3nc(=O)[nH][nH]3)C2)nnn1-c1cccc2ccccc12
vNsp16-as1-118	Z2158387743	-11.2	0.431	345.32	REAL	O=c1[nH]c2ccc(-c3noc(-c4nn[nH]c4-c4ccccc4)n3)cc2[nH]1
vNsp16-as1-119	Z2158538047	-11.2	0.350	420.43	REAL	Cc1nnc(-c2cccc(-c3noc(-c4ccc5[nH]c6ccccc6c(=O)c5c4)n3)c2)[nH]1
vNsp16-as1-120	Z2158538668	-11.2	0.386	389.35	REAL	Cc1nnc(-c2cccc(-c3noc(-c4cc(=O)c5ccc(F)cc5o4)n3)c2)[nH]1
vNsp16-as1-121	Z2159358087	-11.2	0.373	396.41	REAL	O=C(Cc1noc(-c2c[nH]c(=O)c3ccccc23)n1)Nc1ccccc2ccccc12
vNsp16-as1-122	Z2159455398	-11.2	0.339	438.49	REAL	O=C(Cc1noc(-c2cccc3c4c([nH]c23)CCCC4)n1)N1CCn2c1nc1ccccc12
vNsp16-as1-123	Z2167125700	-11.2	0.350	420.48	REAL	Cn1c(-c2n[nH]c(=O)c3ccccc23)nnc1N1C[C@H](c2ccccc2)c2ccccc21
vNsp16-as1-124	Z2192883693	-11.2	0.339	438.48	REAL	O=C(c1cccc(N2C(=O)c3ccccc3C2=O)c1)N1CC[C@]2(CCc3ccccc3O2)C1
vNsp16-as1-125	Z2221676441	-11.2	0.350	430.42	REAL	O=C(NCc1ccc(C(=O)Nc2nnn[nH]2)o1)OCC1c2ccccc2-c2ccccc21
vNsp16-as1-126	Z2225639873	-11.2	0.386	383.41	REAL	Cc1ccc(-c2n[nH]c(=O)[nH]2)cc1NC(=O)c1cc2c(ccc3ccccc32)[nH]1
vNsp16-as1-127	Z2233385027	-11.2	0.373	403.45	REAL	Cc1c(C(=O)N2CCC(c3nnc(N)[nH]3)CC2)nnn1-c1ccccc2ccccc12
vNsp16-as1-128	Z2311242839	-11.2	0.386	398.46	REAL	CCOC(=O)c1ccn(-c2ccccc(NC(=O)NCC[C@H]3C[C@H]4CC[C@H]3O4)c2)n1
vNsp16-as1-129	Z2524820794	-11.2	0.329	454.57	REAL	O=C(c1ccc2c(=O)n3c(nc2c1)CCC3)N1C[C@H]2CC[C@H]1[C@H]1CN(Cc3ccccc3)C[C@H]21
vNsp16-as1-130	Z2635781403	-11.2	0.400	397.45	REAL	O=C(c1cccc(-c2noc(O)n2)c1)N1CCC2(CC1)OCCc1ccsc12
vNsp16-as1-131	Z2651485617	-11.2	0.311	482.54	REAL	C[C@@H](C(=O)Nc1ccc2c(c1)C(=O)c1ccccc1C2=O)N1CCc2ccenc2N2C[C@H](O)C[C@H]2C1
vNsp16-as1-132	Z2893088283	-11.2	0.400	376.42	REAL	O=C(c1cccc(Nc2nnn[nH]2)c1)N1CCC2(CC1)OCc1ccccc12
vNsp16-as1-133	Z366886766	-11.2	0.350	446.49	REAL	O=C1CCc2cc(NC(=O)c3ccc(NC4=NS(=O)(=O)c5ccccc54)cc3)ccc2N1
vNsp16-as1-134	Z448673852	-11.2	0.311	479.54	REAL	Cn1nc(C(=O)NNC(=O)NC[C@H]2CC3c4ccccc4C2c2ccccc23)c2ccccc2c1=O
vNsp16-as1-135	Z466430298	-11.2	0.311	475.55	REAL	O=C(c1cncc(C(=O)N2CCc3[nH]c4ccccc4c3C2)c1)N1CCc2[nH]c3ccccc3c2C1
vNsp16-as1-136	Z605714468	-11.2	0.361	416.44	REAL	Cc1nc(-c2cccc(NC(=O)CN3C(=O)N[C@@]4(CCc5ccccc54)C3=O)c2)n[nH]1
vNsp16-as1-137	Z63697560	-11.2	0.320	468.47	REAL	Cn1nc(C(=O)NNC(=O)c2ccc3c(c2)C[C@H](c2ccccc2)OC3=O)c2ccccc2c1=O
vNsp16-as1-138	Z66805028	-11.2	0.320	466.45	REAL	C[C@H](OC(=O)c1cc2ccccc2c(=O)[nH]1)C(=O)Nc1ccc2c(c1)C(=O)c1ccccc1C2=O
vNsp16-as1-139	Z795029940	-11.2	0.311	480.48	REAL	C[C@@H](OC(=O)c1cc(=O)n(C)c2ccccc12)C(=O)Nc1ccc2c(c1)C(=O)c1ccccc1C2=O
vNsp16-as1-140	Z91830275	-11.2	0.320	467.44	REAL	C[C@H](OC(=O)c1n[nH]c(=O)c2ccccc12)C(=O)Nc1ccc2c(c1)C(=O)c1ccccc1C2=O
vNsp16-as1-141	ZINC000002115916	-11.2	0.339	438.48	ZINC15	Cc1cc(C)cc(COc2ccc3c(-c4cc5ccccc5oc4=O)cc(=O)oc3c2C)c1
vNsp16-as1-142	ZINC000002267002	-11.2	0.361	406.40	ZINC15	O=c1oc2ccc3ccccc3c2cc1-c1nnc(-c2cc3ccccc3cc2O)o1
vNsp16-as1-143	ZINC000003873988	-11.2	0.339	429.43	ZINC15	O=C1c2ccccc2C(=O)c2c(Nc3ccc4c3C(=O)c3ccccc3C4=O)cccc21
vNsp16-as1-144	ZINC000004522785	-11.2	0.329	444.45	ZINC15	Nc1ccccc2c1C(=O)c1cccc(Nc3ccc4c(c3)C(=O)c3ccccc3C4=O)c1C2=O
vNsp16-as1-145	ZINC000008790817	-11.2	0.311	494.42	ZINC15	COc1cccc2cc(-c3cc(=O)oc4cc(OCc5ccccc(C(F)(F)F)c5)ccc43)c(=O)oc21
vNsp16-as1-146	ZINC000013070266	-11.2	0.320	467.57	ZINC15	Cc1cccc(N2CCN([C@H](C)C(=O)Nc3ccc4c(c3)C(=O)c3ccccc3C4=O)CC2)c1C
vNsp16-as1-147	ZINC000013593240	-11.2	0.339	447.53	ZINC15	Cc1ccc(C)c(N2N=C(C(=O)N3CCc4cc5c(cc4[C@@H]3C)OCCCO5)CCC2=O)c1
vNsp16-as1-148	ZINC000014883611	-11.2	0.311	478.60	ZINC15	Cc1ccccc1-c1cc(C(=O)N2CCN([C@H]3CCc4ccccc4C3)CC2)cc(-n2cnnn2)c1
vNsp16-as1-149	ZINC000015999302	-11.2	0.329	471.94	ZINC15	Cc1c2c(ccc1Cl)[C@]1(C(=O)N2)[C@@H]2C(=O)N(c3ccc4ccccc4c3)C(=O)[C@@H]2[C@@H]2CCCN21
vNsp16-as1-150	ZINC000020533850	-11.2	0.295	519.52	ZINC15	O=C(c1cc(-c2ccc3c(c2)OCCO3)nc2ccccc21)N1CCN(c2cccc(C(F)(F)F)c2)CC1
vNsp16-as1-151	ZINC000100414424	-11.2	0.295	499.52	ZINC15	O=C1c2ccccc2C(=O)C12O[C@@H](c1ccccc1)[C@@H]1C(=O)N(c3ccc(-c4ccccc4)cc3)C(=O)[C@H]12
vNsp16-as1-152	ZINC000100505726	-11.2	0.303	488.54	ZINC15	O=C1[C@@H]2[C@H]3C=C[C@@H](C3)[C@@H]2C(=O)N1c1ccc2c(c1)-c1cc(N3C(=O)[C@@H]4[C@@H]5C=C[C@@H](C5)[C@@H]4C3=O)ccc1C2
vNsp16-as1-153	ZINC000109965942	-11.2	0.320	475.57	ZINC15	O=S1(=O)c2ccccc2-c2cc(-c3nc(C4=CN[C@@H]5C=CC=C[C@H]45)[nH]c3-c3ccccc3)ccc21
vNsp16-as1-154	ZINC000257197297	-11.2	0.373	396.49	ZINC15	O=C(c1ccc2ncccc2c1)N1CCC2(CC1)NCCc1c3ccccc3[nH]c12
vNsp16-as1-155	ZINC000257315128	-11.2	0.320	478.52	ZINC15	Cc1nn(C)c2ccc(C(=O)N3CCC[C@H](c4cccc(-c5ccccc(C(F)(F)F)c5)n4)C3)cc12
vNsp16-as1-156	ZINC000408733648	-11.2	0.303	485.54	ZINC15	Cc1ccc2c(c1)OC(=O)[C@@H]1C2=C[C@H](c2ccccc2)[C@@H]2C(=O)N(c3ccc4ccccc4c3)C(=O)[C@@H]21
vNsp16-as1-157	PV-000067512910	-11.1	0.411	365.44	REAL	O=C([C@H]1[C@H]2Cc3ccccc3[C@@H]21)N1C[C@H]2CCN(Cc3nc(=O)[nH][nH]3)C[C@H]21
vNsp16-as1-158	PV-001819607694	-11.1	0.383	459.26	REAL	C[C@@H](C(=O)Nc1cccc(C(=O)NC(N)=O)c1)N1C(=O)c2ccc(Br)cc2C1=O
vNsp16-as1-159	PV-001827827279	-11.1	0.383	385.47	REAL	CNC(=O)Nc1cccc(C(=O)N2CC=C(c3cccc4ccccc34)CC2)c1
vNsp16-as1-160	PV-001849703681	-11.1	0.347	430.51	REAL	CC(=O)Nc1cc(NC(C)=O)cc(C(=O)N2CCC(c3ccnc4ccccc34)CC2)c1
vNsp16-as1-161	PV-001855725522	-11.1	0.358	427.39	REAL	CNc1ncnc2cc(C(=O)Nc3cc(-c4n[nH]c(C)n4)cc(C(F)(F)F)c3)ccc12
vNsp16-as1-162	PV-001855725658	-11.1	0.347	444.37	REAL	Cc1nc(-c2cc(NC(=O)c3ccc4c(c3)NC(=O)CNC4=O)cc(C(F)(F)F)c2)n[nH]1
vNsp16-as1-163	PV-001871264419	-11.1	0.358	425.49	REAL	CNC(=O)N[C@@H]1CCCN(C(=O)c2cccc(NN3C(=O)[C@H]4CC=CC[C@@H]4C3=O)c2)C1
vNsp16-as1-164	PV-001875532156	-11.1	0.358	454.32	REAL	Cc1c(C(=O)N2C[C@@H]3[C@H](C2)C(F)(F)C(F)(F)C(F)(F)C3(F)F)[nH]c(=O)c2ccccc12
vNsp16-as1-165	PV-001922309539	-11.1	0.347	434.49	REAL	CNC(=O)N[C@@H]1CCCN([C@@H](C)C(=O)Nc2ccc3c(c2)C(=O)c2ccccc2C3=O)C1
vNsp16-as1-166	PV-001943072115	-11.1	0.396	422.29	REAL	O=C(NCc1nc(C(F)(F)F)n[nH]1)Nc1nc2cc3c(cc2s1)OC(F)(F)O3
vNsp16-as1-167	PV-001948672381	-11.1	0.336	454.41	REAL	Cc1nc(-c2cc(NC(=O)NNC(=O)c3cccc4ccccc34)cc(C(F)(F)F)c2)n[nH]1
vNsp16-as1-168	PV-001948675298	-11.1	0.347	446.39	REAL	Cc1nc(-c2cc(NC(=O)N[C@@H](C)c3ccc4[nH]c(=O)oc4c3)cc(C(F)(F)F)c2)n[nH]1
vNsp16-as1-169	PV-001948780035	-11.1	0.370	440.29	REAL	O=C(Nc1cc2ccccc2nn1)N1C[C@H]2[C@H](C1)C(F)(F)C(F)(F)C(F)(F)C2(F)F
vNsp16-as1-170	PV-001952317032	-11.1	0.370	409.45	REAL	Cc1ncccnc1NC(=O)N1CCC(C(=O)c2ccc3c(c2)NC(=O)[C@H](C)O3)CC1
vNsp16-as1-171	Z1071336848	-11.1	0.370	408.46	REAL	Cc1ccccnc1NC(=O)N1CCC(C(=O)c2ccc3c(c2)NC(=O)[C@H](C)O3)CC1
vNsp16-as1-172	Z1102637178	-11.1	0.326	476.53	REAL	O=C1O[C@H](c2ccccc2)Cc2cc(C(=O)N3CSC[C@@H]3C(=O)Nc3cccc(F)c3)ccc21
vNsp16-as1-173	Z1117098552	-11.1	0.308	488.57	REAL	O=C1Nc2ccccc2[C@H]1C1CCN(C(=O)Nc2cc(-c3nnc4n3CCCCC4)ccc2F)CC1
vNsp16-as1-174	Z1121634825	-11.1	0.326	452.47	REAL	O=C(Nc1cccc(-c2noc(=O)[nH]2)c1)[C@H]1CC(=O)N(c2ccc3c(c2)Cc2ccccc2-3)C1
vNsp16-as1-175	Z1169877991	-11.1	0.370	405.37	REAL	O=C(Cc1noc(-c2n[nH]c(=O)c3ccccc23)n1)Nc1ccc2c(c1)OCCO2
vNsp16-as1-176	Z1232083743	-11.1	0.396	418.86	REAL	O=C(Nc1nnn[nH]1)c1cc(S(=O)(=O)N2CCc3ccccc3C2)ccc1Cl
vNsp16-as1-177	Z1270035870	-11.1	0.358	436.50	REAL	Cc1cc(C(=O)NC2CCN(c3nc4ccccc4s3)CC2)nc2nc(O)[nH]c(=O)c12
vNsp16-as1-178	Z1311220604	-11.1	0.336	445.48	REAL	Cc1ccc(-c2nnc3n2CCCCC3)cc1NC(=O)c1cc(C)c2c(=O)[nH]c(O)nc2n1
vNsp16-as1-179	Z132917176	-11.1	0.326	447.46	REAL	Cc1ccc(N2C(=O)/C(=C\Nc3nc4ccccc4n4nnnc34)c3ccccc3C2=O)cc1
vNsp16-as1-180	Z1347909154	-11.1	0.336	448.57	REAL	Cc1cccC(=O)N2C[C@@H](C)C[C@H](C)C2)cc1NC(=O)c1ccc2c(c1)NC(=O)[C@H](C)N2C
vNsp16-as1-181	Z1383805436	-11.1	0.358	414.39	REAL	O=C1C[C@@H](C(=O)Nc2ccc3c(c2)C(=O)c2cccc2C3=O)c2ccc(F)cc2N1
vNsp16-as1-182	Z1383807552	-11.1	0.370	399.40	REAL	C[C@H]1Oc2ccccc2O[C@H]1C(=O)Nc1ccc2c(c1)C(=O)c1ccccc1C2=O
vNsp16-as1-183	Z1383817718	-11.1	0.336	440.41	REAL	Cn1c(=O)c2ccc(C(=O)Nc3ccc4c(c3)C(=O)c3ccccc3C4=O)nc2n(C)c1=O
vNsp16-as1-184	Z1421893269	-11.1	0.336	443.51	REAL	Cc1nc([C@H]2CCCN([C@@H](C)C(=O)Nc3cccc4c3C(=O)c3ccccc3C4=O)C2)n[nH]1
vNsp16-as1-185	Z14229668	-11.1	0.347	432.48	REAL	CC1(C)C(=O)Nc2ccccc2N1C(=O)CN1C(=O)N[C@@]2(CCc3ccccc3C2)C1=O
vNsp16-as1-186	Z1453324339	-11.1	0.383	398.46	REAL	Cc1cc(C(=O)N2CCCCC[C@H]2[C@@H]2CCCCC2=O)nc2nc(O)[nH]c(=O)c12
vNsp16-as1-187	Z1461552102	-11.1	0.336	441.49	REAL	Cn1ncc2c(=O)[nH]c(NNC(=O)NC[C@@H]3CC4c5ccccc5C3c3ccccc34)nc21
vNsp16-as1-188	Z1498283742	-11.1	0.370	394.48	REAL	O=c1[nH]c(N2CCN(C3c4ccccc4-c4ccccc43)CC2)nc2ccccc12
vNsp16-as1-189	Z1518719462	-11.1	0.370	404.43	REAL	Cc1cc(C(=O)N2CCC[C@H]2Cn2cnc3ccccc32)nc2nc(O)[nH]c(=O)c12
vNsp16-as1-190	Z1531740169	-11.1	0.358	417.37	REAL	O=C(Nc1ccn(-c2ncccc2F)n1)c1ccc2noc(-c3ccc(F)cc3)c2c1
vNsp16-as1-191	Z1552593243	-11.1	0.347	432.53	REAL	CC(=O)N1CCN(C(=O)c2nnn(-c3cccc4cnccc34)c2C)CC12CCCCC2
vNsp16-as1-192	Z1563751055	-11.1	0.336	442.48	REAL	C[C@@H]1CN(C(=O)c2cccc(-c3ncn[nH]3)c2)CCN1C(=O)c1cccc(-c2ncn[nH]2)c1
vNsp16-as1-193	Z1603534066	-11.1	0.347	431.50	REAL	CC1(C)CC[C@@H]2C[C@@H](NC(=O)NNC(=O)c3n[nH]c(=O)c4ccccc34)c3cccc1c32
vNsp16-as1-194	Z1603536335	-11.1	0.370	407.48	REAL	Cn1ncc2c(=O)[nH]c(NNC(=O)N[C@H]3C[C@@H]4CCC(C)(C)c5cccc3c54)nc21
vNsp16-as1-195	Z1632951313	-11.1	0.336	447.51	REAL	O=C(N[C@@H]1CCc2nnc(-c3ccc(F)cc3)n2C1)N1CCO[C@@]2(CCc3ccccc32)C1
vNsp16-as1-196	Z1671920238	-11.1	0.358	414.47	REAL	Cc1cnn(-c2ccc(C(N)=O)cc2NC(=O)N2CCc3c([nH]c4ccccc34)C2)c1
vNsp16-as1-197	Z1682437003	-11.1	0.383	409.38	REAL	O=C1c2ccccc2S(=O)(=O)N1Cc1noc(-c2n[nH]c(=O)c3ccccc23)n1
vNsp16-as1-198	Z1684579693	-11.1	0.370	404.43	REAL	C[C@]1(c2cccc(-c3noc(-c4cc5c(cc4O)CCCC5)n3)c2)NC(=O)NC1=O
vNsp16-as1-199	Z1685087138	-11.1	0.336	439.47	REAL	O=C(c1cccc2ccccc12)N1CCC(c2nc(-c3ccc4[nH]c(=O)[nH]c4c3)no2)CC1
vNsp16-as1-200	Z1685319347	-11.1	0.383	386.39	REAL	Cc1nnc(-c2cccc(-c3noc(-c4cc5ccc(F)cc5nc4C)n3)c2)[nH]1

Supplementary Table 76. Virtual screening hits 101 to 200 of the screen against the active site of nsp16 (Screen ID: 41). Compounds were filtered so that hits had MW < 600 dalton, cLogP < 6, number of hydrogen bond acceptors < 11, and no reactive functional groups. A few compounds unsuitable for drug discovery were removed by visual inspection. The name of each compound consists of the initial letter 'v' for virtual hit, followed by the target protein name and the target site ('as' for active site, 1 for docking scenario 1). The score is the docking score given by QuickVina 2 in kcal/mol. The ligand efficiency (LE) is computed as LE = -score/#NonH, where #NonH is the number of heavy (i.e. non hydrogen) atoms.

Name	Catalog ID	Score	LE	MW	Library	SMILES
vNsp16-nsp10.1-1	PV-001866716609	-10.2	0.378	408.585	REAL	CSCC[C@@H](NS(=O)(=O)c1ccccc1)C(=O)NC[C@@H]1C[C@@H]2C[C@@H]1[C@@H]1C[C@@H]21
vNsp16-nsp10.1-2	Z46616205	-10	0.294	490.555	REAL	O=C1/C(=C/c2ccc(/C=C3/CS(=O)(=O)c4ccccc4C3=O)cc2)CS(=O)(=O)c2ccccc21
vNsp16-nsp10.1-3	ZINC000408679811	-10	0.263	498.58	ZINC15	Cc1cc(C)cc(NC(=O)c2cccc(N3C(=O)[C@H]4[C@@H](C3=O)C3c5ccccc5C4c4ccccc43)c2)c1
vNsp16-nsp10.1-4	Z2002795192	-9.9	0.367	387.862	REAL	CCOCCOc1c(Cl)cccc1NC(=O)[C@]12[C@@H]3C(=O)[C@H]4[C@@H]5[C@H]([C@H]41)[C@@H]2[C@@H]53
vNsp16-nsp10.1-5	Z510365356	-9.9	0.283	470.484	REAL	CC(=O)N1C[C@H](C(=O)Nc2ccc(C(=O)N3CC(=O)Nc4ccccc43)cc2)Oc2ccccc21
vNsp16-nsp10.1-6	Z1161529919	-9.8	0.288	455.513	REAL	O=C(Cc1ccc(N[C@@H]2CC(=O)N(c3cccc(O)c3)C2=O)cc1)N1CCCc2ccccc21
vNsp16-nsp10.1-7	Z1165732852	-9.8	0.306	438.458	REAL	O=C(Cc1ccc(NC(=O)C2CCC3(CC2)NC(=O)NC3=O)cc1)Nc1ccccc1F
vNsp16-nsp10.1-8	Z1559283665	-9.8	0.297	437.502	REAL	O=C(Nc1ccc(CC(=O)N2CCCc3ccccc32)cc1)c1cccc(-c2ncn[nH]2)c1
vNsp16-nsp10.1-9	Z998874814	-9.8	0.265	499.569	REAL	O=C(c1ccc2[nH]ncc2c1)N1CCC[C@H](C(=O)N2CCC(CN3C(=O)c4ccccc4C3=O)CC2)C1
vNsp16-nsp10.1-10	Z1075646216	-9.7	0.285	453.584	REAL	Cc1ccc(C(=O)N2CCC(NC(=O)N3Cc4ccccc4[C@@H](c4ccccc4)C3)CC2)cc1
vNsp16-nsp10.1-11	Z1094946006	-9.7	0.269	477.479	REAL	O=C(Cc1noc2ccccc12)Nc1ccc2nc(NC(=O)Cc3noc4ccccc34)ccc2c1
vNsp16-nsp10.1-12	Z1684170407	-9.7	0.294	440.458	REAL	NC(=O)c1ccccc(Cc2noc(-c3cccc(NC(=O)[C@@H]4Cc5ccccc5O4)c3)n2)c1
vNsp16-nsp10.1-13	Z1684693872	-9.7	0.303	423.471	REAL	O=C(Nc1cccc(-c2nc(C3Cc4ccccc4C3)no2)c1)[C@@H]1Cc2ccccc2O1
vNsp16-nsp10.1-14	Z1728627932	-9.7	0.285	448.477	REAL	O=C1C/C(=C/c2ccc(/C=C3\CC(=O)Nc4ccccc4C3=O)cc2)C(=O)c2ccccc2N1
vNsp16-nsp10.1-15	Z1827808809	-9.7	0.294	442.478	REAL	Cc1n[nH]c(-c2ccc(NC(=O)c3cccc(NN4C(=O)[C@@H]5CC=CC[C@@H]5C4=O)c3)cc2)n1
vNsp16-nsp10.1-16	Z1869819485	-9.7	0.303	442.542	REAL	O=C(Nc1ccc(CC(=O)N2CCCc3ccccc32)cc1)c1ccc(-c2cc[nH]n2)s1
vNsp16-nsp10.1-17	Z2067513613	-9.7	0.303	438.545	REAL	CN(C)C(=O)CN1[C@H]2CC[C@H]1CC(N[C@@H](C(=O)Nc1ccc(F)cc1)c1ccccc1)C2
vNsp16-nsp10.1-18	Z2811870539	-9.7	0.373	352.437	REAL	C[C@H](Cn1ncc2ccccc2c1=O)NC(=O)N[C@H]1C[C@@H]2C[C@H]1[C@@H]1C[C@@H]21
vNsp16-nsp10.1-19	ZINC000017862766	-9.7	0.243	520.587	ZINC15	O=C(Nc1ccc2ccccc2c1)c1cccc(N2C(=O)[C@H]3[C@@H](C2=O)C2c4ccccc4C3c3ccccc32)c1
vNsp16-nsp10.1-20	ZINC000409414682	-9.7	0.285	454.524	ZINC15	Cc1oc2cc3oc(=O)c(CC(=O)N[C@@H]4CCCc5c6ccccc6[nH]c54)c(C)c3cc2c1C
vNsp16-nsp10.1-21	Z1101973114	-9.6	0.282	475.568	REAL	O=C1CCCc2cc(NC(=O)c3cccc(S(=O)(=O)N4CCCc5ccccc54)c3)ccc2N1
vNsp16-nsp10.1-22	Z1162075545	-9.6	0.267	490.562	REAL	CN1CC(=O)N(c2cccc(NC(=O)N3CCN(CC(=O)N4CCCc5ccccc54)CC3)c2)C1=O
vNsp16-nsp10.1-23	Z1266331370	-9.6	0.3	419.483	REAL	O=C(Nc1ccc2nc(NC(=O)[C@@H]3Cc4ccccc43)ccc2c1)[C@H]1Cc2ccccc21
vNsp16-nsp10.1-24	Z1449094151	-9.6	0.282	448.564	REAL	O=C(NC[C@H]1[C@H]2Cc3ccccc3[C@@H]12)c1ccc(C(=O)NC[C@H]2[C@@H]3Cc4ccccc4[C@@H]23)cc1
vNsp16-nsp10.1-25	Z1666177453	-9.6	0.291	439.518	REAL	O=C(NCc1ccc(Cn2cnc3ccccc32)cc1)NCc1ccc2c(c1)C(=O)NCC2
vNsp16-nsp10.1-26	Z1685223778	-9.6	0.291	437.502	REAL	O=c1[nH]c2ccc(NCc3ccc(-c4noc([C@H]5CCCc6ccccc65)n4)cc3)cc2[nH]1
vNsp16-nsp10.1-27	Z1864295572	-9.6	0.291	447.508	REAL	C[C@H](NC(=O)N[C@H]1Cc2cccc(O)c2C1)c1cccc(NC(=O)Cc2ccccc2F)c1
vNsp16-nsp10.1-28	Z1865902276	-9.6	0.31	419.455	REAL	O=C(Cc1ccc(NC(=O)N[C@H]2Cc3cccc(O)c3C2)cc1)Nc1ccccc1F
vNsp16-nsp10.1-29	Z1867843510	-9.6	0.3	428.487	REAL	O=C(N[C@H]1Cc2cccc(O)c2C1)c1ccc(C(=O)N[C@H]2Cc3cccc(O)c3C2)cc1
vNsp16-nsp10.1-30	Z1891179081	-9.6	0.291	437.458	REAL	O=C(Nc1cccc(-c2nc(Cc3ccc4cn[nH]c4c3)no2)c1)[C@@H]1Cc2ccccc2O1
vNsp16-nsp10.1-31	Z1907681358	-9.6	0.331	414.524	REAL	C=CCNS(=O)(=O)c1ccc(C(=O)NC[C@]2(O)[C@H]3[C@@H]4[C@@H]5[C@@H]6[C@H]4[C@H]3[C@H]6[C@H]52)cc1
vNsp16-nsp10.1-32	Z2021542666	-9.6	0.291	443.462	REAL	O=C(Nc1ccc(-c2cc(=O)[nH][nH]2)cc1)c1cccc(NN2C(=O)[C@@H]3CC=CC[C@@H]3C2=O)c1
vNsp16-nsp10.1-33	Z2158178078	-9.6	0.3	421.459	REAL	CN1C[C@H](c2nc(-c3ccc(-c4nc5ccccc5[nH]4)cc3)no2)c2ccccc2C1=O
vNsp16-nsp10.1-34	Z2174533720	-9.6	0.291	445.517	REAL	O=C1C[C@]2(CCN(C(=O)C3[C@@H]4[C@@H]5C=C[C@@H]([C@H]6C(=O)N(Cc7ccccc7)C(=O)[C@H]56)[C@H]34)C2)CN1
vNsp16-nsp10.1-35	Z2785110607	-9.6	0.356	365.428	REAL	CCCOc1ccccc1C(=O)CNC(=O)[C@]12[C@@H]3C(=O)[C@@H]4[C@H]5C[C@@H]([C@@H]41)[C@@H]2[C@H]53
vNsp16-nsp10.1-36	Z512238600	-9.6	0.274	476.507	REAL	C[C@@H]1Oc2ccc(NC(=O)N[C@H](C)c3cccc(NC(=O)Cc4ccccc4F)c3)cc2NC1=O
vNsp16-nsp10.1-37	Z859085676	-9.6	0.282	460.464	REAL	C[C@@H](NC(=O)Nc1ccc2c(c1)C(=O)NC2=O)c1cccc(NC(=O)Cc2ccccc2F)c1
vNsp16-nsp10.1-38	ZINC000004015296	-9.6	0.253	493.477	ZINC15	O=c1nc2c3cccc4cccc(c(=O)n2c2cc(N5C(=O)c6cccc7cccc(c76)C5=O)ccc12)c43
vNsp16-nsp10.1-39	PV-001809418707	-9.5	0.288	441.573	REAL	Cc1cccc(-c2cccc(C(=O)NCc3ccc(CN4CCC(C(N)=O)CC4)cc3)c2)c1
vNsp16-nsp10.1-40	PV-001949217361	-9.5	0.279	458.492	REAL	C[C@@H](NC(=O)Nc1ccc2c(=O)[nH]ccc2c1)c1cccc(NC(=O)Cc2ccccc2F)c1
vNsp16-nsp10.1-41	PV-001954449705	-9.5	0.279	456.588	REAL	Cc1ccc(-c2cccc(CNC(=O)NCc3ccc(N4CCC[C@@H](C(N)=O)C4)cc3)c2)cc1
vNsp16-nsp10.1-42	PV-001955903293	-9.5	0.297	445.483	REAL	Cc1ccc(C(=O)N2CCC(NC(=O)N3CCc4c(cccc4C(F)(F)F)C3)CC2)cc1
vNsp16-nsp10.1-43	Z1003529826	-9.5	0.279	477.496	REAL	O=C(c1cccc(OS(=O)(=O)c2ccc3[nH]c(=O)[nH]c(=O)c3c2)c1)N1CCc2ccccc2C1
vNsp16-nsp10.1-44	Z1014477988	-9.5	0.264	482.582	REAL	C[C@@H](NC(=O)[C@H]1C[C@@H]2CCCC[C@H]2N1C(=O)c1ccc2ccccc2c1)c1ccc2[nH]c(=O)[nH]c2c1
vNsp16-nsp10.1-45	Z1023507394	-9.5	0.264	491.565	REAL	Cc1cccc(NC(=O)N2CCC[C@H](C(=O)N3CCC[C@H](c4nc(-c5cccc(F)c5)no4)C3)C2)c1
vNsp16-nsp10.1-46	Z1024051824	-9.5	0.257	491.589	REAL	O=C1Nc2ccccc2[C@@H]1C1CCN(C(=O)[C@H]2CC(=O)N(c3ccc4c(c3)Cc3ccccc3-4)C2)CC1
vNsp16-nsp10.1-47	Z1131828782	-9.5	0.279	461.51	REAL	O=C(c1cncc(C(=O)N2CC[C@H](c3cccc(F)c3)C2)c1)N1CC[C@H](c2cccc(F)c2)C1
vNsp16-nsp10.1-48	Z1155470360	-9.5	0.279	454.572	REAL	Cc1ccc(-n2nc(C(=O)N3CCC([C@H]4C(=O)Nc5ccccc54)CC3)c3c2CCC3)cc1
vNsp16-nsp10.1-49	Z1157949085	-9.5	0.271	485.606	REAL	Cc1cnc2c(S(=O)(=O)N3CCN(C(=O)[C@H]4C[C@@H]4c4ccc5ccccc5c4)CC3)cccc2c1
vNsp16-nsp10.1-50	Z1427996452	-9.5	0.288	448.428	REAL	CC(=O)N1C[C@H](C(=O)Nc2ccc(-c3nc4cc(F)c(F)cc4[nH]3)cc2)Oc2ccccc21
vNsp16-nsp10.1-51	Z1452691933	-9.5	0.288	445.493	REAL	O=C(NC[C@H]1[C@@H]2Cc3ccccc3[C@H]12)NNC(=O)c1ccccc1OCc1ccc(F)cc1
vNsp16-nsp10.1-52	Z1494967585	-9.5	0.297	445.585	REAL	Cc1c(NC(=O)[C@H]2CCN(C)c3ccccc32)cccc1C(=O)N1CCc2ccc2C1
vNsp16-nsp10.1-53	Z1499501732	-9.5	0.317	401.508	REAL	O=C(Cc1ccc(NC(=O)N2[C@H]3C=CC[C@H]2CC3)cc1)N1CCCc2ccccc21
vNsp16-nsp10.1-54	Z1610529936	-9.5	0.288	436.47	REAL	O=C(NNc1ccccn1)c1c2c(nc3ccccc13)/C(=C/c1ccc3c(c1)OCO3)CC2
vNsp16-nsp10.1-55	Z1663744099	-9.5	0.288	447.581	REAL	Cc1ccc(C(=O)N2CCC(NC(=O)[C@@H]3C[C@@H]4CCCC[C@@H]4N3c3nccn3)CC2)cc1
vNsp16-nsp10.1-56	Z1683031745	-9.5	0.317	400.441	REAL	O=C(Nc1ccccc1)Nc1ccc(-c2noc([C@H]3CCc4cn[nH]c4C3)n2)cc1
vNsp16-nsp10.1-57	Z1683032795	-9.5	0.297	426.431	REAL	O=C(Nc1ccccc1)Nc1ccc(-c2noc([C@H]3Cc4ccccc4C(=O)O3)n2)cc1
vNsp16-nsp10.1-58	Z1685223830	-9.5	0.279	449.513	REAL	O=c1[nH]c2ccc(NCc3ccc(-c4noc([C@@H]5C[C@@]56CCc5ccccc56)n4)cc3)cc2[nH]1
vNsp16-nsp10.1-59	Z1827712413	-9.5	0.306	417.424	REAL	O=C(Nc1ccc2[nH]c(=O)[nH]c2c1)c1cccc(NN2C(=O)[C@@H]3CC=CC[C@@H]3C2=O)c1
vNsp16-nsp10.1-60	Z1827756688	-9.5	0.306	418.408	REAL	O=C(Nc1ccc2oc(=O)[nH]c2c1)c1cccc(NN2C(=O)[C@@H]3CC=CC[C@H]3C2=O)c1
vNsp16-nsp10.1-61	Z1891181711	-9.5	0.297	445.502	REAL	Cc1ccccc1NS(=O)(=O)c1ccc(-c2nc(Cc3ccc4cn[nH]c4c3)no2)cc1
vNsp16-nsp10.1-62	Z1951507006	-9.5	0.288	445.434	REAL	O=C(Nc1ccc(-c2noc(=O)[nH]2)cc1)c1cccc(NN2C(=O)[C@@H]3CC=CC[C@@H]3C2=O)c1
vNsp16-nsp10.1-63	Z2001073403	-9.5	0.288	437.458	REAL	O=C(Nc1ccccc(-c2nc(Cc3ccc4[nH]ncc4c3)no2)c1)[C@@H]1Cc2ccccc2O1
vNsp16-nsp10.1-64	Z2002848514	-9.5	0.288	438.525	REAL	O=C1[C@@H]2[C@@H]3C[C@H]4[C@@H]2[C@@]2(C(=O)Nc5cccc(CC(=O)N6CCCc7ccccc76)cc5)[C@H]1[C@@H]3[C@@H]42
vNsp16-nsp10.1-65	Z2003428823	-9.5	0.317	426.535	REAL	O=C1[C@H]2[C@H]3C[C@H]4[C@@H]2[C@]2(C(=O)NCc5ccccc5CS(=O)(=O)N5CCCC5)[C@H]1[C@@H]3[C@H]42
vNsp16-nsp10.1-66	Z203623824	-9.5	0.279	452.513	REAL	CC(=O)N1C[C@H](C(=O)Nc2cc(-c3cccc(C)c3)nn2-c2ccccc2)Oc2ccccc21
vNsp16-nsp10.1-67	Z2141231638	-9.5	0.288	442.478	REAL	CC(=O)N1C[C@H](C(=O)Nc2cc(-c3ccn(Cc4ccccc4)n3)n[nH]2)Oc2ccccc21
vNsp16-nsp10.1-68	Z2142478224	-9.5	0.288	446.441	REAL	O=C(Nc1ccc(-c2nc[nH]n2)cc1F)c1cccc(NN2C(=O)[C@@H]3CC=CC[C@H]3C2=O)c1
vNsp16-nsp10.1-69	Z220348464	-9.5	0.264	499.633	REAL	O=C(c1cccc(S(=O)(=O)N2CCc3ccccc3C2)c1)N1CCC(c2c[nH]c3ccccc23)CC1
vNsp16-nsp10.1-70	Z2231941851	-9.5	0.288	442.557	REAL	O=C(C1[C@H]2[C@@H]3C=C[C@@H]([C@H]4C(=O)N(Cc5ccccc5)C(=O)[C@H]34)[C@@H]12)N1C[C@H]2[C@@H]3CC[C@@H](C3)[C@H]2C1
vNsp16-nsp10.1-71	Z228011870	-9.5	0.257	486.53	REAL	O=C(Cc1cccc2ccccnc12)NNC(=O)c1ccc(CN2C(=O)c3cccc4ccccc3c34)cc1
vNsp16-nsp10.1-72	Z2902753353	-9.5	0.279	471.943	REAL	O=C1[C@@H]2[C@@H]3C=C[C@H]([C@H]2C(=O)N1Cc1ccccc1)[C@H]1C(c2nc(Cc4ccc(Cl)cc4)no2)[C@@H]31
vNsp16-nsp10.1-73	Z2902891866	-9.5	0.279	457.508	REAL	Cc1cccc2c1O[C@@H](c1nc(-c3ccc(N4CCN(c5ccc(F)cc5)CC4)nc3)no1)C2
vNsp16-nsp10.1-74	Z358867962	-9.5	0.317	415.532	REAL	Cc1ccccc([C@@H](CC(=O)O[C@@H](C)C(=O)N[C@@H](C)[C@H]2C[C@H]3CC[C@H]2C3)NC(N)=O)c1
vNsp16-nsp10.1-75	Z364958032	-9.5	0.271	492.598	REAL	Cc1cnc2c(S(=O)(=O)N3CCN(C(=O)CC[C@@H]4Cc5ccccc5NC4=O)CC3)cccc2c1
vNsp16-nsp10.1-76	Z364959588	-9.5	0.271	492.598	REAL	Cc1cnc2c(S(=O)(=O)N3CCN(C(=O)c4ccc(CN5CCCC5=O)cc4)CC3)cccc2c1
vNsp16-nsp10.1-77	Z647509392	-9.5	0.279	477.544	REAL	Cc1cnc2c(S(=O)(=O)N3CCN(C(=O)c4cnc5nc(C)ccc5c4O)CC3)cccc2c1
vNsp16-nsp10.1-78	Z729567092	-9.5	0.279	478.567	REAL	CC(=O)Nc1cccc2c1CCCN2C(=O)c1ccc(OS(=O)(=O)c2cc(C)ccc2C)cc1
vNsp16-nsp10.1-79	Z775632330	-9.5	0.279	477.583	REAL	CC(=O)Nc1cccc2c1CCCN2C(=O)c1ccc(NS(=O)(=O)c2cc(C)ccc2C)cc1
vNsp16-nsp10.1-80	Z787516708	-9.5	0.257	495.581	REAL	O=C(c1ccc2[nH]cnc2c1)N1CCN(C(=O)[C@@H]2CCCN(C(=O)c3cccc4ccccc34)C2)CC1
vNsp16-nsp10.1-81	Z95871346	-9.5	0.271	465.512	REAL	O=C(c1cccc(CN2C(=O)c3ccccc3C2=O)c1)N1CCC(c2nnc3ccccn23)CC1
vNsp16-nsp10.1-82	Z967655690	-9.5	0.306	423.393	REAL	O=C(Cc1nc2ccc(-c3cccc3)cc2c(=O)[nH]1)Nc1ccccc1C(F)(F)F
vNsp16-nsp10.1-83	Z981587398	-9.5	0.279	473.959	REAL	O=C(Cc1ccc(N[C@@H]2CC(=O)N(c3cccc(Cl)c3)C2=O)cc1)N1CCCc2ccccc21
vNsp16-nsp10.1-84	Z988062926	-9.5	0.288	442.517	REAL	NC(=O)c1ccccc(CNC(=O)Nc2ccc(CC(=O)N3CCCc4ccccc43)cc2)c1
vNsp16-nsp10.1-85	ZINC000000727305	-9.5	0.271	459.504	ZINC15	O=C(NNC(=O)c1cccc2ccccc21)c1ccc(NC(=O)c2cccc3ccccc32)cc1
vNsp16-nsp10.1-86	ZINC000008901217	-9.5	0.25	499.521	ZINC15	Cc1cc(NC(=O)c2cccc(-c3cc4ccccc4oc3=O)c2)ccc1-c1cc2ccccc2oc1=O
vNsp16-nsp10.1-87	ZINC000019855340	-9.5	0.264	478.554	ZINC15	Cc1cc(N2CCn3c(nc4ccccc43)C2)ccc1NC(=O)Cn1nc(C)c2ccccc2c1=O
vNsp16-nsp10.1-88	ZINC000020390197	-9.5	0.257	504.656	ZINC15	Cc1nn(-c2ccccc2C)c2sc(C(=O)N3CCN(C4c5ccccc5-c5ccccc54)CC3)cc12
vNsp16-nsp10.1-89	ZINC000096222481	-9.5	0.279	454.524	ZINC15	Cc1coc2c1cc1c(C)c(CC(=O)N[C@@H]3CCCc4c5ccccc5[nH]c43)c(=O)oc1c2C
vNsp16-nsp10.1-90	ZINC000408643959	-9.5	0.279	450.536	ZINC15	Cc1ccc(C)c(N2C[C@H](C(=O)Nc3ccc(Oc4ccc5ccccc5c4)cc3)CC2=O)c1
vNsp16-nsp10.1-91	ZINC000408675226	-9.5	0.25	498.58	ZINC15	Cc1cccc(NC(=O)c2cccc(N3C(=O)[C@H]4[C@@H](C3=O)C3c5ccccc5C4c4ccccc43)c2)c1C
vNsp16-nsp10.1-92	PV-001791724704	-9.4	0.303	442.578	REAL	CO[C@@H](C(=O)Nc1ccc(S(=O)(=O)N[C@@H](C)[C@H]2C[C@H]3CC[C@H]2C3)cc1)c1ccccc1
vNsp16-nsp10.1-93	PV-001825863042	-9.4	0.303	423.486	REAL	Cc1cc(C(=O)N2CCC(C)CC2)ccc1NC(=O)[C@@H]1Cc2cc(F)ccc2NC1=O
vNsp16-nsp10.1-94	PV-001854861785	-9.4	0.348	380.874	REAL	O=C(N[C@@H]1CCC[C@@H](c2ncc(Cl)cc2)C1)c1cc2ccccc2c(=O)[nH]1
vNsp16-nsp10.1-95	PV-001867570214	-9.4	0.362	356.464	REAL	CC(C)[C@H](NC(=O)COc1ccccc1)C(=O)N[C@H]1C[C@@H]2C[C@H]1[C@@H]2[C@H]1C[C@@H]21
vNsp16-nsp10.1-96	PV-001936962679	-9.4	0.348	412.573	REAL	CCCCS(=O)(=O)Nc1ccc(S(=O)(=O)NC[C@H]2C[C@H]3C=C[C@H]2CC3)cc1
vNsp16-nsp10.1-97	PV-001942144066	-9.4	0.294	433.482	REAL	Cc1cccc2c1C[C@@H](NC(=O)Nc1ccc(C(=O)NCc3ccc(F)cc3)cc1)CO2
vNsp16-nsp10.1-98	PV-001942434692	-9.4	0.294	431.509	REAL	O=C(Nc1ccc(C(=O)NCCc2ccccc2)cc1)N[C@H]1c2ccccc2CC[C@@H]1F
vNsp16-nsp10.1-99	PV-001942977424	-9.4	0.285	452.528	REAL	O=C(Cc1ccc(NC(=O)N2CCC[C@@H](N3CCCCC3=O)C2)cc1)Nc1ccccc1F
vNsp16-nsp10.1-100	PV-001942977775	-9.4	0.294	437.445	REAL	O=C(Cc1ccc(NC(=O)N2CCOc3cc(F)ccc3C2)cc1)Nc1ccccc1F

Supplementary Table 77. Top 100 virtual hits of the screen against the nsp10 binding site of nsp16 (Screen ID: 40). Compounds were filtered so that hits had MW < 600 dalton, cLogP < 6, number of hydrogen bond acceptors < 11, and no reactive functional groups. A few compounds unsuitable for drug discovery were removed by visual inspection. The name of each compound consists of the initial letter 'v' for virtual hit, followed by the target protein name and the target site ('nsp10' for nsp10 binding site, 1 for docking scenario 1). The score is the docking score given by QuickVina 2 in kcal/mol. The ligand efficiency (LE) is computed as LE = -score/#NonH, where #NonH is the number of heavy (i.e. non hydrogen) atoms.

