

ID30B at the ESRF

Andrew McCarthy (EMBL) and Christoph Mueller-Dieckmann (ESRF)

05/02/2021



ID30B – A versatile MX beamline (re-opened August 2020)

Characteristics


- Tunable (6-20 keV) ⚠
- Beamsize: $\sim 30 \mu\text{m}^2$
- Flux: $\sim 3 \times 10^{13}$ ph/sec (~ 15 MGy/s)
 - $20 \mu\text{m}^2 \sim 1 \times 10^{13}$ ph/sec (~ 11 MGy/s)
 - $10 \mu\text{m}^2 \sim 7 \times 10^{12}$ ph/sec (~ 8 MGy/s)
- Recommend EDNA characterisation but if you must:
 - 0.1° oscillation; 20 ms exposure; 1-10% transmission

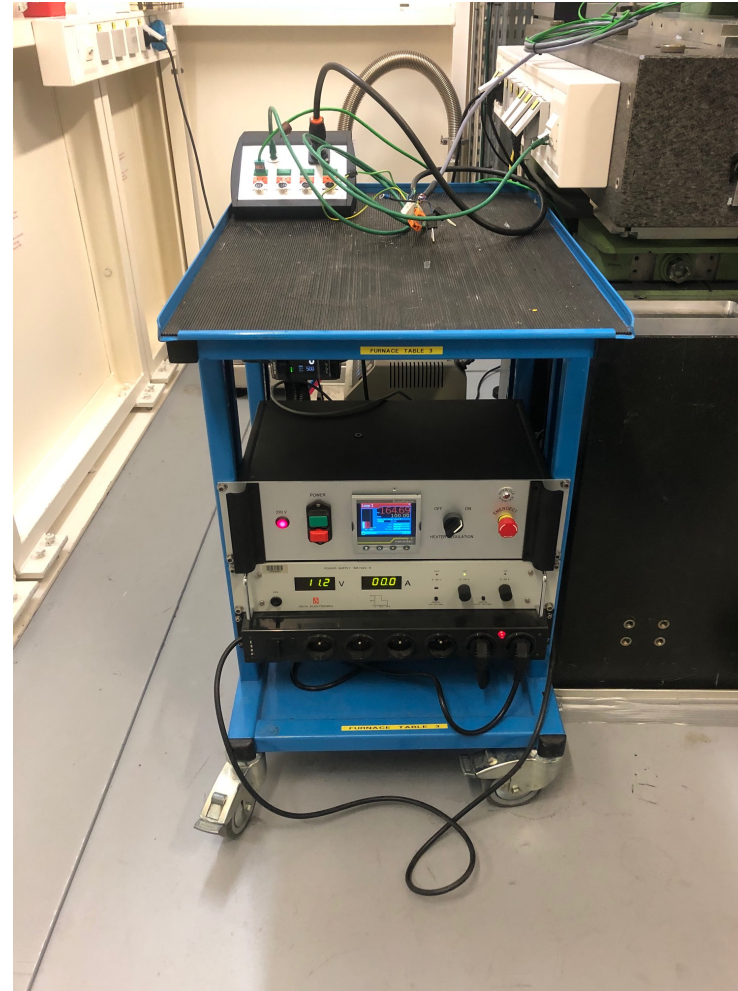
Experimental setup

- MD2-S (MK3 and Plate manipulator heads)
 - New electronics (Power PMAC)
 - New B-ZOOM installed
- FlexHCD sample changer (SPINE and Unipuck)
 - RFID puck detection
- PILATUS3 6M (1000 μm Si sensor)
- Software
 - BLISS (beamline control)
 - MxCuBE³
 - Beamline Expert System (inhouse automation WFs)
 - Extended ISPyB (Exi)



ID30B – Monochromator interventions (Oct 2020 – Jan 2021)

Tunable (6-20 keV)  - 30-50 μm drift over 20-30 mins
- Patience + Centre beam



ID30B – Coming soon

Beam characteristics

- Further stabilise the monochromator.
- Variable focused beamsize:
 - Explore the possibility of using 2D lenses (H x V)

Experimental setup

- Further stabilise software
- Finalise plate manipulator setup
- Facilitate dehydration/RT experiments
- *Implement Global Phasing Crystal re-alignment in MxCuBE³*
- *Implement Raman spectroscopy (icOS)*



