



Elettra Sincrotrone Trieste



Elettra
Sincrotrone
Trieste

Status of the diffraction beamlines at Elettra



Elettra – Sincrotrone Trieste





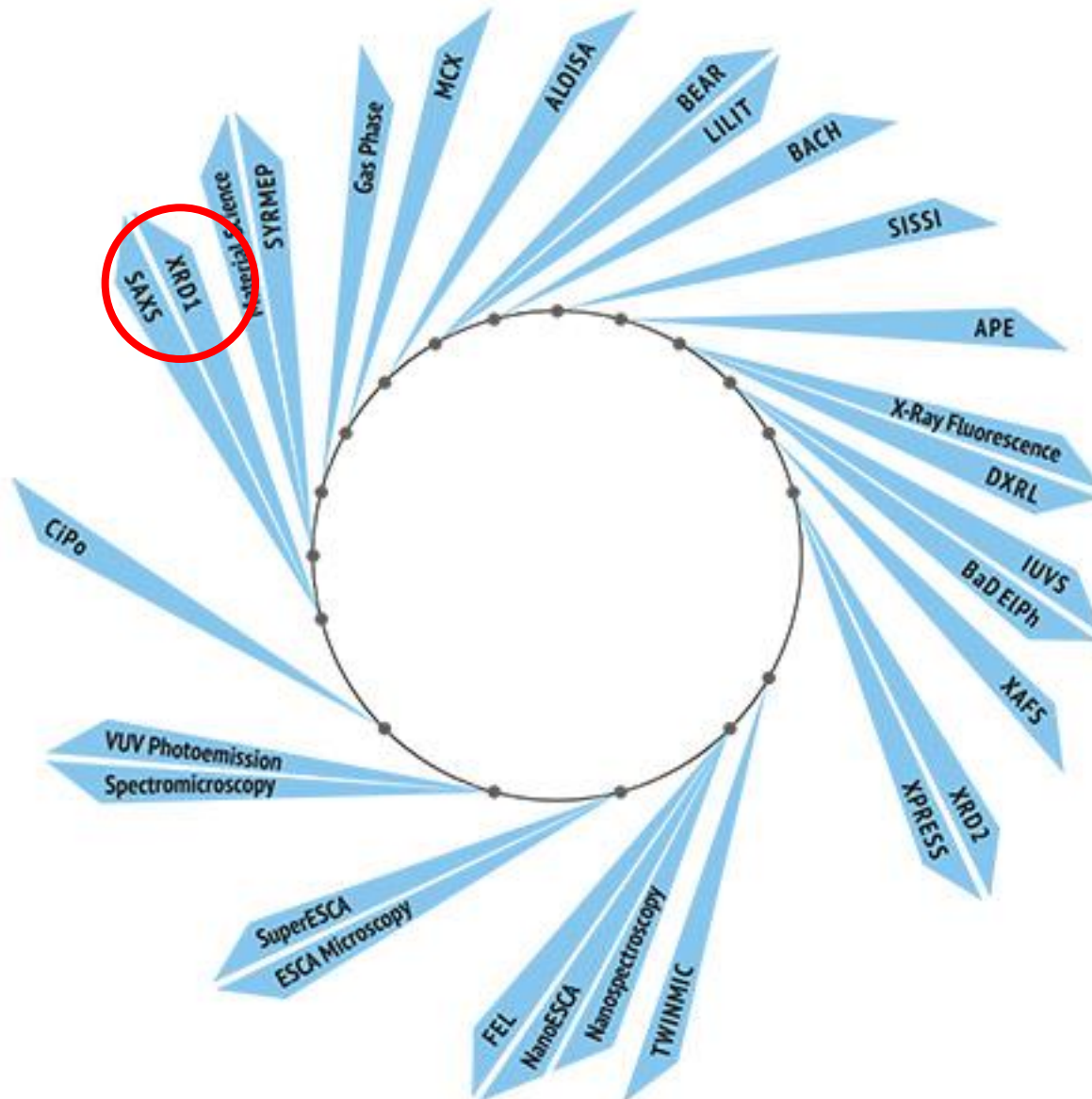
Elettra
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Trieste

