Recent progress of robot based systems for crystallography on synchrotron beamlines and in the laboratories

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IBS/Synchrotron Group (Grenoble, France)

UT Southwest, October 2013

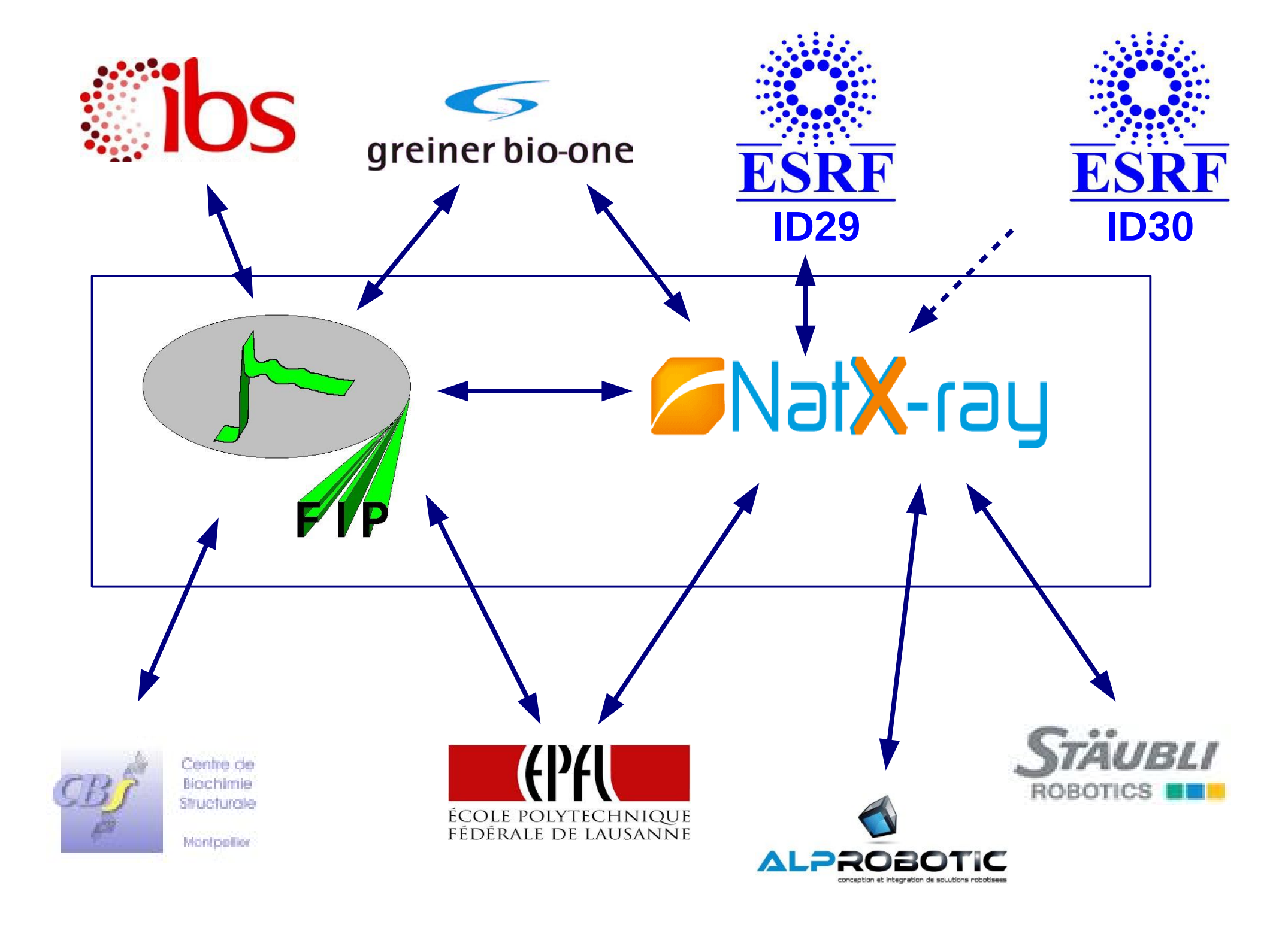
1 – Generalities about G-Rob

2 – G-Rob functionalities

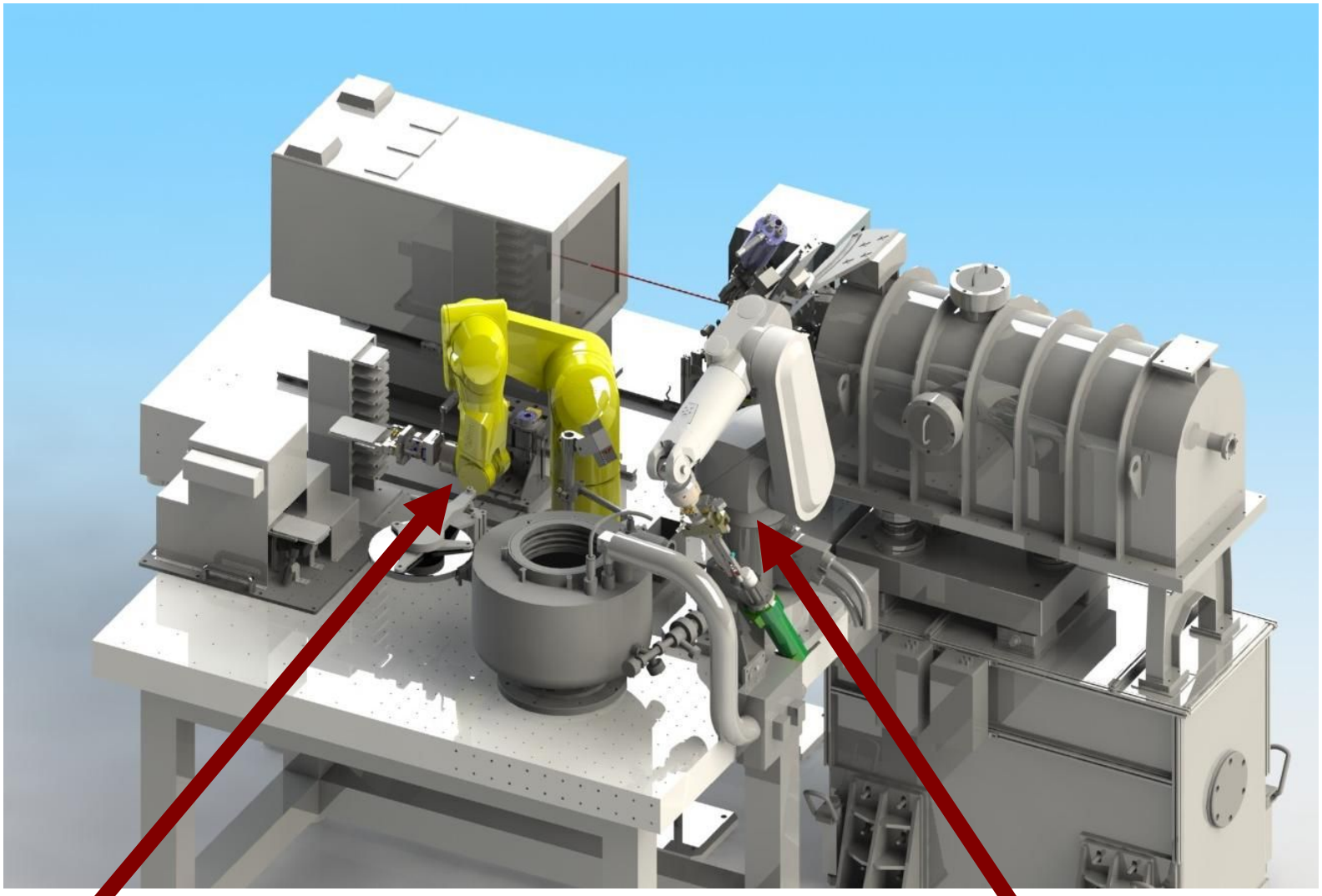
3 – Peripheral equipments

4 – Consumables for PX

1 – Generalities about G-Rob


ibs
greiner bio-one
ESRF
ID29
ESRF
ID30
FIP
NatX-ray
Centre de Biochimie Structurale
Montpellier
ÉCOLE POLYTECHNIQUE FÉDÉRALE DE LAUSANNE
ALPROBOTIC
conception et integration de solutions robotisees
STÄUBLI
ROBOTICS

G-Rob: a robot with goniometer capability



G-Rob (sample changer +goniometer) **CATS** (sample changer)

Robot with goniometer capability

Our problem:

Flexibility → complexity → automation made difficult
(reliability and communication issues, steric constrains)

The solution:

A **fully robotized system** for crystallography

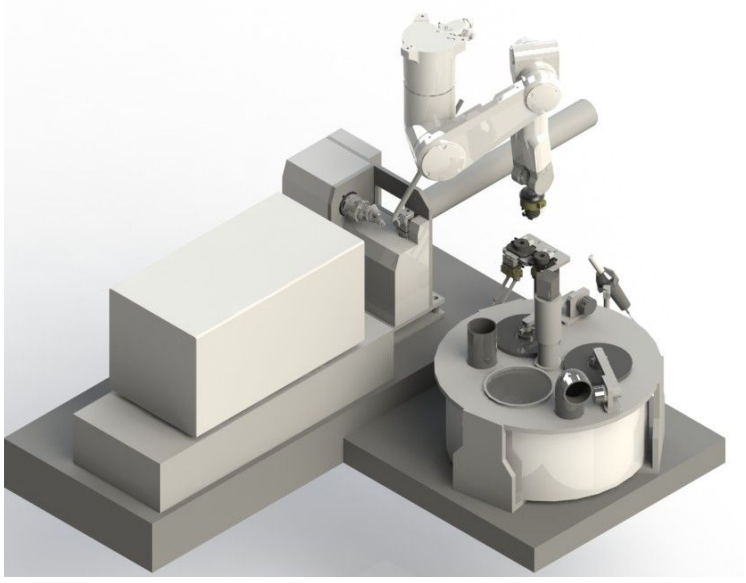
→ **automation**: setup reconfiguration, remote control
→ **flexibility**: multi-task, evolution, upgrading
→ **reliability**: simple, compact, industrial standard
→ **new possibilities**: phi data collection, *in situ*, HP...
→ **open architecture** (published mechanical interface)

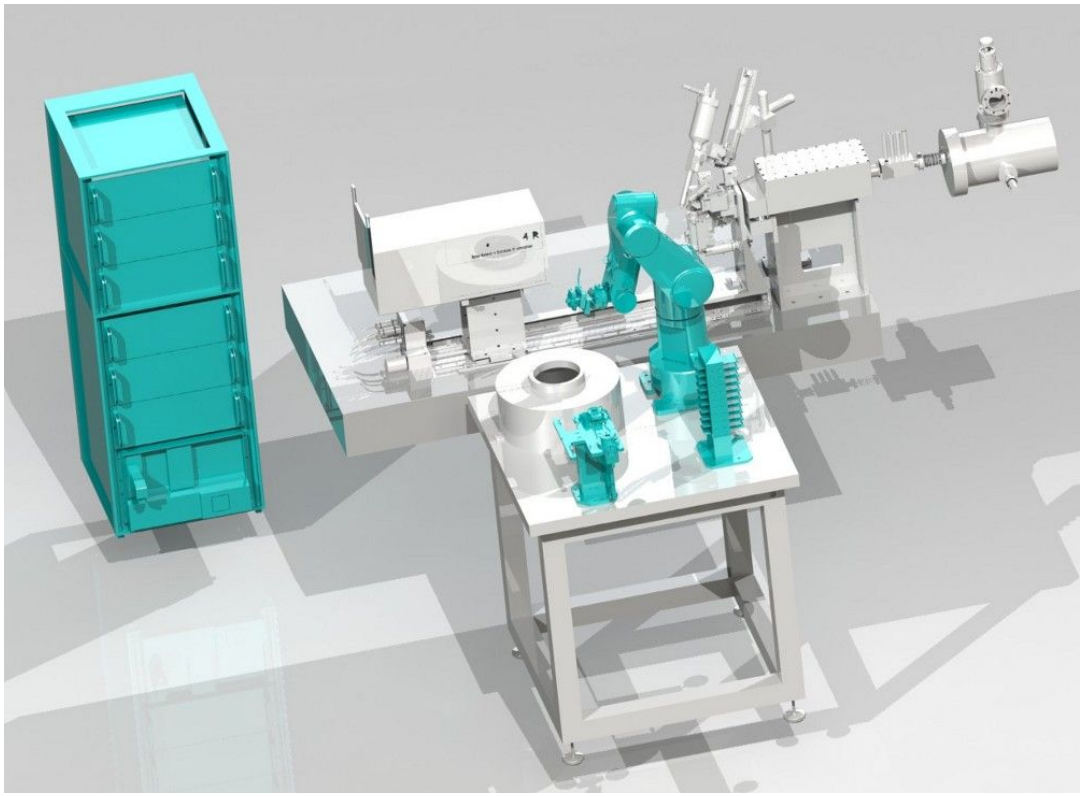
Main limitation: mechanical accuracy

G-Rob for beamlines

Usually including

- G-Rob functionalities
- (Sample environment)
- Supporting frame





G-Rob for beamlines

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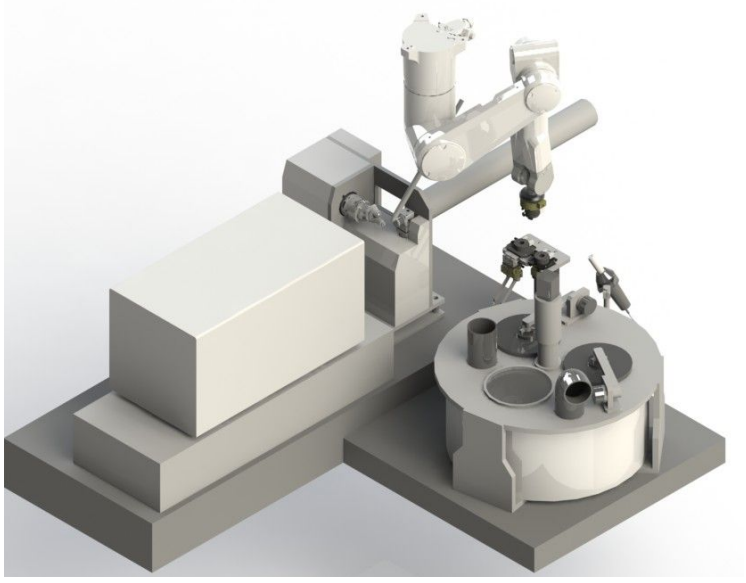
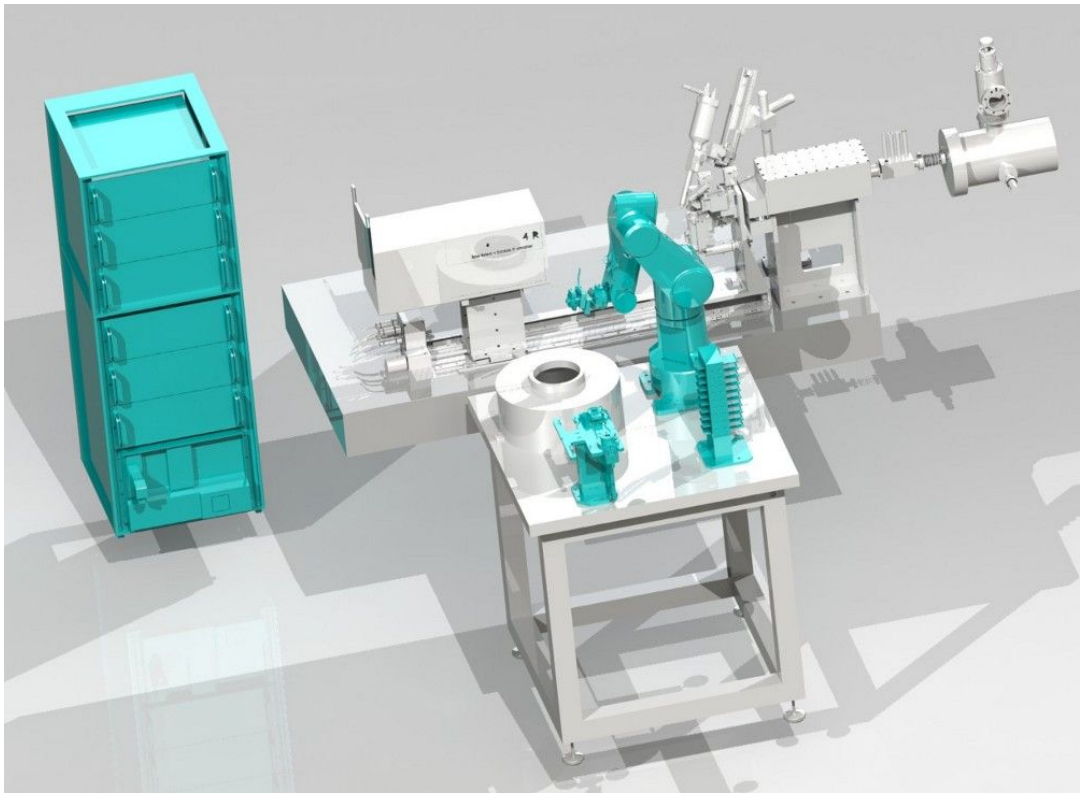
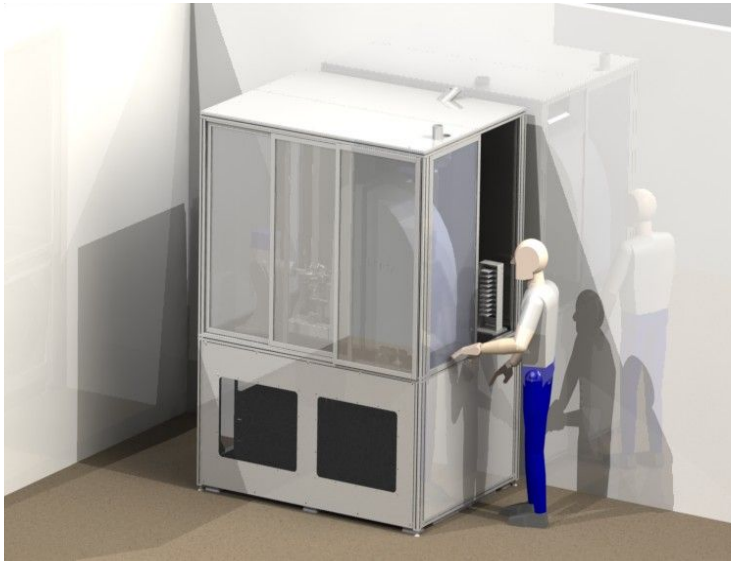


