MXCuBE at LNLS / Sirius

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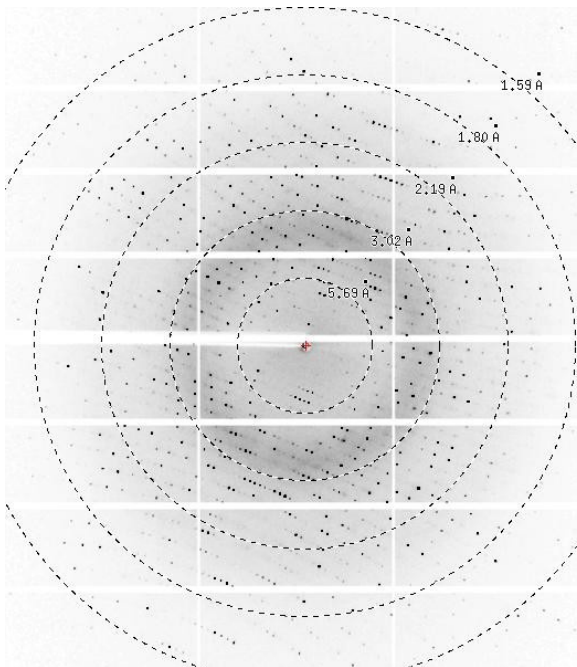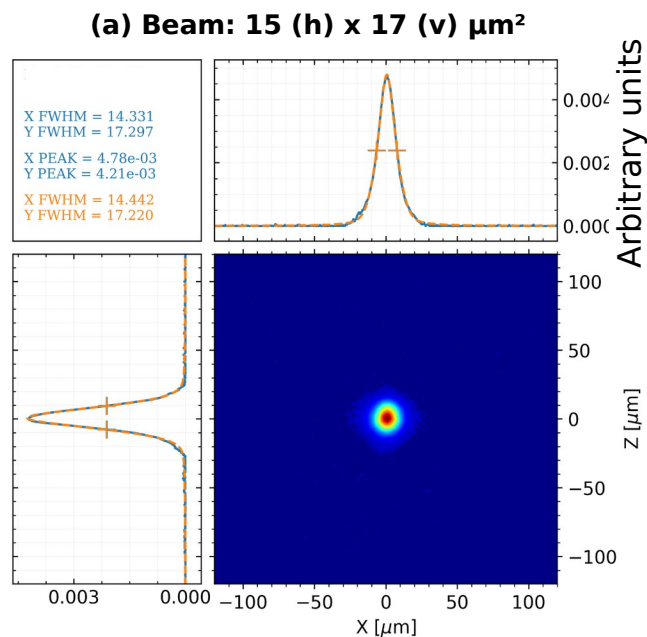
Virtual MXCuBE & ISPyB Meeting