Elettra – Sincrotrone Trieste





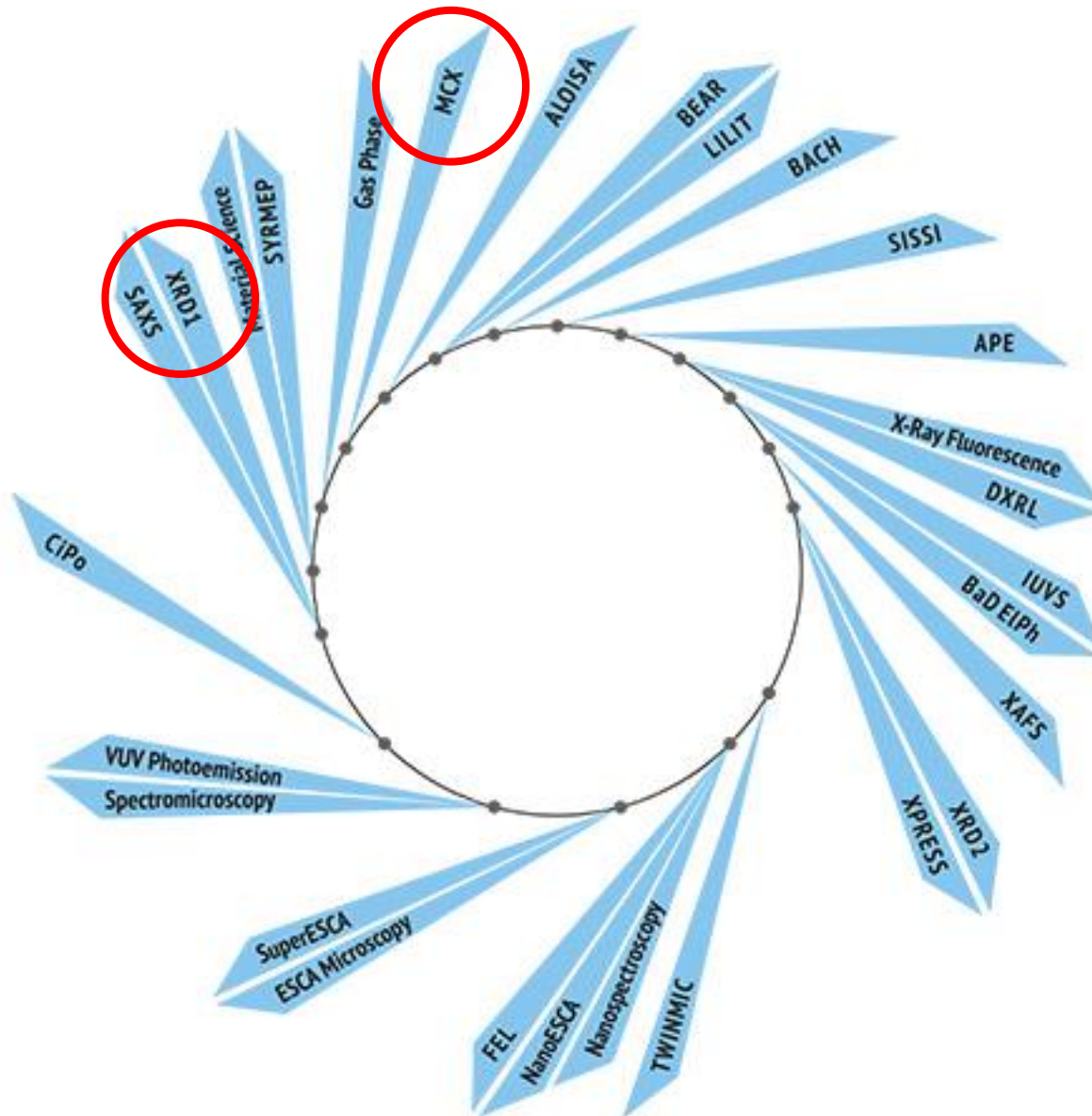
Diffraction beamlines at Elettra



- XRD1 (1997)



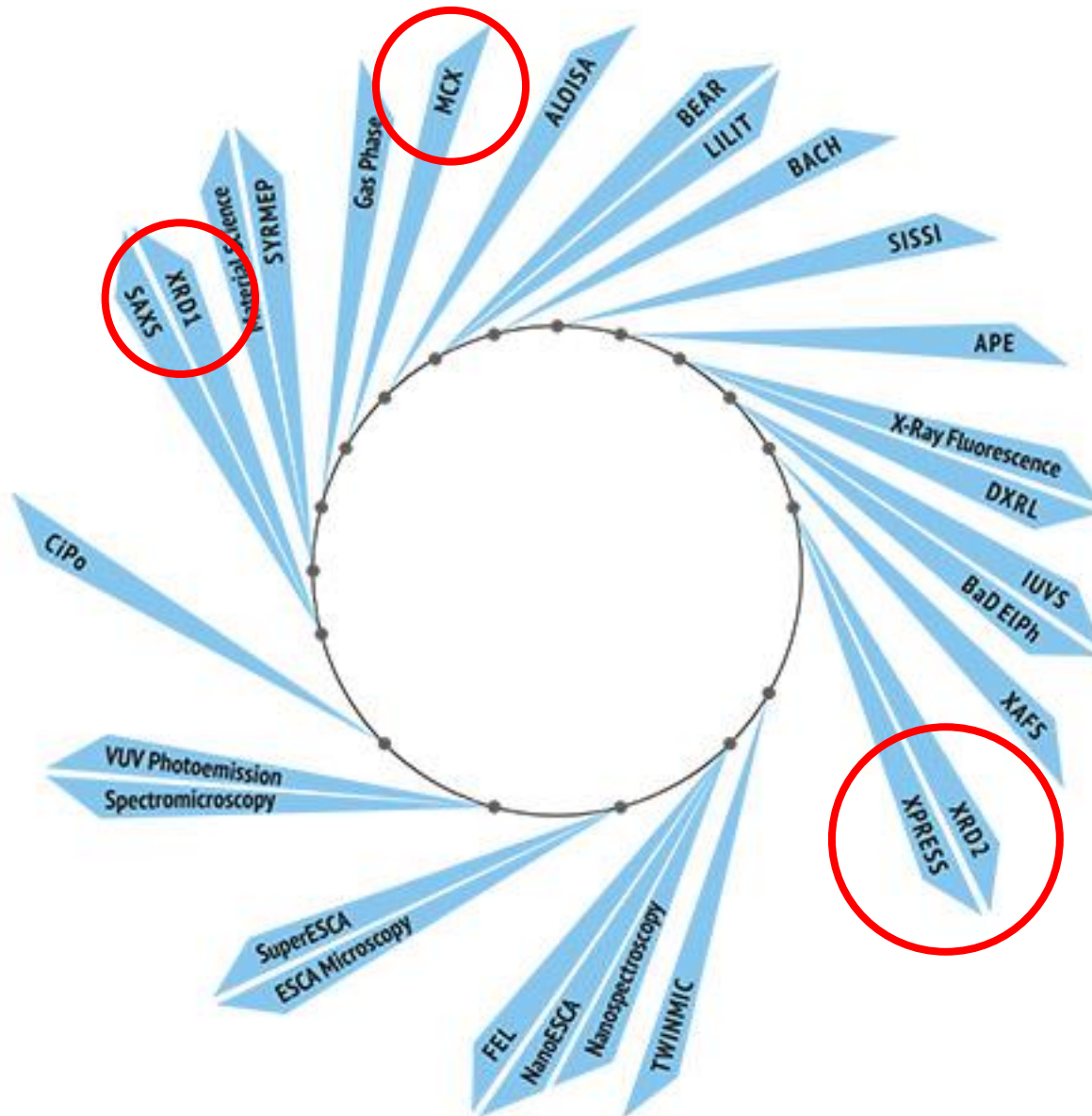
Diffraction beamlines at Elettra



- XRD1 (1997)
- MCX (2007)



Diffraction beamlines at Elettra

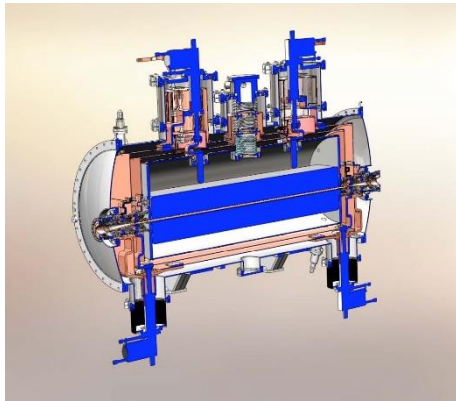


- XRD1 (1997)
- MCX (2007)
- Xpress (2016)
- XRD2 (2018)

XRD2 – Macromolecular Crystallography

Beamline

Source: superconducting wiggler
Fully tunable 8-20 KeV (35 KeV)
Optimized for SeMet
Native beam 300 μm x 100 μm



