BL13-XALOC, MX EXPERIMENTS AT ALBA: CURRENT STATUS AND ONGOING IMPROVEMENTS

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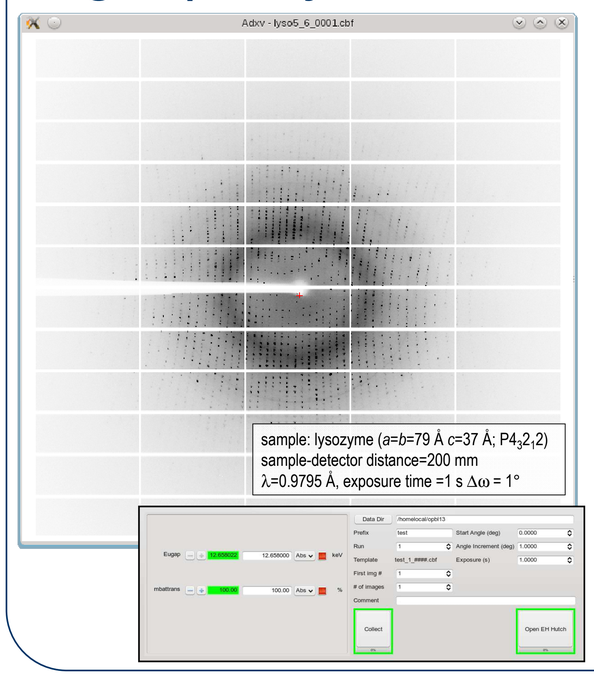
Scientific case

ALBA synchrotron is a third generation 3-GeV storage ring, feeding 7 beamlines in first phase, built near Barcelona and the Universitat Autònoma de Barcelona.

BL13-XALOC beamline is dedicated to Macromolecular Crystallography. It has been tested with different protein crystals provided from friendly users, allowing to perform successfully the more usual experiments (SAD/MAD), and more difficult ones as crystals with large units cells. XALOC is receiving users since July 2012.

High quality data

XALOC produces high quality data due to high beam stability and high quality instrumentation

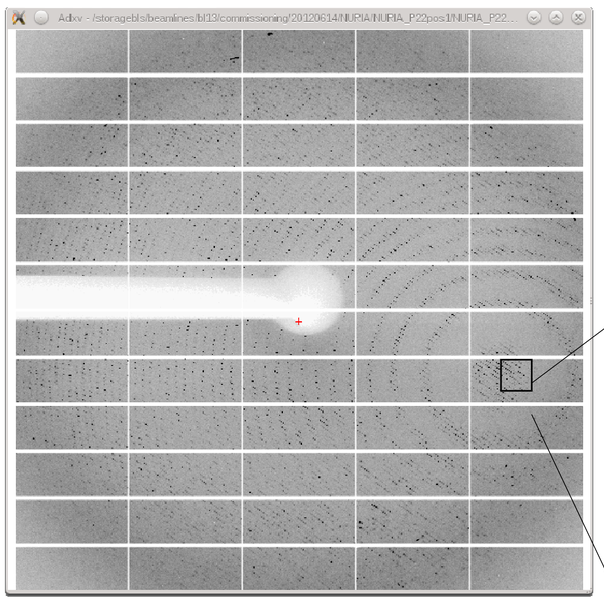


- First full dataset at XALOC 25/04/12.
- Test lysozyme crystal cryogenically cooled.
- Excellent overall statistics: **R_{sym} = 3.8 %.** (90˚ rotation).
- Also at the lowest resolution shell: **R_{sym}= 2 %.**
- Resolution 1.26 Å.
- Molecular replacement phase determination rendered exceptionally good ED maps.

RESOLUTION LIMIT	NUMBER OBSERVED	OF REFLECTIONS UNIQUE	POSSIBLE	COMPLETENESS OF DATA	R-FACTOR observed	R-FACTOR expected	COMPARED	I/SIGMA
3.76	7563	1351	1359	99.4%	2.0%	2.4%	7550	64.62
2.67	13848	2277	2282	99.8%	2.4%	2.5%	13841	61.47
2.18	18104	2888	2895	99.8%	3.2%	3.0%	18092	50.06
1.89	21215	3388	3390	99.9%	4.1%	3.9%	21202	37.67
1.69	24546	3795	3797	99.9%	6.8%	6.8%	24531	23.78
1.54	25959	4193	4193	100.0%	11.0%	11.2%	25949	15.11
1.43	27802	4511	4514	99.9%	18.3%	19.5%	27790	9.19
1.34	28455	4862	4864	100.0%	30.8%	34.2%	28442	5.23
1.26	28810	5124	5154	99.4%	45.2%	52.1%	28746	3.41
total	196302	32389	32448	99.8%	3.8%	4.0%	196143	22.77