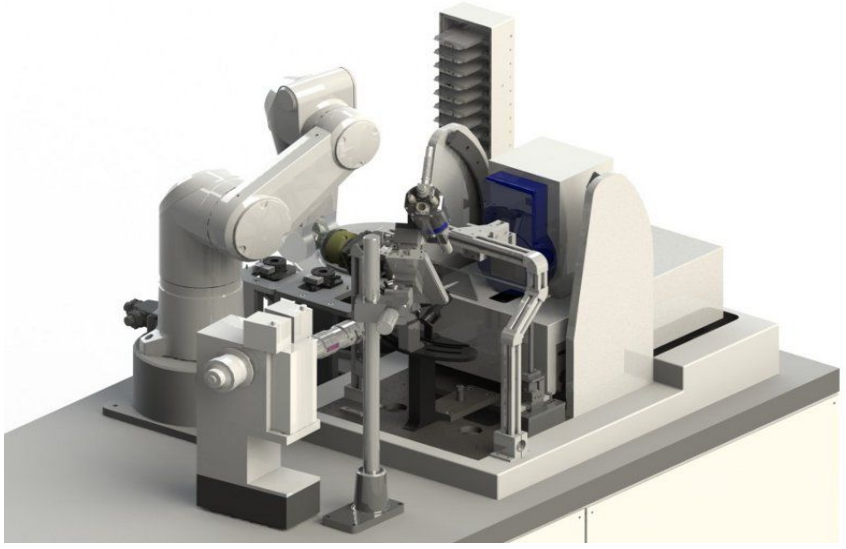


G-Rob lab systems

All-in-One laboratory solution, with

- G-Rob functionalities
- X-ray source
- Detector
- Sample environment
- Table and X-ray shielding





Available as

- A complete system
- An upgrade for existing lab diffraction systems

G-Rob configurations

A large variety of X-ray sources

Sealed tube, rotating anode

A large variety of detectors

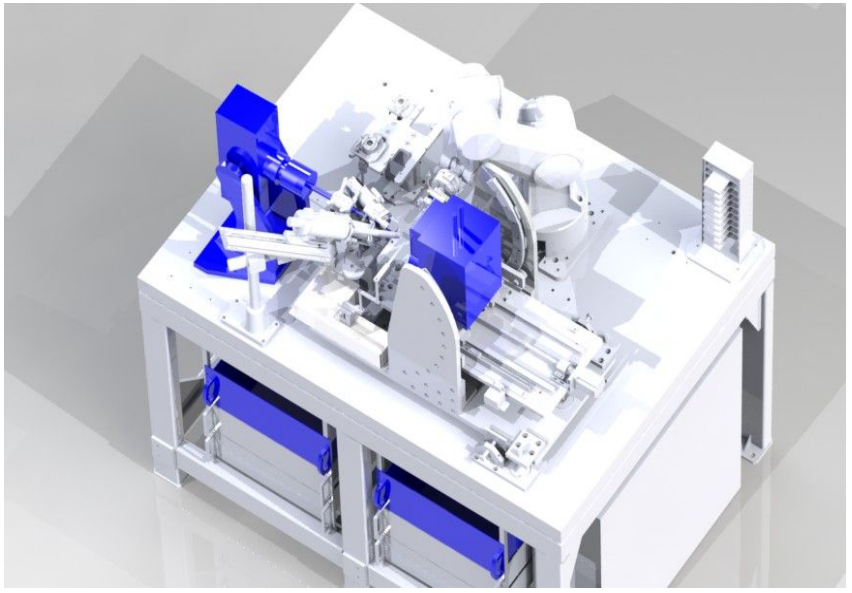
IP, CCD, Solid-State detectors

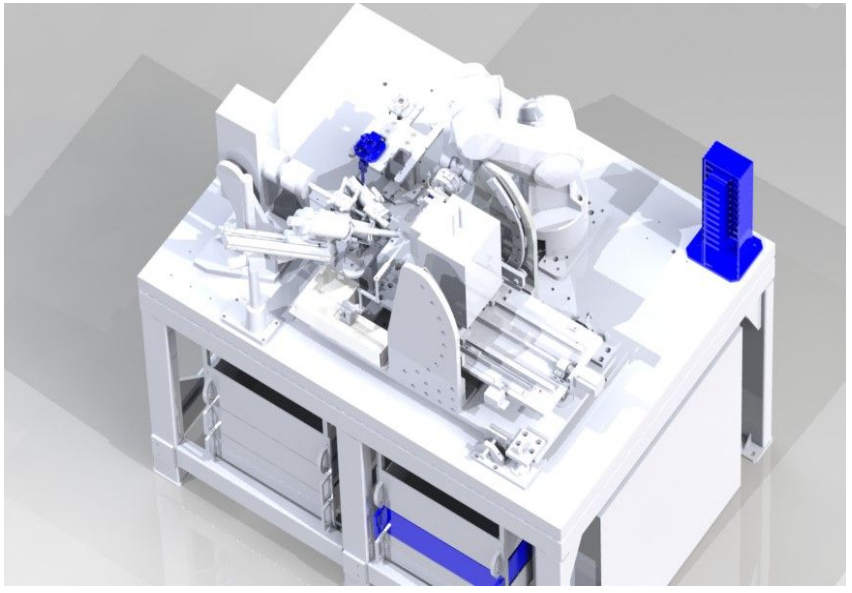
A large choice of options

- cryo-cane
- Etc.

A choice of G-Rob functionalities

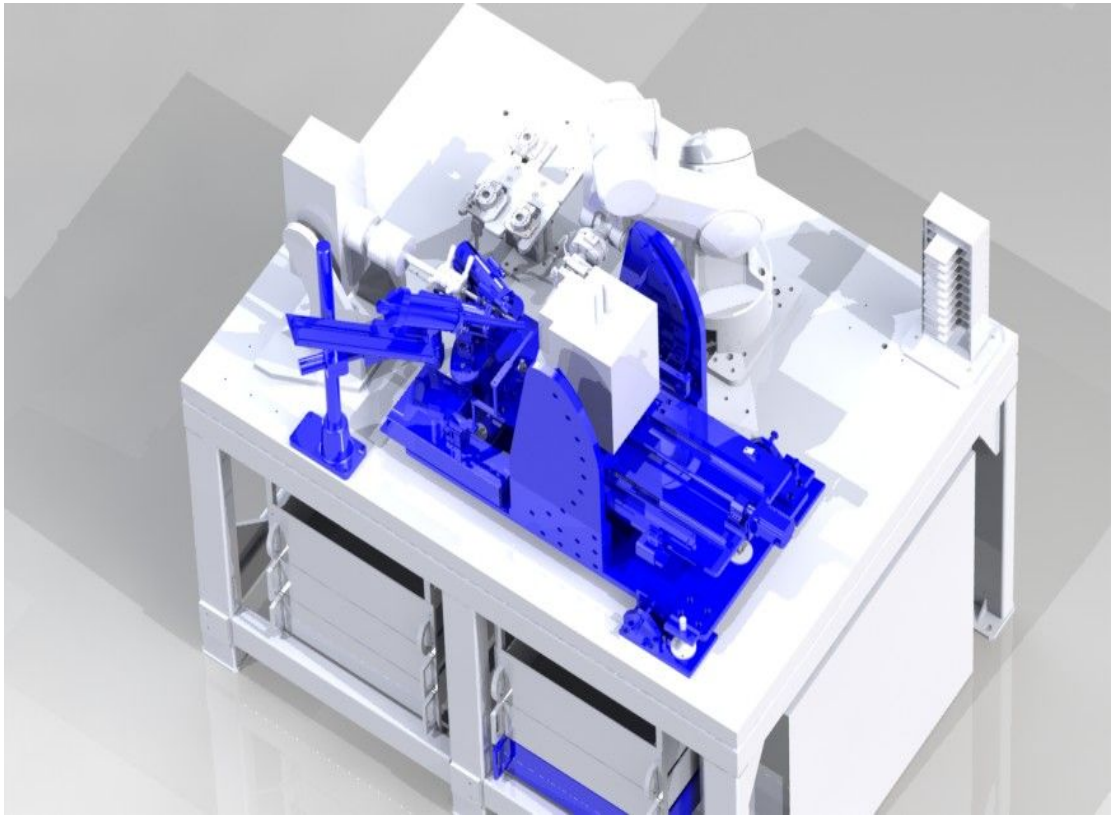
- G-Rob 1D/1D+ (single samples)
- G-Rob 2D (*in situ*)
- G-Rob 1DT (sample transfer)
- G-Rob Monitoring (beam monitoring)



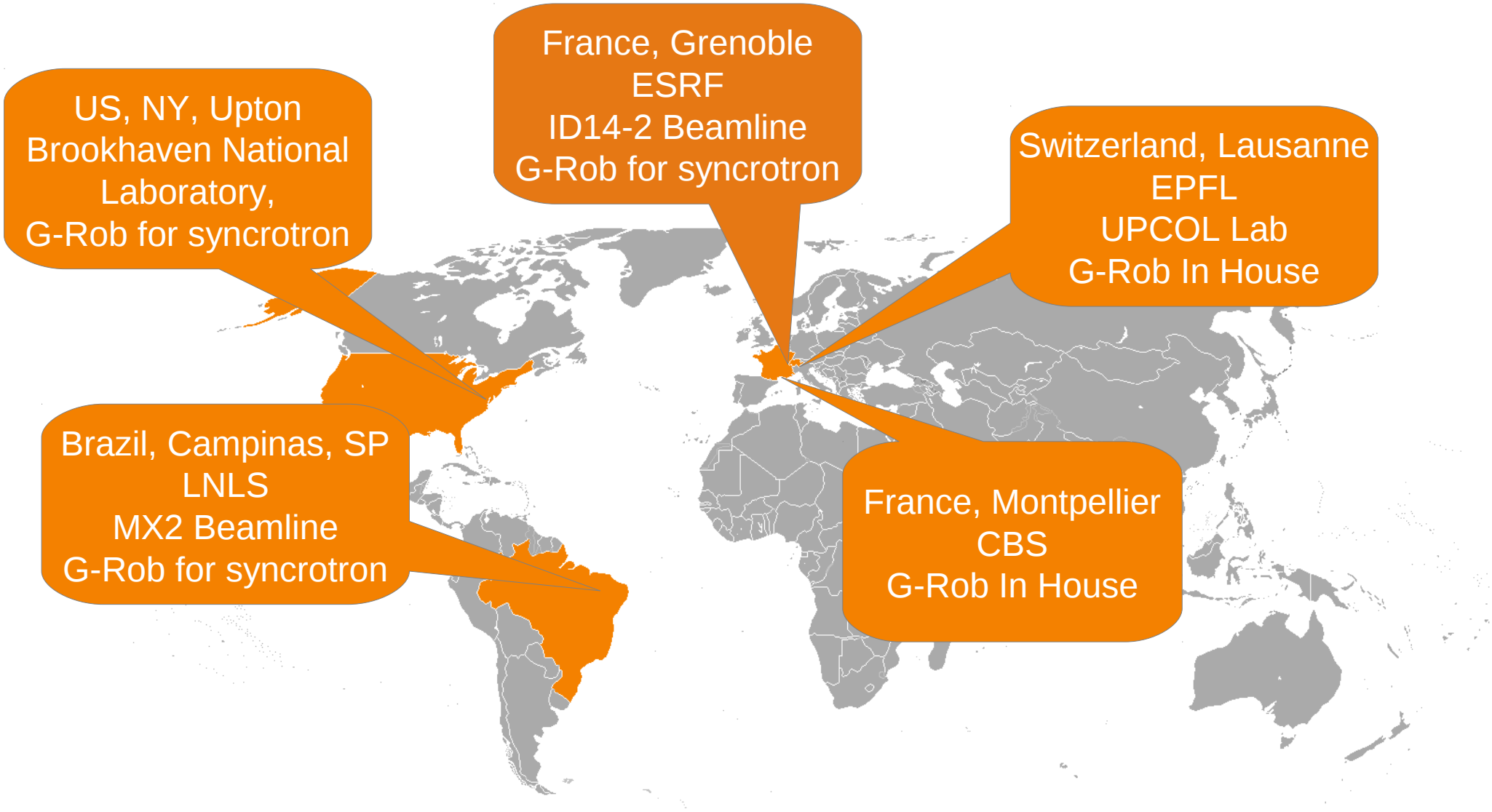


Sample environment

- Sample microscope with motorized zoom
- Motorized detector translation
- Motorized 2-Theta detector rotation
- Motorized beam stop
- Cryo-cane translation



5 G-Rob systems in operation



LNLS Laboratório Nacional de Luz Síncrotron

A light for science ESRF

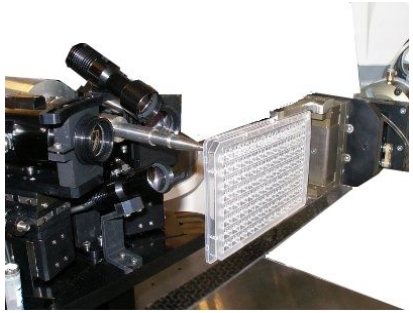
CBS Centre de Biochimie Structurale Montpellier

BROOKHAVEN NATIONAL LABORATORY

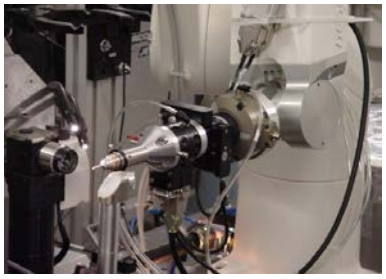
EPFL ÉCOLE POLYTECHNIQUE FÉDÉRALE DE LAUSANNE

2 – G-Rob functionalities

Cryo-sample transfer



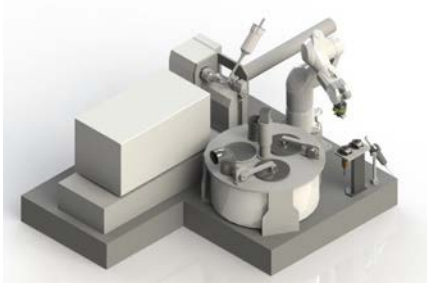
Plates, microchips
(*in situ* screening & datacoll.)