Diffractometer

MD2 \rightarrow kappa
Apertures (μm)
20, 50, 75, 100

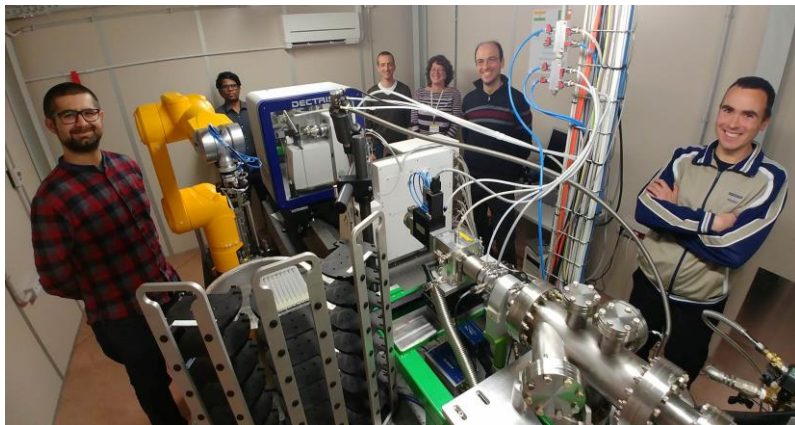
Detector Pilatus 6M
Shutterless



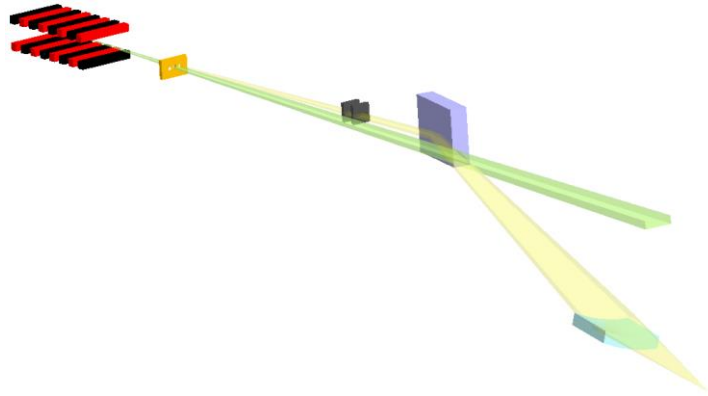
SampleChanger

UNIPUCKS automation

Capacity 188 samples
Dryer, lid, barcode



XPress – High pressure diffraction

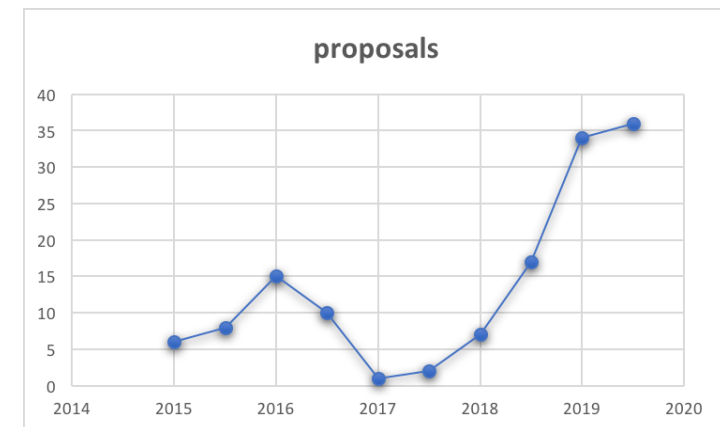
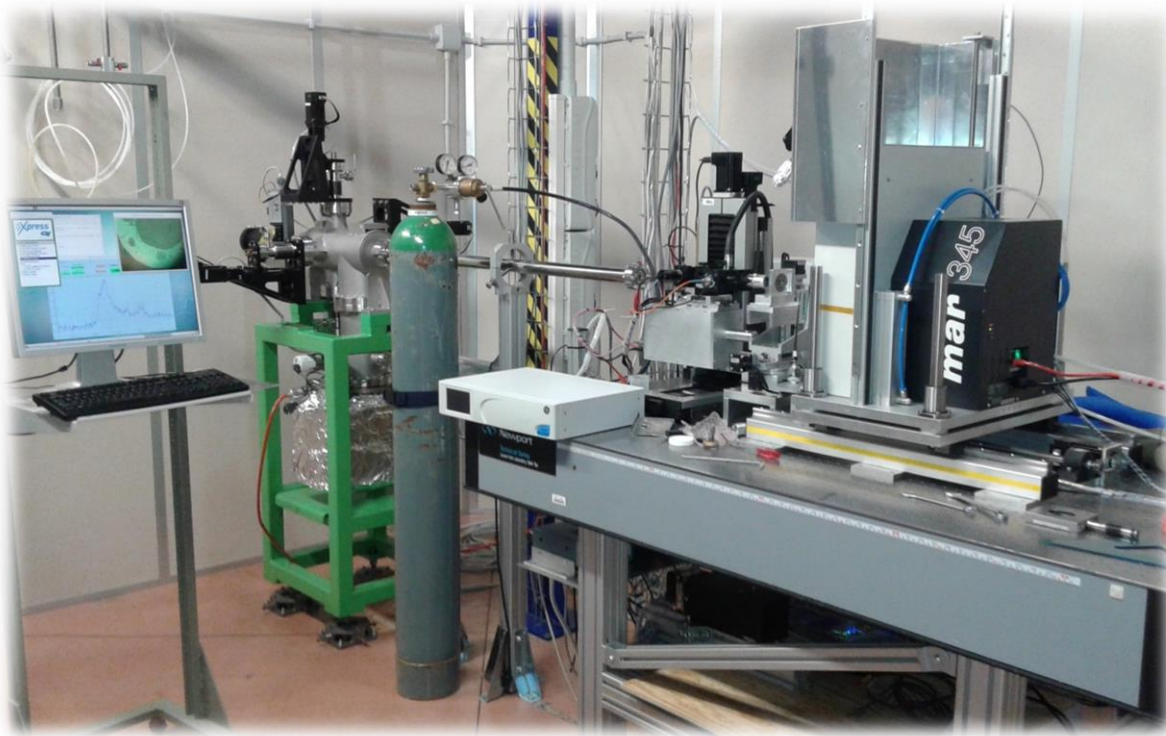