17 - 18 November, 2020

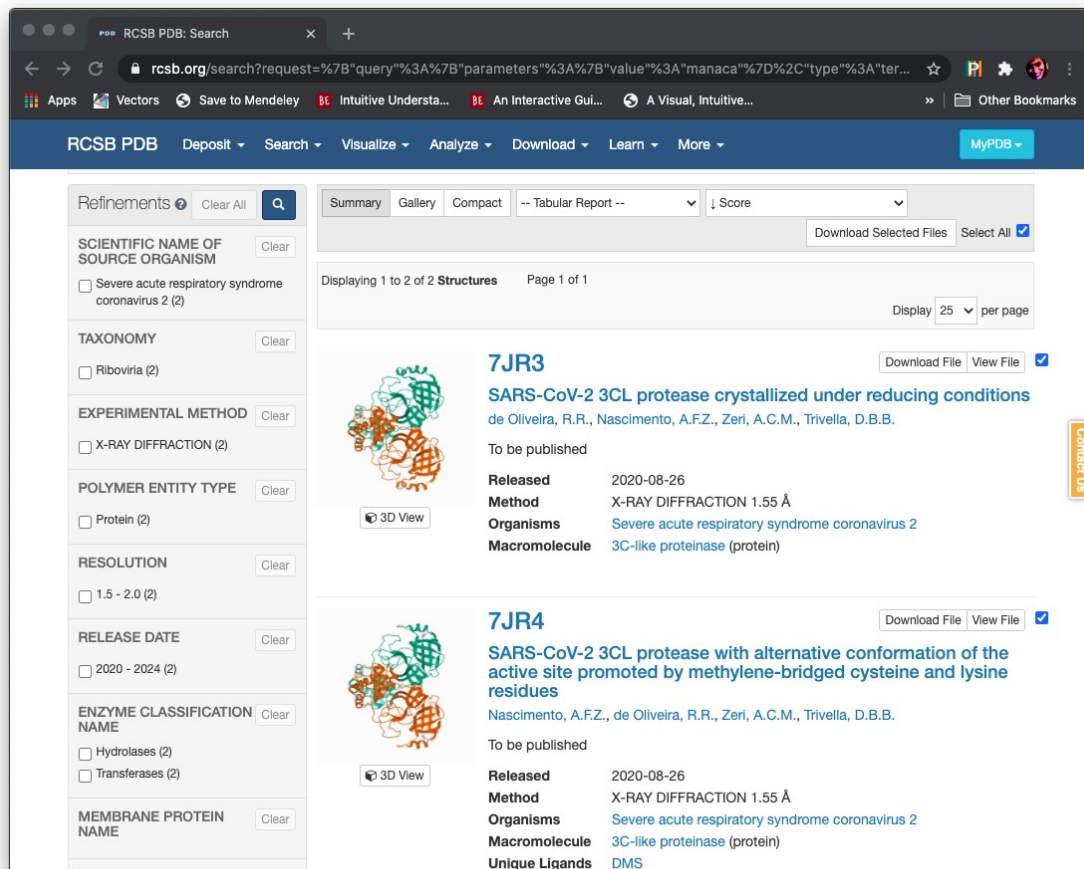# MANACÁ micro station - 1st data collection

- July:

(b) Protein diffraction

(a) Beam: 15 (h) x 17 (v) μm²

X FWHM = 14.331
Y FWHM = 17.297

X PEAK = 4.78e-03
Y PEAK = 4.21e-03

X FWHM = 14.442
Y FWHM = 17.220

*Beam size and protein diffraction at Manaca. (a) Despite undergoing commissioning, a beam size of 15 (h) x 17 (v) μm² was reached, very close to the **nominal size of 10 (h) x 7 (v) μm².** (b) Diffraction pattern from the first hen egg-white lysozyme crystal diffracted at MANACA, showing good data processing statistics (source: Andrey Nascimento, PhD, Manaca 2020).*

|	HEWL
Wavelength (Å)	1.36697
Ring current (mA)	14
Beam size (μm)	~100 x 90
Exposure time (s)	0.1
Transmission (frac.)	0.75
Oscillation/image (°)	0.1
Total oscillation (°)	360
Images	3600
Resolution range	35.29 - 1.48 (1.53 - 1.48)
Space group	P 4$_3$ 2$_1$ 2
Unit cell (Å, °) (a=b, c, α=β=γ=90°)	78.90 36.81
Total reflections	416141 (7202)
Unique reflections	19160 (1336)
Multiplicity	21.7 (5.4)
Completeness (%)	96.13 (68.51)
Mean I/sigma(I)	77.16 (24.07)
Wilson B-factor	10.70
R-meas	0.0378 (0.0495)
CC1/2	1 (0.997)

MANACÁ micro station - LNBio

- August:

  1st real-world samples measured at the beamline and deposited at the PDB.

- Even at low current, using circa 20 % transmission, fixed energy at 9keV, beam at 60 μm².

