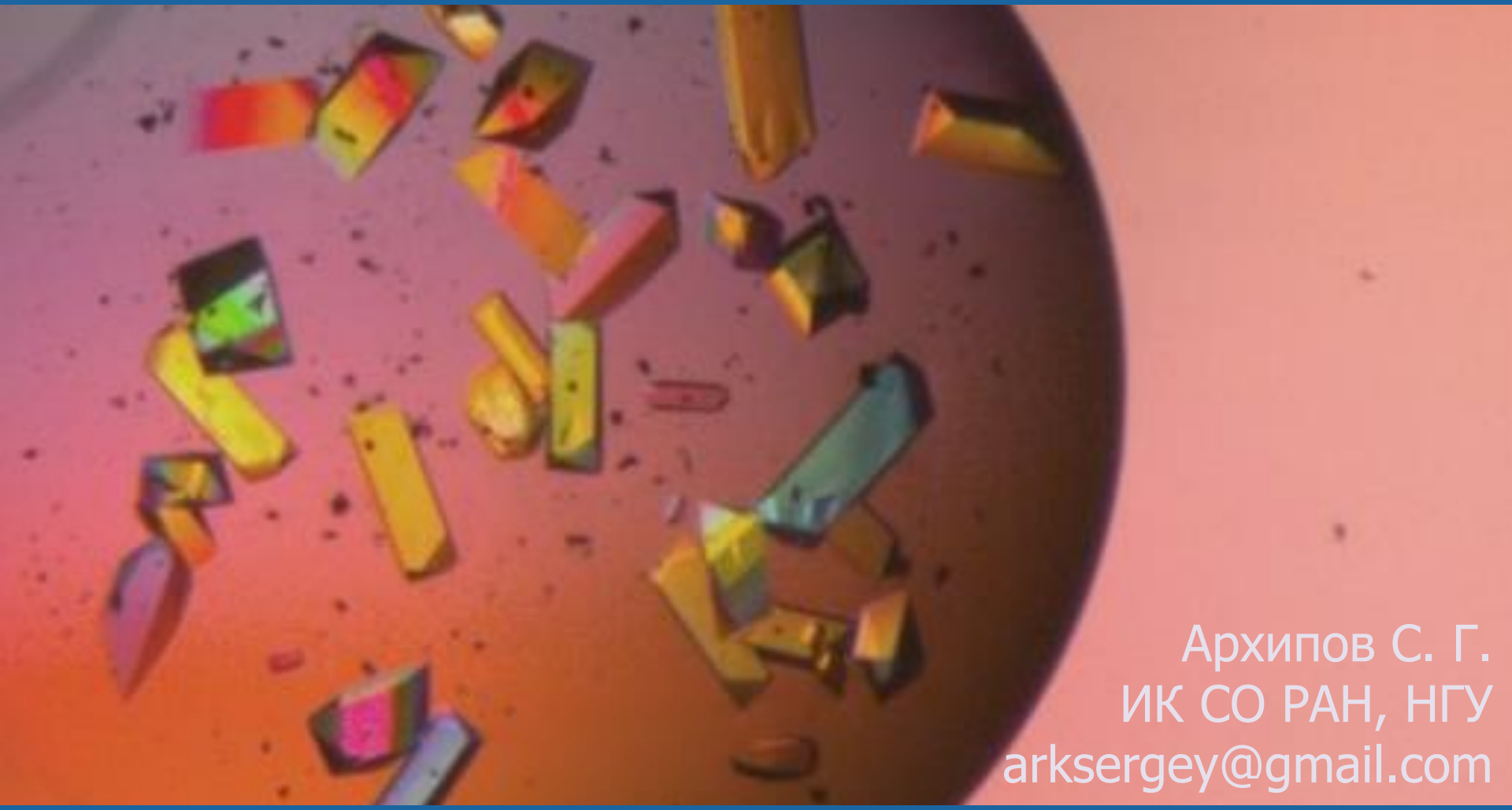
Synchrotron and Free electron laser Radiation: generation and application (SFR-2020)