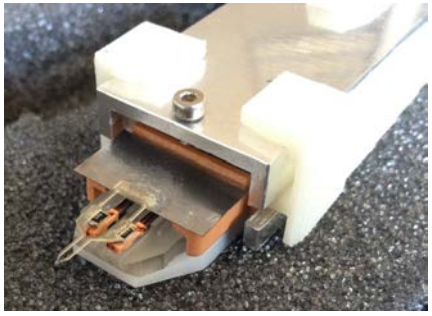
Frozen crystals,
capillaries, powder

Beam monitoring,
quick-realign

G-Rob Sample Changer



Sample changer



Sample harvesting

Cryo-frozen samples transfer

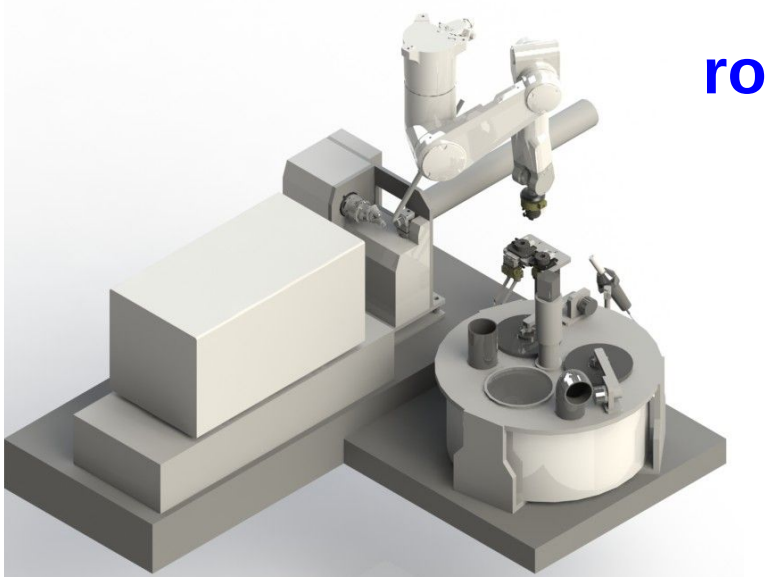
- Automated transfer of frozen samples
- 90 to 240 samples storage Dewar
- SPINE & Unipuck standard formats

Applications

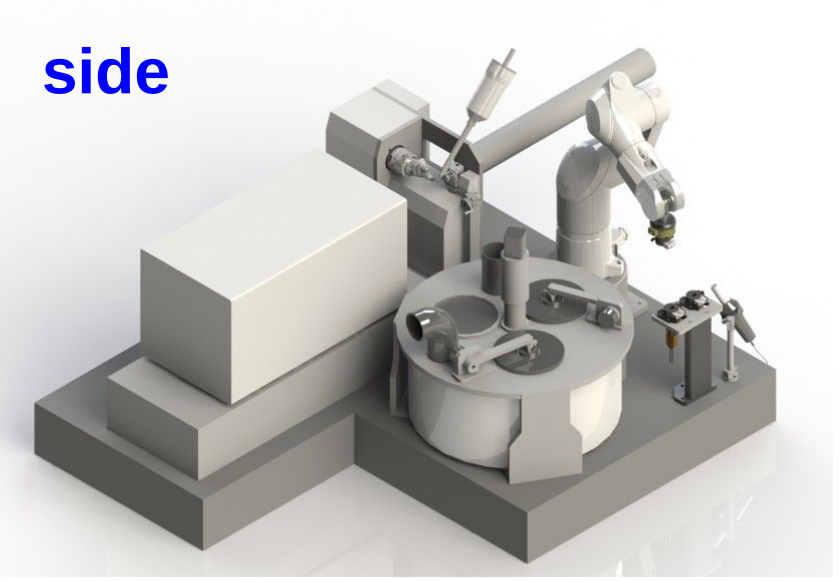
- high throughput screening of frozen crystals
- remote controlled experiments

G-Rob Sample Changer: 2 configurations

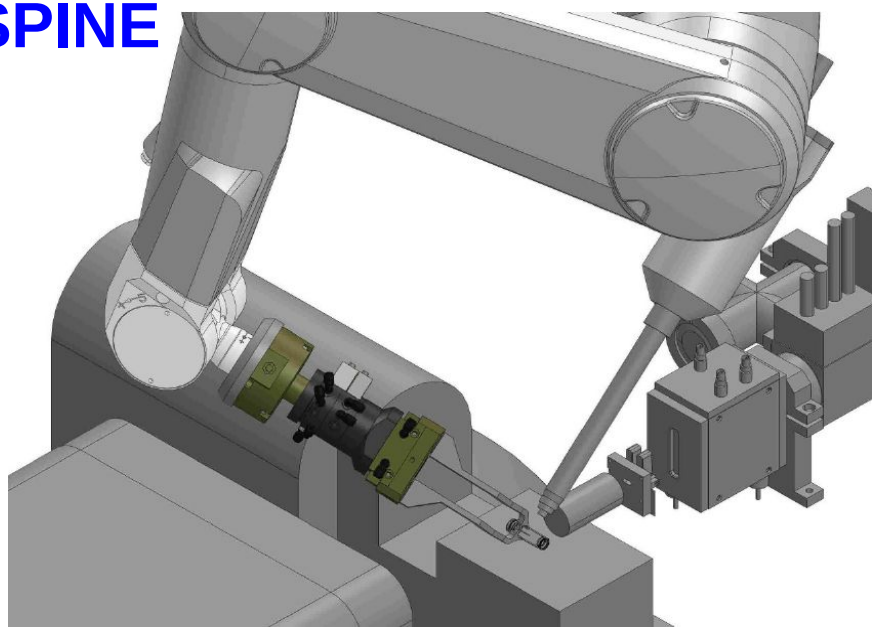
roof



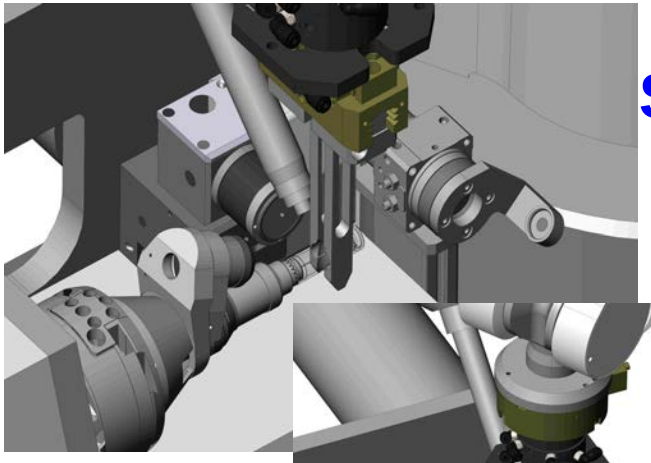
side



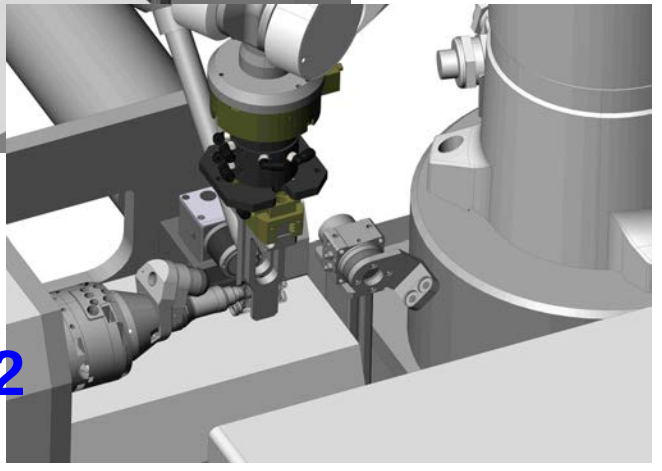
SPINE



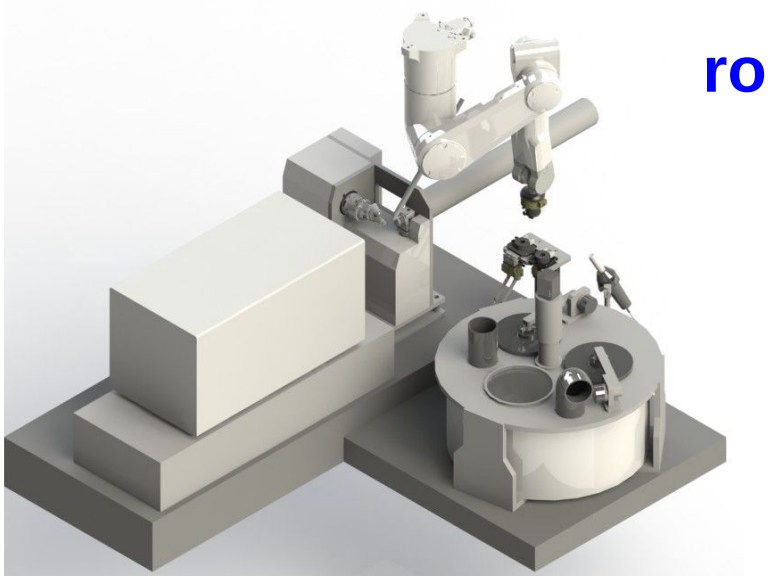
SPINE



SPINE x2

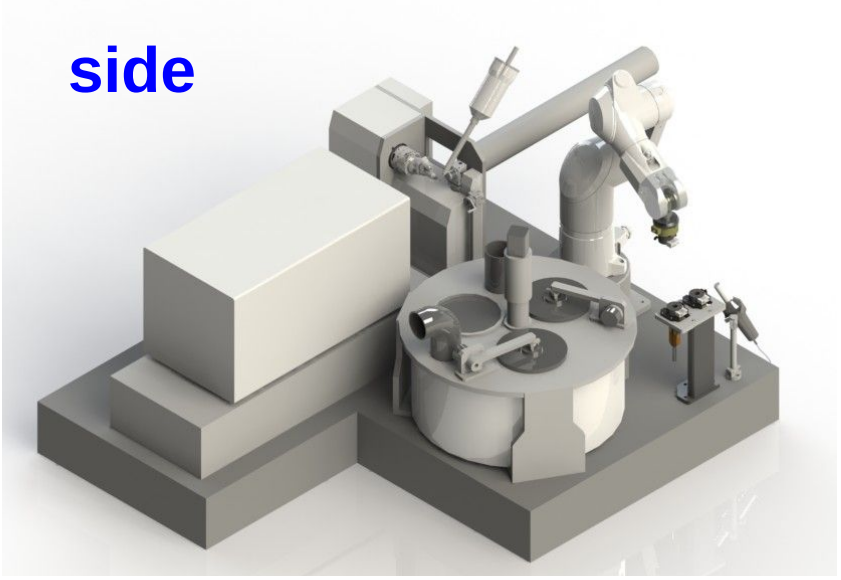


G-Rob Sample Changer: 2 configurations

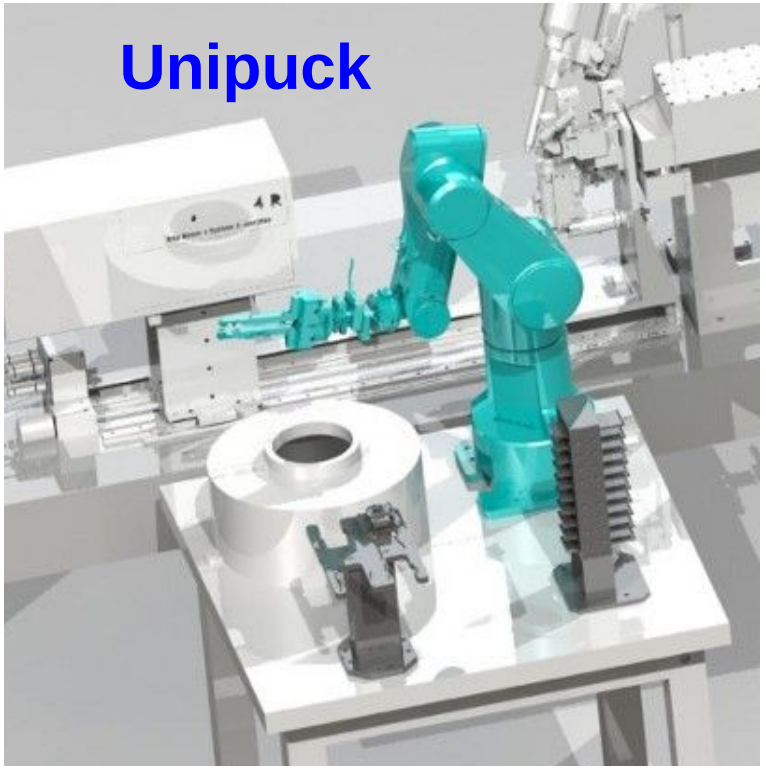


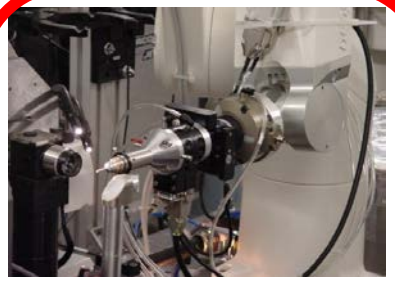
roof

side



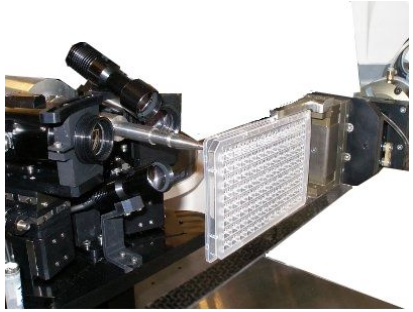
Unipuck





Frozen crystals, capillaries, powder

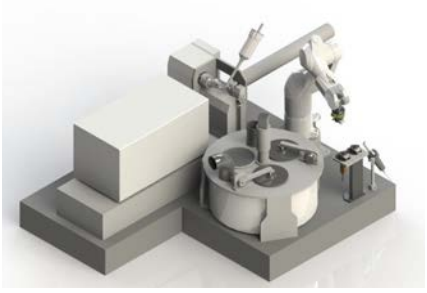
Cryo-sample transfer



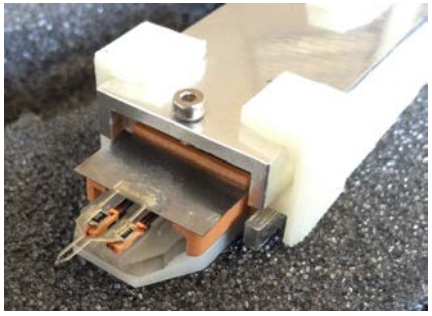
Plates, microchips (*in situ* screening & datacoll.)