MANACÁ micro station - LNBr

Iodine SAD @ MANACA – SGM_086 hydrolase – Mario Murakami / LNBR

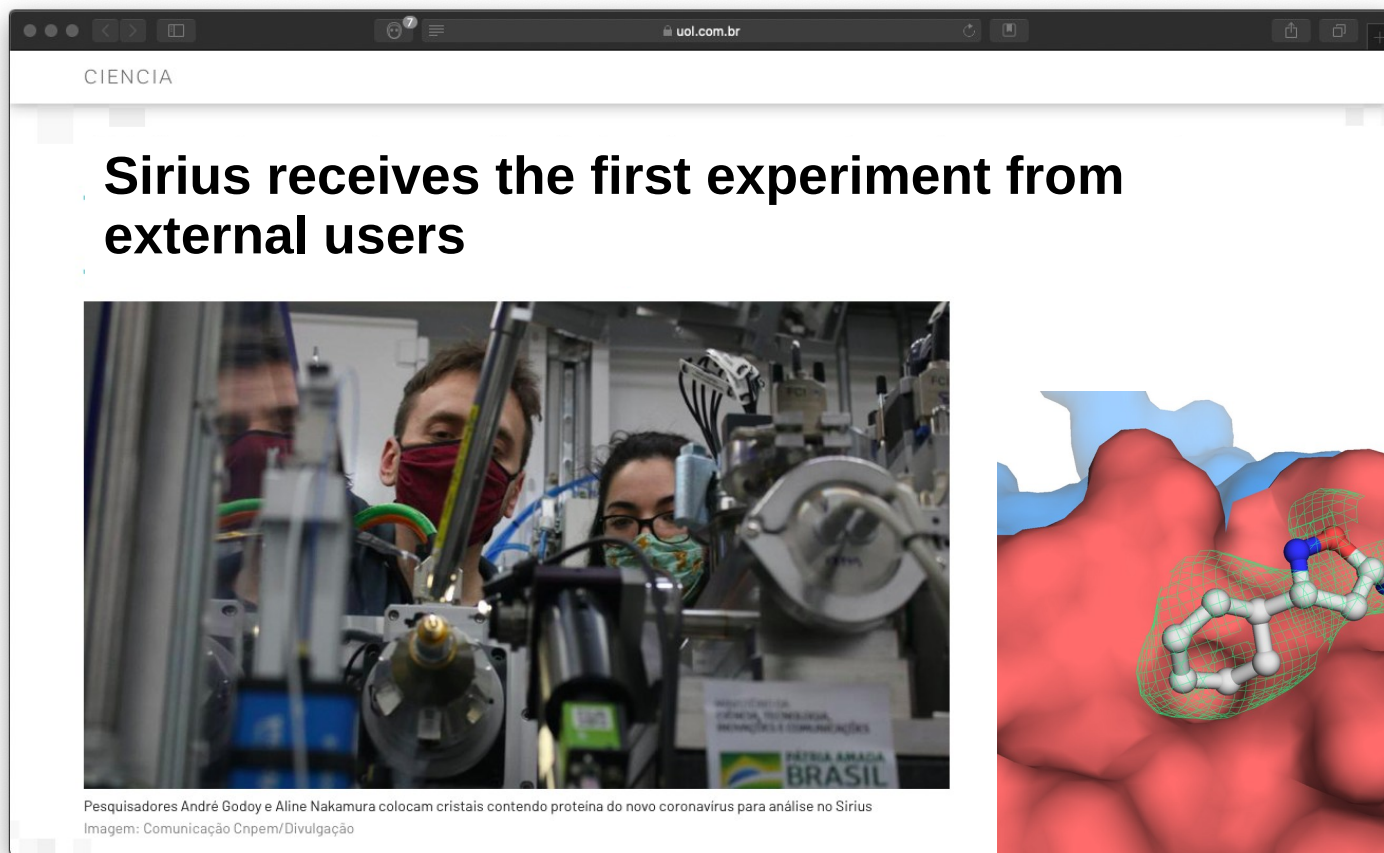Even using an energy very far from the iodine L-I edge was possible to solve the structure by SAD.

