EDITORIAL

Applications of chem-bioinformatic, chemometric and machine learning approaches for COVID-19 related research

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At the end of 2019, a cluster of pneumonia cases occurred in Wuhan, China. It then quickly spread to other parts of the world causing a pandemic situation popularly termed as Coronavirus (CoV) Disease-2019 (COVID2019). Globally, as of 29 June 2022, there have been 543,352,927 confirmed cases of COVID-19, including 6,331,059 deaths, reported to the World Health Organization (https://covid19.who.int/). As per the records of WHO, United States, India and Brazil have topped in terms of cumulative case numbers and cumulative deaths. As of 26 June 2022, a total of 11,981,689,168 vaccine doses have been administered. Currently there are no antiviral drugs with proven efficacy against COVID-19 although a number of vaccines have now been available and several small molecules from the antiviral and other therapeutic categories have been placed in different stages of clinical trial against the COVID-19 infections [1]. The devastating impact of the current COVID-19 outbreak and possibility of future similar epidemics strongly require for the rapid development of new treatments and fast intervention protocols. Three new oral antiviral treatments (molnupiravir, fluvoxamine and Paxlovid) have shown improvement in mortality or hospitalization rates and adverse events among COVID-19 patients [2]. Although CoVs have undergone substantial genetic evolution, they still have considerable similarities. This can be a basis for the identification of promising targets for antiviral therapies against 2019-nCoV. Computational drug design and drug repurposing strategies can efficiently be implemented to identify suitable drugs for different identified targets. Different chem-bioinformatic approaches including structure-based (homology modeling, molecular docking, molecular dynamics, protein–protein interaction network, etc.) and ligand-based modeling strategies (pharmacophore mapping, quantitative structure–activity relationships or QSARs and chemometric models in addition to similarity-based unsupervised techniques like read-across [3, 4]) may be used for this purpose with an objective to prioritize the candidate drugs for further experiments [5, 6]. Drug repurposing is an effective and economic approach to find new indications for already known drugs within a short period which can be used to overcome the emergence of resistance to existing antiviral drugs and re-emerging viral infections [7]. This approach typically relies on an integrated pipeline including a virtual screening of drug libraries to find suitable drug-target pairs using molecular similarity methods and molecular docking and binding free energy calculations used to predict drug-target interactions and binding affinity. This special issue of *Structural Chemistry* presents review articles and research papers describing computational modeling of drug candidates and computational repurposing of the existing drugs and drug candidates collected from different databases for the different targets like coronavirus main protease (3CLpro), papain-like protease (PLpro), RNA-dependent RNA polymerase (RdRp), viral spike glycoprotein (S protein), transmembrane protease serine 2 (TMPRSS2), etc. We hope that the reviews and research works presented in this special issue showcasing the structural aspects of drug research against the coronavirus pandemic will be of value to the researchers in the field.

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