Beam monitoring, quick-realign

G-Rob 1D/1D+



Sample changer



Sample harvesting

a goniometer for single sample

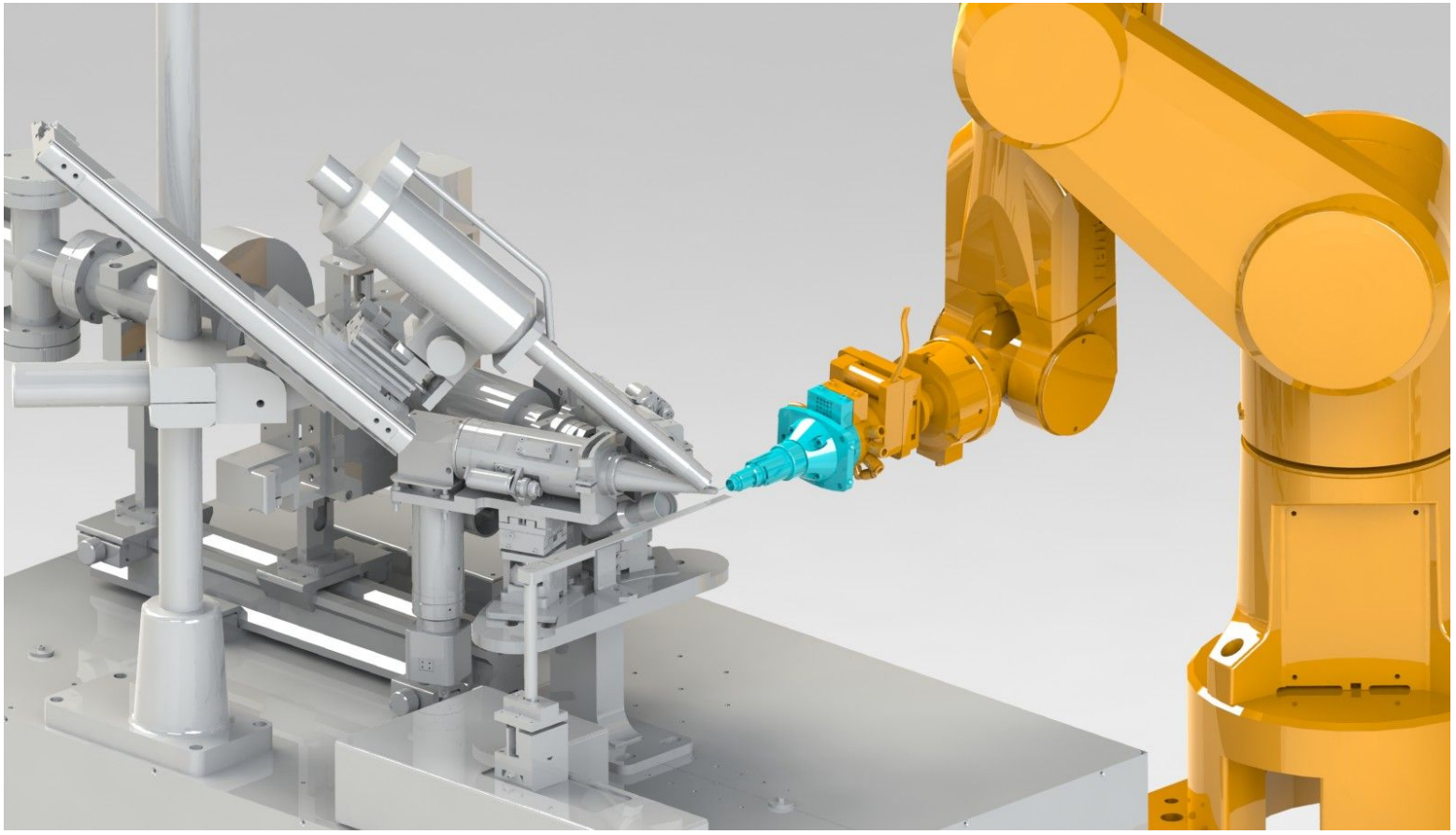
- frozen crystal, capillary

Applications

- classical data collection
- shutter-less data collection
- Phi data collection
- powder diffraction

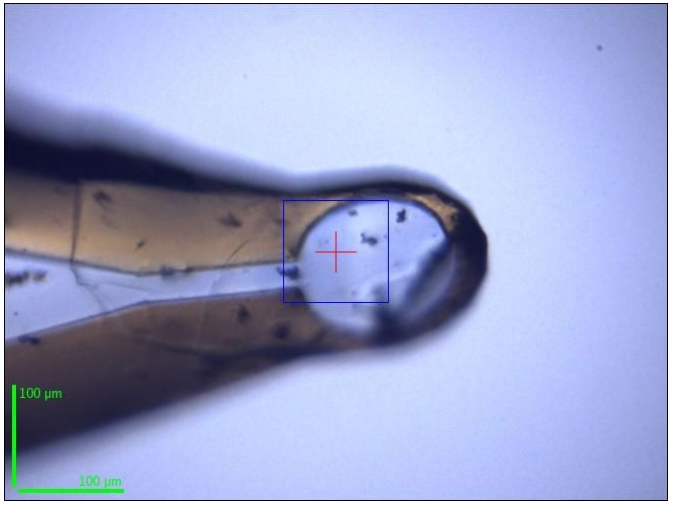
G-Rob function: 1D

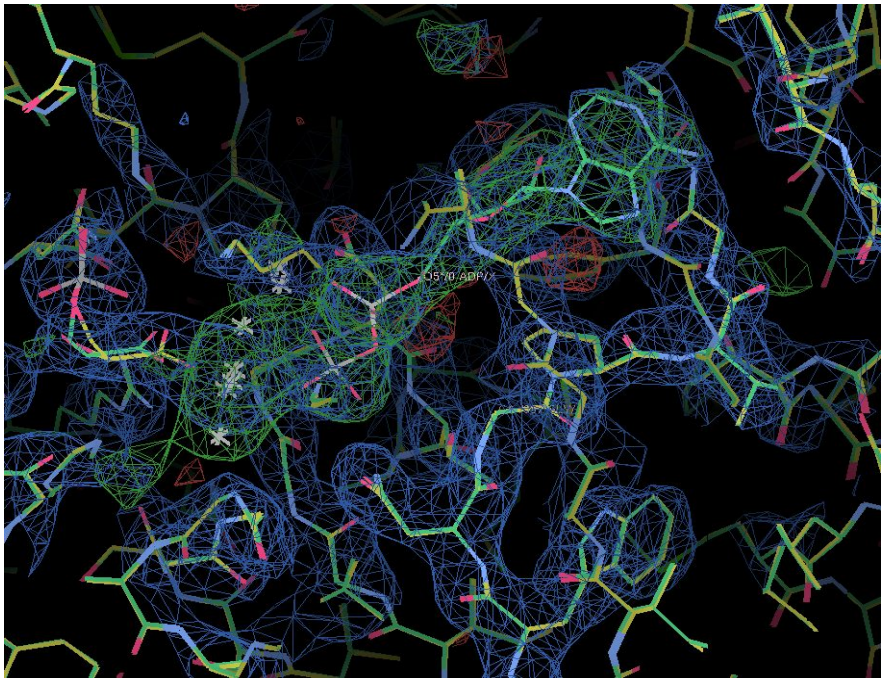
- Goniometer capability
- Validated with beam down to 90 µm
- Exposure time as short as 0.1s for 1° oscillation



Structure of PGK at 2.7 Å, solved on ID14 (ESRF)

M. Bowler, ESRF (ID14-1 and ID14-2)

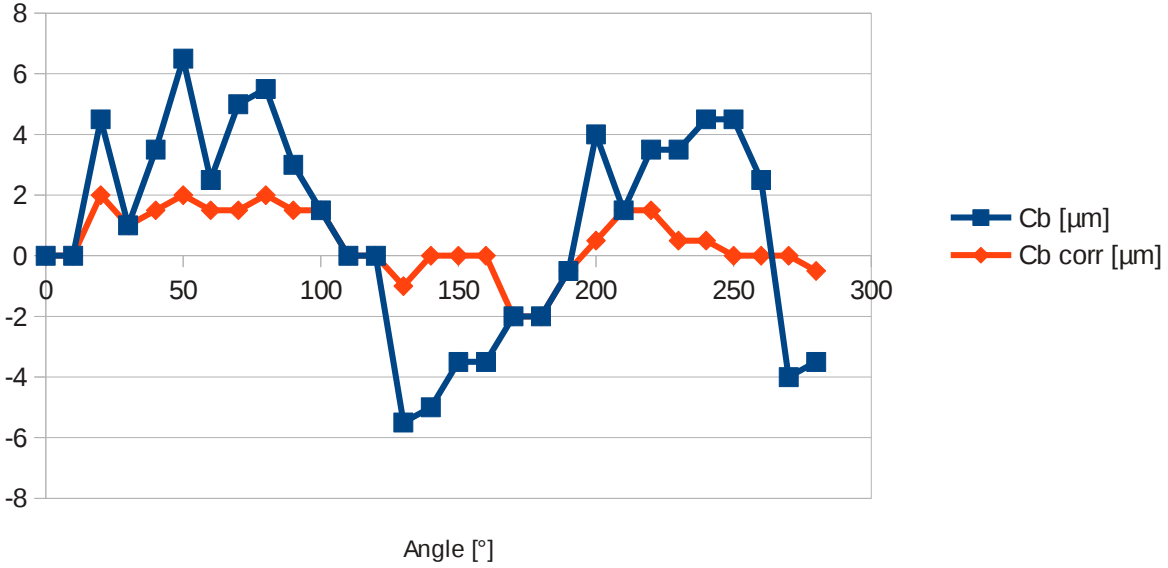


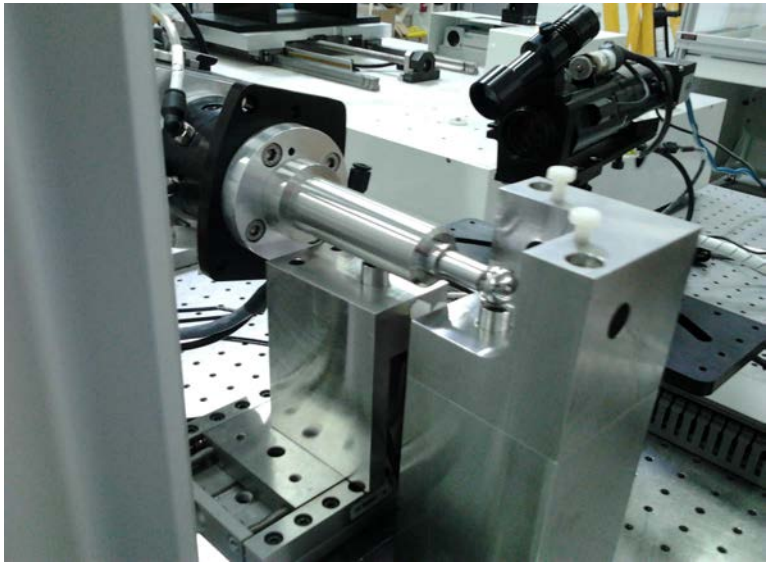


	Overall	Inner shell	Outer shell
Rmerge	0.09	0.05	0.39
Rmerge in top intensity bin	0.04	-	-
Rmeas	0.12	0.07	0.50
Rpim	0.06	0.03	0.23
Mean <I/sI>	8.10	12.6	3.30

G-Rob function: 1D+

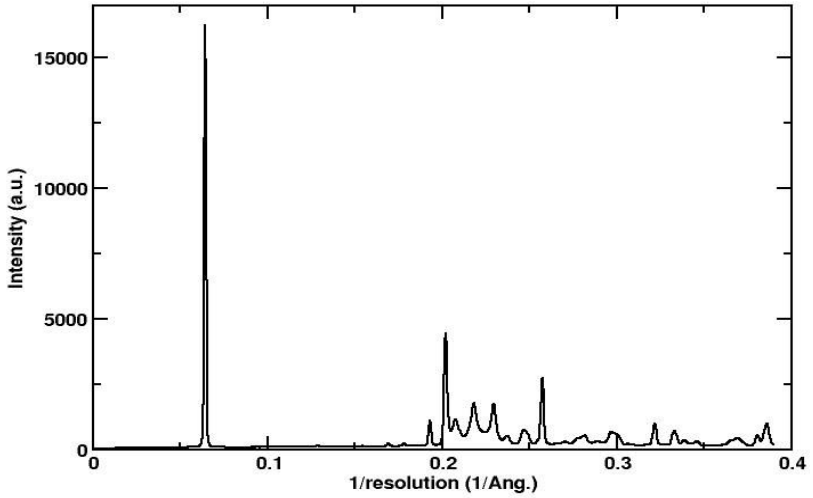
- Improved goniometer capability
- Compatible with beam down to 40 µm diameter !!!!



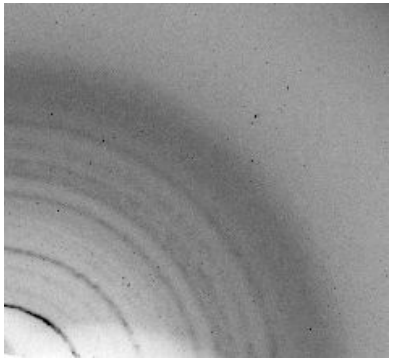


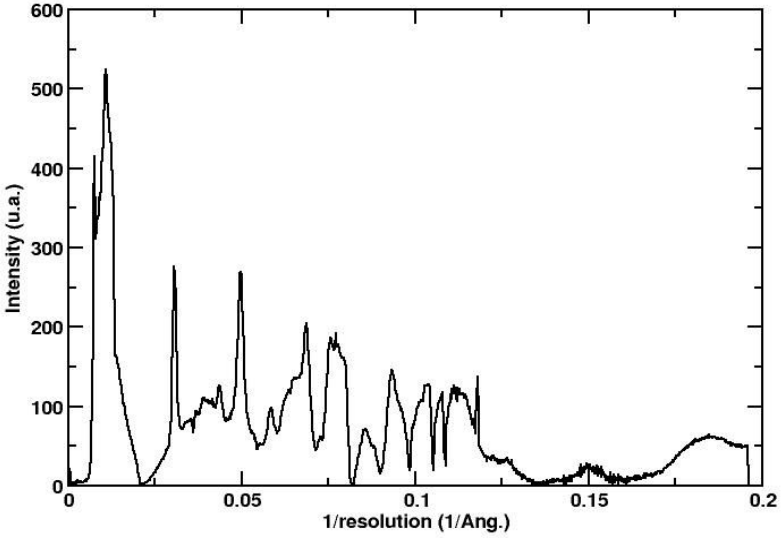
G-Rob function: Powder diffraction

Small molecule powder

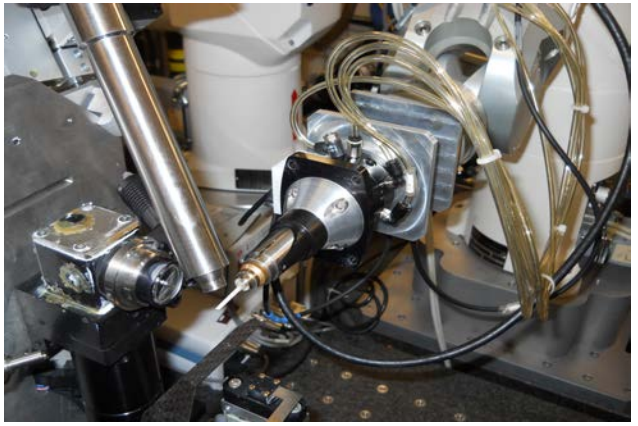


Protein powder

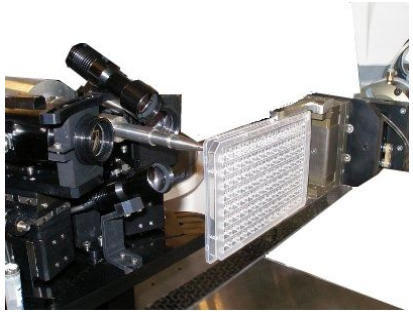




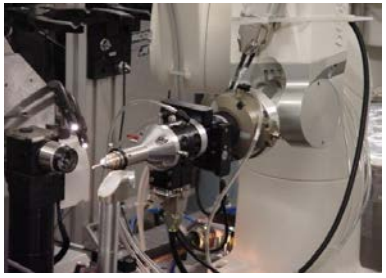
2-4 rotation / sec
Continuous translation



Cryo-sample transfer



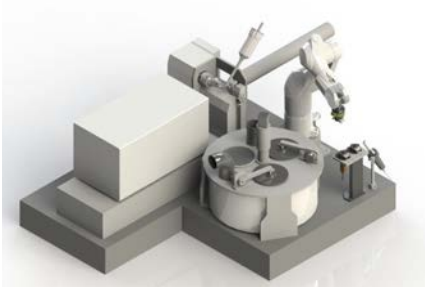
Plates, microchips
(*in situ* screening & datacoll.)