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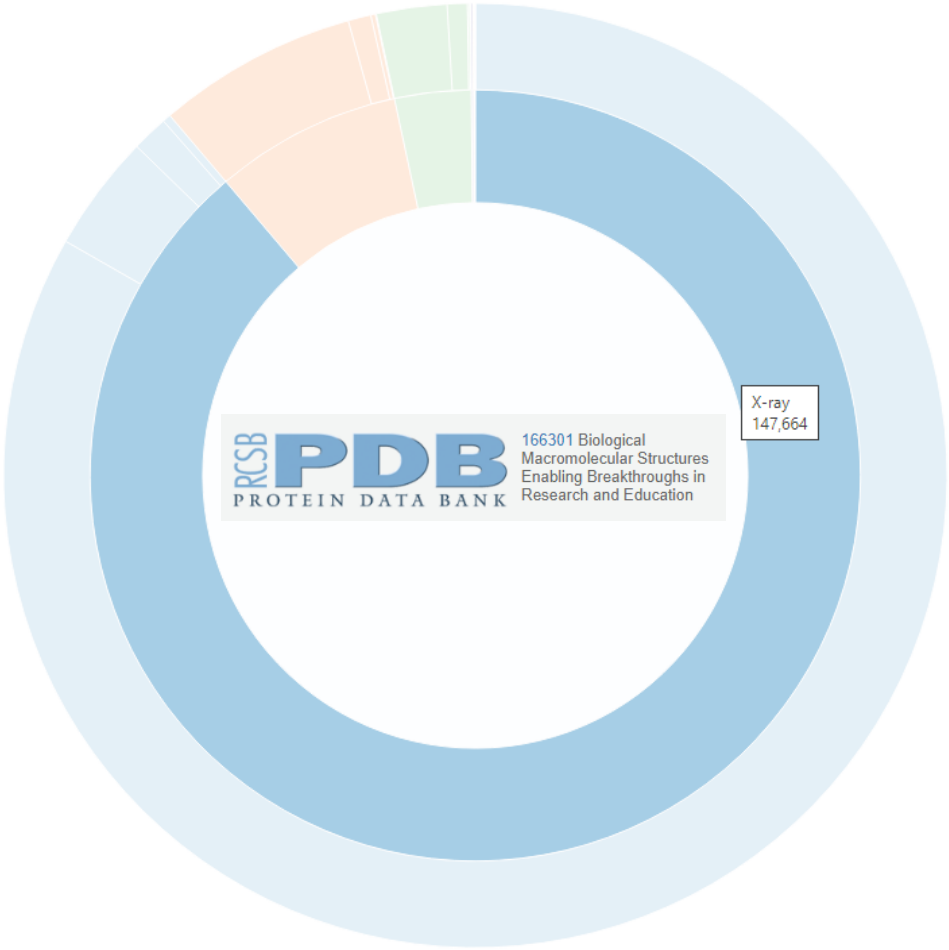
What does the macromolecular crystallography users community expect from the modern synchrotron source?

Where X-ray diffraction data collection from macromolecular single crystals are going on?

X-ray | Count: 147664 | Percentage: 88.8%

120358 datasets were collect under 100K



Total datasets collected using SR	120358 approximately 80%
ESRF	15526
SSRF	4844
Diamond	9537
MAX IV	343
MAX II	1126
Spring-8	5650
EMBL/DESY	2700
SOLEIL	1636
Australian Synchrotron	2622
BESSY	3293
KURCHATOV SNC	39

PDB was analyzed by 12.07.2020

Protein crystal data collection methods

rotating crystal method (1 or several crystals)

- T=100K usual
- crystal harvesting required
- Huge and fast detector/microbeams preferred (PILATUS3 6M; Eiger X 4M/ 10.0 x 10.0 up to 45.0 x 30.0 μm^2(ID23-1))
- spiral rotation is preferred
- time-resolved experiments is impossible