This indicates the data has no major error contribution from beamline instruments/setup (sample rotation, beam stability, energy, etc.), since it was possible to record the intensities with good enough precision to use the small anomalous differences to solve the structure.
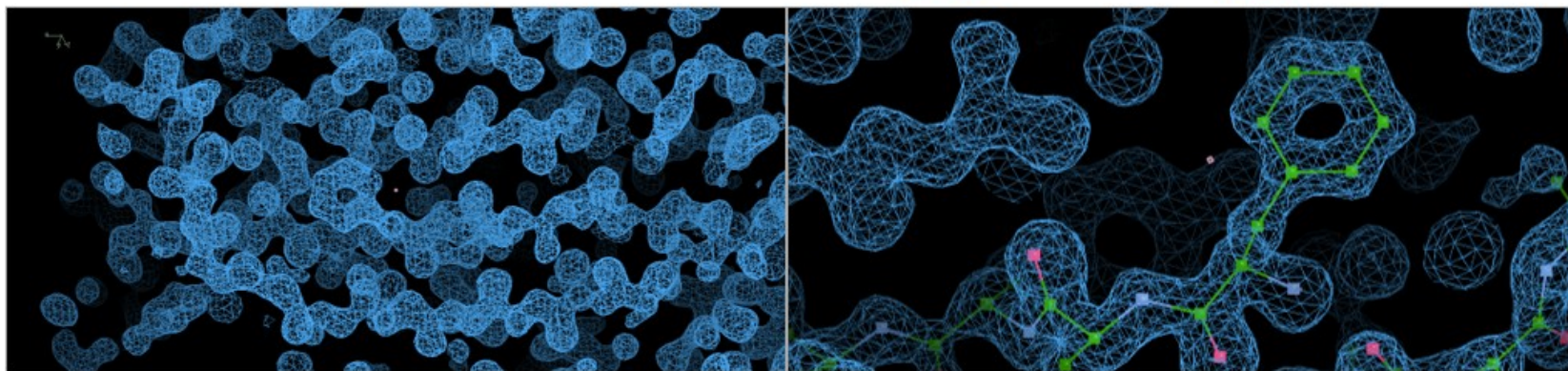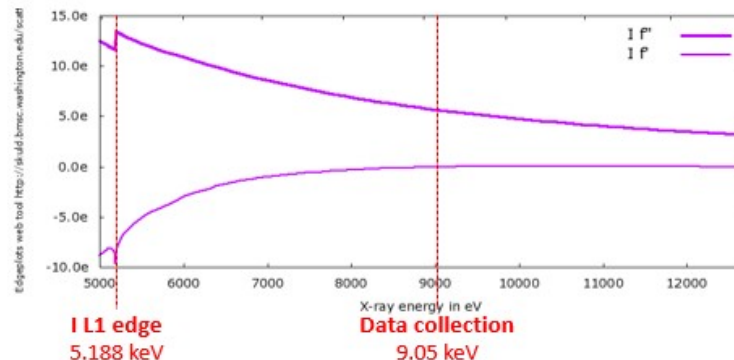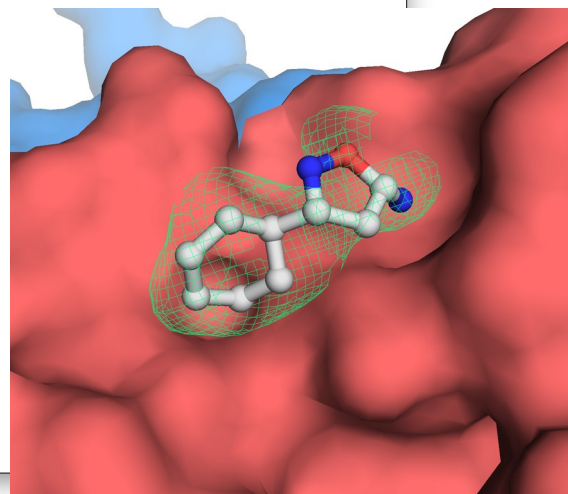

Electron density map obtained only from observed intensities and experimentally determined phases (I-SAD) (High resolution: 1.35 Å; F_o, 1.5 rmsd).