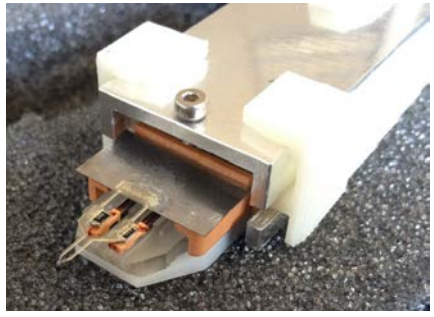
Frozen crystals,
capillaries, powder

Beam monitoring,
quick-realign

G-Rob 1DT



Sample changer



Sample harvesting

Cryo-frozen samples transfer

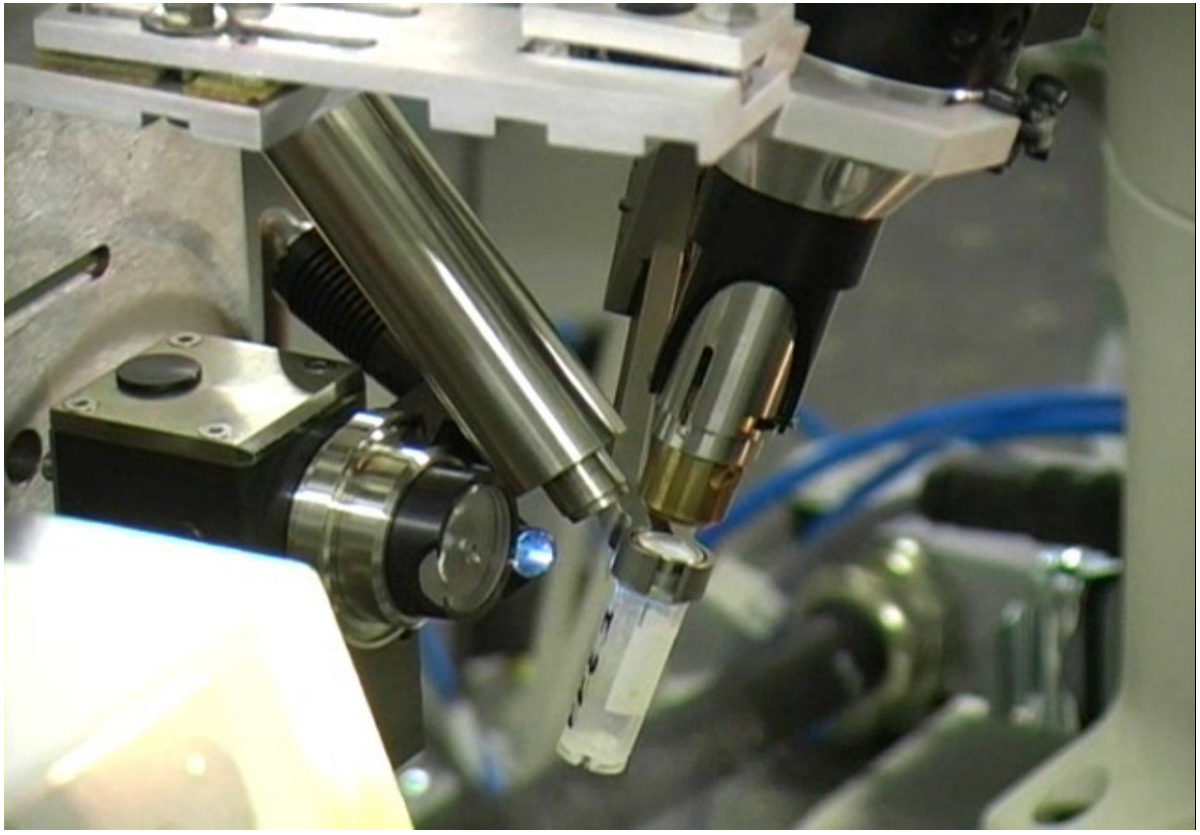
- Automated transfer of frozen samples
- 90 to 240 samples storage Dewar
- SPINE standard format

Applications

- high throughput screening of frozen crystals
- remote controlled experiments

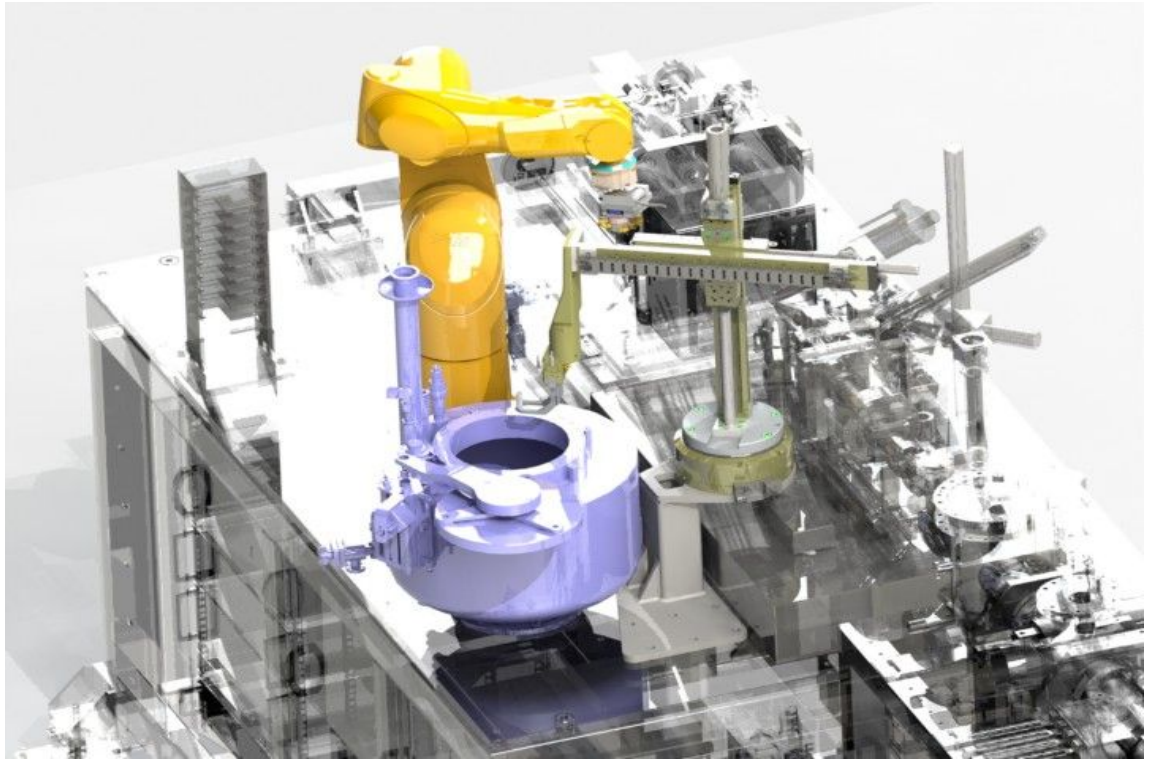
G-Rob 1DT for in-house systems

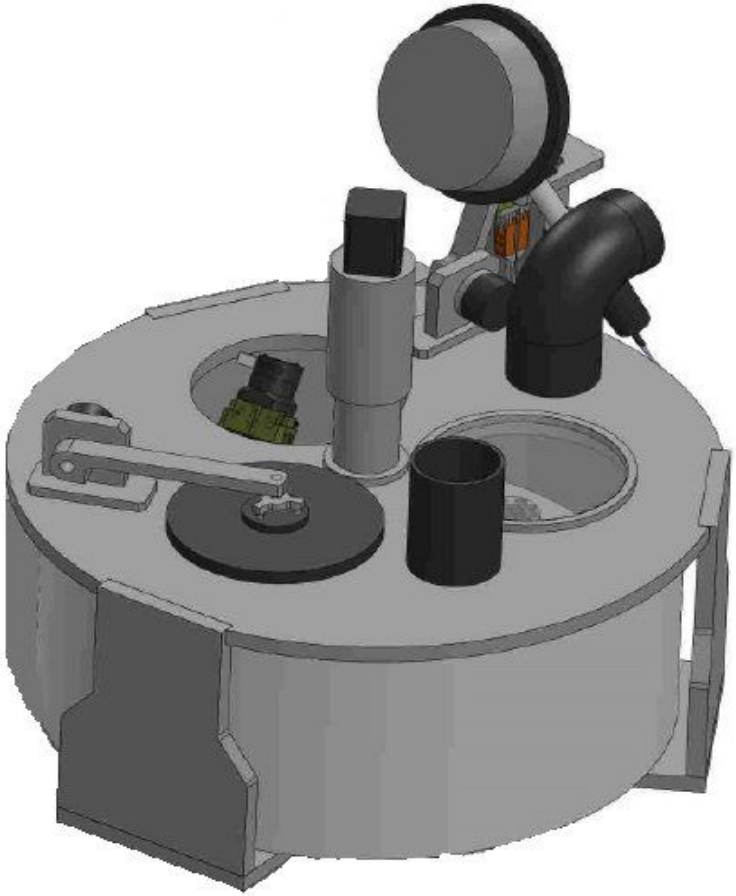
- Rapid sample changer cycle time
- Compatible with SPINE standard
- Storage Dewar for 90 samples



G-Rob 1DT for beamlines

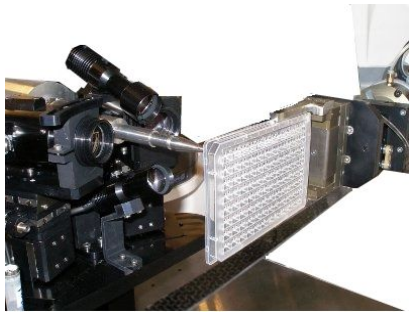
- Very fast: cycle time < 40 sec
- Compatible with SPINE standard
- Storage Dewar for 90 up to 240 samples



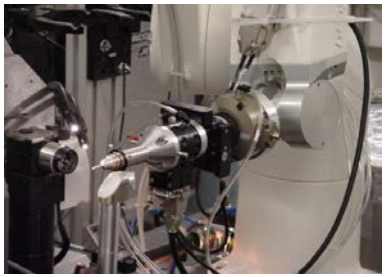



Stäubli
uantum 4R
Detector Systems Corporation

Cryo-sample transfer



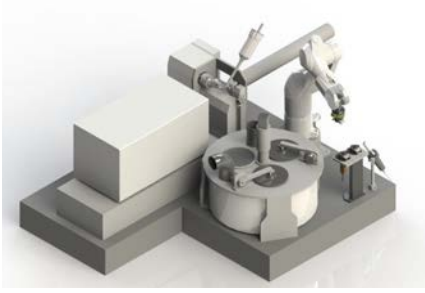
Plates, microchips
(*in situ* screening & datacoll.)



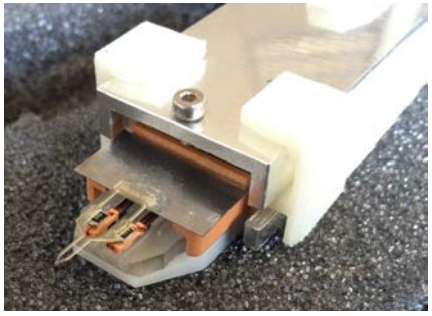
Frozen crystals,
capillaries, powder

Beam monitoring,
quick-realign

G-Rob 2D



Sample changer



Sample harvesting

in situ screening & data collection

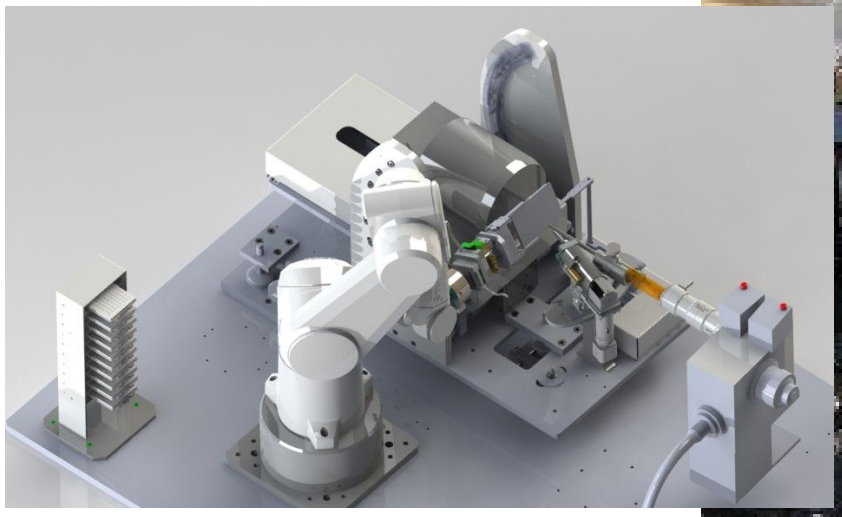
- SBS micro-plates (sitting/hanging drops)
- SBS high density batch plates
- micro-chips
- high pressure cells

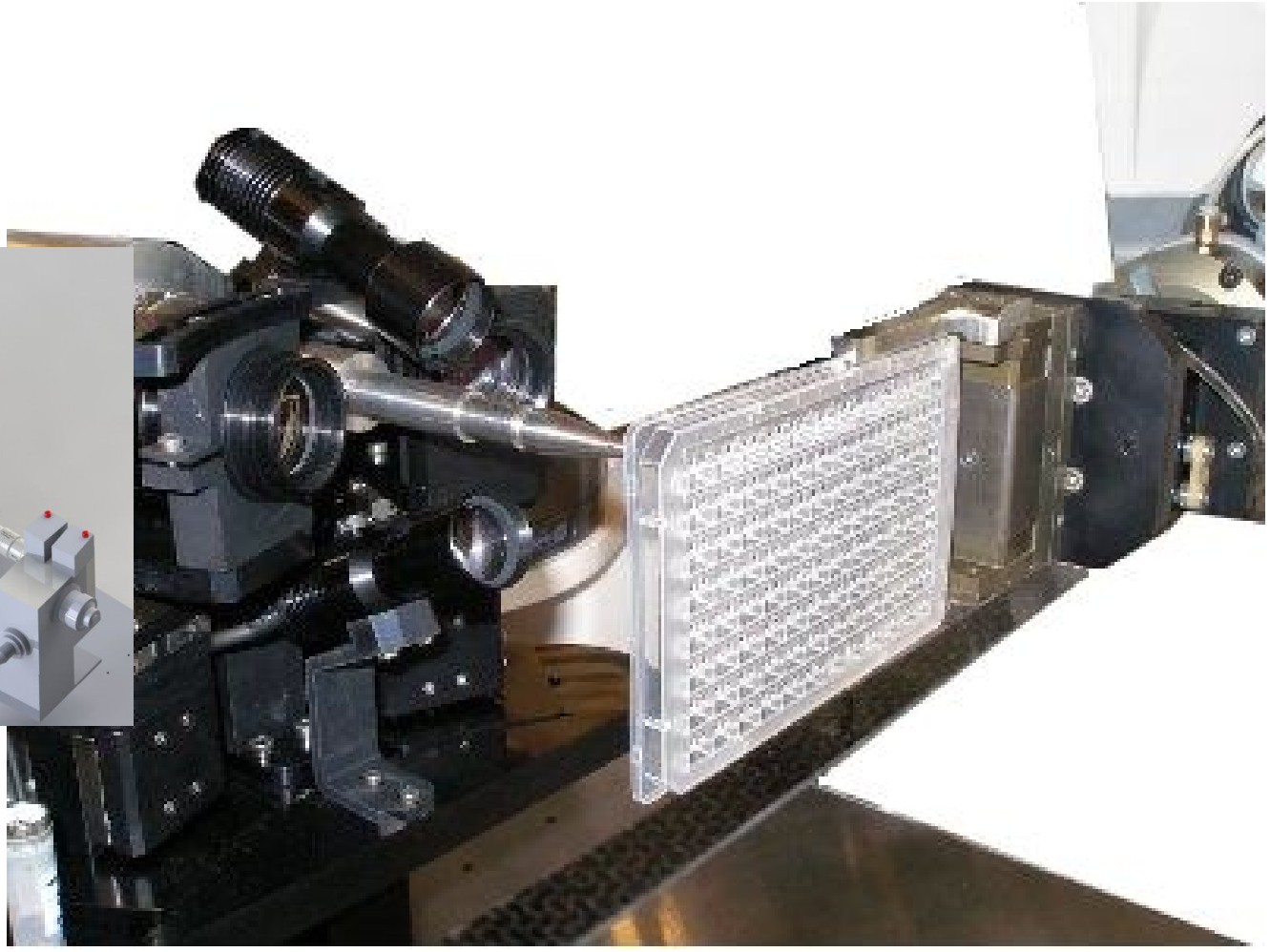
Applications

- rapid crystallization screening
- data collection at room temperature on series of crystals
- automated screening of compounds, fragments, heavy atoms