Name	Catalog ID	Score	LE	MW	Library	SMILES
vNsp16-nsp10.1-101	PV-001950628369	-9.4	0.313	407.51	REAL	CC1(C)COc2cc(NC(=O)N[C@@H]3CCC[C@@H](c4ccccc4)C3)ccc2NC1=O
vNsp16-nsp10.1-102	PV-001953309153	-9.4	0.276	456.54	REAL	C[C@@H](NC(=O)N1CCc2c(CC(N)=O)cccc2C1)c1cccc(NC(=O)c2ccccc2)c1
vNsp16-nsp10.1-103	PV-001953313640	-9.4	0.294	449.45	REAL	O=C(NC1CCN(C(=O)c2ccccc2F)CC1)N1CCc2c(cccc2C(F)(F)F)C1
vNsp16-nsp10.1-104	PV-001958944108	-9.4	0.285	441.57	REAL	CCc1ccc(C(=O)N2CCN(C(=O)NCc3cccc(-c4ccc(C)cc4)c3)CC2)cc1
vNsp16-nsp10.1-105	Z1011412822	-9.4	0.269	463.54	REAL	CN(Cc1ccccc1-c1ccccc1)C(=O)Nc1cccc(Cn2nc3ccccn3c2=O)c1
vNsp16-nsp10.1-106	Z1011495784	-9.4	0.276	464.56	REAL	Cc1cc(C(=O)N2CCCC[C@@H]2C)ccc1NC(=O)N1CCN(C(=O)c2cccc(O)c2)CC1
vNsp16-nsp10.1-107	Z1013915400	-9.4	0.254	488.55	REAL	Cc1ccc2c(CC(=O)NNC(=O)c3ccc(CN4C(=O)c5cccc6cccc4c56)cc3)c[nH]c2c1
vNsp16-nsp10.1-108	Z1024052650	-9.4	0.269	471.56	REAL	O=C1Nc2ccccc2[C@H]1C1CCN(C(=O)[C@H]2CCCN(C(=O)c3ccc4[nH]ncc4c3)C2)CC1
vNsp16-nsp10.1-109	Z1032455496	-9.4	0.269	463.54	REAL	Cc1cccc(-c2cccc(CNC(=O)Nc3cccc(Cn4nc5ccccn5c4=O)c3)c2)c1
vNsp16-nsp10.1-110	Z1033355262	-9.4	0.261	484.60	REAL	Cc1cccc(NC(=O)N2CCN(C(=O)[C@@H]3CCCN(C(=O)c4cccc5ccccc45)C3)CC2)c1
vNsp16-nsp10.1-111	Z1071491534	-9.4	0.261	487.52	REAL	C[C@H]1Oc2ccc(C(=O)C3CCN(C(=O)NNC(=O)c4cccc5ccccc45)CC3)cc2NC1=O
vNsp16-nsp10.1-112	Z1075527660	-9.4	0.261	488.59	REAL	Cc1cc(CNC(=O)N2CCC(C(=O)c3ccc4c(c3)NC(=O)[C@H](C)O4)CC2)c2[nH]c(C)c(C)c2c1
vNsp16-nsp10.1-113	Z1084980652	-9.4	0.324	420.58	REAL	CNS(=O)(=O)c1ccccc1N1CCN(C(=O)NCC[C@H]2C[C@H]3CC[C@H]2C3)CC1
vNsp16-nsp10.1-114	Z1101974232	-9.4	0.285	439.47	REAL	O=C1CCCc2cc(NC(=O)c3cccc(CN4C(=O)c5ccccc5C4=O)c3)ccc2N1
vNsp16-nsp10.1-115	Z1118604420	-9.4	0.254	488.55	REAL	Cc1cccc2[nH]cc(CC(=O)NNC(=O)c3ccc(CN4C(=O)c5cccc6cccc4c56)cc3)c12
vNsp16-nsp10.1-116	Z1132550961	-9.4	0.269	474.53	REAL	C[C@@H](NC(=O)Nc1ccc2c(c1)CCC(=O)N2C)c1cccc(NC(=O)Cc2ccccc2F)c1
vNsp16-nsp10.1-117	Z1139998342	-9.4	0.294	430.44	REAL	CC(=O)N1C[C@H](C(=O)Nc2ccc(-c3nc4cc(F)ccc4[nH]3)cc2)Oc2ccccc21
vNsp16-nsp10.1-118	Z1161349624	-9.4	0.285	448.48	REAL	O=C(c1cnc2[nH]c(=O)[nH]c(=O)c2c1)N1CCN(CC(=O)N2CCCc3ccccc32)CC1
vNsp16-nsp10.1-119	Z1169860637	-9.4	0.294	427.51	REAL	Cc1ccc(-n2nc(-c3nc(CC(=O)Nc4ccccc4C)no3)c3c2CCCC3)cc1
vNsp16-nsp10.1-120	Z1169981038	-9.4	0.276	448.48	REAL	O=C(Nc1cccc(-c2nc(Cc3cccc4ccncn34)no2)c1)[C@@H]1Cc2ccccc2O1
vNsp16-nsp10.1-121	Z118351396	-9.4	0.254	499.61	REAL	O=C(c1cccc2ccccc12)N1CCC[C@@H](C(=O)N2CCN(Cc3ccc4c(c3)OCCO4)CC2)C1
vNsp16-nsp10.1-122	Z1199916922	-9.4	0.294	422.45	REAL	Cc1cccc(-c2nnc(-c3ccc(C(=O)NNc4cnnc5ccccc45)cc3)o2)c1
vNsp16-nsp10.1-123	Z1273504437	-9.4	0.285	446.52	REAL	Cc1cc2c(cc1C)O[C@H](C(=O)N[C@@H](C)c1cccc(NC(=O)Cc3ccccc3F)c1)C2
vNsp16-nsp10.1-124	Z1360225712	-9.4	0.294	426.51	REAL	C[C@@H]1[C@H](c2ccccc2)CCN1C(=O)c1cccc(NC(=O)[C@H]2Cc3ccccc3O2)c1
vNsp16-nsp10.1-125	Z1383805109	-9.4	0.269	488.56	REAL	O=C(Cc1ccc(S(=O)(=O)N2CCCCC2)cc1)Nc1ccc2c(c1)C(=O)c1ccccc1C2=O
vNsp16-nsp10.1-126	Z1411656822	-9.4	0.294	435.50	REAL	C[C@H](NC(=O)N[C@H]1CCc2cn[nH]c2C1)c1cccc(NC(=O)Cc2ccccc2F)c1
vNsp16-nsp10.1-127	Z1416425849	-9.4	0.294	425.49	REAL	O=C(NNC(=O)[C@@H]1CC12CCC2)c1ccc(CN2C(=O)c3cccc4ccccc2c34)cc1
vNsp16-nsp10.1-128	Z1474433863	-9.4	0.285	438.53	REAL	O=C(N[C@@H]1[C@H]2CCc3ccccc3[C@H]21)c1ccc(C(=O)N[C@H]2[C@@H]3CCc4ccccc4[C@H]32)o1
vNsp16-nsp10.1-129	Z1529152590	-9.4	0.313	405.54	REAL	Cc1ccc(C(=O)N2CCC(NC(=O)N3Cc4ccccc4C(C)(C)C3)CC2)cc1
vNsp16-nsp10.1-130	Z1576194542	-9.4	0.285	441.53	REAL	Cc1ccc(-n2nc(C(=O)N3CC=C(c4ccc5c(c4)OCCO5)CC3)c3c2CCC3)cc1
vNsp16-nsp10.1-131	Z1576194738	-9.4	0.285	445.49	REAL	O=C(c1nn(-c2ccc(F)cc2)c2c1CCC2)N1CC=C(c2ccc3c(c2)OCCO3)CC1
vNsp16-nsp10.1-132	Z1590267830	-9.4	0.313	406.48	REAL	Cc1ccc(-c2cccc(CNC(=O)N3CCC4(CC3)NC(=O)N(C)C4=O)c2)cc1
vNsp16-nsp10.1-133	Z1663162572	-9.4	0.276	448.48	REAL	O=C1[C@@H]2[C@H]3C=C[C@@H](C3)[C@H]2C(=O)N1Cc1nnc(-c2cc(-c3ccccc3)nc3ccccc23)o1
vNsp16-nsp10.1-134	Z1684253847	-9.4	0.285	439.47	REAL	O=C(Nc1cccc(-c2nc(Cc3ccc4c(c3)CCO4)no2)c1)[C@H]1Cc2ccccc2O1
vNsp16-nsp10.1-135	Z1685223501	-9.4	0.285	439.47	REAL	O=c1[nH]c2ccc(NCc3ccc(-c4noc([C@H]5CCOc6ccccc65)n4)cc3)cc2[nH]1
vNsp16-nsp10.1-136	Z1685321062	-9.4	0.276	449.47	REAL	Cc1nnc(-c2cccc(-c3noc(-c4ccc5c(c4)C[C@H](c4ccccc4)OC5=O)n3)c2)[nH]1
vNsp16-nsp10.1-137	Z1696509806	-9.4	0.285	447.54	REAL	O=C(Nc1ccc(CC(=O)N2CCc3ccccc32)cc1)N1CCC[C@H](N2CCNC2=O)C1
vNsp16-nsp10.1-138	Z1723433994	-9.4	0.254	494.55	REAL	Cn1c(=O)[nH]c2ncc(-c3cccc(C(=O)N4CCN(C(=O)Cc5c[nH]c6ccccc56)CC4)c3)cc21
vNsp16-nsp10.1-139	Z1827747986	-9.4	0.276	449.51	REAL	O=C(Nc1ccc2c(c1)Cc1ccccc1-2)c1cccc(NN2C(=O)[C@@H]3CC=CC[C@H]3C2=O)c1
vNsp16-nsp10.1-140	Z1827823783	-9.4	0.294	428.45	REAL	O=C(Nc1ccc(-c2nnc[nH]2)cc1)c1cccc(NN2C(=O)[C@@H]3CC=CC[C@H]3C2=O)c1
vNsp16-nsp10.1-141	Z1836096633	-9.4	0.303	416.44	REAL	O=C1Cc2cc(NC(=O)c3cccc(NN4C(=O)[C@@H]5CC=CC[C@@H]5C4=O)c3)ccc2N1
vNsp16-nsp10.1-142	Z1851870716	-9.4	0.276	448.53	REAL	Cc1ccc(-n2cnc3c2CCN(C(=O)c2cnc4c(c2)c(C)nn4-c2ccccc2)C3)cc1
vNsp16-nsp10.1-143	Z1865889088	-9.4	0.294	427.50	REAL	O=C(Nc1ccc(CC(=O)N2CCc3ccccc32)cc1)N[C@H]1Cc2ccccc(O)c2C1
vNsp16-nsp10.1-144	Z1866978296	-9.4	0.294	434.53	REAL	O=C(N[C@H]1Cc2ccccc(O)c2C1)[C@H]1CC[C@H](C(=O)N[C@H]2Cc3cccc(O)c3C2)CC1
vNsp16-nsp10.1-145	Z1870706196	-9.4	0.294	447.52	REAL	C[C@]1(c2ccc(C(=O)Nc3nnc([C@H]4CCCc5ccccc54)s3)cc2)NC(=O)NC1=O
vNsp16-nsp10.1-146	Z1900453516	-9.4	0.285	435.49	REAL	CN1C[C@H](c2nc(-c3cccc(Cn4cnc5ccccc54)c3)no2)c2ccccc2C1=O
vNsp16-nsp10.1-147	Z1907683378	-9.4	0.303	423.51	REAL	O=C(CCCC(=O)c1ccc2c(c1)OCCO2)NC[C@]1(O)[C@@H]2[C@H]3C[C@H]4[C@@H]5[C@H]3C[C@H]2[C@@H]5[C@H]41
vNsp16-nsp10.1-148	Z1927662205	-9.4	0.294	428.57	REAL	O=C(NC1Cc2ccccc2C1)C12CCC(C(=O)NC3Cc4ccccc4C3)(CC1)CC2
vNsp16-nsp10.1-149	Z1948952868	-9.4	0.294	441.39	REAL	O=C(Nc1ccc2c(c1)OC(F)(F)O2)c1cccc(NN2C(=O)[C@@H]3CC=CC[C@H]3C2=O)c1
vNsp16-nsp10.1-150	Z1950365994	-9.4	0.285	438.49	REAL	O=C(Nc1ccc(-c2ccccc2)cn1)c1cccc(NN2C(=O)[C@@H]3CC=CC[C@@H]3C2=O)c1
vNsp16-nsp10.1-151	Z1951504039	-9.4	0.294	429.44	REAL	O=C(Nc1ccc(-c2nnn[nH]2)cc1)c1cccc(NN2C(=O)[C@@H]3CC=CC[C@@H]3C2=O)c1
vNsp16-nsp10.1-152	Z1952918213	-9.4	0.285	444.48	REAL	O=C(NCc1ccc2c(c1)CN(C(=O)[C@H]1Cc3ccc(F)cc31)C2)[C@@H]1Cc2ccc(F)cc21
vNsp16-nsp10.1-153	Z1952918807	-9.4	0.285	440.50	REAL	O=C(NCc1ccc2c(c1)CN(C(=O)[C@@H]1Cc3cccc3O1)C2)[C@@H]1Cc2ccccc2O1
vNsp16-nsp10.1-154	Z2002423492	-9.4	0.294	425.48	REAL	O=C1[C@@H]2[C@@H]3C[C@H]4[C@@H]2[C@]2(C(=O)Oc5cccc(C(=O)N6CCc7ccccc7C6)c5)[C@H]1[C@@H]3[C@@H]42
vNsp16-nsp10.1-155	Z2006390547	-9.4	0.313	409.50	REAL	Cc1ccc(C(=O)N2CCC(NC(=O)N3CCc4cc(F)ccc(C)c4C3)CC2)cc1
vNsp16-nsp10.1-156	Z203540946	-9.4	0.285	464.55	REAL	CC(=O)N1C[C@H](C(=O)Nc2ccc(-c3csc(N4CCOCC4)n3)cc2)Oc2ccccc21
vNsp16-nsp10.1-157	Z2078222895	-9.4	0.294	426.48	REAL	O=C(NCCc1ccc2cn[nH]c2c1)c1cccc(NC(=O)[C@H]2Cc3ccccc3O2)c1
vNsp16-nsp10.1-158	Z2157851786	-9.4	0.285	442.47	REAL	O=C(Nc1cccc(C(=O)N2CCC3(C2)Oc2ccccc2O3)c1)[C@H]1Cc2ccccc2O1
vNsp16-nsp10.1-159	Z216974970	-9.4	0.294	426.48	REAL	CC(=O)N1C[C@H](C(=O)Nc2ccc(-c3cn4ccc(C)cc4n3)cc2)Oc2ccccc21
vNsp16-nsp10.1-160	Z2174584187	-9.4	0.285	446.55	REAL	O=C(C1[C@H]2[C@@H]3C=C[C@@H]([C@H]4C(=O)N(Cc5ccccc5)C(=O)[C@H]34)[C@@H]12)N1CC[C@]2(CCCOC2)C1
vNsp16-nsp10.1-161	Z2176722244	-9.4	0.313	412.53	REAL	CC(C)CC(=O)N[C@@H](Cc1c[nH]cn1)C(=O)NC[C@@]1(O)[C@@H]2[C@H]3C[C@H]4[C@H]5[C@H]3C[C@@H]2[C@H]5[C@H]41
vNsp16-nsp10.1-162	Z2198738154	-9.4	0.294	429.48	REAL	O=C(N[C@H]1Cc2cccc(O)c2C1)c1ccc(C(=O)N[C@H]2Cc3cccc(O)c3C2)nc1
vNsp16-nsp10.1-163	Z227888978	-9.4	0.276	472.61	REAL	CC(=O)N1c2ccc(S(=O)(=O)NC[C@H]3CC4c5ccccc5C3c3ccccc34)cc2C[C@@H]1C
vNsp16-nsp10.1-164	Z229654036	-9.4	0.269	461.52	REAL	O=C(c1cccc(CN2C(=O)c3ccccc3C2=O)c1)N1CC=C(c2c[nH]c3ccccc23)CC1
vNsp16-nsp10.1-165	Z229659808	-9.4	0.261	497.62	REAL	O=C(c1cccc(S(=O)(=O)N2CCc3ccccc3C2)c1)N1CC=C(c2c[nH]c3ccccc23)CC1
vNsp16-nsp10.1-166	Z241510988	-9.4	0.276	470.55	REAL	O=C1CNC(=O)N1Cc1ccc(-c2nc3sc4c(c3c(=O)[nH]2)CC[C@H](c2ccccc2)C4)cc1
vNsp16-nsp10.1-167	Z2902509734	-9.4	0.276	455.49	REAL	Cc1ccc(-c2noc(C3[C@H]4[C@@H]5C=C[C@@H]([C@H]6C(=O)N(Cc7ccccc7)C(=O)[C@H]56)[C@H]34)n2)cc1F
vNsp16-nsp10.1-168	Z2902894125	-9.4	0.254	497.53	REAL	Cn1nc(Cc2nc(-c3ccc(N4CCN(c5ccc(F)cc5)CC4)nc3)no2)c2ccccc2c1=O
vNsp16-nsp10.1-169	Z2903054677	-9.4	0.261	477.52	REAL	O=C1[C@@H]2[C@@H]3C=C[C@H]([C@H]2C(=O)N1Cc1ccccc1)[C@H]1C(=O)c2nc(Cn4cnc5ccccc54)no2)[C@@H]31
vNsp16-nsp10.1-170	Z319051598	-9.4	0.285	437.46	REAL	O=C(NNc1nccnn1)c1c2c(nc3ccccc13)/C(=C/c1ccc3c(c1)OCO3)CC2
vNsp16-nsp10.1-171	Z367230668	-9.4	0.269	493.59	REAL	Cc1cnc2c(S(=O)(=O)N3CCN(C(=O)c4cc(C)n(-c5cc(C)on5)c4C)CC3)cccc2c1
vNsp16-nsp10.1-172	Z368084964	-9.4	0.261	485.58	REAL	COc1ccc(C(=O)N2CCC(C(=O)Nc3cccc(N4CCCCC4=O)c3)CC2)c2ccccc12
vNsp16-nsp10.1-173	Z424332426	-9.4	0.269	470.53	REAL	C[C@@]1(c2cccc(NC(=O)[C@@H]3CCCN(C(=O)c4cccc5cccc45)C3)c2)NC(=O)NC1=O
vNsp16-nsp10.1-174	Z424740926	-9.4	0.261	485.56	REAL	Cc1ccc(CNC(=O)C2CCN(C(=O)c3cnc4c(c3)c(C)nn4-c3ccccc3)CC2)cc1F
vNsp16-nsp10.1-175	Z433464890	-9.4	0.269	494.57	REAL	Cc1cnc2c(S(=O)(=O)N3CCN(C(=O)Nc4cccc(N5CCNC5=O)c4)CC3)cccc2c1
vNsp16-nsp10.1-176	Z453949732	-9.4	0.269	482.51	REAL	Cc1ccc(-n2nc(C(=O)N3CCN(C(=O)c4cccc(C(F)(F)F)c4)CC3)c3cccc3)cc1
vNsp16-nsp10.1-177	Z648211698	-9.4	0.276	474.54	REAL	O=C(Nc1ccc(-c2cc(=O)[nH][nH]2)cc1)c1cccc(S(=O)(=O)N2CCCc3ccccc32)c1
vNsp16-nsp10.1-178	Z653565760	-9.4	0.261	488.49	REAL	O=C(c1cc(F)ccc1F)C1CCN(C(=O)c2cccc(CN3C(=O)c4ccccc4C3=O)c2)CC1
vNsp16-nsp10.1-179	Z666280244	-9.4	0.294	426.48	REAL	CC(=O)N1C[C@H](C(=O)Nc2ccc(-c3cn4cccc(C)c4n3)cc2)Oc2ccccc21
vNsp16-nsp10.1-180	Z738648476	-9.4	0.261	476.54	REAL	O=C(NCc1nn(-c2ccccc2)c2c1CCC2)c1cccc(CN2C(=O)c3ccccc3C2=O)c1
vNsp16-nsp10.1-181	Z747436736	-9.4	0.276	456.54	REAL	CC(=O)Nc1cccc2c1CCN(C(=O)N[C@H](C)c1ccccc(NC(=O)c3ccccc3)c1)C2
vNsp16-nsp10.1-182	Z748887232	-9.4	0.261	486.53	REAL	COc1ccc(C(=O)N2CCC(C(=O)Nc3cccc(N4C(=O)CNC4=O)c3)CC2)c2ccccc12
vNsp16-nsp10.1-183	Z787516648	-9.4	0.269	473.58	REAL	Cc1cc(C)cc(C(=O)N2CCC[C@H](C(=O)N3CCN(C(=O)c4ccc5[nH]cnc5c4)CC3)C2)c1
vNsp16-nsp10.1-184	Z806720820	-9.4	0.285	443.50	REAL	CC(=O)N1C[C@H](C(=O)Nc2ccc(C(=O)NCCc3ccccc3)cc2)Oc2ccccc21
vNsp16-nsp10.1-185	Z809649822	-9.4	0.294	429.48	REAL	CC(=O)N1C[C@H](C(=O)Nc2ccc(C(=O)NCc3ccccc3)cc2)Oc2ccccc21
vNsp16-nsp10.1-186	Z878749952	-9.4	0.261	485.52	REAL	O=C(Nc1ccccc(C(=O)N2CCN(C(=O)Cc3ccccc3F)CC2)c1)c1ccc2[nH]cnc2c1
vNsp16-nsp10.1-187	Z966275476	-9.4	0.285	441.49	REAL	CC(=O)N1C[C@H](C(=O)Nc2ccc(C(=O)N3CCc4ccccc43)cc2)Oc2ccccc21
vNsp16-nsp10.1-188	Z967655798	-9.4	0.324	383.45	REAL	Cc1ccc(NC(=O)Cc2nc3ccc(-c4ccccc4)cc3c(=O)[nH]2)c(C)c1
vNsp16-nsp10.1-189	Z967655966	-9.4	0.336	369.42	REAL	Cc1ccccc1NC(=O)Cc1nc2ccc(-c3ccccc3)cc2c(=O)[nH]1
vNsp16-nsp10.1-190	Z978635552	-9.4	0.269	468.56	REAL	C[C@H](NC(=O)Nc1ccc(CC(=O)N2CCc3ccccc32)cc1)c1ccc2c(c1)CCC(=O)N2
vNsp16-nsp10.1-191	Z980408642	-9.4	0.261	497.57	REAL	O=C1Nc2ccc(S(=O)(=O)Nc3ccc(CC(=O)N4CCCc5ccccc54)cc3)c3ccc1c23
vNsp16-nsp10.1-192	Z981587392	-9.4	0.276	457.50	REAL	O=C(Cc1ccc(N[C@@H]2CC(=O)N(c3ccccc3F)C2=O)cc1)N1CCCc2ccccc21
vNsp16-nsp10.1-193	Z996883384	-9.4	0.294	426.51	REAL	Cc1ccccc1[C@H]1CCN(C(=O)c2ccccc(NC(=O)[C@H]3Cc4ccccc4O3)c2)C1
vNsp16-nsp10.1-194	ZINC000002896738	-9.4	0.261	466.49	ZINC15	O=C(C(=O)c1ccc2c(c1)-c1cccc3c1c-2ccc3C(=O)C(=O)c1ccccc1)c1ccccc1
vNsp16-nsp10.1-195	ZINC000007651552	-9.4	0.294	419.57	ZINC15	O=C(Nc1ccc(C23CC4CC(CC(C4)C2)C3)cc1)C1c2ccccc2-c2ccccc21
vNsp16-nsp10.1-196	ZINC000016392012	-9.4	0.285	436.55	ZINC15	O=C(CN1c2cccc3cccc(c23)C1=O)Nc1ccc(C23CC4CC(CC(C4)C2)C3)cc1
vNsp16-nsp10.1-197	ZINC000016544965	-9.4	0.261	474.56	ZINC15	O=C(NCc1cccc(CNC(=O)Nc2cccc3ccccc32)c1)Nc1ccc2ccccc21
vNsp16-nsp10.1-198	ZINC000018117591	-9.4	0.285	431.45	ZINC15	O=C(Nc1cccc2c1C(=O)[C@H]1C=CC=C[C@@H]1C2=O)c1cccc2c1C(=O)c1ccccc1-2
vNsp16-nsp10.1-199	ZINC000039742926	-9.4	0.285	434.45	ZINC15	O=C(Nc1nnc(-c2ccccc2)o1)c1cccc(NC(=O)c2cccc3ccccc32)c1
vNsp16-nsp10.1-200	ZINC000048368120	-9.4	0.261	482.67	ZINC15	O=C(CC12CC3CC(C1)CC(CC(=O)N1CCc4ccccc4C1)(C3)C2)N1CCc2ccccc2C1

Supplementary Table 78. Virtual screening hits 101 to 200 of the screen against the nsp10 binding site of nsp16 (Screen ID: 40). Compounds were filtered so that hits had MW < 600 dalton, cLogP < 6, number of hydrogen bond acceptors < 11, and no reactive functional groups. A few compounds unsuitable for drug discovery were removed by visual inspection. The name of each compound consists of the initial letter 'v' for virtual hit, followed by the target protein name and the target site ('nsp10' for nsp10 binding site, 1 for docking scenario 1). The score is the docking score given by QuickVina 2 in kcal/mol. The ligand efficiency (LE) is computed as LE = -score/#NonH, where #NonH is the number of heavy (i.e. non hydrogen) atoms.

Name	Catalog ID	Score	LE	MW	Library	SMILES
vOrf7a-ppi1-1	Z1314038522	-9.4	0.285	441.529	REAL	CN1CCC(=O)Nc2cc(C(=O)NCc3ccc(-c4ccc5c(c4)CCCO5)cc3)cccc21
vOrf7a-ppi1-2	Z1413840855	-9.4	0.285	443.502	REAL	Cn1cc(/C=C/C(=O)c2ccc3c(c2)C(C)(C)C(=O)N3)c(-c2ccc3c(c2)OCCCO3)n1
vOrf7a-ppi1-3	ZINC000001099260	-9.4	0.261	474.427	ZINC	O=C1NC(=O)c2cc(N3C(=O)c4cc5oc6ccccc6c6ccccc6oc5cc4C3=O)ccc21
vOrf7a-ppi1-4	Z119684146	-9.3	0.251	498.533	REAL	O=C1O[C@H](c2ccccc2)Cc2cc(C(=O)N3C[C@@H](C(=O)N4CCOCC4)Oc4ccccc43)ccc21
vOrf7a-ppi1-5	Z443975892	-9.3	0.258	490.465	REAL	O=C1CCc2cc(F)c(NC(=O)c3cccc(C(=O)Nc4cc5c(cc4F)CCC(=O)N5)c3)cc2N1
vOrf7a-ppi1-6	Z749631200	-9.3	0.282	476.939	REAL	O=C1c2ccccc2S(=O)(=O)c2cc(C(=O)N3CCc4[nH]c5ccc(Cl)cc5c4C3)ccc21
vOrf7a-ppi1-7	ZINC000002832254	-9.3	0.266	473.507	ZINC	O=c1oc2ccc3ccccc3c2cc1-c1csc(-c2cc3c(ccc4ccccc43)oc2=O)n1
vOrf7a-ppi1-8	ZINC000408827077	-9.3	0.291	421.451	ZINC	O=C(O)c1ccc([C@@H]2Nc3ccc4c(c3[C@@H]3C=CC[C@@H]32)C(=O)c2ccccc2C4=O)cc1
vOrf7a-ppi1-9	PV-001830534322	-9.2	0.287	448.415	REAL	O=C(C1=CCc2ccccc2O[C@H]1C(F)(F)F)N1CCCN(C(=O)c2ccc(F)cc2)CC1
vOrf7a-ppi1-10	Z1335131363	-9.2	0.287	425.487	REAL	C[C@@]1(c2ccc(C(=O)N3CC=C(c4cccc5ccccc45)CC3)cc2)NC(=O)NC1=O
vOrf7a-ppi1-11	Z1682392311	-9.2	0.297	421.387	REAL	C[C@@]1(c2ccc(-c3noc(-c4cc5c(cc4F)NC(=O)CC5)n3)cc2)NC(=O)NC1=O
vOrf7a-ppi1-12	Z1684581689	-9.2	0.287	439.377	REAL	C[C@@]1(c2ccccc(-c3noc([C@H]4CC(c5cc(F)ccc5F)=NO4)n3)c2)NC(=O)NC1=O
vOrf7a-ppi1-13	Z1684582129	-9.2	0.297	421.387	REAL	C[C@]1(c2ccccc(-c3noc(-c4cc5c(cc4F)NC(=O)CC5)n3)c2)NC(=O)NC1=O
vOrf7a-ppi1-14	Z2160286354	-9.2	0.279	436.43	REAL	Cn1c(=O)[nH]c2ncc(-c3cccc(-c4nc(-c5cc(=O)[nH]c6ccccc56)no4)c3)cc21
vOrf7a-ppi1-15	ZINC000002121309	-9.2	0.287	417.423	ZINC	O=C1c2cc3oc4ccccc4c3cc2N=C1NNc1ccc2oc3ccccc3c2c1
vOrf7a-ppi1-16	ZINC000409336379	-9.2	0.263	451.488	ZINC	O=C(Nc1cccc2ccccc21)c1ccc2nc3c4ncccc4c4ccenc4c3nc2c1
vOrf7a-ppi1-17	Z110100908	-9.1	0.268	477.54	REAL	C[C@H]1Oc2ccc(NC(=O)c3cccc(S(=O)(=O)N4c5ccccc5C[C@@H]4C)c3)cc2NC1=O
vOrf7a-ppi1-18	Z1451968763	-9.1	0.303	402.496	REAL	Cc1ccc2[nH]c([C@H]3CCCN(C(=O)c4ccc5c(c4)C(C)(C)C(=O)N5)C3)nc2c1
vOrf7a-ppi1-19	Z1523896184	-9.1	0.284	427.503	REAL	C[C@H]1Cc2cc(-c3ccc(CNC(=O)Nc4ccc5c(c4)NC(=O)CC5)cc3)ccc2O1
vOrf7a-ppi1-20	Z1682662164	-9.1	0.314	415.807	REAL	O=C1CCc2cc(-c3nc(-c4ccc(Cl)c5c(c4)OCCCO5)no3)c(F)cc2N1
vOrf7a-ppi1-21	Z1684579932	-9.1	0.303	400.393	REAL	C[C@@]1(c2cccc(-c3noo(-c4cc5ccccc5cc4O)n3)c2)NC(=O)NC1=O
vOrf7a-ppi1-22	Z1684582773	-9.1	0.303	400.437	REAL	C[C@]1(c2cccc(-c3noo([C@H]4C[C@]45CCc4ccccc45)n3)c2)NC(=O)NC1=O
vOrf7a-ppi1-23	Z1684583182	-9.1	0.276	439.474	REAL	Cc1ccc2nc(C3CC3)cc(-c3nc(-c4cccc([C@]5(C)NC(=O)NC5=O)c4)no3)c2c1
vOrf7a-ppi1-24	Z1764266200	-9.1	0.284	426.431	REAL	C[C@@]1(c2cccc(NC(=O)c3ccc4[nH]c5ccccc5c(=O)c4c3)c2)NC(=O)NC1=O
vOrf7a-ppi1-25	Z1765224786	-9.1	0.314	383.45	REAL	CN1CCN(C(=O)c2ccc3[nH]c4ccccc4c(=O)c3c2)Cc2ccccc21
vOrf7a-ppi1-26	Z2073839861	-9.1	0.284	428.447	REAL	Cn1c(=O)[nH]c2ncc(-c3cccc(C(=O)Oc4cccc5c4CCCC(=O)N5)c3)cc21
vOrf7a-ppi1-27	ZINC000001588362	-9.1	0.268	440.509	ZINC	Nc1nc(-c2ccc3ccccc3c2)cc(-c2cc(-c3ccc4ccccc4c3)nc(N)n2)n1
vOrf7a-ppi1-28	ZINC000004175991	-9.1	0.294	398.464	ZINC	O=C1[C@@H]2[C@@H](c3nc4cccc5ccccc(c54)n31)C1c3ccccc3C2c2ccccc21
vOrf7a-ppi1-29	ZINC000013639683	-9.1	0.303	405.388	ZINC	Cc1cc(O)nc(-n2[nH]c3ncc4c(c3c2=O)C[C@H](c2ccc(F)cc2)CC4=O)n1
vOrf7a-ppi1-30	ZINC000022606981	-9.1	0.294	418.495	ZINC	CC(C)c1ccc([C@@H]2CC(=O)c3cnc4nc(N5CCOCC5)nc(O)c4c3C2)cc1
vOrf7a-ppi1-31	ZINC000100485501	-9.1	0.284	410.431	ZINC	O=C1c2ccc3c4c(ccc(c24)C2=Nc4ccccc4[C@H]21)C1=Nc2ccccc2[C@@H]1C3=O
vOrf7a-ppi1-32	ZINC000103269040	-9.1	0.268	477.54	ZINC	C[C@H]1Cc2ccccc2N1S(=O)(=O)c1cccc(C(=O)Nc2ccc3c(c2)NC(=O)[C@@H](C)O3)c1
vOrf7a-ppi1-33	ZINC000408733643	-9.1	0.246	485.538	ZINC	Cc1ccc2c(c1)OC(=O)[C@@H]1C2=C[C@H](c2ccccc2)[C@@H]2C(=O)Nc3ccc4ccccc4c3)C(=O)[C@H]21
vOrf7a-ppi1-34	PV-001793372083	-9	0.321	374.414	REAL	Cc1cccc(-c2ccccc(C(=O)Nc3cc4c(cc3F)CCC(=O)N4)c2)c1
vOrf7a-ppi1-35	PV-001872294966	-9	0.3	416.398	REAL	O=C1CCC[C@@H](c2ccccc(NC(=O)C3=Cc4ccccc4O[C@@H]3C(F)(F)F)c2)N1
vOrf7a-ppi1-36	Z1000938554	-9	0.281	430.506	REAL	C[C@@]1(c2cccc(CNC(=O)c3ccc4[nH]c5c(c4c3)CCCCC5)c2)NC(=O)NC1=O
vOrf7a-ppi1-37	Z1066065960	-9	0.273	476.536	REAL	O=C1CCc2cc(-c3csc(NS(=O)(=O)c4ccc5c6c(cccc46)C(=O)N5)n3)ccc2N1
vOrf7a-ppi1-38	Z109823584	-9	0.243	496.561	REAL	O=C1O[C@H](c2ccccc2)Cc2cc(C(=O)N3C[C@@H](C(=O)N4CCCCC4)Oc4ccccc43)ccc21
vOrf7a-ppi1-39	Z1101970934	-9	0.25	482.538	REAL	O=C1CCCc2cc(NC(=O)c3cccc(C(=O)Nc4ccc5c(c4)CCCC(=O)N5)c3)ccc2N1
vOrf7a-ppi1-40	Z1129794550	-9	0.29	415.463	REAL	O=C1O[C@H](c2ccccc2)Cc2cc(C(=O)N3CC[C@@H](c4cccc(F)c4)C3)ccc21
vOrf7a-ppi1-41	Z1162537090	-9	0.273	436.47	REAL	O=C(Nc1nc2ccccc2c(=O)[nH]1)[C@@H]1CC(=O)N(c2ccc3c(c2)Cc2ccccc2-3)C1
vOrf7a-ppi1-42	Z1256087617	-9	0.29	427.425	REAL	O=C([C@@H]1C[C@H]1c1ccccc1OC(F)(F)F)N1CC=C(c2c[nH]c3ncccc23)CC1
vOrf7a-ppi1-43	Z1413841768	-9	0.3	401.421	REAL	CC1(C)C(=O)Nc2ccc(C(=O)/C=C\c3c[nH]nc3-c3ccc4c(c3)OCO4)cc21
vOrf7a-ppi1-44	Z1450615957	-9	0.3	403.433	REAL	CC1(C)C(=O)Nc2ccc(C(=O)OCc3cc(=O)oc4cc5c(cc34)CCC5)cc21
vOrf7a-ppi1-45	Z1451926979	-9	0.281	425.487	REAL	C[C@@]1(c2cccc(C(=O)N3CC=C(c4cccc5ccccc45)CC3)c2)NC(=O)NC1=O
vOrf7a-ppi1-46	Z1451968788	-9	0.281	431.495	REAL	Cc1ccc2[nH]c([C@H]3CCCN(C(=O)c4cccc([C@]5(C)NC(=O)NC5=O)c4)C3)nc2c1
vOrf7a-ppi1-47	Z1602670418	-9	0.29	417.507	REAL	CC1(C)CC[C@H]2C[C@H](NC(=O)c3cccc([C@]4(C)NC(=O)NC4=O)c3)c3cccc1c32
vOrf7a-ppi1-48	Z1651242662	-9	0.273	440.458	REAL	O=C(Cc1ccc2c(c1)NC(=O)C2)Nc1ccc(C(=O)N2CC(=O)Nc3ccccc32)cc1
vOrf7a-ppi1-49	Z1663154013	-9	0.281	420.427	REAL	O=C1COc2cc(-c3nnc(-c4cc(-c5ccccc5)nc5ccccc45)o3)ccc2N1
vOrf7a-ppi1-50	Z1663469957	-9	0.281	419.443	REAL	O=C1CCc2cc(-c3nnc(-c4cc(-c5cccc5)nc5ccccc45)o3)ccc2N1
vOrf7a-ppi1-51	Z1682661745	-9	0.31	411.844	REAL	CC1(C)C(=O)Nc2ccc(-c3nc(-c4cc(Cl)c5c(c4)OCCCO5)no3)cc21
vOrf7a-ppi1-52	Z1683685247	-9	0.281	431.495	REAL	CN1CCN(C(=O)c2ccc(-c3noc(-c4ccc5c(c4)C(C)(C)C(=O)N5)n3)cc2)CC1
vOrf7a-ppi1-53	Z1683729579	-9	0.273	446.412	REAL	O=C1CCc2cc(-c3nc(-c4cccc(NC(=O)c5ccccc5F)c4)no3)c(F)cc2N1
vOrf7a-ppi1-54	Z1684580621	-9	0.29	415.408	REAL	C[C@@]1(c2ccccc(-c3noc(Cc4cc5ccccc5[nH]c4=O)n3)c2)NC(=O)NC1=O
vOrf7a-ppi1-55	Z1684580686	-9	0.29	417.424	REAL	CC(=O)N1c2ccccc2C[C@H]1c1nc(-c2cccc([C@]3(C)NC(=O)NC3=O)c2)no1
vOrf7a-ppi1-56	Z1684580765	-9	0.281	432.435	REAL	C[C@]1(c2ccccc(-c3noc([C@H]4C[C@@H]4c4ccc5c(c4)OCCO5)n3)c2)NC(=O)NC1=O
vOrf7a-ppi1-57	Z1684581548	-9	0.3	401.425	REAL	Cc1[nH]c2ccc(-c3nc(-c4cccc([C@]5(C)NC(=O)NC5=O)c4)no3)cc2c1C
vOrf7a-ppi1-58	Z1684581602	-9	0.3	402.453	REAL	Cc1cc(C)cc(C2(c3nc(-c4cccc([C@]5(C)NC(=O)NC5=O)c4)no3)CC2)c1
vOrf7a-ppi1-59	Z1684582725	-9	0.3	399.409	REAL	Cc1ccc2cccc(-c3nc(-c4cccc([C@]5(C)NC(=O)NC5=O)c4)no3)c2n1
vOrf7a-ppi1-60	Z1685242159	-9	0.281	421.463	REAL	Cc1cc(-c2noc(-c3cc(-c4cccc4)nc4c3c(C)nn4C)n2)cc2nc[nH]c12
vOrf7a-ppi1-61	Z1685439490	-9	0.273	436.474	REAL	Cc1nn(C)c2nc(-c3ccccc3)cc(-c3nc(-c4ccc5c(c4)CCC(=O)N5)no3)c12
vOrf7a-ppi1-62	Z1739747160	-9	0.273	438.446	REAL	Cn1c(=O)[nH]c2ncc(-c3cccc(-c4nc(-c5ccc6c(c5)CCC(=O)N6)no4)c3)cc21
vOrf7a-ppi1-63	Z1766451513	-9	0.273	436.514	REAL	Cc1ccc2[nH]c([C@H]3CCCN(C(=O)c4ccc5[nH]c6ccccc6c(=O)c5c4)C3)nc2c1
vOrf7a-ppi1-64	Z1988035038	-9	0.281	438.57	REAL	C[C@H]1CC[C@H](O)[C@H]([C@H]2CCCN2C(=O)[C@H]2CCCN(C(=O)c3ccc4[nH]ncc4c3)C2)C1
vOrf7a-ppi1-65	Z2117057514	-9	0.281	437.513	REAL	C[C@H]1CCc2cF)cccc2[C@H]1NC(=O)N1C[C@@H](C[C@@H]2COCC(=O)N2)c2ccccc21
vOrf7a-ppi1-66	Z2157310224	-9	0.273	437.458	REAL	O=C1CN(c2ccc(-c3noc(-c4ccc5[nH]c6ccccc6c(=O)c5c4)n3)cc2)CCN1
vOrf7a-ppi1-67	Z2157917647	-9	0.281	429.435	REAL	C[C@@H](c1nc(-c2cccc([C@]3(C)NC(=O)NC3=O)c2)no1)n1ccc2ccccc2c1=O
vOrf7a-ppi1-68	Z2171979283	-9	0.29	416.436	REAL	C[C@@]1(c2ccccc(-c3noc(-c4ccc5c(c4)CCCCC5=O)n3)c2)NC(=O)NC1=O
vOrf7a-ppi1-69	Z2265466591	-9	0.31	385.47	REAL	Cc1ccccc(-c2nnc3n2C[C@@H](C(=O)Nc2ccc4[nH]c(C)cc4c2)CC3)c1
vOrf7a-ppi1-70	Z442663522	-9	0.265	490.563	REAL	O=C1CSc2ccc(NC(=O)c3cccc(C(=O)Nc4ccc5c(c4)NC(=O)CS5)c3)cc2N1
vOrf7a-ppi1-71	Z448918812	-9	0.257	464.528	REAL	Cc1ccc(-c2cc(C(=O)NNC(=O)N[C@H](C)c3nc4ccccc4[nH]3)c3ccccc3n2)cc1
vOrf7a-ppi1-72	Z770162286	-9	0.265	449.509	REAL	O=C(c1ccccc(N2C(=O)c3ccccc3C2=O)c1)N1CCC[C@@H](c2cc3ccccc3[nH]2)C1
vOrf7a-ppi1-73	Z998852352	-9	0.273	436.514	REAL	O=C(c1ccc2[nH]ncc2c1)N1CCC[C@H](C(=O)N2Cc3ccccc3-c3ccccc32)C1
vOrf7a-ppi1-74	ZINC000002831958	-9	0.25	470.531	ZINC	Cc1cc(-c2ccc(/N=C3/c4ccccc4NC3=O)c(C)c2)ccc1/N=C1/c2ccccc2NC1=O
vOrf7a-ppi1-75	ZINC000004522785	-9	0.265	444.445	ZINC	Nc1ccccc2c1C(=O)c1cccc(Nc3ccc4c(c3)C(=O)c3ccccc3C4=O)c1C2=O
vOrf7a-ppi1-76	ZINC000006444984	-9	0.273	444.505	ZINC	O=C(O)CNC(=O)c1cc2c3c(c1)[C@H]1C=CC[C@@H]1CN3[C@@H](c1ccc(F)cc1)[C@@H]1CC=C[C@H]21
vOrf7a-ppi1-77	ZINC000012436788	-9	0.273	431.446	ZINC	O=C(Nc1cccc2c1C(=O)[C@@H]1C=CC=C[C@H]1C2=O)c1cccc2c1C(=O)c1ccccc1-2
vOrf7a-ppi1-78	ZINC000015080442	-9	0.273	437.494	ZINC	O=C(c1ccc2c3c(cccc31)CC2)[C@@H]1CCCN(C(=O)c2cc(=O)c3ccccc3o2)C1
vOrf7a-ppi1-79	ZINC000018117591	-9	0.273	431.446	ZINC	O=C(Nc1cccc2c1C(=O)[C@H]1C=CC=C[C@@H]1C2=O)c1cccc2c1C(=O)c1ccccc1-2
vOrf7a-ppi1-80	ZINC000019973984	-9	0.29	416.523	ZINC	CC(C)c1ccc([C@@H]2CC(=O)c3cnc4nc(N5CCCCC5)nH]c(=O)c4c3C2)cc1
vOrf7a-ppi1-81	ZINC000100737710	-9	0.273	431.446	ZINC	O=C(Nc1cccc2c1C(=O)[C@H]1C=CC=C[C@H]1C2=O)c1cccc2c1C(=O)c1ccccc1-2
vOrf7a-ppi1-82	ZINC000229542679	-9	0.265	477.54	ZINC	C[C@@H]1Cc2ccccc2N1S(=O)(=O)c1cccc(C(=O)Nc2ccc3c(c2)NC(=O)[C@@H](C)O3)c1
vOrf7a-ppi1-83	ZINC000257198807	-9	0.281	428.578	ZINC	O=C(c1n[nH]c2c1CCc1ccccc1-2)N1CCCC2=C[C@H]3C[C@H](CN4CCCC[C@@H]34)[C@H]21
vOrf7a-ppi1-84	ZINC000408826920	-9	0.3	391.469	ZINC	Cc1ccc([C@@H]2Nc3ccc4c(c3[C@@H]3C=CC[C@@H]32)C(=O)c2ccccc2C4=O)cc1
vOrf7a-ppi1-85	ZINC000408831744	-9	0.3	411.887	ZINC	O=C1c2ccccc2C(=O)c2c1ccc1c2[C@@H]2C=CC[C@@H]2[C@H](c2ccc(Cl)cc2)N1
vOrf7a-ppi1-86	PV-001793587453	-8.9	0.27	457.455	REAL	CC(=O)Nc1ccc(NC(=O)[C@H]2CCc3nnc(-c4cccc(C)c4)n3C2)c(C(F)(F)F)c1
vOrf7a-ppi1-87	PV-001800444863	-8.9	0.287	437.901	REAL	C[C@@H]1C(=O)Nc2cc(C(=O)NCc3ccc(-c4ccc(Cl)cc4)cc3F)ccc2N1C
vOrf7a-ppi1-88	PV-001834031082	-8.9	0.342	358.484	REAL	O=C1C[C@H](C(=O)Nc2cc(C3CCCCCC3)[nH]n2)[C@H]2CCCC[C@H]2N1
vOrf7a-ppi1-89	PV-001836932620	-8.9	0.287	437.901	REAL	CN1CCC(=O)Nc2cc(C(=O)NCc3ccc(-c4ccc(Cl)cc4)cc3F)ccc21
vOrf7a-ppi1-90	PV-001850179638	-8.9	0.307	387.398	REAL	O=C(Nc1cccc1)Nc1ccc(C(=O)Nc2n[nH]c3cc(O)ccc23)cc1
vOrf7a-ppi1-91	PV-001856498358	-8.9	0.33	366.463	REAL	Cc1cc(C)cc(-c2cc(NC(=O)[C@H]3CC(=O)N[C@@H]4CCCC[C@@H]43)[nH]n2)c1
vOrf7a-ppi1-92	PV-001869140399	-8.9	0.297	404.429	REAL	Cc1cc(C)c(-c2cc(NC(=O)c3cc(C)c4c(=O)[nH]c(O)nc4n3)[nH]n2)cc1C
vOrf7a-ppi1-93	PV-001945884979	-8.9	0.27	453.419	REAL	O=C(NNC(=O)c1cc2ccccc2cc1O)N[C@H](c1cccc2ccccc12)C(F)(F)F
vOrf7a-ppi1-94	PV-001947448281	-8.9	0.33	367.383	REAL	NC(=O)Nc1cc(NC(=O)N2CCc3c([nH]c4ccccc34)C2)ccc1F
vOrf7a-ppi1-95	Z1069479288	-8.9	0.287	418.491	REAL	C[C@@H]1Oc2ccc(C(=O)C3CCN(C(=O)c4cccc5c4CCC5)CC3)cc2NC1=O
vOrf7a-ppi1-96	Z1123944616	-8.9	0.254	495.53	REAL	C[C@@H]1Oc2ccc(NC(=O)c3cc(S(=O)(=O)N4c5ccccc5C[C@H]4C)ccc3F)cc2NC1=O
vOrf7a-ppi1-97	Z1129123713	-8.9	0.27	445.565	REAL	NC(=O)C1CCN(c2nccc2CNC(=O)c2ccc3[nH]c4c(c3c2)CCCC4)CC1
vOrf7a-ppi1-98	Z1148382838	-8.9	0.254	465.512	REAL	Cc1ccc2nc(-c3cccnc3)cc(C(=O)NCc3cccc([C@]4(C)NC(=O)NC4=O)c3)c2c1
vOrf7a-ppi1-99	Z1172365392	-8.9	0.27	443.506	REAL	COc1cc2nc(N3CCN(C(=O)c4cccc5ccccc45)CC3)nc(N)c2cc1OC
vOrf7a-ppi1-100	Z1175482539	-8.9	0.297	402.496	REAL	Cc1ccc2c(c1)N(C(=O)[C@H]1CCCN(C(=O)c3ccc4[nH]ncc4c3)C1)CCC2

Supplementary Table 79. Top 100 virtual hits of the screen against the surface of ORF7a (Screen ID: 9). Compounds were filtered so that hits had MW < 600 dalton, cLogP < 6, number of hydrogen bond acceptors < 11, and no reactive functional groups. A few compounds unsuitable for drug discovery were removed by visual inspection. The name of each compound consists of the initial letter 'v' for virtual hit, followed by the target protein name and the target site ('ppi' for protein-protein interface, 1 for docking scenario 1). The score is the docking score given by QuickVina 2 in kcal/mol. The ligand efficiency (LE) is computed as LE = -score/#NonH, where #NonH is the number of heavy (i.e. non hydrogen) atoms.

Name	Catalog ID	Score	LE	MW	Library	SMILES
vOrf7a-ppi1-101	Z1314038517	-8.9	0.270	442.47	REAL	Cc1cc(C(=O)NCc2ccc(-c3ccc4c(c3)CCCO4)cc2)nc2nc(O)[nH]c(=O)c12
vOrf7a-ppi1-102	Z1344205818	-8.9	0.270	440.59	REAL	O=C([C@H]1C[C@@]12CCc1ccccc12)N1CCCN(C(=O)[C@H]2C[C@@]23CCc2ccccc23)CC1
vOrf7a-ppi1-103	Z1447518399	-8.9	0.297	406.46	REAL	Cc1ccc2[nH]c([C@H]3CCCN(C(=O)c4cc5c(cc4F)NC(=O)CC5)C3)nc2c1
vOrf7a-ppi1-104	Z1452822444	-8.9	0.330	366.44	REAL	C[C@@H]1CCc2c(F)cccc2[C@@H]1NC(=O)c1ccc2c(c1)C(C)(C)C(=O)N2
vOrf7a-ppi1-105	Z1472744572	-8.9	0.287	418.45	REAL	Cc1n[nH]c(NC(=O)c2ccc3c(c2)C(C)(C)C(=O)N3)c1-c1ccc2c(c1)OCCO2
vOrf7a-ppi1-106	Z1522533358	-8.9	0.278	433.51	REAL	C[C@H]1Cc2cc(-c3ccc(CNC(=O)C4CCC5(CC4)NC(=O)NC5=O)cc3)ccc2O1
vOrf7a-ppi1-107	Z1601183738	-8.9	0.287	417.47	REAL	NC(=O)c1n[nH]c2ccc(N[C@@H]3CCCC[C@H](N4C(=O)c5ccccc5C4=O)C3)cc12
vOrf7a-ppi1-108	Z1610573477	-8.9	0.278	443.48	REAL	Cc1cc2ccccc2nc1NNC(=O)c1ccc2c(c1)S(=O)(=O)c1ccccc1C2=O
vOrf7a-ppi1-109	Z1683817915	-8.9	0.278	432.48	REAL	CC(=O)N1CCN(c2cc(-c3noc(-c4ccc5c(c4)C(C)(C)C(=O)N5)n3)ccn2)CC1
vOrf7a-ppi1-110	Z1684062486	-8.9	0.297	403.44	REAL	CC1(C)C(=O)Nc2ccc(-c3nc(-c4ccc(N5CCNC(=O)C5)cc4)no3)cc21
vOrf7a-ppi1-111	Z1684064363	-8.9	0.287	413.48	REAL	O=C1CN(c2ccc(-c3noc(-c4ccc5[nH]c6c(c5c4)CCCC6)n3)cc2)CCN1
vOrf7a-ppi1-112	Z1684199339	-8.9	0.307	388.39	REAL	Cc1[nH]c2ccc(-c3noc(-c4cnc5c(c4)c(=O)[nH]c(=O)n5C)n3)cc2c1C
vOrf7a-ppi1-113	Z1684199417	-8.9	0.342	349.35	REAL	Cc1[nH]c2ccc(-c3noc(-c4cc5c(cc4O)OCO5)n3)cc2c1C
vOrf7a-ppi1-114	Z1684579693	-8.9	0.297	404.43	REAL	C[C@]1(c2cccc(-c3noc(-c4cc5c(cc4O)CCCC5)n3)c2)NC(=O)NC1=O
vOrf7a-ppi1-115	Z1684579912	-8.9	0.297	403.40	REAL	C[C@@]1(c2cccc(-c3noc(Cc4ccc5c(c4)NC(=O)C5)n3)c2)NC(=O)NC1=O
vOrf7a-ppi1-116	Z1684580156	-8.9	0.287	415.41	REAL	Cn1c(=O)ccc(-c2nc(-c3cccc([C@]4(C)NC(=O)NC4=O)c3)no2)c2ccccc21
vOrf7a-ppi1-117	Z1684580280	-8.9	0.287	414.46	REAL	C[C@@]1(c2cccc(-c3noc([C@@H]4C[C@]45CCCc4ccccc45)n3)c2)NC(=O)NC1=O
vOrf7a-ppi1-118	Z1684580286	-8.9	0.270	443.44	REAL	C[C@@]1(c2cccc(-c3noc(-c4cc(C5CC5)nc5ccc(F)cc45)n3)c2)NC(=O)NC1=O
vOrf7a-ppi1-119	Z1684580444	-8.9	0.297	399.41	REAL	Cc1cc(-c2nc(-c3cccc([C@]4(C)NC(=O)NC4=O)c3)no2)c2ccccc2n1
vOrf7a-ppi1-120	Z1684581049	-8.9	0.287	417.40	REAL	Cc1cc(-c2nc(-c3cccc([C@]4(C)NC(=O)NC4=O)c3)no2)c2ccc(F)cc2n1
vOrf7a-ppi1-121	Z1684581074	-8.9	0.307	392.39	REAL	C[C@@]1(c2cccc(-c3noc([C@H]4C[C@@H]4c4ccc(F)cc4)n3)c2)NC(=O)NC1=O
vOrf7a-ppi1-122	Z1684581455	-8.9	0.278	427.46	REAL	CC(C)c1cc(-c2nc(-c3cccc([C@]4(C)NC(=O)NC4=O)c3)no2)c2ccccc2n1
vOrf7a-ppi1-123	Z1684581792	-8.9	0.270	438.44	REAL	C[C@@]1(c2cccc(-c3noc(Cc4cc5c(ccc6ccccc65)o4)n3)c2)NC(=O)NC1=O
vOrf7a-ppi1-124	Z1684582483	-8.9	0.307	406.47	REAL	Cc1ccc2c(c1)S[C@H](c1nc(-c3cccc([C@]4(C)NC(=O)NC4=O)c3)no1)C2
vOrf7a-ppi1-125	Z1684582608	-8.9	0.287	440.84	REAL	C[C@@]1(c2cccc(-c3noc(-c4cc(Cl)c5c(c4)OCCCO5)n3)c2)NC(=O)NC1=O
vOrf7a-ppi1-126	Z1684583348	-8.9	0.297	401.39	REAL	C[C@@]1(c2cccc(-c3noc(-c4cccc(-c5ncn[nH]5)c4)n3)c2)NC(=O)NC1=O
vOrf7a-ppi1-127	Z1684853587	-8.9	0.330	361.40	REAL	CC1(C)C(=O)Nc2ccc(-c3nc([C@@H]4CCOc5ccccc54)no3)cc21
vOrf7a-ppi1-128	Z1685086980	-8.9	0.297	395.38	REAL	O=c1[nH]c2ccc(-c3noc(-c4cc(-c5ccco5)ne5ccccc45)n3)cc2[nH]1
vOrf7a-ppi1-129	Z1685375198	-8.9	0.297	401.39	REAL	CN(C)c1cc(-c2noc(-c3cnc4[nH]c(=O)[nH]c(=O)c4c3)n2)c2ccccc2n1
vOrf7a-ppi1-130	Z1685436842	-8.9	0.318	374.36	REAL	CN1C(=O)c2ccc(-c3nc(-c4ccc5c(c4)CCC(=O)N5)no3)cc2C1=O
vOrf7a-ppi1-131	Z1685438276	-8.9	0.307	390.36	REAL	Cn1c(=O)[nH]c(=O)c2cc(-c3nc(-c4ccc5c(c4)CCC(=O)N5)no3)cnc21
vOrf7a-ppi1-132	Z1685438656	-8.9	0.318	374.40	REAL	CC1(C)C(=O)Nc2ccc(-c3nc(-c4ccc5c(c4)CCC(=O)N5)no3)cc21
vOrf7a-ppi1-133	Z1723436569	-8.9	0.247	475.51	REAL	Cn1c(=O)[nH]c2ncc(-c3cccc(C(=O)NCc4ccc(-n5cnc6ccccc65)nc4)c3)cc21
vOrf7a-ppi1-134	Z1723437103	-8.9	0.247	479.54	REAL	Cn1c(=O)[nH]c2ncc(-c3cccc(C(=O)N4CCC(c5nc(-c6ccccc6)n[nH]5)CC4)c3)cc21
vOrf7a-ppi1-135	Z1723442804	-8.9	0.287	417.47	REAL	Cc1nc([C@H]2CCCN(C(=O)c3cccc(-c4cnc5[nH]c(=O)n(C)c5c4)c3)C2)n[nH]1
vOrf7a-ppi1-136	Z1744659652	-8.9	0.318	372.40	REAL	O=C1CCc2cc(NC(=O)c3ccc4c(c3)-c3ccccc3C4)c(F)cc2N1
vOrf7a-ppi1-137	Z1750748345	-8.9	0.270	440.50	REAL	Cc1ccc(NC(=O)c2ccccc2)cc1NC(=O)N1CC[C@]2(C1)C(=O)Nc1ccccc12
vOrf7a-ppi1-138	Z1763722201	-8.9	0.278	423.48	REAL	O=C(c1ccc2[nH]c3ccccc3c(=O)c2c1)N1CCC[C@H](c2nnc3ccccn23)C1
vOrf7a-ppi1-139	Z1767358997	-8.9	0.307	447.33	REAL	Cc1cc(Br)c2c(c1)CN(C(=O)c1ccc3[nH]c4ccccc4c(=O)c3c1)CC2
vOrf7a-ppi1-140	Z1767888779	-8.9	0.270	437.45	REAL	O=C(OCc1cc(=O)oc2cc3c(cc12)CCC3)c1ccc2[nH]c3ccccc3c(=O)c2c1
vOrf7a-ppi1-141	Z1771195936	-8.9	0.287	416.39	REAL	O=C(Nc1cc(-c2cccc(F)c2F)n[nH]1)c1ccc2[nH]c3ccccc3c(=O)c2c1
vOrf7a-ppi1-142	Z1772036337	-8.9	0.287	412.42	REAL	Cc1ccc(F)c(-c2cc(NC(=O)c3ccc4[nH]c5ccccc5c(=O)c4c3)[nH]n2)c1
vOrf7a-ppi1-143	Z1890551840	-8.9	0.278	428.45	REAL	CC1(C)C(=O)Nc2cccc(-c3nc(CC(=O)N4CCn5c4nc4ccccc45)no3)cc21
vOrf7a-ppi1-144	Z1897796092	-8.9	0.297	401.51	REAL	Cc1[nH]c2ccccc2c1C1=CCN(C(=O)N[C@@H]2CCc3cc(O)ccc3C2)CC1
vOrf7a-ppi1-145	Z1934679339	-8.9	0.307	393.42	REAL	CN1CCC(=O)Nc2cc(C(=O)NCc3ccc(-c4ccco4)cc3F)ccc21
vOrf7a-ppi1-146	Z1940876310	-8.9	0.297	423.47	REAL	Cc1ccc(F)cc1-c1nnc(NC(=O)N2CC[C@]3(C2)C(=O)Nc2ccccc23)s1
vOrf7a-ppi1-147	Z1949761967	-8.9	0.270	448.45	REAL	O=C1CCc2cc(F)c(NC(=O)c3cccc(NN4C(=O)[C@H]5CC=CC[C@@H]5C4=O)c3)cc2N1
vOrf7a-ppi1-148	Z1956676322	-8.9	0.330	354.41	REAL	O=C1CCCCc2cc(-c3nc4ccc5ccccc5cc4c(=O)[nH]3)ccc21
vOrf7a-ppi1-149	Z2155928866	-8.9	0.287	431.83	REAL	O=c1c2ccccc2[nH]c2ccc(-c3nc(-c4cc(Cl)c5c(c4)OCCO5)no3)cc12
vOrf7a-ppi1-150	Z2157699278	-8.9	0.270	435.44	REAL	Cc1c[nH]c(=O)n1-c1cccc(-c2noc(-c3ccc4[nH]c5ccccc5c(=O)c4c3)n2)c1
vOrf7a-ppi1-151	Z2157918411	-8.9	0.297	402.41	REAL	C[C@]1(c2cccc(-c3noc([C@H]4CCC(=O)c5ccccc54)n3)c2)NC(=O)NC1=O
vOrf7a-ppi1-152	Z2158388125	-8.9	0.270	436.43	REAL	Cc1c(-c2ccccc2)oc2c(-c3nc(-c4ccc5[nH]c(=O)[nH]c5c4)no3)ccc2c1=O
vOrf7a-ppi1-153	Z2158588243	-8.9	0.278	420.43	REAL	COc1cc(-c2noc(-c3ccc4[nH]c5ccccc5c(=O)c4c3)n2)c2ccccc2n1
vOrf7a-ppi1-154	Z2170585290	-8.9	0.297	404.47	REAL	O=C(Nc1ccc2[nH]c(N3CCOCC3)nc2c1)c1ccc2c(c1)CCCCC2=O
vOrf7a-ppi1-155	Z2171660643	-8.9	0.297	406.44	REAL	O=C1COc2c(cccc2NC(=O)N2CCC([C@@H]3C(=O)Nc4ccccc43)CC2)N1
vOrf7a-ppi1-156	Z2171893341	-8.9	0.287	416.44	REAL	C[C@]1(c2cccc(-c3noc(-c4ccc5c(c4)CCCCC5=O)n3)cc2)NC(=O)NC1=O
vOrf7a-ppi1-157	Z2171979271	-8.9	0.297	404.43	REAL	CC1(C)COc2ccc(-c3nc(-c4cccc[C@]5(C)NC(=O)NC5=O)c4)no3)cc21
vOrf7a-ppi1-158	Z2171986052	-8.9	0.330	355.40	REAL	O=C1CCCCc2cc(-c3nc(-c4ccccc5ncccc45)no3)ccc21
vOrf7a-ppi1-159	Z2172136505	-8.9	0.330	355.40	REAL	O=C1CCCCc2cc(-c3nc(-c4cccc5ncccc45)no3)ccc21
vOrf7a-ppi1-160	Z2193902171	-8.9	0.278	421.42	REAL	Cc1c(-c2ccccc2)oc2c(-c3nc(-c4ccc5[nH]nnc5c4)no3)cccc2c1=O
vOrf7a-ppi1-161	Z2221930694	-8.9	0.287	421.36	REAL	C[C@@]1(c2cccc(-c3noc(-c4cnc5c(F)ccc(F)c5c4)n3)c2)NC(=O)NC1=O
vOrf7a-ppi1-162	Z2232448624	-8.9	0.270	443.55	REAL	O=C(c1ccc2[nH]ncc2c1)N1CCC[C@H](C(=O)N2C[C@@H]3CCCCN3c3ccccc32)C1
vOrf7a-ppi1-163	Z230809316	-8.9	0.247	491.58	REAL	C[C@H]1c2cc3c(cc2C2(CCCC2)CN1C(=O)CCC(=O)c1ccc2c(c1)OCCCO2)OCCO3
vOrf7a-ppi1-164	Z24127003	-8.9	0.287	418.45	REAL	O=C1CN(C(=O)COc2ccc3c4c(c(=O)oc3c2)CCCCC4)c2ccccc2N1
vOrf7a-ppi1-165	Z2691526808	-8.9	0.318	370.45	REAL	C[C@@H]1C(=O)Nc2ccccc2CN1C(=O)[C@H]1C[C@@H]1c1ccc2ccccc2c1
vOrf7a-ppi1-166	Z2902676431	-8.9	0.254	464.48	REAL	C[C@@]1(c2cccc(-c3nc(-c4cccc(Cn5cnc6ccccc65)c4)no3)c2)NC(=O)NC1=O
vOrf7a-ppi1-167	Z2902893029	-8.9	0.247	484.53	REAL	CC1(C)C(=O)Nc2ccc(-c3nc(-c4ccc(N5CCN(c6ccc(F)cc6)CC5)nc4)no3)cc21
vOrf7a-ppi1-168	Z2903520995	-8.9	0.297	400.40	REAL	Cc1c(-c2noc(-c3cc(-c4ccc5ccccc5c4)[nH]n3)n2)c(=O)[nH]c(=O)n1C
vOrf7a-ppi1-169	Z297252242	-8.9	0.241	487.52	REAL	O=C(CNC(=O)c1cc(-c2cccc3ccccc23)nc2ccccc12)Nc1ccc2[nH]c(=O)[nH]c2c1
vOrf7a-ppi1-170	Z767063666	-8.9	0.287	410.43	REAL	C[C@@]1(c2cccc(NC(=O)c3cc4ccccc4c4ccnc34)c2)NC(=O)NC1=O
vOrf7a-ppi1-171	Z988062428	-8.9	0.241	494.60	REAL	O=C(Nc1ccc(CC(=O)N2CCCc3ccccc32)cc1)N1CCC(c2nnc3ccccn23)CC1
vOrf7a-ppi1-172	Z998960316	-8.9	0.254	469.59	REAL	Cc1[nH]c2ccccc2c1C1CCN(C(=O)[C@H]2CCCN(C(=O)c3ccc4[nH]ncc4c3)C2)CC1
vOrf7a-ppi1-173	ZINC000003182996	-8.9	0.278	439.45	ZINC	O=c1oc2cc(O)ccc2cc1-c1csc(-c2cc3c(ccc4ccccc43)oc2=O)n1
vOrf7a-ppi1-174	ZINC000003257351	-8.9	0.270	449.54	ZINC	Oc1nc2sc3c(c2c2nc(-c4cc(-c5ccccc5)nc5ccccc54)nn21)CCCC3
vOrf7a-ppi1-175	ZINC000009059757	-8.9	0.262	457.53	ZINC	Cc1c2cc3c(cc2oc(=O)c1CC(=O)N=c1[nH]c2ccccc2[nH]1)OC1(CCCCC1)CC3
vOrf7a-ppi1-176	ZINC000009561286	-8.9	0.247	477.57	ZINC	Cc1cccc(N2CCN(C(=O)c3cccc(Nc4nc5ccccc5n5cnnc45)c3)C[C@H]2C)c1
vOrf7a-ppi1-177	ZINC000013590233	-8.9	0.254	470.57	ZINC	Cc1ccc(N2C(=O)C[C@H]([C@H]3C=C(C)[C@H]4C(=O)N(c5ccc(C)c(C)c5)C(=O)[C@@H]4C3)C2=O)cc1C
vOrf7a-ppi1-178	ZINC000013639687	-8.9	0.297	401.43	ZINC	Cc1cccc([C@@H]2CC(=O)c3cnc4[nH]n(-c5nc(C)cc(O)n5)c(=O)c4c3C2)c1
vOrf7a-ppi1-179	ZINC000019973970	-8.9	0.307	390.44	ZINC	Cc1ccc([C@@H]2CC(=O)c3cnc4nc(N5CCOCC5)[nH]c(=O)c4c3C2)cc1
vOrf7a-ppi1-180	ZINC000038704217	-8.9	0.254	492.56	ZINC	Cc1cc(C)nc(NS(=O)(=O)c2ccc(NC(=O)c3cc(-c4ccc(C)c(C)c4O)n[nH]3)cc2)n1
vOrf7a-ppi1-181	ZINC000049947087	-8.9	0.270	427.51	ZINC	O=C1N(Cc2cccc3ccccc32)c2ccccc2C12Nc1ccc3ccccc(c31)N2
vOrf7a-ppi1-182	ZINC000057709837	-8.9	0.262	450.46	ZINC	O=c1[nH]c2cc3c(cc2cc1CNc1ccc2nc(-c4ccc5[nH]cnc5c4)[nH]c2c1)OCO3
vOrf7a-ppi1-183	ZINC000098023339	-8.9	0.234	541.35	ZINC	O=C(c1ccc2c(c1)C(=O)N(c1ccc(Cl)c1)C2=O)c1ccc2c(c1)C(=O)N(c1cccc(Cl)c1)C2=O
vOrf7a-ppi1-184	ZINC000100688954	-8.9	0.228	511.58	ZINC	Cc1ccc(N2C(=O)[C@@H]3[C@H](C2=O)[C@H]2c4ccccc4C=NN2[C@@H]3C(=O)c2ccc(-c3ccccc3)cc2)cc1
vOrf7a-ppi1-185	ZINC000101344116	-8.9	0.241	489.51	ZINC	O=C(c1ccc(F)cc1)[C@@H]1[C@@H]2C(=O)N(c3ccc4ccccc4c3)C(=O)[C@H]2[C@@H]2c3ccccc3C=NN21
vOrf7a-ppi1-186	ZINC000104480052	-8.9	0.247	490.95	ZINC	O=C(NC1=CC=C[C@@H]2C(=O)c3ccccc3C(=O)[C@H]12)c1cc(-c2ccccc2Cl)nc2ccccc21
vOrf7a-ppi1-187	ZINC000248341954	-8.9	0.262	451.53	ZINC	Cc1ccc2c(c1C)NC(=O)[C@@]21[C@@H]2C(=O)N(c3ccc4ccccc4c3)C(=O)[C@H]2[C@@H]2CCCN21
vOrf7a-ppi1-188	ZINC000257198481	-8.9	0.270	444.58	ZINC	O=C(c1cc(-c2ccc3c(c2)CCO3)n[nH]1)N1CCCC2=C[C@H]3C[C@H](CN4CCCC[C@@H]34)[C@H]21
vOrf7a-ppi1-189	ZINC000257198806	-8.9	0.278	428.58	ZINC	O=C(c1n[nH]c2c1CCc1ccccc1-2)N1CCCC2=C[C@H]3C[C@H](CN4CCCC[C@H]34)[C@H]21
vOrf7a-ppi1-190	ZINC000524729079	-8.9	0.241	491.50	ZINC	O=C1C[C@H](c2cc3cccc4c3n(c2=O)CCC4)c2c(cc(O)c3c(=O)c(-c4ccccc4)coc32)O1
vOrf7a-ppi1-191	PV-001796027985	-8.8	0.314	374.48	REAL	Cc1cc(CNC(=O)c2ccc3c(c2)CCCCC3=O)c2[nH]c(C)c(C)c2c1
vOrf7a-ppi1-192	PV-001798023552	-8.8	0.326	356.42	REAL	Cc1cccc(-c2cccc(C(=O)Nc3ccc4c(c3)NC(=O)CC4)c2)c1
vOrf7a-ppi1-193	PV-001856498559	-8.8	0.314	373.46	REAL	Cc1cc(C)cc(-c2cc(NC(=O)c3ccc4c(c3)CCCC4=O)[nH]n2)c1
vOrf7a-ppi1-194	PV-001867470273	-8.8	0.303	400.36	REAL	O=C(NCc1cc(O)c2ccccc2n1)C1=Cc2ccccc2O[C@H]1C(F)(F)F
vOrf7a-ppi1-195	PV-001913003467	-8.8	0.303	394.57	REAL	CC(C)c1ccc2c(c1)CC[C@H]1[C@@](C)(CNc3nc(N)nc(N)n3)CCC[C@@]21C
vOrf7a-ppi1-196	PV-001947319179	-8.8	0.338	346.43	REAL	Cc1cc(NC(=O)N[C@@H]2CCc3cc(O)ccc3C2)c2ccccc2c1
vOrf7a-ppi1-197	Z1413841078	-8.8	0.314	371.44	REAL	Cc1ccc(-c2n[nH]cc2/C=C/C(=O)c2ccc3c(c2)C(C)(C)CC(=O)N3)cc1
vOrf7a-ppi1-198	Z1448126436	-8.8	0.303	394.36	REAL	O=C1CCc2cc(C(=O)Nc3[nH]ncc3-c3ccc4c(c3)OCO4)c(F)cc2N1
vOrf7a-ppi1-199	Z1542482556	-8.8	0.338	348.45	REAL	C[C@@H]1CCc2ccccc2[C@@H]1NC(=O)c1ccc2c(c1)C(C)(C)C(=O)N2
vOrf7a-ppi1-200	Z1684200041	-8.8	0.314	374.36	REAL	Cc1[nH]c2ccc(-c3noc(-c4cnc5[nH]c(=O)[nH]c(=O)c5c4)n3)cc2c1C

Supplementary Table 80. Virtual screening hits 101 to 200 of the screen against the surface of ORF7a (Screen ID: 9). Compounds were filtered so that hits had MW < 600 dalton, cLogP < 6, number of hydrogen bond acceptors < 11, and no reactive functional groups. A few compounds unsuitable for drug discovery were removed by visual inspection. The name of each compound consists of the initial letter 'v' for virtual hit, followed by the target protein name and the target site ('ppi' for protein-protein interface, 1 for docking scenario 1). The score is the docking score given by QuickVina 2 in kcal/mol. The ligand efficiency (LE) is computed as LE = -score/#NonH, where #NonH is the number of heavy (i.e. non hydrogen) atoms.

