

Getting the Most from SC-XRD During the COVID-19 Lockdown

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With many X-ray labs in lockdown and synchrotron beamtime operations suspended, we look at how you can continue to get the most from your single crystal X-ray diffraction instrument during and after the COVID-19 lockdown period.

Crystallography at the forefront of SARS-CoV-2 Research

There are several targets identified as potential sites of action of antiviral therapeutics. One of the key

targets in SARS-CoV-2 is the main protease (MPro). Inhibiting the activity of this enzyme would block viral replication. Since no human proteases with a similar cleavage specificity are known, inhibitors are unlikely to be toxic ([Science, 20 March 2020](#)). As of 1st April, over 80 crystal structures of this protease in complex with ligands of interest have been published in the Protein Data Bank (PDB).

Other SARS-CoV-2 structures solved by crystallography include other proteases, RNA polymerase and other RNA binding proteins, receptor binding domains and nucleocapsid protein. A full list of released structures is maintained at the [PDB COVID-19/SARS-CoV-2 Resources](#) page.

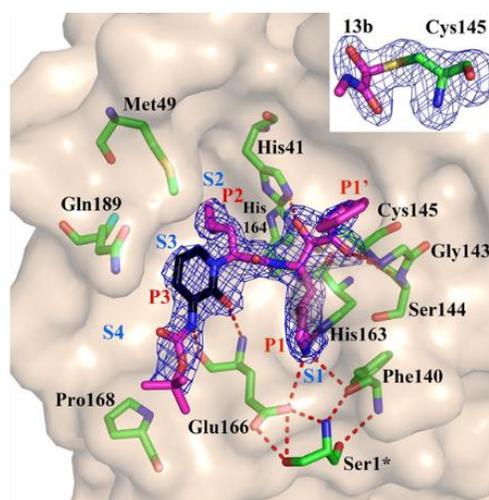
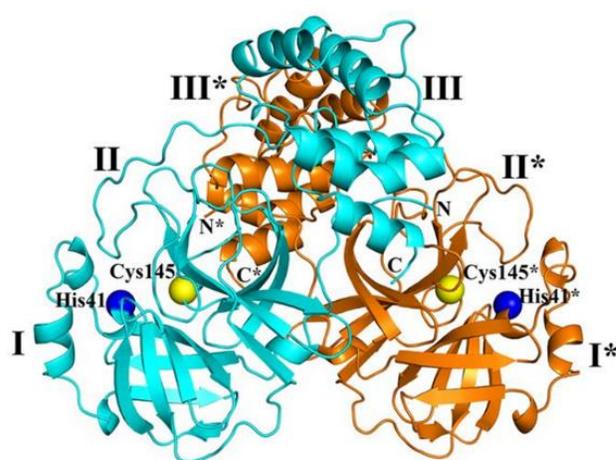


Figure 1: (a) Three-dimensional structure of SARS-CoV-2 Mpro, (b) Compound 13b in the substrate-binding cleft located between domains I and II of the Mpro (Linlin Zhang et al. Science 2020; science.abb3405)

Getting the most from your instrument during lockdown

Bruker AXS will continue to provide all the support possible to help you continue getting the most from your instruments during lockdown. Our support specialists remain available to provide advice on how to continue your work, whether it is with limited instrument access or entirely from home. A program of webinars will be announced in the coming days, so keep an eye on the [Bruker Webinars webpage](#) for announcements. We have also introduced [Bruker Training Office Hours](#), a unique opportunity to receive training free-of-charge on processing challenging datasets in real time using real-life examples.

Maximizing the productivity of your facility

Automating your instrument to provide remote data collection is one of the clearest ways to maintain the productivity of your instrument during lockdown. But beyond lockdown, there will be a lot of measurements to be made and, the risk that beamtime will be in heavy demand. Here are a few suggestions (Fig. 2) for how you can enhance the productivity of your instrument. For more information visit www.bruker.com/scd or contact your local sales representative.

Upgrade your X-ray detector

The photon counting **PHOTON III** CPAD can collect data more than ten times faster than your CCD or PHOTON 100 detector.

Upgrade your X-ray source

Our latest range of X-ray sources provide the brightest beams whatever your budget, from the latest **1 μ S 3.0**, to the peerless **1 μ S DIAMOND** and **METALJET**. And a second source can be added to the **D8 VENTURE** to expand the applications of the system.

Automate your remote data collection

The **SCOUT** automated sample changer can significantly extend the available beamtime of your system and enables data to be collected remotely from up to 48 samples at a time. Get the most from your synchrotron trips by screening and characterizing your crystals in advance.

Automate your goniometer head

Why waste valuable time centering crystals by hand when you can quickly and accurately use 2-click centering with the AGH?

In situ crystallography

Quickly identify good crystal leads and discard false leads. Screening crystals in plates with the **ISX STAGE** will significantly reduce the time from protein to structure.

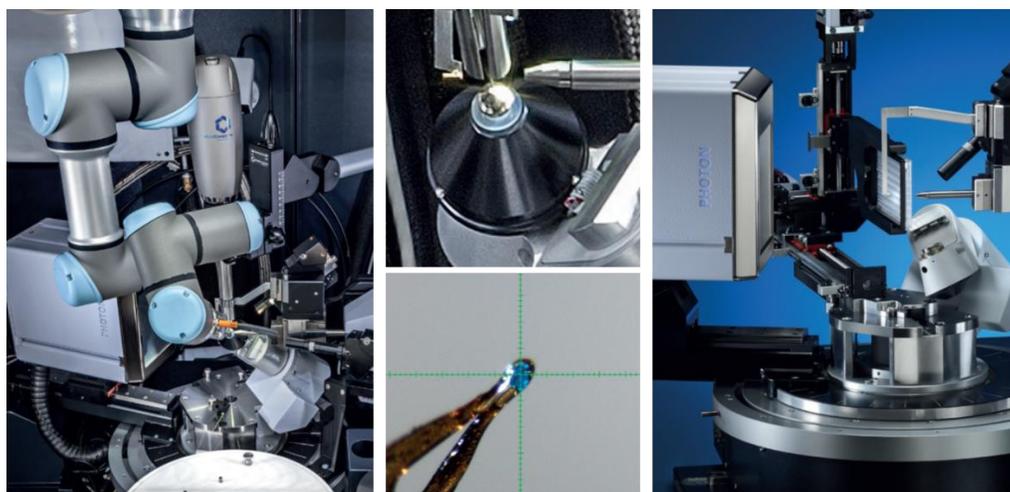


Figure 2: Automating your D8 VENTURE will significantly reduce time-to-structure and increase productivity. SCOUT (l), AGH (c), ISX STAGE (r).