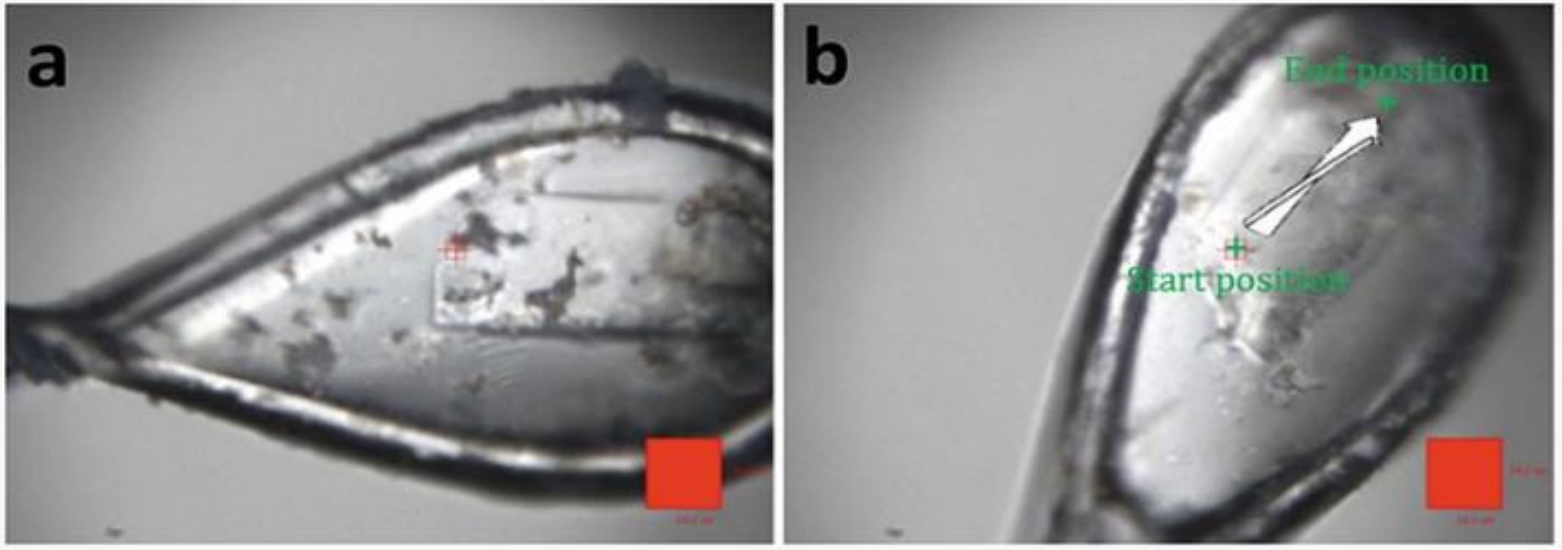


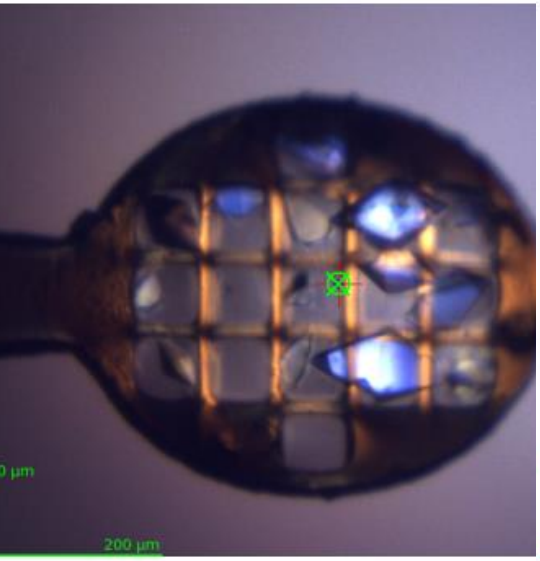
Fig. 8.5
Plate-like crystal of ABCB10 before (**a**) and after (**b**) the loop was bent for data collection. (**b**) Shows the centered start and end positions for the line scan data collection

The Next Generation in Membrane Protein Structure Determination pp 105-117| Cite as
Exploiting Microbeams for Membrane Protein Structure Determination

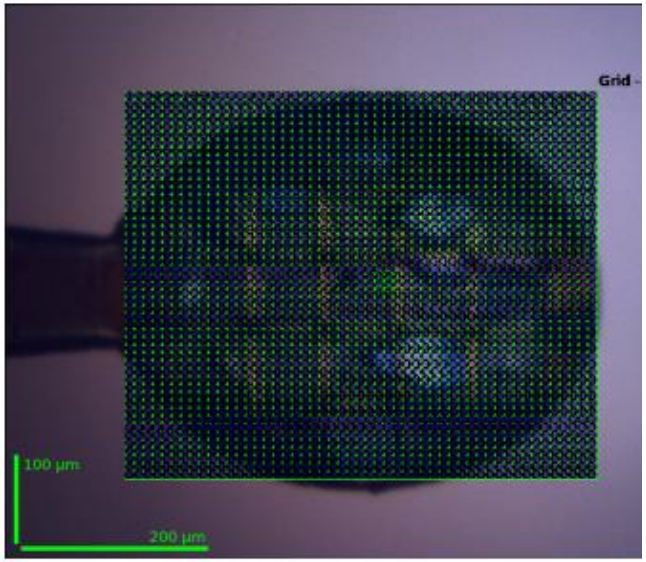
Protein crystal data collection methods

small-wedge (5–10°) crystallography (10-100 crystals)