G-Rob function: 2D

- *In situ* screening for crystallization plates
- Up to 80 degree rotation range for *in situ* data collection





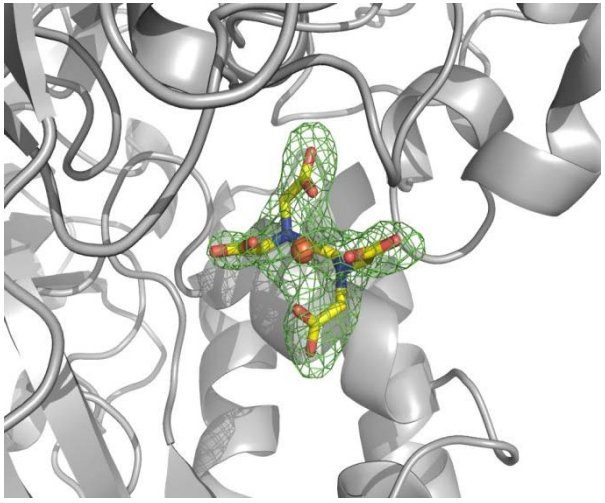
Crystal Listing

Position off all crystals on a plate can be recorded by single clicks.
Then data can be recorded in a row on these crystals, in a fully automated way.

Listing on:	G-Rob
Number of samples	79
<|X|> error (µm)	3
<|Y|> error (µm)	3
<|radius|> error (µm)	5
X standard deviation (µm)	2
X standard deviation (µm)	2
radius standard deviation (µm)	3

Experiments performed on the
in-house G-Rob system
of the the EPFL crystallography platform
(Prof. S. Cole laboratory, Lausanne).

	Lysozyme	NikA-FeEDTA
Data collection		
Resolution (last shell) (Å)	2.10	2.45
Completeness (last shell) (%)	71.6 (75.0)	68.4 (71.4)
R_{sym}[a] (last shell) (%)	13.9 (38.5)	13.8 (41.6)
I/σ (last shell) (I)	5.61 (2.75)	4.45 (2.20)
Refinement		
R_{work}[b] (%)	18.82	17.39
R_{free}[c] (%)	23.11	25.07



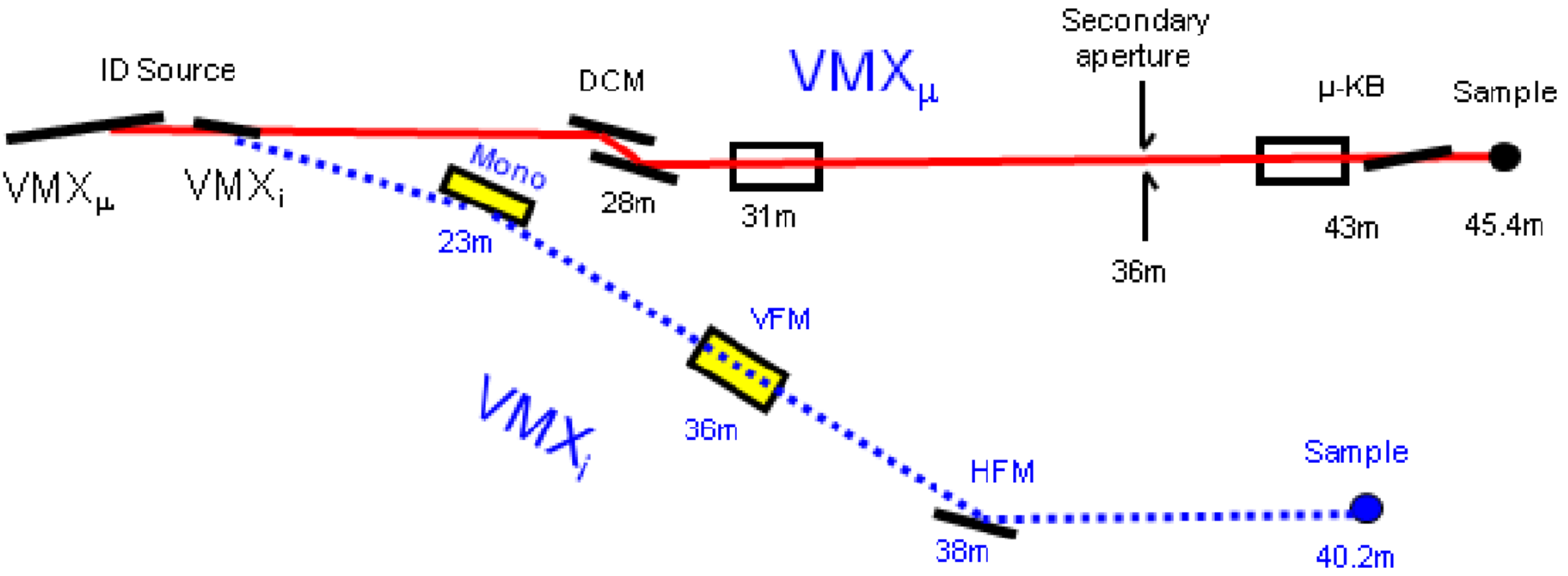
Fe(III)-EDTA binding site in NikA.
Omit Fourier electron density map
of Fe-EDTA contoured at 3 sigma

In situ on synchrotron beamlines

Synchrotron	Beamline	Equipment	Availability
ESRF	FIP-BM30A	G-Rob	in operation
ESRF	BM14	home made	in operation
ESRF	ID30	G-Rob	in project
SLS	?	CATS	in operation
LNLS	MX2	G-Rob	in operation
DLS	I5	home made	in operation
SSRF	u-focus	CATS	end of 2013
APS	LS-CAT	CATS	in operation
BESSY	BL14.1	CATS	in operation
BNL	X12B	G-Rob	end of 2013

Etc...

The VMX project at DLS



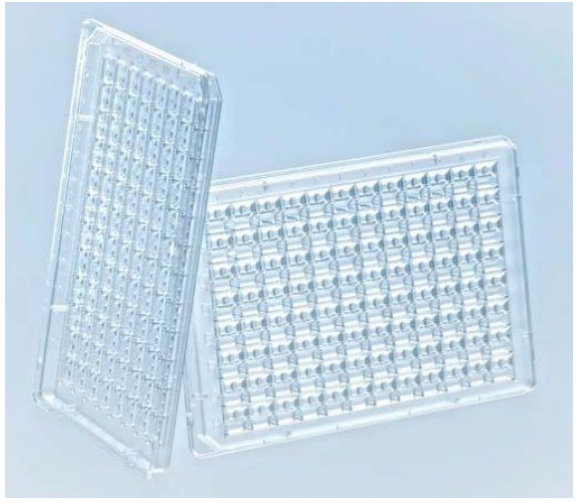
Endstation	Sub microfocus (VMXu)	In situ (VMXi)
Energy range (keV)	5 – 30	Nominally ~14 keV
Beamsize (μm)	0.5 – 5 (300)	5 – 50
Flux (phs/s)	~ 1e12 at 20 keV	>1e12

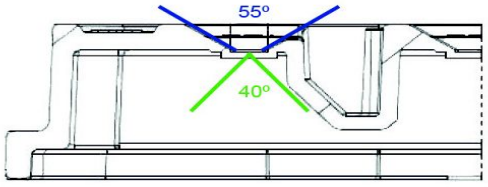
96-well sitting-drop crystallization trays for *in situ* diffraction

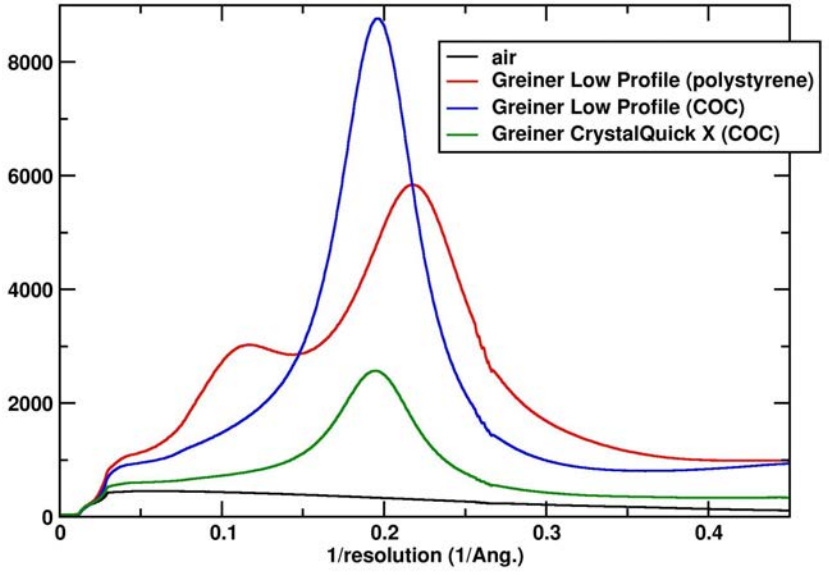
Manufacturer (distributor)	Reference	Preferred orientation	Scattering	Angular range (deg)
MRC (Mol. Dimensions)	MD11-003/003U	(Both)	High	~30
MRC (Mol. Dimensions)	MD11-00	Portrait	High	~30
Greiner BioOne	609101	Lanscape	High	~30
Greiner BioOne	609120	Lanscape	High	~30
Greiner BioOne	609171	Lanscape	High	~50
Greiner BioOne	**609890/895**	**Lanscape**	**Low**	**~80**
Mitegen	**InSitu-01CL**	**Both**	**Low**	**~90**
Art Robbins Instruments	102-0001-00/10	Portrait	High	~30
Art Robbins Instruments	102-0001-03/13	Portrait	High	~30
Art Robbins Instruments	102-0001-01	Portrait	High	~30
Corning	Crystal*EX, 1-well*	(Both)	High	~30
Corning	Crystal*EX, 3-well*	(Both)	High	~30

CrystalQuick™X plate

- Made with "low birefringence" COC
- 80 degrees of angular range
- Compatible with any crystallization robot
- Reduced bottom thickness
  - 250-300 µm instead of 1000 µm for other plates
  - Lower X or UV scattering
  - Higher brightness in visible range

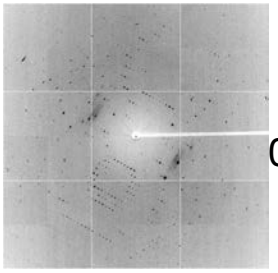






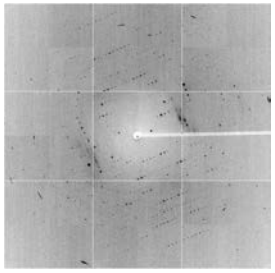
greiner bio-one

High pressure cell
(R. Kahn *et al*., IBS, Grenoble)

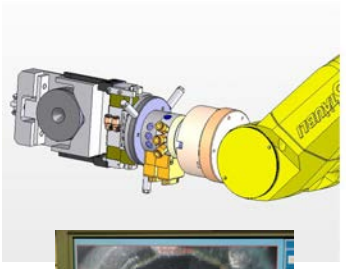


Z-DNA

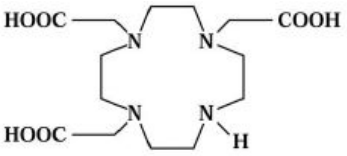
0 Mpa



540 MPa

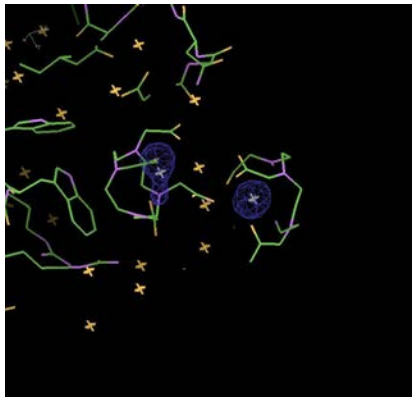


Anomalous data of Yb-DO3A / lysozyme complex solved "in the drop"



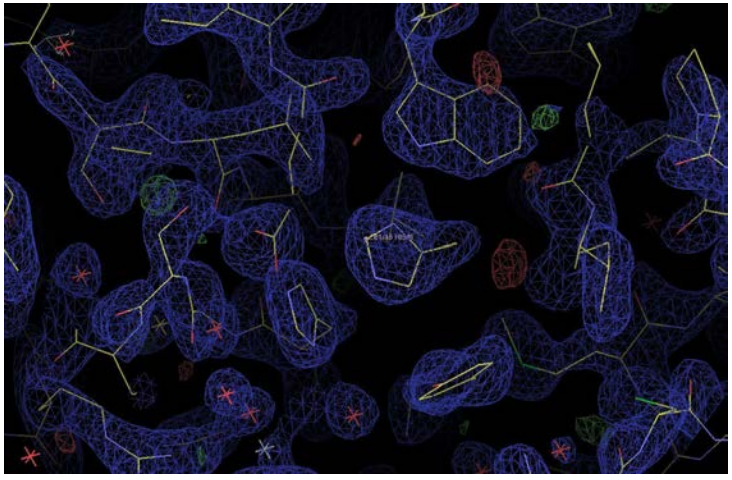
resolution: 1.8 Å
complet.: 90 %
(anomalous)

Anomalous diff. map (threshold: 6 σ)

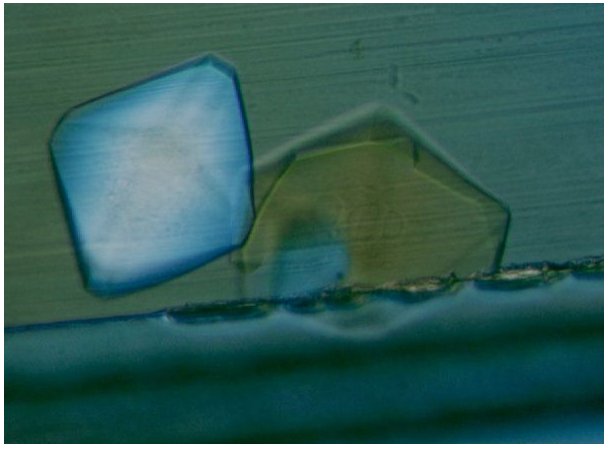


Structure of NDK from *A. Polyphaga* Mimivirus solved "in the drop"
(C. Abergel, CNRS)

space group: p6(3)
a/b/c: 70.8/70.8/106.3
resolution: 2.3 Å
completness: 80 %, I/σ(I): 3.3
Rsym: 19.6 %, Rfree: 27.4 %