X-ray Energy 25 keV

Acceptance $500 \times 120 \mu\text{rad}^2$

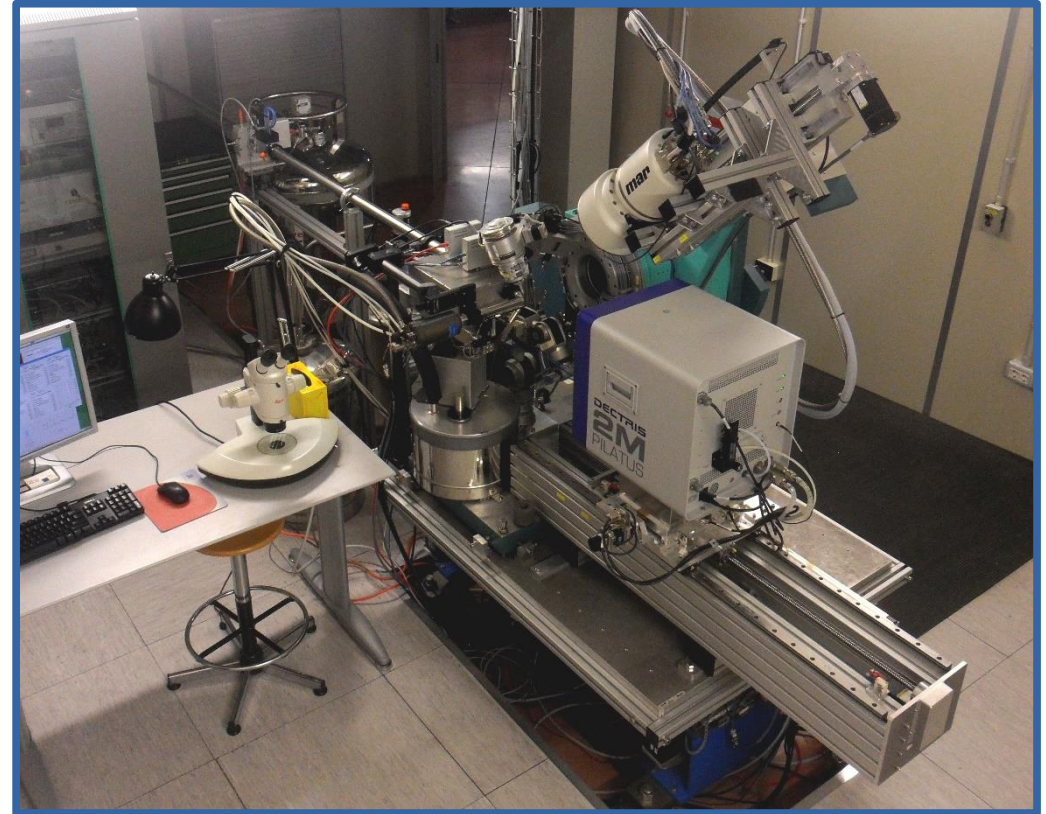
Flux in $80 \times 80 \mu\text{m}^2$ aperture at sample:

10^{11} ph/s @ 2.4 GeV, 100mA



XRD1 – General purpose diffraction

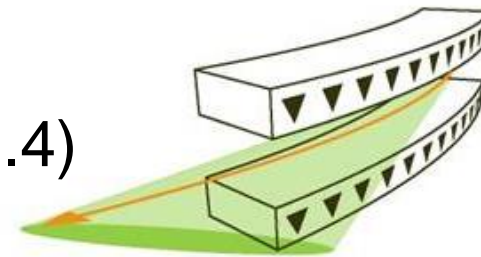
- Wiggler as source ($5 \cdot 10^{12}$ ph/s)
- Wide spectrum 4-21.5 keV
- Beam size: $200\mu\text{m}$ – $30\mu\text{m}$
- Huber k-geometry goniometer
- Spine compliant robotic arm for automatic sample mounting, 50 samples capacity (ESRF puck)
- Large single photon counting area detector (Dectris 2M)
- 9mm^2 fluorescence detector



- At the present mainly used for: (i) single crystal for molecular structural solution (small molecules, supramolecular chemistry), (ii) grazing incidence diffraction (in-plane and out-of-plane), (iii) material science (phase transitions)

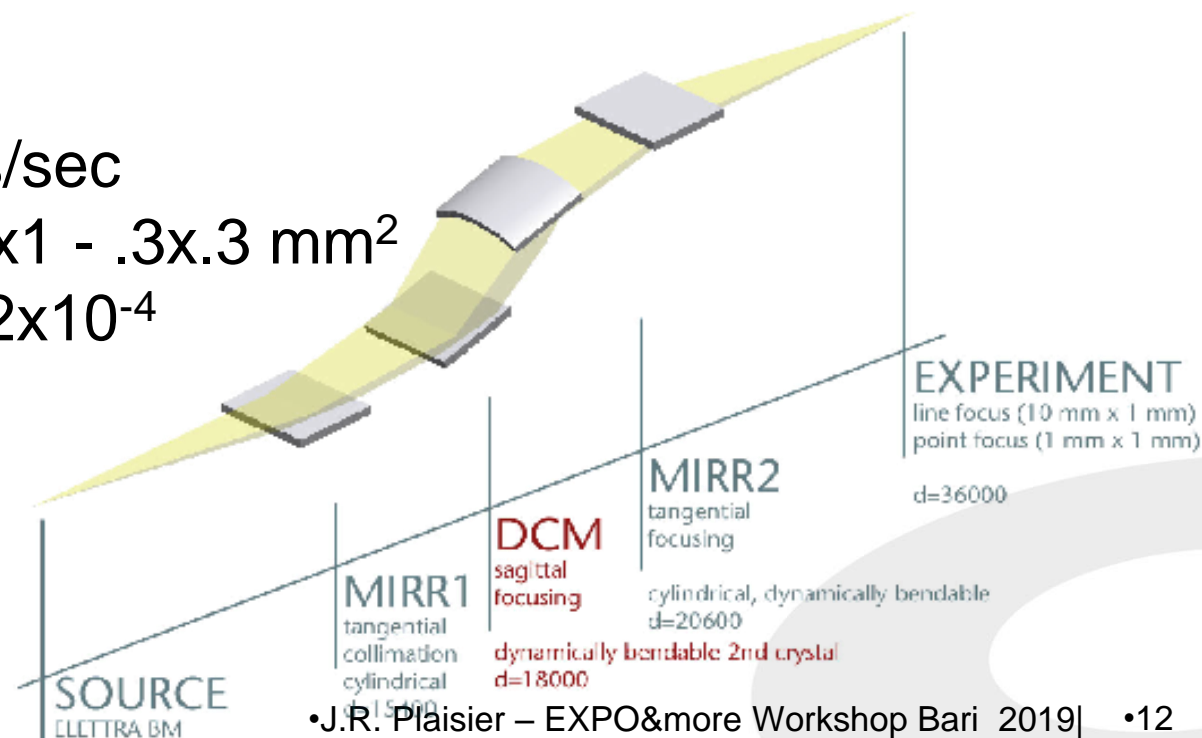
Light Source:

- Bending magnet
- Critical energy : 3.2keV (2.0) , 5.5keV (2.4)



X-rays at sample:

- Energy range : 6-22 keV
- Photon flux : 10^{11} photons/sec
- Beam size at sample : $10 \times 1 - .3 \times .3 \text{ mm}^2$
- Energy resolution : $\Delta E/E \ 2 \times 10^{-4}$