Name	Catalog ID	Score	LE	MW	Library	SMILES
vN-rna1-1	Z100370010	-10.8	0.318	9	REAL	C/C(=N/Nc1nc2ccccc2c(=O)n1-c1ccc(C)cc1C)c1ccc(-n2cnnn2)c1
vN-rna1-2	Z916986696	-10.7	0.306	8	REAL	C/C(=N/Nc1nc2ccccc2c(=O)n1-c1ccc(C)cc1C)c1ccc(N2CCOC2=O)c1
vN-rna1-3	ZINC000230013090	-10.7	0.306	7	ZINC	Cc1ccc(N2C(=O)[C@]3(Cc4ccccc4N4CCN(c5ccccc5)C[C@H]43)C(=O)N=C2O)cc1
vN-rna1-4	Z916986700	-10.6	0.303	8	REAL	C/C(=N\Nc1nc2ccccc2c(=O)n1-c1ccc(C)cc1C)c1ccc(N2CCOC2=O)c1
vN-rna1-5	ZINC000002840892	-10.6	0.321	7	ZINC	O=C1[C@@H]2[C@@H](C(=O)N1c1nc3ccccc3s1)C1c3ccccc3C2([N+](=O)[O-])c2ccccc21
vN-rna1-6	Z2007564992	-10.5	0.339	6	REAL	Cn1c(-c2cc3c(s2)CCCCCC3)nnc1N1CC[C@@]2(C1)C(=O)Nc1ccccc12
vN-rna1-7	Z363547144	-10.5	0.292	9	REAL	O=C(Nc1nnc2ccc(Cl)nn12)c1c2c(nc3ccccc13)/C(=C/c1ccc3c(c1)OCO3)CC2
vN-rna1-8	Z448673858	-10.5	0.3	8	REAL	O=C(NC[C@@H]1CC2c3ccccc3C1c1ccccc12)NNC(=O)c1n[nH]c(=O)c2ccccc12
vN-rna1-9	Z1039647126	-10.4	0.306	7	REAL	O=C([C@@H]1CCCN(c2nc3ccccc3s2)C1)N1CCC(c2nc(-c3ccccc3)n[nH]2)CC1
vN-rna1-10	Z104027022	-10.4	0.335	7	REAL	Cc1c(-c2nnc(-c3cccc(S(=O)(=O)N4CCCCC4)c3)o2)oc2c(F)cccc12
vN-rna1-11	Z449520874	-10.4	0.306	7	REAL	C/C(=N\Nc1nc2ccccc2c(=O)n1-c1ccc(C)cc1C)c1ccc2c(c1)CCC(=O)N2
vN-rna1-12	ZINC000011171943	-10.4	0.281	10	ZINC	CC(=O)Nc1ccc(N2C(=O)c3ccc(C(=O)O[C@@H](C)c4nc5ccccc5c(=O)[nH]4)cc3C2=O)cc1
vN-rna1-13	ZINC000016038169	-10.4	0.281	6	ZINC	O=C(c1ccc(Cl)cc1)[C@@H]1[C@@H]2C(=O)N(c3cccc4ccccc43)C(=O)[C@@H]2[C@H]2c3ccccc3C=NN12
vN-rna1-14	ZINC000020533997	-10.4	0.306	5	ZINC	O=C(O)C12c3ccccc3C(c3ccccc31)[C@H]1C(=O)N(c3cccc4ccccc43)C(=O)[C@H]12
vN-rna1-15	ZINC000020533999	-10.4	0.306	5	ZINC	O=C(O)C12c3ccccc3C(c3ccccc31)[C@@H]1C(=O)N(c3cccc4ccccc43)C(=O)[C@H]12
vN-rna1-16	ZINC000248140721	-10.4	0.289	8	ZINC	COc1ccc(N2C(=O)NC(=O)[C@@]3(Cc4ccccc4N4CCN(c5ccccc5)C[C@H]43)C2=O)cc1
vN-rna1-17	ZINC000408730080	-10.4	0.274	5	ZINC	Cc1ccc(N2C(=O)[C@H]3[C@H](C2=O)[C@@H]2C(=O)Oc4c5ccccc5ccc4C2=C[C@H]3c2ccccc2)c(C)c1
vN-rna1-18	Z1039650188	-10.3	0.286	8	REAL	O=C1c2ccccc2S(=O)(=O)c2cc(C(=O)N3CCC(c4nc(-c5ccccc5)n[nH]4)CC3)ccc21
vN-rna1-19	Z1417814945	-10.3	0.312	7	REAL	O=C(c1ccc2[nH]ncc2c1)N1CCC[C@@H](C(=O)N2CCC3(CC2)OCc2ccccc23)C1
vN-rna1-20	Z1685280116	-10.3	0.343	10	REAL	O=c1nc2c(-c3nc(-c4cccc(-n5cccn5)n4)no3)c[nH]n2c2ccccc12
vN-rna1-21	Z1834348123	-10.3	0.322	8	REAL	O=C(Nc1n[nH]c2cc(F)ccc12)c1ccccc(C(=O)Nc2n[nH]c3cc(F)ccc23)c1
vN-rna1-22	Z2087182409	-10.3	0.312	8	REAL	CC1(C)CC(=O)c2cc(NC(=O)[C@@H]3CCCN(C(=O)c4ccc5[nH]ncc5c4)C3)ccc2O1
vN-rna1-23	Z286572294	-10.3	0.286	9	REAL	CC(=O)Nc1ccc(N2C(=O)c3ccc(C(=O)OCc4nc(C)c5ccccc5n4)cc3C2=O)cc1
vN-rna1-24	Z449521112	-10.3	0.303	7	REAL	C/C(=N\Nc1nc2ccccc2c(=O)n1-c1ccc(C)cc1C)c1ccc2c(c1)CCC(=O)N2
vN-rna1-25	Z991833002	-10.3	0.286	9	REAL	O=C(CN1C(=O)N[C@]2(CCc3ccccc32)C1=O)N1CCC[C@H](c2nc(-c3cccc(F)c3)no2)C1
vN-rna1-26	ZINC000008845457	-10.3	0.303	8	ZINC	Cc1cccc(NC(=O)c2oc3ccccc3c2NC(=O)c2cc(-c3ccccc3O)n[nH]2)c1
vN-rna1-27	ZINC000015972032	-10.3	0.278	7	ZINC	Cc1cccc(N2C(=O)[C@@H]3[C@H](C2=O)[C@@H](Cc2c[nH]c4ccccc24)N[C@]32C(=O)Nc3ccc(F)cc32)c1
vN-rna1-28	ZINC000035944116	-10.3	0.264	7	ZINC	C[C@@H]1CC[C@H](C)[C@H](N2C(=O)c3ccc(Oc4ccc5c(c4)C(=O)N([C@@H]4C[C@@H](C)CC[C@H]4C)C5=O)cc3C2=O)C1
vN-rna1-29	ZINC000229930169	-10.3	0.24	7	ZINC	CC1=C[C@@H]2N(c3ccccc31)[C@H](C(=O)c1ccc(Cl)cc1)[C@@H](C(=O)c1ccc3c(c1)OCO3)[C@@]21C(=O)Nc2ccccc21
vN-rna1-30	ZINC000408730041	-10.3	0.278	5	ZINC	Cc1ccc(N2C(=O)[C@@H]3[C@H](C2=O)[C@@H]2C(=O)Oc4c5ccccc5ccc4C2=C[C@H]3c2ccccc2)cc1
vN-rna1-31	ZINC000408730075	-10.3	0.271	5	ZINC	Cc1ccc(N2C(=O)[C@@H]3[C@H](C2=O)[C@@H]2C(=O)Oc4c5ccccc5ccc4C2=C[C@H]3c2ccccc2)c(C)c1
vN-rna1-32	ZINC000409330841	-10.3	0.271	7	ZINC	O=C(Nc1ccc2nc3c4ccccc4c4ccccc4c3nc2c1)c1ccc(N2C(=O)C=CC2=O)cc1
vN-rna1-33	PV-001935764998	-10.2	0.34	8	REAL	NC(=O)N1CCCc2ccc(NS(=O)(=O)c3cc4c(cc3Cl)CCCC(=O)N4)cc21
vN-rna1-34	Z1037873764	-10.2	0.283	8	REAL	Cc1ccccc1NC(=O)[C@@H]1CCc2ccccc2N1C(=O)c1ccc(N2NC(=O)CCC2=O)cc1
vN-rna1-35	Z1037876612	-10.2	0.291	7	REAL	Cc1ccccc1NC(=O)[C@@H]1CCc2ccccc2N1C(=O)c1ccc(N2C(=O)CCC2=O)cc1
vN-rna1-36	Z1155286490	-10.2	0.3	6	REAL	O=C(Nc1nnc(Cc2ccccc2F)s1)[C@@H]1CCCN(C(=O)c2cccc3ccccc23)C1
vN-rna1-37	Z1161212003	-10.2	0.291	8	REAL	O=C(c1csc(-c2ccc3c(c2)OCCO3)n1)N1CCC[C@H](c2nc(-c3ccc(F)cc3)no2)C1
vN-rna1-38	Z165051166	-10.2	0.378	9	REAL	O=C1NC(=O)c2ccccc2/C1=C/Nc1nc2ccccc2n2nnnc12
vN-rna1-39	Z193545508	-10.2	0.309	10	REAL	Cc1ccc(C)c(N2C(=O)c3ccc(C(=O)OCc4nc(N)nc(N(C)C)n4)cc3C2=O)c1
vN-rna1-40	Z1983282382	-10.2	0.309	9	REAL	Cc1ccc2c(c1)c(=O)n(C)c1nnc(CN3C(=O)N[C@@]4(C[C@H]5C[C@@H]4[C@@H]4CCC[C@H]54)C3=O)n21
vN-rna1-41	Z3094262567	-10.2	0.34	7	REAL	Cc1ccc2cc(-c3nnc(N4CC[C@@]5(C4)C(=O)Nc4ccccc45)n3C)[nH]c2c1
vN-rna1-42	Z424333592	-10.2	0.283	9	REAL	Cc1ccc(C)c(N2C(=O)c3ccc(C(=O)Nc4cccc([C@@]5(C)NC(=O)NC5=O)c4)cc3C2=O)c1
vN-rna1-43	Z441413092	-10.2	0.309	6	REAL	C[C@]1(c2cccc(C(F)(F)F)c2)NC(=O)N(Cc2cc(=O)oc3cc4c(cc23)CCC4)C1=O
vN-rna1-44	Z448673098	-10.2	0.291	6	REAL	Cc1cc(C(=O)NNC(=O)NC[C@@H]2CC3c4ccccc4C2c2ccccc23)c2ccccc2n1
vN-rna1-45	Z448673850	-10.2	0.276	8	REAL	CCn1nc(C(=O)NNC(=O)NC[C@@H]2CC3c4ccccc4C2c2ccccc23)c2ccccc2c1=O
vN-rna1-46	Z449520116	-10.2	0.309	8	REAL	C/C(=N/Nc1nc2ccccc2c(=O)n1C)c1cccc(OCc2cn3ccccc3n2)c1
vN-rna1-47	Z764667804	-10.2	0.291	7	REAL	O=C(Nc1nc2ccccc2nc1N1CCCC1)c1ccc2c(c1)C[C@@H](c1ccccc1)OC2=O
vN-rna1-48	Z812555872	-10.2	0.291	8	REAL	O=C(CCC12C[C@H]3C[C@@H](C1)CC(C(=O)Nc1nc4ccccc4[nH]1)(C3)C2)Nc1nc2ccccc2[nH]1
vN-rna1-49	ZINC000000658060	-10.2	0.309	9	ZINC	O=C(NN1C(=O)[C@@H]2[C@@H](C1=O)C1c3ccccc3C2([N+](=O)[O-])c2ccccc21)c1ccncc1
vN-rna1-50	ZINC000002326623	-10.2	0.309	4	ZINC	O=C1C[C@H](c2cn(Cc3ccccc3)c3ccccc23)C(=O)N1c1ccc2ccccc21
vN-rna1-51	ZINC000002366044	-10.2	0.283	6	ZINC	O=C(c1ccccc1)[C@H]1[C@H]2C(=O)N(c3ccc4ccccc4c3)C(=O)[C@@H]2[C@H]2c3ccccc3C=NN12
vN-rna1-52	ZINC000049916776	-10.2	0.283	7	ZINC	O=C(c1ccc2c(c1)OCO2)[C@H]1[C@H]2C(=O)N(c3ccc(F)cc3)C(=O)[C@@H]2[C@H]2c3ccccc3C=CN12
vN-rna1-53	ZINC000101344120	-10.2	0.276	6	ZINC	O=C(c1ccc(F)cc1)[C@@H]1[C@@H]2C(=O)N(c3ccc4ccccc4c3)C(=O)[C@H]2[C@H]2c3ccccc3C=NN12
vN-rna1-54	ZINC000408675226	-10.2	0.268	5	ZINC	Cc1cccc(NC(=O)c2ccccc(N3C(=O)[C@H]4[C@@H](C3=O)C3c5ccccc5C4c4ccccc43)c2)c1C
vN-rna1-55	ZINC000408733646	-10.2	0.276	5	ZINC	Cc1ccc2c(c1)OC(=O)[C@@H]1C2=C[C@H](c2ccccc2)[C@H]2C(=O)N(c3ccc4ccccc4c3)C(=O)[C@H]21
vN-rna1-56	Z1039646216	-10.1	0.281	9	REAL	O=C(c1ccc2[nH]ncc2c1)N1CCC[C@H](C(=O)N2CCC(c3nc(-c4ccccc4)n[nH]3)CC2)C1
vN-rna1-57	Z104018388	-10.1	0.326	8	REAL	Cc1c(-c2nnc(-c3cccc(S(=O)(=O)N4CCOCC4)c3)o2)oc2c(F)cccc12
vN-rna1-58	Z1069484124	-10.1	0.289	7	REAL	C[C@@H]1Oc2ccc(C(=O)C3CCN(C(=O)c4cccc5c6c([nH]c45)CCCC6)CC3)cc2NC1=O
vN-rna1-59	Z1074946920	-10.1	0.281	9	REAL	CC(=O)N1CCCc2cc(NC(=O)N3CCC(C(=O)c4ccc5c(c4)NC(=O)[C@@H](C)O5)CC3)ccc21
vN-rna1-60	Z1118913879	-10.1	0.273	10	REAL	Cc1ccc(C)c(N2C(=O)c3ccc(C(=O)NNC(=O)C4CCN(c5ncccn5)CC4)cc3C2=O)c1
vN-rna1-61	Z1132553661	-10.1	0.289	9	REAL	C[C@@H]1Oc2ccc(C(=O)C3CCN(C(=O)Nc4ccc5c(c4)CCC(=O)N5C)CC3)cc2NC1=O
vN-rna1-62	Z1137170717	-10.1	0.297	8	REAL	C/C(=N\Nc1nc2ccccc2c(=O)n1-c1ccc(C)cc1C)c1cccc(NS(C)(=O)=O)c1
vN-rna1-63	Z1263760208	-10.1	0.337	9	REAL	C/C(=N\Nc1nc(-c2cccn2)nc2c1CCC2)c1cccc(-n2cnnn2)c1
vN-rna1-64	Z14076292	-10.1	0.306	6	REAL	C[C@]1(c2cccc3ccccc23)NC(=O)N(Cc2cc(=O)oc3cc4c(cc23)CCC4)C1=O
vN-rna1-65	Z1645879510	-10.1	0.337	8	REAL	O=S(=O)(c1cccc(-c2nnc([C@H]3COc4ccccc4O3)o2)c1)N1CCCCC1
vN-rna1-66	Z1685241667	-10.1	0.316	8	REAL	Cc1cc(-c2noc(-c3ccc4c(c3)S(=O)(=O)c3ccccc3C4=O)n2)cc2nc[nH]c12
vN-rna1-67	Z1685279260	-10.1	0.297	10	REAL	O=c1[nH]c2cc(-c3nc(-c4cccc(-n5cccn5)n4)no3)ccc2c(=O)n1-c1ccccc1
vN-rna1-68	Z1685320758	-10.1	0.326	10	REAL	Cc1nnc(-c2cccc(-c3noc(-c4c[nH]n5c4nc(=O)c4ccccc45)n3)c2)[nH]1
vN-rna1-69	Z1685325821	-10.1	0.337	10	REAL	O=c1nc2c(-c3nc(-c4cccc(-n5ccnc5)n4)no3)c[nH]n2c2ccccc12
vN-rna1-70	Z1685687614	-10.1	0.316	7	REAL	CN1CCN(c2ccnc(-c3noc(-c4cc(Cc5ccccc5)ccc4O)n3)c2)CC1
vN-rna1-71	Z18052785	-10.1	0.316	8	REAL	Cc1ccc2c(CN3C(=O)N[C@](C)(c4ccc5c(c4)OCCO5)C3=O)cc(=O)oc2c1C
vN-rna1-72	Z1820405953	-10.1	0.316	8	REAL	Cc1nc2ccccn2c1[C@H]1C(=O)NCCN1C(=O)[C@@H]1CC(c2cc(F)ccc2F)=NO1
vN-rna1-73	Z1891087676	-10.1	0.361	6	REAL	Oc1ccc(Cc2ccccc2)cc1-c1nc(-c2ccc3cc[nH]c3n2)no1
vN-rna1-74	Z1891829064	-10.1	0.316	7	REAL	Cc1cc(C)cc([C@H]2NC(=O)N(c3ccc(-c4nnc5n4CCCCC5)cc3)C2=O)c1
vN-rna1-75	Z2007963978	-10.1	0.337	7	REAL	Cn1c(-c2ccc3ccccc3n2)nnc1N1CC[C@@]2(C1)C(=O)Nc1ccccc12
vN-rna1-76	Z2167680249	-10.1	0.316	9	REAL	N\#Cc1ccccnc1-n1cc(NC(=O)N2CCC(c3noc4cc(F)ccc34)CC2)cn1
vN-rna1-77	Z2190297067	-10.1	0.306	7	REAL	CC1(C)NC(=O)N(c2ccccc(NC(=O)N3CCC[C@]4(CCCc5ccccc54)C3)c2)C1=O
vN-rna1-78	Z2193966758	-10.1	0.306	9	REAL	Cc1ccc(C)c(N2C(=O)c3ccc(-c4nc(-c5ccnc6ccnn56)no4)cc3C2=O)c1
vN-rna1-79	Z25741554	-10.1	0.289	8	REAL	O=C(CN1C(=O)N[C@@]2(CCc3ccccc32)C1=O)Nc1ccc2c(c1)C(=O)c1ccccc1C2=O
vN-rna1-80	Z286720458	-10.1	0.281	10	REAL	Cc1nc2ccccc2c2c(NC(=O)C3CCN(c4ccc5nnnn5n4)CC3)c3ccccc3n12
vN-rna1-81	Z2902676637	-10.1	0.289	8	REAL	Cc1c(-c2nc(-c3cccc(Cn4cnc5ccccc54)c3)no2)nnn1-c1ccc(F)c(F)c1
vN-rna1-82	Z2902704246	-10.1	0.281	9	REAL	Cc1cc(C)n(Cc2ccccc(-c3noc(CN4C(=O)c5ccccc5N5C(=O)CC[C@@]45C)n3)c2)n1
vN-rna1-83	Z3094784978	-10.1	0.348	8	REAL	Cn1c([C@@H]2CCc3cn[nH]c3C2)nnc1N1CC[C@@]2(C1)C(=O)Nc1ccccc12
vN-rna1-84	Z448673106	-10.1	0.297	7	REAL	Cc1nc2ccccn2c1C(=O)NNC(=O)NC[C@@H]1CC2c3ccccc3C1c1ccccc12
vN-rna1-85	Z685839178	-10.1	0.326	10	REAL	Cc1cc(C)n2nc(-c3nnc(-c4cccc(S(=O)(=O)N5CCCCC5)c4)o3)nc2n1
vN-rna1-86	Z767777902	-10.1	0.281	8	REAL	O=C(Nc1cccc(-c2n[nH]c3c2CCCC3)c1)c1ccc(NC2=NS(=O)(=O)c3ccccc32)cc1
vN-rna1-87	Z80629029	-10.1	0.306	8	REAL	Cc1ccc2c(CN3C(=O)N[C@](C)(c4ccc5c(c4)OCCCO5)C3=O)cc(=O)oc2c1C
vN-rna1-88	Z941450350	-10.1	0.281	7	REAL	O=C1NCc2ccc(NC(=O)c3c4c(nc5ccccc35)/C(=C\c3ccc5c(c3)OCO5)CC4)cc21
vN-rna1-89	Z992146912	-10.1	0.273	8	REAL	O=C(c1cccc(CN2C(=O)c3ccccc3C2=O)c1)N1CCC(c2nc(-c3ccccc3)n[nH]2)CC1
vN-rna1-90	Z995482396	-10.1	0.297	9	REAL	Cc1ccc2c(CN3C(=O)N[C@](C)(c4cccc(N5CCOC5=O)c4)C3=O)cc(=O)oc2c1C
vN-rna1-91	Z998728844	-10.1	0.289	7	REAL	O=C(c1ccc2[nH]ncc2c1)N1CCC[C@@H](C(=O)N2CC=C(c3c[nH]c4cc(F)ccc34)CC2)C1
vN-rna1-92	Z99991476	-10.1	0.289	8	REAL	C/C(=N\Nc1ccc2ccccc2n1)c1ccc(NC(=O)C[C@@H]2Nc3ccccc3NC2=O)cc1
vN-rna1-93	ZINC000001099260	-10.1	0.281	8	ZINC	O=C1NC(=O)c2cc(N3C(=O)c4cc5oc6ccccc6c6ccccc6oc5cc4C3=O)ccc21
vN-rna1-94	ZINC000001717023	-10.1	0.316	5	ZINC	O=c1oc2ccc(-n3c(=O)c4ccccc4c4ccccc4c3=O)cc2c2ccccc12
vN-rna1-95	ZINC000002908937	-10.1	0.273	6	ZINC	O=c1oc(-c2cccc(F)c2)nc2cc(Cc3ccc4nc(-c5cccc(F)c5)oc(=O)c4c3)ccc12
vN-rna1-96	ZINC000003190476	-10.1	0.316	3	ZINC	CC12c3ccccc3C(c3ccccc31)[C@H]1C(=O)N(c3cccc4ccccc43)C(=O)[C@@H]12
vN-rna1-97	ZINC000003437040	-10.1	0.306	8	ZINC	C[C@]1(c2ccc3c(c2)OCCO3)NC(=O)N(Cc2cc(=O)oc3cc4c(cc23)CCC4)C1=O
vN-rna1-98	ZINC000011316532	-10.1	0.316	8	ZINC	Cc1ccc2c(CN3C(=O)N[C@](C)(c4ccc5c(c4)OCCO5)C3=O)cc(=O)oc2c1C
vN-rna1-99	ZINC000012086093	-10.1	0.316	7	ZINC	O=C(c1cc(-c2ccc(F)cc2)on1)N1C[C@H]2[C@H](CC[C@]23NC(=O)c2ccccc2N3)C1
vN-rna1-100	ZINC000013129767	-10.1	0.281	10	ZINC	Cc1ccc(C)c(N2C(=O)c3ccc(C(=O)OCC(=O)Nc4ccc5[nH]c(=O)[nH]c5c4)cc3C2=O)c1

Supplementary Table 81. Top 100 virtual hits of the screen against the RNA binding region of the nucleoprotein (Screen ID: 42). Compounds were filtered so that hits had MW < 600 dalton, cLogP < 6, number of hydrogen bond acceptors < 11, and no reactive functional groups. A few compounds unsuitable for drug discovery were removed by visual inspection. The name of each compound consists of the initial letter 'v' for virtual hit, followed by the target protein name and the target site ('rna' for RNA binding site, 1 for docking scenario 1). The score is the docking score given by QuickVina 2 in kcal/mol. The ligand efficiency (LE) is computed as LE = -score/#NonH, where #NonH is the number of heavy (i.e. non hydrogen) atoms.

Name	Catalog ID	Score	LE	MW	Library	SMILES
vN-rna1-101	ZINC000013729659	-10.1	0.273	7.00	ZINC	O=C1[C@H]2[C@@H]3CCCN3[C@]3(c4ccccc4-n4c3nc3ccccc3c4=O)[C@H]2C(=O)N1c1ccc(F)cc1
vN-rna1-102	ZINC000016037199	-10.1	0.273	5.00	ZINC	O=C(c1ccc(Cl)cc1)[C@@H]1[C@@H]2C(=O)N(c3ccc4ccccc4c3)C(=O)[C@@H]2[C@H]2c3ccccc3C=CN12
vN-rna1-103	ZINC000020533996	-10.1	0.297	5.00	ZINC	O=C(O)C12c3ccccc3C(c3ccccc31)[C@H]1C(=O)N(c3ccc4ccccc43)C(=O)[C@@H]12
vN-rna1-104	ZINC000020572281	-10.1	0.273	7.00	ZINC	O=C1Nc2ccc(F)cc2[C@@]12N[C@H](Cc1c[nH]c3ccccc13)[C@H]1C(=O)N(c3ccc(F)cc3)C(=O)[C@H]12
vN-rna1-105	ZINC000034856480	-10.1	0.297	6.00	ZINC	Cc1cc2c(c(C)c1)NC(=O)[C@@]21[C@@H]2C(=O)N(c3ccc4ccccc4c3)C(=O)[C@@H]2[C@H]2CCCN21
vN-rna1-106	ZINC000059503350	-10.1	0.297	6.00	ZINC	O=C1[C@@H]2[C@@H](C(=O)N1c1ccccc3ccccc31)C1c3ccccc3C2([N+](=O)[O-])c2ccccc21
vN-rna1-107	ZINC000065111374	-10.1	0.273	8.00	ZINC	Cc1cccc(-c2noc(-c3nn(CC(=O)N4CCN(c5ccccc5F)CC4)c4ccccc43)n2)c1
vN-rna1-108	ZINC000101262757	-10.1	0.289	9.00	ZINC	O=C1[C@H]2N=NN(Cc3nc(-c4cccc(C(F)(F)F)c4)no3)[C@@H]2C(=O)N1c1ccc2c(c1)CCC2
vN-rna1-109	ZINC000101262763	-10.1	0.289	9.00	ZINC	O=C1[C@@H]2N=NN(Cc3nc(-c4cccc(C(F)(F)F)c4)no3)[C@@H]2C(=O)N1c1ccc2c(c1)CCC2
vN-rna1-110	ZINC000254722125	-10.1	0.281	7.00	ZINC	O=C(N=C1N=C2C=CC(Br)=CN2Cc2ccccc21)c1ccc2c(c1)S(=O)(=O)c1ccccc1C2=O
vN-rna1-111	ZINC000408731315	-10.1	0.266	5.00	ZINC	Cc1ccc(C)c(N2C(=O)[C@H]3[C@H](C2=O)[C@@H]2C(=O)Oc4c5ccccc5ccc4C2=C[C@H]3c2ccccc2)c1
vN-rna1-112	ZINC000409367716	-10.1	0.281	6.00	ZINC	O=C1[C@@H]2[C@@H](C(=O)N1c1ccc(-c3ccccc3)cc1)C1c3ccccc3C2([N+](=O)[O-])c2ccccc21
vN-rna1-113	Z1000936770	-10.0	0.278	9.00	REAL	C[C@]1(c2cccc(CNC(=O)c3cccc(NC(=O)[C@@H]4Cc5ccccc5O4)c3)c2)NC(=O)NC1=O
vN-rna1-114	Z100348282	-10.0	0.345	8.00	REAL	C/C(=N/Nc1nc(C(F)(F)F)nc2ccccc12)c1cccc(-n2cnnn2)c1
vN-rna1-115	Z1022554804	-10.0	0.286	9.00	REAL	Cc1cccc(NC(=O)N2CCC[C@H](C(=O)N3CCC(c4nc(-c5ccccn5)no4)CC3)C2)c1
vN-rna1-116	Z1037876966	-10.0	0.294	6.00	REAL	Cc1ccccc1NC(=O)[C@@H]1CCc2ccccc2N1C(=O)c1ccc(N2CCCC2=O)cc1
vN-rna1-117	Z1037877046	-10.0	0.278	7.00	REAL	Cc1ccccc1NC(=O)[C@@H]1CCc2ccccc2N1C(=O)c1ccc2c(=O)n3c(nc2c1)CCC3
vN-rna1-118	Z1043026382	-10.0	0.278	8.00	REAL	Cc1ccc(NC(=O)[C@@H]2CCc3ccccc3N2C(=O)c2ccc(N3NC(=O)CCC3=O)cc2)cc1
vN-rna1-119	Z1069484738	-10.0	0.278	7.00	REAL	C[C@H]1CCc2[nH]c3ccc(C(=O)N4CCC(C(=O)c5ccc6c(c5)NC(=O)[C@@H](C)O6)CC4)cc3c2C1
vN-rna1-120	Z1069484924	-10.0	0.278	9.00	REAL	Cc1cc(=O)oc2cc(OCC(=O)N3CCC(C(=O)c4ccc5c(c4)NC(=O)[C@H](C)O5)CC3)ccc12
vN-rna1-121	Z1071336660	-10.0	0.294	9.00	REAL	C[C@H]1Oc2cccc(C(=O)C3CCN(C(=O)Nc4ccc5oc(=O)ccc5c4)CC3)cc2NC1=O
vN-rna1-122	Z1075593418	-10.0	0.303	10.00	REAL	Cc1nc2n(n1)C[C@@H](NC(=O)N1CCC(C(=O)c3ccc4c(c3)NC(=O)[C@@H](C)O4)CC1)CC2
vN-rna1-123	Z1095050586	-10.0	0.286	10.00	REAL	Cc1cc(-c2cc(C(=O)Nc3nc(-c4ccc5ccccc5n4)n[nH]3)c3c(C)noc3n2)c(C)o1
vN-rna1-124	Z109829510	-10.0	0.286	8.00	REAL	CNC(=O)[C@@H]1CN(C(=O)c2cccc(S(=O)(=O)N3CCCc4ccccc43)c2)c2ccccc2O1
vN-rna1-125	Z1160993086	-10.0	0.286	9.00	REAL	Cc1c(C(=O)N2CCCC[C@@H]2c2nc(-c3ccccc3)no2)nnn1-c1ccc2ncccc2c1
vN-rna1-126	Z1161178562	-10.0	0.278	9.00	REAL	Cc1c(C(=O)Nc2ccccc2-c2nc(-c3ccccc3)n[nH]2)nnn1-c1ccc2ncccc2c1
vN-rna1-127	Z1161365763	-10.0	0.294	8.00	REAL	O=C(Nc1cccc(NC(=O)c2n[nH]c(=O)c3ccccc23)c1)Nc1ccccc2c1CCCC2
vN-rna1-128	Z1273151877	-10.0	0.323	9.00	REAL	Cc1cc(Cl)cc(C)c1O[C@H](C)C(=O)NNC(=O)CN1C(=O)[C@H]2[C@H]3CC[C@@H](O3)[C@H]2C1=O
vN-rna1-129	Z14076580	-10.0	0.313	6.00	REAL	Cc1cc2oc(=O)cc(CN3C(=O)N[C@](C)(c4cccc5cccc45)C3=O)c2cc1C
vN-rna1-130	Z144835264	-10.0	0.294	7.00	REAL	Cc1c(C(=O)NNC(=O)c2cc(-c3ccccc3Cl)nc3ccccc23)[nH]c2c1C(=O)CCC2
vN-rna1-131	Z1506268298	-10.0	0.303	7.00	REAL	Cc1c(C(=O)N2CCO[C@@]3(CCc4ccccc43)C2)nnn1-c1ccc2c1CCN(C)C2
vN-rna1-132	Z1518206238	-10.0	0.323	7.00	REAL	O=C(NCCC1Cc2ccccc2C1)N1CCN(C2=NS(=O)(=O)c3ccccc32)CC1
vN-rna1-133	Z1531730465	-10.0	0.313	8.00	REAL	O=C(Nc1ccn(-c2nccc2F)n1)c1ccc2c(c1)C(=O)N(C1CCCCC1)C2=O
vN-rna1-134	Z16336950	-10.0	0.345	7.00	REAL	Cc1ccc2c(CN3C(=O)N[C@@]4(CCOc5ccccc54)C3=O)ccc(=O)oc2c1
vN-rna1-135	Z1663343305	-10.0	0.345	8.00	REAL	CC(=O)N1CCC[C@H](c2nnc(-c3cccc(S(=O)(=O)N4CCCCC4)c3)o2)C1
vN-rna1-136	Z1663347538	-10.0	0.313	7.00	REAL	O=S(=O)(c1cccc(-c2nnc(/C=C\c3ccnc4ccccc34)o2)c1)N1CCCCC1
vN-rna1-137	Z1690104786	-10.0	0.313	10.00	REAL	O=C(NNC(=O)[C@@H]1C[C@@H]2CCCC[C@H]2N1c1ncccn1)c1n[nH]c(=O)c2ccccc12
vN-rna1-138	Z1763534852	-10.0	0.345	10.00	REAL	O=C1c2ccccc2C(=O)N1C1CCC(=NNc2nc3[nH]ncc3c(=O)[nH]2)CC1
vN-rna1-139	Z1763536530	-10.0	0.333	10.00	REAL	Cn1ncc2c(=O)[nH]c(NN=C3CCC(N4C(=O)c5ccccc5C4=O)CC3)nc21
vN-rna1-140	Z1890914262	-10.0	0.357	7.00	REAL	Cc1nc2c(cc1-c1nc(-c3cc(C)c4ccccc4n3)no1)c(C)nn2C
vN-rna1-141	Z1891089508	-10.0	0.303	8.00	REAL	Cc1ccc(C)c(N2C(=O)c3ccc(-c4nc(-c5ccc6cc[nH]c6n5)no4)cc3C2=O)c1
vN-rna1-142	Z1907886413	-10.0	0.313	9.00	REAL	Cc1c(C(=O)Nc2ccc3c(c2)N(C(N)=O)CCC3)nnn1-c1cccc2cnccc12
vN-rna1-143	Z1907890391	-10.0	0.357	7.00	REAL	Cc1c(C(=O)Nc2ccc3c(c2)N(C(N)=O)CCC3)c(O)nc2ccccc12
vN-rna1-144	Z1959809610	-10.0	0.294	7.00	REAL	CC(=O)N1Cc2ccccc2C[C@@H]1c1nc(-c2cccc(Cn3cnc4ccccc43)c2)no1
vN-rna1-145	Z1963622330	-10.0	0.303	7.00	REAL	Cc1ccc2c(c1)[C@H]1CN(C)CC[C@H]1N2C(=O)CN1C(=O)N[C@@]2(CCc3ccccc32)C1=O
vN-rna1-146	Z2041541983	-10.0	0.313	8.00	REAL	Cc1nc2c(-c3noc(-c4ccc5c(c4)S(=O)(=O)c4ccccc4C5=O)n3)ccnc2[nH]1
vN-rna1-147	Z2041573042	-10.0	0.303	8.00	REAL	Cc1cccc(C)c(N2C(=O)c3ccc(-c4nc(-c5nccc6[nH]ccc56)no4)cc3C2=O)c1
vN-rna1-148	Z2090581044	-10.0	0.303	7.00	REAL	Cc1c(C(=O)N2C[C@H](c3ccccc3)[C@H]3COCC[C@@H]32)nnn1-c1cccc2cccnc12
vN-rna1-149	Z2090603094	-10.0	0.313	5.00	REAL	CN(C)c1ccc(-c2ncc(C(=O)N3C[C@@H](c4ccccc4)[C@@H]4COCC[C@@H]43)c2)cc1
vN-rna1-150	Z2142506450	-10.0	0.370	8.00	REAL	C/C(=N\Nc1nc2ccccc2c(=O)n1C)c1cccc(-n2ccnn2)c1
vN-rna1-151	Z2159645141	-10.0	0.303	8.00	REAL	Cc1cc(-c2noc(CN3C(=O)c4ccccc4N4C(=O)CC[C@@]34C)n2)nc2ccccc12
vN-rna1-152	Z2167301598	-10.0	0.357	6.00	REAL	O=C(Nc1nc2ccccc2s1)N1CCC(c2noc3cc(F)ccc23)CC1
vN-rna1-153	Z2167663170	-10.0	0.357	8.00	REAL	O=C(Nc1nc2ccccn2n1)N1CCC(c2noc3cc(F)ccc23)CC1
vN-rna1-154	Z2178247271	-10.0	0.303	6.00	REAL	O=C(c1cccc2c(=O)c3ccccc3[nH]c12)N1CCC(c2noc3cc(F)ccc23)CC1
vN-rna1-155	Z220351324	-10.0	0.313	7.00	REAL	NC(=O)[C@@H]1Cc2ccccc2CN1C(=O)c1ccc2c(c1)S(=O)(=O)c1ccccc1C2=O
vN-rna1-156	Z2206456474	-10.0	0.313	10.00	REAL	O=C(CN1C(=O)C(F)(F)Oc2ccccc21)NNC(=O)C1CCN(c2ncccn2)CC1
vN-rna1-157	Z2233035507	-10.0	0.313	8.00	REAL	Cc1nc2ccccn2c1[C@H]1C(=O)NCCN1C(=O)[C@@H]1CC(c2c(F)cccc2F)=NO1
vN-rna1-158	Z2296193683	-10.0	0.357	8.00	REAL	O=C(Nc1nc2n(n1)CCCC2)N1CCC(c2noc3cc(F)ccc23)CC1
vN-rna1-159	Z24514298	-10.0	0.313	6.00	REAL	C[C@]1(c2ccc3c(c2)CCC3)NC(=O)N(Cc2cc(=O)oc3cc4c(cc23)CCC4)C1=O
vN-rna1-160	Z301910150	-10.0	0.294	8.00	REAL	O=C([C@@H]1CCCN(S(=O)(=O)c2ccc(F)cc2)C1)N1CCC[C@@H](c2nnc3n2CCCCC3)C1
vN-rna1-161	Z3095156613	-10.0	0.357	6.00	REAL	Cc1cc(F)cc(-c2nnc(N3CC[C@@]4(C3)C(=O)Nc3ccccc34)n2C)c1
vN-rna1-162	Z3095561900	-10.0	0.345	9.00	REAL	Cn1c(-c2cc3nccn3cn2)nnc1N1CC[C@@]2(C1)C(=O)Nc1ccccc12
vN-rna1-163	Z32994301	-10.0	0.278	8.00	REAL	Cc1cc(C(=O)NNC(=O)c2ccc3c(c2)S(=O)(=O)c2ccccc2C3=O)c(C)n1-c1ccccc1
vN-rna1-164	Z383456236	-10.0	0.263	8.00	REAL	Cc1cc(N2CCN(C(=O)c3cc(-c4cccc5ccccc45)nc4ccccc34)CC2)n2ncnc2n1
vN-rna1-165	Z595981632	-10.0	0.303	7.00	REAL	O=C(Nc1nnc(C23CC4CC(CC(C4)C2)C3)s1)NC1CCN(C(=O)c2ccccc2)CC1
vN-rna1-166	Z605475312	-10.0	0.294	10.00	REAL	Cc1c(C)c(C)c(S(=O)(=O)N2CCN(C(=O)c3cnc4[nH]c(=O)[nH]c(=O)c4c3)CC2)c(C)c1C
vN-rna1-167	Z605598772	-10.0	0.270	8.00	REAL	C[C@H](Oc1ccc2ccccc2c1)C(=O)NNC(=O)c1cccc(NC(=O)[C@@H]2Cc3ccccc3O2)c1
vN-rna1-168	Z748733888	-10.0	0.286	9.00	REAL	O=C(Nc1ccc(Cl)cc1NC(=O)c1ccco1)c1ccc2c(c1)C(=O)N(C[C@H]1CCCO1)C2=O
vN-rna1-169	Z806248884	-10.0	0.286	7.00	REAL	O=C([C@H]1CC(=O)N(c2ccc3c(c2)Cc2ccccc2-3)C1)N1CCC[C@@H](c2nnc3n2CCC3)C1
vN-rna1-170	Z87764900	-10.0	0.294	9.00	REAL	CN1C(=O)c2ccc(NC(=O)CN3C(=O)N[C@](C)(c4cccc5ccccc45)C3=O)cc2C1=O
vN-rna1-171	Z920784194	-10.0	0.286	9.00	REAL	O=C(NNC(=O)N1CCOCC1)c1c2c(nc3ccccc13)/C(=C/c1ccc3c(c1)OCO3)CC2
vN-rna1-172	Z941406048	-10.0	0.294	7.00	REAL	Cc1nc(N2CCOCC2)[nH]c(=O)c1CCC(=O)N1CCC(c2cccc3ccccc23)CC1
vN-rna1-173	Z966749662	-10.0	0.294	7.00	REAL	O=C(NNC(=O)[C@@H]1Cc2ccccc2O1)c1c2c(nc3ccccc13)/C(=C\c1ccco1)CC2
vN-rna1-174	Z980042734	-10.0	0.303	7.00	REAL	O=C(Nc1nnc(-c2ccccn2)s1)[C@H]1C[C@H]2CCCC[C@@H]2N1C(=O)c1ccc(F)cc1F
vN-rna1-175	Z998231366	-10.0	0.270	6.00	REAL	O=C(NC[C@@H]1CC2c3ccccc3C1c1ccccc12)[C@H]1CCCN(C(=O)c2ccc3[nH]ncc3c2)C1
vN-rna1-176	ZINC000000990899	-10.0	0.286	5.00	ZINC	O=C(c1ccc(N2C(=O)[C@H]3[C@H](C2=O)C2c4ccccc4C3c3ccccc32)cc1)N1CCCCC1
vN-rna1-177	ZINC000001380707	-10.0	0.286	8.00	ZINC	Cc1ccc2c(c1)nnn2C1CCN(S(=O)(=O)c2ccc(C(=O)N[C@H]3CCCC[C@@H]3C)cc2)CC1
vN-rna1-178	ZINC000001641983	-10.0	0.278	9.00	ZINC	O=C1C(/C=C/c2ccc(Cl)cc2)=NN[C@H]2N1N=C1N=C(O)C3(NN12)c1ccccc1-c1ccccc13
vN-rna1-179	ZINC000002267002	-10.0	0.323	6.00	ZINC	O=c1oc2ccc3ccccc3c2cc1-c1nnc(-c2cc3ccccc3cc2O)o1
vN-rna1-180	ZINC000004846183	-10.0	0.238	8.00	ZINC	O=c1[nH]c2ccccc2n1C1CCN(Cc2ccc(-c3nc4cc5ncccc5[nH]c5c4nc3-c3ccccc3)cc2)CC1
vN-rna1-181	ZINC000005955032	-10.0	0.278	9.00	ZINC	O=C1NC2=NN3C(=O)C(/C=C\c4ccc(Cl)cc4)=NN[C@@H]3N2NC12c1ccccc1-c1ccccc12
vN-rna1-182	ZINC000015972607	-10.0	0.270	7.00	ZINC	Cc1ccc(N2C(=O)[C@@H]3[C@H](C2=O)[C@@H](Cc2c[nH]c4ccccc24)N[C@]32C(=O)Nc3ccccc32)cc1C
vN-rna1-183	ZINC000016038238	-10.0	0.270	6.00	ZINC	O=C(c1ccc(Cl)cc1)[C@@H]1[C@@H]2C(=O)N(c3ccc4ccccc4c3)C(=O)[C@@H]2[C@H]2c3ccccc3C=NN12
vN-rna1-184	ZINC000035375706	-10.0	0.270	7.00	ZINC	Cc1cc(C)cc(N2C(=O)[C@@H]3[C@H](C2=O)[C@H](Cc2c[nH]c4ccccc24)N[C@@]32C(=O)Nc3ccccc32)c1
vN-rna1-185	ZINC000064566615	-10.0	0.286	9.00	ZINC	Cc1ccc(-c2nnc(-c3nn(C)c4c3CN(S(=O)(=O)c3ccc5ccenc53)CC4)o2)cc1
vN-rna1-186	ZINC000067262736	-10.0	0.303	6.00	ZINC	Fc1ccc(N2CCN(c3nc4c(-c5cccc(Cl)c5)nnn4c4ccccc43)CC2)cc1
vN-rna1-187	ZINC000096115782	-10.0	0.286	7.00	ZINC	C[C@H]1Oc2ccccc2C=C1[C@@H]1CC(=O)Oc2cc(O)c3c(=O)c(-c4ccc(O)cc4)coc3c21
vN-rna1-188	ZINC000096582005	-10.0	0.303	7.00	ZINC	O=C1Nc2ccccc2C12c1c(=O)oc3ccccc3c1Oc1c3ccccc3oc(=O)c12
vN-rna1-189	ZINC000230021243	-10.0	0.286	7.00	ZINC	O=C1N=C(O)N(c2ccc(Cl)cc2)C(=O)[C@]12Cc1ccccc1N1CCN(c3ccccc3)C[C@H]12
vN-rna1-190	ZINC000408679814	-10.0	0.263	5.00	ZINC	Cc1cc(C)cc(NC(=O)c2ccc(N3C(=O)[C@H]4[C@H](C3=O)C3c5ccccc5C4c4ccccc43)c2)c1
vN-rna1-191	ZINC000408730071	-10.0	0.270	5.00	ZINC	Cc1ccc(N2C(=O)[C@@H]3[C@H](C2=O)[C@@H]2C(=O)Oc4ccc5ccccc5c4C2=C[C@H]3c2ccccc2)cc1
vN-rna1-192	ZINC000409333463	-10.0	0.263	7.00	ZINC	O=C(Oc1ccc2nc3ccc4ccccc4c3nc2c1)c1ccc(N2C(=O)c3ccccc3C2=O)cc1
vN-rna1-193	ZINC000409334997	-10.0	0.278	7.00	ZINC	O=C(Nc1ccc2ccccc2c1)Nc1ccc2nc3c4ccccnc4c4nccc4c3nc2c1
vN-rna1-194	ZINC000409337259	-10.0	0.263	5.00	ZINC	Cc1ccc(N2C(=O)[C@H]3[C@H](C2=O)[C@@H]2C(=O)Oc4ccc5ccccc5c4C2=C[C@H]3c2ccccc2)c(C)c1
vN-rna1-195	PV-000375602024	-9.9	0.309	5.00	REAL	O=C(N[C@H]1C[C@H]2CC[C@@H]1N2C(=O)c1ccc2c3c(cccc13)CC2)[C@@H]1C[C@@H]2O[C@H]1[C@H]1C[C@@H]21
vN-rna1-196	PV-000381289172	-9.9	0.354	7.00	REAL	NC(=O)c1ccc(C(=O)N[C@@H]2C[C@H]3CC[C@@H]2N3C(=O)[C@H]2Cc3ccccc32)[nH]1
vN-rna1-197	PV-001824937252	-9.9	0.291	9.00	REAL	Cc1ccc(CNC(=O)c2cccc(CNC(=O)c3cc(C)c4c(=O)[nH]c(O)nc4n3)c2)cc1
vN-rna1-198	PV-001826824399	-9.9	0.319	8.00	REAL	NC(=O)c1ccc(C(=O)Nc2cccc(NC(=O)Nc3cccc(C(F)(F)F)c3)c2)[nH]1
vN-rna1-199	PV-001846618860	-9.9	0.341	7.00	REAL	Cc1ccc2c(c1)C(=O)O[C@@](C)(C)C(=O)Nc1ccc3c(c1)N(C(N)=O)CCC3)C2
vN-rna1-200	PV-001868280957	-9.9	0.300	7.00	REAL	Cc1ccc(C(=O)N[C@@H]2CC3(CCOCC3)Oc3ccccc32)cc1NC(=O)NC(C)(C)C

Supplementary Table 82. Virtual screening hits 101 to 200 of the screen against the RNA binding region of the nucleoprotein (Screen ID: 42). Compounds were filtered so that hits had MW < 600 dalton, cLogP < 6, number of hydrogen bond acceptors < 11, and no reactive functional groups. A few compounds unsuitable for drug discovery were removed by visual inspection. The name of each compound consists of the initial letter 'v' for virtual hit, followed by the target protein name and the target site ('rna' for RNA binding site, 1 for docking scenario 1). The score is the docking score given by QuickVina 2 in kcal/mol. The ligand efficiency (LE) is computed as LE = -score/#NonH, where #NonH is the number of heavy (i.e. non hydrogen) atoms.

