

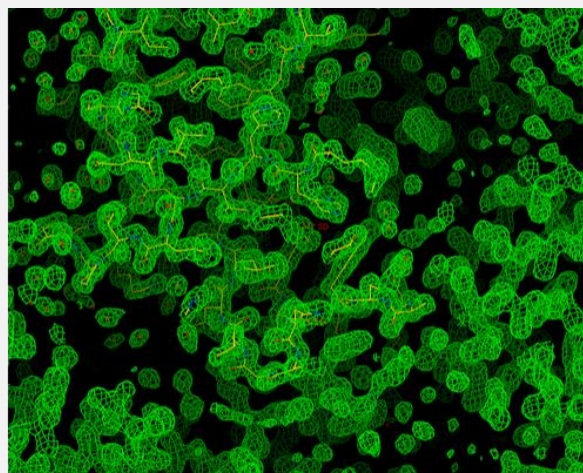
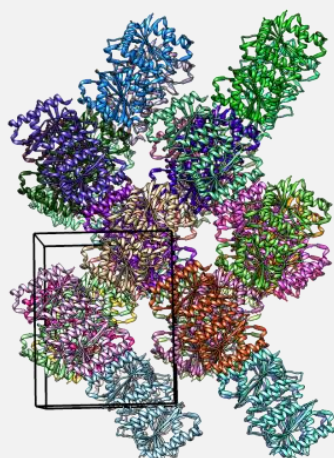
XtaLAB Synergy + Actor

Single crystal X-ray diffraction

Rigaku OD (Oxford Diffraction) XtaLAB Synergy Custom with robotics ACTOR, set of instruments optimized for 'home lab' diffraction experiments with single crystals of macromolecules: proteins, nucleic acids, etc. Single crystal X-ray diffraction is very powerful technique allowing to obtain 3D structure of molecules with atomic resolution. In standard experiment, X-rays are diffracted on single crystal of macromolecular sample. Set of diffraction images is recorded and used for structure determination. Obtained atomic models and electron density maps are used for unraveling the structural and functional properties of studied macromolecules, understanding mechanisms of action on atomic level and creating rational basis for further molecular design. The XtaLAB Synergy diffractometer configuration incorporates ACTOR robotics for automated routine crystal screening and unattended serial data collection for up to 50 frozen crystals.

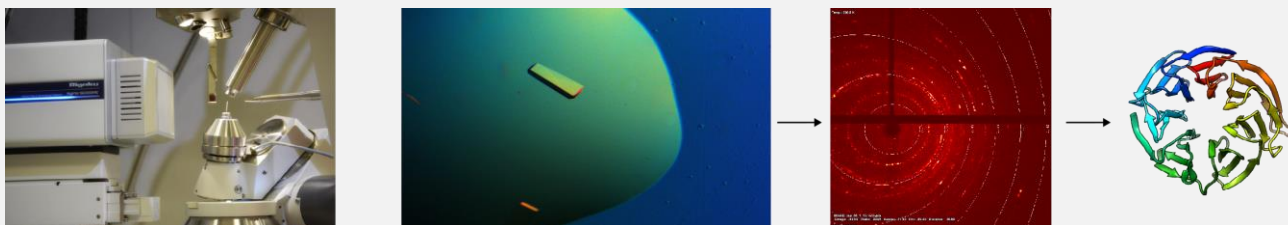
● Single crystal X-ray diffraction can be used for:

- Structure determination with atomic resolution
- Macromolecules: proteins, nucleic acids and complexes
- Protein engineering
- Drug design
- Ligand screening
- Crystallization condition screening
- Diffraction quality testing
- Cryo-condition testing



● Technical specifications

Instrument: XtaLAB Synergy (Rigaku)



Features:

- Rigaku MicroMax-007HF - rotating anode generator of Cu K α X-ray ($\lambda=1.54 \text{ \AA}$)
- Rigaku VariMax VHF optics for intense monochromatic X-ray beam with adjustable divergence
- 4-circle kappa geometry goniometer
- Intelligent Goniometer Head (IGH), motorized goniometer head with automated optical object centering
- Rigaku HyPix-6000HE, hybrid photon counting X-ray detector
- ACTOR, robotics for automated sample cryomanipulation
- Sample storage for up to 50 crystals under liquid nitrogen
- Oxford Cryosystems Cryostream 700, low-temperature device for cryotemperature experiments
- CrysAlis Pro, software for single crystal X-ray data collection and processing

Operational mode:

X-ray diffraction data acquisition is performed by core facility staff only

● **Provided Services and Established Methodologies**

● **Provided services:**

PX diffraction – user obtains set of 2D diffraction images and/or reduced HKL dataset and/or crystal structure (atomic model – PDB, electron density maps).

● **Established Methodologies:**

PX diffraction data collection - standard single crystal X-ray diffraction data collection. The strategy of data collection and parameters of rotational images could be intervened by user upon request.

X-ray diffraction data reduction – single crystal X-ray diffraction data reduction is performed using XDS program package (Kabsch).

Crystal structure determination – determination of crystal structures of biological macromolecules from single crystal diffraction data is performed using CCP4 program suite package.

● **Sample requirements**

- Minimum crystal dimensions 20 x 20 x 20 microM
- Crystals could be delivered to CF frozen or in crystallization plates
- Frozen crystals should be delivered in SPINE pucks
- Mounting loops or MicroMounts with standard BR-5 base and 18mm rod length could be provided by CF

● **Contacts**

Biomolecular Interactions and Crystallization Core Facility

bic@ceitec.cz



Core Facility Leader: JOSEF HOUSER

josef.houser@ceitec.cz

Method Responsible Person: JAROMÍR MAREK / TOMÁŠ KLUMPLER

jaromir.marek@ceitec.cz / tomas.klumpler@ceitec.cz

Instrument Location:

CEITEC MU Campus Bohunice, pavilion C12/115 laboratory, Kamenice 5, 62500 Brno