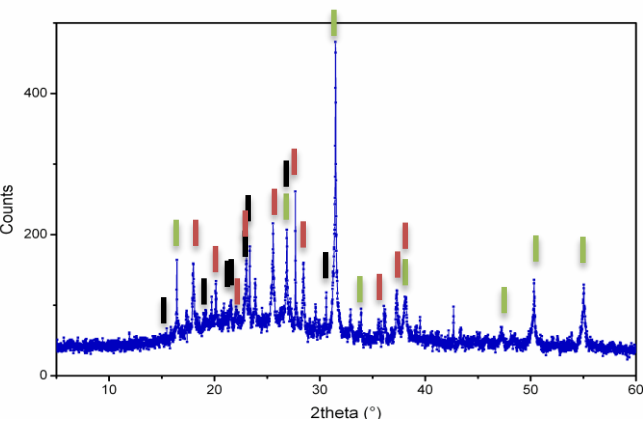
MCX - Experimental station

- Huber 4 circle diffractometer ($.0001^\circ$ precision in 2θ)
- Analyzer crystal / scintillator detection system or CCD
- Transmission geometry, reflection geometry, grazing incidence diffraction
- Temperature control from 100 K to 1273 K
- Fluorescence detector

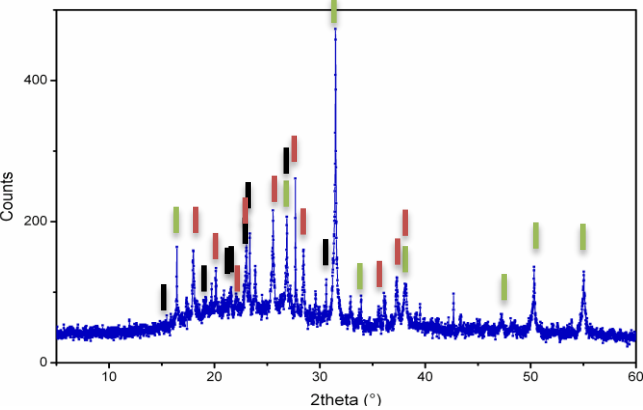


Diffraction experiments at MCX

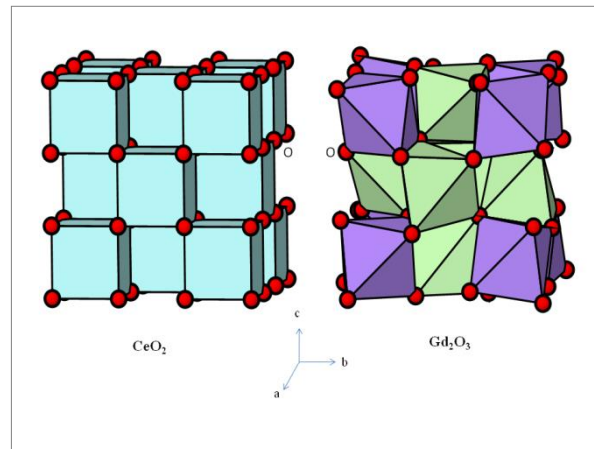
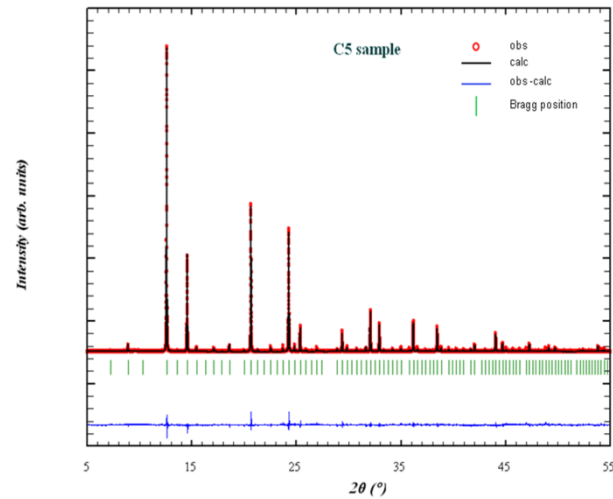
Phase Identification



Phase Identification

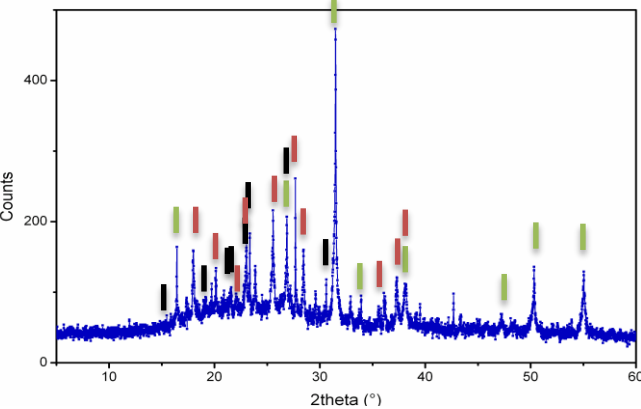


Structure Determination

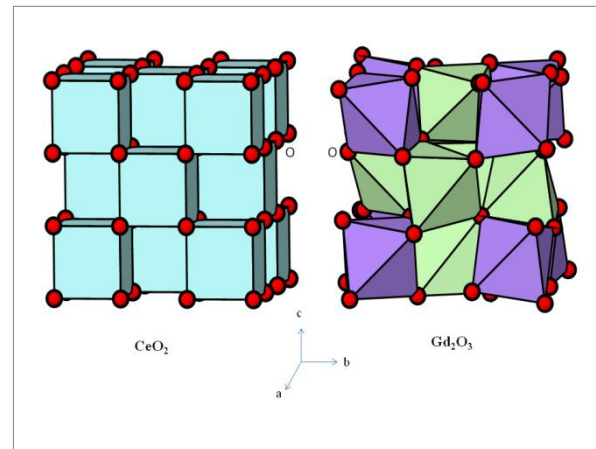
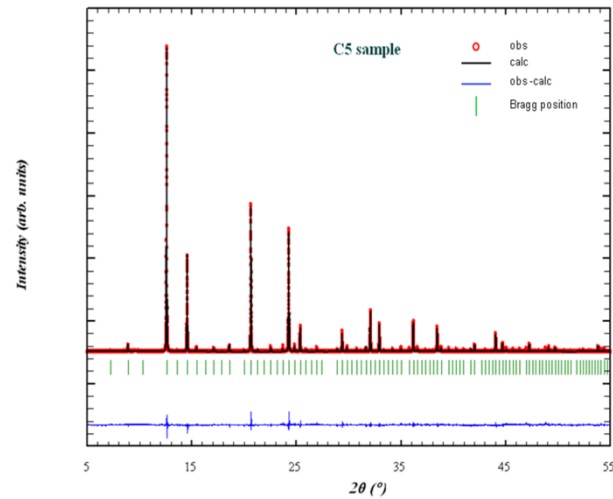