Name	Catalog ID	Score	LE	MW	Library	SMILES
vN-ppi1-1	ZINC000004015296	-10.9	0.287	493.477	ZINC	O=c1nc2c3cccc4cccc(c(=O)n2c2cc(N5C(=O)c6cccc7cccc(c76)C5=O)ccc12)c43
vN-ppi1-2	ZINC000003954537	-10.4	0.281	481.466	ZINC	O=C(Nc1cccc2c1C(=O)c1cccc1C2=O)c1ccc2c3c1ncnc3-c1ccccc1C2=O
vN-ppi1-3	ZINC000097945320	-10.2	0.255	522.559	ZINC	O=C(Oc1cccc2ccccnc21)c1cccc(N2C(=O)[C@H]3[C@H](C2=O)C2c4ccccc4C3c3ccccc32)c1
vN-ppi1-4	ZINC000097945321	-10.2	0.255	522.559	ZINC	O=C(Oc1cccc2ccccnc21)c1cccc(N2C(=O)[C@H]3[C@@H](C2=O)C2c4ccccc4C3c3ccccc32)c1
vN-ppi1-5	Z1370892539	-10.1	0.374	426.323	REAL	C[C@@H]1c2c(Cl)cc(Cl)cc2CCN1C(=O)[C@@H]1Nc2ccccc2S(=O)(=O)N1
vN-ppi1-6	Z1684582607	-10.1	0.316	448.506	REAL	Cc1ccc(C)n1-c1nc(Cc2nc(-c3cccc([C@]4(C)NC(=O)NC4=O)c3)no2)cs1
vN-ppi1-7	ZINC000018101483	-10.1	0.316	416.439	ZINC	O=C1Nc2ccccc2/C1=N\c1cccc2c(/N=C3/c4ccccc4NC3=O)cccc12
vN-ppi1-8	ZINC000097945322	-10.1	0.252	522.559	ZINC	O=C(Oc1cccc2ccccnc21)c1cccc(N2C(=O)[C@@H]3[C@@H](C2=O)C2c4ccccc4C3c3ccccc32)c1
vN-ppi1-9	ZINC000100504092	-10.1	0.326	404.512	ZINC	O=c1cccc2n1C[C@H]1C[C@H]2CN(Cc2ccc3ccc4ccc5ccc2c3c45)C1
vN-ppi1-10	Z1094946006	-10	0.278	477.479	REAL	O=C(Cc1noc2ccccc12)Nc1ccc2nc(NC(=O)Cc3noc4ccccc34)ccc2c1
vN-ppi1-11	Z1452979797	-10	0.345	406.828	REAL	O=C(NNc1nc2ccccc2c(=O)[nH]1)c1cc(-c2ccccc2)cc(Cl)c1O
vN-ppi1-12	Z1684580621	-10	0.323	415.408	REAL	C[C@@]1(c2cccc(-c3noc(Cc4cc5ccccc5[nH]c4=O)n3)c2)NC(=O)NC1=O
vN-ppi1-13	Z1684580915	-10	0.313	427.463	REAL	Cc1nc2ccccc2c(C)c1Cc1nc(-c2cccc([C@]3(C)NC(=O)NC3=O)c2)no1
vN-ppi1-14	Z1684581792	-10	0.303	438.442	REAL	C[C@@]1(c2cccc(-c3noc(Cc4cc5c(ccc6ccccc65)o4)n3)c2)NC(=O)NC1=O
vN-ppi1-15	Z281552112	-10	0.313	430.423	REAL	Cc1nnc(NNC(=O)c2cc(-c3ccc4c(c3)OCCO4)nc3ccccc23)[nH]c1=O
vN-ppi1-16	ZINC000003146351	-10	0.313	458.477	ZINC	O=C1c2ccc(-c3ccc4c(c3)C(=O)N(c3nccs3)C4=O)cc2C(=O)N1c1nccs1
vN-ppi1-17	ZINC000004522786	-10	0.278	486.506	ZINC	Nc1c(-c2nc3ccc4c(c3s2)C(=O)c2ccccc2C4=O)ccc2c1C(=O)c1ccccc1C2=O
vN-ppi1-18	Z1014754852	-9.9	0.268	496.522	REAL	Cc1ccc(C)c(N2C(=O)c3ccc(C(=O)NCc4ccc([C@]5(C)NC(=O)NC5=O)cc4)cc3C2=O)c1
vN-ppi1-19	Z1070904338	-9.9	0.268	497.549	REAL	C[C@@H]1Oc2ccc(C(=O)C3CCN([C@H]4CC(=O)N(c5cccc6ccccc56)C4=O)CC3)cc2NC1=O
vN-ppi1-20	Z1116902231	-9.9	0.268	489.486	REAL	Cc1cccc2c(=O)[nH]c(COC(=O)c3ccc(N4C(=O)c5cccc6cccc(c56)C4=O)cc3)nc12
vN-ppi1-21	Z1173530296	-9.9	0.33	399.445	REAL	C[C@H]1CN(C(=O)c2ccc3c(c2)C[C@@H](c2ccccc2)OC3=O)c2ccccc2O1
vN-ppi1-22	Z1213581804	-9.9	0.319	439.873	REAL	O=C1C[C@H](C(=O)N2CCC(=C3C(=O)Nc4cc(Cl)ccc43)CC2)c2ccc(F)cc2N1
vN-ppi1-23	Z1372583545	-9.9	0.3	444.49	REAL	C[C@@]1(c2ccc(CNC(=O)N3CCc4cc(-c5ccccc5)oc4C3)cc2)NC(=O)NC1=O
vN-ppi1-24	Z1410517883	-9.9	0.367	380.79	REAL	O=C(NNc1nc2ccccc2c(=O)[nH]1)c1cc(Cl)c2ccccc2c1O
vN-ppi1-25	Z1410520849	-9.9	0.309	428.534	REAL	Cc1ccc(C23C[C@@H]4C[C@H](CC(C(=O)NNc5nc6ccccc6c(=O)[nH]5)(C4)C2)C3)cc1
vN-ppi1-26	Z1716062271	-9.9	0.309	424.455	REAL	O=C(c1ccccc(N2C(=O)c3ccccc3C2=O)c1)N1CC[C@]2(C1)OCc1ccccc12
vN-ppi1-27	Z2224499046	-9.9	0.381	345.397	REAL	O=C1CCCc2cc(C(=O)N3C[C@@H]4CCC(=O)c5cccc3c54)ccc21
vN-ppi1-28	Z223105634	-9.9	0.309	433.502	REAL	C[C@@H]1c2cc3c(cc2C2(CCCC2)CN1C(=O)[C@@H]1Cc2ccccc2C(=O)O1)OCCO3
vN-ppi1-29	Z316831980	-9.9	0.275	480.566	REAL	O=C(c1ccc2c(=O)n3c(nc2c1)CCCCC3)N1CCN(C(=O)c2cccc3ccccc23)CC1
vN-ppi1-30	ZINC000001855719	-9.9	0.367	356.464	ZINC	O=C1c2c(ccc3c2CCCC3)CC12Cc1ccc3c(c1C2=O)CCCC3
vN-ppi1-31	ZINC000002154274	-9.9	0.291	444.445	ZINC	O=c1oc(-c2cccc(-n3c(=O)c4ccccc4c4ccccc4c3=O)c2)nc2ccccc21
vN-ppi1-32	ZINC000002232892	-9.9	0.354	366.415	ZINC	Cc1cc2oc(=O)c3c(c2c2occ(-c4ccc5ccccc5c4)c21)CCC3
vN-ppi1-33	ZINC000005607051	-9.9	0.275	470.439	ZINC	Nc1c(-c2nc3cc4c(cc3o2)C(=O)c2ccccc2C4=O)ccc2c1C(=O)c1ccccc1C2=O
vN-ppi1-34	ZINC000005955034	-9.9	0.275	495.929	ZINC	O=C1NC2=NN3C(=O)C(/C=C\c4ccc(Cl)cc4)=NN[C@H]3N2NC12c1ccccc1-c1ccccc12
vN-ppi1-35	PV-001828573882	-9.8	0.327	407.448	REAL	CC(C)(C)c1ccc(-c2nnc(NC(=O)[C@@H]3Cc4cc(F)ccc4NC3=O)[nH]2)cc1
vN-ppi1-36	PV-001950627204	-9.8	0.306	434.451	REAL	CC1(C)COc2cc(NC(=O)NNC(=O)c3cc4ccccc4cc3O)ccc2NC1=O
vN-ppi1-37	Z1323785308	-9.8	0.288	449.513	REAL	O=C(Cc1ccc2ccccc2c1)NCc1nc(NC(=O)Cc2ccc3ccccc3c2)n[nH]1
vN-ppi1-38	Z137333280	-9.8	0.288	451.485	REAL	Cc1nc2ccccc2c(=O)n1-c1ccc(C(=O)NNC(=O)Cc2c[nH]c3ccccc23)cc1
vN-ppi1-39	Z1410513874	-9.8	0.377	350.377	REAL	O=C(NNc1nc2ccccc2c(=O)[nH]1)c1cc2c(cc1O)CCCC2
vN-ppi1-40	Z1410515355	-9.8	0.377	346.345	REAL	O=C(NNc1nc2ccccc2c(=O)[nH]1)c1ccc2ccccc2c1O
vN-ppi1-41	Z15458061	-9.8	0.265	489.486	REAL	C[C@H](OC(=O)c1ccc(N2C(=O)c3cccc4cccc(c34)C2=O)cc1)c1nc2ccccc2c(=O)[nH]1
vN-ppi1-42	Z1559726405	-9.8	0.363	383.834	REAL	NC(=O)[C@H](NC(=O)CCc1cc2ccccc2[nH]c1=O)c1ccc(Cl)cc1
vN-ppi1-43	Z1684579933	-9.8	0.316	417.38	REAL	C[C@@]1(c2cccc(-c3noc(CN4C(=O)c5ccccc5C4=O)n3)c2)NC(=O)NC1=O
vN-ppi1-44	Z1684580887	-9.8	0.338	408.844	REAL	C[C@@]1(c2cccc(-c3noc([C@H]4CCc5c(Cl)cccc54)n3)c2)NC(=O)NC1=O
vN-ppi1-45	Z1684581156	-9.8	0.306	435.414	REAL	C[C@@]1(c2cccc(-c3noc([C@@H]4CC(=O)N(c5ccc(F)cc5)C4)n3)c2)NC(=O)NC1=O
vN-ppi1-46	Z1684581901	-9.8	0.297	438.442	REAL	C[C@@]1(c2cccc(-c3noc(Cc4coc5ccc6ccccc6c45)n3)c2)NC(=O)NC1=O
vN-ppi1-47	Z1823391654	-9.8	0.316	417.468	REAL	Cc1ccnc(-n2nccc2NC(=O)N2CC=C(c3ccc4c(c3)OCCO4)CC2)c1
vN-ppi1-48	Z2066084353	-9.8	0.297	435.442	REAL	O=C(NNC(=O)c1n[nH]c(=O)c2ccccc12)c1ccc(-c2cccc3ccnc23)cc1
vN-ppi1-49	Z2189099689	-9.8	0.338	388.509	REAL	Cc1ccc2c(c1)[C@H]1CN(C)CC[C@H]1N2C(=O)c1ccc2c(c1)CCCCC2=O
vN-ppi1-50	Z749455328	-9.8	0.288	470.508	REAL	O=C(NNC(=O)c1ccc2ccccc2c1)c1ccc(NC2=NS(=O)(=O)c3ccccc32)cc1
vN-ppi1-51	Z976283494	-9.8	0.306	423.471	REAL	O=C1NC(=O)c2ccccc2/C1=C/Nc1ccc(CC(=O)N2CCc3ccccc32)cc1
vN-ppi1-52	ZINC000001225262	-9.8	0.251	553.36	ZINC	O=C1c2cccc(Cl)c2C(=O)N1c1ccc(-c2nc3ccc(N4C(=O)c5cccc(Cl)c5C4=O)cc3[nH]2)cc1
vN-ppi1-53	ZINC000001641985	-9.8	0.272	495.929	ZINC	O=C1C(/C=C/c2ccc(Cl)cc2)=NN[C@@H]2N1N=C1N=C(O)C3(NN12)c1ccccc1-c1ccccc13
vN-ppi1-54	ZINC000002212711	-9.8	0.297	429.474	ZINC	O=C(Nc1ccc2c(c1)Cc1ccccc1-2)c1ccccc(-c2cc3ccccc3oc2=O)c1
vN-ppi1-55	ZINC000002652048	-9.8	0.288	443.461	ZINC	O=C(Nc1ccc(N2C(=O)c3cccc4cccc(c43)C2=O)cc1)c1ccc2ccccc2n1
vN-ppi1-56	ZINC000006885885	-9.8	0.316	406.396	ZINC	O=C1c2cccc3cccc(c32)C(=O)N1c1ccc2c(c1)C(=O)Nc1ccccc1O2
vN-ppi1-57	ZINC000098042868	-9.8	0.239	570.752	ZINC	O=C(Nc1ccc2c(c1)S(=O)(=O)c1cc(NC(=O)C34CC5CC(CC(C5)C3)C4)ccc1-2)C12CC3CC(CC(C3)C1)C2
vN-ppi1-58	ZINC000100737708	-9.8	0.297	431.446	ZINC	O=C(Nc1cccc2c1C(=O)[C@@H]1C=CC=C[C@@H]1C2=O)c1cccc2c1C(=O)c1ccccc1-2
vN-ppi1-59	ZINC000146057035	-9.8	0.233	566.639	ZINC	CCc1cc(O)c(F)cc1-c1ccc2c(c1)[nH]nc2-c1nc2c([nH]1)CCN(C(=O)c1cnc(N3CCCC3)cn1)C2
vN-ppi1-60	ZINC000263588750	-9.8	0.265	509.512	ZINC	O=C1C[C@H](c2cccc(-c3nc4ccccc4s3)o2)c2c(ccc3c(=O)c(-c4ccccc4F)coc32)O1
vN-ppi1-61	PV-001850778928	-9.7	0.294	445.449	REAL	Cc1ccc(-c2ccc(C(=O)NNC(=O)[C@@H]3C(=O)Nc4ccccc4C3=O)cc(F)c2)cc1C
vN-ppi1-62	PV-001950482035	-9.7	0.294	450.537	REAL	Cc1ccc(C(=O)N2CCC(NC(=O)Nc3ccc4c(c3)NC(=O)C(C)(C)CO4)CC2)cc1
vN-ppi1-63	PV-001950627242	-9.7	0.313	418.452	REAL	CC1(C)COc2cc(NC(=O)NNC(=O)c3ccc4ccccc4c3)ccc2NC1=O
vN-ppi1-64	Z100372608	-9.7	0.269	481.511	REAL	Cc1cccc(-n2c(N/N=C3\C(=O)Nc4cc5c(cc43)OCCCO5)nc3ccccc3c2=O)c1C
vN-ppi1-65	Z1072129990	-9.7	0.262	495.581	REAL	Cc1ccc2[nH]c([C@H]3CCCN(C(=O)CN4C(=O)N[C@@](C)(c5ccc6ccccc6c5)C4=O)C3)nc2c1
vN-ppi1-66	Z1082330214	-9.7	0.313	440.523	REAL	C[C@@H]1C[C@@H](C)CN(S(=O)(=O)c2cccc(C(=O)Nc3nc4ccccc4c(=O)[nH]3)c2)C1
vN-ppi1-67	Z1094946018	-9.7	0.285	451.481	REAL	O=C(Nc1ccc2nc(NC(=O)[C@H]3Cc4ccccc4O3)ccc2c1)[C@@H]1CCc2ccccc2O1
vN-ppi1-68	Z113593176	-9.7	0.269	482.495	REAL	Cc1nc2ccccc2c(=O)n1-c1ccc(C(=O)O[C@@H](C)C(=O)N2CC(=O)Nc3ccccc32)cc1
vN-ppi1-69	Z1165732167	-9.7	0.303	427.467	REAL	O=C(Nc1ccc2nc(NC(=O)c3n[nH]c4c3CCC4)ccc2c1)c1n[nH]c2c1CCC2
vN-ppi1-70	Z1213581716	-9.7	0.303	448.909	REAL	NC(=O)c1cn(CC(=O)N2CCC(=C3C(=O)Nc4cc(Cl)cc43)CC2)c2ccccc12
vN-ppi1-71	Z1231995924	-9.7	0.334	389.493	REAL	C[C@@H]1C[C@H]2CCCC[C@H]2N1C(=O)c1ccc2c(c1)C[C@@H](c1ccccc1)OC2=O
vN-ppi1-72	Z1315090992	-9.7	0.294	444.498	REAL	Cc1nc2c(c(C)c1CCC(=O)Nc1n[nH]c3c1c(-c1ccccc1)nn3C)c(=O)[nH]n2C
vN-ppi1-73	Z1410520271	-9.7	0.346	378.391	REAL	C[C@H]1C(=O)Nc2cc(C(=O)NNc3nc4ccccc4c(=O)[nH]3)ccc2N1C
vN-ppi1-74	Z1451959293	-9.7	0.294	449.509	REAL	C[C@@]1(c2cccc(C(=O)Nc3ccc(NC(=O)N4CCCCC4)cc3)c2)NC(=O)NC1=O
vN-ppi1-75	Z1452579296	-9.7	0.303	434.494	REAL	CC1CCN(C(=O)c2ccc(NC(=O)c3ccc([C@]4(C)NC(=O)NC4=O)cc3)cc2)CC1
vN-ppi1-76	Z1463874745	-9.7	0.303	432.526	REAL	Cc1ccc(C23C[C@@H]4C[C@H](CC(C(=O)NNc5nc6c(cnn6C)c(=O)[nH]5)(C4)C2)C3)cc1
vN-ppi1-77	Z165047412	-9.7	0.262	487.47	REAL	O=C1NC(=O)c2ccccc2/C1=C\NN1C(=O)c2cccc3c(C(=O)c4ccccc4)ccc(c23)C1=O
vN-ppi1-78	Z1684579553	-9.7	0.313	431.475	REAL	C[C@@]1(c2cccc(-c3noc(Cc4cxc(-c5ccccc5)n4)n3)c2)NC(=O)NC1=O
vN-ppi1-79	Z1684579644	-9.7	0.294	442.478	REAL	Cc1cc(C)n(-c2ccc(Cc3nc(-c4cccc([C@]5(C)NC(=O)NC5=O)c4)no3)cc2)n1
vN-ppi1-80	Z1684579929	-9.7	0.313	416.436	REAL	Cc1ccc2c(Cc3nc(-c4cccc([C@]5(C)NC(=O)NC5=O)c4)no3)coc2c1C
vN-ppi1-81	Z1684580204	-9.7	0.323	402.413	REAL	Cc1cccn2cc(Cc3nc(-c4cccc([C@]5(C)NC(=O)NC5=O)c4)no3)nc12
vN-ppi1-82	Z1684580724	-9.7	0.303	424.459	REAL	C[C@@]1(c2cccc(-c3noc([C@H]4C[C@H]4c4ccc5ccccc5c4)n3)c2)NC(=O)NC1=O
vN-ppi1-83	Z1684581478	-9.7	0.294	444.49	REAL	C[C@@]1(c2cccc(-c3noc(CCC(=O)c4ccc5c(c4)CCCC5)n3)c2)NC(=O)NC1=O
vN-ppi1-84	Z1892834134	-9.7	0.323	394.429	REAL	O=C1CC[C@@H]2CN(C(=O)c3cccc4c(=O)c5ccccc5[nH]c34)c3ccc1c32
vN-ppi1-85	Z192486970	-9.7	0.269	480.483	REAL	Cc1nc2ccccc2c(=O)n1-c1ccc(C(=O)NNC(=O)c2nn(-c3ccccc3)cc2O)cc1
vN-ppi1-86	Z1929427925	-9.7	0.313	419.436	REAL	O=C1NC(=O)[C@@]2(CCCN(C(=O)c3ccc4c(c3)C[C@H](c3ccccc3)OC4=O)C2)N1
vN-ppi1-87	Z1956676322	-9.7	0.359	354.408	REAL	O=C1CCCCc2cc(-c3nc4cc5ccccc5cc4c(=O)[nH]3)ccc21
vN-ppi1-88	Z1969747560	-9.7	0.346	373.459	REAL	CN(C)c1ccnc(NC(=O)N2CC=C(c3cccc4ccccc34)CC2)n1
vN-ppi1-89	Z2157916546	-9.7	0.313	417.424	REAL	C[C@@]1(c2cccc(-c3noc(CN4CCc5ccccc5C4=O)n3)c2)NC(=O)NC1=O
vN-ppi1-90	Z2157918107	-9.7	0.303	428.447	REAL	C[C@H](Oc1ccc2ccccc2c1)c1nc(-c2cccc([C@]3(C)NC(=O)NC3=O)c2)no1
vN-ppi1-91	Z2177413288	-9.7	0.334	389.493	REAL	O=C1CCCCc2cc(C(=O)N3C[C@H](c4ccccc4)[C@@H]4COCC[C@H]43)ccc21
vN-ppi1-92	Z2192883693	-9.7	0.294	438.482	REAL	O=C(c1cccc(N2C(=O)c3ccccc3C2=O)c1)N1CC[C@@]2(CCc3ccccc3O2)C1
vN-ppi1-93	Z220541322	-9.7	0.285	471.536	REAL	O=C1c2ccccc2S(=O)(=O)c2cc(C(=O)N3CCC[C@H](c4nc5ccccc5[nH]4)C3)ccc21
vN-ppi1-94	Z2225658838	-9.7	0.346	367.447	REAL	O=C1CCCc2cc(C(=O)N3C[C@H](c4ccccc4)c4ccccc43)ccc21
vN-ppi1-95	Z230808608	-9.7	0.277	475.543	REAL	C[C@H]1c2cc3c(cc2C2(CCCC2)CN1C(=O)CCn1c(=O)[nH]c(=O)c2ccccc21)OCCO3
vN-ppi1-96	Z2500351010	-9.7	0.346	371.435	REAL	O=C1CCCc2cc(C(=O)N3CC(O)(c4cccc5ccccc45)C3)ccc21
vN-ppi1-97	Z280311184	-9.7	0.323	407.448	REAL	CC(C)(C)c1ccc(-c2nnc(NC(=O)[C@@H]3CC(=O)Nc4cc(F)ccc43)[nH]2)cc1
vN-ppi1-98	Z424332108	-9.7	0.277	485.421	REAL	Cc1cc(=O)c(C(=O)Nc2cccc([C@]3(C)NC(=O)NC3=O)c2)nn1-c1cccc(C(F)(F)F)c1
vN-ppi1-99	Z64808849	-9.7	0.277	466.456	REAL	Cc1nc2ccccc2c(=O)n1-c1ccc(C(=O)NNC(=O)c2n[nH]c(=O)c3ccccc23)cc1
vN-ppi1-100	Z64808992	-9.7	0.269	480.483	REAL	Cc1nc2ccccc2c(=O)n1-c1ccc(C(=O)NNC(=O)c2nn(C)c(=O)c3ccccc23)cc1

Supplementary Table 83. Top 100 virtual hits of the screen against the oligomerization interface of the NTD of the nucleoprotein (Screen ID: 43). Compounds were filtered so that hits had MW < 600 dalton, cLogP < 6, number of hydrogen bond acceptors < 11, and no reactive functional groups. A few compounds unsuitable for drug discovery were removed by visual inspection. The name of each compound consists of the initial letter 'v' for virtual hit, followed by the target protein name and the target site ('ppi' for protein-protein interface, 1 for docking scenario 1). The score is the docking score given by QuickVina 2 in kcal/mol. The ligand efficiency (LE) is computed as LE = -score/#NonH, where #NonH is the number of heavy (i.e. non hydrogen) atoms.

Name	Catalog ID	Score	LE	MW	Library	SMILES
vN-ppi1-101	Z738255284	-9.7	0.277	480.50	REAL	O=C(Nc1cccc(-c2cn3ccenc3n2)c1)c1ccc2c(c1)S(=O)(=O)c1ccccc1C2=O
vN-ppi1-102	Z771183888	-9.7	0.294	440.50	REAL	O=C1C[C@@H](c2ccccc2)N(C(=O)c2ccc3c(c2)C[C@@H](c2ccccc2)OC3=O)CCN1
vN-ppi1-103	Z966751854	-9.7	0.294	440.46	REAL	Cc1nc2ccccc2c(=O)n1-c1ccc(C(=O)NNC(=O)[C@@H]2Cc3ccccc3O2)cc1
vN-ppi1-104	Z976183842	-9.7	0.269	482.55	REAL	O=C(Nc1ccc(CC(=O)N2CCc3ccccc32)cc1)C1CCN(c2ccc3nnnn3n2)CC1
vN-ppi1-105	Z976185340	-9.7	0.285	453.50	REAL	Cc1ccc2c(c1)C(=O)N(CC(=O)Nc1ccc(CC(=O)N3CCc4ccccc43)cc1)C2=O
vN-ppi1-106	Z976186264	-9.7	0.294	438.49	REAL	O=C(Cc1n[nH]c(=O)c2ccccc12)Nc1ccc(CC(=O)N2CCc3ccccc32)cc1
vN-ppi1-107	Z988053508	-9.7	0.285	453.50	REAL	CN(Cc1nc2ccccc2c(=O)[nH]1)C(=O)Nc1cccc(C(=O)N2CCc3ccccc32)c1
vN-ppi1-108	ZINC000000111271	-9.7	0.359	349.39	ZINC	O=C1c2cccc3cccc(c32)C(=O)N1c1ccc2c3c(cccc31)CC2
vN-ppi1-109	ZINC000000704991	-9.7	0.285	451.39	ZINC	Cc1ccc2nc(-c3ccc4c(c3)C(=O)N(N3C(=O)c5ccccc5C3=O)C4=O)oc(=O)c2c1
vN-ppi1-110	ZINC000000988780	-9.7	0.303	415.41	ZINC	O=c1c2ccc3c(=O)n(-c4ccccc4)c(=O)c4ccc(c5nc6ccccc6n51)c2c43
vN-ppi1-111	ZINC000002125371	-9.7	0.285	446.51	ZINC	CCn1c2ccccc2c2cc(N3COc4ccc5c6ccccc6c(=O)oc5c4C3)ccc21
vN-ppi1-112	ZINC000002145885	-9.7	0.359	354.40	ZINC	Cc1cc2oc(=O)c(C)c(C)c2c2occ(-c3ccc4ccccc4c3)c21
vN-ppi1-113	ZINC000002170289	-9.7	0.334	378.47	ZINC	CN1c2ccccc2C(C)(C)[C@]12C=Nc1c3ccccc3c3ccccc3c1O2
vN-ppi1-114	ZINC000006513294	-9.7	0.359	356.46	ZINC	O=C1CCCc2cc3c(cc21)C[C@]1(Cc2ccc4c(c2C1)C(=O)CCC4)C3
vN-ppi1-115	ZINC000008921457	-9.7	0.255	498.54	ZINC	O=C(NN1C(=O)[C@H]2[C@H](C1=O)C1c3ccccc3C2c2ccccc21)C1(O)c2ccccc2-c2ccccc21
vN-ppi1-116	ZINC000012444294	-9.7	0.269	475.51	ZINC	Cc1cc(NC(=O)Cc2ccc3ccccc32)n(-c2nc3c(cnn3-c3ccccc3)c(=O)[nH]2)n1
vN-ppi1-117	ZINC000015670427	-9.7	0.294	460.88	ZINC	Cc1nn(-c2nncc(-c3ccc(Cl)cc3)n2)c2c1[C@@H](c1ccc3c(c1)OCO3)CC(=O)N2
vN-ppi1-118	ZINC000015670617	-9.7	0.294	444.43	ZINC	Cc1nn(-c2nncc(-c3ccc(F)cc3)n2)c2c1[C@@H](c1ccc3c(c1)OCO3)CC(=O)N2
vN-ppi1-119	ZINC000018021374	-9.7	0.255	498.54	ZINC	O=C(NN1C(=O)[C@H]2[C@@H](C1=O)C1c3ccccc3C2c2ccccc21)C1(O)c2ccccc2-c2ccccc21
vN-ppi1-120	ZINC000019926200	-9.7	0.303	412.49	ZINC	O=C1C[C@]2(c3ccccc31)c1ccccc1[C@]1(c3ccccc3)c3ccccc3C(=O)[C@@H]21
vN-ppi1-121	ZINC000019926202	-9.7	0.303	412.49	ZINC	O=C1C[C@]2(c3ccccc31)c1ccccc1[C@]1(c3ccccc3)c3ccccc3C(=O)[C@H]21
vN-ppi1-122	ZINC000021867166	-9.7	0.269	482.52	ZINC	Cc1cccc(-c2nnn3c2nc(O)c2ccc(C(=O)N4CCN(c5ccccc5F)CC4)cc23)c1
vN-ppi1-123	ZINC000022636400	-9.7	0.334	375.38	ZINC	O=C1c2ccccc2C(=O)N1c1ccc2c3c(cccc13)C(=O)c1ccccc1-2
vN-ppi1-124	ZINC000033271405	-9.7	0.313	409.45	ZINC	Cc1nn(-c2ccc3nnc(C)n3n2)c2c1[C@@H](c1cccc3ccccc31)CC(=O)N2
vN-ppi1-125	ZINC000034253221	-9.7	0.255	494.55	ZINC	CCn1nc2c3c1-c1ccccc1C(=O)c3ccc2-c1ccc2c3c1nn(CC)c3-c1ccccc1C2=O
vN-ppi1-126	ZINC000095471041	-9.7	0.334	379.37	ZINC	O=c1c2ccc3oc4ccccc4c4ccc(c(=O)n1-c1cccc(O)c1)c2c34
vN-ppi1-127	ZINC000169684223	-9.7	0.262	487.51	ZINC	Cc1cccc([C@@H]2OC3(C(=O)c4ccccc4C3=O)[C@H]3C(=O)N(c4ccc5ccccc54)C(=O)[C@@H]23)c1
vN-ppi1-128	ZINC000253623742	-9.7	0.262	493.47	ZINC	O=C1c2ccc3c(c2O/C1=C/c1ccc2c(c1)OCCO2)[C@H](c1cc2ccccc2nc1O)CC(=O)O3
vN-ppi1-129	ZINC000408997474	-9.7	0.303	417.51	ZINC	O=C(O)c1cccc2c1N[C@H](c1ccc3c4c(ccc41)CC3)[C@H]1Cc3ccccc3[C@H]21
vN-ppi1-130	PV-001807670974	-9.6	0.356	361.48	REAL	Cc1ccc2c(c1)CN(C(=O)c1ccc3c(c1)CCCCC3=O)C(C)(C)C2
vN-ppi1-131	PV-001810031067	-9.6	0.356	389.78	REAL	Cc1c(F)cc(Cl)c2c1CCCN2C(=O)c1cc(=O)c2ccc(F)cc2o1
vN-ppi1-132	PV-001810938644	-9.6	0.384	398.26	REAL	O=C(Nc1ncc2[nH]ccc2c1Br)c1ccc2c(c1)CCCCC2=O
vN-ppi1-133	PV-001825780512	-9.6	0.291	451.57	REAL	Cc1cccc(NC(=O)[C@H]2CCCN(C(=O)[C@]3(C)CCc4c(C)c(O)c(C)c(C)c4O3)C2)n1
vN-ppi1-134	PV-001950627240	-9.6	0.310	418.45	REAL	CC1(C)COc2cc(NC(=O)NNC(=O)c3ccc4ccccc34)cc2NC1=O
vN-ppi1-135	Z100374338	-9.6	0.259	495.54	REAL	CC(C)c1ccc(-n2c(N/N=C3\C(=O)Nc4cc5c(cc43)OCCCO5)nc3ccccc3c2=O)cc1
vN-ppi1-136	Z1021036198	-9.6	0.274	483.95	REAL	O=C1Nc2cc(Cl)ccc2C1=C1CCN(C(=O)Cn2c3ccccc3c(=O)c3ccccc32)CC1
vN-ppi1-137	Z1030001348	-9.6	0.282	470.51	REAL	O=C(Nc1ccccc(-c2nc(C3CC3)n[nH]2)c1)c1ccc2c(c1)S(=O)(=O)c1ccccc1C2=O
vN-ppi1-138	Z1134799337	-9.6	0.310	430.89	REAL	Cc1cccc2c1CC[C@H]2NC(=O)c1ccc2c(c1)C(=O)N(c1ccccc1Cl)C2=O
vN-ppi1-139	Z1155697954	-9.6	0.267	498.51	REAL	O=C(Nc1ccccc(-c2ccc3c(c2)OCCO3)n1)c1ccc2c(c1)S(=O)(=O)c1ccccc1C2=O
vN-ppi1-140	Z1157972316	-9.6	0.267	482.59	REAL	Cc1ccc(C(=O)N2C[C@H](C)C[C@H](C)C2)cc1NC(=O)c1nnn(-c2cccc3ccncc23)c1C
vN-ppi1-141	Z1160971603	-9.6	0.267	482.59	REAL	Cc1ccc(C(=O)N2C[C@H](C)C[C@H](C)C2)cc1NC(=O)c1nnn(-c2cccc3ncccc23)c1C
vN-ppi1-142	Z1276029491	-9.6	0.310	416.45	REAL	CN1CCN(C(=O)c2ccc3c(c2)C[C@@H](c2ccccc2)OC3=O)c2ccc(F)cc21
vN-ppi1-143	Z1335515246	-9.6	0.310	412.44	REAL	CN1C(=O)CN(C(=O)c2ccc3c(c2)C[C@H](c2ccccc2)OC3=O)c2ccccc21
vN-ppi1-144	Z1401767183	-9.6	0.331	391.47	REAL	O=C1O[C@@H](c2ccccc2)Cc2cc(C(=O)N3CCC[C@@H]4COCC[C@H]43)ccc21
vN-ppi1-145	Z1410514678	-9.6	0.369	370.37	REAL	O=C(NNc1nc2ccccc2c(=O)[nH]1)c1cc(F)cc2nc(S)[nH]c12
vN-ppi1-146	Z1410515700	-9.6	0.331	387.44	REAL	C[C@H]1CCc2[nH]c3ccc(C(=O)NNc4nc5ccccc5c(=O)[nH]4)cc3c2C1
vN-ppi1-147	Z1410518999	-9.6	0.356	381.42	REAL	C[C@@H]1Sc2ccc(C(=O)NNc3nc4ccccc4c(=O)[nH]3)cc2NC1=O
vN-ppi1-148	Z1410519206	-9.6	0.300	421.46	REAL	Cc1ccc2nc(-c3ccccc3)cc(C(=O)NNc3nc4ccccc4c(=O)[nH]3)c2c1
vN-ppi1-149	Z1410521266	-9.6	0.300	421.46	REAL	Cc1ccc(-c2cc(C(=O)NNc3nc4ccccc4c(=O)[nH]3)c3ccccc3n2)cc1
vN-ppi1-150	Z1410521735	-9.6	0.384	334.34	REAL	Cc1cc(C(=O)NNc2nc3ccccc3c(=O)[nH]2)c2n[nH]cc2c1
vN-ppi1-151	Z1410522821	-9.6	0.300	425.42	REAL	O=C(NNc1nc2ccccc2c(=O)[nH]1)c1cc(-c2ccccc2)nc2cc(F)ccc12
vN-ppi1-152	Z1440949385	-9.6	0.291	447.48	REAL	O=C(Nc1ccc(CC(=O)N2CCc3ccccc32)cc1)N1CCc2c(F)cc(F)cc2C1
vN-ppi1-153	Z1460682890	-9.6	0.291	439.47	REAL	O=C(NNC(=O)c1n[nH]c(=O)c2ccccc12)c1ccc(N2CCCc3ccccc32)cc1
vN-ppi1-154	Z1463880202	-9.6	0.291	446.55	REAL	Cc1ccc(C23C[C@H]4C[C@@H](CC(C(=O)NNc5nc6c(cnn6C)c(=O)[nH]5)(C4)C2)C3)cc1C
vN-ppi1-155	Z1486231674	-9.6	0.343	367.41	REAL	O=C1CCc2cc(-c3nc4ccc(-c5ccccc5)cc4c(=O)[nH]3)ccc2N1
vN-ppi1-156	Z1488528286	-9.6	0.291	440.50	REAL	CC(=O)N[C@@H]1Cc2ccccc2N(C(=O)c2ccc3c(c2)C[C@H](c2ccccc2)OC3=O)C1
vN-ppi1-157	Z1492672049	-9.6	0.310	416.44	REAL	C[C@H]1CN(Cc2nc3c(oc4ccccc43)c(=O)[nH]2)CCN1c1nccn2cnnc12
vN-ppi1-158	Z1533909865	-9.6	0.310	428.47	REAL	CN(C(=O)c1ccc2c(c1)S(=O)(=O)c1ccccc1C2=O)c1ccc2ncccc12
vN-ppi1-159	Z1575694745	-9.6	0.310	417.47	REAL	Cc1cc(NC(=O)N2CC=C(c3ccc4c(c3)OCCO4)CC2)n(-c2ccccn2)n1
vN-ppi1-160	Z1684579562	-9.6	0.291	440.46	REAL	C[C@@]1(c2cccc(-c3noc(CCC(=O)c4ccc5ccccc5c4)n3)c2)NC(=O)NC1=O
vN-ppi1-161	Z1684580310	-9.6	0.300	424.46	REAL	C[C@]1(c2cccc(-c3noc([C@H]4C[C@H]4c4cccc5ccccc45)n3)c2)NC(=O)NC1=O
vN-ppi1-162	Z1684582054	-9.6	0.310	416.40	REAL	C[C@@]1(c2cccc(-c3noc(Cn4ncc5ccccc5c4=O)n3)c2)NC(=O)NC1=O
vN-ppi1-163	Z1684582563	-9.6	0.310	432.36	REAL	C[C@@]1(c2cccc(-c3noc(Cc4ccc(OC(F)(F)F)cc4)n3)c2)NC(=O)NC1=O
vN-ppi1-164	Z1684582896	-9.6	0.300	432.41	REAL	Cc1cc(F)ccc1-n1ccc(-c2nc(-c3cccc([C@]4(C)NC(=O)NC4=O)c3)no2)n1
vN-ppi1-165	Z1684583103	-9.6	0.300	433.42	REAL	C[C@@]1(c2cccc(-c3noc(CN4C(=O)[C@@H]5[C@H]6C=C[C@@H](C6)[C@H]5C4=O)n3)c2)NC(=O)NC1=O
vN-ppi1-166	Z1685319274	-9.6	0.291	439.48	REAL	Cc1nnc(-c2cccc(-c3noc(-c4ccc5c(=O)n6c(nc5c4)CCCCC6)n3)c2)[nH]1
vN-ppi1-167	Z1697483552	-9.6	0.300	423.47	REAL	O=C1O[C@H](c2ccccc2)Cc2cc(C(=O)N3C[C@H]4CCC(=O)c5cccc3c54)ccc21
vN-ppi1-168	Z1697991271	-9.6	0.310	435.43	REAL	Cn1c(NC(=O)c2ccc3c(c2)S(=O)(=O)c2ccccc2C3=O)nc2ccc(F)cc21
vN-ppi1-169	Z1716066639	-9.6	0.300	445.49	REAL	O=C1c2ccccc2S(=O)(=O)c2cc(C(=O)N3CC[C@]4(C3)OCc3ccccc34)ccc21
vN-ppi1-170	Z1723434460	-9.6	0.267	479.58	REAL	CCc1ccc2c(C3CCN(C(=O)c4ccc(-c5cnc6[nH]c(=O)n(C)c6c5)c4)CC3)c[nH]c12
vN-ppi1-171	Z1767252402	-9.6	0.320	394.43	REAL	O=C1CC[C@H]2CN(C(=O)c3ccc4[nH]c5ccccc5c(=O)c4c3)c3cccc1c32
vN-ppi1-172	Z1845117519	-9.6	0.310	413.44	REAL	O=C(NNc1nc2ccccn2n1)Nc1cccc(C(=O)N2CCc3ccccc32)c1
vN-ppi1-173	Z184756012	-9.6	0.274	486.51	REAL	O=C(NNC(=O)c1cc2ccccc2cc1O)c1ccc(NC2=NS(=O)(=O)c3ccccc32)cc1
vN-ppi1-174	Z188890184	-9.6	0.282	456.46	REAL	Cc1nc2ccccc2c(=O)n1-c1ccc(C(=O)NNC(=O)c2ccc3c(c2)OCCO3)cc1
vN-ppi1-175	Z1899438537	-9.6	0.300	432.43	REAL	CN1C[C@H](C(=O)Nc2ccc3[nH]c(-c4cc(F)ccc4F)nc3c2)c2ccccc21=O
vN-ppi1-176	Z2011507278	-9.6	0.310	408.42	REAL	O=C(Nc1nccn1-c1ccccc1)c1ccc(N2C(=O)c3ccccc3C2=O)cc1
vN-ppi1-177	Z2014694104	-9.6	0.310	420.47	REAL	Cc1ccc(C2=NO[C@@H](CNC(=O)c3cccc([C@]4(C)NC(=O)NC4=O)c3)C2)cc1C
vN-ppi1-178	Z2067945206	-9.6	0.343	383.33	REAL	O=C(Nc1nnc(C(F)(F)F)[nH]1)c1ccc(-c2ccccc3ccenc23)cc1
vN-ppi1-179	Z2069070673	-9.6	0.310	409.44	REAL	O=C(NNC(=O)[C@@H]1Cc2ccccc2O1)c1ccc(-c2ccccc3ccenc23)cc1
vN-ppi1-180	Z2087359694	-9.6	0.310	419.46	REAL	Cc1c(N2C(=O)N[C@H](C[C@@H]3CCCc4ccccc43)C2=O)nocc1-c1ccccc1F
vN-ppi1-181	Z2118684028	-9.6	0.343	383.31	REAL	O=C(NNc1nc2ccccc2c(=O)[nH]1)c1cnc2c(F)cc(F)cc2c1O
vN-ppi1-182	Z2147520661	-9.6	0.331	383.39	REAL	O=C(Nc1nc2ccc(F)cn2n1)c1ccc(-c2cccc3ccenc23)cc1
vN-ppi1-183	Z2148399989	-9.6	0.331	399.84	REAL	O=C(Nc1nc2ccc(Cl)cn2n1)c1ccc(-c2cccc3ccenc23)cc1
vN-ppi1-184	Z2167695493	-9.6	0.310	420.45	REAL	Cc1ccnc(-n2nccc2NC(=O)N2CCC(c3noc4cc(F)ccc34)CC2)c1
vN-ppi1-185	Z2171979179	-9.6	0.291	447.45	REAL	C[C@@](O)(CN1Cc2ccccc2C1=O)c1nc(-c2cccc([C@]3(C)NC(=O)NC3=O)c2)no1
vN-ppi1-186	Z2194277339	-9.6	0.310	415.41	REAL	Cc1cc(=O)n2nc(NC(=O)c3ccc4c(c3)C[C@@H](c3ccccc3)OC4=O)nH]c2n1
vN-ppi1-187	Z2225645671	-9.6	0.291	444.49	REAL	O=C([C@@H]1CC(=O)N(c2ccc3c(c2)Cc2ccccc2-3)C1)N1CCC[C@H](c2n[nH]c(=O)o2)C1
vN-ppi1-188	Z226529812	-9.6	0.267	476.54	REAL	Cc1nc2ccccc2c(=O)n1-c1ccc(C(=O)Nc2nc3ccccc3nc2N2CCC2)cc1
vN-ppi1-189	Z2717395028	-9.6	0.331	387.48	REAL	O=C1O[C@H](c2ccccc2)Cc2cc(C(=O)N3[C@H]4CC[C@@H]3CC3(CC3)C4)ccc21
vN-ppi1-190	Z2879729906	-9.6	0.356	361.40	REAL	O=C1CCCCc2cc(-c3nc(-c4cc5c([nH]c4=O)CCC5)no3)ccc21
vN-ppi1-191	Z30085028	-9.6	0.274	488.57	REAL	CN(Cc1nc2ccccc2c(=O)[nH]1)C(=O)c1cccc(S(=O)(=O)N2CCc3ccccc3C2)c1
vN-ppi1-192	Z383608842	-9.6	0.274	468.47	REAL	C[C@@]1(c2cccc(NC(=O)c3cccc(CN4C(=O)c5ccccc5C4=O)c3)cc2)NC(=O)NC1=O
vN-ppi1-193	Z385057680	-9.6	0.282	475.57	REAL	NC(=O)c1cccc2c1CCCN2C(=O)c1cccc(S(=O)(=O)N2CCc3ccccc3C2)c1
vN-ppi1-194	Z424333592	-9.6	0.267	482.50	REAL	Cc1ccc(C)c(N2C(=O)c3ccc(C(=O)Nc4cccc([C@]5(C)NC(=O)NC5=O)c4)cc3C2=O)c1
vN-ppi1-195	Z64798584	-9.6	0.282	456.54	REAL	Cc1nc2ccccc2c(=O)n1-c1ccc(C(=O)NNC(=O)C23CC4CC(CC(C4)C2)C3)cc1
vN-ppi1-196	Z652492728	-9.6	0.267	487.49	REAL	Cc1nn(Cc2ccc(F)cc2)c2[nH]nc(NC(=O)CN3C(=O)N[C@@]4(CCc5ccccc54)C3=O)c12
vN-ppi1-197	Z70895836	-9.6	0.291	442.43	REAL	Cc1nc2ccccc2c(=O)n1-c1ccc(C(=O)NNC(=O)c2ccc3c(c2)OCO3)cc1
vN-ppi1-198	Z737388578	-9.6	0.291	468.52	REAL	O=C(c1cccc(S(=O)(=O)N2CCc3ccccc3C2)c1)N1CCCc2cc(F)cc(F)c21
vN-ppi1-199	Z901882616	-9.6	0.274	478.43	REAL	C[C@]1(c2ccc(-c3nc4ccc(-c5cccc(C(F)(F)F)c5)cc4c(=O)[nH]3)cc2)NC(=O)NC1=O
vN-ppi1-200	Z955663406	-9.6	0.282	471.50	REAL	O=C(NNC(=O)c1cccc2ccenc12)c1ccc(NC2=NS(=O)(=O)c3ccccc32)cc1

Supplementary Table 84. Virtual screening hits 101 to 200 of the screen against the oligomerization interface of the NTD of the nucleoprotein (Screen ID: 43). Compounds were filtered so that hits had MW < 600 dalton, cLogP < 6, number of hydrogen bond acceptors < 11, and no reactive functional groups. A few compounds unsuitable for drug discovery were removed by visual inspection. The name of each compound consists of the initial letter 'v' for virtual hit, followed by the target protein name and the target site ('ppi' for protein-protein interface, 1 for docking scenario 1). The score is the docking score given by QuickVina 2 in kcal/mol. The ligand efficiency (LE) is computed as LE = -score/#NonH, where #NonH is the number of heavy (i.e. non hydrogen) atoms.

Name	Catalog ID	Score	LE	MW	Library	SMILES
vN-ctd1-1	ZINC000002412360	-13.5	0.365	485.494	ZINC	O=C(Nc1ccc(-c2cc3ccccc3oc2=O)cc1)c1cccc(-c2cc3ccccc3oc2=O)c1
vN-ctd1-2	ZINC000004015296	-13.2	0.347	493.477	ZINC	O=c1nc2c3cccc4cccc(c(=O)n2c2cc(N5C(=O)c6cccc7cccc(c76)C5=O)ccc12)c43
vN-ctd1-3	ZINC000005220992	-13.1	0.364	468.427	ZINC	O=c1nc2c3cccc4c(=O)n5c(=O)c6ccccc6nc5c5ccc(c(=O)n2c2ccccc12)c3c45
vN-ctd1-4	ZINC000017862766	-13.1	0.327	520.587	ZINC	O=C(Nc1ccc2ccccc2c1)c1cccc(N2C(=O)[C@H]3[C@@H](C2=O)C2c4ccccc4C3c3ccccc32)c1
vN-ctd1-5	ZINC000002832254	-13	0.371	473.507	ZINC	O=c1oc2ccc3ccccc3c2cc1-c1csc(-c2cc3c(ccc4ccccc43)oc2=O)n1
vN-ctd1-6	ZINC000016757167	-13	0.342	498.537	ZINC	Cc1ccc(N2C(=O)c3ccccc3/C(=C/Nc3ccc4c(c3)C(=O)c3ccccc3C4=O)C2=O)c(C)c1
vN-ctd1-7	Z1066669856	-12.9	0.349	495.621	REAL	O=C(c1cccc2ccccc12)N1CCN(C(=O)[C@H]2C[C@@H]3CCCC[C@H]3N2C(=O)c2ccccc2)CC1
vN-ctd1-8	Z91060830	-12.9	0.358	496.586	REAL	O=C1c2ccccc2S(=O)(=O)c2cc(C(=O)N3CCN(Cc4cccc5ccccc45)CC3)ccc21
vN-ctd1-9	ZINC000037246229	-12.9	0.369	465.591	ZINC	O=C1c2ccccc2C(=O)c2cc3c(cc21)N[C@H]1CC[C@H]2[C@@H]4CCCC[C@@H]4C(=O)[C@H]4CC[C@H]3[C@H]1[C@@H]42
vN-ctd1-10	Z367327618	-12.8	0.356	481.55	REAL	Cc1ccc(C(=O)C2CCN(C(=O)c3ccc4c(=O)n(-c5ccccc5)c(=O)[nH]c4c3)CC2)c(C)c1
vN-ctd1-11	Z383456236	-12.8	0.337	499.577	REAL	Cc1cc(N2CCN(C(=O)c3cc(-c4cccc5ccccc45)nc4ccccc34)CC2)n2ncnc2n1
vN-ctd1-12	Z758345806	-12.8	0.376	473.548	REAL	Cc1ccc(C(=O)C2CCN(C(=O)c3ccc4c(c3)S(=O)(=O)c3ccccc3C4=O)CC2)cc1
vN-ctd1-13	ZINC000001266504	-12.8	0.366	456.456	ZINC	O=C1c2cc3oc4ccccc4c4ccccc4oc3cc2C(=O)N1c1cccc2ccccnc21
vN-ctd1-14	ZINC000008826512	-12.8	0.376	441.485	ZINC	O=C1[C@H]2[C@H](C(=O)N1c1ccc3c(c1)oc1ccccc13)C1c3ccccc3C2c2ccccc21
vN-ctd1-15	ZINC000017988176	-12.8	0.32	521.571	ZINC	O=C(Oc1ccc2ccccc2c1)c1cccc(N2C(=O)[C@H]3[C@@H](C2=O)C2c4ccccc4C3c3ccccc32)c1
vN-ctd1-16	ZINC000018021374	-12.8	0.337	498.537	ZINC	O=C(NN1C(=O)[C@H]2[C@@H](C1=O)C1c3ccccc3C2c2ccccc21)C1(O)c2ccccc2-c2ccccc21
vN-ctd1-17	ZINC000408731626	-12.8	0.337	499.565	ZINC	Cc1ccc(N2C(=O)[C@H]3[C@H](C2=O)[C@@H]2C(=O)Oc4c5ccccc5ccc4C2=C[C@H]3c2ccccc2)cc1C
vN-ctd1-18	ZINC000408731630	-12.8	0.337	499.565	ZINC	Cc1ccc(N2C(=O)[C@@H]3[C@H](C2=O)[C@@H]2C(=O)Oc4c5ccccc5ccc4C2=C[C@H]3c2ccccc2)cc1C
vN-ctd1-19	Z1260000954	-12.7	0.385	436.466	REAL	O=C(NNC(=O)c1cccc2ccccc12)c1ccc2c(c1)C[C@@H](c1ccccc1)OC2=O
vN-ctd1-20	Z1452691933	-12.7	0.385	445.493	REAL	O=C(NC[C@H]1[C@@H]2Cc3ccccc3[C@H]12)NNC(=O)c1ccccc1OCc1ccc(F)cc1
vN-ctd1-21	Z1472866131	-12.7	0.374	449.552	REAL	O=C(N[C@H]1[C@@H]2CCc3ccccc3[C@@H]21)c1cncc(C(=O)N[C@H]2[C@@H]3CCc4ccccc4[C@@H]32)c1
vN-ctd1-22	Z1529686811	-12.7	0.385	437.541	REAL	CN1C(=O)CCc2cc(C(=O)N3CCN(C4c5ccccc5-c5ccccc54)CC3)ccc21
vN-ctd1-23	Z770161618	-12.7	0.374	470.548	REAL	O=C1c2ccccc2S(=O)(=O)c2cc(C(=O)N3CCC[C@@H](c4cc5ccccc5[nH]4)C3)ccc21
vN-ctd1-24	ZINC000000826899	-12.7	0.353	468.467	ZINC	O=C1c2cccc3cccc(c32)C(=O)N1c1ccc(N2C(=O)c3cccc4ccccc(c43)C2=O)cc1
vN-ctd1-25	ZINC000100414424	-12.7	0.334	499.521	ZINC	O=C1c2ccccc2C(=O)C12O[C@@H](c1ccccc1)[C@@H]1C(=O)N(c3ccc(-c4ccccc4)cc3)C(=O)[C@H]12
vN-ctd1-26	ZINC000101076130	-12.7	0.334	499.521	ZINC	O=C1c2ccccc2C(=O)C12O[C@@H](c1ccccc1)[C@@H]1C(=O)N(c3ccc(-c4ccccc4)cc3)C(=O)[C@@H]12
vN-ctd1-27	Z1024046328	-12.6	0.371	453.54	REAL	O=C1Nc2ccccc2[C@H]1C1CCN(C(=O)[C@@H]2CC(=O)N(c3cccc4ccccc34)C2)CC1
vN-ctd1-28	Z1449091221	-12.6	0.382	436.51	REAL	Cc1ccc(C)c(N2C(=O)c3ccc(C(=O)NC[C@H]4[C@H]5Cc6ccccc6[C@H]45)cc3C2=O)c1
vN-ctd1-29	Z165047412	-12.6	0.341	487.47	REAL	O=C1NC(=O)c2ccccc2/C1=C/NN1C(=O)c2ccc3c(C(=O)c4ccccc4)ccc(c23)C1=O
vN-ctd1-30	Z316831980	-12.6	0.35	480.566	REAL	O=C(c1ccc2c(=O)n3c(nc2c1)CCCCC3)N1CCN(C(=O)c2ccc3ccccc23)CC1
vN-ctd1-31	Z941405732	-12.6	0.36	487.622	REAL	O=C(C1CCN(C2=NS(=O)(=O)c3ccccc32)CC1)N1CCC(c2ccc3ccccc23)CC1
vN-ctd1-32	ZINC000001269423	-12.6	0.323	554.65	ZINC	Cc1nc2ccccc2n1S(=O)(=O)c1ccc2c(c1)Cc1cc(S(=O)(=O)n3c(C)nc4ccccc43)ccc1-2
vN-ctd1-33	ZINC000003954537	-12.6	0.341	481.466	ZINC	O=C(Nc1ccc2c1C(=O)c1ccccc1C2=O)c1ccc2c3c1ncnc3-c1ccccc1C2=O
vN-ctd1-34	ZINC000004542487	-12.6	0.332	497.553	ZINC	O=C(c1ccc(-c2ccccc2)cc1)[C@@H]1[C@@H]2C(=O)N(c3cccc3)C(=O)[C@@H]2[C@H]2c3ccccc3C=NN12
vN-ctd1-35	ZINC000008901217	-12.6	0.332	499.521	ZINC	Cc1cc(NC(=O)c2ccc(-c3cc4ccccc4oc3=O)c2)ccc1-c1cc2ccccc2oc1=O
vN-ctd1-36	ZINC000016037690	-12.6	0.332	519.987	ZINC	O=C(Nc1ccc(Cl)cc1)[C@@H]1[C@@H]2C(=O)N(c3cccc4ccccc43)C(=O)[C@@H]2[C@H]2c3ccccc3C=CN12
vN-ctd1-37	ZINC000033358359	-12.6	0.3	567.613	ZINC	O=C(c1cc2nc3c(c(C(F)(F)F)n2n1)CCc1ccccc1-3)N1CCN(C(=O)c2ccccc2)c2ccccc2)CC1
vN-ctd1-38	ZINC000100485510	-12.6	0.394	410.431	ZINC	O=C1c2ccc3c4c(ccc(c24)C2=Nc4ccccc4[C@H]21)C1=Nc2ccccc2[C@H]1C3=O
vN-ctd1-39	ZINC000101076136	-12.6	0.332	499.521	ZINC	O=C1c2ccccc2C(=O)C12O[C@@H](c1ccccc1)[C@H]1C(=O)N(c3ccc(-c4ccccc4)cc3)C(=O)[C@@H]12
vN-ctd1-40	ZINC000107765190	-12.6	0.341	480.585	ZINC	O=C(/C=C\c1cc[n+](CC(=O)c2ccc3ccccc4c3c2CC4)cc1)c1ccc2ccc3c2c1CC3
vN-ctd1-41	ZINC000409337159	-12.6	0.332	494.509	ZINC	O=C(Nc1ccc2nc3ccc4ccccc4c3nc2c1)c1ccc(N2C(=O)c3ccccc3C2=O)cc1
vN-ctd1-42	Z1102068504	-12.5	0.357	463.496	REAL	Cc1cc2nc(-c3ccccc3)cc(C(=O)NNC(=O)c3n[nH]c(=O)c4ccccc34)c2cc1C
vN-ctd1-43	Z165048186	-12.5	0.357	459.46	REAL	O=C1NC(=O)c2ccccc2/C1=C\Nc1ccc(N2C(=O)c3cccc4ccccc34)C2=O)cc1
vN-ctd1-44	Z1833542217	-12.5	0.379	442.513	REAL	O=C1C[C@H](C(=O)N2C[C@@H]3CCCN(C(=O)[C@@H]4CC(=O)c5ccccc54)[C@@H]3C2)c2ccccc21
vN-ctd1-45	Z1888493741	-12.5	0.368	447.536	REAL	O=C(c1ccc2c(=O)c3cccc3[nH]c12)N1CCN(Cc2cccc3ccccc23)CC1
vN-ctd1-46	Z2008707791	-12.5	0.379	436.518	REAL	Cn1c(-c2c[nH]c3ccccc23)nnc1N1CCN(C(=O)c2cccc3ccccc23)CC1
vN-ctd1-47	Z2008725225	-12.5	0.379	437.545	REAL	Cn1c(-c2cccc3ccccc23)nnc1N1CCC(C(=O)N2CCc3ccccc32)CC1
vN-ctd1-48	Z2167429497	-12.5	0.368	448.529	REAL	Cn1c(-c2nn(C)c(=O)c3ccccc23)nnc1N1CC=C(c2cccc3ccccc23)CC1
vN-ctd1-49	Z2174372362	-12.5	0.379	432.526	REAL	O=C(c1cnnc(-c2ccccc2)c1)N1CCN(C2c3ccccc3-c3ccccc32)CC1
vN-ctd1-50	Z26848700	-12.5	0.357	467.567	REAL	Cc1ccc(C)c(N2C(=O)c3ccc(C(=O)N4CCN(c5cccc(C)c5C)CC4)cc3C2=O)c1
vN-ctd1-51	Z28562030	-12.5	0.368	488.587	REAL	O=C1c2ccccc2S(=O)(=O)c2cc(C(=O)N3CCC[C@@H](c4nc5ccccc5s4)C3)ccc21
vN-ctd1-52	Z728494648	-12.5	0.379	461.512	REAL	O=C1c2ccccc2S(=O)(=O)c2cc(C(=O)N3CCC(=Cc4cccc(F)c4)CC3)ccc21
vN-ctd1-53	Z810425188	-12.5	0.357	469.539	REAL	Cc1cccc(NC(=O)[C@H]2CCCN(C(=O)c3ccc4c(c3)C[C@@H](c3ccccc3)OC4=O)C2)n1
vN-ctd1-54	Z920796876	-12.5	0.357	485.606	REAL	O=C(C1CCN(C2=NS(=O)(=O)c3ccccc32)CC1)N1CC=C(c2cccc3ccccc23)CC1
vN-ctd1-55	ZINC000001862466	-12.5	0.357	455.468	ZINC	Cc1nc(-c2cc3c(ccc4ccccc43)oc2=O)cc2c1c(=O)oc1ccc3ccccc3c12
vN-ctd1-56	ZINC000008449795	-12.5	0.329	493.561	ZINC	O=C1[C@@H]2[C@@H](C(=O)N1c1ccc(Oc3ccc4ccccc4c3)cc1)C1c3ccccc3C2c2ccccc21
vN-ctd1-57	ZINC000008832077	-12.5	0.347	472.499	ZINC	Cc1ccccc1-c1nc2cc(NC(=O)c3cccc(-c4ec5ccccc5oc4=O)c3)ccc2o1
vN-ctd1-58	ZINC000009087807	-12.5	0.347	470.527	ZINC	O=C(c1ccccc1)[C@H]1[C@H]2C(=O)N(c3cccc4ccccc43)C(=O)[C@@H]2[C@H]2c3ccccc3C=CN12
vN-ctd1-59	ZINC000009389051	-12.5	0.368	448.477	ZINC	C[C@]1(c2ccc3ccccc3c2)NC(=O)N(Cc2cc(=O)oc3ccc4ccccc4c23)C1=O
vN-ctd1-60	ZINC000012847897	-12.5	0.379	436.51	ZINC	O=C(CN1C(=O)N[C@]2(CCCCc3ccccc32)C1=O)c1ccc2c(c1)-c1ccccc1C2
vN-ctd1-61	ZINC000029491187	-12.5	0.298	569.629	ZINC	Cc1ccc(-c2cc(C(F)(F)F)n3nc(C(=O)N4CCN(C(c5ccccc5)c5ccccc5)CC4)cc3n2)cc1C
vN-ctd1-62	ZINC000035241256	-12.5	0.347	470.527	ZINC	O=C(c1ccccc1)[C@H]1[C@@H]2C(=O)N(c3cccc4ccccc43)C(=O)[C@@H]2[C@H]2c3ccccc3C=CN12
vN-ctd1-63	ZINC000037246227	-12.5	0.357	465.591	ZINC	O=C1c2ccccc2C(=O)c2cc3c(cc21)N[C@H]1CC[C@@H]2[C@@H]4CCCC[C@@H]4C(=O)[C@H]4CC[C@H]3[C@H]1[C@H]24
vN-ctd1-64	ZINC000229940499	-12.5	0.298	573.09	ZINC	Cc1ccc(C(=O)[C@@H]2[C@H](C(=O)c3ccccc3Cl)[C@]3(C(=O)Nc4ccccc43)[C@@H]3C=C(C)c4cc(C)ccc4N32)cc1
vN-ctd1-65	ZINC000409336230	-12.5	0.329	499.565	ZINC	Cc1ccc(N2C(=O)[C@H]3[C@H](C2=O)[C@@H]2C(=O)Oc4ccc5ccccc5c4C2=C[C@H]3c2ccccc2)cc1C
vN-ctd1-66	Z1024046034	-12.4	0.365	456.544	REAL	O=C1Nc2ccccc2[C@H]1C1CCN(C(=O)c2ccc3c(=O)n4c(nc3c2)CCCCC4)CC1
vN-ctd1-67	Z1095050588	-12.4	0.365	447.457	REAL	Cc1noc2nc(-c3ccccc3)cc(C(=O)Nc3nc(-c4ccc5ccccc5n4)n[nH]3)c12
vN-ctd1-68	Z1129794489	-12.4	0.376	442.489	REAL	Cc1ccc(C)c(N2C(=O)c3ccc(C(=O)N4CC[C@H](c5cccc(F)c5)C4)cc3C2=O)c1
vN-ctd1-69	Z131821778	-12.4	0.344	496.633	REAL	O=C(c1ccc2c(c1)-c1ccccc1C2)N1CCN(Cc2nc3sc4c(c3c(=O)[nH]2)CCCC4)CC1
vN-ctd1-70	Z1383816512	-12.4	0.365	453.461	REAL	O=C1c2ccccc2C(=O)c2cc(NC(=O)C3CCN(c4ccc5nnnn5n4)CC3)ccc21
vN-ctd1-71	Z1383818315	-12.4	0.354	458.472	REAL	O=C(Cn1c2ccccc2c(=O)c2ccccc21)Nc1ccc2c(c1)C(=O)c1ccccc1C2=O
vN-ctd1-72	Z1404436268	-12.4	0.387	444.554	REAL	CC1(C)CN(C(=O)c2cc(-c3cccc4ccccc34)nc3ccccc23)CCS1(=O)=O
vN-ctd1-73	Z1473414262	-12.4	0.365	448.525	REAL	O=C(NNC(=O)c1cc(-c2ccccc2)nc2ccccc12)N[C@H]1[C@@H]2CCc3ccccc3[C@@H]21
vN-ctd1-74	Z1626782444	-12.4	0.376	437.498	REAL	O=C(CN1C(=O)N[C@@]2(CCc3ccccc32)C1=O)N1CC=C(c2cccc3ccccc23)C1
vN-ctd1-75	Z2085937346	-12.4	0.387	443.522	REAL	O=C1c2ccccc2S(=O)(=O)c2cc(C(=O)N3Cc4ccccc4C4(CCC4)C3)ccc21
vN-ctd1-76	Z2166788972	-12.4	0.376	434.502	REAL	Cn1c(-c2n[nH]c(=O)c3ccccc23)nnc1N1CC=C(c2cccc3ccccc23)CC1
vN-ctd1-77	Z220408188	-12.4	0.335	491.55	REAL	Cc1ccc(C)c(N2C(=O)c3ccc(C(=O)Nc4nc5ccccc5nc4N4CCCC4)cc3C2=O)c1
vN-ctd1-78	Z2524832653	-12.4	0.344	481.642	REAL	Cc1cccc(-c2nnc3n2C[C@@H](C(=O)N2C[C@@H]4CC[C@H]2[C@H]2CN(Cc5ccccc5)C[C@H]42)CC3)c1
vN-ctd1-79	Z298645214	-12.4	0.354	464.567	REAL	O=C(c1ccccc2ccccc12)N1CCC(C(=O)N2CC=C(c3c[nH]c4ncccc34)CC2)CC1
vN-ctd1-80	Z367578612	-12.4	0.365	472.52	REAL	O=C1c2ccccc2S(=O)(=O)c2cc(C(=O)N3CCC[C@@H](c4nc5ccccc5o4)C3)ccc21
vN-ctd1-81	Z652498744	-12.4	0.335	495.513	REAL	Cc1nn(Cc2ccc(F)cc2)c2[nH]nc(NC(=O)c3ccc4c(c3)C[C@@H](c3ccccc3)OC4=O)c12
vN-ctd1-82	Z654041216	-12.4	0.365	450.493	REAL	O=C(Cc1ccc2ccccc2c1)NNC(=O)c1ccc2c(c1)C[C@@H](c1ccccc1)OC2=O
vN-ctd1-83	Z791415724	-12.4	0.335	494.506	REAL	Cc1ccc2c(c1)c(=O)n(C)c1nnc(COC(=O)c3ccc4c(c3)C[C@@H](c3ccccc3)OC4=O)n21
vN-ctd1-84	Z998375970	-12.4	0.335	495.581	REAL	O=C(c1ccc2[nH]ncc2c1)N1CCC[C@@H](C(=O)N2CCN(C(=O)c3cccc4ccccc34)CC2)C1
vN-ctd1-85	ZINC000002212711	-12.4	0.376	429.474	ZINC	O=C(Nc1ccc2c(c1)Cc1ccccc1-2)c1ccc(-c2cc3ccccc3oc2=O)c1
vN-ctd1-86	ZINC000002294074	-12.4	0.365	446.501	ZINC	Cc1c(OCC(=O)c2ccc(-c3ccccc3)cc2)ccc2c(-c3ccccc3)cc(=O)oc12
vN-ctd1-87	ZINC000002466512	-12.4	0.387	419.483	ZINC	O=C(Nc1cnc2ccccc2c1)[C@H]1c2ccccc2C(=O)N2CCc3ccccc3[C@H]12
vN-ctd1-88	ZINC000002865873	-12.4	0.318	515.52	ZINC	COc1ccc(-c2cc3ccccc3oc2=O)cc1NC(=O)c1ccccc(-c2cc3ccccc3oc2=O)c1
vN-ctd1-89	ZINC000008449797	-12.4	0.326	493.561	ZINC	O=C1[C@H]2[C@H](C(=O)N1c1ccc(Oc3ccc4ccccc4c3)cc1)C1c3ccccc3C2c2ccccc21
vN-ctd1-90	ZINC000008792183	-12.4	0.335	486.573	ZINC	Cc1ccccc(N2CCN(C(=O)c3cc4c5ccccc5n5c4c(n3)c3ccccc3c5=O)CC2)c1C
vN-ctd1-91	ZINC000009224387	-12.4	0.354	466.587	ZINC	Cc1c2c(nn1-c1ccc(C)cc1)c(N1CCC[C@@H](C(=O)N3CCc4ccccc43)C1)nnc2C
vN-ctd1-92	ZINC000009762378	-12.4	0.344	480.475	ZINC	CC1=CC(C)(C)N2C(=O)C(=O)c3cc(OC(=O)CN4C(=O)c5ccc6cccc(c65)C4=O)cc1c32
vN-ctd1-93	ZINC000016037828	-12.4	0.335	504.972	ZINC	O=C(c1ccc(Cl)cc1)[C@@H]1[C@@H]2C(=O)N(c3cccc4ccccc43)C(=O)[C@@H]2[C@H]2c3ccccc3C=CN12
vN-ctd1-94	ZINC000016038169	-12.4	0.335	505.96	ZINC	O=C(c1ccc(Cl)cc1)[C@@H]1[C@@H]2C(=O)N(c3cccc4ccccc43)C(=O)[C@@H]2[C@H]2c3ccccc3C=NN12
vN-ctd1-95	ZINC000018181101	-12.4	0.335	487.51	ZINC	Cc1cccc([C@H]2OC3(C(=O)c4ccccc4C3=O)[C@@H]3C(=O)N(c4ccc5ccccc54)C(=O)[C@H]32)c1
vN-ctd1-96	ZINC000020759059	-12.4	0.326	498.584	ZINC	O=C(c1cc2c3ccccc3n3c2c(n1)c1ccccc1c3=O)N1CCN(C/C=C/c2ccccc2)CC1
vN-ctd1-97	ZINC000029748612	-12.4	0.318	560.65	ZINC	C[C@@H]1CN(S(=O)(=O)c2ccc3oc4ccccc4c3c2)CCN1S(=O)(=O)c1ccc2oc3ccccc3c2c1
vN-ctd1-98	ZINC000037246228	-12.4	0.354	465.591	ZINC	O=C1c2ccccc2C(=O)c2cc3c(cc21)N[C@@H]1CC[C@H]2[C@@H]4CCCC[C@@H]4C(=O)[C@H]4CC[C@H]3[C@H]1[C@@H]42
vN-ctd1-99	ZINC000052955754	-12.4	0.288	581.671	ZINC	CN1C[C@H](C(=O)N[C@]2(C)O[C@@]3(O)[C@@H]4CCCN4C(=O)[C@H](Cc4ccccc4)N3C2=O)C=C2c3ccccc4[nH]cc(c43)C[C@H]21
vN-ctd1-100	ZINC000085392553	-12.4	0.318	520.606	ZINC	O=C([C@@H]1CC(=O)N(c2ccc(F)cc2)C1)N1CCC(c2c[nH]c3ccccc32)(c2c[nH]c3ccccc32)CC1