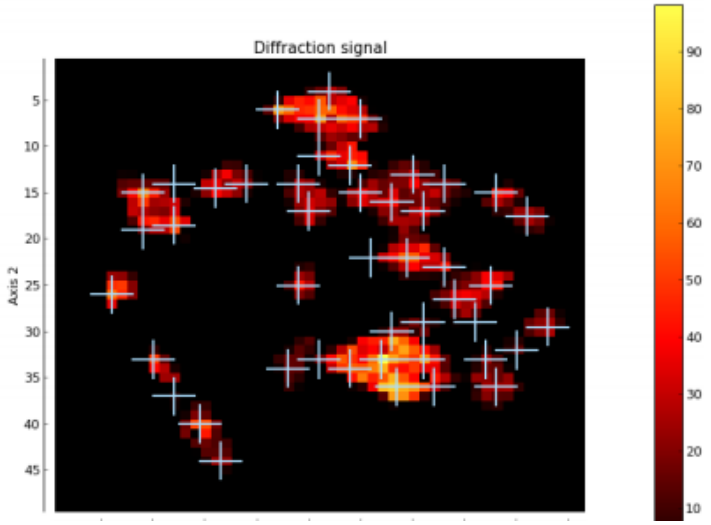
- T=100K usual and compatible with room-temperature experiments
- crystal harvesting required (if 100K). Chips,microfluidic devices,crystallization plates can be used too (RT)
- Huge and fast detector/microbeams necessary
- X/Y scan of the sample
- time-resolved experiments is impossible



☐ Sample on mesh loop



☐ Sample on mesh loop
☐ Mesh scan of sample



☐ Sample on mesh loop
☐ Mesh scan of sample
☐ Detection of protein diffraction
☐ Series of partial data collection

Protein crystal data collection methods

rotating crystal method (1 or several crystals)

- T=100K usual
- crystal harvesting required
- microbeams preferred
- spiral rotation is preferred
- time-resolved experiments is impossible

small-wedge (5–10°) crystallography (10-100 crystals)

- T=100K usual and compatible with room-temperature experiments
- crystal harvesting required (if 100K). Chips,microfluidic devices,crystallization plates can be used too (RT)
- microbeams necessary
- X/Y scan of the sample
- time-resolved experiments is impossible

serial crystallography (1000-10000 crystals)

- room-temperature experiments
- crystal harvesting not applicable. **Delivery systems** (fixed target, liquid get, tape) or chips should be used
- microbeams necessary
- X/Y scan of the sample
- Time-resolved experiments is possible(!)

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HTCC4
Structural biology
Dubrovnik, Croatia Oct. 1-6, 2019

How to deliver crystals to a synchrotron from home or host lab?

Dewar

A dry-transporter/shipper must be used to transport the samples safely. The most common one is the **Taylor-Wharton CP100 dry shipper** (see these articles for more details on temperature measurements: paper1, paper2)

ESRF The European Synchrotron

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DEWAR SENDING

PREPARE YOUR EXPERIMENT

DEWAR SENDING

When to send your Dewar

It is important to leave **at least 3 days** between sending the dewar and experiment start. If a problem occurs on a 24 hour delivery, it will NOT arrive on time and your trip will be wasted.

Be certain that the delivery takes place during **week days 08:30-12:00 and 13:00-17.00**. The ESRF stores are **closed at the weekends and for French and ESRF holidays**: No deliveries can take place on any of these days.

Sending your dewar

Warning !! Please use dewars for sample transport only. A number of dewars have been found to contain scissors, syringes and even hard disks. Please do NOT transport such articles within a dewar transport box.

ESRF staff will now top up your dewars with liquid nitrogen on arrival at the ESRF and empty them before they are returned. If you would like staff to do this please DO NOT close your dewars with cable ties.