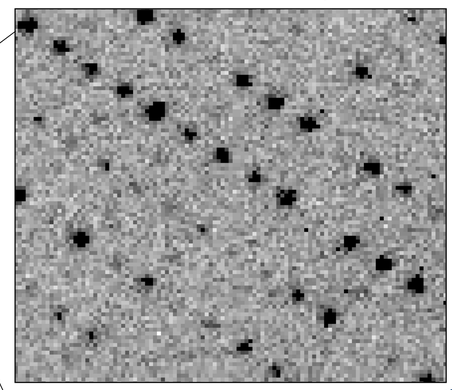
Large unit cell crystals

Low beam divergence and high monochromaticity



Crystal from Nuria Verdeguer (IBMB-Park Cientific de Barcelona)

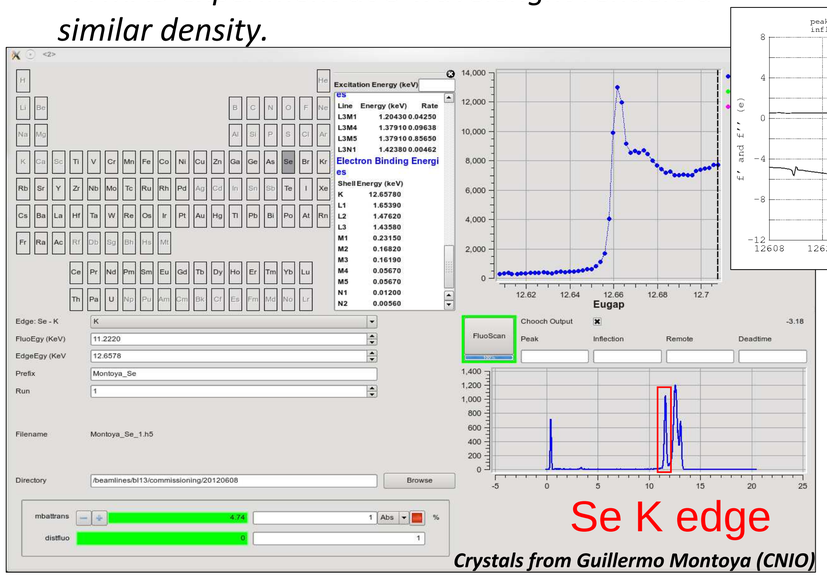
- **Human Rhinovirus 2**
- Monoclinic cell
- **a= 470 Å, b= 376 Å, c= 465 Å** α= 90˚, β= 99˚, γ= 90˚
- Diffraction to ~4 Å.
- Crystal-detector distance 750 cm (max. distance 1350 cm)



Se SAD/MAD

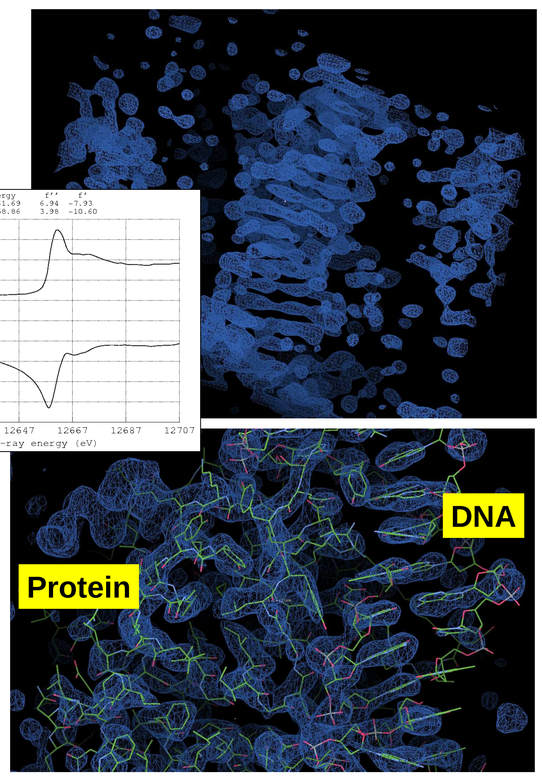
XALOC may solve structures by SAD/MAD due to full tunability

- *First ab initio solved structure by Se K-edge SAD*
- ***Protein-DNA complex (PDB 2VS8)***
- *Se-Met SAD 360˚, 2.4 Å resolution*
- *A MAD experiment at 3 wavelenght renders a similar density.*