Diffraction experiments at MCX

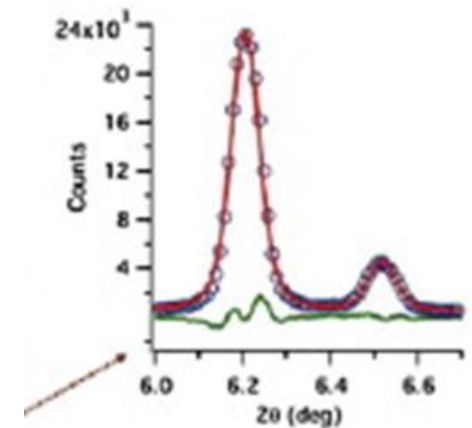
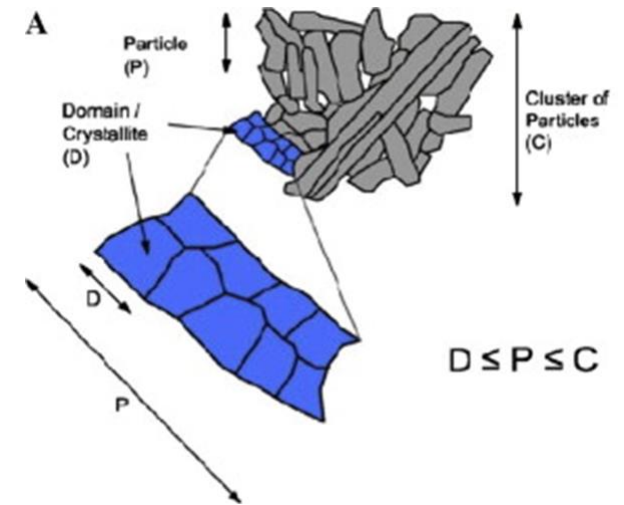
Phase Identification



Structure Determination

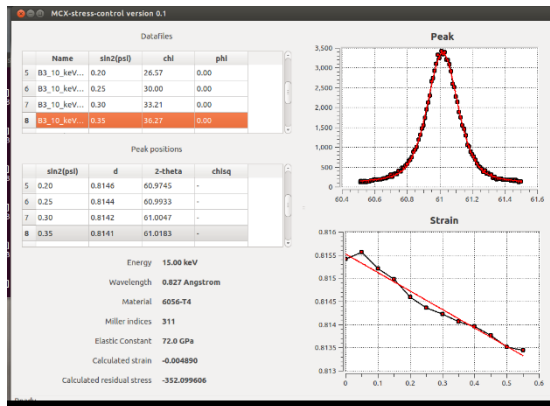
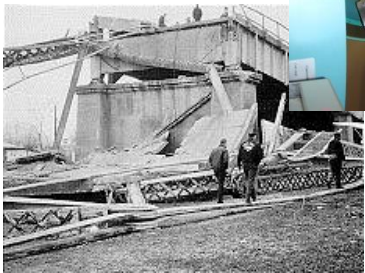
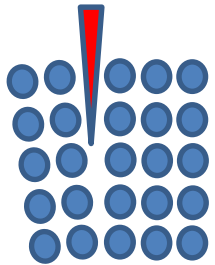


Line Profile Analysis

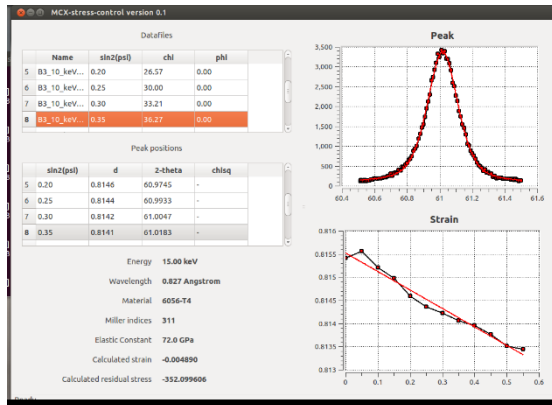
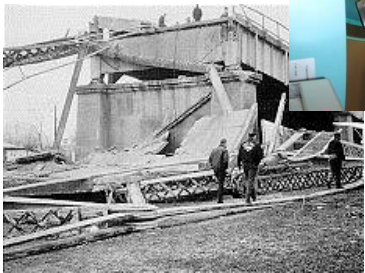
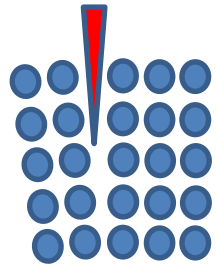


Diffraction experiments at MCX

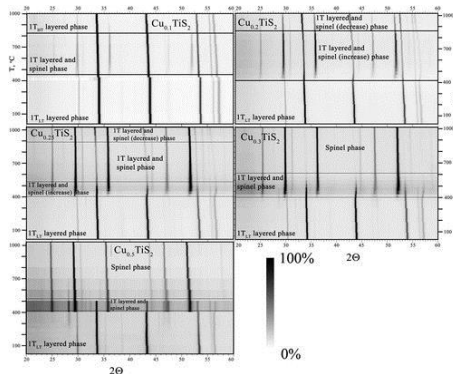
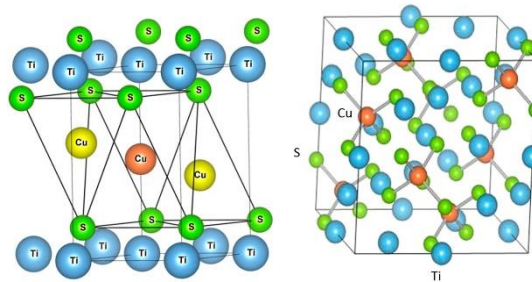
Residual Stress Analysis



Residual Stress Analysis

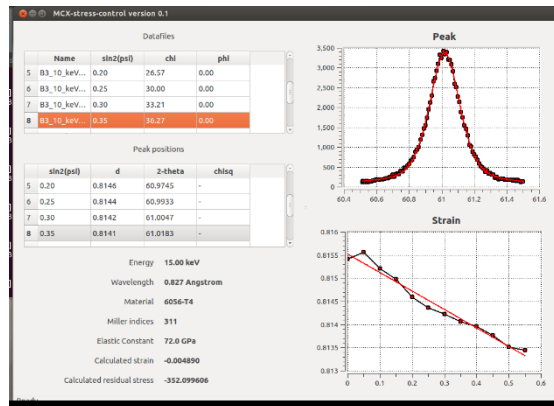
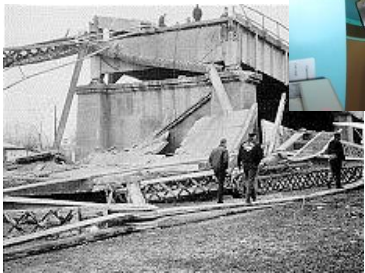
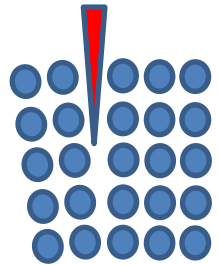