When to send your dewar

Paperwork

Not all customs / airport / traffic police officers are sympathetic to dewar with liquid nitrogen. Despite the fact that the dewar has a sponge into which liquid nitrogen is absorbed.

https://www.esrf.eu/UsersAndScience/Experiments/MX/How_to_use_our_beamlines/Prepare_Your_Experiment/Sample_support#Dewar

Send samples by mail / to go to a synchrotron with samples?

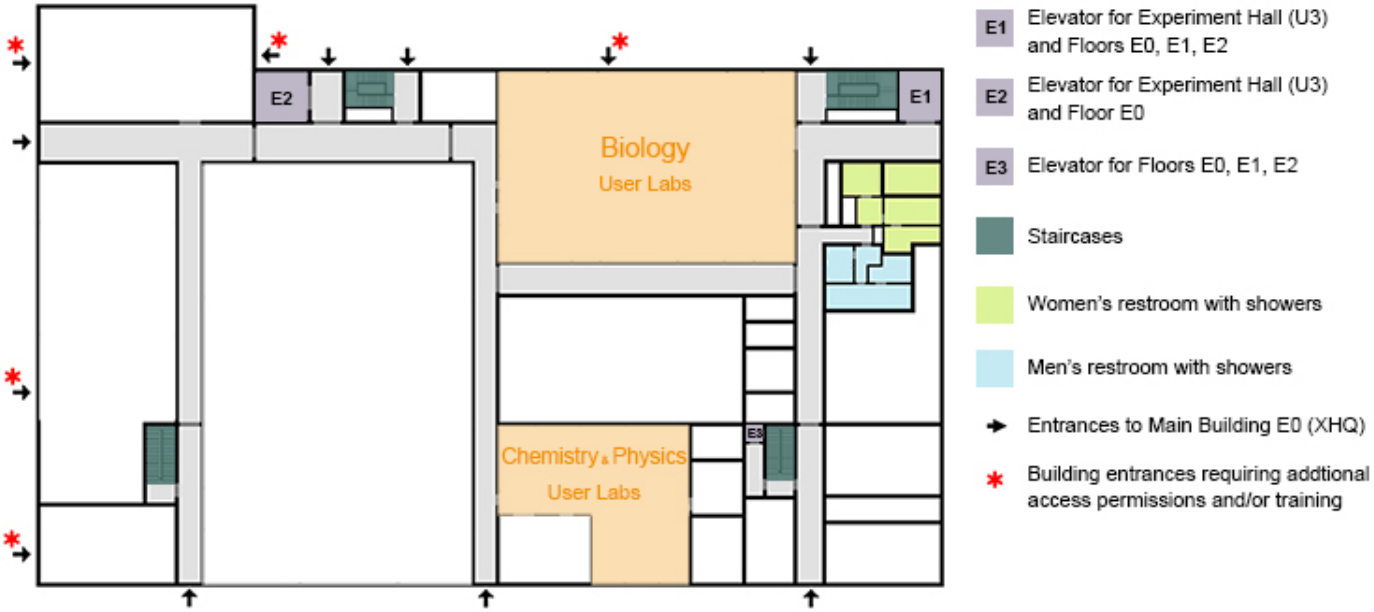
user send samples by mail	user goes to the synchrotron with samples
The user has equipment for protein crystallization	The user does not have equipment for protein crystallization. Usually, the synchrotron has department for MX crystallization or interacts with organizations engaged in MX crystallization.
There is a technical opportunity and infrastructure at the synchrotron (contacts with customs and postal services are established, there are responsible people at the synchrotron, delivery is possible in a short time)	There is no technical possibility to send by mail and the corresponding infrastructure at the synchrotron. Then synchrotrons lose potential users.
Routine experiment	Protein crystals break down during harvesting or transportation
Automated experiment (often used by pharmaceutical companies)	The experiment is not routine, requires the attention of a scientist, including for mounting delivery systems (serial crystallography).

What to do to users who cannot deliver crystals to the synchrotron?

Laboratories

European XFEL

A variety of laboratories are available at the ground level of the European XFEL headquarters building (XHQ) for users to prepare samples at the facility's scientific instruments in the underground Experiment hall. The laboratories are specialized for preparation of solid samples, chemical samples, gaseous samples, and liquid and aerosol samples. A suite of labs for biological samples has been contributed by the XBI user consortium.