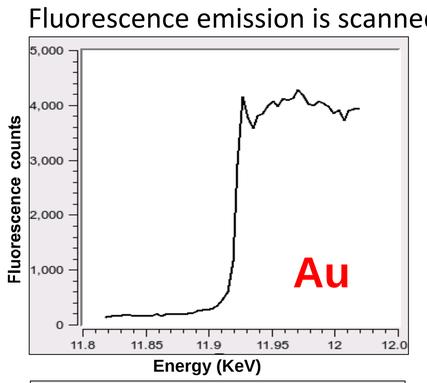
Se K edge

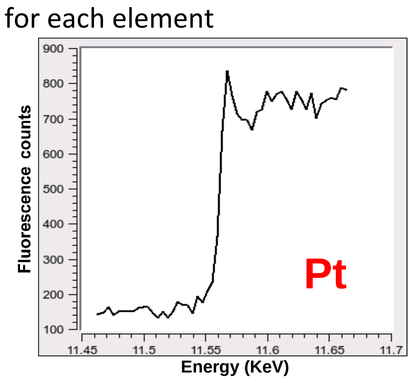
Crystals from Guillermo Montoya (CNIO)

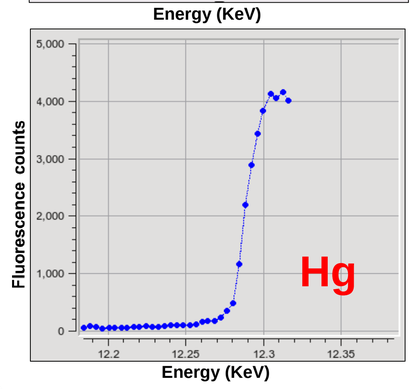


…and SAD/MAD with other heavy atoms

Fluorescence emission is scanned for each element

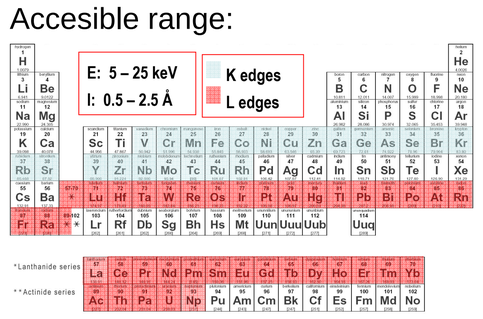






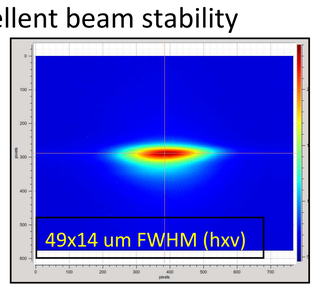
Crystals from David Reverter (IBB-UAB)

Accesible range:

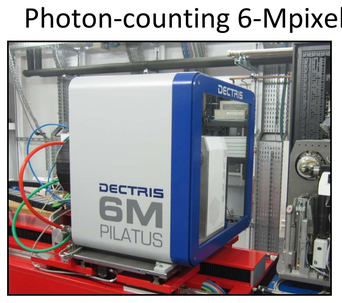


XALOC is ready for users, and improvements are ongoing

- XALOC opened to users on **July 18 2013**.
- Fully tunable beamline from 5 keV to 25 keV.
- Excellent beam stability

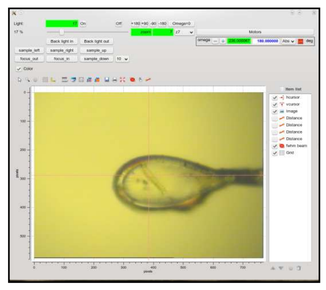


- High accuracy single axis diffractometer.
- Photon-counting 6-Mpixel detector.



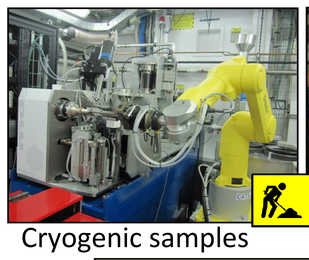
- **High dynamic range**
- **Low background noise**
- **Fast read-out**
- **Thin w-slicing**
- **Fast frame collection**

- Two operation modes: focused and unfocused/defocused



- **Small crystals: focused** mode (**~50×14 μm^2**) (h×v)
- **Larger crystals: unfocused mode (~300×300 μm^2)** (h×v)
- Mini-kappa goniometer head

- Automated mounting robot (CATS)



Cryogenic samples

Crystallization plates

- *Ongoing: EDNA completely integrated*
- *Ongoing: Collect queues*
- *Next: Integrated applications for Samples+Collect+…*
- *Long-term features: workflows + autoproc + …*

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