

The Bragg Crystallography Facility

Structure determination for small and large molecules

Description of Technology

The main capabilities of the Bragg Crystallography Facility include:

- High throughput small molecule structure determination
- Protein and macromolecule structure determination
- Screening of large protein samples for subsequent synchrotron data collection
- Powder diffraction analysis

From 2010, the Bragg Crystallography Facility will be equipped with two state-of-the-art diffractometers; a Mo-target Oxford Diffraction X-Calibur X-ray diffractometer for small molecule structure determination, and a Cu-target Rigaku Hiflux Homelab rotating anode X-ray diffractometer for large molecule structure determination.

Commercial Applications

1) High throughput small molecule structure determination (SMX)

SMX is used to determine the structures of inorganic, organic and mineralogical species (i.e. compounds with a few atoms to those containing a thousand atoms) and to define the absolute structure and configuration of chiral (asymmetric) compounds. SMX can be used to identify and characterise potential drug leads, protein inhibitors/activators and nanoscale/catalytic homogeneous systems.

2) Protein and macromolecule structure determination (PX)

PX structure determination offers industries with a research focus in biotechnology, (stem) cell biology, biochemistry, biomedicine and biotechnology single step access to the 3-D structure of a protein or enzyme. This information can be used to further

understand drug targets or biological activity, for example. Our PX capable instrument can also be used for other macromolecular structure determination, e.g. polynucleic acids, polymers and supramolecular extended network materials. The services provided under items 1 and 2 can include:

- Selection and mounting of crystal specimens
- X-ray data collection
- Digital movies of crystals
- Face-indexed numerical absorption corrections (when needed)
- Structure solution and refinement
- Full crystallographic report with experimental details, figures, files, and tables of crystallographic data

3) Screening of weakly diffracting protein samples prior to synchrotron access

Samples that require more intense X-ray sources due to inherently weak X-ray diffraction using conventional sources can only be structurally determined using the intense X-ray beams provided by a synchrotron. Examples of these samples include membrane bound proteins and biomacromolecules with dimensions greater than $60 \times 10^{-10}\text{m}$. The Bragg Crystallography Facility will be able to screen samples locally, thereby allowing more sensitive species to be screened for the first time and providing a rapid screening facility for other weakly diffracting samples.

4) Powder

Powder samples can be run on the Xcalibur (Mo radiation only). However, only homogeneous powder samples with at most two chemical components are appropriate for the CCD diffractometer.

Summary

Single-crystal X-ray structure determination provides the single most important means of unambiguously characterising molecules in the solid state. Using this technique an experimenter can determine the exact 3-D arrangement of atoms in a structure – this includes the relative positions, bonding and interactions of all atoms in a structure. No single step can provide more information about the way a biological/chemical agent works than its three dimensional structure.

Key People



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