Source: Andrey Nascimento, PhD, and Evandro Araujo, PhD.

MANACÁ micro station - USP

Sirius receives the first experiment from external users

Pesquisadores André Godoy e Aline Nakamura colocam cristais contendo proteína do novo coronavírus para análise no Sirius
Imagem: Comunicação Cnpem/Divulgação

- September
- University of São Paulo (USP)
- SARS-CoV virus + ligands

Source: Andre Godoy, PhD.

# MANACÁ

	microMANACA	**nanoMANACA**
2020	Energy and position controls refinement MXCube3 - new features and support Data processing pipelines development	Research on sample delivery methods at XFELs and other SRS
2021	Automated sample delivery commissioning Remote access for data acquisition and treatment	Optical and Mechanical designs for sample table and jet injector M3 base design Hutch design
2022	Faster detector (Pi-Mega)	Liquid jet tests

CATERETÊ

- Long beamline for imaging and coherence experiments (CXDI, XPCS, TR-SAXS, USAXS)
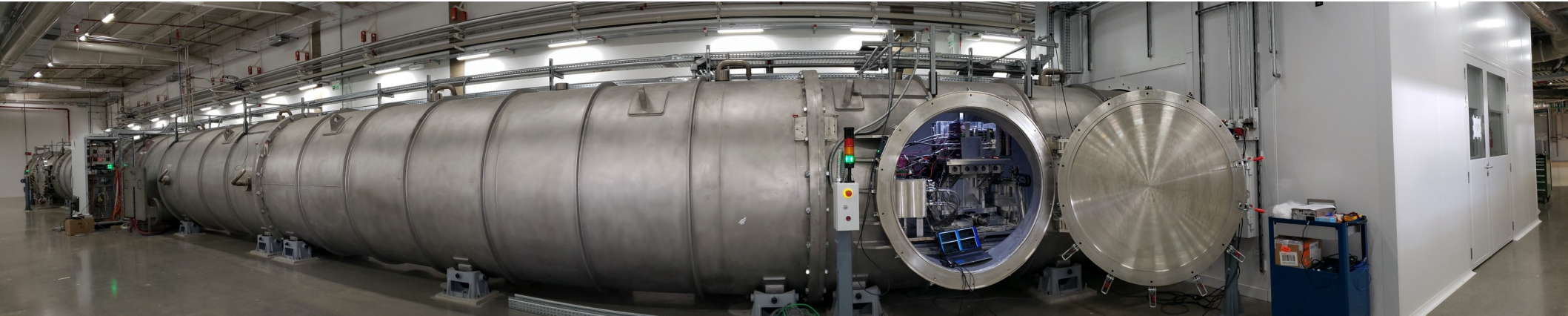
- July
    - **1st beam at sample,**