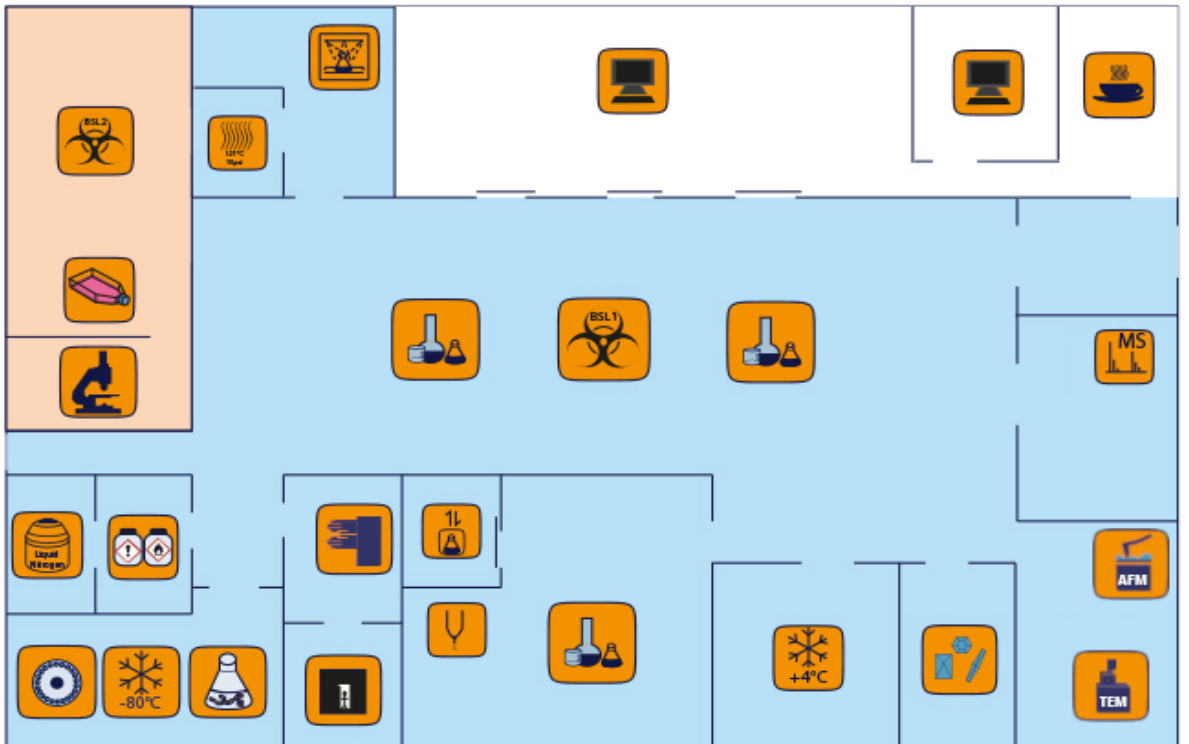
What to do to users who cannot deliver crystals to the synchrotron?

Laboratories | Samples processing | Access | About us

Biology lab (XBI) | Chemistry labs | Material Science

Facility > User Laboratories > Laboratories > **Biology lab (XBI)**

The biological laboratories are located directly above the experiment hall. They host a large state-of-the-art wet lab area surrounded by specialized rooms and allow for sample preparation starting from cell culture, through centrifugation, protein purification and finally crystallisation, as well as the subsequent sample analysis.



What does the macromolecular crystallography users community expect from the modern synchrotron source?

- huge, fast and sensitive 2D detector
- microbeam
- spiral rotation, X/Y scan of the sample
- biological labs and MX crystal growth labs
- ability to conduct remote and automated experiments
  sample delivery support department
- automatic sample changer
- cooling system
- place for users deliveries systems
- intellectual property protection (for companies)

optimum variant

- huge, superfast and sensitive 2D detector
- submicrobeam
- development and optimization of deliveries systems for SSX
- energy range pink beam
- background reduction systems
- BSL3 or BSL4 level labs

extended variant

CCP4 Online Automated Webservices

The CCP4-online webserver is now available. Users can make use of **BALBES**, **MrBUMP** and **MoRDa**, the automated molecular replacement services. **Zanuda**, the refinement result checking software and **PISA** for the calculation and analysis of macromolecular surfaces and interfaces ar
experimental phasing. To

MoRDa - Automatic Molecular Replacement Pipeline

Authors: A.Vagin, A.Lebedev

Thanks for your attention!