Non ambient conditions

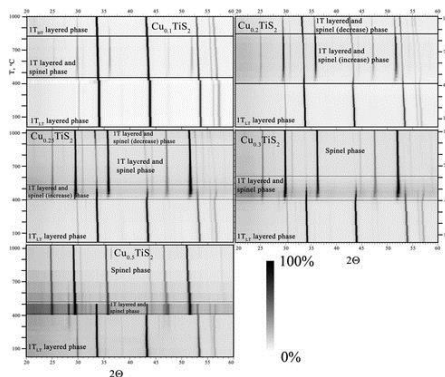
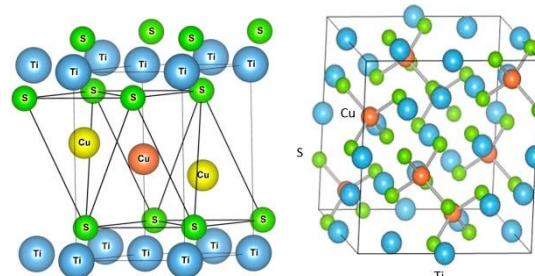


Diffraction experiments at MCX

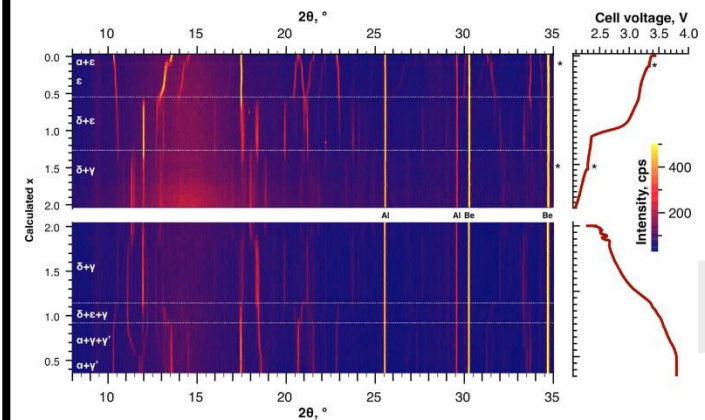
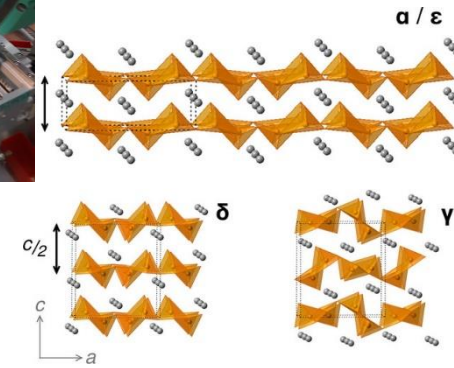
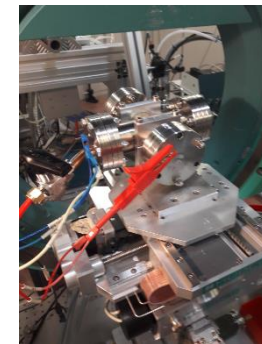
Residual Stress Analysis



