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Editors Letter

Scientific Response to the Coronavirus Crisis in Spain: Collaboration and Multidisciplinarity

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We have been contacting chemical biology researchers throughout the world to ask about how they are coping with the COVID-19 pandemic. We have heard from researchers in China and Italy on how the virus is impacting research but also how researchers are forming new alliances to contribute to understanding and curbing the virus. In this installment, we learn about how researchers in Spain have been coping. The authors are on the front line. For example, a team of researchers at CIC-bioGUNE in partnership with BIOLAN, a biotechnology company located in the Basque region of Spain, are engaged in several projects focused on improving the speed and accuracy of COVID-19 diagnosis. Among these projects are the development of serological tests (based on a lateral flow immunochromatographic assay), which yield rapid results. They also are validating laboratory protocols for automated extraction of RNA from human samples and PCR-based detection of SARS-CoV-2 viral RNA.[1,2] We hope that you enjoy these reports from multidisiplinary scientists around the world. **—Laura L. Kiessling, Editor in Chief, *ACS Chemical Biology***

SCIENTIFIC RESPONSE TO THE CORONAVIRUS CRISIS IN SPAIN: COLLABORATION AND MULTIDISCIPLINARITY

Coronavirus infectious disease 2019 (COVID-19), caused by severe acute respiratory syndrome coronavirus 2 (SARS-CoV-2), has quickly spread globally, resulting in the ongoing coronavirus pandemic. While the majority of cases result in mild symptoms, some patients progress to viral pneumonia and multiorgan failure, constituting a global threat. As of April 28, 2020, more than 230 000 cases have been reported in Spain, resulting in about 24 000 deaths in the country.[3]

Our scientific community has quickly and responsibly reacted to this challenge. A plethora of scientific projects have thrived, and many laboratories and research institutes have partially or completely changed their research focuses to address the new demands. Two words may well summarize the current effort in the country: collaboration and multidisciplinarity.

Of course, the main goal in tackling this pandemic is to find an effective vaccine for the virus. Among the more than 50 reported initiatives currently running worldwide, at least four of them take place partially or totally in Spain, including one centered on the genetic manipulation of the entire virus to obtain attenuated vaccines, conducted at the National Center for Biotechnology of the Spanish Research Council (CNB-CSIC). Alternatively, the Center for Research in Biological Chemistry and Molecular Materials (CiQUS) is using a proprietary technology based on micro- and nanoparticles to develop a vaccine that would avoid the use of adjuvants or genetic material. The same center is also exploring a mRNA anti-COVID-19 vaccine based on gene delivery vehicles as a tool to facilitate the entry of the viral proteins encoded in the mRNA cargo. Finally, another research group at CNB-CSIC is using the smallpox virus as a scaffold to develop a vaccine against SARS-CoV-2.

The development of reliable tools for testing the disease progression constitutes another holy grail. Among the efforts, CIC bioGUNE is exploring different testing methods to detect antibodies, focusing on antigen selection and including an innovative reading method based on cell sorting. On the other hand, researchers at CIC biomaGUNE are using protein-stabilized metal nanoclusters as a novel detection technology for antibodies. In line, IMDEA-Nanociencia is using a similar approach using gold nanoparticles, and researchers at ICN2 and CIBER-BBN are exploring the use of nanotechnology to develop SARS-CoV-2 monitoring devices based on optical biosensors. Due to the shortage of reagents and the high mutation rate of the virus, it is expected that these initiatives will complement rather than compete with the already commercially available products.

Computational studies constitute an important part of the chemical biology community in Spain, with the utmost reputation. Unraveling the fundamental mechanisms behind SARS-CoV-2 pathogenesis is envisioned as an essential step toward effectively tackling this and future coronavirus-related pandemics, and many researchers have switched gears to address specific problems of the SARS-CoV-2 virus using docking and molecular dynamics simulations. Such efforts include studies to understand the proteolysis reaction catalyzed by the virus (for instance, at the Universities of Valencia and Jaume I) or the mechanism by which the SARS-CoV-2 virus penetrates human cells by interacting with the host receptors, especially hACE2 (IRB, the University of Barcelona, CSIC, and the Institute for Computational Chemistry and Catalysis in Girona). Other, more applied computational efforts are

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dedicated to the discovery of inhibitors that abrogate the viral recognition and that could be translated to the clinic later on. As a leading example, docking studies are being carried out at the Barcelona Supercomputing Center (BSC), to understand interaction events associated with multiple SARS-CoV-2 targets. They are also part of a consortium involving many local institutions funded by the pharmaceutical company Grifols to develop small molecules and antibodies and to design mutations to stabilize the closed state of the S protein for vaccine development. Other studies include a large cooperative effort at CSIC, including different institutes at Madrid (IQM, CIB) and Valencia (I2SysBio and IBV), as well as some independent studies at CIC bioGUNE, CiQUS, and Universities of Valencia and Jaume I, among others.

Still *in silico*, researchers at the Institute for Research in Biomedicine (IRB) use network biology and structural bioinformatics to provide solutions for the challenges associated with the COVID-19 pandemic, including the use of artificial intelligence and systematic literature mining to repurpose currently approved compounds to fight the disease. Also at IRB, biomolecular simulations are being employed to identify alternative strategies to treat COVID-19 such as inhibiting the viral RNA polymerase.

Finally, when considering experiments oriented toward therapy, we just refer to a couple of examples that account for the myriad of different ongoing initiatives: the use of proteomics and computational methods to shed light on the potential interactions of key viral proteins with repurposed drugs (CiQUS), the use of CRISPR/Cas13d technologies for prophylactic purposes, carried on at the same institute, the investigation of metabolic pathways with therapeutic potential (ATLAS Molecular Pharma), and the design and synthesis of oligonucleotides aimed to bind SARS-CoV-2 RNA (IQAC−CSIC).

In summary, chemical biology is currently used by many groups and in many ways to fight the SARS-CoV-2 virus. It is important to emphasize that this briefing does not aim to be fully comprehensive. The goal here was to illustrate how these emerging projects are quickly and profoundly reshaping the scientific landscape in Spain with important implications for the years to come.

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Notes

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