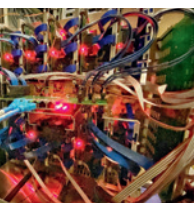
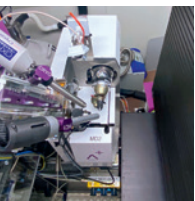
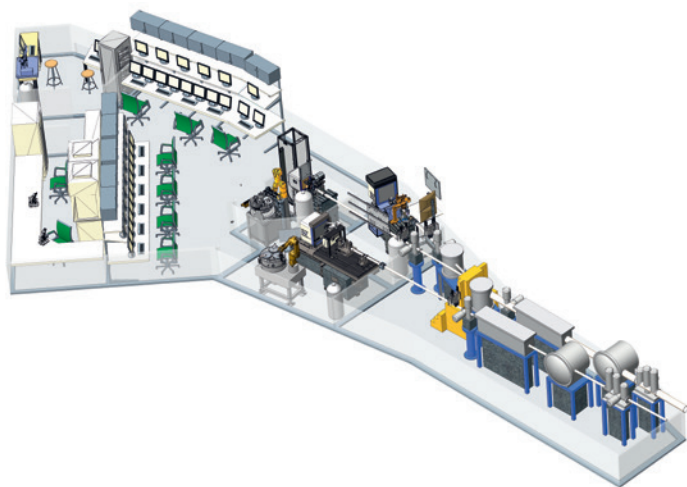


Introduction



Macromolecular Crystallography (MX) is one of the key disciplines in modern biological, biochemical and bio-medical research. It is the most important technique to provide atomic level descriptions of the bio-molecules involved in intra- and extracellular processes. At the BESSY II storage ring, Germany's first third-generation synchrotron source, three state-of-the-art synchrotron beamlines for MX are operated by the HZB-MX group.

With more than 4000 PDB depositions, the beamlines are very productive and hence also very popular among academic and industrial users [1,2].



Characteristics of the HZB-MX beamlines

	Experimental Station BL14.1	Experimental Station BL14.2	Experimental Station BL14.3
Wavelength range [Å]	0.8–2.25	0.8–2.25	0.89
Photon flux at sample [Phot / s x 100 mA x 0.05% BW]	1.6×10^{11} (at $\lambda = 0.92$ Å)	1.5×10^{11} (at $\lambda = 0.92$ Å)	2.3×10^{10}
Energy resolution [eV]	<2	<2	<5
Beam size [μ m diameter]	50–100	100	50–200
Goniometry	MD2-microdiffractometer with MK3	Nanodiffractometer	MD2S-microdiffractometer with MK3
X-ray detector	PILATUS3 S 6M	PILATUS3 S 2M	PILATUS2 6M
Sample mounting	CATS robot	G-ROB robot (ISARA robot*)	manual
No. of samples in sample dewar	144 Unipuck	50 SPINE (464 Unipuck*)	–
Exposure times [s / °]	0.4–10	0.4–10	0.9–20
Detector distance range [mm]	140–649	57–800	110–501
Achievable resolution [Å]	0.84	0.71	0.85
Maximum unit cell length [Å]	600 (at $d_{\min} = 2.0$ Å)	400 (at $d_{\min} = 2.0$ Å)	600 (at $d_{\min} = 2.0$ Å)
Remote operation	YES	YES	NO
Special equipment and operations	<ul style="list-style-type: none"> • Helical data collection • Crystal annealing • UV-pulsed laser for UV-RIP 	<ul style="list-style-type: none"> • Long wavelength and atomic resolution data collection • Safe light conditions 	<ul style="list-style-type: none"> • RT data collection • Controlled dehydration • REX nozzle exchanger • <i>In situ</i> crystal screening

* after 2022/2 upgrade

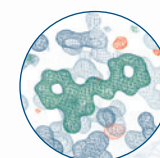
Unique opportunities



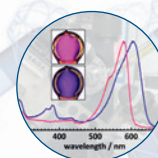
Crystal improvement by controlled dehydration



Kappa-goniometry



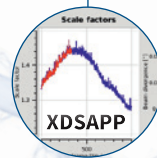
Crystallographic fragment-screening [4]



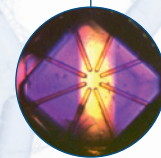
In crystallo micro-spectro-photometry



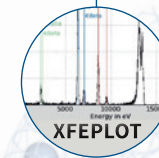
In situ crystal screening



Automatic data processing using XDSAPP [3]



Radiation damage



X-ray fluorescence based element identification using XFEPLLOT

- [1] Mueller *et al.* (2012). *J. Synchr. Rad.* **19**, 442–449.
 [2] Mueller *et al.* (2015). *Eur. Phys. J. Plus* **130**, 141–150.
 [3] Sparta *et al.* (2016). *J. Appl. Cryst.* **49**, 1085–1092.
 [4] Wollenhaupt *et al.* (2021). *J. Vis. Exp.* **169**, e62208.