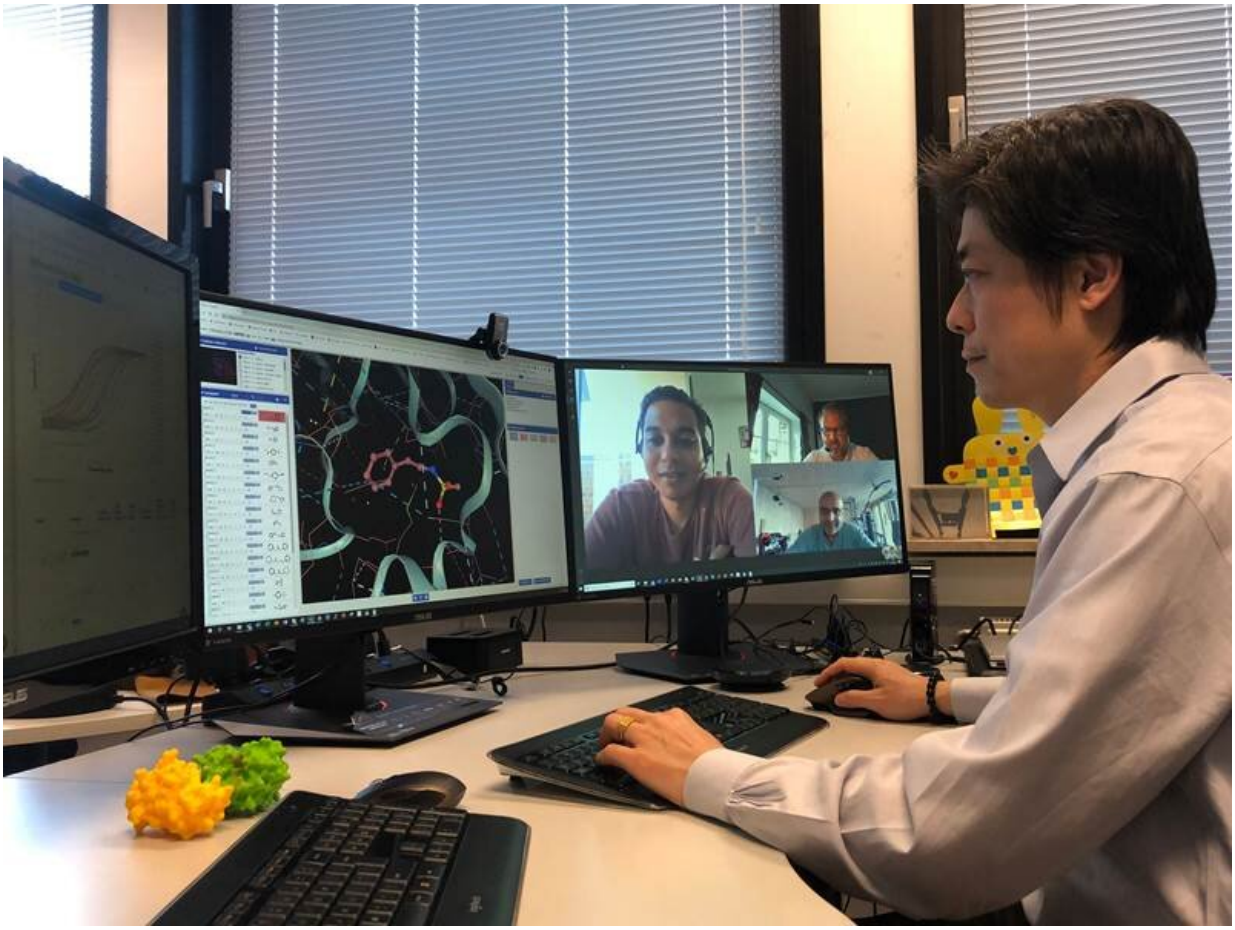
Computer-aided drug design added to global fight against COVID-19

July 3 2020



Credit: Royal Society of Chemistry

Life sciences company UCB is the first pharma company to join the

COVID Moonshot crowdsourcing initiative, which involves the Diamond Light Source synchrotron facility in Oxfordshire and the Weizmann Institute of Science in Israel among others—encouraging anyone to submit designs to be synthesized and tested.

Like many similar companies, UCB rapidly pivoted its business to lend its scientific expertise and experience to the cause, dedicating teams in its discovery research labs in Slough, UK and Braine-l'Alleud, Belgium along with the expertise of its team across the world, including its Medicinal Chemistry team, to produce a highly targeted drug that aims to counteract the viral replication element of the SARS-COV-2 virus.

The data from the studies, successful or otherwise, is then made public and incorporated in the next design cycle until the most effective solutions are found.

Jiye Shi, UCB's Senior Director, CADD said: "We are excited to be part of the COVID Moonshot and join the fight against COVID-19 together with volunteers around the world. Using UCB's proprietary molecular simulation and design technologies, our computational chemists are working hand in hand with medicinal chemists to design novel compounds aimed at not only SARS-COV-2 inhibition, but also broad-spectrum inhibition of multiple coronaviruses to better protect our future."

So far more than 5,000 molecular designs have been crowdsourced, out of which more than 400 compounds have been synthesized. The first new compounds are being tested in biochemical assays with encouraging results emerging. And the global learning has been immense.

Dr. Mark Calmiano, Principal Scientist, CADD at UCB, says: "I feel privileged to be part of a truly global team of scientists who have come together at short notice and worked so hard to get the Moonshot project

off the ground. My role in bringing together a diverse, global team of medicinal chemists and computational chemists on the project has been both hugely challenging and hugely inspiring. I am learning a lot from so many talented individuals across the worlds of medicinal chemistry and CADD and am proud that UCB can contribute our own expertise to such an important project with the potential to help so many people across our planet."

Dr. Calmiano and Dr. Shi are joined by their colleagues Drs Jag Heer, Director, Medicinal Chemistry, Eric Jnoff, Associate Director, Medicinal Chemistry and Daniel Brookings, Director, Medicinal Chemistry, in being intimately involved in the strategic development of the initiative—e.g. leading the computational chemistry activities critical to assessing and triaging of chemical design submissions for synthesis and testing—but also in coordinating internal efforts to contribute computational analysis and insightful inhibitor designs from the CADD and Medicinal Chemistry communities at UCB.

Eric Jnoff said: "As a medicinal chemist working at UCB, it is for me a privilege to have the opportunity to contribute to this project in bringing medicinal chemistry expertise and coordinating drug design efforts amongst other UCB scientists who are volunteering their time for this cause. Exchanging ideas and learning from others in the team is really inspiring and I'm proud that UCB is actively taking part in this initiative."

Provided by Royal Society of Chemistry