

# MXCuBE at the Brazilian Synchrotron Light Laboratory – LNLS/Sirius Status Report

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Computing Platforms (COMP)

MXCuBE Meeting – MAX IV, 29 May 2024

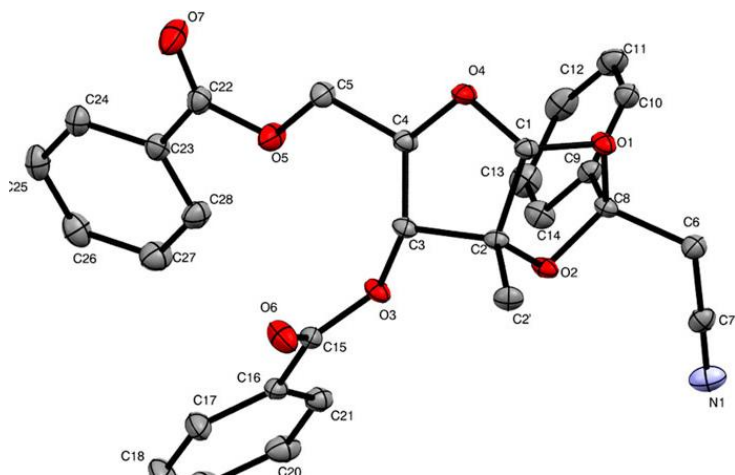


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# MXCuBE at Manacá beamline

- Chemical Crystallography
  - Small Molecules



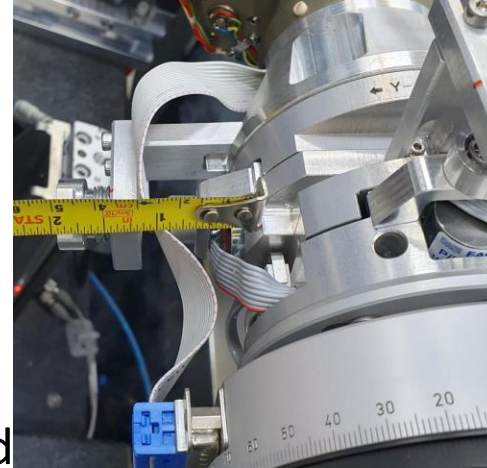
First structure of a small molecule solved at MANACÁ beamline (Naciuk et al., Front. Chem. 11, 2023).



Small molecule data collection by advanced users. After an one-week intensive work several high-quality data sets were collected, confirming the potential of MANACÁ beamline for Chemical crystallography Community. From left to right: Prof. Javier Ellena (USP, São Carlos), Prof. Leopoldo Suescun (Udelar, Montevideo), Dr. Andrey Nascimento (MANACÁ, LNLs), Prof. Alejandro Ayala (UFC, Fortaleza) and Prof. Florencia Di Salvo (UBA, Buenos Aires).

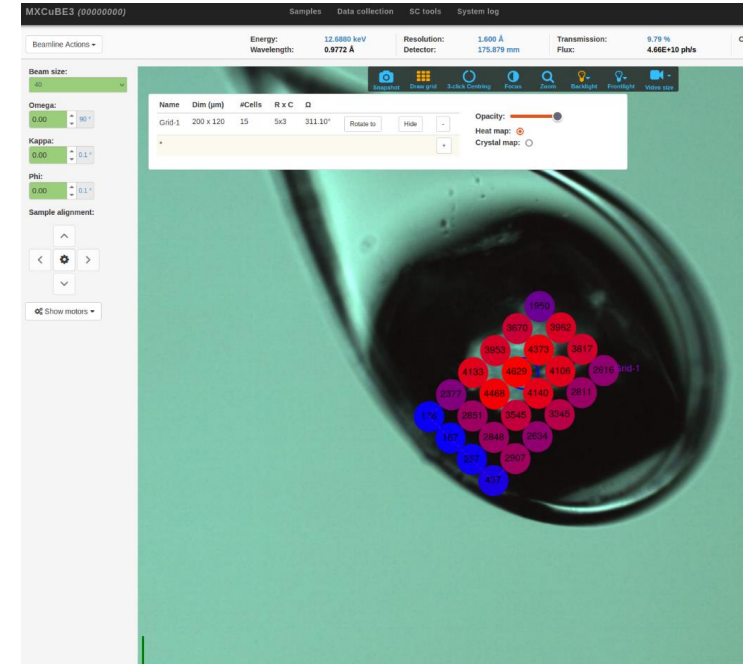
# MXCuBE at Manacá beamline - Improvements

- Reduction of sample-detector distance (112 mm).
  - A part of goniometer (spring load) was refurbished to allow shorter distances.
- Real-time photon flux monitoring on MXCuBE.
  - The flux used on data collection can be checked on MXCuBE for all energies and transmissions.
- Multi-axis goniometry available (mini-kappa).
  - The mini-kappa (from MX2) was repaired and now are available for all users.



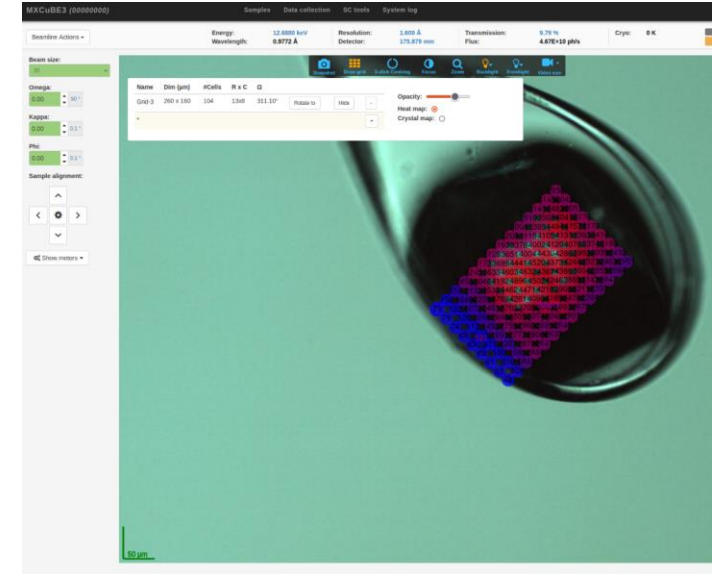
# MXCuBE status

- Version MXCube 3, updating to mxcube core and version 4
- In house scripts to:
  - Auto Align (3 click center).
  - Auto processing heat map grid scan.



# Developments since last meeting

- Fix bug grid Scan (fast shutter).
- Heat map, intensity GridScan.
- Align beam to best intensity, found in heat map.
- Fix EPICS.py (timeout(0.01) to timeout(0.1))
- New class to safety shutter and fast shutter.
- Add new motors (Kinematics) samp-z and samp-y
- Script auto align sample (Auto 3 click centering).



# Plans for the next six months

- Updates GridScan
- Tests first version Energy Scan
- Updates LNLSEpics Class.
- Update transmission
  - Now set and get by script, transform into ALU epics IOC, and integrate to MXCuBE
- Change Energy by MXCuBE.
  - Change Energy and Phase, using script.

# Thank you all!

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