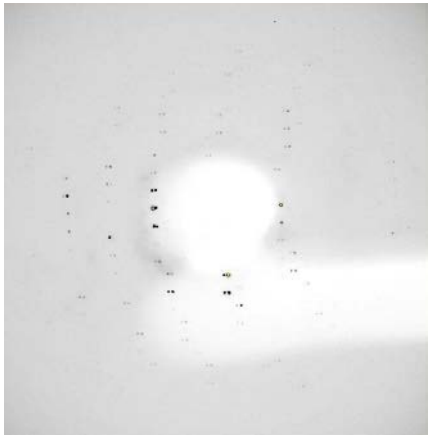


Extra-cellular domain of a membrane protein
(A. Haouz, Inst. Pasteur, Paris)



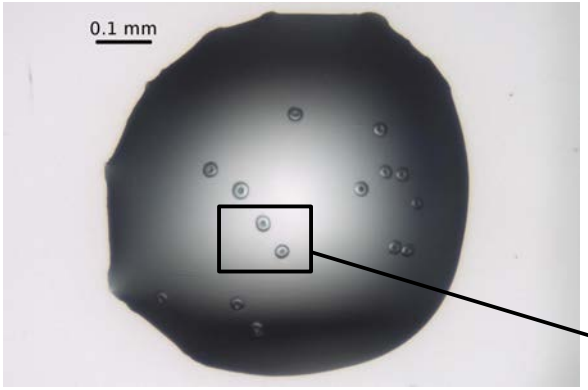
>300 um crystals
No diffraction when frozen

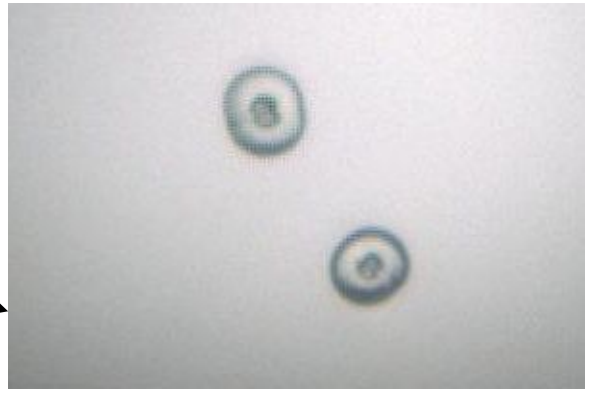
Beamline: FIP-BM30A
Plate: X-ray plate
Resolution: ~ 10 Å

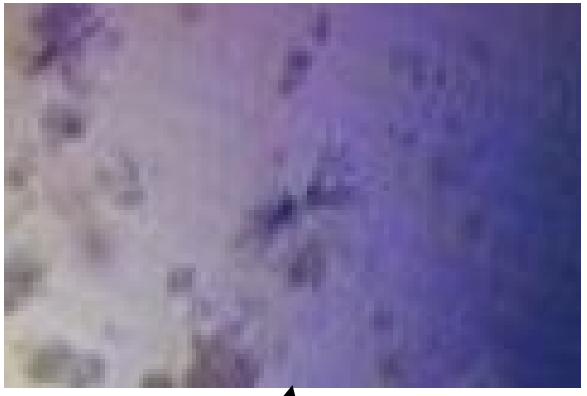


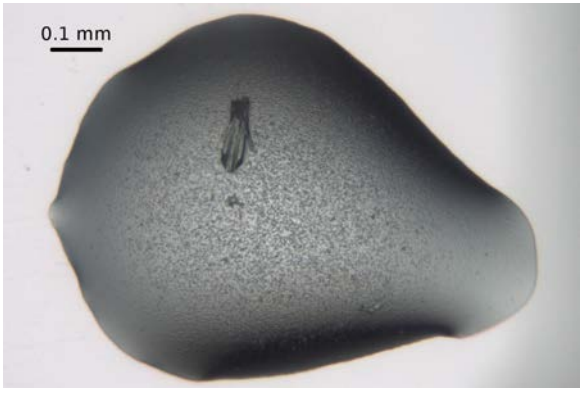
In situ screening

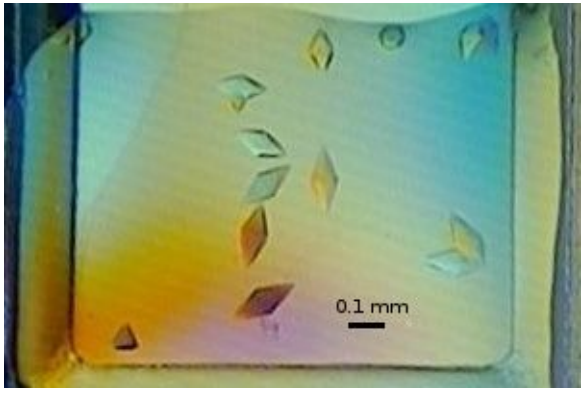
Samples recently proved to be diffracting protein crystals using G-Rob 2D ("*in situ*") screening

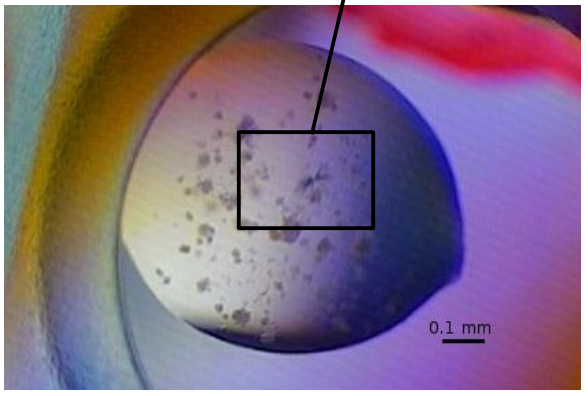








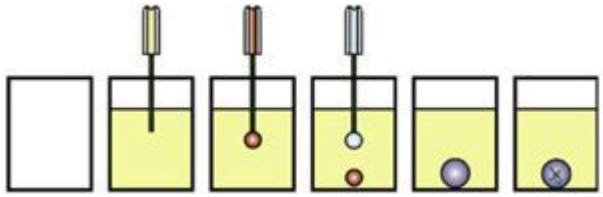




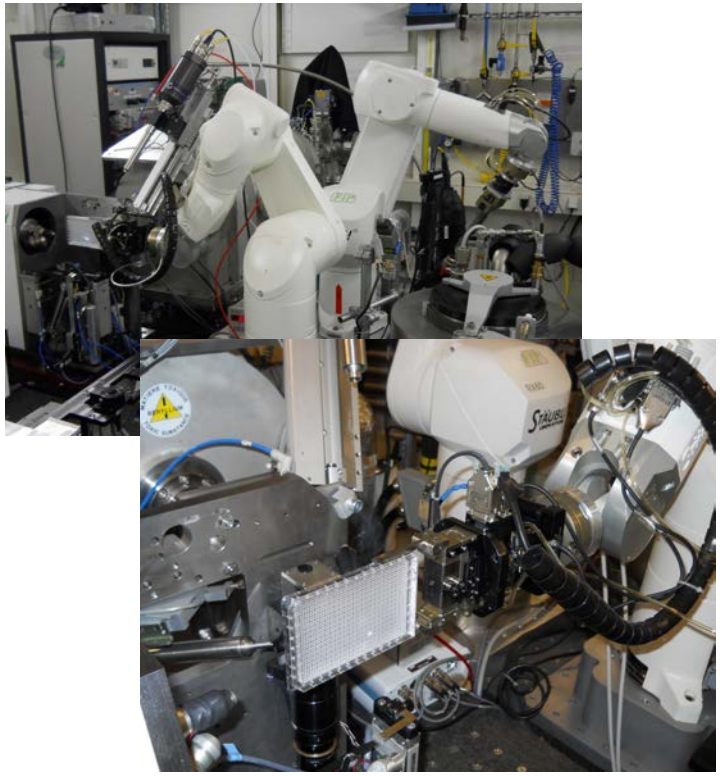
Adenovirus surface protein in complex with its receptor

In situ experiment performed on FIP-BM30A (5 Oct 2012)

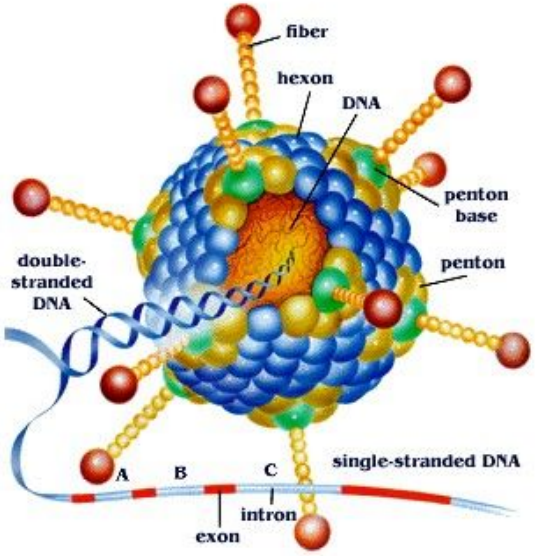
C. Zubieta, P. Fender (EMBL-Grenoble), A. Lieber (Washington Univ., Seattle)



Microbatch crystallization assay (HT platform, HWI Buffalo)

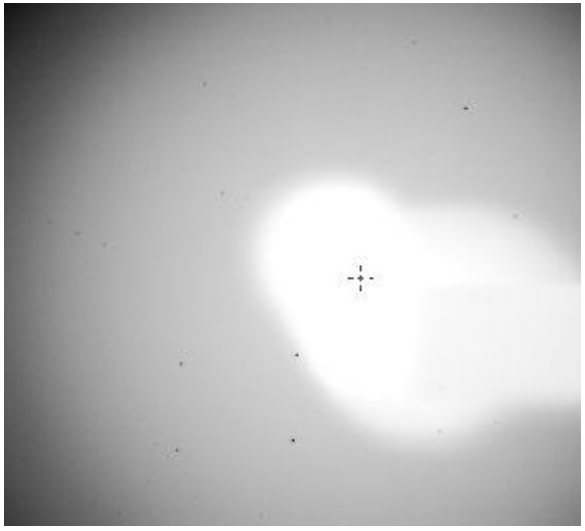


situ screening in 1536-well plate with G-Rob on FIP-BM30A



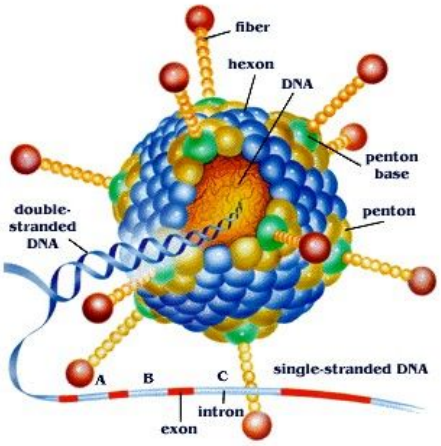
Aim of the experiment: study of the complex between the virus capside fiber and the human Desmoglein-2 receptor. This interaction leads to the opening of epithelial cells inter-cellular junctions, responsible for virus entry.