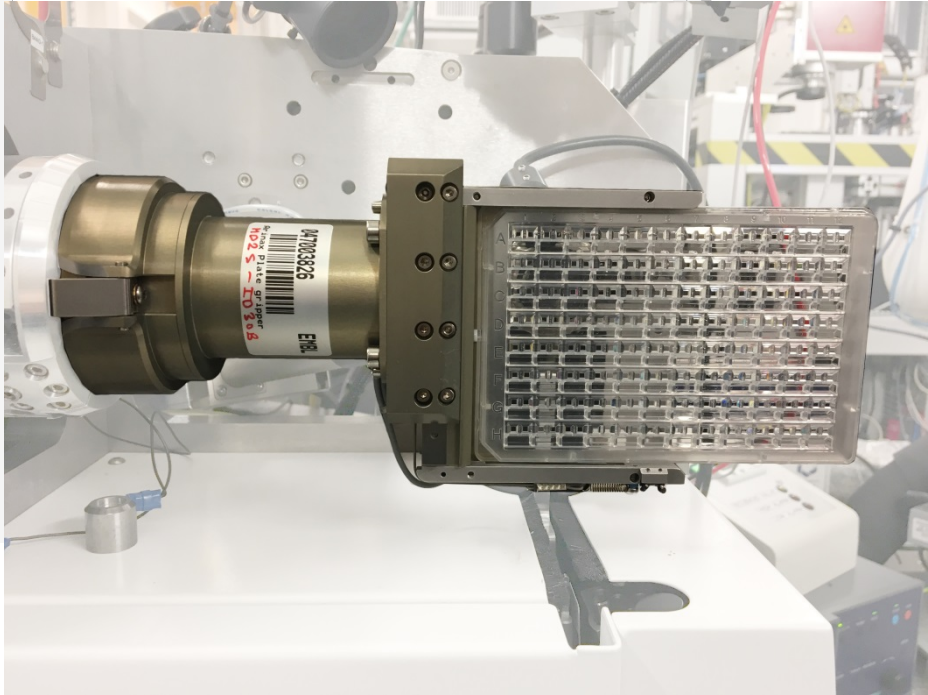
ID30B – Plate manipulator integration into MxCuBE³

The screenshot shows the MxCuBE3 web interface. At the top, there are browser tabs and a URL bar. Below that, a navigation bar includes 'MXCuBE3 (opid30b collecting)', 'Samples', 'Data collection', 'SC tools', and 'System log'. A status bar displays experimental parameters: Energy: 11.5600 keV, Wavelength: 1.0725 Å, Resolution: 3.674 Å, Detector: 700.050 mm, Transmission: -%, Flux: 0 ph/s, and Cryo: 0 K. On the right, there are status indicators for Detector (READY), Sample Changer (READY), Fast Shutter (CLOSED), Capillary (UNKNOWN), Beamstop (UNKNOWN), and Ring Current (-0.1 mA).

