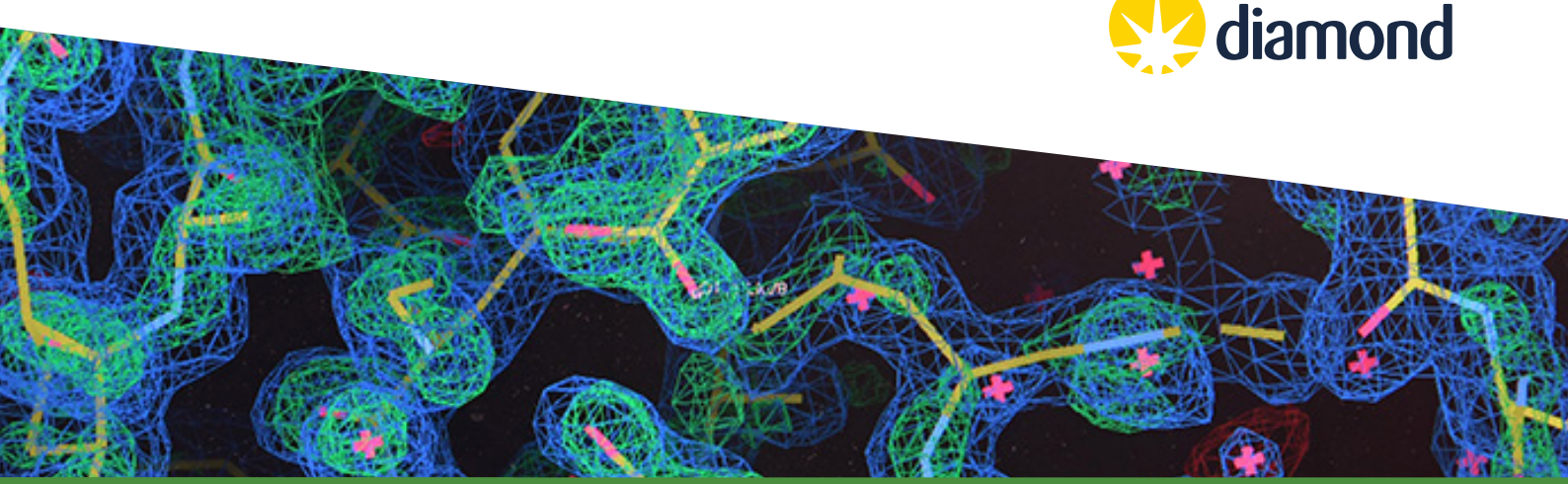


XCHEM FOR INDUSTRY

Crystallographic Fragment Screening

The XChem platform at Diamond enables users to exploit the capabilities of fragment-based lead discovery and accelerate their drug discovery pipeline.

Fragment-based drug design has revolutionised the pharmaceutical industry, providing valuable and cost-effective insights for rational drug design in the early stages. It allows scientists to explore a larger part of the existing chemical space from the drug targets of interest, providing new entry routes for the development of lead compounds.

With the co-location of the XChem laboratory and beamline I04-1, we can significantly reduce the time to structural determination. Our unique processes, tailored software, and automated systems enable us to record and securely track your data seamlessly from initial crystal cultivation through to data analysis. Our expert scientists are on hand throughout your research to advise, train and support you.

Applications

Fragment screening provides a cost effective process for early drug discovery, enabling you to:

- isolate new chemical information at the binding site of interest for drug targets
- quickly develop follow-up compounds with high affinity against the target of interest

Benefits

Fragment screening via X-ray crystallography provides an effective and rapid route to the early stages of rational drug design. It provides:

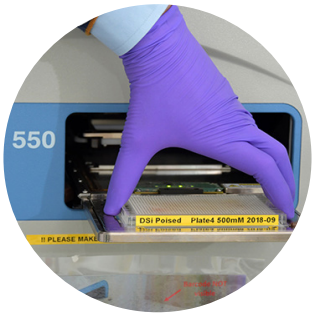
- High resolution, robust and reliable results, with hit rates of between 3-10%
- Direct structural feedback of the ligand-target interaction at atomic level
- Fragment validation, to enable quick progression through the research pipeline
- Fast and cost effective structural determination

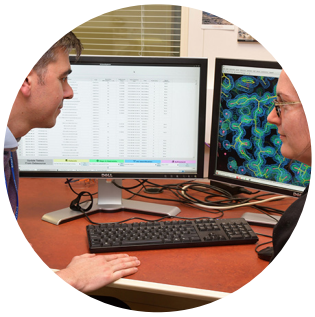
Here at Diamond, our unique facilities provide:

- Cost-effective access to innovative (first of its kind) facilities
- Co-location of lab and beamline speeding up time to results
- Secure sample tracking and data management
- Readily available libraries of compounds
- Support and on-the-job training from XChem experts
- Optimised processes and automation for screening up to 700 compounds a day

Innovative Resources

Through Diamond's innovative instruments and streamlined processes, we can not only deliver your research from initial stages through to full structural determination, but also securely track and record the data. This ensures that vast amounts of fragments can be investigated within a short amount of time, made even speedier through the co-location of beamline and XChem lab.





Readily available libraries of compounds developed for the XChem platform.

TexRank provides rapid high-resolution crystallisation plate images to identify the likely location of crystals. The graphical interface allows this information to be easily transferred for use on the Echo.

Echo Acoustic Liquid Handler enables compounds to be quickly dispensed from one of our fragment libraries.

Shifter speeds up the process of crystal harvesting while recording the tracking of samples.

SoakDB database manages the entire soak/harvest experiment.

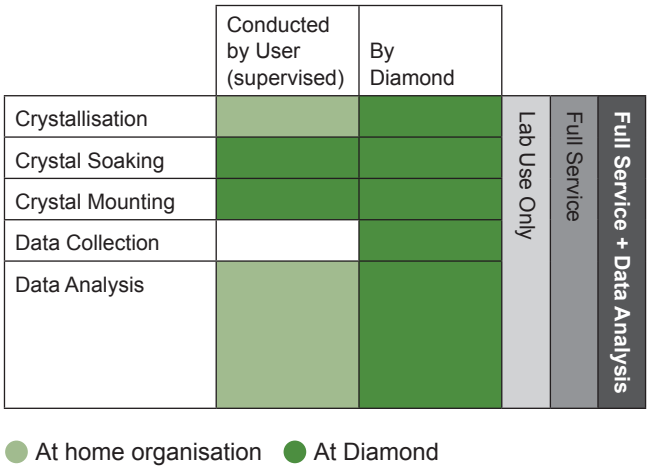
Beamline I04-1 is co-located alongside the XChem lab, enabling quick lab to beamtime transition. It can collect up to 700 datasets in 24 hours, using fully automated/ unattended data collection capabilities.

XChem Explorer manages large-scale processing and analysis of X-ray data from the beamline.

PanDDA is used to analyse large sets of X-ray data to efficiently identify bound fragments.

Experienced scientific support and full service offerings

Our experienced staff can provide support and on-the-job training throughout your research at Diamond. They can provide different levels of service, dependent upon your requirements and level of experience.



For further information

Diamond Industrial Liaison Team

+44 1235 778797
industry@diamond.ac.uk
diamond.ac.uk/industry
@DiamondILO

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