Supplementary Table 85. Top 100 virtual hits of the screen against the dimerization interface of the CTD of the nucleoprotein (Screen ID: 44). Compounds were filtered so that hits had MW < 600 dalton, cLogP < 6, number of hydrogen bond acceptors < 11, and no reactive functional groups. A few compounds unsuitable for drug discovery were removed by visual inspection. The name of each compound consists of the initial letter 'v' for virtual hit, followed by the target protein name and the target site ('ctd' for CTD binding interface, 1 for docking scenario 1). The score is the docking score given by QuickVina 2 in kcal/mol. The ligand efficiency (LE) is computed as LE = -score/#NonH, where #NonH is the number of heavy (i.e. non hydrogen) atoms.

Name	Catalog ID	Score	LE	MW	Library	SMILES
vN-ctd1-101	ZINC000100485501	-12.4	0.387	410.43	ZINC	O=C1c2ccc3c4c(ccc(c24)C2=Nc4ccccc4[C@H]21)C1=Nc2ccccc2[C@@H]1C3=O
vN-ctd1-102	ZINC000100688954	-12.4	0.318	511.58	ZINC	Cc1ccc(N2C(=O)[C@@H]3[C@H](C2=O)[C@H]2c4ccccc4C=NN2[C@@H]3C(=O)c2ccc(-c3ccccc3)cc2)cc1
vN-ctd1-103	ZINC000216298986	-12.4	0.387	412.49	ZINC	O=C1C[C@]2(c3ccccc31)c1ccccc1[C@@]1(c3ccccc3)c3ccccc3C(=O)[C@@H]21
vN-ctd1-104	ZINC000229890704	-12.4	0.295	552.67	ZINC	Cc1ccc(C(=O)[C@H]2[C@@H](C(=O)c3ccc(C)cc3)N3c4ccc(C)cc4C(C)=C[C@H]3[C@@]23C(=O)Nc2ccccc23)cc1
vN-ctd1-105	ZINC000254513605	-12.4	0.365	473.55	ZINC	CN1c2ccccc2C(C)(C)[C@]12CC(c1ccc3c(c1)S(=O)(=O)c1ccccc1C3=NO)=NO2
vN-ctd1-106	ZINC000254722125	-12.4	0.344	558.41	ZINC	O=C(N=C1N=C2C=CC(Br)=CN2Cc2ccccc21)c1ccc2c(c1)S(=O)(=O)c1ccccc1C2=O
vN-ctd1-107	ZINC000408686155	-12.4	0.326	498.58	ZINC	Cc1cc(C)cc(NC(=O)c2ccc(N3C(=O)[C@@H]4[C@@H](C3=O)C3c5ccccc5C4c4ccccc43)cc2)c1
vN-ctd1-108	PV-001957449472	-12.3	0.397	409.49	REAL	Cc1cccc(-c2ccc(CNC(=O)NNC(=O)c3cccc4ccccc34)cc2)c1
vN-ctd1-109	Z1000674394	-12.3	0.342	481.55	REAL	Cc1ccc(C)c(N2C(=O)c3ccc(C(=O)N[C@@H]4CCCN(C(=O)c5ccccc5)C4)cc3C2=O)c1
vN-ctd1-110	Z1005784094	-12.3	0.332	492.58	REAL	O=C(N[C@@H]1CCc2nc(-c3ccccc3)ncc2C1)[C@H]1CCCN1C(=O)c1ccc2ccccc2c1O
vN-ctd1-111	Z1069429018	-12.3	0.342	474.52	REAL	O=C(N[C@@H]1CCc2nc(-c3ccccc3)ncc2C1)c1cccc(N2C(=O)c3ccccc3C2=O)c1
vN-ctd1-112	Z1070217308	-12.3	0.351	490.99	REAL	O=C1Nc2ccc(Cl)ccc2[C@@H]1C1CCN(C(=O)c2ccc3c(=O)n4c(nc3c2)CCCCC4)CC1
vN-ctd1-113	Z1104727050	-12.3	0.342	498.61	REAL	O=C(Nc1ccc2c(c1)Cc1ccccc1-2)N1CCCN(S(=O)(=O)c2cccc3cnccc23)CC1
vN-ctd1-114	Z1314558973	-12.3	0.384	425.53	REAL	C[C@@H]1c2ccccc2CCN1C(=O)c1ccnc(C(=O)N2CCc3ccccc3[C@@H]2C)c1
vN-ctd1-115	Z1449094407	-12.3	0.362	449.55	REAL	O=C(NC[C@H]1[C@H]2Cc3ccccc3[C@@H]12)c1cncc(C(=O)N[C@H]2[C@H]3Cc4ccccc4[C@@H]23)c1
vN-ctd1-116	Z1581473271	-12.3	0.373	440.59	REAL	O=C(NC[C@H]1CCCN1C(=O)[C@@H]1C[C@@]12CCc1ccccc12)[C@H]1C[C@@]12CCc1ccccc12
vN-ctd1-117	Z1610587670	-12.3	0.373	434.50	REAL	Cc1cc2ccccc2nc1NNC(=O)c1nnn(-c2ccc(-c3ccccc3)cc2)c1C
vN-ctd1-118	Z1752022802	-12.3	0.362	449.55	REAL	O=C(NC[C@H]1CC2c3ccccc3C1c1ccccc12)N1CC[C@@]2(C1)C(=O)Nc1ccccc12
vN-ctd1-119	Z2002423492	-12.3	0.384	425.48	REAL	O=C1[C@@H]2[C@@H]3C[C@H]4[C@@H]2[C@]2(C(=O)Oc5ccccc(C(=O)N6CCc7ccccc7C6)c5)[C@H]1[C@@H]3[C@@H]42
vN-ctd1-120	Z2008325723	-12.3	0.373	436.52	REAL	Cn1c(-c2n[nH]c(=O)c3ccccc23)nnc1N1CCC(c2cccc3ccccc23)CC1
vN-ctd1-121	Z220541322	-12.3	0.362	471.54	REAL	O=C1c2ccccc2S(=O)(=O)c2cc(C(=O)N3CCC[C@@H](c4nc5ccccc5[nH]4)C3)ccc21
vN-ctd1-122	Z2524830102	-12.3	0.332	499.56	REAL	O=C(c1cc(F)cc2c(=O)c3cc(F)ccc3[nH]c12)N1C[C@@H]2CC[C@H]1[C@H]1CN(Cc3ccccc3)C[C@H]21
vN-ctd1-123	Z288378426	-12.3	0.342	482.59	REAL	Cc1ccc(-c2nnc3n2CCCCC3)cc1NC(=O)c1ccc2c(=O)n3c(nc2c1)CCCCC3
vN-ctd1-124	Z344096624	-12.3	0.351	470.50	REAL	C[C@]1(c2ccc3ccccc3c2)NC(=O)N(CC(=O)N2CCc3[nH]c4ccc(F)cc4c3C2)C1=O
vN-ctd1-125	Z344132624	-12.3	0.351	466.54	REAL	Cc1ccc2[nH]c3c(c2c1)CN(C(=O)CN1C(=O)N[C@](C)(c2cc4ccccc4c2)C1=O)CC3
vN-ctd1-126	Z383879656	-12.3	0.373	438.53	REAL	CN(C)C(=O)N1CCN(C(=O)c2cc(-c3cccc4ccccc34)nc3ccccc23)CC1
vN-ctd1-127	Z415220808	-12.3	0.351	481.58	REAL	O=C(c1cc2ccccc2c2cccnc12)N1CCN(S(=O)(=O)c2ccc3ccccc3c2)CC1
vN-ctd1-128	Z62471841	-12.3	0.342	493.49	REAL	O=C(Nc1ccc2c(c1)C(=O)c1ccccc1C2=O)c1ccc2c(c1)S(=O)(=O)c1ccccc1C2=O
vN-ctd1-129	Z749464616	-12.3	0.373	436.47	REAL	O=C(NNC(=O)c1ccc2ccccc2c1)c1ccc2c(c1)C[C@H](c1ccccc1)OC2=O
vN-ctd1-130	Z764667804	-12.3	0.351	464.52	REAL	O=C(Nc1nc2ccccc2nc1N1CCCC1)c1ccc2c(c1)C[C@@H](c1ccccc1)OC2=O
vN-ctd1-131	Z770165242	-12.3	0.351	484.58	REAL	O=C(c1ccc(NC2=NS(=O)(=O)c3ccccc32)cc1)N1CCC[C@@H](c2cc3ccccc3[nH]2)C1
vN-ctd1-132	Z852297896	-12.3	0.373	441.57	REAL	C[C@@H]1CCc2[nH]c3ccc(C(=O)N4CCC(C(=O)N5CCc6ccccc65)CC4)cc3c2C1
vN-ctd1-133	ZINC000001213051	-12.3	0.286	589.62	ZINC	O=C(c1cnn2c1N[C@H](c1ccc3c(c1)OCO3)C[C@@H]2C(F)(F)F)N1CCN(C(c2ccccc2)c2ccccc2)CC1
vN-ctd1-134	ZINC000001228911	-12.3	0.324	498.53	ZINC	Cc1ccc([C@H]2OC3(C(=O)c4ccccc4C3=O)[C@@H](c3ccccc3)C23C(=O)c2ccccc2C3=O)cc1
vN-ctd1-135	ZINC000001588362	-12.3	0.362	440.51	ZINC	Nc1nc(-c2ccc3ccccc3c2)cc(-c2cc(-c3ccc4ccccc4c3)nc(N)n2)n1
vN-ctd1-136	ZINC000002267002	-12.3	0.397	406.40	ZINC	O=c1oc2ccc3ccccc3c2cc1-c1nnc(-c2cc3ccccc3cc2O)o1
vN-ctd1-137	ZINC000002592693	-12.3	0.351	473.41	ZINC	O=C1c2cc3oc4ccccc4c4ccccc4oc3cc2C(=O)N1c1ccccC(C(F)(F)F)c1
vN-ctd1-138	ZINC000002933884	-12.3	0.332	494.45	ZINC	O=c1oc(-c2cccc(F)c2)nc2cc(Cc3ccc4c(=O)oc(-c5cccc(F)c5)nc4c3)ccc12
vN-ctd1-139	ZINC000003845263	-12.3	0.373	444.47	ZINC	O=C1c2cccc3ccccc23)/C1=C1\Sc2ccc3c(c2C1=O)C(=O)c1ccccc1C3=O
vN-ctd1-140	ZINC000004522763	-12.3	0.342	472.46	ZINC	Nc1c(C(=O)Nc2cccc3c2C(=O)c2ccccc2C3=O)ccc2c1C(=O)c1ccccc1C2=O
vN-ctd1-141	ZINC000004542488	-12.3	0.324	497.55	ZINC	O=C(c1ccc(-c2ccccc2)cc1)[C@H]1[C@@H]2C(=O)N(c3ccccc3)C(=O)[C@@H]2[C@H]2c3ccccc3C=NN12
vN-ctd1-142	ZINC000004831167	-12.3	0.384	412.49	ZINC	O=C1C[C@]2(c3ccccc31)c1ccccc1[C@@]1(c3ccccc3)c3ccccc3C(=O)[C@H]12
vN-ctd1-143	ZINC000008442893	-12.3	0.332	489.53	ZINC	C[C@H](C(=O)OCC(=O)c1ccc(-c2ccccc2)cc1)N1C(=O)c2ccc3c4c(ccc(c42)C1=O)CC3
vN-ctd1-144	ZINC000008444221	-12.3	0.351	482.97	ZINC	Cc1ccc2occ([C@H]3Nc4ccccc4NC4=C3C(=O)C[C@@H](c3ccccc3Cl)C4)c(=O)c2c1
vN-ctd1-145	ZINC000009776995	-12.3	0.332	493.65	ZINC	Cc1cccc(CN2CCC(CNC(=O)[C@@H]3c4ccccc4C(=O)N4CCc5ccccc5[C@@H]34)CC2)c1
vN-ctd1-146	ZINC000013513993	-12.3	0.324	515.57	ZINC	O=c1/c(=C/c2cn(-c3ccccc3)nc2-c2ccc3ccccc3c2)sc2nc(-c3ccc(F)cc3)nn12
vN-ctd1-147	ZINC000014883609	-12.3	0.342	478.60	ZINC	Cc1ccccc1-c1cc(C(=O)N2CCN([C@@H]3CCc4ccccc4C3)CC2)cc(-n2cnnn2)c1
vN-ctd1-148	ZINC000016525610	-12.3	0.373	429.47	ZINC	O=C(Nc1ccc2c(c1)Cc1ccccc1-2)c1ccc(-c2cc3ccccc3oc2=O)cc1
vN-ctd1-149	ZINC000019795177	-12.3	0.362	437.45	ZINC	O=C1c2ccccc2C2=C1C1(c3cccc4cccc(c34)C1=O)C1=C(N2)c2ccccc2C1=O
vN-ctd1-150	ZINC000059475095	-12.3	0.384	412.54	ZINC	c1ccc2c(c1)ccc2N1Cc2cc3c(cc2C1)CN(c1ccc2ccccc21)C3
vN-ctd1-151	ZINC000059932650	-12.3	0.308	527.62	ZINC	Cc1ccc2c(c1C)NC(=O)[C@@]21N2CCC[C@@H]2[C@@H](C(=O)c2ccc3ccccc3c2)[C@]12c1ccccc1NC2=O
vN-ctd1-152	ZINC000096358934	-12.3	0.362	448.53	ZINC	O=C(NCc1ccc2c(c1)CCN2C(=O)c1ccccc1)c1n[nH]c2c1CCc1ccccc1-2
vN-ctd1-153	ZINC000097945322	-12.3	0.308	522.56	ZINC	O=C(Oc1ccc2ccenc21)c1cccc(N2C(=O)[C@@H]3[C@@H](C2=O)C2c4ccccc4C3c3ccccc32)c1
vN-ctd1-154	ZINC000100688930	-12.3	0.324	497.55	ZINC	O=C(c1ccc(-c2ccccc2)cc1)[C@@H]1[C@H]2C(=O)N(c3ccccc3)C(=O)[C@@H]2[C@H]2c3ccccc3C=NN12
vN-ctd1-155	ZINC000103568480	-12.3	0.362	450.58	ZINC	O=C(NC[C@@H]1CCC[C@@H]1c1ccccc1)[C@@H]1c2ccccc2C(=O)N2CCc3ccccc3[C@@H]12
vN-ctd1-156	ZINC000104480060	-12.3	0.342	490.95	ZINC	O=C(NC1=CC=C[C@@H]2C(=O)c3ccccc3C(=O)[C@@H]12)c1cc(-c2ccccc2Cl)nc2ccccc21
vN-ctd1-157	ZINC000245238194	-12.3	0.332	487.56	ZINC	C[C@@H]1N[C@@]2(c3ccccc3N(Cc3ccccc3)C2=O)[C@H]2C(=O)N(c3ccc4ccccc43)C(=O)[C@@H]12
vN-ctd1-158	ZINC000247797224	-12.3	0.324	497.55	ZINC	O=C(c1ccc(-c2ccccc2)cc1)[C@@H]1[C@@H]2C(=O)N(c3ccccc3)C(=O)[C@H]2[C@H]2c3ccccc3C=NN12
vN-ctd1-159	ZINC000408733650	-12.3	0.332	485.54	ZINC	Cc1ccc2c(c1)OC(=O)[C@@H]1C2=C[C@H](c2ccccc2)[C@H]2C(=O)N(c3ccc4ccccc4c3)C(=O)[C@@H]21
vN-ctd1-160	ZINC000408754547	-12.3	0.332	479.58	ZINC	O=C1[C@@H]2[C@H]3C=C[C@@H](C3=C(c3ccccc3)c3ccccc3)[C@H]2C(=O)N1c1ccc(-c2ccccc2)cc1
vN-ctd1-161	ZINC000408978119	-12.3	0.324	495.49	ZINC	O=C(Oc1ccc2nc3c4ccccc4c4ccccc4c3nc2c1)c1ccc(N2C(=O)C=CC2=O)cc1
vN-ctd1-162	ZINC000409367719	-12.3	0.342	472.50	ZINC	O=C1[C@H]2[C@H](C(=O)N1c1ccc(-c3ccccc3)cc1)C1([N+](=O)[O-])c3ccccc3C2c2ccccc21
vN-ctd1-163	PV-001841361759	-12.2	0.381	424.50	REAL	Cc1cccc(-c2cccc(C(=O)NNC(=O)c3cc(-c4cc(C)ccc4C)n[nH]3)c2)c1
vN-ctd1-164	Z1069481792	-12.2	0.339	485.58	REAL	C[C@H]1Oc2ccc(C(=O)C3CCN(C(=O)e4ccc5[nH]c6c(c5c4)CCCCC6)CC3)cc2NC1=O
vN-ctd1-165	Z1138432459	-12.2	0.370	462.53	REAL	O=C(NS(=O)(=O)N1CCc2ccccc2C1)c1ccc2c(c1)C[C@@H](c1ccccc1)OC2=O
vN-ctd1-166	Z1143873046	-12.2	0.370	436.51	REAL	Cc1ccc2c(c1)[C@H](NC(=O)NNC(=O)c1cc(-c3ccccc3)nc3ccccc13)CC2
vN-ctd1-167	Z1147999214	-12.2	0.370	442.49	REAL	Cc1ccc(C)c(N2C(=O)c3ccc(C(=O)N4CC[C@H](c5ccccc5F)C4)cc3C2=O)c1
vN-ctd1-168	Z1239389230	-12.2	0.381	426.47	REAL	CN1C(=O)CCN(C(=O)c2ccc3c(c2)C[C@@H](c2ccccc2)OC3=O)c2ccccc21
vN-ctd1-169	Z1620445351	-12.2	0.381	447.93	REAL	Cc1cc2ccc(Cl)cc2nc1NNC(=O)c1ccc2c(=O)n3c(nc2c1)CCCCC3
vN-ctd1-170	Z1664060976	-12.2	0.370	437.46	REAL	Cn1nc(-c2nnc([C@H]3CC(=O)N(c4ccccc5ccccc45)C3)o2)c2ccccc2c1=O
vN-ctd1-171	Z1698172573	-12.2	0.381	443.48	REAL	O=C1c2ccccc2S(=O)(=O)c2cc(C(=O)N3C[C@@H]4CCC(=O)c5cccc3c54)ccc21
vN-ctd1-172	Z1708479469	-12.2	0.370	449.50	REAL	O=C(c1ccc2c(=O)n3c(nc2c1)CCCCC3)N1CCC(=Cc2ccc(F)c(F)c2)CC1
vN-ctd1-173	Z1846550710	-12.2	0.381	421.42	REAL	O=C(Nc1nnc(-c2cc3ccccc3o2)[nH]1)c1ccc2[nH]c3ccccc3c(=O)c2c1
vN-ctd1-174	Z2065978494	-12.2	0.359	448.48	REAL	Cn1c(C(=O)NNC(=O)c2cc(-c3ccccc3)nc3ccccc23)cc2ccccc2c1=O
vN-ctd1-175	Z2087363551	-12.2	0.370	438.49	REAL	O=C1N[C@H](C[C@@H]2CCCc3ccccc32)C(=O)N1c1cc(-c2ccc3nccc3c2)on1
vN-ctd1-176	Z2164604253	-12.2	0.370	435.53	REAL	Cc1cc(=O)[nH]c2cc(C(=O)N3CCN(C4c5ccccc5-c5ccccc54)CC3)ccc12
vN-ctd1-177	Z2215633083	-12.2	0.359	449.56	REAL	O=C(CN1CCc2c(nnn2-c2ccccc2)C1)N1Cc2ccccc2[C@@H](c2ccccc2)C1
vN-ctd1-178	Z2223517426	-12.2	0.370	439.56	REAL	O=C([C@H]1CCc2nnc(C3CC3)n2C1)N1CCN(C2c3ccccc3-c3ccccc32)CC1
vN-ctd1-179	Z229950998	-12.2	0.359	454.57	REAL	O=C(c1ccccc1)C1CCN(C(=O)[C@@H]2CCCN(C(=O)c3ccce4ccccc34)C2)CC1
vN-ctd1-180	Z25741554	-12.2	0.349	465.46	REAL	O=C(CN1C(=O)N[C@@]2(CCc3ccccc32)C1=O)Nc1ccc2c(c1)C(=O)c1ccccc1C2=O
vN-ctd1-181	Z26445406	-12.2	0.359	445.53	REAL	O=C(c1cc(-c2ccccc3ccccc23)nc2ccccc12)N1CCN(c2nccn2)CC1
vN-ctd1-182	Z275522396	-12.2	0.330	493.56	REAL	O=C(OCC(=O)N1c2ccccc2CCc2ccccc21)c1ccc2c(=O)n3c(nc2c1)CCCCC3
vN-ctd1-183	Z2902673259	-12.2	0.330	490.53	REAL	O=C(c1ccc2[nH]ncc2c1)N1CCC[C@@H](c2nc(-c3ccc(-n4cnc5ccccc54)nc3)no2)C1
vN-ctd1-184	Z297252242	-12.2	0.330	487.52	REAL	O=C(CNC(=O)c1cc(-c2cccc3ccccc23)nc2ccccc12)Nc1ccc2[nH]c(=O)[nH]c2c1
vN-ctd1-185	Z320095592	-12.2	0.349	463.54	REAL	O=C(c1ccc2ccccc12)N1CCN([C@H]2CC(=O)N(c3ccc4ccccc4c3)C2=O)CC1
vN-ctd1-186	Z397589742	-12.2	0.349	483.55	REAL	O=C1c2ccccc2S(=O)(=O)c2cc(C(=O)N3CCN(c4ccc5ccccc5n4)CC3)ccc21
vN-ctd1-187	Z412577390	-12.2	0.339	499.64	REAL	O=C(Nc1ccc2c3c(cccc13)CC2)N1CCN(Cc2nc3sc4c(c3c(=O)[nH]2)CCCC4)CC1
vN-ctd1-188	Z63721304	-12.2	0.359	454.44	REAL	O=C(NNC(=O)c1n[nH]c(=O)c2ccccc12)c1ccc2c(c1)C[C@@H](c1ccccc1)OC2=O
vN-ctd1-189	Z67740146	-12.2	0.339	478.59	REAL	O=C(CN1CCN(C(=O)c2cc(-c3cccc4ccccc34)nc3ccccc23)CC1)N1CCCC1
vN-ctd1-190	Z746230784	-12.2	0.381	431.47	REAL	O=C(c1ccc2ccccc12)N1CCN(C(=O)[C@H]2CC(c3cccc(F)c3)=NO2)CC1
vN-ctd1-191	Z746544906	-12.2	0.339	477.52	REAL	O=C(c1ccc2c(=O)n(-c3ccccc3)c(=O)[nH]c2e1)N1CCN(c2ccc3ccccc3n2)CC1
vN-ctd1-192	Z758344776	-12.2	0.370	443.55	REAL	Cc1ccc(C(=O)C2CCN(C(=O)c3ccc4c(=O)n5c(nc4c3)CCCCC5)CC2)cc1
vN-ctd1-193	Z758347616	-12.2	0.349	467.52	REAL	Cc1ccc(C(=O)C2CCN(C(=O)c3ccc4c(=O)n(-c5ccccc5)c(=O)[nH]c4c3)CC2)cc1
vN-ctd1-194	Z785316544	-12.2	0.349	464.53	REAL	O=C(c1cccc2ccccc12)N1CCN(Cc2nc3c(cnn3-c3ccccc3)c(=O)[nH]2)CC1
vN-ctd1-195	Z787515358	-12.2	0.349	467.53	REAL	O=C(c1ccc2[nH]cnc2c1)N1CCN(C(=O)[C@H]2CC(=O)N(c3cccc4ccccc34)C2)CC1
vN-ctd1-196	Z804800684	-12.2	0.359	455.49	REAL	O=C1CCc2ec(F)c(NC(=O)[C@@H]3CC(=O)N(c4ccc5c(c4)Cc4ccccc4-5)C3)cc2N1
vN-ctd1-197	Z814174956	-12.2	0.370	436.51	REAL	Cc1ccc2c(c1)CC[C@H]2NC(=O)NNC(=O)c1cc(-c2ccccc2)nc2ccccc12
vN-ctd1-198	Z852298000	-12.2	0.349	464.57	REAL	Cc1nc2cc(C(=O)N3CCC(C(=O)N4CCc5ccccc54)CC3)ccc2n1-c1ccccc1
vN-ctd1-199	Z973898440	-12.2	0.339	477.53	REAL	Cc1n[nH]c(NC(=O)c2cccc(C(=O)Nc3[nH]nc(C)c3-c3ccccc3)n2)c1-c1ccccc1
vN-ctd1-200	Z995711582	-12.2	0.330	495.62	REAL	O=C(c1ccccc1)N1CCN(C(=O)[C@@H]2C[C@@H]3CCCC[C@@H]3N2C(=O)c2ccc3ccccc3c2)CC1

Supplementary Table 86. Virtual screening hits 101 to 200 of the screen against the dimerization interface of the CTD of the nucleoprotein (Screen ID: 44). Compounds were filtered so that hits had MW < 600 dalton, cLogP < 6, number of hydrogen bond acceptors < 11, and no reactive functional groups. A few compounds unsuitable for drug discovery were removed by visual inspection. The name of each compound consists of the initial letter 'v' for virtual hit, followed by the target protein name and the target site ('ctd' for CTD binding interface, 1 for docking scenario 1). The score is the docking score given by QuickVina 2 in kcal/mol. The ligand efficiency (LE) is computed as LE = -score/#NonH, where #NonH is the number of heavy (i.e. non hydrogen) atoms.

Name	Catalog ID	Score	LE	MW	Library	SMILES
vN-ctd2-1	ZINC000012436788	-10.8	0.327	431.446	ZINC	O=C(Nc1cccc2c1C(=O)[C@@H]1C=CC=C[C@H]1C2=O)c1cccc2c1C(=O)c1ccccc1-2
vN-ctd2-2	Z1081850494	-10.7	0.324	495.97	REAL	O=C(Nc1nnc(-c2cccc(Cl)c2)s1)c1ccc(NC2=NS(=O)(=O)c3ccccc32)cc1
vN-ctd2-3	Z2902585038	-10.7	0.315	471.5	REAL	Cc1cc(C)n2ncc(-c3noc(-c4ccc(NC5=NS(=O)(=O)c6ccccc65)cc4)n3)c2n1
vN-ctd2-4	ZINC000036610867	-10.7	0.315	446.421	ZINC	O=C1Nc2ccccc2/C1=C1\C(=O)Nc2cc3c(cc21)NC(=O)/C3=C1/C(=O)Nc2ccccc21
vN-ctd2-5	ZINC000408827077	-10.7	0.334	421.451	ZINC	O=C(O)c1ccc([C@@H]2Nc3ccc4c(c3[C@@H]3C=CC[C@@H]32)C(=O)c2ccccc2C4=O)cc1
vN-ctd2-6	Z1766649313	-10.6	0.331	430.413	REAL	Cc1cc2ccccc2nc1NNC(=O)c1cc(F)cc2c(=O)c3cc(F)ccc3[nH]c12
vN-ctd2-7	Z1846549780	-10.6	0.366	387.398	REAL	CC1(C)C(=O)Nc2ccc(C(=O)Nc3nnc(-c4cc5ccccc5o4)[nH]3)cc21
vN-ctd2-8	Z63721304	-10.6	0.312	454.441	REAL	O=C(NNC(=O)c1n[nH]c(=O)c2ccccc12)c1ccc2c(c1)C[C@H](c1ccccc1)OC2=O
vN-ctd2-9	ZINC000001225262	-10.6	0.272	553.36	ZINC	O=C1c2ccc(Cl)c2C(=O)N1c1ccc(-c2nc3ccc(N4C(=O)c5ccccc5)C(=O)c5C4=O)cc3[nH]2)cc1
vN-ctd2-10	ZINC000017094385	-10.6	0.331	425.422	ZINC	O=c1[nH]c2ccccc2c2c1[C@@H](c1ccc(F)cc1)N/C(=N\c1nc3ccccc3o1)N2
vN-ctd2-11	ZINC000100737710	-10.6	0.321	431.446	ZINC	O=C(Nc1cccc2c1C(=O)[C@H]1C=CC=C[C@H]1C2=O)c1cccc2c1C(=O)c1ccccc1-2
vN-ctd2-12	ZINC000245380417	-10.6	0.303	470.567	ZINC	Cc1ccc(N2C(=O)C[C@@H]([C@H]3C=C(C)[C@@H]4C(=O)N(c5ccc(C)c(C)c5)C(=O)[C@H]4C3)C2=O)cc1C
vN-ctd2-13	Z1449291474	-10.5	0.375	385.369	REAL	C[C@]1(c2ccc(C(=O)N3CCc4ccc(F)c(F)c4C3)cc2)NC(=O)NC1=O
vN-ctd2-14	ZINC000002935991	-10.5	0.292	480.425	ZINC	O=c1oc(-c2cccc(F)c2)nc2ccc(-c3ccc4nc(-c5cccc(F)c5)oc(=O)c4c3)cc21
vN-ctd2-15	ZINC000003878239	-10.5	0.292	499.542	ZINC	CC1(C)Cc2oc3ccc(NS(=O)(=O)c4ccc5c4C(=O)c4ccccc4C5=O)cc3c2C(=O)C1
vN-ctd2-16	ZINC000021867397	-10.5	0.284	496.545	ZINC	Cc1cccc(N2CCN(C(=O)c3ccc4c(O)nc5c(-c6ccccc6F)nnn5c4c3)CC2)c1C
vN-ctd2-17	ZINC000100737708	-10.5	0.318	431.446	ZINC	O=C(Nc1cccc2c1C(=O)[C@@H]1C=CC=C[C@@H]1C2=O)c1cccc2c1C(=O)c1ccccc1-2
vN-ctd2-18	ZINC000239302914	-10.5	0.309	452.552	ZINC	O=C(Nc1ccc2c(c1)OCCO2)c1ccc2c(c1)[C@H]1[C@@H]([C@H]3CC[C@H]1C3)[C@H](c1ccccc1)N2
vN-ctd2-19	Z1618330958	-10.4	0.347	408.388	REAL	Cc1cc(F)c2nc(O)cc(C(=O)Nc3cccc([C@@]4(C)NC(=O)NC4=O)c3)c2c1
vN-ctd2-20	Z1664715974	-10.4	0.325	444.514	REAL	O=S1(=O)N=C(Nc2ccc(-c3nnc(CCCc4ccccc4)o3)cc2)c2ccccc21
vN-ctd2-21	Z1673511399	-10.4	0.315	440.502	REAL	C[C@@]1(c2cccc(CNC(=O)N3CC=C(c4cccc5ccccc45)C3)c2)NC(=O)NC1=O
vN-ctd2-22	Z1764003566	-10.4	0.315	447.415	REAL	O=C(c1cc(F)cc2c(=O)c3cc(F)ccc3[nH]c12)N1CCc2[nH]c3ccc(F)cc3c2C1
vN-ctd2-23	Z811745926	-10.4	0.315	495.97	REAL	O=C(Nc1nnc(-c2ccccc2Cl)s1)c1ccc(NC2=NS(=O)(=O)c3ccccc32)cc1
vN-ctd2-24	Z951982548	-10.4	0.315	441.533	REAL	Cc1ccc2[nH]c([C@H]3CCCN3C(=O)c3ccc4c(=O)n5c(nc4c3)CCCCC5)nc2c1
vN-ctd2-25	ZINC000001516031	-10.4	0.248	583.549	ZINC	O=C(Nc1ccc2c3c1cccc3C(=O)N(c1ccccc1)C2=O)c1cc2nc(-c3ccs3)cc(C(F)(F)F)n2n1
vN-ctd2-26	ZINC000002201660	-10.4	0.325	460.319	ZINC	O=C1c2ccccc2C2=C1[C@@H](c1ccc(Cl)cc1Cl)c1c(O)n(-c3ccccc3)nc1N2
vN-ctd2-27	ZINC000005607051	-10.4	0.289	470.439	ZINC	Nc1c(-c2nc3cc4c(cc3o2)C(=O)c2ccccc2C4=O)ccc2c1C(=O)c1ccccc1C2=O
vN-ctd2-28	ZINC000009332188	-10.4	0.297	460.488	ZINC	O=C(c1ccco1)[C@@H]1[C@@H]2C(=O)N(c3cccc4ccccc43)C(=O)[C@H]2[C@@H]2c3ccccc3C=CN21
vN-ctd2-29	ZINC000009781971	-10.4	0.281	484.47	ZINC	O=C1c2ccccc2C(=O)N1c1ccc(-c2nc3ccc(N4C(=O)c5ccccc5C4=O)cc3[nH]2)cc1
vN-ctd2-30	ZINC000018117591	-10.4	0.315	431.446	ZINC	O=C(Nc1cccc2c1C(=O)[C@H]1C=CC=C[C@@H]1C2=O)c1cccc2c1C(=O)c1ccccc1-2
vN-ctd2-31	ZINC000059436990	-10.4	0.347	395.432	ZINC	O=C1c2ccccc2C(=O)c2c1ccc1c2[C@@H]2C=CC[C@@H]2[C@H](c2cccc2F)N1
vN-ctd2-32	ZINC000100504092	-10.4	0.335	404.512	ZINC	O=c1cccc2n1C[C@H]1C[C@H]2CN(Cc2ccc3ccc4cccc5ccc2c3c45)C1
vN-ctd2-33	ZINC000102553907	-10.4	0.289	480.562	ZINC	CC1=CC[C@@H]2C(=O)N(c3ccc(-c4ccc(N5C(=O)[C@@H]6CC=C(C)C[C@@H]6C5=O)cc4)cc3)C(=O)[C@@H]2C1
vN-ctd2-34	ZINC000104529567	-10.4	0.297	468.551	ZINC	Cc1ccc(N2C(=O)C3=C(C2=O)C(C)=C[C@@H]([C@@H]2CC(=O)N(c4ccc(C)c(C)c4)C2=O)C3)cc1C
vN-ctd2-35	ZINC000408826920	-10.4	0.347	391.469	ZINC	Cc1ccc([C@@H]2Nc3ccc4c(c3[C@@H]3C=CC[C@@H]32)C(=O)c2ccccc2C4=O)cc1
vN-ctd2-36	ZINC000408831744	-10.4	0.347	411.887	ZINC	O=C1c2ccccc2C(=O)c2c1ccc1c2[C@@H]2C=CC[C@@H]2[C@H](c2ccc(Cl)cc2)N1
vN-ctd2-37	ZINC000409336379	-10.4	0.297	451.488	ZINC	O=C(Nc1cccc2ccccc21)c1ccc2nc3c4ncccc4c4ccnc4c3nc2c1
vN-ctd2-38	PV-001874906597	-10.3	0.332	454.424	REAL	O=C(c1cc2c(C(F)(F)F)cc(=O)[nH]c2o1)N1CCCS(=O)(=O)C[C@@H]1c1ccccc1
vN-ctd2-39	Z1024047020	-10.3	0.294	466.535	REAL	O=C1O[C@H](c2ccccc2)Cc2cc(C(=O)N3CCC([C@H]4C(=O)Nc5ccccc54)CC3)ccc21
vN-ctd2-40	Z1192946650	-10.3	0.312	437.502	REAL	Cc1ccc(-n2c(NNC(=O)Cc3c[nH]c4ccccc34)nc3ccccc3c2=O)c(C)c1
vN-ctd2-41	Z1472736345	-10.3	0.312	446.505	REAL	CC(=O)N1CCc2ccccc2[C@@H]1CC(=O)Nc1[nH]nc(C)c1-c1ccc2c(c1)OCCO2
vN-ctd2-42	Z1472862510	-10.3	0.343	399.493	REAL	O=C(N[C@@H]1[C@H]2CCc3ccccc3[C@H]21)c1ccc2c(=O)n3c(nc2c1)CCCCC3
vN-ctd2-43	Z1505419243	-10.3	0.322	430.51	REAL	Cc1ccc2[nH]c([C@H]3CCCN(C(=O)C4=NN(c5ccccc5)C(=O)[C@@H](C)N4)C3)nc2c1
vN-ctd2-44	Z165047412	-10.3	0.278	487.47	REAL	O=C1NC(=O)c2ccccc2/C1=C\NN1C(=O)c2ccc3c(C(=O)c4ccccc4)ccc(c23)C1=O
vN-ctd2-45	Z1684428213	-10.3	0.303	445.441	REAL	O=c1nc2c(-c3nc(-c4ccc(-n5cnc6ccccc65)cc4)no3)c[nH]n2c2ccccc12
vN-ctd2-46	Z1704441279	-10.3	0.322	447.514	REAL	C[C@H]1CCN(C(=O)c2ccc(NC3=NS(=O)(=O)c4ccccc43)cc2)c2c(O)cccc21
vN-ctd2-47	Z1731217817	-10.3	0.355	391.43	REAL	O=C(NNc1ccc2ccccc2n1)Nc1cccc(C(=O)N2CCOCC2)c1
vN-ctd2-48	Z1764004735	-10.3	0.312	443.452	REAL	Cc1ccc2[nH]c3c(c2c1)CN(C(=O)c1cc(F)cc2c(=O)c4cc(F)ccc4[nH]c12)CC3
vN-ctd2-49	Z1891953576	-10.3	0.343	399.449	REAL	CC(=O)N1CCCc2cc(N3C(=O)N[C@@H](c4cccc5ccccc45)C3=O)ccc21
vN-ctd2-50	Z243910572	-10.3	0.294	485.567	REAL	O=C(Nc1ccc2c(c1)nc1n2CCCCC1)c1ccc(NC2=NS(=O)(=O)c3ccccc32)cc1
vN-ctd2-51	Z283971412	-10.3	0.303	451.485	REAL	Cc1cccc(-c2nnc(-c3ccc(C(=O)N(C)Cc4nc5ccccc5c(=O)[nH]4)cc3)o2)c1
vN-ctd2-52	Z298639830	-10.3	0.303	469.52	REAL	O=C1c2ccccc2S(=O)(=O)c2cc(C(=O)N3CC=C(c4c[nH]c5ncccc45)CC3)ccc21
vN-ctd2-53	Z424331542	-10.3	0.343	408.457	REAL	Cc1c(C(=O)Nc2cccc([C@]3(C)NC(=O)NC3=O)c2)[nH]c2c1C(=O)CC(C)(C)C2
vN-ctd2-54	Z839960534	-10.3	0.294	481.429	REAL	O=C1c2ccccc2N[C@@]2(C(=O)Nc3cc4c(cc32)OCCCO4)N1c1cccc(C(F)(F)F)c1
vN-ctd2-55	Z966268928	-10.3	0.286	478.55	REAL	O=C(Nc1cccc(C(=O)N2CCc3ccccc32)c1)c1ccc2c(=O)n3c(nc2c1)CCCC3
vN-ctd2-56	ZINC000003671066	-10.3	0.294	459.5	ZINC	O=C(O)[C@@H]1C2c3ccccc3C(c3ccccc32)[C@@H]1C(=O)Nc1ccc2c(c1)oc1ccccc12
vN-ctd2-57	ZINC000008694925	-10.3	0.294	452.472	ZINC	O=C1c2ccccc2C(=O)c2c3[nH]nc(-c4nc5ccccc5nc4-c4ccccc4)c3ccc21
vN-ctd2-58	ZINC000100968105	-10.3	0.286	491.532	ZINC	C[C@@H]1CCc2cc(F)cc3c(O)c(CCC4=C(O)c5cc(F)cc6c5[C@H](C4=O)[C@@H](C)CC6)c(=O)n1c23
vN-ctd2-59	PV-001818621537	-10.2	0.329	454.316	REAL	Cc1cc(=O)[nH]c2cc(C(=O)N3C[C@H]4[C@H](C3)C(F)(F)C(F)(F)C(F)(F)C4(F)F)ccc12
vN-ctd2-60	PV-001818621863	-10.2	0.329	455.304	REAL	Cc1nc2cc(C(=O)N3C[C@H]4[C@H](C3)C(F)(F)C(F)(F)C(F)(F)C4(F)F)ccc2c(=O)[nH]1
vN-ctd2-61	PV-001869783920	-10.2	0.319	455.534	REAL	Cc1ccc(S(=O)(=O)C2CCN(C(=O)c3cccc([C@@]4(C)NC(=O)NC4=O)c3)CC2)cc1
vN-ctd2-62	PV-001940740368	-10.2	0.319	456.609	REAL	C[C@H](CNC(=O)Nc1ccc(S(=O)(=O)N[C@H](C)[C@@H]2C[C@H]3CC[C@H]2C3)cc1)c1ccncc1
vN-ctd2-63	PV-001945831122	-10.2	0.392	356.371	REAL	Cc1oc2ccc(NC(=O)N3CCc4cc(F)c(F)cc4C3)cc2c1C
vN-ctd2-64	Z1160637727	-10.2	0.291	491.571	REAL	Cc1cc(N2CCC[C@@H](OC(=O)c3ccc(NC4=NS(=O)(=O)c5ccccc54)cc3)C2)nc(C)n1
vN-ctd2-65	Z1260000954	-10.2	0.309	436.466	REAL	O=C(NNC(=O)c1cccc2ccccc12)c1ccc2c(c1)C[C@H](c1ccccc1)OC2=O
vN-ctd2-66	Z1312754180	-10.2	0.309	445.482	REAL	Cc1cc(C(=O)Nc2ccc(-c3nnc4n3CCCCCC4)cc2)nc2nc(O)[nH]c(=O)c12
vN-ctd2-67	Z1360025790	-10.2	0.34	403.489	REAL	O=C(C1CCN(c2ccc3nnnn3n2)CC1)N1CC2(CCCC2)c2ccccc21
vN-ctd2-68	Z139983810	-10.2	0.3	471.536	REAL	O=C(Nn1cnc2sc3c(c2c1=O)CCCC3)c1ccc2c(c1)C[C@@H](c1ccccc1)OC2=O
vN-ctd2-69	Z1684583135	-10.2	0.319	438.486	REAL	C[C@@]1(c2cccc(-c3noc([C@@H]4CCCN(C(=O)N5CCCC5)C4)n3)c2)NC(=O)NC1=O
vN-ctd2-70	Z1697480705	-10.2	0.392	348.376	REAL	Cc1cc(F)cc2[nH]c(C(=O)N3C[C@@H]4CCC(=O)c5cccc3c54)cc12
vN-ctd2-71	Z1698172573	-10.2	0.319	443.478	REAL	O=C1c2ccccc2S(=O)(=O)c2cc(C(=O)N3C[C@@H]4CCC(=O)c5cccc3c54)ccc21
vN-ctd2-72	Z1698181628	-10.2	0.34	398.421	REAL	Cn1c(C(=O)N2C[C@@H]3CCC(=O)c4cccc2c43)cc2c(=O)n3ccccc3nc21
vN-ctd2-73	Z1764266200	-10.2	0.319	426.431	REAL	C[C@@]1(c2cccc(NC(=O)c3ccc4[nH]c5ccccc5c(=O)c4c3)c2)NC(=O)NC1=O
vN-ctd2-74	Z1863983108	-10.2	0.352	390.398	REAL	Cn1cc(C(=O)Nc2cccc([C@@]3(C)NC(=O)NC3=O)c2)c2ccccc2c1=O
vN-ctd2-75	Z1891089698	-10.2	0.319	442.458	REAL	O=S1(=O)N=C(Nc2ccc(-c3nc(-c4ccc5cc[nH]c5n4)no3)cc2)c2ccccc21
vN-ctd2-76	Z1891122660	-10.2	0.319	442.458	REAL	O=S1(=O)N=C(Nc2ccc(-c3nc(-c4cccn5ccnc45)no3)cc2)c2ccccc21
vN-ctd2-77	Z1907872362	-10.2	0.309	442.478	REAL	Cn1c(=O)[nH]c2ncc(-c3cccc(C(=O)Nc4ccc5c(c4)N(C(N)=O)CCC5)c3)cc21
vN-ctd2-78	Z2066084353	-10.2	0.309	435.442	REAL	O=C(NNC(=O)c1n[nH]c(=O)c2ccccc12)c1ccc(-c2cccc3ccccn23)cc1
vN-ctd2-79	Z2141478755	-10.2	0.319	434.47	REAL	C[C@]1(c2cccc(C(=O)N3CCC(c4c[nH]c5ccc(F)cc45)CC3)c2)NC(=O)NC1=O
vN-ctd2-80	Z2154604015	-10.2	0.352	386.493	REAL	Cc1cc(=O)[nH]c2cc(C(=O)N3CCC[C@]4(CCCc5ccccc54)C3)ccc12
vN-ctd2-81	Z2155692118	-10.2	0.319	427.463	REAL	C[C@@]1(c2ccc(-c3noc(-c4cccc5c6c([nH]c45)CCCC6)n3)cc2)NC(=O)NC1=O
vN-ctd2-82	Z2188335143	-10.2	0.364	374.439	REAL	Cc1cc(C)c2ncc(C(=O)N3Cc4ccc(O)cc4C4(CC4)C3)c(O)c2c1
vN-ctd2-83	Z2285099282	-10.2	0.364	378.431	REAL	Cc1cccc2c1CC(C)(C)N(C(=O)c1cnc3c(c1)c(=O)[nH]c(=O)n3C)C2
vN-ctd2-84	Z52370516	-10.2	0.291	479.515	REAL	O=C(Nc1cccc(-c2nc3ccccc3[nH]2)c1)c1ccc2c(c1)S(=O)(=O)c1ccccc1C2=O
vN-ctd2-85	Z728738796	-10.2	0.309	462.572	REAL	C[C@H]1CCc2[nH]c3ccc(C(=O)N4CCN(C5=NS(=O)(=O)c6ccccc65)CC4)cc3c2C1
vN-ctd2-86	Z79674176	-10.2	0.309	440.541	REAL	Cc1cccc(N2CCN(C(=O)c3ccc4c(c3)C[C@@H](c3ccccc3)OC4=O)CC2)c1C
vN-ctd2-87	Z851522220	-10.2	0.283	488.63	REAL	Cc1cc(C(=O)N2CCC(C)CC2)ccc1NC(=O)N1CCC(C(=O)N2CCc3ccccc32)CC1
vN-ctd2-88	Z977298470	-10.2	0.3	455.556	REAL	Cc1c(C(=O)Nc2ccc(CC(=O)N3CCc4ccccc43)cc2)[nH]c2c1C(=O)CC(C)(C)C2
vN-ctd2-89	ZINC000004107418	-10.2	0.276	478.558	ZINC	C(=c1/c(-c2ccccc2)nn2c3ccccc3nc12)\[C@@H]1C(c2ccccc2)=NN2c3ccccc3N[C@@H]12
vN-ctd2-90	ZINC000004175980	-10.2	0.329	398.464	ZINC	O=C1[C@@H]2[C@H](c3nc4ccnc5ccccc5nc4)n31)C1c3ccccc3C2c2ccccc21
vN-ctd2-91	ZINC000004522763	-10.2	0.283	472.455	ZINC	Nc1c(C(=O)Nc2ccccc3c2C(=O)c2ccccc2C3=O)ccc2c1C(=O)c1ccccc1C2=O
vN-ctd2-92	ZINC000004794272	-10.2	0.283	529.538	ZINC	Cc1[nH]c(=O)[nH]c(=O)c1S(=O)(=O)N1CCC[C@@H](C(=O)N2CCN(c3cccc(C(F)(F)F)c3)CC2)C1
vN-ctd2-93	ZINC000008612447	-10.2	0.319	423.423	ZINC	Cc1ccc2c(=O)cc(C(=O)Nc3c4ccccc4oc3C(=O)c3ccccc3)oc2c1
vN-ctd2-94	ZINC000021867386	-10.2	0.283	486.481	ZINC	O=C(c1ccc2c(O)nc3c(-c4ccccc4F)nnn3c2c1)N1CCN(c2ccc(F)cc2)CC1
vN-ctd2-95	ZINC000022528214	-10.2	0.3	449.513	ZINC	CC(C)c1ccc([C@H]2N/C(=N\c3nc4ccccc4o3)Nc3c4ccccc4[nH]c(=O)c32)cc1
vN-ctd2-96	ZINC000035538889	-10.2	0.319	422.443	ZINC	CN1c2ccccc2[C@H](c2c(-c3ccc4ccccc4c3)[nH]c3[nH]c(=O)[nH]c(=O)c32)C1=O
vN-ctd2-97	ZINC000100485510	-10.2	0.319	410.431	ZINC	O=C1c2ccc3c4c(ccc(c24)C2=Nc4ccccc4[C@H]21)C1=Nc2ccccc2[C@H]1C3=O
vN-ctd2-98	ZINC000101094157	-10.2	0.34	400.473	ZINC	Cc1ec2c(cc1C)C(=O)[C@@H]1C[C@@H]3C(=O)c4cc(C)c(C)cc4C(=O)[C@H]3C[C@H]1C2=O
vN-ctd2-99	ZINC000103225698	-10.2	0.3	457.572	ZINC	Cc1cccc(N2CCN(C(=O)c3cccc(N4C(=O)[C@@H]5CC=C[C@@H](C)[C@H]5C4=O)c3)CC2)c1C
vN-ctd2-100	ZINC000239310051	-10.2	0.283	481.613	ZINC	O=C(c1ccc2c(c1)[C@H]1[C@@H]([C@H]3CC[C@H]1C3)[C@H](c1ccccc1)N2)N1CCN(c2ccccc2F)CC1

Supplementary Table 87. Top 100 virtual hits of the screen against the oligomerization interface of the CTD of the nucleoprotein (Screen ID: 45). Compounds were filtered so that hits had MW < 600 dalton, cLogP < 6, number of hydrogen bond acceptors < 11, and no reactive functional groups. A few compounds unsuitable for drug discovery were removed by visual inspection. The name of each compound consists of the initial letter 'v' for virtual hit, followed by the target protein name and the target site ('ctd' for CTD binding interface, 2 for docking scenario 2). The score is the docking score given by QuickVina 2 in kcal/mol. The ligand efficiency (LE) is computed as LE = -score/#NonH, where #NonH is the number of heavy (i.e. non hydrogen) atoms.