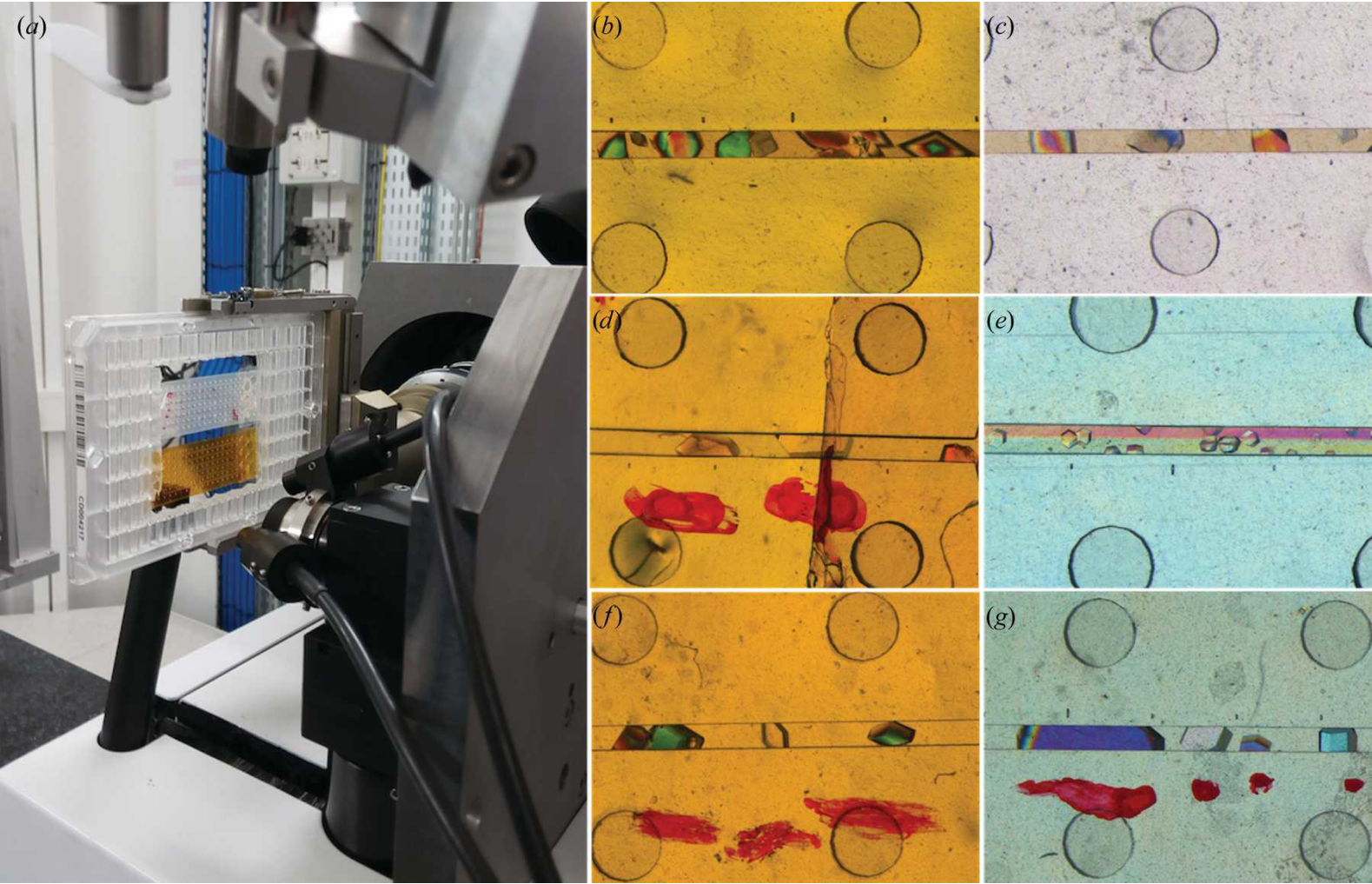
The main area features a 2D diffraction pattern. A '2D-Point-1' label is visible. A 'Plate Navigation' window is overlaid, showing a grid of 12 columns and 8 rows (A-H). The grid contains colored squares indicating the status of each well. A 'Currently loaded: E7:1-0' window shows a list of wells: 3 (grey), 2 (grey), and 1 (red). The 'Plate Navigation' window also includes buttons for 'Cristal Direct', 'Refresh', 'CRYMS', and 'Scan all containers'.

On the right side, there is a 'Run Queue' section with a 'Next Sample (Sample:E7:1-0)' button and a 'Settings' dropdown. Below it, a 'Sample: Sample:E7:1-0' section shows 'Queued Samples (1)' and a 'Mesh Scan' section. A table below the 'Mesh Scan' section displays data collection parameters:

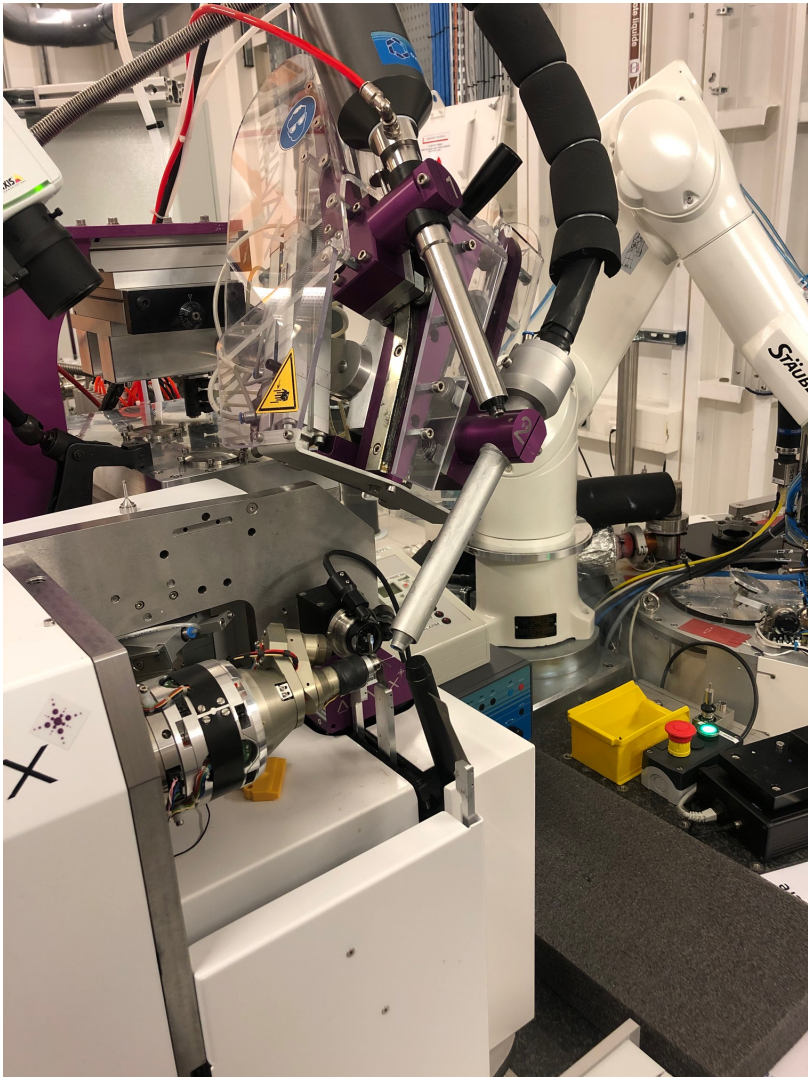
Start *	Osc. *	t (s)	# Img	T (%)	Res. (Å)	E (KeV)	ϕ *	κ *
311.45	0.02	0.031	234	97.40	3.674	11.5600	0.00	0.00