Non ambient conditions



Operando

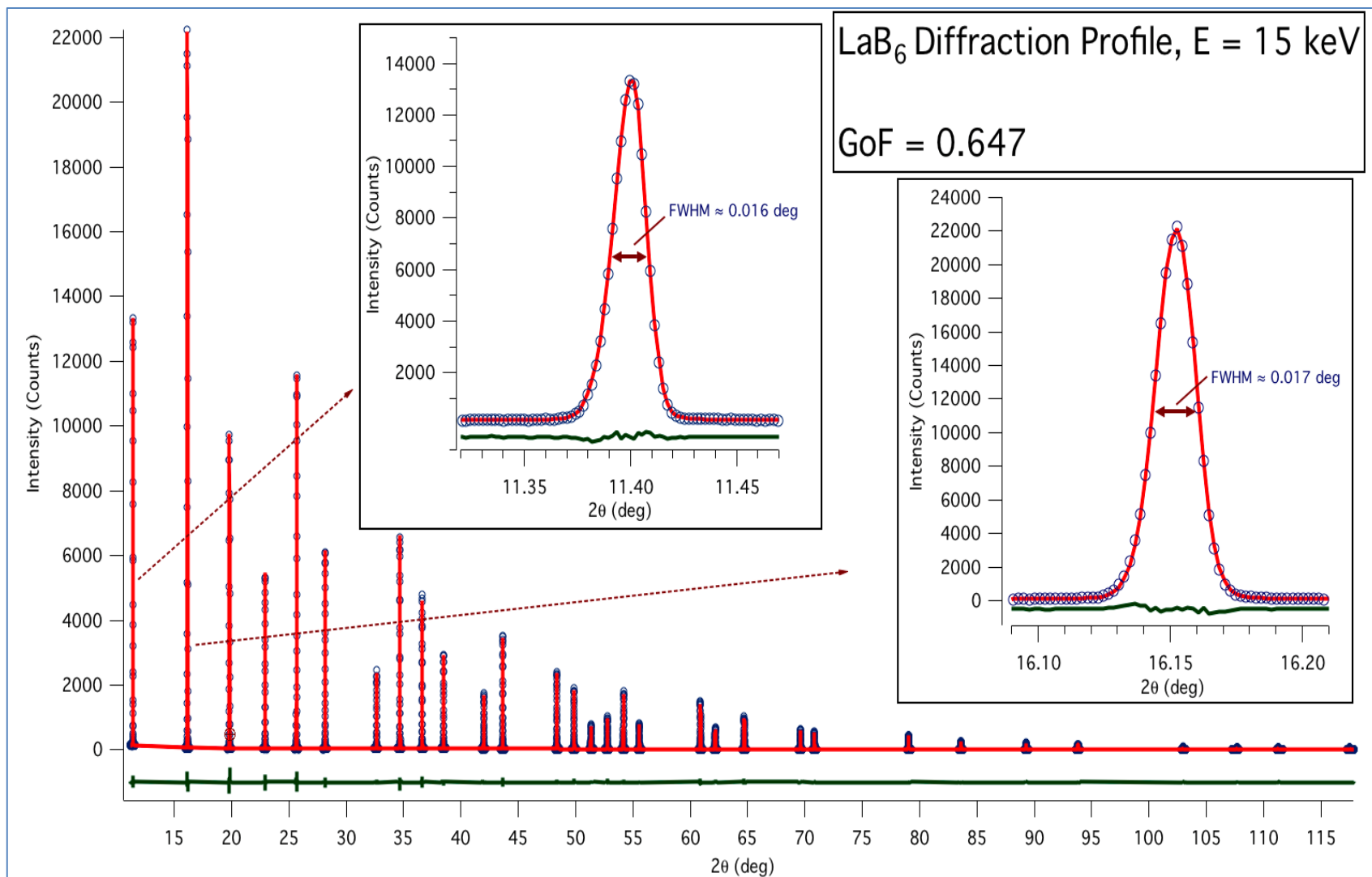




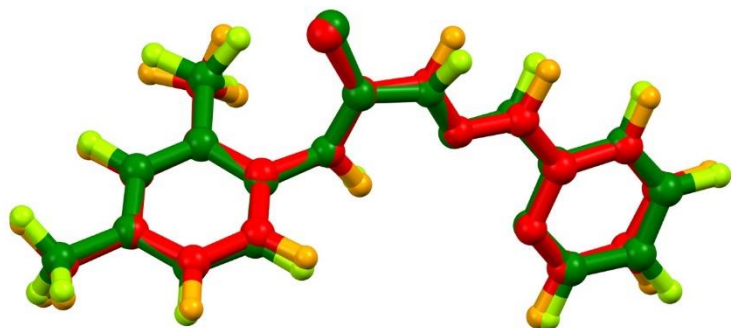
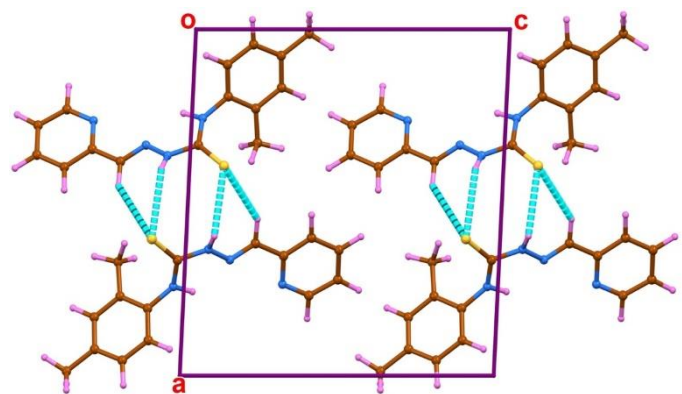
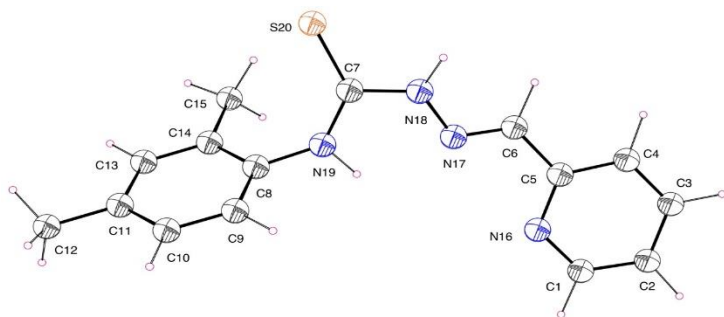
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MCX and EXPO?

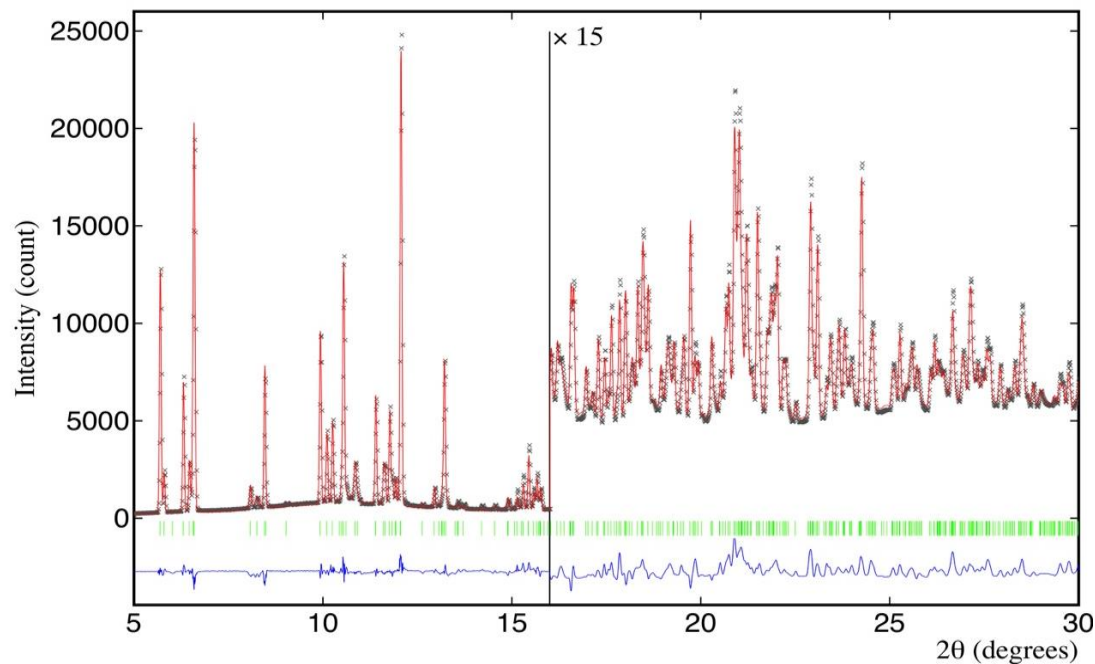
MCX and EXPO?



MCX and EXPO?



M Ibrahim *et al.*, *Future Medicinal Chemistry*, 10, 2507 (2018)



Chemical formula	$C_{15}H_{16}SN_4$
a, b, c (Å)	14.1186(5), 7.9535(2), 13.3615(7)
b (°)	92.8285(2)
V (Å ³)	1498.58
Z	4
Space group / system	C2 / Monoclinic
Radiation type	Synchrotron, $\lambda = 0.7 \text{ \AA}$
2 θ values (°)	2 $\theta_{\min} = 5^\circ$, 2 $\theta_{\max} = 30^\circ$, 2 $\theta_{\text{step}} = 0.01^\circ$
R _{wp} , R _p , R _{exp} , S	0.0655, 0.0455, 0.0338, 1.937
No. of data peaks/parameters	356/45

General info

- Deadline for proposals every six months: March 15th and September 15th
- For more info visit our website:
 - www.elettra.eu/elettra-beamlines/mcx.html
- Contact us!
 - jasper.plaisier@elettra.eu
 - lara.gigli@elettra.eu
 - mattia.gaboardi@elettra.eu



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