Name	Catalog ID	Score	LE	MW	Library	SMILES
vN-ctd2-101	PV-001809069814	-10.1	0.326	416.48	REAL	Cc1cccc(CNC(=O)c2ccc(C(=O)Nc3nc(O)c4c(n3)CCCC4)cc2)c1
vN-ctd2-102	PV-001811072406	-10.1	0.361	436.26	REAL	Cc1c(C(=O)Nc2ccnc(-c3cccc(Br)c3)n2)oc(=O)c2ccccc12
vN-ctd2-103	PV-001811757658	-10.1	0.316	445.48	REAL	O=C(c1cncc(-c2ccccc2)c1)N1CCCC[C@H]1[C@@H]1CCCN(C(=O)C(F)(F)F)C1
vN-ctd2-104	PV-001838861973	-10.1	0.374	363.35	REAL	Cc1c(C(=O)Nc2ccn(-c3nccc3F)n2)[nH]c(=O)c2ccccc12
vN-ctd2-105	PV-001858361756	-10.1	0.306	455.44	REAL	Cc1cc2c(NC(=O)[C@@H]3CCC(=O)N(C)[C@@H]3c3ccc(C(F)(F)F)cc3)n[nH]c2cc1C\#N
vN-ctd2-106	PV-001885289599	-10.1	0.348	458.29	REAL	CN1C(=O)C(C)(C)c2cc(C(=O)Nc3nc(-c4ccc(Br)cc4F)n[nH]3)ccc21
vN-ctd2-107	Z1021229948	-10.1	0.306	447.42	REAL	O=c1[nH]c(Cc2nc(-c3ccccc3)n[nH]2)nc2ccc(-c3cccc(C(F)(F)F)c3)cc12
vN-ctd2-108	Z1043030904	-10.1	0.273	495.59	REAL	Cc1ccc(NC(=O)[C@H]2CCc3ccccc3N2C(=O)C2CCN(c3ccc4nncn4n3)CC2)cc1
vN-ctd2-109	Z1075647338	-10.1	0.281	488.59	REAL	Cc1ccc(C(=O)N2CCC(NC(=O)N3CCN(Cc4nc5ccccc5c(=O)[nH]4)CC3)CC2)cc1
vN-ctd2-110	Z1134220569	-10.1	0.281	471.52	REAL	O=C1/C(=C/c2cnn3ccccc23)CC2(C/C1=C\c1cnn3ccccc13)C(=O)Nc1ccccc12
vN-ctd2-111	Z1161084575	-10.1	0.289	484.54	REAL	O=C(Nc1ccc(-c2nnc3n2CCCC3)cc1)c1ccc2c(c1)S(=O)(=O)c1ccccc1C2=O
vN-ctd2-112	Z1170162723	-10.1	0.297	446.43	REAL	O=c1nc2c(-c3nc(-c4ccc(-n5cnc6ccccc65)nc4)no3)c[nH]n2c2ccccc12
vN-ctd2-113	Z1174758868	-10.1	0.306	442.48	REAL	O=C(c1c2c(nc3ccccc13)/C(=C\c1ccco1)CCC2)N1CCO[C@H](c2nnn[nH]2)C1
vN-ctd2-114	Z1199002097	-10.1	0.306	436.51	REAL	O=C(Nc1ccc2c(c1)CCN2C(=O)c1cccnc1)c1ccc2[nH]c3c(c2c1)CCCC3
vN-ctd2-115	Z1240727240	-10.1	0.316	449.51	REAL	C[C@H]1c2c(F)cccc2CCN1C(=O)c1ccc(NC2=NS(=O)(=O)c3ccccc32)cc1
vN-ctd2-116	Z133656968	-10.1	0.306	467.54	REAL	CC(=O)N1CCCc2cc(S(=O)(=O)Oc3ccc4c5c(c(=O)oc4c3)CCCC5)ccc21
vN-ctd2-117	Z1383810362	-10.1	0.337	397.39	REAL	O=C1O[C@H](C(=O)Nc2ccc3c(c2)C(=O)c2ccccc2C3=O)Cc2ccccc21
vN-ctd2-118	Z1391596126	-10.1	0.316	429.48	REAL	Cc1ccc(-c2cc(C(=O)N3CCC[C@H](NC(=O)c4cc5ccccc5o4)C3)on2)cc1
vN-ctd2-119	Z1411806918	-10.1	0.316	427.44	REAL	Cc1cccc(-c2nnc(-c3ccc(C(=O)Nc4nc5c(F)cccc5n4C)cc3)o2)c1
vN-ctd2-120	Z1451348456	-10.1	0.316	429.52	REAL	CC1(C)C(=O)Nc2ccc(C(=O)Nc3ccc(-c4nnc5n4CCCCCC5)cc3)cc21
vN-ctd2-121	Z1452677455	-10.1	0.316	429.45	REAL	C[C@]1(c2cccc(C(=O)N3CCc4cc(-c5ccc(F)c5)ccc43)c2)NC(=O)NC1=O
vN-ctd2-122	Z1481412627	-10.1	0.306	444.42	REAL	C[C@]1(c2cccc(NC(=O)c3ccc4noc(-c5ccc(F)cc5)c4c3)c2)NC(=O)NC1=O
vN-ctd2-123	Z1521939402	-10.1	0.306	449.46	REAL	C[C@@H]1Oc2ccc(C(=O)C3CCN(C(=O)c4cccc5c4oc(=O)n5C)CC3)cc2NC1=O
vN-ctd2-124	Z1627364166	-10.1	0.348	390.40	REAL	Cn1cnc(-c2ccc(C(=O)Nc3cccc([C@@]4(C)NC(=O)NC4=O)c3)cc2)n1
vN-ctd2-125	Z1683364048	-10.1	0.316	441.47	REAL	O=S1(=O)N=C(Nc2ccc(-c3nc(-c4ccc5[nH]ccc5c4)no3)cc2)c2ccccc21
vN-ctd2-126	Z1684856266	-10.1	0.316	442.50	REAL	O=S1(=O)N=C(Nc2ccc(-c3nc([C@@H]4CCc5ccccc54)no3)cc2)c2ccccc21
vN-ctd2-127	Z1685320529	-10.1	0.316	427.47	REAL	Cc1nnc(-c2cccc(-c3noc(C4CCN(c5nc6ccccc6o5)CC4)n3)c2)[nH]1
vN-ctd2-128	Z1685321062	-10.1	0.297	449.47	REAL	Cc1nnc(-c2cccc(-c3noc(-c4ccc5c(c4)C[C@@H](c4ccccc4)OC5=O)n3)c2)[nH]1
vN-ctd2-129	Z1723434789	-10.1	0.337	398.47	REAL	Cc1ccc2c(c1)CC[C@@H]2NC(=O)c1cccc(-c2cnc3[nH]c(=O)n(C)c3c2)c1
vN-ctd2-130	Z1752608634	-10.1	0.306	446.49	REAL	O=C(N[C@H]1CCc2nnc(-c3ccc(F)cc3)n2C1)N1CC[C@@]2(C1)C(=O)Nc1ccccc12
vN-ctd2-131	Z1765110758	-10.1	0.306	437.50	REAL	O=C1Nc2ccccc2[C@H]1C1CCN(C(=O)c2ccc3[nH]c4ccccc4c(=O)c3c2)CC1
vN-ctd2-132	Z1890914883	-10.1	0.374	355.36	REAL	Cc1cc(-c2noc(-c3n[nH]c(=O)c4ccccc34)n2)nc2ccccc12
vN-ctd2-133	Z1892015761	-10.1	0.361	392.43	REAL	O=C1N[C@H](c2cccc3ccccc23)C(=O)N1c1ccc2c(c1)S(=O)(=O)CC2
vN-ctd2-134	Z2004206136	-10.1	0.306	438.49	REAL	Cn1c(=O)[nH]c2ncc(-c3cccc(C(=O)N4CCC(C\#N)(c5ccccn5)CC4)c3)cc21
vN-ctd2-135	Z202253278	-10.1	0.326	430.53	REAL	O=C(Cc1nc(-c2ccccc2)cs1)NNC(=O)c1ccc2[nH]c3c(c2c1)CCCC3
vN-ctd2-136	Z2167006606	-10.1	0.306	447.47	REAL	Cn1c(-c2n[nH]c(=O)c3ccccc23)nnc1N1CCCN(C(=O)c2cccc(F)c2)CC1
vN-ctd2-137	Z2170271478	-10.1	0.348	387.44	REAL	O=C(Nc1ccc2nc3n(c(=O)c2c1)CCC3)c1ccc2c(c1)CCCCC2=O
vN-ctd2-138	Z2902834347	-10.1	0.306	453.48	REAL	O=S1(=O)N=C(Nc2ccc(-c3nc(-c4nccc5cccc45)no3)cc2)c2ccccc21
vN-ctd2-139	Z2902892909	-10.1	0.273	499.55	REAL	CN1CCC(=O)Nc2cc(-c3nc(-c4ccc(N5CCN(c6ccc(F)cc6)CC5)nc4)no3)ccc21
vN-ctd2-140	Z311871846	-10.1	0.306	436.52	REAL	Nc1nc(CN2CCN(C(=O)c3cc4c(ccc5ccccc54)[nH]3)CC2)nc2ccccc12
vN-ctd2-141	Z654776498	-10.1	0.316	429.52	REAL	C[C@H]1CCc2[nH]c3ccc(C(=O)Nc4ccc5[nH]c(N6CCOCC6)nc5c4)cc3c2C1
vN-ctd2-142	Z73939098	-10.1	0.297	452.47	REAL	Cn1c(=O)c2ccccc2n2c(CN3C(=O)N[C@@](C)(c4ccc5ccccc5c4)C3=O)nnc12
vN-ctd2-143	Z771078902	-10.1	0.326	431.52	REAL	C[C@H]1CCN(C(=O)c2ccc(NC3=NS(=O)(=O)c4ccccc43)cc2)c2ccccc21
vN-ctd2-144	Z810731188	-10.1	0.281	499.59	REAL	Cn1c([C@H]2CCCCN2C(=O)c2ccc(NC3=NS(=O)(=O)c4ccccc43)cc2)nc2ccccc21
vN-ctd2-145	Z846287900	-10.1	0.306	439.51	REAL	Cc1ccc([C@H]2CCCN2C(=O)c2ccc3c(c2)C(=O)N(Cc2ccncc2)C3=O)cc1C
vN-ctd2-146	Z952446382	-10.1	0.289	485.57	REAL	Cc1ccc2[nH]c([C@H]3CCCN3C(=O)c3ccc(NC4=NS(=O)(=O)c5ccccc54)cc3)nc2c1
vN-ctd2-147	ZINC000001714458	-10.1	0.289	462.46	ZINC	O=C1c2ccccc2C(=O)C(C(/C=C/c2ccccc2)C2=C(O)C(=O)c3ccccc3C2=O)=C1O
vN-ctd2-148	ZINC000002371636	-10.1	0.316	418.41	ZINC	O=C1c2ccc(-c3nc4ccccc4c(=O)o3)cc2C(=O)N1c1ccc2ccccc2c1
vN-ctd2-149	ZINC000002896234	-10.1	0.281	472.50	ZINC	Cc1ccccc1-c1nc2ccc(-c3ccc4nc(-c5ccccc5C)oc(=O)c4c3)cc2c(=O)o1
vN-ctd2-150	ZINC000003056675	-10.1	0.297	453.54	ZINC	Cc1ccccc1N1CCN(C(=O)c2ccc(/C=C3\Oc4ccccc4NC3=O)cc2)[C@H](C)C1
vN-ctd2-151	ZINC000004091241	-10.1	0.289	457.44	ZINC	O=C(Nc1eccc2c1C(=O)c1ccccc1C2=O)c1ccc2c1C(=O)c1ccccc1C2=O
vN-ctd2-152	ZINC000007613840	-10.1	0.374	359.38	ZINC	O=C(Nc1nnc(-c2ccc3c(c2)CCCC3)o1)c1cc2ccccc2o1
vN-ctd2-153	ZINC000008648258	-10.1	0.281	474.48	ZINC	O=C(O)c1ccc(-c2nc3ccc(-c4ccc5[nH]c(-c6ccc(C(=O)O)cc6)nc5c4)cc3[nH]2)cc1
vN-ctd2-154	ZINC000012752096	-10.1	0.306	438.45	ZINC	O=C(NNC(=O)c1cccc2cn[nH]c21)c1ccc(Cn2nnc(-c3ccccc3)n2)cc1
vN-ctd2-155	ZINC000015887215	-10.1	0.316	450.56	ZINC	C[C@H]1CCc2[nH]c3ccc(C(=O)Nc4cccc(S(=O)(=O)/N=C5/CCCN5)c4)cc3c2C1
vN-ctd2-156	ZINC000017093521	-10.1	0.316	423.44	ZINC	Cc1[nH]nc2c1[C@@H](c1cnn(C)c1)c1c3nc(-c4c[nH]c5ccccc45)nn3cnc1O2
vN-ctd2-157	ZINC000021655264	-10.1	0.273	491.55	ZINC	Cc1cccc(-c2noc(-c3cn(CC(=O)Nc4ccc5c(c4)CCC5)c4nc(C)ccc4c3=O)n2)c1
vN-ctd2-158	ZINC000021867174	-10.1	0.273	492.58	ZINC	Cc1cccc(-c2nnn3c2nc(O)c2ccc(C(=O)N4CCN(c5cc(C)ccc5C)CC4)cc23)c1
vN-ctd2-159	ZINC000021867378	-10.1	0.289	468.49	ZINC	O=C(c1ccc2c(O)nc3c(-c4ccccc4F)nnn3c2c1)N1CCN(c2ccccc2)CC1
vN-ctd2-160	ZINC000021867393	-10.1	0.273	496.55	ZINC	Cc1ccc(C)c(N2CCN(C(=O)c3ccc4c(O)nc5c(-c6ccccc6F)nnn5c4c3)CC2)c1
vN-ctd2-161	ZINC000077406513	-10.1	0.337	402.47	ZINC	Cc1c2cc(CNC(=O)c3n[nH]c4c3CCCC4)ccc2[nH]c1-c1ccc(F)cc1
vN-ctd2-162	ZINC000101025561	-10.1	0.281	479.49	ZINC	O=C1C[C@H](N(O)[C@H]2CC(=O)N(c3ccc4ccccc4c3)C2=O)C(=O)N1c1ccc2ccccc2c1
vN-ctd2-163	ZINC000102635692	-10.1	0.348	389.41	ZINC	Cc1nc2nc(N3C(=O)[C@H]4CC=CC[C@@H]4C3=O)nn2c(O)c1Cc1ccccc1
vN-ctd2-164	ZINC000257198806	-10.1	0.316	428.58	ZINC	O=C(c1n[nH]c2c1CCc1ccccc1-2)N1CCCC2=C[C@H]3C[C@H](CN4CCCC[C@H]34)[C@H]21
vN-ctd2-165	ZINC000299738308	-10.1	0.289	477.51	ZINC	C[C@@H]1CCc2cc(F)cc3c2[C@H]1C(=O)C(Cc1c(O)c2cc(F)cc4c2n(c1=O)[C@@H](C)CC4)=C3O
vN-ctd2-166	ZINC000408864607	-10.1	0.337	395.43	ZINC	O=C1c2ccccc2C(=O)c2c1ccc1c2[C@@H]2C=CC[C@@H]2[C@H](c2ccc(F)cc2)N1
vN-ctd2-167	ZINC000409337159	-10.1	0.266	494.51	ZINC	O=C(Nc1ccc2nc3ccc4ccccc4c3nc2c1)c1ccc(N2C(=O)c3ccccc3C2=O)cc1
vN-ctd2-168	PV-001801797994	-10.0	0.323	428.41	REAL	CN1C(=O)C(C)(C)c2cc(C(=O)Nc3ccn(-c4cccc(C(F)(F)F)c4)n3)ccc21
vN-ctd2-169	PV-001809069531	-10.0	0.385	354.34	REAL	O=C(Nc1nc(O)c2c(n1)CCCC2)c1cc(=O)[nH]c2cc(F)ccc12
vN-ctd2-170	PV-001822237837	-10.0	0.357	372.38	REAL	Cc1ccc(C(=O)NNC(=O)c2n[nH]c(=O)c3ccccc23)c2ccccc12
vN-ctd2-171	PV-001822247080	-10.0	0.303	455.39	REAL	O=C1CCc2cc(F)c(NC(=O)c3ccc(NC(=O)c4cc(F)cc(F)c4)c3O)cc2N1
vN-ctd2-172	PV-001833853142	-10.0	0.370	356.38	REAL	O=C(NNC(=O)c1cccc2ccccc12)c1cc2ccccc2cc1O
vN-ctd2-173	PV-001833853427	-10.0	0.357	371.40	REAL	Cc1c(C(=O)NNC(=O)c2cccc3ccccc23)c(O)nc2ccccc12
vN-ctd2-174	PV-001839839282	-10.0	0.385	349.34	REAL	O=C1CCOc2c(NC(=O)c3ccc4ccc(O)cc4c3O)cccc21
vN-ctd2-175	PV-001842161697	-10.0	0.385	345.44	REAL	C[C@H]1CCCc2ccccc2[C@@H]1NC(=O)c1ccc2ccccc2c1O
vN-ctd2-176	PV-001848790643	-10.0	0.323	421.40	REAL	C[C@@]1(c2cccc(C(=O)Nc3cccc(-c4ccc(F)c(F)c4)c3)c2)NC(=O)NC1=O
vN-ctd2-177	PV-001850120211	-10.0	0.345	390.40	REAL	Cc1noc(-c2ccc(C(=O)Nc3cccc(C4CC(=O)NC(=O)C4)c3)cc2)n1
vN-ctd2-178	PV-001871871051	-10.0	0.385	344.37	REAL	Cc1cc(C)c2cc(NC(=O)c3n[nH]c4ccccc4c3=O)ccc2n1
vN-ctd2-179	PV-001948704330	-10.0	0.313	444.39	REAL	O=C(NNC(=O)c1cccc2ccccc12)N[C@@H](c1c[nH]c2cccc(F)c12)C(F)(F)F
vN-ctd2-180	Z1024049144	-10.0	0.286	465.51	REAL	O=C1Nc2ccccc2[C@@H]1C1CCN(C(=O)c2cccc(N3C(=O)c4ccccc4C3=O)c2)CC1
vN-ctd2-181	Z1074896398	-10.0	0.303	480.51	REAL	CN1CCC/C1=N\S(=O)(=O)c1ccc(NC(=O)NC2(c3cccc(C(F)(F)F)c3)CC2)cc1
vN-ctd2-182	Z1095049186	-10.0	0.357	365.40	REAL	O=C(Nc1nc(-c2ccc3ccccc3n2)n[nH]1)c1ccc2ccccc2c1
vN-ctd2-183	Z1096186020	-10.0	0.294	491.59	REAL	C[C@@]1(c2cccc3ccccc23)NC(=O)N(Cc2csc(-c3ccc(S(C)(=O)=O)cc3)n2)C1=O
vN-ctd2-184	Z1098707397	-10.0	0.385	344.35	REAL	O=C(Nc1n[nH]c2ccc(F)cc12)c1cc2c(ccc3ccccc32)[nH]1
vN-ctd2-185	Z110096356	-10.0	0.278	486.48	REAL	C[C@H]1Oc2ccc(NC(=O)c3ccc(C(=O)Nc4ccc5c(c4)NC(=O)[C@@H](C)O5)cc3)cc2NC1=O
vN-ctd2-186	Z1101835892	-10.0	0.303	440.43	REAL	Cc1nc2cc(F)cc(C(=O)Nc3ccc(N4C(=O)c5ccccc5C4=O)cc3)c2nc1C
vN-ctd2-187	Z1129405406	-10.0	0.303	439.47	REAL	CN1C(=O)CCc2cc(NC(=O)c3cccc(NC(=O)c4ccc5[nH]cnc5c4)c3)ccc21
vN-ctd2-188	Z1171598131	-10.0	0.313	425.45	REAL	Cc1nnc2[nH]nc(NC(=O)c3cccc4c(=O)c(C)c(-c5ccccc5)oc34)c2c1C
vN-ctd2-189	Z1177435038	-10.0	0.370	355.35	REAL	O=C(Nc1ccc2oc3ccccc3c2c1)c1n[nH]c2ccccc2c1=O
vN-ctd2-190	Z1239265137	-10.0	0.345	392.37	REAL	Cc1cc(C(=O)Nc2nc3ccccc3c(=O)[nH]2)nc2c1c(=O)n(C)c(=O)n2C
vN-ctd2-191	Z1304269314	-10.0	0.313	425.45	REAL	O=C1c2ccccc2C(=O)N1[C@@H]1CCC/C(=N/Nc2ncnc3c2oc2ccccc23)C1
vN-ctd2-192	Z1347710577	-10.0	0.313	430.51	REAL	C[C@H]1C(=O)Nc2cc(C(=O)Nc3ccc(-c4nnc5n4CCCCC5)cc3)ccc2N1C
vN-ctd2-193	Z1347774863	-10.0	0.303	444.54	REAL	C[C@H]1C(=O)Nc2cc(C(=O)Nc3ccc(-c4nnc5n4CCCCCC5)cc3)ccc2N1C
vN-ctd2-194	Z139984444	-10.0	0.286	483.55	REAL	Cc1ccc(-c2nnc(-c3ccc(C(=O)Nn4cnc5sc6c(c5c4=O)CCCC6)cc3)o2)cc1
vN-ctd2-195	Z1441537213	-10.0	0.385	350.42	REAL	Cc1cccc2c1CCN(C(=O)Nc1ccc3oc(N(C)C)nc3c1)C2
vN-ctd2-196	Z1577041855	-10.0	0.313	430.51	REAL	C1=C(c2ccc3c(c2)OCCO3)CCN(c2nc3ccccc3nc2N2CCOCC2)C1
vN-ctd2-197	Z1612411734	-10.0	0.303	437.50	REAL	O=C(Cc1ccc(N2C(=O)[C@@H]3c4ccccc4CCN3C2=O)cc1)N1CCc2ccccc21
vN-ctd2-198	Z165129150	-10.0	0.313	426.51	REAL	Cc1cccc(N2CCN(C(=O)c3ccc4c(c3)C[C@@H](c3ccccc3)OC4=O)CC2)c1
vN-ctd2-199	Z1682437947	-10.0	0.313	448.50	REAL	C[C@H]1CCc2[nH]c3ccc(-c4nc(CN5C(=O)c6ccccc6S5(=O)=O)no4)cc3c2C1
vN-ctd2-200	Z1683177695	-10.0	0.370	355.36	REAL	Oc1cc2ccccc2cc1-c1nc(-c2ccnc(-n3cccn3)c2)no1

Supplementary Table 88. Virtual screening hits 101 to 200 of the screen against the oligomerization interface of the CTD of the nucleoprotein (Screen ID: 45). Compounds were filtered so that hits had MW < 600 dalton, cLogP < 6, number of hydrogen bond acceptors < 11, and no reactive functional groups. A few compounds unsuitable for drug discovery were removed by visual inspection. The name of each compound consists of the initial letter 'v' for virtual hit, followed by the target protein name and the target site ('ctd' for CTD binding interface, 2 for docking scenario 2). The score is the docking score given by QuickVina 2 in kcal/mol. The ligand efficiency (LE) is computed as LE = -score/#NonH, where #NonH is the number of heavy (i.e. non hydrogen) atoms.

Name	Catalog ID	Score	LE	MW	Library	SMILES
vSpike-ace2.1-1	ZINC000100688954	-10.3	0.264	511.58	ZINC	Cc1ccc(N2C(=O)[C@@H]3[C@H](C2=O)[C@H]2c4ccccc4C=NN2[C@@H]3C(=O)c2ccc(-c3ccccc3)cc2)cc1
vSpike-ace2.1-2	Z1452691933	-10.1	0.306	445.493	REAL	O=C(NC[C@H]1[C@@H]2Cc3ccccc3[C@H]12)NNC(=O)c1ccccc1OCc1ccc(F)cc1
vSpike-ace2.1-3	Z2087363989	-10	0.313	420.427	REAL	O=C1N[C@H](c2ccc3ccccc3c2)C(=O)N1c1ccc(-c2ccc3nccc3c2)on1
vSpike-ace2.1-4	Z1948615421	-9.9	0.367	361.444	REAL	O=C(Cc1c[nH]c2ccccc12)NNC(=O)[C@@H]1[C@@H]2[C@H]3C[C@@H]4[C@@H]5[C@H]3C[C@H]2[C@@H]5[C@H]41
vSpike-ace2.1-5	Z1524785469	-9.7	0.323	394.473	REAL	O=C(c1cc2ccccc2c(=O)[nH]1)N1CCc2ccccc2[C@H]1Cc1ccccc1
vSpike-ace2.1-6	Z1541121209	-9.7	0.313	433.531	REAL	O=C([C@@H]1Nc2ccccc2S(=O)(=O)N1)N1CCc2ccccc2[C@H]1Cc1ccccc1
vSpike-ace2.1-7	Z2633153141	-9.7	0.346	392.538	REAL	CCCC[C@@H](CNC(=O)[C@@]1(C)C[C@@H]2CC[C@H]1O2)NC(=O)[C@@]1(C)C[C@@H]2CC[C@@H]1O2
vSpike-ace2.1-8	Z511797774	-9.7	0.303	443.526	REAL	O=C(c1ccc2c(c1)-c1ccccc1C2)N1CCN(C2=NS(=O)(=O)c3ccccc32)CC1
vSpike-ace2.1-9	Z973896126	-9.7	0.285	448.525	REAL	Cc1n[nH]c(NC(=O)[C@H]2CC(=O)N(c3ccc4c(c3)Cc3ccccc3-4)C2)c1-c1ccccc1
vSpike-ace2.1-10	ZINC000008449797	-9.7	0.255	493.561	ZINC	O=C1[C@H]2[C@H](C(=O)N1c1ccc(Oc3ccc4ccccc4c3)cc1)C1c3ccccc3C2c2ccccc21
vSpike-ace2.1-11	ZINC000101835650	-9.7	0.269	493.59	ZINC	Cc1ccc([C@H]2C=C(c3ccccc3)Nc3nc(NS(=O)(=O)c4ccc5ccccc5c4)nn32)cc1
vSpike-ace2.1-12	ZINC000102709703	-9.7	0.269	491.532	ZINC	C[C@H]1CCc2cc(F)cc3c2[C@@H]1C(=O)C(CCc1c(O)c2cc(F)cc4c2n(c1=O)[C@@H](C)CC4)=C3O
vSpike-ace2.1-13	ZINC000102709709	-9.7	0.269	491.532	ZINC	C[C@H]1CCc2cc(F)cc3c2[C@H]1C(=O)C(CCc1c(O)c2cc(F)cc4c2n(c1=O)[C@@H](C)CC4)=C3O
vSpike-ace2.1-14	ZINC000408730040	-9.7	0.262	485.538	ZINC	Cc1ccc(N2C(=O)[C@H]3[C@H](C2=O)[C@@H]2C(=O)Oc4c5ccccc5ccc4C2=C[C@H]3c2ccccc2)cc1
vSpike-ace2.1-15	Z1603395474	-9.6	0.31	421.543	REAL	Cn1ccc(N2CCC[C@H](NC(=O)N[C@H]3C[C@H]4CCC(C)(C)c5ccc3c54)C2=O)n1
vSpike-ace2.1-16	Z2902672278	-9.6	0.259	486.494	REAL	Cn1c(=O)[nH]c2ncc(-c3cccc(-c4nc(-c5ccc(-n6cnc7ccccc76)nc5)no4)c3)cc21
vSpike-ace2.1-17	ZINC000102083157	-9.6	0.274	463.531	ZINC	CC1=C[C@H]2[C@H](1[C@H]1C(=O)N(c3cccc(OCC(=O)c4ccc(-c5ccccc5)cc4)c3)C(=O)[C@H]21
vSpike-ace2.1-18	ZINC000247797224	-9.6	0.253	497.553	ZINC	O=C(c1ccc(-c2ccccc2)cc1)[C@@H]1[C@@H]2C(=O)N(c3cccc3)C(=O)[C@H]2[C@H]2c3cccc3C=NN12
vSpike-ace2.1-19	ZINC000408731626	-9.6	0.253	499.565	ZINC	Cc1ccc(N2C(=O)[C@H]3[C@H](C2=O)[C@@H]2C(=O)Oc4c5ccccc5ccc4C2=C[C@H]3c2ccccc2)cc1C
vSpike-ace2.1-20	PV-001962375352	-9.5	0.297	441.52	REAL	C[C@H](NC(=O)N1CC[C@@H](c2ccc(F)c(F)c2)C1(C)C)C(=O)N1c2ccccc2C[C@@H]1C
vSpike-ace2.1-21	Z1021140402	-9.5	0.297	430.467	REAL	Cc1cc(=O)n2nc(NC(=O)[C@@H]3CCCN(C(=O)c4ccc5ccccc45)C3)[nH]c2n1
vSpike-ace2.1-22	Z1389963584	-9.5	0.288	441.529	REAL	O=C(NCCN1C(=O)[C@H]2[C@@H]3C=C[C@@H](C3)[C@H]2C1=O)N1Cc2ccccc2[C@H](c2ccccc2)C1
vSpike-ace2.1-23	Z1603403958	-9.5	0.317	401.508	REAL	CC1(C)CC[C@@H]2C[C@H](NC(=O)NCc3cc(=O)[nH]c4ccccc34)c3ccc1c32
vSpike-ace2.1-24	Z1723437098	-9.5	0.257	498.517	REAL	Cn1c(=O)[nH]c2ncc(-c3cccc(C(=O)N4CCC[C@H](c5nc(-c6ccc(F)cc6)no5)C4)c3)cc21
vSpike-ace2.1-25	Z1870480213	-9.5	0.317	404.44	REAL	O=C1N[C@@H](c2ccc3ccccc3c2)C(=O)N1[C@@H]1CCO[C@@H](c2ccc(F)cc2)C1
vSpike-ace2.1-26	Z2004574187	-9.5	0.297	430.546	REAL	CC1(C)C(=O)N(C[C@@](C)(O)C(=O)N2[C@H]3C=C(c4ccccc4)C[C@H]2CC3)c2ccccc21
vSpike-ace2.1-27	Z2086535021	-9.5	0.339	372.423	REAL	O=C1N[C@@H](c2ccc3ccccc23)C(=O)N1[C@H]1CCc2ccccc2OC1
vSpike-ace2.1-28	Z71170329	-9.5	0.306	406.484	REAL	O=C(NC[C@@H]1CC2c3ccccc3C1c1ccccc12)c1cc2ccccc2c(=O)[nH]1
vSpike-ace2.1-29	ZINC000001717021	-9.5	0.297	417.419	ZINC	O=c1oc2cc(-n3c(=O)c4ccccc4c4ccccc4c3=O)ccc2c2ccccc12
vSpike-ace2.1-30	ZINC000002299954	-9.5	0.306	410.468	ZINC	Cc1c(OCC(=O)c2ccc(-c3cccc3)cc2)ccc2c3c(c(=O)oc12)CCC3
vSpike-ace2.1-31	ZINC000002908937	-9.5	0.257	494.452	ZINC	O=c1oc(-c2cccc(F)c2)nc2cc(Cc3ccc4nc(-c5cccc(F)c5)oc(=O)c4c3)ccc12
vSpike-ace2.1-32	ZINC000012436788	-9.5	0.288	431.446	ZINC	O=C(Nc1cccc2c1C(=O)[C@@H]1C=CC=C[C@H]1C2=O)c1cccc2c1C(=O)c1ccccc1-2
vSpike-ace2.1-33	ZINC000015957613	-9.5	0.264	481.507	ZINC	O=C1Nc2ccccc2[C@@]12N[C@@H](Cc1ccccc1)[C@H]1C(=O)N(c3ccc4c(c3)OCCO4)C(=O)[C@H]12
vSpike-ace2.1-34	ZINC000101835370	-9.5	0.297	421.503	ZINC	Cc1ccc(C2=C[C@H](c3ccccc3)n3nc(NC(=O)c4ccccc4)c4)nc3N2)cc1
vSpike-ace2.1-35	ZINC000408733650	-9.5	0.257	485.538	ZINC	Cc1ccc2c(c1)OC(=O)[C@@H]1C2=C[C@H](c2ccccc2)[C@H]2C(=O)N(c3ccc4ccccc4c3)C(=O)[C@@H]21
vSpike-ace2.1-36	ZINC000409336230	-9.5	0.25	499.565	ZINC	Cc1ccc(N2C(=O)[C@H]3[C@H](C2=O)[C@@H]2C(=O)Oc4ccc5ccccc5c4C2=C[C@H]3c2ccccc2)cc1C
vSpike-ace2.1-37	ZINC000409336236	-9.5	0.25	499.565	ZINC	Cc1ccc(N2C(=O)[C@@H]3[C@H](C2=O)[C@@H]2C(=O)Oc4ccc5ccccc5c4C2=C[C@H]3c2ccccc2)cc1C
vSpike-ace2.1-38	PV-001801798150	-9.4	0.303	432.401	REAL	CC1(C)CNC(=O)c2c(C(=O)Nc3ccn(-c4cccc(C(F)(F)F)c4)n3)coc2C1
vSpike-ace2.1-39	PV-001813318786	-9.4	0.324	392.404	REAL	NC(=O)c1cccc2c1CCN(C(=O)c1ccc(-c3ccc(F)cc3)cc1F)C2
vSpike-ace2.1-40	PV-001955148032	-9.4	0.324	388.509	REAL	CC1(C)CC[C@H](NC(=O)NC[C@H](O)c2ccc3ccccc3c2)c2ccccc21
vSpike-ace2.1-41	PV-001955148372	-9.4	0.294	437.557	REAL	CC1(C)CC[C@H](NC(=O)N2CCCN(C(=O)Cc3cccc(F)c3)CC2)c2ccccc21
vSpike-ace2.1-42	Z1188975473	-9.4	0.313	415.839	REAL	O=C(NNc1nc(-c2ccc(Cl)cc2)no1)c1cc2ccccc2c2cccnc12
vSpike-ace2.1-43	Z119762790	-9.4	0.276	473.556	REAL	Cc1ccc(-c2nnc(NC(=O)c3cccc(S(=O)(=O)N4CCc5ccccc5C4)c3)[nH]2)cc1
vSpike-ace2.1-44	Z1336613669	-9.4	0.285	442.474	REAL	CN1C(=O)CN(C(=O)CN2C(=O)N[C@](C)(c3ccc4ccccc4c3)C2=O)c2ccccc21
vSpike-ace2.1-45	Z1374245383	-9.4	0.324	411.525	REAL	O=C([C@@H]1Nc2ccccc2S(=O)(=O)N1)N1CCC[C@@]2(CCCc3ccccc32)C1
vSpike-ace2.1-46	Z144731708	-9.4	0.294	420.423	REAL	O=C1NC(=O)c2ccccc2/C1=C/c1ccc(/C=C2/C(=O)NC(=O)c3ccccc32)cc1
vSpike-ace2.1-47	Z1452696604	-9.4	0.276	448.525	REAL	O=C(NC[C@H]1[C@H]2Cc3ccccc3[C@H]12)NNC(=O)c1cc(-c2ccccc2)nc2ccccc12
vSpike-ace2.1-48	Z1473414262	-9.4	0.276	448.525	REAL	O=C(NNC(=O)c1cc(-c2ccccc2)nc2ccccc12)N[C@H]1[C@@H]2CCc3ccccc3[C@@H]21
vSpike-ace2.1-49	Z1537126265	-9.4	0.313	395.461	REAL	O=C(c1nc2ccccc2c(=O)[nH]1)N1CCc2ccccc2[C@H]1Cc1ccccc1
vSpike-ace2.1-50	Z1571944836	-9.4	0.294	427.546	REAL	Cc1cc(C)cc(C2=CCN(C(=O)c3ccc4c(=O)n5c(nc4c3)CCCC5)CC2)c1
vSpike-ace2.1-51	Z1629272954	-9.4	0.324	384.434	REAL	O=C(Nc1ccc2c(c1)Cc1ccccc1-2)NC1(C(=O)O)Cc2ccccc2C1
vSpike-ace2.1-52	Z1682893334	-9.4	0.294	423.431	REAL	O=C1CNC(=O)N1Cc1ccccc1-c1noc(-c2cc3c(ccc4ccccc43)[nH]2)n1
vSpike-ace2.1-53	Z1698176044	-9.4	0.336	365.431	REAL	O=C1CC[C@@H]2CN(C(=O)c3cc4c(c3)Cc3ccccc3-4)c3ccc1c32
vSpike-ace2.1-54	Z1864554237	-9.4	0.313	394.473	REAL	Cn1cc(C(=O)N2CCCc3cc(-c4ccccc4)ccc32)c2ccccc2c1=O
vSpike-ace2.1-55	Z1891946720	-9.4	0.276	447.493	REAL	O=C(c1cccc(N2C(=O)N[C@@H](c3cccc4ccccc34)C2=O)c1)N1CCc2ccccc21
vSpike-ace2.1-56	Z1983287835	-9.4	0.324	392.454	REAL	Cc1ccc2c(CN3C(=O)N[C@]4(C[C@@H]5C[C@@H]4[C@@H]4CCC[C@@H]54)C3=O)cc(=O)oc2c1
vSpike-ace2.1-57	Z2001436960	-9.4	0.324	388.466	REAL	CC(=O)N1C[C@@H](C(=O)N2[C@@H]3C=C(c4ccccc4)C[C@H]2CC3)Oc2ccccc21
vSpike-ace2.1-58	Z2004579732	-9.4	0.348	357.412	REAL	O=C(c1n[nH]c(=O)c2ccccc12)N1[C@@H]2C=C(c3ccccc3)C[C@@H]1CC2
vSpike-ace2.1-59	Z2119931797	-9.4	0.303	410.476	REAL	O=C(NNc1ccc2c(=O)[nH]ccc2c1)N[C@@H]1CCc2ccc(-c3ccccc3)cc21
vSpike-ace2.1-60	Z226821924	-9.4	0.276	456.497	REAL	Cc1ccc(OC(=O)CN2C(=O)N[C@](C)(c3ccc4ccccc4c3)C2=O)c2c1[C@H](C)CC2=O
vSpike-ace2.1-61	Z358867962	-9.4	0.313	415.532	REAL	Cc1cccc([C@@H](CC(=O)O[C@@H](C)C(=O)N[C@@H](C)[C@H]2C[C@H]3CC[C@H]2C3)NC(N)=O)c1
vSpike-ace2.1-62	Z749462654	-9.4	0.276	471.536	REAL	O=C(NNC(=O)c1ccc2ccccc2c1)c1cccc(S(=O)(=O)N2CCc3ccccc32)c1
vSpike-ace2.1-63	Z804390806	-9.4	0.254	495.625	REAL	O=C([C@H]1CC(=O)N(c2ccc3c(c2)Cc2ccccc2-3)C1)N1CCC[C@@H](c2nnc3n2CCCCC3)C1
vSpike-ace2.1-64	Z845324458	-9.4	0.261	495.5	REAL	Cc1cccc(C(=O)Nc2ccccc2C(=O)N2CCN(C(=O)c3ccc(C(F)(F)F)cc3)CC2)c1
vSpike-ace2.1-65	Z941524362	-9.4	0.313	398.504	REAL	Cc1ccc2c(c1)N(C(=O)C1CCN(C(=O)c3cccc4ccccc34)CC1)CC2
vSpike-ace2.1-66	Z988053964	-9.4	0.261	486.545	REAL	Cc1ccc(C(=O)N2CCN(C(=O)Nc3cccc(C(=O)N4CCc5ccccc54)c3)CC2)cc1F
vSpike-ace2.1-67	Z998375970	-9.4	0.254	495.581	REAL	O=C(c1ccc2[nH]ncc2c1)N1CCC[C@@H](C(=O)N2CCN(C(=O)c3cccc4ccccc34)CC2)C1
vSpike-ace2.1-68	ZINC000002956443	-9.4	0.276	441.529	ZINC	CC12c3ccccc3C(c3ccccc31)[C@@H]1C(=O)N(c3ccc(-c4ccccc4)cc3)C(=O)[C@@H]12
vSpike-ace2.1-69	ZINC000002956445	-9.4	0.276	441.529	ZINC	CC12c3ccccc3C(c3ccccc31)[C@H]1C(=O)N(c3ccc(-c4ccccc4)cc3)C(=O)[C@@H]12
vSpike-ace2.1-70	ZINC000008826511	-9.4	0.276	441.485	ZINC	O=C1[C@@H]2[C@@H](C(=O)N1c1ccc3c(c1)oc1ccccc13)C1c3ccccc3C2c2ccccc21
vSpike-ace2.1-71	ZINC000018117591	-9.4	0.285	431.446	ZINC	O=C(Nc1ccc2c1C(=O)[C@H]1C=CC=C[C@@H]1C2=O)c1ccc2c1C(=O)c1ccccc1-2
vSpike-ace2.1-72	ZINC000100504092	-9.4	0.303	404.512	ZINC	O=c1ccc2n1C[C@H]1C[C@H]2CN(Cc2ccc3ccc4cccc5ccc2c3c45)C1
vSpike-ace2.1-73	ZINC000100737710	-9.4	0.285	431.446	ZINC	O=C(Nc1cccc2c1C(=O)[C@H]1C=CC=C[C@H]1C2=O)c1cccc2c1C(=O)c1ccccc1-2
vSpike-ace2.1-74	ZINC000100968114	-9.4	0.261	491.532	ZINC	C[C@@H]1CCc2cc(F)cc3c(O)c(CCC4=C(O)c5cc(F)cc6c5[C@@H](C4=O)[C@@H](C)CC6)c(=O)n1c23
vSpike-ace2.1-75	ZINC000101836267	-9.4	0.285	459.911	ZINC	Cc1cccc(C(=O)Nc2nc3n(n2)[C@@H](c2ccc(F)cc2)C=C(c2ccc(Cl)cc2)N3)c1
vSpike-ace2.1-76	ZINC000109965938	-9.4	0.269	475.571	ZINC	O=S1(=O)c2ccccc2-c2cc(-c3nc(C4=CN[C@H]5C=CC=C[C@H]45)[nH]c3-c3ccccc3)ccc21
vSpike-ace2.1-77	PV-001799751743	-9.3	0.332	376.415	REAL	CC1(C)CNC(=O)c2c(C(=O)Nc3ccc(-c4ccccc4)nn3)coc2C1
vSpike-ace2.1-78	PV-001800924123	-9.3	0.291	448.585	REAL	Cc1cc(C(=O)N2CCCc3cc(-c4ccccc4)ccc32)cc(S(=O)(=O)N(C)C)c1C
vSpike-ace2.1-79	PV-001825814403	-9.3	0.291	422.483	REAL	Cc1ccc(C(=O)c2ccccc2C(=O)NNC(=O)c2ccc3ccccc3c2)cc1C
vSpike-ace2.1-80	PV-001828769439	-9.3	0.291	448.585	REAL	Cc1cc(C)c(C)c(S(=O)(=O)NCC(=O)N2Cc3ccccc3-c3ccccc3C2)c1C
vSpike-ace2.1-81	PV-001841361759	-9.3	0.291	424.503	REAL	Cc1cccc(-c2cccc(C(=O)NNC(=O)c3cc(-c4cc(C)ccc4C)n[nH]3)c2)c1
vSpike-ace2.1-82	PV-001847910255	-9.3	0.291	441.412	REAL	Cc1ccccc1C1=NO[C@@H](C(=O)NNc2ccc(-c3cccc(C(F)(F)F)c3)nn2)C1
vSpike-ace2.1-83	PV-001866698388	-9.3	0.282	459.471	REAL	Cc1cc(C)nc(-n2[nH]c(C(=O)N3CC[C@H](c4cccc(C(F)(F)F)c4)C3(C)C)cc2=O)n1
vSpike-ace2.1-84	PV-001954720811	-9.3	0.332	381.45	REAL	C[C@@H](NC(=O)N[C@H]1CCc2cc(F)ccc21)C(=O)N1c2ccccc2C[C@@H]1C
vSpike-ace2.1-85	PV-001962374248	-9.3	0.31	425.958	REAL	C[C@@H](NC(=O)N[C@@H]1CC[C@@H](c2ccc(Cl)cc2)C1)C(=O)N1c2ccccc2C[C@@H]1C
vSpike-ace2.1-86	Z1023504634	-9.3	0.251	496.497	REAL	O=C(c1cccc(N2C(=O)c3ccccc3C2=O)c1)N1CCC[C@H](c2nc(-c3cccc(F)c3)no2)C1
vSpike-ace2.1-87	Z1162535574	-9.3	0.344	355.396	REAL	O=C(Nc1nc2ccccc2c(=O)[nH]1)[C@H]1C[C@H]1c1ccc2ccccc2c1
vSpike-ace2.1-88	Z1313836871	-9.3	0.332	369.463	REAL	O=C(N1CC=C(c2cccc3ccccc23)CC1)C1(O)Cc2ccccc2C1
vSpike-ace2.1-89	Z131407602	-9.3	0.291	424.542	REAL	CN1CCC2(CC1)C[C@@H](NC(=O)c1ccc3c(c1)-c1ccccc1C3)c1ccccc1O2
vSpike-ace2.1-90	Z1329924307	-9.3	0.3	413.472	REAL	Cc1ccc2c(c1)N(C(=O)c1ccc3c(c1)C[C@@H](c1ccccc1)OC3=O)C[C@@H](C)O2
vSpike-ace2.1-91	Z14075666	-9.3	0.3	412.444	REAL	Cc1ccc2c(CN3C(=O)N[C@@](C)(c4cccc5ccccc45)C3=O)cc(=O)oc2c1
vSpike-ace2.1-92	Z14076292	-9.3	0.282	438.482	REAL	C[C@@]1(c2cccc3ccccc23)NC(=O)N(Cc2cc(=O)oc3cc4c(cc23)CCC4)C1=O
vSpike-ace2.1-93	Z14136476	-9.3	0.282	438.482	REAL	C[C@@]1(c2ccc3ccccc3c2)NC(=O)N(Cc2cc(=O)oc3cc4c(cc23)CCC4)C1=O
vSpike-ace2.1-94	Z1420929016	-9.3	0.31	394.473	REAL	Cn1c(=O)cc(C(=O)N2CCCc3cc(-c4ccccc4)ccc32)c2ccccc21
vSpike-ace2.1-95	Z1472866131	-9.3	0.274	449.552	REAL	O=C(N[C@@H]1[C@H]2CCc3ccccc3[C@H]21)c1cncc(C(=O)N[C@@H]2[C@H]3CCc4ccccc4[C@H]32)c1
vSpike-ace2.1-96	Z1662361581	-9.3	0.282	438.486	REAL	C[C@]12CCC(=O)N1c1ccccc1C(=O)N2Cc1nnc(Cc2ccc3ccccc3c2)o1
vSpike-ace2.1-97	Z1733801359	-9.3	0.291	427.55	REAL	Cc1nc([C@H]2CCCN(C(=O)NC[C@@H]3CC4c5ccccc5C3c3ccccc34)C2)n[nH]1
vSpike-ace2.1-98	Z1742516546	-9.3	0.282	442.561	REAL	C[C@@H]1CN(c2ccc(CNC(=O)N[C@H]3CCc4ccc(-c5ccccc5)cc43)cn2)CCO1
vSpike-ace2.1-99	Z1744509596	-9.3	0.282	443.545	REAL	O=C([C@@H]1C[C@H]2CCCC[C@@H]2N1C(=O)c1ccccc1)N1CC[C@@]2(C1)C(=O)Nc1ccccc12
vSpike-ace2.1-100	Z1748297099	-9.3	0.321	381.434	REAL	O=C(c1cc2c(ccc3ccccc32)[nH]1)N1CC[C@@]2(C1)C(=O)Nc1ccccc12

Supplementary Table 89. Top 100 virtual hits of the screen against the ACE2 binding site of the spike protein (Screen ID: 7). Compounds were filtered so that hits had MW < 600 dalton, cLogP < 6, number of hydrogen bond acceptors < 11, and no reactive functional groups. A few compounds unsuitable for drug discovery were removed by visual inspection. The name of each compound consists of the initial letter 'v' for virtual hit, followed by the target protein name and the target site ('ace2' for ACE2 binding site, 1 for docking scenario 1). The score is the docking score given by QuickVina 2 in kcal/mol. The ligand efficiency (LE) is computed as LE = -score/#NonH, where #NonH is the number of heavy (i.e. non hydrogen) atoms.