    92.5 (h) x 30 (v) µm²
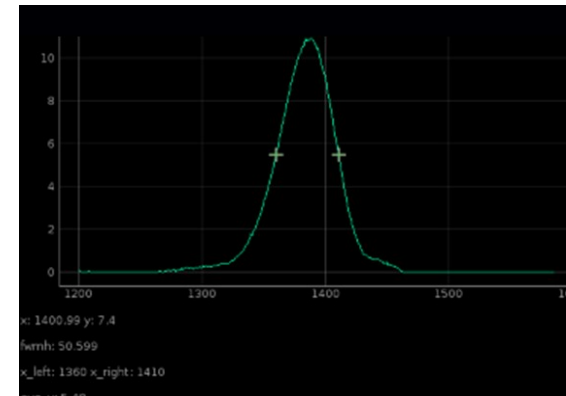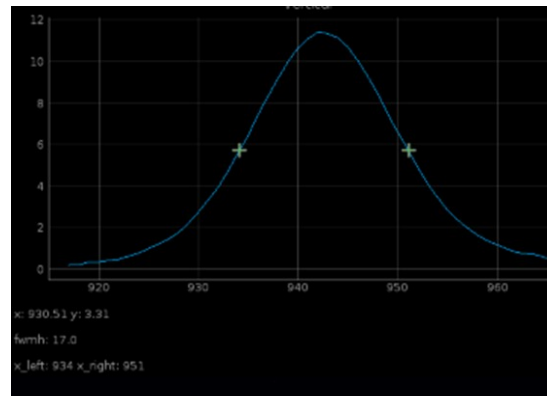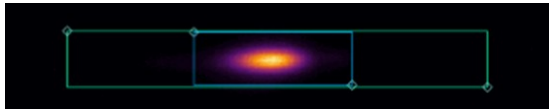
CATERETÊ

- September
 - **1st data collections with Pi-Mega detector**

- 2.4 megapixel x-ray detector module, based on 6 x HEXA sensors.
- Total of 36 Medipix3 chips
- Stack of HEXA modules in a stairs shape
- This assembly covers the wirebonding
- No detection gaps neither rows nor columns
- 85x85mm 100% active area
- In vacuum 10^{-3} mbar
- Simple exchange modules for maintenance
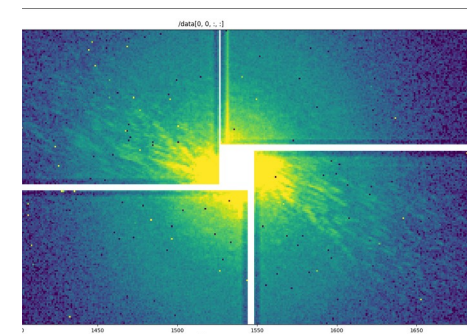- 2 kHz frame rate
- 12 and 24 bits
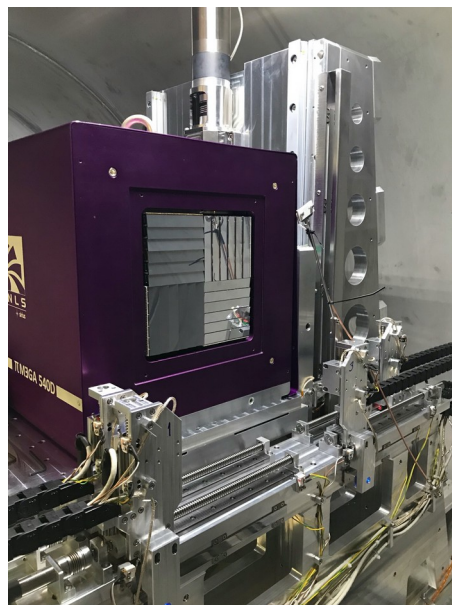
Detector from Pi-Mega Project at Cateretê (in-house development of LNLS Detectors Group).