ID30B – Plate manipulator facilitates microfluidic chip data collection



ID30B – Dehydration device available



ID30B – Incorporate Global phasing MK3 routines in MxCuBE³

mxcube (opid-30b) Expert mode

Machine current: 39.3 mA, 4 bunch, 00:15

Flux: 9.05e+10 ph/s

Current: 12.7000 keV, 0.976 Å

Resolution: 1.994 Å, 392.35 mm

Transmission: 9.83%

Cryo: 100.00 K

Beamstop distance: 38.0

Safety shutter: opened

Fast shutter: closed

Beamstop: in

Capillary: in

Current users: [empty]

Selecting gives control, Allow timeout control, Take control

My name: bacon

Sample centring: Omega: 308.80, Kappa: 17.92, Phi: 273.25

Holder length: 22.803, samp: 0.14, samp: 0.33

Back Light: 0.50, Focus: -0.21, Front Light: 2.0, Zoom: 5

Collection method: Standard Collection, Characterisation, Helical Collection, Energy Scan, XRF Spectrum

Workflows: SingleWavelengthAcquisition

Data location: Folder: /data/id30b/inhouse/opid30b/20180501/RAW_DATA, Prefix: opid30b

Crystal data: Space group: P41212, Unit cell: a: 0, b: 0, c: 0, alpha: 0, beta: 0, gamma: 0

Acquisition: Expected resolution (Å): 2.1, Beam energies (keV): Acquisition energy: 12.7

Sample is centred! Aperture diameter: 50

100 µm, 100 µm

Collect Queue, Pause

[2018-05-01 11:34:56] OPID workflow completed.
[2018-05-01 11:34:56] Finishing workflow SingleWavelengthAcquisition
[2018-05-01 11:40:02] May 1 11:40 Refilling
[2018-05-01 11:40:22] May 1 11:40 Delivery:Next Refill at 12:00;

Adxv Co

File Edit View Terminal Go Help

```
bacon:~/Desktop % Hi, Global phasing remote t
```

11:44

Acknowledgements

EMBL Grenoble

Stephen Cusack

Matthew Bowler

Shibom Basu

Jean Baptiste Florial

Gergely Papp

Franck Felisaz

Robert Janocha

Marcos Lopez-Marrero

Christopher Rossi

Jeremy Sinoir

Victor Manuel Armijo Gomez

Raphael Cohen-Aberdam

Florent Cipriani

ESRF

Jean Susini

Harald Reichert

Gordon Leonard

Christoph Müller-Dieckmann

Daniele de Sanctis

David Flot

Max Nanao

Didier Nurizzo

Sasha Popov

Gianluca Santoni

Igor Melnikov

Romain Talon

Pascal Theveneau

Hugo Caserotto

Fabien Dobias

Thierry Giraud

John Surr

Antonia Beteva

Marcus Oscarsson

Olof Svensson

Alejandro de Maria

Solange Delageniere

Carole Clavel

UVHCI/IBS

Eva Pebay-Peyroula

Winfried Weissenhorn

Sandrine Vignon

Sylvie Costa

Corinne Iodice