Name	Catalog ID	Score	LE	MW	Library	SMILES
vSpike-ace2.1-101	Z1869886653	-9.3	0.300	417.44	REAL	O=C1[C@H](N2C(=O)N[C@@H](c3cec4ccccc4c3)C2=O)CCCN1c1ccccc1F
vSpike-ace2.1-102	Z1891182475	-9.3	0.274	449.47	REAL	Cc1ccc(C)c(N2C(=O)c3ccc(-c4nc(Cc5ccc6cn[nH]c6c5)no4)cc3C2=O)c1
vSpike-ace2.1-103	Z1983285837	-9.3	0.300	421.50	REAL	CC1(C)C(=O)Nc2ccc(C(=O)CN3C(=O)N[C@]4(C[C@H]5C[C@@H]4[C@@H]4CCC[C@H]54)C3=O)cc21
vSpike-ace2.1-104	Z2087363242	-9.3	0.300	412.40	REAL	O=C1N[C@H](c2ccc3c(c2)CCO3)C(=O)N1c1cc(-c2ccc3ncccc3c2)on1
vSpike-ace2.1-105	Z2179839522	-9.3	0.332	372.42	REAL	Cc1cccc2c1OC[C@@H](N1C(=O)N[C@@H](c3ccc4ccccc4c3)C1=O)C2
vSpike-ace2.1-106	Z2209285463	-9.3	0.332	389.47	REAL	O=C(c1ccc2c(c1)-c1ccccc1C2)N1CC[C@H](c2ccccc2)S1(=O)=O
vSpike-ace2.1-107	Z2232119751	-9.3	0.291	421.50	REAL	O=C(c1ccc2c(=O)n3c(nc2c1)CCC3)N1CCc2ccccc2[C@@H]1c1ccccc1
vSpike-ace2.1-108	Z226874468	-9.3	0.258	500.00	REAL	C[C@@H]1c2[nH]c3ccccc3c2[C@H](c2ccccc2Cl)CN1C(=O)CN1C(=O)[C@H]2[C@@H]3C=C[C@@H](C3)[C@H]2C1=O
vSpike-ace2.1-109	Z2524818882	-9.3	0.251	491.59	REAL	O=C1c2ccccc2C(=O)N1c1cccc(C(=O)N2C[C@H]3CC[C@H]2[C@H]2CN(Cc4ccccc4)C[C@H]32)c1
vSpike-ace2.1-110	Z286954404	-9.3	0.251	490.57	REAL	Cc1ccc(-c2cc(NC(=O)C3CCN(c4ccc5nnnn5n4)CC3)nc(-c3ccccc3)c2)cc1
vSpike-ace2.1-111	Z2902673259	-9.3	0.251	490.53	REAL	O=C(c1ccc2[nH]ncc2c1)N1CCC[C@@H](c2nc(-c3ccc(-n4cnc5ccccc54)nc3)no2)C1
vSpike-ace2.1-112	Z29403053	-9.3	0.258	499.59	REAL	O=C(Nc1ccccc1C(=O)N1CCN(S(=O)(=O)c2ccc3ccccc3c2)CC1)c1ccccc1
vSpike-ace2.1-113	Z397589568	-9.3	0.258	498.61	REAL	O=C(c1cccc(S(=O)(=O)N2CCc3ccccc32)c1)N1CCN(c2ccc3ccccc3n2)CC1
vSpike-ace2.1-114	Z454312366	-9.3	0.274	448.48	REAL	Cn1c(=O)cc(C(=O)NNC(=O)c2cc(-c3ccccc3)nc3ccccc23)c2ccccc21
vSpike-ace2.1-115	Z654034888	-9.3	0.258	499.59	REAL	O=C(Cc1ccc2ccccc2c1)NNC(=O)c1cccc(S(=O)(=O)N2CCCc3ccccc32)c1
vSpike-ace2.1-116	Z767777520	-9.3	0.282	458.54	REAL	O=C(CN1c2ccccc3cccc(c23)S1(=O)=O)Nc1cccc(-c2n[nH]c3c2CCCC3)c1
vSpike-ace2.1-117	Z852301348	-9.3	0.258	479.58	REAL	Cc1nn(C)c2nc(-c3ccccc3)cc(C(=O)N3CCC(C(=O)N4CCc5ccccc54)CC3)c12
vSpike-ace2.1-118	Z941524442	-9.3	0.300	413.48	REAL	Cc1ccc2c(c1)N(C(=O)CN1C(=O)N[C@](C)(c3ccc4ccccc4c3)C1=O)CC2
vSpike-ace2.1-119	Z966271352	-9.3	0.266	468.52	REAL	O=C(Nc1cccc(C(=O)N2CCc3ccccc32)c1)C1CCN(c2ccc3nnnn3n2)CC1
vSpike-ace2.1-120	Z979337226	-9.3	0.274	458.60	REAL	Cc1cc(C)cc(C(=O)N2CCC[C@@H](C(=O)N3CCC[C@H](c4nc5cc(C)ccc5[nH]4)C3)C2)c1
vSpike-ace2.1-121	ZINC000002297329	-9.3	0.282	430.51	ZINC	O=C1C[C@H](c2cn(Cc3ccccc3)c3ccccc23)C(=O)N1c1ccc2ccccc2c1
vSpike-ace2.1-122	ZINC000002978046	-9.3	0.274	491.93	ZINC	O=C1Nc2ccc(F)cc2[C@@]12Nc1ccccc1-c1nnc(SCc3ccccc3Cl)nc1O2
vSpike-ace2.1-123	ZINC000004237097	-9.3	0.274	453.52	ZINC	O=C(Nc1cccc(F)c1)N1C[C@H]2C[C@@H](C1)Cn1c(=O)c(-c3ccc4ccccc4c3)ccc12
vSpike-ace2.1-124	ZINC000004741578	-9.3	0.332	369.47	ZINC	O=C1C[C@H](c2ccccc2)CC2=C1C1(CCCC1)n1c3ccccc3nc1N2
vSpike-ace2.1-125	ZINC000005092449	-9.3	0.321	377.40	ZINC	O=C(Nc1ccc2c(c1)C(=O)c1ccccc1C2=O)c1ccc2ccccc2c1
vSpike-ace2.1-126	ZINC000008449795	-9.3	0.245	493.56	ZINC	O=C1[C@@H]2[C@@H](C(=O)N1c1ccc(Oc3ccc4ccccc4c3)cc1)C1c3ccccc3C2c2ccccc21
vSpike-ace2.1-127	ZINC000008901217	-9.3	0.245	499.52	ZINC	Cc1cc(NC(=O)c2ccccc(-c3cc4ccccc4oc3=O)c2)ccc1-c1cc2ccccc2oc1=O
vSpike-ace2.1-128	ZINC000033821753	-9.3	0.291	442.90	ZINC	O=C1[C@H]2[C@@H]3C[C@@H]([C@H]4C(c5ccccc5Cl)=NO[C@H]34)[C@@H]2C(=O)N1c1ccc2ccccc2c1
vSpike-ace2.1-129	ZINC000040388522	-9.3	0.291	422.53	ZINC	CC(C)c1ccc(/C=C/c2ccnc3nc(N4CCc5ccccc5C4)[nH]c(=O)c23)cc1
vSpike-ace2.1-130	ZINC000067262716	-9.3	0.274	468.99	ZINC	Cc1ccc(N2CCN(c3nc4c(-c5cccc(Cl)c5)nnn4c4ccccc43)CC2)c(C)c1
vSpike-ace2.1-131	ZINC000100737708	-9.3	0.282	431.45	ZINC	O=C(Nc1cccc2c1C(=O)[C@@H]1C=CC=C[C@@H]1C2=O)c1cccc2c1C(=O)c1ccccc1-2
vSpike-ace2.1-132	ZINC000100968105	-9.3	0.258	491.53	ZINC	C[C@@H]1CCc2cc(F)cc3c(O)c(CCC4=C(O)c5cc(F)cc6c5[C@H](C4=O)[C@@H](C)CC6)c(=O)n1c23
vSpike-ace2.1-133	ZINC000101012333	-9.3	0.291	462.34	ZINC	O=C(Nc1nc2n(n1)[C@@H](c1ccccc1)C=C(c1ccccc1)N2)c1ccc(Cl)cc1Cl
vSpike-ace2.1-134	ZINC000101094157	-9.3	0.310	400.47	ZINC	Cc1cc2c(cc1C)C(=O)[C@@H]1C[C@@H]3C(=O)c4cc(C)c(C)cc4C(=O)[C@H]3C[C@H]1C2=O
vSpike-ace2.1-135	ZINC000101094159	-9.3	0.310	400.47	ZINC	Cc1cc2c(cc1C)C(=O)[C@H]1C[C@@H]3C(=O)c4cc(C)c(C)cc4C(=O)[C@H]3C[C@H]1C2=O
vSpike-ace2.1-136	ZINC000101464346	-9.3	0.258	492.50	ZINC	O=C(Nc1ccccc1C(F)(F)F)c1cccc(N2C(=O)[C@@H]3CC[C@@H](c4ccccc4)C[C@@H]3C2=O)c1
vSpike-ace2.1-137	ZINC000101835174	-9.3	0.300	407.48	ZINC	Cc1cccc(C(=O)Nc2nc3n(n2)[C@@H](c2ccccc2)C=C(c2ccccc2)N3)c1
vSpike-ace2.1-138	ZINC000101835312	-9.3	0.291	421.50	ZINC	Cc1ccc(C(=O)Nc2nc3n(n2)[C@@H](c2ccccc2)C=C(c2ccc(C)cc2)N3)cc1
vSpike-ace2.1-139	ZINC000101836373	-9.3	0.282	459.91	ZINC	Cc1ccc(C2=C[C@H](c3ccc(F)cc3)n3nc(NC(=O)c4ccc(Cl)cc4)nc3N2)cc1
vSpike-ace2.1-140	ZINC000408733646	-9.3	0.251	485.54	ZINC	Cc1ccc2c(c1)OC(=O)[C@@H]1C2=C[C@H](c2ccccc2)[C@H]2C(=O)N(c3ccc4ccccc4c3)C(=O)[C@H]21
vSpike-ace2.1-141	ZINC000952856206	-9.3	0.251	499.61	ZINC	CC(C)c1ccc(C(=O)N2CCC3(CC2)Cc2ccccc2)Oc2ccccc2)CCNC3=O)c(O)n1
vSpike-ace2.1-142	PV-001796053059	-9.2	0.297	419.52	REAL	Cc1ccc([C@]2(C)NC(=O)N(CC(=O)N[C@H]3CCC(C)(C)c4ccccc43)C2=O)cc1
vSpike-ace2.1-143	PV-001796055641	-9.2	0.329	376.50	REAL	Cc1ccc(C)c(C2=NO[C@@H](C(=O)N[C@H]3CCC(C)(C)c4ccccc43)C2)c1
vSpike-ace2.1-144	PV-001806848950	-9.2	0.317	386.49	REAL	C[C@@H](NC(=O)[C@H](C)c1ccc2ccccc2c1)C(=O)N1c2ccccc2C[C@@H]1C
vSpike-ace2.1-145	PV-001819655835	-9.2	0.317	393.48	REAL	COC(=O)[C@]1(NC(=O)[C@H]2COc3cc(C)c(C)cc32)CC[C@@H](C)c2ccccc21
vSpike-ace2.1-146	PV-001825815596	-9.2	0.329	371.40	REAL	Cc1c(C(=O)NNC(=O)c2ccc3ccccc3c2)[nH]c(=O)c2ccccc12
vSpike-ace2.1-147	PV-001842839623	-9.2	0.317	400.40	REAL	Cc1c(C(=O)N2CC[C@@H](c3cccc(C(F)(F)F)c3)C2)[nH]c(=O)c2ccccc12
vSpike-ace2.1-148	PV-001852605125	-9.2	0.287	434.51	REAL	Cc1cc(C)cc(C(=O)N2CCC[C@@H](C(=O)Nc3cc(-c4cc(C)ccc4F)n[nH]3)C2)c1
vSpike-ace2.1-149	PV-001855674807	-9.2	0.287	428.47	REAL	Cc1ccc(C)c(C(=O)c2ccccc2C(=O)Nc2n[nH]c(Cc3cccc(F)c3)n2)c1
vSpike-ace2.1-150	PV-001856495923	-9.2	0.287	430.55	REAL	Cc1cc(C)cc(C(=O)N2CCC[C@H](C(=O)Nc3cc(-c4cc(C)cc(C)c4)n[nH]3)C2)c1
vSpike-ace2.1-151	PV-001865661451	-9.2	0.354	411.30	REAL	C[C@@H]1C[C@@H](c2ccc(Br)cc2)CN1C(=O)c1cc2ccccc2c(=O)[nH]1
vSpike-ace2.1-152	PV-001944972139	-9.2	0.297	413.48	REAL	Cc1cc(C)cc(-n2nc(NC(=O)NNC(=O)c3ccc4ccccc4c3)cc2C)c1
vSpike-ace2.1-153	PV-001955148436	-9.2	0.341	362.52	REAL	CC1(CNC(=O)N[C@H]2CCC(C)(C)c3ccccc32)Cc2ccccc2C1
vSpike-ace2.1-154	PV-001955149424	-9.2	0.307	405.54	REAL	Cc1ccc(C2=NO[C@@H](CNC(=O)N[C@H]3CCC(C)(C)c4ccccc43)C2)cc1C
vSpike-ace2.1-155	PV-001966039611	-9.2	0.307	423.49	REAL	O=C(Cc1ccc2ccccc12)NNC(=O)N[C@H]1CS(=O)(=O)Cc2ccccc21
vSpike-ace2.1-156	PV-001969235131	-9.2	0.317	387.48	REAL	Cc1cc(C)cc(C2=CCN(C(=O)NCc3c[nH]c(=O)c4ccccc34)CC2)c1
vSpike-ace2.1-157	Z1144325540	-9.2	0.287	427.50	REAL	Cc1ccc2c(c1)[C@@H](NC(=O)CN1C(=O)N[C@@](C)(c3ccc4ccccc4c3)C1=O)CC2
vSpike-ace2.1-158	Z1162535189	-9.2	0.317	387.41	REAL	Cc1ccc(-c2ccc(C(=O)Nc3nc4ccccc4c(=O)[nH]3)c(F)c2)cc1C
vSpike-ace2.1-159	Z1172231620	-9.2	0.317	379.46	REAL	O=c1[nH]c(NC[C@@H]2CC3c4ccccc4C2c2ccccc23)nc2ccccc12
vSpike-ace2.1-160	Z1314149838	-9.2	0.287	423.43	REAL	Cc1cc(C(=O)Nc2cccc(-c3ccc4ccccc4c3)n2)nc2nc(O)[nH]c(=O)c12
vSpike-ace2.1-161	Z1389971656	-9.2	0.307	407.51	REAL	O=C(NCCN1C(=O)[C@H]2[C@@H]3C=C[C@@H](C3)[C@H]2C1=O)N1CCC[C@H](c2ccccc2)CC1
vSpike-ace2.1-162	Z14076286	-9.2	0.287	426.47	REAL	CCc1ccc2c(CN3C(=O)N[C@@](C)(c4cccc5ccccc45)C3=O)cc(=O)oc2c1
vSpike-ace2.1-163	Z14135947	-9.2	0.297	412.44	REAL	Cc1ccc2c(CN3C(=O)N[C@@](C)(c4ccc5ccccc5c4)C3=O)cc(=O)oc2c1
vSpike-ace2.1-164	Z14136470	-9.2	0.287	426.47	REAL	CCc1ccc2c(CN3C(=O)N[C@](C)(c4ccc5ccccc5c4)C3=O)cc(=O)oc2c1
vSpike-ace2.1-165	Z1429363779	-9.2	0.329	370.45	REAL	O=C(Nc1ccc2c(c1)Cc1ccccc1-2)N1CCc2ccccc2[C@H]1CO
vSpike-ace2.1-166	Z1431635582	-9.2	0.287	431.49	REAL	CC1(C)C(=O)Nc2ccc(C(=O)CN3C(=O)N[C@@]4(CCCCc5ccccc54)C3=O)cc21
vSpike-ace2.1-167	Z1473412632	-9.2	0.329	371.44	REAL	O=C(NNC(=O)c1ccc2ccccc12)N[C@H]1[C@@H]2CCc3ccccc3[C@@H]21
vSpike-ace2.1-168	Z1547587469	-9.2	0.287	423.52	REAL	Cc1cc(C)nc(-n2nc(C(=O)N3CCCc4cc(-c5ccccc5)ccc43)ce2C)n1
vSpike-ace2.1-169	Z1571946543	-9.2	0.317	390.44	REAL	Cc1cc(C)cc(C2=CCN(C(=O)c3cc(C)c4c(=O)[nH]c(O)nc4n3)CC2)c1
vSpike-ace2.1-170	Z1603533364	-9.2	0.287	427.55	REAL	CC1(C)CC[C@@H]2C[C@H](NC(=O)N3CCn4c(nnc4-c4ccccc4)C3)c3cccc1c32
vSpike-ace2.1-171	Z1674169958	-9.2	0.307	399.49	REAL	O=C1NCCc2ccc(CNC(=O)N3CCC[C@H]3c3cccc4ccccc34)cc21
vSpike-ace2.1-172	Z1682391572	-9.2	0.287	424.46	REAL	C[C@]1(c2cccc(-c3noc(Cc4ccc(-c5ccccc5)cc4)n3)cc2)NC(=O)NC1=O
vSpike-ace2.1-173	Z1684581876	-9.2	0.297	410.43	REAL	C[C@]1(c2cccc(-c3noc(-c4ccc(-c5ccccc5)cc4)n3)c2)NC(=O)NC1=O
vSpike-ace2.1-174	Z1698172573	-9.2	0.287	443.48	REAL	O=C1c2ccccc2S(=O)(=O)c2cc(C(=O)N3C[C@H]4CCC(=O)c5cccc3c54)ccc21
vSpike-ace2.1-175	Z1726979893	-9.2	0.307	401.47	REAL	O=C(NNC(=O)N1CCC[C@@]2(C1)OCc1ccccc12)c1ccc2ccccc12
vSpike-ace2.1-176	Z1727068597	-9.2	0.297	409.48	REAL	O=C1O[C@H](c2ccccc2)Cc2cc(C(=O)N3Cc4ccccc4C4(CC4)C3)ccc21
vSpike-ace2.1-177	Z1740089529	-9.2	0.287	441.45	REAL	Cc1cc(C)c2c(c1)CN(C(=O)c1nn(-c3cccc(C(F)(F)F)c3)c(C)cc1=O)CC2
vSpike-ace2.1-178	Z1742548866	-9.2	0.297	411.50	REAL	C[C@@H](NC(=O)N[C@@H]1CCc2ccc(-c3ccccc3)cc21)c1ccc2c(c1)CC(=O)N2
vSpike-ace2.1-179	Z1752292521	-9.2	0.279	439.51	REAL	O=C(NCc1ccc(-c2ccc3c(c2)CCO3)cc1)N1CC[C@]2(C1)C(=O)Nc1ccccc12
vSpike-ace2.1-180	Z1752602875	-9.2	0.297	415.54	REAL	CC1(C)CC[C@@H]2C[C@@H](NC(=O)N3CC[C@]4(C3)C(=O)Nc3ccccc34)c3ccc1c32
vSpike-ace2.1-181	Z1752851247	-9.2	0.279	436.51	REAL	Cc1cc(C(=O)NNC(=O)N[C@@H]2CCc3ccc(-c4ccccc4)cc32)c2ccccc2n1
vSpike-ace2.1-182	Z1763374630	-9.2	0.279	444.40	REAL	O=C(NNC(=O)c1cc(F)cc2c(=O)c3cc(F)ccc3[nH]c12)c1ccc2ccccc2n1
vSpike-ace2.1-183	Z1816108318	-9.2	0.317	380.45	REAL	O=C(c1c[nH]c(=O)c2ccccc12)N1CC=C(c2ccccc3ccccc23)CC1
vSpike-ace2.1-184	Z1846603747	-9.2	0.297	412.53	REAL	Cc1ccc2c(c1)CCN(C(=O)[C@H]1CCCN(C(=O)c3cccc4ccccc34)C1)C2
vSpike-ace2.1-185	Z1869553990	-9.2	0.307	399.45	REAL	Cc1ccc(N2CC[C@@H](N3C(=O)N[C@@H](c4ccc5ccccc5c4)C3=O)C2=O)cc1
vSpike-ace2.1-186	Z1870480661	-9.2	0.297	422.50	REAL	O=C1N[C@@H](C[C@H]2CCCc3ccccc32)C(=O)N1[C@@H]1CCO[C@@H](c2ccc(F)cc2)C1
vSpike-ace2.1-187	Z1972507579	-9.2	0.287	429.49	REAL	Cn1cc(C(=O)N2CCC[C@H](NC(=O)c3ccc4ccccc4c3)C2)c2cc(F)ccc21
vSpike-ace2.1-188	Z1988867451	-9.2	0.287	435.44	REAL	Cn1c(C(F)F)nc2cc(C(=O)NNc3nc(-c4ccccn4)nc4c3CCC4)ccc21
vSpike-ace2.1-189	Z2033164844	-9.2	0.279	448.56	REAL	O=C(N1CCCN(C(=O)[C@@]2(O)CCc3ccccc3C2)CC1)[C@]1(O)CCc2ccccc2C1
vSpike-ace2.1-190	Z2087236883	-9.2	0.297	410.48	REAL	Cc1cc(C)cc(-n2nc(N3C(=O)N[C@@H](c4ccc5ccccc45)C3=O)cc2C)c1
vSpike-ace2.1-191	Z2107788659	-9.2	0.279	436.51	REAL	O=C(NC[C@H]1CC2c3ccccc3C1c1ccccc12)NNc1ccc2c(=O)[nH]ccc2c1
vSpike-ace2.1-192	Z2154914109	-9.2	0.317	391.47	REAL	CC(=O)N1C[C@H]2CCC[C@H](N3C(=O)N[C@@H](c4ccc5ccccc5c4)C3=O)[C@@H]2C1
vSpike-ace2.1-193	Z2176721349	-9.2	0.287	425.53	REAL	O=C1CCc2ccccC(=O)N3CCC(O)(c4ccc(-c5ccccc5)cc4)CC3)c2C1
vSpike-ace2.1-194	Z2232120680	-9.2	0.297	412.45	REAL	Cc1cc(C(=O)N2CCc3ccccc3[C@@H]2c2ccccc2)nc2nc(O)[nH]c(=O)c12
vSpike-ace2.1-195	Z2234599015	-9.2	0.297	411.46	REAL	Cn1c(=O)c(CN2C(=O)N[C@@](C)(c3cccc4ccccc34)C2=O)cc2ccccc21
vSpike-ace2.1-196	Z2782420202	-9.2	0.317	387.48	REAL	CN1CCC2(CC1)CN(C(=O)c1c[nH]c(=O)c3ccccc13)Cc1ccccc12
vSpike-ace2.1-197	Z2902754938	-9.2	0.297	410.43	REAL	C[C@]1(c2cccc(-c3nc(-c4ccc(-c5ccccc5)cc4)no3)c2)NC(=O)NC1=O
vSpike-ace2.1-198	Z383303418	-9.2	0.287	424.54	REAL	CN1CCC2(CC1)C[C@@H](NC(=O)c1ccc3c(c1)Cc1ccccc1-3)c1ccccc1O2
vSpike-ace2.1-199	Z654045360	-9.2	0.297	405.46	REAL	O=C(Cc1ccc2ccccc2c1)NNC(=O)c1cc2ccccc2c2cccnc12
vSpike-ace2.1-200	Z917573322	-9.2	0.297	417.51	REAL	CC1(C)CC[C@H](NC(=O)CN2C(=O)N[C@@]3(CCc4ccccc43)C2=O)c2ccccc21

Supplementary Table 90. Virtual screening hits 101 to 200 of the screen against the ACE2 binding site of the spike protein (Screen ID: 7). Compounds were filtered so that hits had MW < 600 dalton, cLogP < 6, number of hydrogen bond acceptors < 11, and no reactive functional groups. A few compounds unsuitable for drug discovery were removed by visual inspection. The name of each compound consists of the initial letter 'v' for virtual hit, followed by the target protein name and the target site ('ace2' for ACE2 binding site, 1 for docking scenario 1). The score is the docking score given by QuickVina 2 in kcal/mol. The ligand efficiency (LE) is computed as LE = -score/#NonH, where #NonH is the number of heavy (i.e. non hydrogen) atoms.

Name	Catalog ID	Score	LE	MW	Library	SMILES
vSpike-hr2.1-1	Z1952918462	-10.8	0.327	436.553	REAL	O=C(NCc1ccc2c(c1)CN(C(=O)C1Cc3ccccc3C1)C2)C1Cc2ccccc2C1
vSpike-hr2.1-2	Z1038827768	-10.6	0.393	367.491	REAL	O=C1NCCN1c1cccc(C(=O)N2CCC[C@H]2C[C@H]2C[C@H]3CC[C@H]2C3)c1
vSpike-hr2.1-3	Z2158178895	-10.6	0.342	406.444	REAL	O=C1[C@H]2[C@H]3C[C@@H]4[C@H]2[C@]2(c5nc(-c6ccc(-c7nc8ccccc8[nH]7)cc6)no5)[C@H]1[C@H]3[C@H]42
vSpike-hr2.1-4	PV-001936962679	-10.5	0.389	412.573	REAL	CCCCS(=O)(=O)Nc1ccc(S(=O)(=O)NC[C@H]2C[C@H]3C=C[C@H]2CC3)cc1
vSpike-hr2.1-5	Z1095049172	-10.5	0.309	449.473	REAL	O=C(Nc1ccccc1)Nc1ccc(CC(=O)Nc2nc(-c3ccc4ccccc4n3)n[nH]2)cc1
vSpike-hr2.1-6	Z1443318096	-10.5	0.328	439.4	REAL	Cc1nc(C(=O)N2CCc3cc(-c4ccccc4)ccc32)nn1-c1nnc(C(F)(F)F)[nH]1
vSpike-hr2.1-7	Z1452691933	-10.5	0.318	445.493	REAL	O=C(NC[C@H]1[C@@H]2Cc3ccccc3[C@H]12)NNC(=O)c1ccccc1OCc1ccc(F)cc1
vSpike-hr2.1-8	Z1589889555	-10.5	0.35	410.516	REAL	Cc1cc(NC(=O)Nc2ccc(OC[C@@H]3CCCO3)cc2)n([C@H]2C[C@H]3CC[C@H]2C3)n1
vSpike-hr2.1-9	Z358867962	-10.5	0.35	415.532	REAL	Cc1cccc([C@@H](CC(=O)O[C@@H](C)C(=O)N[C@@H](C)[C@H]2C[C@H]3CC[C@H]2C3)NC(N)=O)c1
vSpike-hr2.1-10	Z901882444	-10.5	0.309	462.43	REAL	O=c1[nH]c(CCn2cnc3ccccc3c2=O)nc2ccc(-c3cccc(C(F)(F)F)c3)cc12
vSpike-hr2.1-11	PV-000960238301	-10.4	0.433	336.474	REAL	C=CCOCCNCC1(NC(=O)[C@@H]2C[C@H]3CC[C@H]2C3)CCOCC1
vSpike-hr2.1-12	Z1685794424	-10.4	0.315	446.505	REAL	C[C@H]1CCCN1C(=O)c1ccc(-c2noc(-c3cc4c([nH]c3=O)CC(C)(C)CC4=O)n2)cc1
vSpike-hr2.1-13	Z1983290694	-10.4	0.359	392.458	REAL	O=C1N[C@]2(C[C@H]3C[C@H]2[C@H]2CCC[C@H]32)C(=O)N1Cc1nc(C(=O)c2ccccc2)no1
vSpike-hr2.1-14	Z966276628	-10.4	0.289	473.535	REAL	O=C(Nc1ccc(C(=O)N2CCc3ccccc32)cc1)c1cnc2c(cnn2Cc2ccccc2)c1
vSpike-hr2.1-15	ZINC000002935991	-10.4	0.289	480.425	ZINC	O=c1oc(-c2cccc(F)c2)nc2ccc(-c3ccc4nc(-c5cccc(F)c5)oc(=O)c4c3)cc21
vSpike-hr2.1-16	ZINC000195528747	-10.4	0.289	476.531	ZINC	O=C1[C@@H]2[C@@H]3C=C[C@@H](C3)[C@@H]2C(=O)N1c1ccc(-c2ccc(N3C(=O)[C@@H]4[C@@H]5C=C[C@@H](C5)[C@@H]4C3=O)cc2)cc1
vSpike-hr2.1-17	Z1727132737	-10.3	0.355	391.517	REAL	O=C(NC[C@H]1[C@H]2Cc3ccccc3[C@H]12)N1CCC(c2nnc3n2CCCC3)CC1
vSpike-hr2.1-18	Z1728627739	-10.3	0.303	448.477	REAL	O=C1C/C(=C\c2ccccc(/C=C3\CC(=O)Nc4ccccc4C3=O)c2)C(=O)c2ccccc2N1
vSpike-hr2.1-19	Z1907686599	-10.3	0.343	430.567	REAL	CC(C)N(C)S(=O)(=O)c1ccc(C(=O)NC[C@@]2(O)[C@H]3[C@@H]4C[C@H]5[C@H]6[C@@H]4C[C@H]3[C@@H]6[C@H]52)cc1
vSpike-hr2.1-20	Z1940864458	-10.3	0.343	414.5	REAL	COCCC[C@@H](Cc1ccccc1)NC(=O)[C@H](C)N1C(=O)[C@H]2[C@@H]3CC[C@H](O3)[C@@H]2C1=O
vSpike-hr2.1-21	Z1952918807	-10.3	0.312	440.498	REAL	O=C(NCc1ccc2c(c1)CN(C(=O)[C@@H]1Cc3ccccc3O1)C2)[C@H]1Cc2ccccc2O1
vSpike-hr2.1-22	Z753588730	-10.3	0.286	492.568	REAL	O=C(NC1CCN(Cc2ccc(F)c(F)c2)CC1)N1CCN(C(=O)c2ccc3ccccc23)CC1
vSpike-hr2.1-23	ZINC000009427922	-10.3	0.294	494.614	ZINC	C[C@@H]1C[C@@H](C)CN(S(=O)(=O)c2ccc(C(=O)Nc3nnc(-c4ccc5c(c4)CCCC5)o3)cc2)C1
vSpike-hr2.1-24	ZINC000014272522	-10.3	0.286	472.499	ZINC	Cc1ccc(-c2nc3cc(NC(=O)c4cccc(-c5cc6ccccc6oc5=O)c4)ccc3o2)cc1
vSpike-hr2.1-25	ZINC000014278977	-10.3	0.271	499.521	ZINC	Cc1cc(NC(=O)c2ccc(-c3cc4ccccc4oc3=O)cc2)ccc1-c1cc2ccccc2oc1=O
vSpike-hr2.1-26	ZINC000245245776	-10.3	0.322	424.499	ZINC	O=C(c1ccccc(N2C(=O)[C@@H]3[C@H]4C=C[C@@H](C4)[C@H]3C2=O)c1)N1CC=C(c2ccccc2)CC1
vSpike-hr2.1-27	ZINC000408682918	-10.3	0.278	493.561	ZINC	Cc1ccc(C(=O)Nc2ccc(NC(=O)c3ccc(N4C(=O)[C@@H]5CC=C(C)C[C@H]5C4=O)cc3)cc2)cc1
vSpike-hr2.1-28	ZINC000409173886	-10.3	0.257	549.693	ZINC	O=C(Nc1ccc(S(=O)(=O)Nc2ccccc2)cc1)c1ccc2c(c1)[C@@H]1[C@H]3CC[C@@H](C3)[C@@H]1[C@@H](c1ccccc1)N2
vSpike-hr2.1-29	Z1023507394	-10.2	0.283	491.565	REAL	Cc1cccc(NC(=O)N2CCC[C@H](C(=O)N3CCC[C@@H](c4nc(-c5cccc(F)c5)no4)C3)C2)c1
vSpike-hr2.1-30	Z1297309213	-10.2	0.309	438.461	REAL	Cn1c(C(=O)N2CCc3cc(-c4ccccc(F)c4)ccc32)cc2c(=O)n3ccccc3nc21
vSpike-hr2.1-31	Z1314536557	-10.2	0.329	412.427	REAL	Cc1nnc(-c2ccc(C(=O)Nc3ccc(-c4nc5cc(F)ccc5[nH]4)cc3)cc2)[nH]1
vSpike-hr2.1-32	Z1314609893	-10.2	0.329	413.411	REAL	Cc1nnc(-c2ccc(C(=O)Nc3ccc(-c4nc5c(F)cccc5[nH]4)cc3)cc2)o1
vSpike-hr2.1-33	Z1335294199	-10.2	0.319	429.45	REAL	C[C@@]1(c2ccc(C(=O)N3CCc4cc(-c5cccc(F)c5)ccc43)cc2)NC(=O)NC1=O
vSpike-hr2.1-34	Z1523624492	-10.2	0.309	446.481	REAL	CC(=O)N1CC[C@H](NC(=O)Nc2ccccc(C(=O)Nc3cccc(F)c3)c2)c2ccccc21
vSpike-hr2.1-35	Z1683033219	-10.2	0.319	423.431	REAL	O=C(Nc1ccccc1)Nc1ccc(-c2noc(-c3cc4ccccc4[nH]c3=O)n2)cc1
vSpike-hr2.1-36	Z1685363160	-10.2	0.309	442.517	REAL	CC(=O)N1CCC[C@H](c2noc([C@H]3CC(=O)N(c4ccc5c(c4)Cc4ccccc4-5)C3)n2)C1
vSpike-hr2.1-37	Z1723444417	-10.2	0.283	477.523	REAL	Cn1c(=O)[nH]c2ncc(-c3cccc(C(=O)Nc4cccc(C(=O)NCc5ccccc5)c4)c3)ccc21
vSpike-hr2.1-38	Z192487054	-10.2	0.3	456.461	REAL	O=C(Nc1ccccc1)Nc1ccc(C(=O)NNC(=O)c2nn(-c3ccccc3)c2O)cc1
vSpike-hr2.1-39	Z2002848514	-10.2	0.309	438.525	REAL	O=C1[C@H]2[C@@H]3C[C@@H]4[C@H]2[C@]2(C(=O)Nc5ccc(CC(=O)N6CCCc7ccccc76)cc5)[C@H]1[C@H]3[C@H]42
vSpike-hr2.1-40	Z2003510133	-10.2	0.352	383.446	REAL	O=C1[C@@H]2[C@@H]3C[C@H]4[C@H]2[C@]2(C(=O)Nc5cccc(-c6ccc7c(c6)CCO7)c5)[C@H]1[C@H]3[C@@H]42
vSpike-hr2.1-41	Z2041378968	-10.2	0.34	401.396	REAL	O=C1[C@H]2[C@@H]3C[C@@H]4[C@H]2[C@@]2(c5nc(-c6ccc(Oc7ccc(F)cc7)nc6)no5)[C@H]1[C@@H]3[C@@H]42
vSpike-hr2.1-42	Z2079983063	-10.2	0.309	436.47	REAL	Cc1cccc(-c2nnc(-c3ccc(C(=O)Nc4ccc5ccn(C)c(=O)c5c4)cc3)o2)c1
vSpike-hr2.1-43	Z2476264366	-10.2	0.34	397.437	REAL	O=C1N[C@]2(c3nc(-c4ccc(-c5nc6ccccc6[nH]5)cc4)no3)C[C@@H]3C[C@H]1[C@H]2C3
vSpike-hr2.1-44	Z413443986	-10.2	0.291	474.607	REAL	O=C(Nc1ccc(CC(=O)N2CCN(c3nccn3)CC2)cc1)N[C@H]1C[C@H]2C[C@H]1[C@H]1CCC[C@H]21
vSpike-hr2.1-45	Z654035428	-10.2	0.291	484.535	REAL	O=C(Cc1ccc2ccccc2c1)NNC(=O)c1ccc(NC2=NS(=O)(=O)c3ccccc32)cc1
vSpike-hr2.1-46	Z73254763	-10.2	0.276	492.49	REAL	O=C1COc2cc(C(=O)NNC(=O)c3ccc(CN4C(=O)c5cccc6cccc4c56)cc3)ccc2N1
vSpike-hr2.1-47	Z907864316	-10.2	0.309	438.49	REAL	O=C(Nc1ccc2[nH]c([C@@H]3CCCO3)nc2c1)c1cnc2c(cnn2Cc2ccccc2)c1
vSpike-hr2.1-48	ZINC000002053169	-10.2	0.34	391.425	ZINC	O=C(Nc1cccc(-c2cc3ccccc3oc2=O)c1)c1ccc2ccccc2c1
vSpike-hr2.1-49	ZINC000002412360	-10.2	0.276	485.494	ZINC	O=C(Nc1ccc(-c2cc3ccccc3oc2=O)cc1)c1cccc(-c2cc3ccccc3oc2=O)c1
vSpike-hr2.1-50	ZINC000002956437	-10.2	0.3	441.529	ZINC	CC12c3ccccc3C(c3cccc31)[C@@H]1C(=O)N(c3ccc(-c4ccccc4)cc3)C(=O)[C@H]12
vSpike-hr2.1-51	ZINC000006792372	-10.2	0.329	407.476	ZINC	Cc1nnc2c(Nc3cc(C)cc(C)c3)nc3ccc(C(=O)c4ccccc4)cc3n12
vSpike-hr2.1-52	ZINC000008832077	-10.2	0.283	472.499	ZINC	Cc1ccccc1-c1nc2cc(NC(=O)c3cccc(-c4cc5ccccc5oc4=O)c3)ccc2o1
vSpike-hr2.1-53	ZINC000010220594	-10.2	0.291	488.567	ZINC	Cc1ccc(-c2nnc(NC(=O)c3ccc(S(=O)(=O)N4CCc5ccccc5C4)cc3)o2)cc1C
vSpike-hr2.1-54	ZINC000239339157	-10.2	0.276	490.557	ZINC	O=C1[C@@H]2[C@H]3C=C[C@@H](C3)[C@H]2C(=O)N1c1ccc(Cc2ccc(N3C(=O)[C@@H]4[C@H]5C=C[C@@H](C5)[C@H]4C3=O)cc2)cc1
vSpike-hr2.1-55	ZINC000240824835	-10.2	0.262	516.556	ZINC	O=C1[C@@H]2[C@H]3C=C[C@@H](C3)[C@H]2C(=O)N1c1ccc2nc(-c3ccc(N4C(=O)[C@@H]5[C@H]6C=C[C@@H](C6)[C@@H]5C4=O)cc3)[nH]c2c1
vSpike-hr2.1-56	PV-001806072119	-10.1	0.361	424.37	REAL	CN(C)C(=O)CN1[C@@H]2CC[C@@H]1CC(NC(=O)[C@@H]1C[C@H]1c1ccc(Cl)c(Cl)c1)C2
vSpike-hr2.1-57	PV-001814387156	-10.1	0.337	409.46	REAL	CC1(C)[C@@H](c2cccc(F)c2)CCN1C(=O)c1ccc(N2NC(=O)CCC2=O)cc1
vSpike-hr2.1-58	PV-001963350596	-10.1	0.316	445.483	REAL	Cc1ccc2c(c1)[C@@H](NC(=O)N1CCN(C(=O)c3ccc(C(F)(F)F)c3)CC1)CCC2
vSpike-hr2.1-59	Z1022495902	-10.1	0.289	465.551	REAL	O=C(NCC(=O)N1CCc2ccccc2C1)[C@@H]1CC(=O)N(c2ccc3c(c2)Cc2ccccc2-3)C1
vSpike-hr2.1-60	Z1039648538	-10.1	0.281	478.55	REAL	O=C1OI[C@H](c2ccccc2)Cc2cc(C(=O)N3CCC(c4nc(-c5ccccc5)n[nH]4)CC3)ccc21
vSpike-hr2.1-61	Z1069484002	-10.1	0.281	484.55	REAL	COc1ccc2cc(/C=C\C(=O)N3CCC(C(=O)c4ccc5c(c4)NC(=O)[C@@H](C)O5)CC3)ccc2c1
vSpike-hr2.1-62	Z1075651470	-10.1	0.306	444.577	REAL	Cc1ccc(C(=O)N2CCC(NC(=O)N3CCC[C@@H](c4cc5ccccc5[nH]4)C3)CC2)cc1
vSpike-hr2.1-63	Z1127251375	-10.1	0.306	473.48	REAL	O=C(c1cc(O)nc2ccc(S(=O)(=O)Nc3ccc(F)cc3)cc12)N1CCC2(C1)OCCO2
vSpike-hr2.1-64	Z1158436379	-10.1	0.281	477.566	REAL	Cc1c(C(=O)N2CCC([C@@H]3C(=O)Nc4ccccc43)CC2)nnn1-c1ccc(-c2ccccc2)cc1
vSpike-hr2.1-65	Z1158447916	-10.1	0.281	489.57	REAL	C[C@H]1Oc2ccc(C(=O)C3CCN(C(=O)[C@H]4CCCN(C(=O)c5ccccc5)C4)CC3)cc2NC1=O
vSpike-hr2.1-66	Z1170482380	-10.1	0.316	428.422	REAL	O=C(Nc1nc(-c2ccccc2F)n[nH]1)c1ccc2c(c1)C[C@@H](c1ccccc1)OC2=O
vSpike-hr2.1-67	Z1197755968	-10.1	0.297	446.469	REAL	O=c1[nH]c(-c2ccccn2)ccc1-c1nc(-c2cccc(Cn3cnc4ccccc43)c2)no1
vSpike-hr2.1-68	Z1205121203	-10.1	0.326	431.515	REAL	Cc1ccc2c1CCCN2C(=O)c1ccc(NC2=NS(=O)(=O)c3ccccc32)cc1
vSpike-hr2.1-69	Z1240723100	-10.1	0.316	449.505	REAL	C[C@H]1c2ccc(F)cc2CCN1C(=O)c1ccc(NC2=NS(=O)(=O)c3ccccc32)cc1
vSpike-hr2.1-70	Z1274012069	-10.1	0.306	446.545	REAL	C[C@H]1IOc2ccc(C(=O)C3CCN(C(=O)[C@@]4(C)CCc5ccccc5C4)CC3)cc2NC1=O
vSpike-hr2.1-71	Z1276023393	-10.1	0.306	443.477	REAL	O=C1CN(C(=O)CCC(=O)N2CCc3cc(-c4ccccc(F)c4)ccc32)c2ccccc2N1
vSpike-hr2.1-72	Z1276024682	-10.1	0.326	420.439	REAL	O=C1[C@@H]2[C@@H]3CC[C@@H](O3)[C@H]2C(=O)N1CC(=O)N1CCc2cc(-c3cccc(F)c3)ccc21
vSpike-hr2.1-73	Z1314609895	-10.1	0.326	412.427	REAL	Cc1nnc(-c2ccc(C(=O)Nc3ccc(-c4nc5c(F)cccc5[nH]4)cc3)cc2)[nH]1
vSpike-hr2.1-74	Z1428902290	-10.1	0.316	430.417	REAL	Cc1nnc(-c2ccc(C(=O)Nc3ccc(-c4nc5cc(F)c(F)cc5[nH]4)cc3)cc2)[nH]1
vSpike-hr2.1-75	Z1443315028	-10.1	0.337	424.52	REAL	O=C([C@H]1CC(=O)N([C@@H]2CCS(=O)(=O)C2)C1)N1CCc2cc(-c3cccc3)ccc21
vSpike-hr2.1-76	Z1532499794	-10.1	0.306	446.456	REAL	C[C@H]1CN(C(=O)c2cnc3ccc(F)cc3c2)CCN1C(=O)c1cnc2ccc(F)cc2c1
vSpike-hr2.1-77	Z1567994687	-10.1	0.306	443.458	REAL	O=C(CN1C(=O)[C@@H]2[C@H]3CC[C@@H](O3)[C@H]2C1=O)Nc1nc(-c2ccccc2)c(-c2ccccc2)o1
vSpike-hr2.1-78	Z1645924039	-10.1	0.306	434.454	REAL	O=C(Nc1cccc(-c2nnc(-c3cccc4ccccn34)o2)c1)[C@@H]1Cc2ccccc2O1
vSpike-hr2.1-79	Z1686058002	-10.1	0.297	449.513	REAL	Cc1nc2cc(-c3nc([C@H]4CC(=O)N(Cc5ccccc5)C4)no3)ccc2n1-c1ccccc1
vSpike-hr2.1-80	Z1723437105	-10.1	0.289	470.488	REAL	Cn1c(=O)[nH]c2ncc(-c3cccc(C(=O)NCc4cccc([C@@]5(C)NC(=O)NC5=O)c4)c3)cc21
vSpike-hr2.1-81	Z1763423365	-10.1	0.297	449.513	REAL	O=C(Nc1ccc(-c2nnc3n2CCCCC3)cc1)c1ccc2[nH]c3ccccc3c(=O)c2c1
vSpike-hr2.1-82	Z1952918213	-10.1	0.306	444.48	REAL	O=C(NCc1ccc2c(c1)CN(C(=O)[C@@H]1Cc3ccc(Fcc31)C2)[C@H]1Cc2ccc(F)cc21
vSpike-hr2.1-83	Z1974565596	-10.1	0.316	440.586	REAL	O=C(Nc1ccc(C(=O)NC2CCCCC2)cc1)N[C@H]1CC[C@@H](C(=O)N2CCCCC2)C1
vSpike-hr2.1-84	Z1983283234	-10.1	0.316	446.428	REAL	O=C1N[C@]2(C[C@H]3C[C@H]2[C@H]2CCC[C@H]32)C(=O)N1Cc1nc(-c2ccc(C(F)(F)F)cc2)no1
vSpike-hr2.1-85	Z2002795192	-10.1	0.374	387.862	REAL	CCOCCOc1c(Cl)cccc1NC(=O)[C@@]12[C@@H]3C(=O)[C@H]4[C@@H]5C[C@H]([C@H]41)[C@H]2[C@H]53
vSpike-hr2.1-86	Z2074160089	-10.1	0.306	437.545	REAL	O=C(c1ccc(-c2cccc3ccenc23)cc1)N1CCC(c2nnc3n2CCCC3)CC1
vSpike-hr2.1-87	Z2098403929	-10.1	0.361	374.37	REAL	O=C(c1ccc2oc(=O)[nH]c2c1)N1CCc2cc(-c3cccc(F)c3)ccc21
vSpike-hr2.1-88	Z2157032951	-10.1	0.374	361.444	REAL	CN(C)C(=O)c1cccc(-c2noc([C@@H]3[C@H]4[C@@H]5C[C@H]6[C@H]7[C@@H]5C[C@@H]4[C@H]7[C@H]63)n2)c1
vSpike-hr2.1-89	Z2158267563	-10.1	0.306	439.47	REAL	O=c1c2ccccc2[nH]c2ccc(-c3nc(-c4ccc(OC5CCOCC5)cc4)no3)cc12
vSpike-hr2.1-90	Z2174554342	-10.1	0.306	438.525	REAL	O=C(N[C@@H]1C[C@H]1c1ccccc1)C1[C@@H]2[C@@H]3C=C[C@@H]([C@H]4C(=O)N(Cc5ccccc5)C(=O)[C@@H]34)[C@H]12
vSpike-hr2.1-91	Z2299370866	-10.1	0.337	395.501	REAL	O=C(c1ccc2c(c1)Cc1ccccc1-2)N1CCC2(CC1)OCCc1ccccc12
vSpike-hr2.1-92	Z237130882	-10.1	0.273	496.565	REAL	O=C(CN1CCC(NC(=O)c2cccc(CN3C(=O)c4ccccc4C3=O)c2)CC1)Nc1ccccc1
vSpike-hr2.1-93	Z325118426	-10.1	0.348	395.497	REAL	Cc1ccc(C23C[C@H]4C[C@@H](CC(C(=O)OCCN5C(=O)CCC5=O)(C4)C2)C3)cc1
vSpike-hr2.1-94	Z372172858	-10.1	0.326	435.547	REAL	O=C(N[C@@H]1C[C@H]2C[C@H]1[C@H]1CCC[C@H]21)c1ccc(NC2=NS(=O)(=O)c3ccccc32)cc1
vSpike-hr2.1-95	Z382990922	-10.1	0.326	409.488	REAL	O=C(c1ccc2c(c1)Cc1ccccc1-2)N1CCC(n2c(=O)[nH]c3ccccc32)CC1
vSpike-hr2.1-96	Z383065896	-10.1	0.337	394.477	REAL	O=C(c1ccc2c(c1)Cc1ccccc1-2)N1CCC(c2nnc3ccccn23)CC1
vSpike-hr2.1-97	Z68839578	-10.1	0.273	495.494	REAL	O=C(NNC(=O)c1nn(-c2ccccc2)cc1O)c1ccc2c(c1)C(=O)N(CCc1ccccc1)C2=O
vSpike-hr2.1-98	Z814170768	-10.1	0.326	435.42	REAL	O=C(N[C@H]1CCc2cc(F)ccc21)N1CCN(C(=O)c2cccc(C(F)(F)F)c2)CC1
vSpike-hr2.1-99	Z966271352	-10.1	0.289	468.52	REAL	O=C(Nc1cccc(C(=O)N2CCc3ccccc32)c1)C1CCN(c2ccc3nnnn3n2)CC1
vSpike-hr2.1-100	Z966782000	-10.1	0.289	470.523	REAL	O=C(CCC(=O)c1ccc2c(c1)OCCCO2)Nc1ccc(C(=O)N2CCc3ccccc32)cc1

Supplementary Table 91. Top 100 virtual hits of the screen against the HR2 binding interface of the HR1 domain of the spike protein (Screen ID: 8). Compounds were filtered so that hits had MW < 600 dalton, cLogP < 6, number of hydrogen bond acceptors < 11, and no reactive functional groups. A few compounds unsuitable for drug discovery were removed by visual inspection. The name of each compound consists of the initial letter 'v' for virtual hit, followed by the target protein name and the target site ('hr2' for HR2 binding site, 1 for docking scenario 1). The score is the docking score given by QuickVina 2 in kcal/mol. The ligand efficiency (LE) is computed as LE = -score/#NonH, where #NonH is the number of heavy (i.e. non hydrogen) atoms.

Name	Catalog ID	Score	LE	MW	Library	SMILES
vSpike-hr2.1-101	Z992145816	-10.1	0.273	493.61	REAL	O=C(c1cccc2ccccc12)N1CCC(C(=O)N2CCC(c3nc(-c4ccccc4)n[nH]3)CC2)CC1
vSpike-hr2.1-102	ZINC000002861242	-10.1	0.337	432.89	ZINC	O=C(Nc1nc2c(cccc2Cl)s1)c1ccc(-c2cc3ccccc3oc2=O)cc1
vSpike-hr2.1-103	ZINC000002896234	-10.1	0.281	472.50	ZINC	Cc1ccccc1-c1nc2ccc(-c3ccc4nc(-c5ccccc5C)oc(=O)c4c3)cc2c(=O)o1
vSpike-hr2.1-104	ZINC000002933884	-10.1	0.273	494.45	ZINC	O=c1oc(-c2cccc(F)c2)nc2cc(Cc3ccc4c(=O)oc(-c5cccc(F)c5)nc4c3)ccc12
vSpike-hr2.1-105	ZINC000008424887	-10.1	0.316	433.38	ZINC	O=C1OC(c2ccc3ccccc3c2)=N/C1=C\c1ccc(-c2cccc(C(F)(F)F)c2)o1
vSpike-hr2.1-106	ZINC000008834428	-10.1	0.297	443.51	ZINC	c1ccc(C2=NN3[C@@H](C2)c2ccccc2O[C@@H]3c2ccc3noc(-c4ccccc4)c3c2)cc1
vSpike-hr2.1-107	ZINC000016047620	-10.1	0.289	488.57	ZINC	Cc1ccc(C)c(-c2nnc(NC(=O)c3ccc(S(=O)(=O)N4CCc5ccccc5C4)cc3)o2)c1
vSpike-hr2.1-108	ZINC000029748612	-10.1	0.259	560.65	ZINC	C[C@@H]1CN(S(=O)(=O)c2ccc3oc4ccccc4c3c2)CCN1S(=O)(=O)c1ccc2oc3ccccc3c2c1
vSpike-hr2.1-109	ZINC000100500728	-10.1	0.273	492.53	ZINC	O=C1[C@@H]2[C@H]3C=C[C@@H](C3)[C@@H]2C(=O)N1c1ccc(Oc2ccc(N3C(=O)[C@@H]4[C@H]5C=C[C@@H](C5)[C@@H]4C3=O)cc2)cc1
vSpike-hr2.1-110	ZINC000225532554	-10.1	0.289	496.65	ZINC	O=C(Nc1ccc(C23CC4CC(CC(C4)C2)C3)cc1)[C@H]1CCCN(S(=O)(=O)c2ccc(F)cc2)C1
vSpike-hr2.1-111	PV-000173288097	-10.0	0.400	344.50	REAL	CO[C@@H](C)CN1[C@H]2CCC[C@H]1CN(C(=O)[C@H](C)Cc1ccccc1)C2
vSpike-hr2.1-112	PV-001814431312	-10.0	0.333	409.46	REAL	CC1(C)[C@@H](c2ccc(F)cc2)CCN1C(=O)c1ccc(N2NC(=O)CCC2=O)cc1
vSpike-hr2.1-113	PV-001820244725	-10.0	0.313	448.55	REAL	O=C(Nc1ccccc1)Nc1ccc(C(=O)NNC(=O)c2cc3c(s2)CCCCC3)cc1
vSpike-hr2.1-114	PV-001841355369	-10.0	0.303	440.50	REAL	Cc1ccc(-c2cc(C(=O)NNC(=O)c3ccc(Oc4ccccc4)cc3C)[nH]n2)cc1C
vSpike-hr2.1-115	PV-001850232915	-10.0	0.357	373.39	REAL	C/C(=C\C(=O)Nc1nc(-c2ccc3ccccc3n2)n[nH]1)c1ccccc(F)c1
vSpike-hr2.1-116	PV-001862202548	-10.0	0.303	443.46	REAL	O=C1C[C@@H](c2ccc(NC(=O)c3ccc(NC(=O)Nc4ccccc4)cc3)cc2)NC(=O)N1
vSpike-hr2.1-117	PV-001864771899	-10.0	0.357	388.35	REAL	O=C(c1cccc(Nc2nnn[nH]2)c1)N1CCc2cc(C(F)(F)F)ccc2C1
vSpike-hr2.1-118	PV-001942704173	-10.0	0.303	452.57	REAL	Cc1cc(C(=O)N2CCCC[C@@H]2C)ccc1NC(=O)N1CCN(c2cccc(F)c2)C[C@@H]1C
vSpike-hr2.1-119	Z1023502786	-10.0	0.303	448.50	REAL	O=C1Nc2ccccc2C[C@@H]1CCC(=O)N1CCC[C@H](c2nc(-c3cccc(F)c3)no2)C1
vSpike-hr2.1-120	Z1040455752	-10.0	0.294	482.65	REAL	Cc1ccccc(C2(CNC(=O)Nc3ccc(S(=O)(=O)/N=C4\CCCCCN4)cc3)CCCC2)c1
vSpike-hr2.1-121	Z1069484462	-10.0	0.286	470.52	REAL	C[C@H]1Oc2ccc(C(=O)C3CCN(C(=O)c4ccc(Oc5ccccc5)cc4)CC3)cc2NC1=O
vSpike-hr2.1-122	Z1069702122	-10.0	0.323	432.83	REAL	O=C(Nc1ccc(-c2nc3c(Cl)cccc3[nH]2)cc1)c1cnc2[nH]c(=O)[nH]c(=O)c2c1
vSpike-hr2.1-123	Z1101970930	-10.0	0.278	483.53	REAL	O=C1CCCc2cc(NC(=O)c3ccc(C(=O)Nc4ccc5c(c4)CCCC(=O)N5)nc3)ccc2N1
vSpike-hr2.1-124	Z1103945576	-10.0	0.294	472.43	REAL	Cc1ccc([C@]2(C)NC(=O)N(CC(=O)Nc3nc(-c4cccc(C(F)(F)F)c4)n[nH]3)C2=O)cc1
vSpike-hr2.1-125	Z1122702353	-10.0	0.286	477.61	REAL	Cc1cc(C(=O)N2CCCC[C@H]2C)ccc1NC(=O)NCC(=O)N1CCN(c2ccccc2)CC1
vSpike-hr2.1-126	Z1161096792	-10.0	0.286	469.54	REAL	O=C(Nc1cccc(NC(=O)c2ccc(N3CCNC3=O)cc2)c1)Nc1ccc2c1CCCC2
vSpike-hr2.1-127	Z1239444736	-10.0	0.303	442.52	REAL	Cc1nc([C@@H]2CCCCN2C(=O)[C@@H]2CC(=O)N(c3ccc4c(c3)Cc3ccccc3-4)C2)no1
vSpike-hr2.1-128	Z1276023806	-10.0	0.345	387.41	REAL	Cn1c(=O)[nH]c2cc(C(=O)N3CCc4cc(-c5cccc(F)c5)ccc43)ccc21
vSpike-hr2.1-129	Z1276024300	-10.0	0.345	385.40	REAL	O=C(c1cc(-c2cccnc2)on1)N1CCc2cc(-c3cccc(F)c3)ccc21
vSpike-hr2.1-130	Z1276024508	-10.0	0.323	416.41	REAL	Cn1c(=O)[nH]c(=O)c2cc(C(=O)N3CCc4cc(-c5cccc(F)c5)ccc43)cnc21
vSpike-hr2.1-131	Z1276024716	-10.0	0.345	389.43	REAL	O=C(c1ccc2c(c1)OCCCO2)N1CCc2cc(-c3cccc(F)c3)ccc21
vSpike-hr2.1-132	Z1281003913	-10.0	0.303	442.45	REAL	O=C1C[C@H](Cc2ccc(C(=O)Nc3ccc(-c4nc5cc(F)ccc5[nH]4)cc3)cc2)C(=O)N1
vSpike-hr2.1-133	Z1315750206	-10.0	0.303	446.48	REAL	O=C([C@@H]1CCCCN1C(=O)c1ccc(=O)[nH]n1)N1CCc2cc(-c3cccc(F)c3)ccc21
vSpike-hr2.1-134	Z1334994284	-10.0	0.313	424.51	REAL	O=C(Nc1ccc(-c2cn3c(n2)CCCC3)cc1)c1ccc(-c2nc(C3CC3)nc3[nH]2)cc1
vSpike-hr2.1-135	Z1360348055	-10.0	0.303	443.48	REAL	O=C(c1ccc(=O)n(-c2cccc(F)c2)c1)N1CCC(c2nc(-c3ccccc3)n[nH]2)CC1
vSpike-hr2.1-136	Z1391613692	-10.0	0.303	435.53	REAL	O=C(N[C@H]1CCCN(C(=O)/C=C/c2ccc3ccccc3n2)C1)c1ccc2ccccc2c1
vSpike-hr2.1-137	Z1410116355	-10.0	0.370	359.36	REAL	O=C(c1ccc2nnnn2c1)N1CCc2cc(-c3cccc(F)c3)ccc21
vSpike-hr2.1-138	Z1428899832	-10.0	0.323	418.36	REAL	O=C(Nc1ccc(-c2nc3cc(F)c(F)cc3[nH]2)cc1)c1ccc2c(c1)C(=O)NC2=O
vSpike-hr2.1-139	Z1447722648	-10.0	0.345	385.51	REAL	O=C(NC[C@H]1[C@H]2CC3ccccc3[C@H]12)N1CCC(c2c[nH]c3ccccc23)CC1
vSpike-hr2.1-140	Z1448565377	-10.0	0.323	417.47	REAL	Cc1ccc(-c2cc(C(=O)NNC(=O)c3ccc4c(c3)CCCC(=O)N4)[nH]n2)cc1C
vSpike-hr2.1-141	Z1449094151	-10.0	0.294	448.56	REAL	O=C(NC[C@@H]1[C@@H]2Cc3ccccc3[C@@H]12)c1ccc(C(=O)NC[C@H]2[C@@H]3Cc4ccccc4[C@@H]23)cc1
vSpike-hr2.1-142	Z1449281955	-10.0	0.345	409.51	REAL	O=C(N[C@H]1CC2CCC1CC2)c1ccc(NC2=NS(=O)(=O)c3ccccc32)cc1
vSpike-hr2.1-143	Z1458999179	-10.0	0.294	448.56	REAL	O=C(NC[C@H]1[C@H]2Cc3ccccc3[C@@H]12)c1ccc(C(=O)NC[C@H]2[C@H]3Cc4ccccc4[C@@H]23)c1
vSpike-hr2.1-144	Z1482218634	-10.0	0.303	441.47	REAL	O=C(c1ccc2noc(-c3ccc(F)cc3)c2c1)N1CCC[C@@H](c2nnc3ccccn23)C1
vSpike-hr2.1-145	Z1504942823	-10.0	0.313	428.49	REAL	O=C(Nc1cccc(NC(=O)[C@@H]2OCCc3ccccc32)c1)[C@H]1OCCc2ccccc21
vSpike-hr2.1-146	Z1521978904	-10.0	0.323	414.44	REAL	O=C(Nc1ccc(-c2nc3cc(F)ccc3[nH]2)cc1)c1ccc(C(=O)NC2CC2)cc1
vSpike-hr2.1-147	Z1523875761	-10.0	0.323	435.91	REAL	CN1Cc2ccccc2[C@@H](NC(=O)Nc2cccc(C(=O)Nc3ccc(Cl)cn3)c2)C1
vSpike-hr2.1-148	Z1575195134	-10.0	0.303	439.47	REAL	O=C(NN1CCc2ccccc2C1=O)c1ccc2c(c1)C(=O)N(CCc1ccccc1)C2=O
vSpike-hr2.1-149	Z1614248827	-10.0	0.313	430.51	REAL	C[C@@H]1C(=O)Nc2cc(C(=O)N3CCC[C@@H](c4n[nH]c(-c5ccccc5)n4)C3)ccc2N1C
vSpike-hr2.1-150	Z1658278065	-10.0	0.323	413.52	REAL	O=C(NC[C@@H]1[C@@H]2Cc3ccccc3[C@H]12)N1CCC[C@H](c2n[nH]c(-c3ccccc3)n2)C1
vSpike-hr2.1-151	Z1672855787	-10.0	0.313	431.47	REAL	Cc1ccc(-c2nc(-c3ccc(N4CCN(c5ccc(F)cc5)CC4)nc3)no2)c(O)c1
vSpike-hr2.1-152	Z1684804818	-10.0	0.303	436.43	REAL	Cc1c(-c2nc(-c3ccc(-c4nc5ccccc5[nH]4)cc3)no2)cnn1-c1ccc(=O)[nH]n1
vSpike-hr2.1-153	Z1685793437	-10.0	0.303	440.46	REAL	C[C@H]1CCCN1C(=O)c1ccc(-c2noc(-c3c[nH]n4c3nc(=O)c3ccccc34)n2)cc1
vSpike-hr2.1-154	Z1723430363	-10.0	0.286	469.54	REAL	Cn1c(=O)[nH]c2ncc(-c3cccc(C(=O)NCc4ccc(C(=O)N5CCCCC5)cc4)c3)cc21
vSpike-hr2.1-155	Z1723444287	-10.0	0.313	423.48	REAL	Cn1c(=O)[nH]c2ncc(-c3cccc(C(=O)N4CCc5c([nH]c6ccccc56)C4)c3)cc21
vSpike-hr2.1-156	Z1728300167	-10.0	0.333	398.51	REAL	O=C(c1ccc2c(c1)Cc1ccccc1-2)N1CCC(c2nnc3n2CCCC3)CC1
vSpike-hr2.1-157	Z1728302983	-10.0	0.303	441.58	REAL	O=C(c1ccc(N2CCCc3ccccc32)cc1)N1CCC(c2nnc3n2CCCC3)CC1
vSpike-hr2.1-158	Z1730347971	-10.0	0.303	441.58	REAL	O=C(c1ccc(N2CCc3ccccc3C2)cc1)N1CCC(c2nnc3n2CCCC3)CC1
vSpike-hr2.1-159	Z183359610	-10.0	0.313	424.42	REAL	Cc1ccc(-c2nnc(-c3ccc(C(=O)NN4C(=O)c5ccccc5C4=O)cc3)o2)cc1
vSpike-hr2.1-160	Z1891946720	-10.0	0.294	447.49	REAL	O=C(c1cccc(N2C(=O)N[C@H](c3ccce4ccccc34)C2=O)c1)N1CCc2ccccc21
vSpike-hr2.1-161	Z1891951269	-10.0	0.303	437.50	REAL	O=C(Cc1ccc(N2C(=O)N[C@@]3(CCc4ccccc43)C2=O)cc1)N1CCc2ccccc21
vSpike-hr2.1-162	Z1975069937	-10.0	0.313	440.52	REAL	O=C(NCc1ccnc(Oc2ccc(F)cc2)c1)N[C@H]1CC[C@@H](C(=O)N2CCCCC2)C1
vSpike-hr2.1-163	Z2004573046	-10.0	0.303	436.51	REAL	Cn1c(=O)[nH]c2ncc(-c3cccc(C(=O)N4[C@@H]5C=C(c6ccccc6)C[C@@H]4CC5)c3)cc21
vSpike-hr2.1-164	Z2021748415	-10.0	0.313	431.50	REAL	O=C(Nc1ccccc1)N1CC[C@@H](NC(=O)N2CCn3c(nnc3-c3ccccc3)C2)C1
vSpike-hr2.1-165	Z2120871249	-10.0	0.303	439.47	REAL	C[C@@]1(c2ccc3ccccc3c2)NC(=O)N(CC(=O)Nc2ncc(-c3ccccc3)[nH]2)C1=O
vSpike-hr2.1-166	Z2156982318	-10.0	0.313	427.43	REAL	O=C(Nc1cccc(-c2noc([C@@]34[C@H]5C(=O)[C@H]6[C@@H]7C[C@H]([C@@H]63)[C@H]4[C@H]75)n2)c1)c1ccccc1F
vSpike-hr2.1-167	Z2159643627	-10.0	0.313	443.32	REAL	Fc1cccc(-n2nnc(-c3nc(-c4ccc(-c5nncs5)cc4)no3)c2C(F)(F)F)c1
vSpike-hr2.1-168	Z2171894126	-10.0	0.303	437.50	REAL	Cc1ccc(-c2noc(C3[C@@H]4[C@@H]5C=C[C@@H]([C@H]6C(=O)N(Cc7ccccc7)C(=O)[C@@H]56)[C@H]34)n2)cc1
vSpike-hr2.1-169	Z2171963536	-10.0	0.303	443.55	REAL	CC1CCC(c2noc(C3[C@@H]4[C@@H]5C=C[C@@H]([C@H]6C(=O)N(Cc7ccccc7)C(=O)[C@@H]56)[C@H]34)n2)CC1
vSpike-hr2.1-170	Z2217760967	-10.0	0.313	442.44	REAL	O=C1CCCc2cc(C(=O)N3CCC[C@H](c4nnc5ccc(C(F)(F)F)cn45)C3)ccc21
vSpike-hr2.1-171	Z2227159726	-10.0	0.333	399.41	REAL	O=C(Nc1nnc2[nH]cnn12)[C@H]1CC(=O)N(c2ccc3c(c2)Cc2ccccc2-3)C1
vSpike-hr2.1-172	Z226202566	-10.0	0.303	458.86	REAL	O=C(Nc1nnc2ccc(Cl)nn12)c1cc(-c2ccc3c(c2)OCCO3)nc2ccccc12
vSpike-hr2.1-173	Z284651570	-10.0	0.345	389.45	REAL	O=C(c1c[nH]nc1-c1ccc2c(c1)OCCO2)N1CCC(c2ccccc2)CC1
vSpike-hr2.1-174	Z2902641389	-10.0	0.286	472.54	REAL	O=C1c2ccc(-c3nc(-c4cccc(CN5CCCCC5)c4)no3)cc2C(=O)N1C[C@H]1CCCO1
vSpike-hr2.1-175	Z367312052	-10.0	0.303	442.45	REAL	Cc1ccc(-c2nnc(-c3ccc(C(=O)Nc4cc5c(cc4F)CCC(=O)N5)cc3)o2)cc1
vSpike-hr2.1-176	Z408892704	-10.0	0.278	482.54	REAL	Cc1cccc(-c2nnc(-c3ccc(C(=O)Nc4ccc(CC(=O)N5CCOCC5)cc4)cc3)o2)c1
vSpike-hr2.1-177	Z412661354	-10.0	0.303	446.55	REAL	C[C@H]1CCCN(C(=O)C2CCN(C(=O)Nc3ccc(-c4nc5ccccc5o4)cc3)CC2)C1
vSpike-hr2.1-178	Z442888540	-10.0	0.303	444.53	REAL	C[C@H]1c2cc3c(cc2C(CCCC2)CN1C(=O)c1cc(=O)n(C)c2ccccc12)OCCO3
vSpike-hr2.1-179	Z647599744	-10.0	0.303	440.50	REAL	O=C(Nc1cccc(N2CCCCC2=O)c1)c1ccc2c(c1)C[C@H](c1ccccc1)OC2=O
vSpike-hr2.1-180	Z771078902	-10.0	0.323	431.52	REAL	C[C@@H]1CCN(C(=O)c2ccc(NC3=NS(=O)(=O)c4ccccc43)cc2)c2ccccc21
vSpike-hr2.1-181	Z872175314	-10.0	0.286	467.57	REAL	Cc1ccc(C(=O)N2CCC[C@H](C)C2)ccc1NC(=O)c1cnc2c(cnn2Cc2ccccc2)c1
vSpike-hr2.1-182	Z966268770	-10.0	0.270	487.51	REAL	O=C(Nc1cccc(C(=O)N2CCc3ccccc32)c1)c1cccc(N2C(=O)c3ccccc3C2=O)c1
vSpike-hr2.1-183	Z966269606	-10.0	0.270	495.53	REAL	O=C(Nc1cccc(C(=O)N2CCc3ccccc32)c1)c1ccc2c(c1)C(=O)N(C[C@H]1CCCO1)C2=O
vSpike-hr2.1-184	Z992145818	-10.0	0.270	493.61	REAL	O=C(c1cccc2ccccc12)N1CCC[C@H](C(=O)N2CCC(c3nc(-c4ccccc4)n[nH]3)CC2)C1
vSpike-hr2.1-185	Z998654248	-10.0	0.313	438.57	REAL	C[C@@H]1CCCN(C(=O)C2CCN(C(=O)c3ccc4c(c3)[nH]c(=O)n4C3CCC3)CC2)C1
vSpike-hr2.1-186	ZINC000000990526	-10.0	0.250	547.99	ZINC	O=C(COC(=O)c1ccc(N2C(=O)[C@H]3[C@@H](C2=O)C2c4ccccc4C3c3ccccc32)cc1)c1ccc(Cl)cc1
vSpike-hr2.1-187	ZINC000001225262	-10.0	0.256	553.36	ZINC	O=C1c2cccc(Cl)c2C(=O)N1c1ccc(-c2nc3ccc(N4C(=O)c5cccc(Cl)c5C4=O)cc3[nH]2)cc1
vSpike-hr2.1-188	ZINC000001664789	-10.0	0.278	468.57	ZINC	O=C1c2ccc3ccccc3c2CC[C@H]1[C@]1([n+]2ccccc2)CCc2c3ccccc3ccc2C1=O
vSpike-hr2.1-189	ZINC000002910998	-10.0	0.286	485.54	ZINC	Cc1c(C(=O)Nc2ccc(Oc3ccccc3)cc2)sc2ncn(Cc3cccc3F)c(=O)c12
vSpike-hr2.1-190	ZINC000002933672	-10.0	0.278	513.34	ZINC	O=c1oc(-c2ccccc2Cl)nc2ccc(-c3ccc4nc(-c5ccccc5Cl)oc(=O)c4c3)ccc21
vSpike-hr2.1-191	ZINC000002935946	-10.0	0.294	456.54	ZINC	O=c1oc(C2CCCCC2)nc2ccc(-c3ccc4nc(C5CCCCC5)oc(=O)c4c3)ccc21
vSpike-hr2.1-192	ZINC000004804594	-10.0	0.270	499.65	ZINC	C[C@]12CC[C@H]3[C@@H](CCC4=CC(=O)CC[C@@]43C)[C@@H]1C[C@@H]1C[C@H]3C(=O)N(Cc4ccccc4)C(=O)[C@@H]3CC(=O)[C@@H]12
vSpike-hr2.1-193	ZINC000009062297	-10.0	0.278	494.57	ZINC	COc1ccc(-c2nnc(NC(=O)c3ccc(NC(=O)Cc4ccc5ccccc54)cc3)s2)cc1
vSpike-hr2.1-194	ZINC000009427939	-10.0	0.286	488.57	ZINC	CN(c1ccccc1)S(=O)(=O)c1ccc(C(=O)Nc2nnc(-c3ccc4c(c3)CCCC4)o2)cc1
vSpike-hr2.1-195	ZINC000009714812	-10.0	0.286	492.53	ZINC	O=C(Nc1nnc(-c2ccc3c(c2)CCCC3)o1)c1cccc(NS(=O)(=O)c2ccc(F)cc2)c1
vSpike-hr2.1-196	ZINC000011912829	-10.0	0.294	453.58	ZINC	O=C(CCc1ccccnc1)N1CC[C@H]2[C@H](CCCN2C(=O)c2ccc(-c3ccccc3)cc2)C1
vSpike-hr2.1-197	ZINC000012524867	-10.0	0.303	438.53	ZINC	Cc1ccc(-c2nnc(-c3ccc(C(=O)Nc4ccc(N5CCCCC5)cc4)cc3)o2)cc1
vSpike-hr2.1-198	ZINC000033254447	-10.0	0.278	487.60	ZINC	Cc1nc(-c2ccc(C(=O)N3CCC(C(=O)Nc4ccc(N5CCC(C)CC5)cc4)CC3)cc2)no1
vSpike-hr2.1-199	ZINC000064439108	-10.0	0.294	471.54	ZINC	Cc1c(-c2nc(-c3ccccc3)no2)sc2ncn(CC(=O)Nc3ccc(C)c(C)c3)c(=O)c12
vSpike-hr2.1-200	ZINC000100485501	-10.0	0.313	410.43	ZINC	O=C1c2ccc3c4c(ccc(c24)C2=Nc4ccccc4[C@H]21)C1=Nc2ccccc2[C@@H]1C3=O