$q_{min} \sim 2 \cdot 10^{-4} A^{-1}$
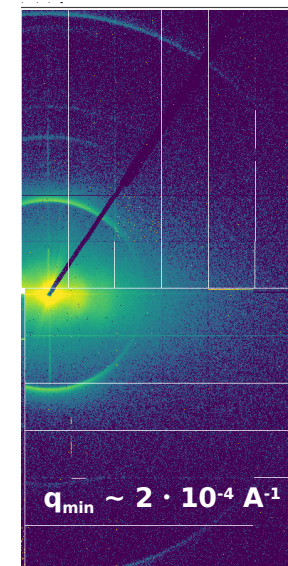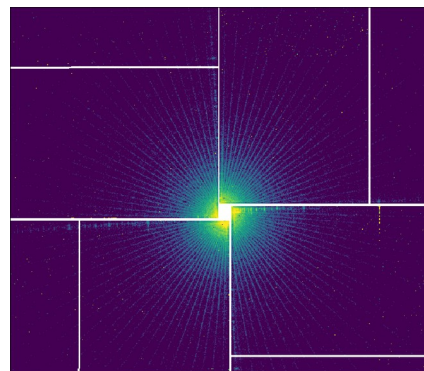
Single fiber of collagen, 67 nm d-spacing.
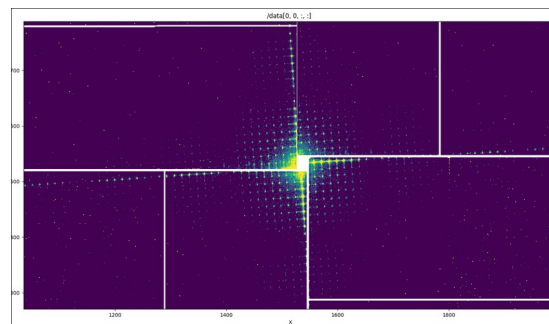
First images (Siemen Star).

Sugar cane.

CATERETÊ

- **In progress**

  - Geometric correction of Pi-Mega images

  - Focusing on SAXS, XPCS experiments (beginning CDI in parallel)

MXCuBE 3

- Done

  - Code camp (MachInfo class PR finished, merged)

  - Classes:

    - New: LNLSBeam, LNLSAperture, LNLSSlits

    - New: LNLSDetDistMotor, LNLSEnergy, LNLSTransmission

    - LNLSDiffractometer: methods and XML for zoom level calibration

    - LNLSPilatusDet: CBF header setting

MXCuBE 3

- **In progress:**

  - User authentication + Proposal details

  - Review of specific code (Next: PR)

  - Back to CATERETÊ configuration (centring routines)
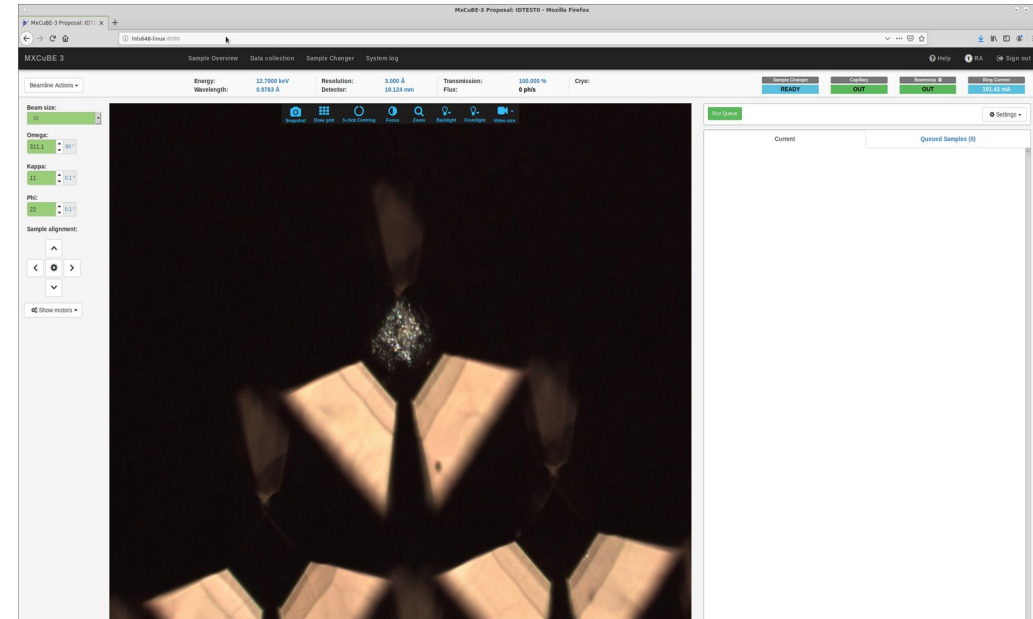
MXCuBE 3 at CATERETÊ beamline

Thank you!

Questions? :)