Supplementary Table 92. Virtual screening hits 101 to 200 of the screen against the HR2 binding interface of the HR1 domain of the spike protein (Screen ID: 8). Compounds were filtered so that hits had MW < 600 dalton, cLogP < 6, number of hydrogen bond acceptors < 11, and no reactive functional groups. A few compounds unsuitable for drug discovery were removed by visual inspection. The name of each compound consists of the initial letter 'v' for virtual hit, followed by the target protein name and the target site ('hr2' for HR2 binding site, 1 for docking scenario 1). The score is the docking score given by QuickVina 2 in kcal/mol. The ligand efficiency (LE) is computed as LE = -score/#NonH, where #NonH is the number of heavy (i.e. non hydrogen) atoms.

Name	Catalog ID	Score	LE	MW	Library	SMILES
vTmprss2-as1-1	Z131645048	-11.7	0.3441176	474.54	REAL	O=C(c1ccc2c(c1)-c1ccccc1C2)N1CCN(S(=O)(=O)c2ccc3[nH]c(=O)[nH]c3c2)CC1
vTmprss2-as1-2	Z2001060769	-11.7	0.3441176	447.497	REAL	O=C1C[C@@H](c2nc(Cc3ccc4[nH]ncc4c3)no2)CN1c1ccc2c(c1)Cc1ccccc1-2
vTmprss2-as1-3	Z1927955742	-11.3	0.3424242	434.498	REAL	Nc1ncc2c(n1)CCN(C(=O)CCC(=O)c1ccc3ccc4ccc5ccc1c3c45)C2
vTmprss2-as1-4	Z2227147910	-11.3	0.353125	424.459	REAL	O=C(Nc1cccc2[nH]c(=O)[nH]c12)[C@@H]1CC(=O)N(c2ccc3c(c2)Cc2ccccc2-3)C1
vTmprss2-as1-5	Z1167185258	-11.2	0.35	427.478	REAL	O=C(c1nn(-c2ccc(F)cc2)ccc1=O)N1CCC(c2cccc3ccccc23)CC1
vTmprss2-as1-6	Z1454726034	-11.2	0.4	413.525	REAL	Nc1nsc(N2CCN(S(=O)(=O)c3ccc4c(c3)Cc3ccccc3-4)CC2)n1
vTmprss2-as1-7	Z2178142149	-11.2	0.35	425.443	REAL	O=C(Nc1cccc2[nH]c(=O)oc12)[C@@H]1CC(=O)N(c2ccc3c(c2)Cc2ccccc2-3)C1
vTmprss2-as1-8	Z806298542	-11.2	0.3027027	494.593	REAL	NC(=O)c1ccc(CN2CCN(C(=O)[C@H]3CC(=O)N(c4ccc5c(c4)Cc4ccccc4-5)C3)CC2)cc1
vTmprss2-as1-9	Z1518156451	-11.1	0.3363636	444.533	REAL	CC(=O)c1ccc2c(c1)CCN(C(=O)[C@@H]1CCCN(C(=O)c3ccc4[nH]ncc4c3)C1)CC2
vTmprss2-as1-10	Z1575962044	-11.1	0.346875	433.554	REAL	Cc1cccc(C2=CCN(C(=O)NCc3ccenc3N3CCC(C(N)=O)CC3)CC2)c1
vTmprss2-as1-11	Z1910609877	-11.1	0.3363636	443.506	REAL	O=C(CCC(=O)N1CCC(c2cccc3ccccc23)CC1)Nc1ccc2[nH]c(=O)[nH]c2n1
vTmprss2-as1-12	Z2053436568	-11.1	0.3827586	387.486	REAL	Cc1cc(-c2ccccc2)ccc1NC(=O)N1CCC[C@H](c2ccnc(N)n2)C1
vTmprss2-as1-13	Z940088872	-11.1	0.3363636	440.502	REAL	CN1CC(=O)N(c2ccc(NC(=O)N3CC=C(c4cccc5ccccc45)CC3)c2)C1=O
vTmprss2-as1-14	ZINC000000991027	-11.1	0.2846154	514.536	ZINC	O=C(O)c1ccc(NC(=O)c2cccc(N3C(=O)[C@H]4[C@@H](C3=O)C3c5ccccc5C4c4ccccc43)c2)cc1
vTmprss2-as1-15	ZINC000000991029	-11.1	0.2846154	514.536	ZINC	O=C(O)c1ccc(NC(=O)c2cccc(N3C(=O)[C@@H]4[C@@H](C3=O)C3c5ccccc5C4c4ccccc43)c2)cc1
vTmprss2-as1-16	ZINC000012360361	-11.1	0.3171429	458.516	ZINC	O=C(Cc1cccc2ccccc21)NN1C(=O)[C@H]2[C@@H](C1=O)C1c3ccccc3C2c2ccccc21
vTmprss2-as1-17	Z131639334	-11	0.3235294	494.595	REAL	O=C(c1cc2c(s1)-c1ccccc1CC2)N1CCN(S(=O)(=O)c2ccc3[nH]c(=O)[nH]c3c2)CC1
vTmprss2-as1-18	Z1391614241	-11	0.3333333	445.493	REAL	O=C1C[C@H](C(=O)N2CCC[C@@H](NC(=O)c3ccc4ccccc4c3)C2)c2ccc(F)cc2N1
vTmprss2-as1-19	Z1395766217	-11	0.3333333	443.506	REAL	O=C(CN1CCC[C@H](NC(=O)c2ccc3ccccc3c2)C1)Nc1ccc2[nH]c(=O)[nH]c2c1
vTmprss2-as1-20	Z1442087775	-11	0.3333333	445.565	REAL	Cc1ccc(C)c(N2CCN(C(=O)[C@@H]3CCCN(C(=O)c4ccc5[nH]ncc5c4)C3)CC2)c1
vTmprss2-as1-21	Z1443316769	-11	0.3333333	439.518	REAL	Cc1nc2c(C(N)=O)cnn2c(C)c1CCC(=O)N1CCc2cc(-c3ccccc3)ccc21
vTmprss2-as1-22	Z1581633558	-11	0.3548387	413.476	REAL	NC(=O)c1cc(OC2CCN(C(=O)c3ccc4c(c3)-c3ccccc3C4)CC2)ccn1
vTmprss2-as1-23	Z1654001326	-11	0.3333333	438.486	REAL	O=C(NCc1ccc2[nH]c(=O)[nH]c2c1)[C@H]1CC(=O)N(c2ccc3c(c2)Cc2ccccc2-3)C1
vTmprss2-as1-24	Z1683768061	-11	0.3333333	436.47	REAL	NC(=O)c1cccc(-c2noc([C@@H]3CC(=O)N(c4ccc5c(c4)Cc4ccccc4-5)C3)n2)c1
vTmprss2-as1-25	Z2027241503	-11	0.3666667	403.485	REAL	NC(=O)c1ncn(C2CCN(C(=O)[C@H]3C[C@@H]3c3ccc4ccccc4c3)CC2)c1N
vTmprss2-as1-26	Z804640398	-11	0.34375	425.443	REAL	O=C(Nc1ccc2oc(=O)[nH]c2c1)[C@H]1CC(=O)N(c2ccc3c(c2)Cc2ccccc2-3)C1
vTmprss2-as1-27	Z806473494	-11	0.3333333	439.47	REAL	O=C1COc2cc(NC(=O)[C@H]3CC(=O)N(c4ccc5c(c4)Cc4ccccc4-5)C3)ccc2N1
vTmprss2-as1-28	Z806562132	-11	0.3333333	442.517	REAL	Cc1noc(C2CCN(C(=O)[C@@H]3CC(=O)N(c4ccc5c(c4)Cc4ccccc4-5)C3)CC2)n1
vTmprss2-as1-29	Z806580470	-11	0.3333333	439.514	REAL	CN(Cc1eccc(C(N)=O)c1)C(=O)[C@@H]1CC(=O)N(c2ccc3c(c2)Cc2ccccc2-3)C1
vTmprss2-as1-30	Z826980228	-11	0.3548387	439.499	REAL	Nc1nn2c(=O)cc(CN3CCN(S(=O)(=O)c4ccc5ccccc5c4)CC3)nc2[nH]1
vTmprss2-as1-31	ZINC000012112313	-11	0.34375	427.459	ZINC	O=C(c1ccc(-c2ccccc2)cc1)[C@@H]1CCCN(C(=O)c2ccc3c(c2)no[n+]3[O-])C1
vTmprss2-as1-32	ZINC000257281890	-11	0.3235294	461.56	ZINC	CC1(C)Oc2ccccc2[C@@H]2O[C@@H]3CCN(CC(=O)N4CCC(=O)Nc5ccccc54)C[C@H]3C[C@H]21
vTmprss2-as1-33	PV-001917095232	-10.9	0.3633333	420.438	REAL	Nc1nn2c(=O)cc(CN3CCC(CCc4cccc(C(F)(F)F)c4)CC3)nc2[nH]1
vTmprss2-as1-34	PV-001966451252	-10.9	0.3758621	391.47	REAL	Cc1cc(C)cc(C2=CCN(C(=O)N[C@H](C)c3ccc4[nH]c(=O)oc4c3)CC2)c1
vTmprss2-as1-35	Z1079361744	-10.9	0.3516129	414.507	REAL	Cn1cc(C(=O)NCC2CCN(C(=O)c3ccc4c(c3)-c3ccccc3C4)CC2)cn1
vTmprss2-as1-36	Z1361235893	-10.9	0.330303	435.53	REAL	O=C(c1c2c(nc3ccccc13)/C(=C\c1ccccc1)CC2)N1CCC(c2nnc[nH]2)CC1
vTmprss2-as1-37	Z1391618928	-10.9	0.3516129	415.448	REAL	O=C(N[C@@H]1CCCN(C(=O)c2ccc3[nH]c(=O)oc3c2)C1)c1ccc2ccccc2c1
vTmprss2-as1-38	Z1392750588	-10.9	0.3633333	399.453	REAL	O=C(N[C@@H]1CCCN(C(=O)c2ccc3[nH]nnc3c2)C1)c1ccc2ccccc2c1
vTmprss2-as1-39	Z1669331888	-10.9	0.3633333	400.441	REAL	O=C(N[C@@H]1CCCN(C(=O)c2cnc3[nH]nnc3c2)C1)c1ccc2ccccc2c1
vTmprss2-as1-40	Z1771159538	-10.9	0.3516129	417.443	REAL	O=C(N[C@H]1CCCN(C(=O)c2cc3[nH]nnc3cc2F)C1)c1ccc2ccccc2c1
vTmprss2-as1-41	Z2075859652	-10.9	0.3516129	430.433	REAL	Cc1[nH]c(-c2cccc(C(F)(F)F)c2)nc1C(=O)N1CCC[C@H](c2ccnc(N)n2)C1
vTmprss2-as1-42	Z2174760155	-10.9	0.3758621	386.454	REAL	Nc1ncc(N2CCC[C@@H](OC(=O)c3ccc4c(c3)Cc3ccccc3-4)C2)n1
vTmprss2-as1-43	Z2174773215	-10.9	0.3758621	386.454	REAL	Nc1ncc(N2CCC[C@@H](OC(=O)c3ccc4c(c3)-c3ccccc3C4)C2)n1
vTmprss2-as1-44	Z2225645671	-10.9	0.330303	444.49	REAL	O=C([C@@H]1CC(=O)N(c2ccc3c(c2)Cc2ccccc2-3)C1)N1CCC[C@@H](c2n[nH]c(=O)o2)C1
vTmprss2-as1-45	Z2225837007	-10.9	0.330303	444.49	REAL	O=C([C@@H]1CC(=O)N(c2ccc3c(c2)Cc2ccccc2-3)C1)N1CCC(c2n[nH]c(=O)o2)CC1
vTmprss2-as1-46	Z382976940	-10.9	0.330303	440.498	REAL	O=C(Nc1ccc2c(c1)OCO2)C1CCN(C(=O)c2ccc3c(c2)Cc2ccccc2-3)CC1
vTmprss2-as1-47	Z460978596	-10.9	0.3114286	487.539	REAL	O=C(c1cc2ccccc2c2ccenc12)N1CCN(S(=O)(=O)c2ccc3[nH]c(=O)[nH]c3c2)CC1
vTmprss2-as1-48	Z757866178	-10.9	0.3516129	406.444	REAL	O=C1CN=C(NC(=O)c2cc(-c3ccc(-c4ccccc4)cc3)nc3ccccc23)N1
vTmprss2-as1-49	ZINC000000944501	-10.9	0.3114286	482.515	ZINC	O=C(O)c1ccc(NC2=C/C(=N\S(=O)(=O)c3ccc4ccccc4c3)c3ccccc3C2=O)cc1
vTmprss2-as1-50	ZINC000103721003	-10.9	0.3114286	482.515	ZINC	O=C(O)c1ccc(NC2=C/C(=N/S(=O)(=O)c3ccc4ccccc4c3)c3ccccc3C2=O)cc1
vTmprss2-as1-51	PV-001948149596	-10.8	0.3375	430.506	REAL	Cc1ccc(NC(=O)NCC(C)(C)c2ccc3ccccc3c2)cc1N1C(=O)CNC1=O
vTmprss2-as1-52	Z1128760223	-10.8	0.3272727	436.474	REAL	O=C(Nc1ccc(-c2nnn[nH]2)cc1)[C@H]1CC(=O)N(c2ccc3c(c2)Cc2ccccc2-3)C1
vTmprss2-as1-53	Z1198954945	-10.8	0.3375	423.471	REAL	O=C1Cc2cc(NC(=O)[C@H]3CC(=O)N(c4ccc5c(c4)Cc4ccccc4-5)C3)ccc2N1
vTmprss2-as1-54	Z1229725100	-10.8	0.3272727	442.474	REAL	C[C@@]1(c2ccc3ccccc3c2)NC(=O)N(CC(=O)N2CCC(=O)Nc3ccccc32)C1=O
vTmprss2-as1-55	Z1233881640	-10.8	0.3375	434.513	REAL	C[C@H]1C[C@@H](c2ccc(F)cc2)CN1C(=O)[C@H]1CCCN(C(=O)c2ccc3[nH]ncc3c2)C1
vTmprss2-as1-56	Z1276146317	-10.8	0.36	395.417	REAL	O=C(Nc1[nH]ncc1-c1ccc2c(c1)OCO2)c1ccc2c(c1)-c1ccccc1C2
vTmprss2-as1-57	Z1276150313	-10.8	0.36	395.417	REAL	O=C(Nc1[nH]ncc1-c1ccc2c(c1)OCO2)c1ccc2c(c1)Cc1ccccc1-2
vTmprss2-as1-58	Z131639554	-10.8	0.3085714	494.527	REAL	CC(=O)c1ccc(-c2ccc(C(=O)N3CCN(S(=O)(=O)c4ccc5[nH]c(=O)[nH]c5c4)CC3)o2)cc1
vTmprss2-as1-59	Z1329850286	-10.8	0.3375	429.45	REAL	NC(=O)c1ccc(NC(=O)[C@H]2CC(=O)N(c3ccc4c(c3)Cc3ccccc3-4)C2)c(F)c1
vTmprss2-as1-60	Z1337296307	-10.8	0.3272727	438.486	REAL	Cc1nc(-c2ccc(C)c(NC(=O)c3ccc4c(c3)C[C@@H](c3ccccc3)OC4=O)c2)n[nH]1
vTmprss2-as1-61	Z1348302641	-10.8	0.3483871	435.507	REAL	O=C(Nc1ccc2[nH]nnc2c1)C1CCN(S(=O)(=O)c2ccc3ccccc3c2)CC1
vTmprss2-as1-62	Z1392745135	-10.8	0.36	401.465	REAL	NC(=O)c1ccc(C(=O)N2CCC[C@H](NC(=O)c3ccc4ccccc4c3)C2)cc1
vTmprss2-as1-63	Z1392753478	-10.8	0.3375	427.459	REAL	O=C(N[C@@H]1CCCN(C(=O)c2ccc3c(c2)C(=O)NC3=O)C1)c1ccc2ccccc2c1
vTmprss2-as1-64	Z1393508577	-10.8	0.3375	434.47	REAL	NC(=O)c1ccc(F)c(NC(=O)N2CCC[C@@H](NC(=O)c3ccc4ccccc4c3)C2)c1
vTmprss2-as1-65	Z1410300309	-10.8	0.36	400.441	REAL	O=C(N[C@@H]1CCCN(C(=O)c2ccc3nnnn3c2)C1)c1ccc2ccccc2c1
vTmprss2-as1-66	Z1487641111	-10.8	0.3483871	417.511	REAL	O=C(NNc1ccce2c1CCCC2)[C@H]1CCCN(C(=O)c2ccc3[nH]ncc3c2)C1
vTmprss2-as1-67	Z1543065403	-10.8	0.3483871	415.452	REAL	O=C(N[C@@H]1CCCN(C(=O)c2ccc3n[nH]c(=O)n3c2)C1)c1ccc2ccccc2c1
vTmprss2-as1-68	Z1620593776	-10.8	0.3483871	414.511	REAL	Cc1ccc2[nH]c3c(c2c1)C[C@H](NC(=O)Nc1cc(-c2n[nH]c(C)n2)cc1C)CC3
vTmprss2-as1-69	Z1626791432	-10.8	0.3483871	414.507	REAL	Cc1ccccc1C1=CCN(C(=O)[C@@H]2CCCN(C(=O)c3ccc4[nH]ncc4c3)C2)C1
vTmprss2-as1-70	Z1627330143	-10.8	0.3272727	442.478	REAL	Cn1cc(-c2nc([C@@H]3COCCN3C(=O)Nc3ccc4c(c3)Cc3ccccc3-4)no2)cn1
vTmprss2-as1-71	Z1643822107	-10.8	0.36	395.465	REAL	Cc1nc(-c2cccc(NC(=O)N3CC=C(c4cccc5ccccc45)C3)c2)n[nH]1
vTmprss2-as1-72	Z1740710352	-10.8	0.3483871	416.523	REAL	Cc1cc(C)c2c(c1)CN(C(=O)[C@@H]1CCCN(C(=O)c3ccc4[nH]ncc4c3)C1)CC2
vTmprss2-as1-73	Z1785648029	-10.8	0.36	397.473	REAL	O=C(O)c1ccccc1C1CCN(C(=O)c2ccc3c(c2)-c2ccccc2C3)CC1
vTmprss2-as1-74	Z1820356932	-10.8	0.36	403.441	REAL	Nc1nc(=O)[nH]cc1N1CCN(C(=O)Cc2cc3c(ccc4ccccc43)o2)CC1
vTmprss2-as1-75	Z1827620903	-10.8	0.3375	429.522	REAL	Nc1nc(=O)[nH]cc1N1CCN(C(=O)CCCc2ccc3c(c2)-c2ccccc2C3)CC1
vTmprss2-as1-76	Z1835892373	-10.8	0.36	418.48	REAL	Nc1ncc2c(n1)CCN(C(=O)CSc1nnc(-c3ccc4ccccc4c3)o1)C2
vTmprss2-as1-77	Z1899606016	-10.8	0.36	402.457	REAL	Cc1nc(Cn2cc(C(=O)N3CCC(c4ccc5ccccc45)CC3)nn2)no1
vTmprss2-as1-78	Z1901061377	-10.8	0.36	400.441	REAL	Cc1nc(Cn2cc(C(=O)N3CC=C(c4cccc5ccccc45)CC3)nn2)no1
vTmprss2-as1-79	Z1948615421	-10.8	0.4	361.444	REAL	O=C(Cc1c[nH]c2ccccc12)NNC(=O)[C@@H]1[C@@H]2[C@H]3C[C@@H]4[C@@H]5[C@H]3C[C@H]2[C@@H]5[C@H]41
vTmprss2-as1-80	Z1953861210	-10.8	0.3272727	446.433	REAL	O=C(Nc1ccc(F)c(N2CCOC2=O)c1)c1ccc2c(c1)C[C@@H](c1ccccc1)OC2=O
vTmprss2-as1-81	Z2004572359	-10.8	0.3272727	440.545	REAL	O=C(c1ccc2[nH]ncc2c1)N1CCC[C@@H](C(=O)N2[C@@H]3C=C(c4ccccc4)C[C@@H]2CC3)C1
vTmprss2-as1-82	Z2015597943	-10.8	0.3272727	441.49	REAL	Nc1nccc([C@H]2CCCN(CC(=O)Nc3ccc4c(c3)C(=O)c3ccccc3C4=O)C2)n1
vTmprss2-as1-83	Z2027111833	-10.8	0.3724138	384.438	REAL	Cc1ccc(-c2n[nH]c(=O)[nH]2)cc1NC(=O)[C@H]1C[C@@H]1c1ccc2ccccc2c1
vTmprss2-as1-84	Z2114995716	-10.8	0.3375	430.482	REAL	O=C(Nc1ccc(F)c(N2CCCNC2=O)c1)N1CC=C(c2cccc3ccccc23)C1
vTmprss2-as1-85	Z2225291359	-10.8	0.3176471	449.509	REAL	O=C(NCc1ccc2c(=O)cc[nH]c2c1)[C@@H]1CC(=O)N(c2ccc3c(c2)Cc2ccccc2-3)C1
vTmprss2-as1-86	Z2226909716	-10.8	0.3483871	406.448	REAL	O=C(NNc1nnc[nH]1)c1cc(-c2ccc(-c3ccccc3)cc2)nc2ccccc12
vTmprss2-as1-87	Z2227159520	-10.8	0.3272727	431.458	REAL	O=C(Nc1nnc2[nH]cnn12)c1cc(-c2ccc(-c3ccccc3)cc2)nc2ccccc12
vTmprss2-as1-88	Z2639648322	-10.8	0.4	359.432	REAL	Nc1nnc(C2CCN(C(=O)c3ccc4c(c3)-c3ccccc3C4)CC2)[nH]1
vTmprss2-as1-89	Z2654576638	-10.8	0.3857143	376.423	REAL	Nc1nn2c(=O)cc(CN3CCN(c4ccc5ccccc5n4)CC3)nc2[nH]1
vTmprss2-as1-90	Z338530490	-10.8	0.3085714	475.543	REAL	O=C([C@@H]1CN(C(=O)[C@H]2CC(=O)N(c3ccc4c(c3)CCC4)C2)c2ccccc2O1)N1CCOCC1
vTmprss2-as1-91	Z338795670	-10.8	0.3483871	447.444	REAL	O=C(Nc1nc2cc(C(F)(F)F)ccc2s1)C1CCN(c2ccc3nncn3n2)CC1
vTmprss2-as1-92	Z605475312	-10.8	0.3176471	485.563	REAL	Cc1c(C)c(C)c(S(=O)(=O)N2CCN(C(=O)c3cnc4[nH]c(=O)[nH]c(=O)c4c3)CC2)c(C)c1C
vTmprss2-as1-93	Z642644784	-10.8	0.3272727	437.502	REAL	Cc1nc2c(C(N)=O)cnn2c(C)c1CCC(=O)Nc1cccc(C\#Cc2ccccc2)c1
vTmprss2-as1-94	Z749458592	-10.8	0.36	394.429	REAL	O=C(NNC(=O)C1c2ccccc2Oc2ccccc21)c1ccc2ccccc2c1
vTmprss2-as1-95	Z847629948	-10.8	0.3176471	455.473	REAL	Cn1ncc2c(=O)[nH]c(COC(=O)[C@@H]3CC(=O)N(c4ccc5c(c4)Cc4ccccc4-5)C3)nc21
vTmprss2-as1-96	Z924788550	-10.8	0.3375	426.475	REAL	O=C(Nc1cccc(N2C(=O)CNC2=O)c1)N1CC=C(c2cccc3ccccc23)CC1
vTmprss2-as1-97	Z998116374	-10.8	0.3272727	438.486	REAL	O=C(Nc1ccc2oc3ccccc3c2c1)[C@@H]1CCCN(C(=O)c2ccc3[nH]ncc3c2)C1
vTmprss2-as1-98	Z998966812	-10.8	0.3176471	458.56	REAL	Cc1ccc(C(=O)C2CCN(C(=O)[C@@H]3CCCN(C(=O)c4ccc5[nH]ncc5c4)C3)CC2)cc1
vTmprss2-as1-99	ZINC000000991026	-10.8	0.2769231	514.536	ZINC	O=C(O)c1ccc(NC(=O)c2cccc(N3C(=O)[C@H]4[C@H](C3=O)C3c5ccccc5C4c4ccccc43)c2)cc1
vTmprss2-as1-100	ZINC000008745390	-10.8	0.3176471	460.445	ZINC	C[C@@]1(c2ccc3ccccc3c2)NC(=O)N(CC(=O)NC(=O)Nc2ccc3c(c2)OCO3)C1=O

Supplementary Table 93. Top 100 virtual hits of the screen against the active site of TMPRSS2 (Screen ID: 6). Compounds were filtered so that hits had MW < 600 dalton, cLogP < 6, number of hydrogen bond acceptors < 11, and no reactive functional groups. A few compounds unsuitable for drug discovery were removed by visual inspection. The name of each compound consists of the initial letter 'v' for virtual hit, followed by the target protein name and the target site ('as' for active site, 1 for docking scenario 1). The score is the docking score given by QuickVina 2 in kcal/mol. The ligand efficiency (LE) is computed as LE = -score/#NonH, where #NonH is the number of heavy (i.e. non hydrogen) atoms.

Name	Catalog ID	Score	LE	MW	Library	SMILES
vTmprss2-as1-101	ZINC000011715672	-10.8	0.318	454.48	ZINC	O=C(Nc1ccc2c(c1)OCO2)C1CCN(C(=O)c2ccc3c(c2)C(=O)c2ccccc2-3)CC1
vTmprss2-as1-102	ZINC000013382030	-10.8	0.318	452.46	ZINC	O=C(c1ccc(F)cc1)c1ccc(-c2[nH]c(-c3ccccc3O)nc2-c2ccc(F)cc2)cc1
vTmprss2-as1-103	ZINC000015675930	-10.8	0.309	465.51	ZINC	COc1ccc(CC(=O)N2Cc3nc[nH]c3C[C@H]2c2nc(-c3ccc4ccccc4c3)no2)cc1
vTmprss2-as1-104	ZINC000020440415	-10.8	0.292	490.57	ZINC	O=C(c1ccccc1)N1CCC[C@H](c2nc(=O)c3nnn(Cc4ccc(-c5ccccc5)cc4)c3[nH]2)C1
vTmprss2-as1-105	ZINC000020714006	-10.8	0.309	475.55	ZINC	O=C(CNC(=O)N1CCc2c3ccccc3[nH]c2C1)N1CCN(Cc2ccc3c(c2)OCO3)CC1
vTmprss2-as1-106	ZINC000085392756	-10.8	0.270	530.67	ZINC	Cc1ccc(N2C[C@@H](C(=O)N3CCC(c4c[nH]c5ccccc54)(c4c[nH]c5ccccc54)CC3)CC2=O)c(C)c1
vTmprss2-as1-107	ZINC000257332760	-10.8	0.327	450.53	ZINC	CC1(C)Oc2ccccc2[C@@H]2O[C@@H]3CCN(CC(=O)Nc4ccc(C(=O)O)cc4)C[C@H]3C[C@H]21
vTmprss2-as1-108	ZINC000257335224	-10.8	0.327	451.45	ZINC	O=C(c1ccc2[nH]nnc2c1)N1CCC[C@@H](c2cccc(-c3cccc(C(F)(F)F)c3)n2)C1
vTmprss2-as1-109	ZINC000409336132	-10.8	0.327	459.97	ZINC	O=C(O)c1ccc2c(c1)[C@@H]1[C@H]3CC[C@@H](C3)[C@@H]1[C@H](c1ccc(OCc3ccc(Cl)cc3)cc1)N2
vTmprss2-as1-110	ZINC000521398113	-10.8	0.318	463.53	ZINC	O=C(O)C1CCN(C(=O)N2CCN(C(=O)OCC3c4ccccc4-c4ccccc43)CC2)CC1
vTmprss2-as1-111	PV-000316113690	-10.7	0.369	391.43	REAL	O=C(N[C@@H]1CN(C(=O)c2c[nH]nn2)C[C@@H]1O)[C@@H]1C[C@H]1c1ccc2ccccc2c1
vTmprss2-as1-112	PV-001803737801	-10.7	0.324	455.40	REAL	O=C(C[C@@H]1NC(=O)c2ccccc2NC1=O)Nc1cnc(-c2cccc(C(F)(F)F)c2)cn1
vTmprss2-as1-113	PV-001813620200	-10.7	0.369	394.43	REAL	Cc1ccc(C(=O)N2CCC[C@H](C(=O)Nc3nc(=O)c4cnn(C)c4[nH]3)C2)cc1
vTmprss2-as1-114	PV-001825816062	-10.7	0.357	402.41	REAL	O=C(C[C@@H]1NC(=O)c2ccccc2NC1=O)NNC(=O)c1ccc2ccccc2c1
vTmprss2-as1-115	PV-001942501849	-10.7	0.334	447.42	REAL	Cc1ccc(NC(=O)c2cccc(C(F)(F)F)c2)cc1NC(=O)NNc1nnc(C)n1C
vTmprss2-as1-116	PV-001951115204	-10.7	0.357	445.52	REAL	NC(=O)c1ncc(NC(=O)N2CCN(S(=O)(=O)c3ccc4ccccc4c3)CC2)s1
vTmprss2-as1-117	PV-001966450996	-10.7	0.382	377.44	REAL	Cc1cccc(C2=CCN(C(=O)N[C@H](C)c3ccc4[nH]c(=O)oc4c3)CC2)c1
vTmprss2-as1-118	PV-001966451451	-10.7	0.369	393.49	REAL	Cc1ccc(CC2CCN(C(=O)N[C@H](C)c3ccc4[nH]c(=O)oc4c3)CC2)cc1
vTmprss2-as1-119	Z1066143110	-10.7	0.345	447.54	REAL	NC(=O)c1ccccc(S(=O)(=O)Nc2nc(-c3ccc4c(c3)Cc3ccccc3-4)cs2)c1
vTmprss2-as1-120	Z1129123902	-10.7	0.334	426.52	REAL	NC(=O)C1CCN(c2nccc2CNC(=O)c2ccc3c(c2)Cc2ccccc2-3)CC1
vTmprss2-as1-121	Z1145893578	-10.7	0.324	439.47	REAL	C[C@]1(c2ccc3ccccc3c2)NC(=O)N(CC(=O)NNc2ccnc3ccccc23)C1=O
vTmprss2-as1-122	Z1167626285	-10.7	0.334	425.46	REAL	O=C(c1nn(-c2ccc(F)cc2)ccc1=O)N1CC=C(c2ccc3ccccc23)CC1
vTmprss2-as1-123	Z1170781979	-10.7	0.324	442.52	REAL	O=C(NC[C@@H](O)c1ccc2ccccc2c1)[C@H]1CCCN(C(=O)c2ccc3[nH]ncc3c2)C1
vTmprss2-as1-124	Z1220967658	-10.7	0.382	378.41	REAL	Cc1cc(C)cc(-c2cc(NC(=O)[C@H]3CC(=O)Nc4cc(F)ccc43)[nH]n2)c1
vTmprss2-as1-125	Z1262711094	-10.7	0.369	385.43	REAL	C/C(=N/NC(=O)Nc1ccc(-c2ccccc2)cc1)c1ccc2[nH]c(=O)[nH]c2c1
vTmprss2-as1-126	Z1266208840	-10.7	0.345	431.92	REAL	O=C(c1cc(N2CCNC2=O)ccc1Cl)N1CC=C(c2ccc3ccccc23)CC1
vTmprss2-as1-127	Z126939246	-10.7	0.289	497.55	REAL	C[C@@]1(c2ccc3ccccc3c2)NC(=O)N(CC(=O)N2CCC(n3c(=O)[nH]c4ccccc43)CC2)C1=O
vTmprss2-as1-128	Z1273982468	-10.7	0.382	368.44	REAL	O=C(Nc1cccc(-c2ccc3ccccc3c2)n1)[C@H]1CCc2cn[nH]c2C1
vTmprss2-as1-129	Z131647642	-10.7	0.315	479.56	REAL	O=C(c1ccc2[nH]c3c(c2c1)CCCC3)N1CCN(S(=O)(=O)c2ccc3[nH]c(=O)[nH]c3c2)CC1
vTmprss2-as1-130	Z1392734612	-10.7	0.334	430.46	REAL	Cc1oc2nc[nH]c(=O)c2c1C(=O)N1CCC[C@@H](NC(=O)c2ccc3ccccc3c2)C1
vTmprss2-as1-131	Z1449094660	-10.7	0.345	414.51	REAL	O=C(NC[C@H]1[C@H]2Cc3ccccc3[C@H]12)[C@@H]1CCCN(C(=O)c2ccc3[nH]ncc3c2)C1
vTmprss2-as1-132	Z1465758956	-10.7	0.334	430.50	REAL	O=C([C@@H]1C[C@]12CCCc1ccccc12)N1CCO[C@H](CN2C(=O)c3ccccc3C2=O)C1
vTmprss2-as1-133	Z1524783606	-10.7	0.345	412.45	REAL	NC(=O)c1ccc(NC(=O)[C@H]2CC(=O)N(c3ccc4c(c3)Cc3ccccc3-4)C2)cn1
vTmprss2-as1-134	Z1578943531	-10.7	0.345	416.48	REAL	NC(=O)c1cc(OC2CCN(C(=O)Nc3ccc(-c4ccccc4)cc3)CC2)ccn1
vTmprss2-as1-135	Z1618652098	-10.7	0.345	417.47	REAL	Cc1ccc2[nH]c3c(c2c1)C[C@H](NC(=O)Nc1cccc(N2C(=O)CNC2=O)c1)CC3
vTmprss2-as1-136	Z1620385394	-10.7	0.334	431.50	REAL	Cc1ccc2[nH]c3c(c2c1)C[C@H](NC(=O)Nc1cccc(N2C(=O)CN(C)C2=O)c1)CC3
vTmprss2-as1-137	Z1620406240	-10.7	0.324	442.52	REAL	Cc1ccc2[nH]c3c(c2c1)C[C@H](NC(=O)CN1C(=O)N[C@@]2(CCc4ccccc42)C1=O)CC3
vTmprss2-as1-138	Z1623720359	-10.7	0.345	413.48	REAL	Cc1ccc2[nH]c3c(c2c1)C[C@@H](NC(=O)NNC(=O)c1ccc2ccccc2n1)CC3
vTmprss2-as1-139	Z1625701189	-10.7	0.324	442.48	REAL	NC(=O)c1cn(C2CN(C(=O)[C@@H]3CC(=O)N(c4ccc5c(c4)Cc4ccccc4-5)C3)C2)nn1
vTmprss2-as1-140	Z1700163581	-10.7	0.357	420.54	REAL	Cc1cc(C(N)=O)ccc1NC(=O)NCc1nc2c(s1)C[C@@H](c1ccccc1)CC2
vTmprss2-as1-141	Z1702714389	-10.7	0.324	440.50	REAL	O=C(Nc1cccc2c1OCC[C@H]2O)[C@@H]1CC(=O)N(c2ccc3c(c2)Cc2ccccc2-3)C1
vTmprss2-as1-142	Z1723003957	-10.7	0.345	409.49	REAL	Cn1cnc(-c2cccc(NC(=O)N3CC=C(c4cccc5ccccc45)CC3)c2)n1
vTmprss2-as1-143	Z1730127207	-10.7	0.324	434.50	REAL	O=C(c1c2c(nc3ccccc13)/C(=C/c1ccccc1)CC2)N1CCc2n[nH]c(=O)cc2C1
vTmprss2-as1-144	Z1744836126	-10.7	0.357	416.50	REAL	O=C1Nc2ccccc2[C@@]12CCN(S(=O)(=O)c1ccc3c(c1)Cc1ccccc1-3)C2
vTmprss2-as1-145	Z1752605895	-10.7	0.345	414.51	REAL	Cc1ccc2[nH]c3c(c2c1)C[C@H](NC(=O)N1CC[C@@]2(C1)C(=O)Nc1ccccc12)CC3
vTmprss2-as1-146	Z1764086666	-10.7	0.357	405.50	REAL	C[C@]1(c2ccc(C(N)=O)cc2)NC(=O)N(CC2CCC(c3ccccc3)CC2)C1=O
vTmprss2-as1-147	Z1937347528	-10.7	0.382	372.47	REAL	Nc1nccc([C@@H]2CCCN(C(=O)[C@@H]3C[C@H]3c3ccc4ccccc4c3)C2)n1
vTmprss2-as1-148	Z2015600762	-10.7	0.324	441.49	REAL	Nc1nccc([C@@H]2CCCN(CC(=O)Nc3cccc4c3C(=O)c3ccccc3C4=O)C2)n1
vTmprss2-as1-149	Z2027111043	-10.7	0.324	440.46	REAL	Cc1ccc(-c2n[nH]c(=O)[nH]2)cc1NC(=O)c1ccc2c(c1)C[C@@H](c1ccccc1)OC2=O
vTmprss2-as1-150	Z2038004085	-10.7	0.324	442.52	REAL	Nc1nccc([C@@H]2CCCN(C(=O)Nc3cccc(C(=O)N4CCc5ccccc54)c3)C2)n1
vTmprss2-as1-151	Z2075856097	-10.7	0.324	437.55	REAL	Cc1ccc(-c2ccc(C(=O)N3CCC[C@H](c4ccnc(N)n4)C3)c3ccccc3n2)c(C)c1
vTmprss2-as1-152	Z2075874636	-10.7	0.357	418.56	REAL	CC1(C)Cc2cc(C(=O)N3CCC[C@H](c4ccnc(N)n4)C3)sc2-c2ccccc21
vTmprss2-as1-153	Z2099254407	-10.7	0.334	424.50	REAL	O=C1COC[C@@H](C[C@H]2CN(C(=O)c3ccc4c(c3)Cc3ccccc3-4)c3ccccc32)N1
vTmprss2-as1-154	Z2114068197	-10.7	0.324	443.48	REAL	O=C(Nc1ccc(F)c(N2C(=O)CCC2=O)c1)N1CC=C(c2ccccc3ccccc23)CC1
vTmprss2-as1-155	Z2127351512	-10.7	0.324	443.46	REAL	O=C(Nc1ccccc(-c2n[nH]c(=O)[nH]2)c1)[C@H]1CCCN1C(=O)c1ccc2ccccc2c1O
vTmprss2-as1-156	Z2171860547	-10.7	0.369	388.47	REAL	Cc1nc(NC(=O)N2CCC[C@@H](c3ccnc(N)n3)C2)ccc1-c1ccccc1
vTmprss2-as1-157	Z2233591120	-10.7	0.315	443.47	REAL	O=C(Nc1nc(-c2ccc3ccccc3n2)n[nH]1)c1cc(-c2ccnc2)nc2ccccc12
vTmprss2-as1-158	Z2524122788	-10.7	0.324	467.55	REAL	O=c1[nH]c(=O)c2cc(S(=O)(=O)N3C[C@H]4CC[C@H]3[C@H]3CN(Cc5ccccc5)C[C@H]43)cnc2[nH]1
vTmprss2-as1-159	Z2524823382	-10.7	0.334	431.50	REAL	O=C(c1cnc2[nH]c(=O)[nH]c(=O)c2c1)N1C[C@H]2CC[C@H]1[C@H]1CN(Cc3ccccc3)C[C@H]21
vTmprss2-as1-160	Z343948804	-10.7	0.324	443.50	REAL	O=C(O)c1ccc2[nH]c3c(c2c1)CN(C(=O)[C@H]1CC(=O)N(c2ccc4c(c2)CCC4)C1)CC3
vTmprss2-as1-161	Z393677994	-10.7	0.334	419.44	REAL	O=C(Nc1ccccc1-n1ncc2c(=O)[nH]cnc21)c1ccc2c(c1)Cc1ccccc1-2
vTmprss2-as1-162	Z444210754	-10.7	0.324	439.56	REAL	O=C(c1ccccc2ccccc12)N1CCC(C(=O)N2C[C@@H]3CCCN3c3ccccc32)CC1
vTmprss2-as1-163	Z749111224	-10.7	0.315	449.56	REAL	Cn1cnnc1[C@@H]1CCCN(C(=O)c2c3c(nc4ccccc24)/C(=C/c2ccccc2)CC3)C1
vTmprss2-as1-164	Z822681034	-10.7	0.345	412.44	REAL	NC(=O)c1cccc(OC(=O)[C@H]2CC(=O)N(c3ccc4c(c3)Cc3ccccc3-4)C2)c1
vTmprss2-as1-165	Z847630610	-10.7	0.289	495.53	REAL	C[C@@H](OC(=O)[C@@H]1CC(=O)N(c2ccc3c(c2)Cc2ccccc2-3)C1)C(=O)N1CC(=O)Nc2ccccc21
vTmprss2-as1-166	Z920833354	-10.7	0.306	490.58	REAL	CC1(C)CC[C@H](NC(=O)c2ccc(NS(=O)(=O)c3ccc4[nH]c(=O)[nH]c4c3)cc2)c2ccccc21
vTmprss2-as1-167	Z998120744	-10.7	0.315	476.56	REAL	O=C(Nn1cnc2sc3c(c2c1=O)CCCC3)[C@@H]1CCCN(C(=O)c2ccc3[nH]ncc3c2)C1
vTmprss2-as1-168	Z999566940	-10.7	0.306	471.60	REAL	C[C@@H]1Cc2ccccc2N1C1CCN(C(=O)[C@@H]2CCCN(C(=O)c3ccc4[nH]ncc4c3)C2)CC1
vTmprss2-as1-169	ZINC000000671507	-10.7	0.289	487.51	ZINC	O=C(NN1C(=O)c2ccccc2N[C@H]1c1c2ccccc2cc2ccccc21)c1ccc2c(c1)OCO2
vTmprss2-as1-170	ZINC000009643195	-10.7	0.324	441.57	ZINC	NC(=O)C1CCN(C(=O)c2cc(-c3ccc(C4CCCCC4)cc3)nc3ccccc32)CC1
vTmprss2-as1-171	ZINC000019691229	-10.7	0.324	443.52	ZINC	Cc1cc(-c2ccc(F)cc2)cc(C2CCN(C(=O)[C@H]3CC(=O)Nc4ccccc43)CC2)n1
vTmprss2-as1-172	ZINC000035598066	-10.7	0.357	398.47	ZINC	Cc1nc(-n2ccnc2)cc(N2CCN(C(=O)c3ccccc4ccccc43)CC2)n1
vTmprss2-as1-173	ZINC000524729098	-10.7	0.297	476.54	ZINC	O=C(CN1C(=O)c2ccccc2N2C(=O)c3ccccc3[C@@H]21)N[C@H]1CCCc2c3ccccc3[nH]c21
vTmprss2-as1-174	ZINC000588225447	-10.7	0.289	498.61	ZINC	O=C1N=C(SCc2ccccc2)NN2C1=c1ccccc1=N[C@H]2c1c2ccccc2cc2ccccc21
vTmprss2-as1-175	PV-001826467597	-10.6	0.342	423.45	REAL	O=C(NCc1cccnc1-n1cccn1)[C@H]1C[C@H](O)CN1C(=O)Cc1ccccc1F
vTmprss2-as1-176	PV-001852607377	-10.6	0.379	378.37	REAL	Cc1ccc(F)c(-c2cc(NC(=O)c3cccc(Nc4nnn[nH]4)c3)[nH]n2)c1
vTmprss2-as1-177	PV-001856500112	-10.6	0.379	374.41	REAL	Cc1cc(C)cc(-c2cc(NC(=O)c3cccc(Nc4nnn[nH]4)c3)[nH]n2)c1
vTmprss2-as1-178	PV-001918003355	-10.6	0.353	421.38	REAL	Nc1nn2c(=O)cc(CN3CCN(C(=O)c4ccc(C(F)(F)F)cc4)CC3)nc2[nH]1
vTmprss2-as1-179	PV-001944822791	-10.6	0.353	409.39	REAL	C[C@H](NC(=O)Nc1ccc(-c2cccc(F)c2)c(F)c1)c1ccc2[nH]c(=O)oc2c1
vTmprss2-as1-180	PV-001948929688	-10.6	0.342	416.41	REAL	C[C@@H](NC(=O)Nc1ncc2oc(=O)[nH]c2cc1F)c1ccc(-c2cccc(C\#N)c2)cc1
vTmprss2-as1-181	PV-001957784398	-10.6	0.353	409.53	REAL	C[C@@H]1C[C@H](NC(=O)N[C@H]2CCC[C@H](c3ccccc3)CC2)C(=O)N1c1cnn(C)c1
vTmprss2-as1-182	PV-001959107455	-10.6	0.342	418.47	REAL	C[C@H](NC(=O)N[C@H](C)c1ccc2[nH]c(=O)[nH]c2c1)c1ccc(-c2ccc(F)cc2)cc1
vTmprss2-as1-183	Z1099281343	-10.6	0.353	403.44	REAL	O=C(NNC(=O)N1CCC[C@H]1c1ccc2e(c1)OCO2)c1ccc2ccccc2c1
vTmprss2-as1-184	Z1158408650	-10.6	0.353	394.48	REAL	Cn1cc(-c2cncc(C(=O)N3CC=C(c4ccc5ccccc45)CC3)c2)cn1
vTmprss2-as1-185	Z1204916977	-10.6	0.342	412.49	REAL	O=C(N[C@@H]1CCc2[nH]ncc2C1)[C@@H]1CC(=O)N(c2ccc3c(c2)Cc2ccccc2-3)C1
vTmprss2-as1-186	Z1250822165	-10.6	0.353	406.48	REAL	Cc1ccc(CCC2CCN(C(=O)c3cc(C)c4c(=O)[nH]c(O)nc4n3)CC2)cc1
vTmprss2-as1-187	Z1275520713	-10.6	0.353	400.44	REAL	C[C@@H](c1ccc(-c2ccccc2)cc1)N(C)C(=O)c1cnc2[nH]c(=O)[nH]c(=O)c2c1
vTmprss2-as1-188	Z1276023412	-10.6	0.353	402.42	REAL	O=C1Nc2ccccc2O[C@H]1CC(=O)N1CCc2cc(-c3cccc(F)c3)ccc21
vTmprss2-as1-189	Z1277897156	-10.6	0.342	409.49	REAL	O=C(Nc1ccn(Cc2ccncc2)n1)N1CC=C(c2ccccc3ccccc23)CC1
vTmprss2-as1-190	Z1286436516	-10.6	0.366	384.43	REAL	Cc1ccc(N2CCOC2=O)cc1NC(=O)c1ccc2c(c1)Cc1ccccc1-2
vTmprss2-as1-191	Z1313837080	-10.6	0.342	438.51	REAL	NC(=O)c1cc(S(=O)(=O)NCC(=O)N2CC=C(c3cccc4ccccc34)CC2)c[nH]1
vTmprss2-as1-192	Z1372283755	-10.6	0.342	434.42	REAL	O=C(N[C@@H]1CC(=O)N(c2ccccc(C(F)(F)F)c2)C1)N[C@H]1CCCc2[nH]c(=O)ccc21
vTmprss2-as1-193	Z1391613824	-10.6	0.342	413.48	REAL	Cn1nnc2cc(C(=O)N3CCC[C@H](NC(=O)c4ccc5ccccc5c4)C3)ccc21
vTmprss2-as1-194	Z1392745172	-10.6	0.353	406.44	REAL	O=C(N[C@H]1CCCN(C(=O)Cn2ccc(=O)[nH]c2=O)C1)c1ccc2ccccc2c1
vTmprss2-as1-195	Z1394790183	-10.6	0.353	410.42	REAL	O=C(N[C@@H]1CCCN(C(=O)c2c(O)cc(F)cc2F)C1)c1ccc2ccccc2c1
vTmprss2-as1-196	Z1414681082	-10.6	0.353	423.54	REAL	Nc1nsc(N2CCN(CC(=O)N3CC=C(c4c[nH]c5ccccc45)CC3)CC2)n1
vTmprss2-as1-197	Z1452022870	-10.6	0.353	395.47	REAL	O=C(Nc1cccc(-n2ccnn2)c1)N1CC=C(c2ccccc3ccccc23)CC1
vTmprss2-as1-198	Z1465755907	-10.6	0.342	416.48	REAL	O=C([C@@H]1C[C@]12CCc1ccccc12)N1CCO[C@H](CN2C(=O)c3ccccc3C2=O)C1
vTmprss2-as1-199	Z151758680	-10.6	0.342	412.44	REAL	C[C@@H](OC(=O)c1ccc2c(c1)-c1ccccc1C2)C(=O)N1CC(=O)Nc2ccccc21
vTmprss2-as1-200	Z1644493659	-10.6	0.342	411.51	REAL	Cc1ncc2c(n1)CCC[C@@H]2NC(=O)N[C@@H](C)c1ccc(-c2cccc(C\#N)c2)cc1

Supplementary Table 94. Virtual screening hits 101 to 200 of the screen against the active site of TMPRSS2 (Screen ID: 6). Compounds were filtered so that hits had MW < 600 dalton, cLogP < 6, number of hydrogen bond acceptors < 11, and no reactive functional groups. A few compounds unsuitable for drug discovery were removed by visual inspection. The name of each compound consists of the initial letter 'v' for virtual hit, followed by the target protein name and the target site ('as' for active site, 1 for docking scenario 1). The score is the docking score given by QuickVina 2 in kcal/mol. The ligand efficiency (LE) is computed as LE = -score/#NonH, where #NonH is the number of heavy (i.e. non hydrogen) atoms.