Diffraction at 6.3 Ang on 30x10 μm² crystals

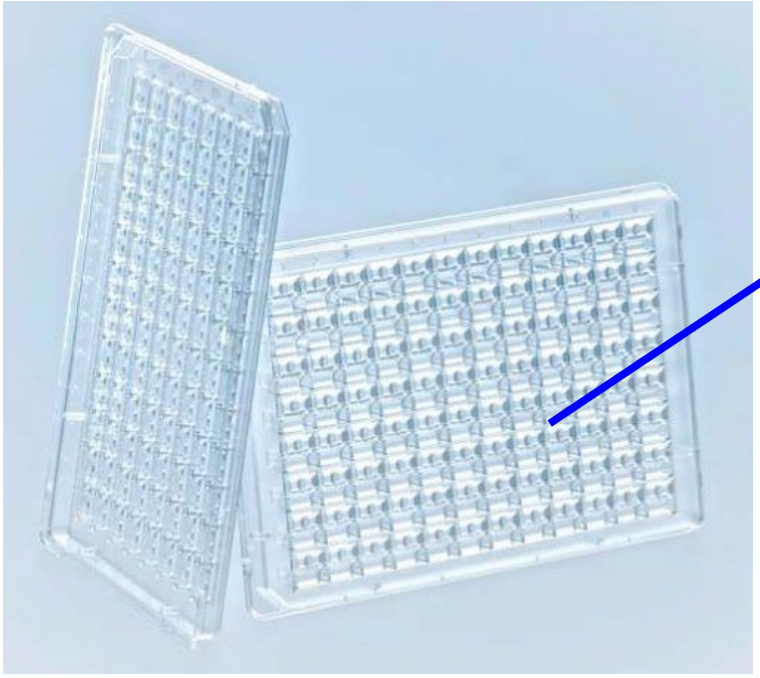


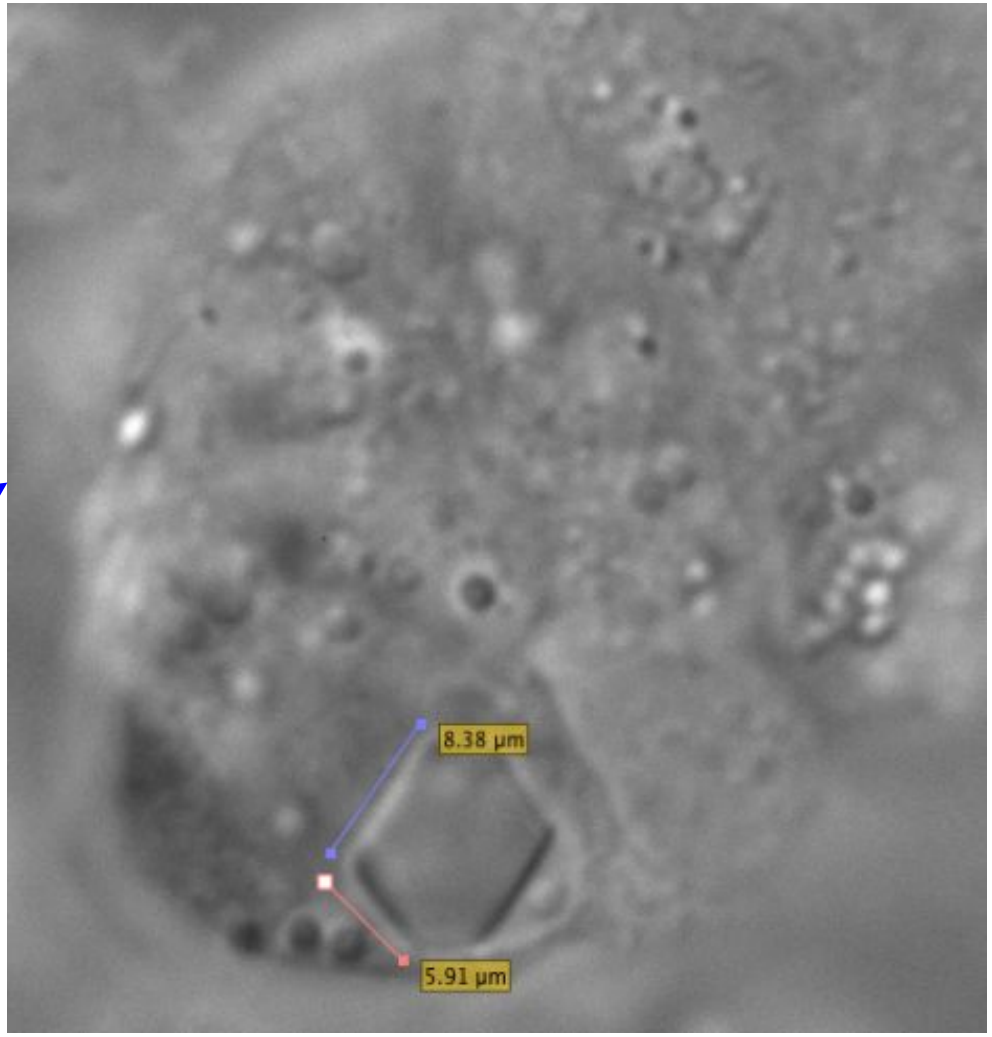
Intranuclear Adenovirus cristals

P. Fender *et al.*, EMBL



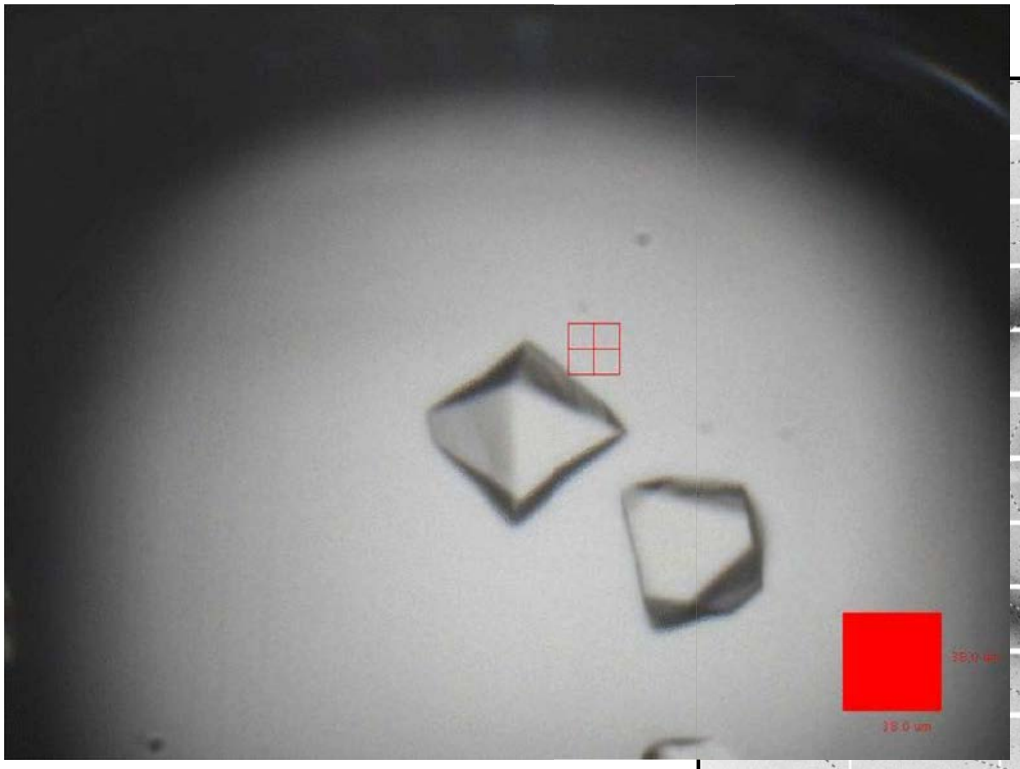
In situ analysis of crystals appeared in the insect cells used for expression.

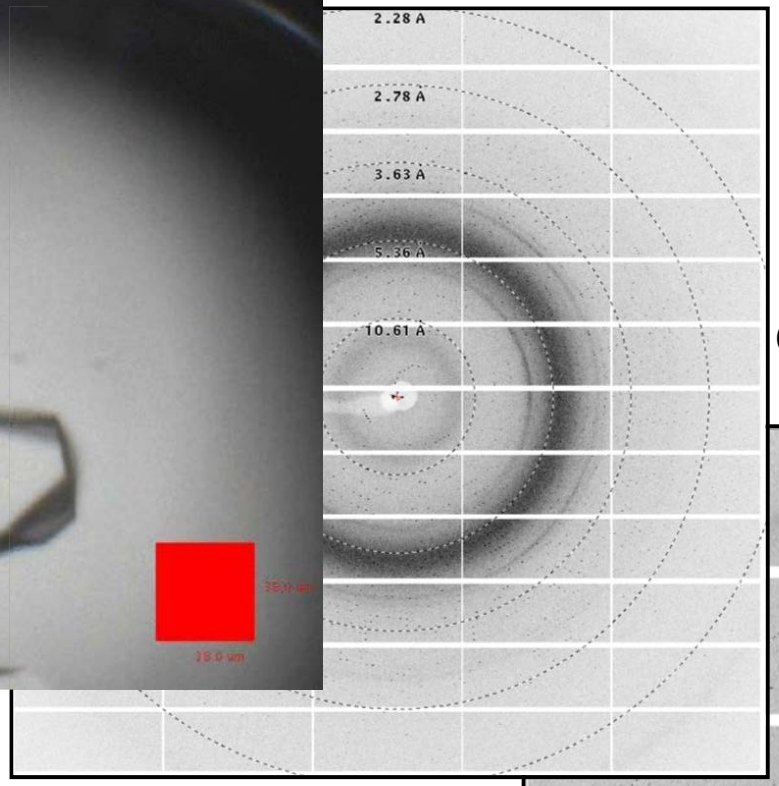


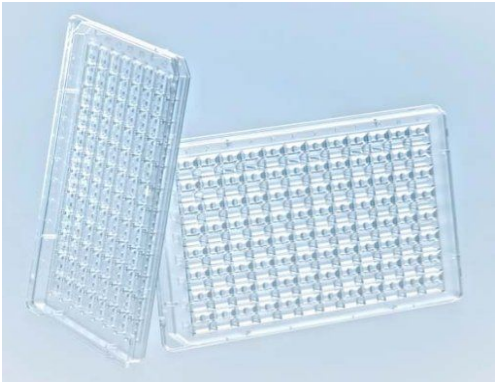


A new virus structure: Bovine enterovirus 2

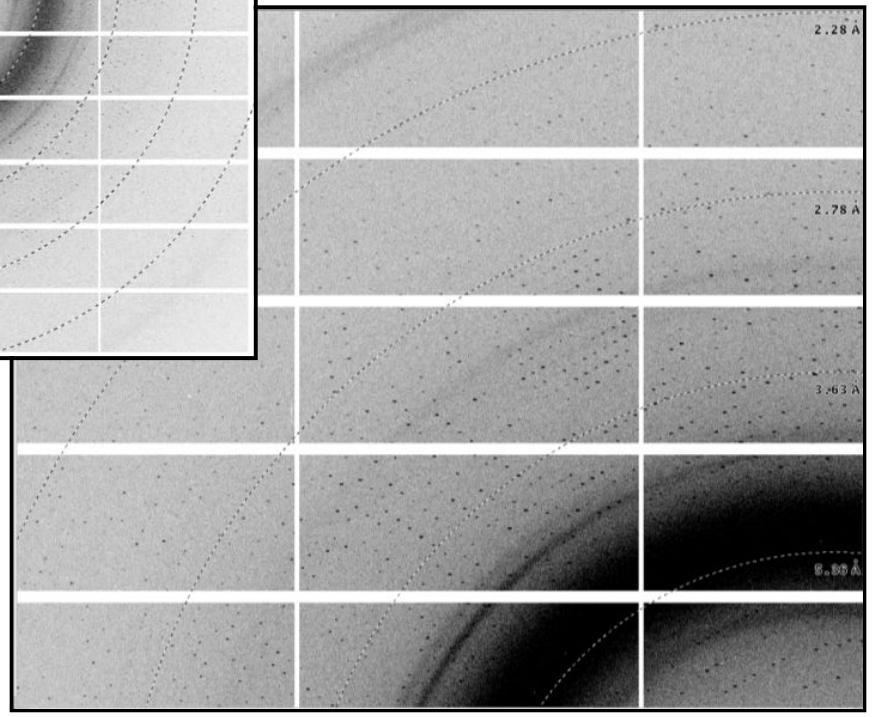
Crystallization plate screening on I24







CrystalQuick X plate

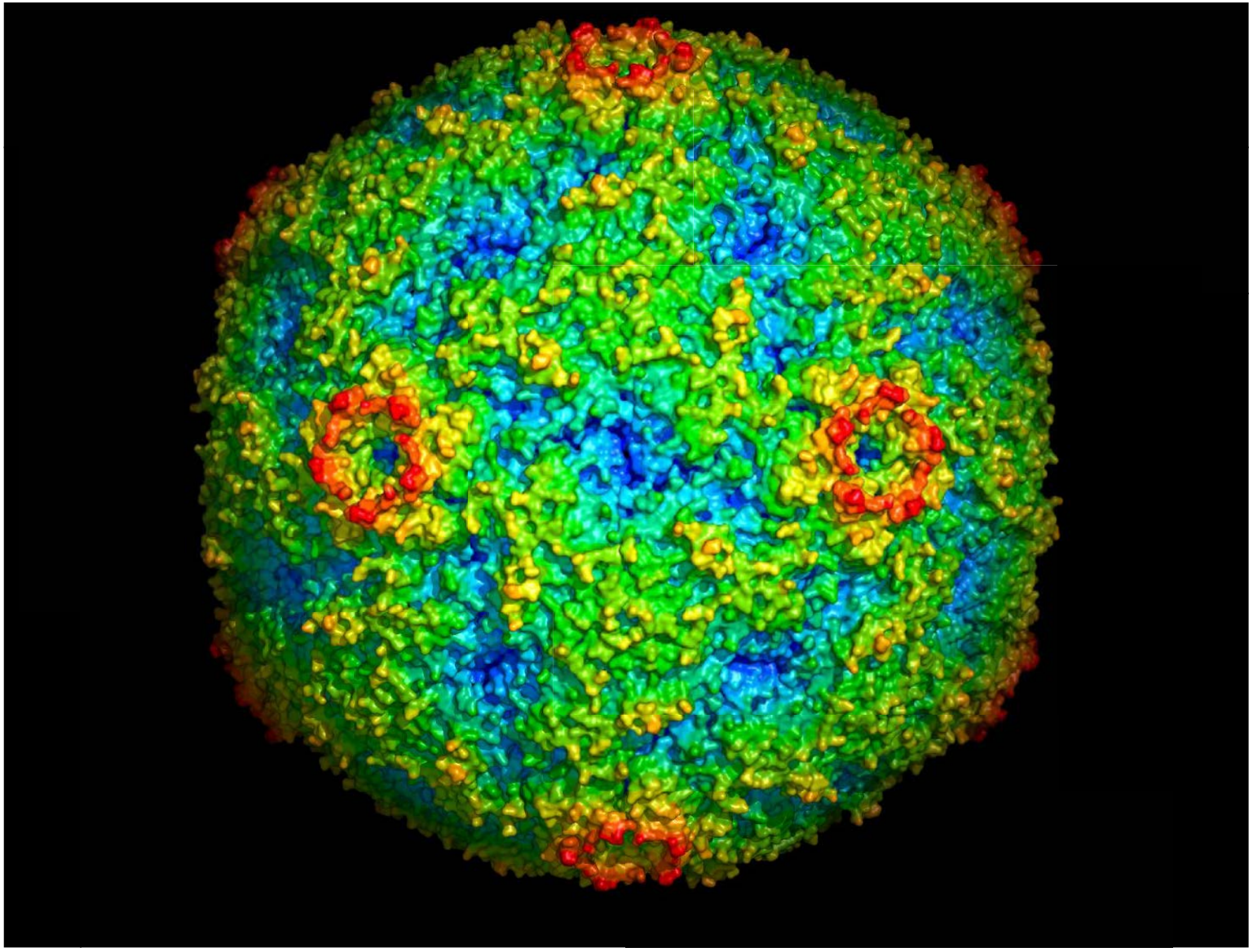


Data collected at DLS, I24
Beam size 20 microns, focus at detector (P6M)
exposure time 0.1 sec, 0.1° oscillation,
detector distance = 480 & 645 mm,
resolution at edge of detector 2.28 & 2.97 Å

E.E. Fry, J.S. Ren, A. Kotecha, T.S. Walter, C. Porta, D.I. Stuart,
The Wellcome Trust Centre for Human Genetics, University of Oxford (UK),
D.J. Rowlands, Institute of Molecular and Cellular Biology, University of Leeds (UK) and
Gwyndaf Evans, Robin Owen, Danny Axford, Jun Ashima, I24, Diamond Light Source (UK)

A new virus structure: Bovine enterovirus 2

Crystallization plate screening on I24

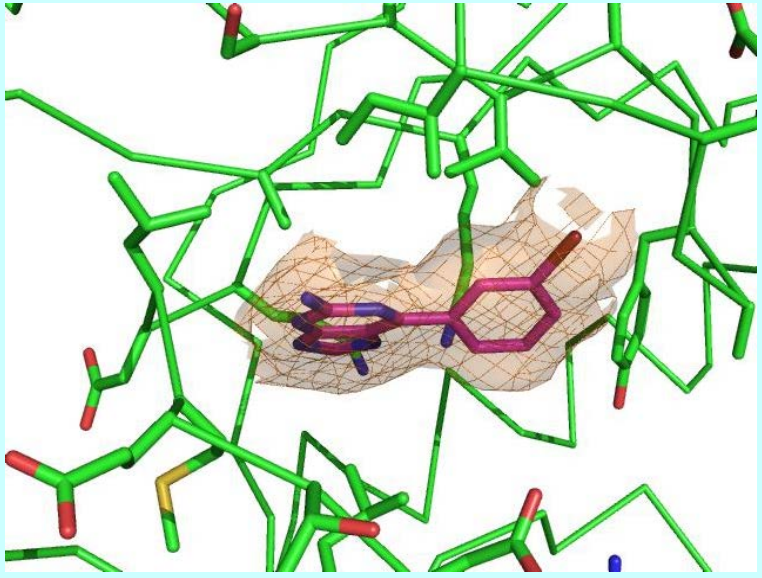


E.E. Fry, J.S. Ren, A. Kotecha, T.S. Walter, C. Porta, D.I. Stuart,
The Wellcome Trust Centre for Human Genetics, University of Oxford (UK),
D.J. Rowlands, Institute of Molecular and Cellular Biology, University of Leeds (UK) and
Gwyndaf Evans, Robin Owen, Danny Axford, Jun Ashima, I24, Diamond Light Source (UK)

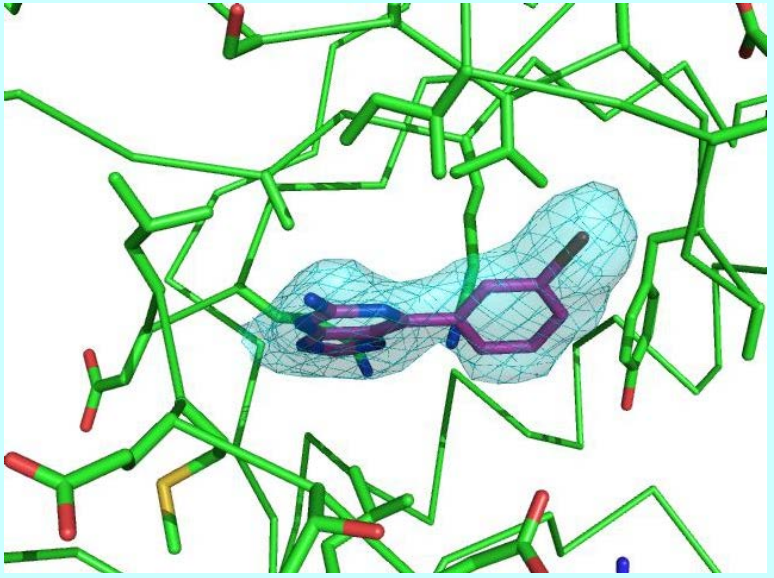
Test of ERK-2 in P21 with bromated ligand

Completness of 83%
by merging 3 dataset (50+50+41 frames)
Rsym ~5.4 at 2.15 Å.
Refinement against the structure of ERK-2, with no ligand.

ERK-2 (6PB)
Refinement: Refmac/Coot
Without ligand (R/Rfree ~ 20.4/25.5)



fo-fc (orange) 0.9 sigma



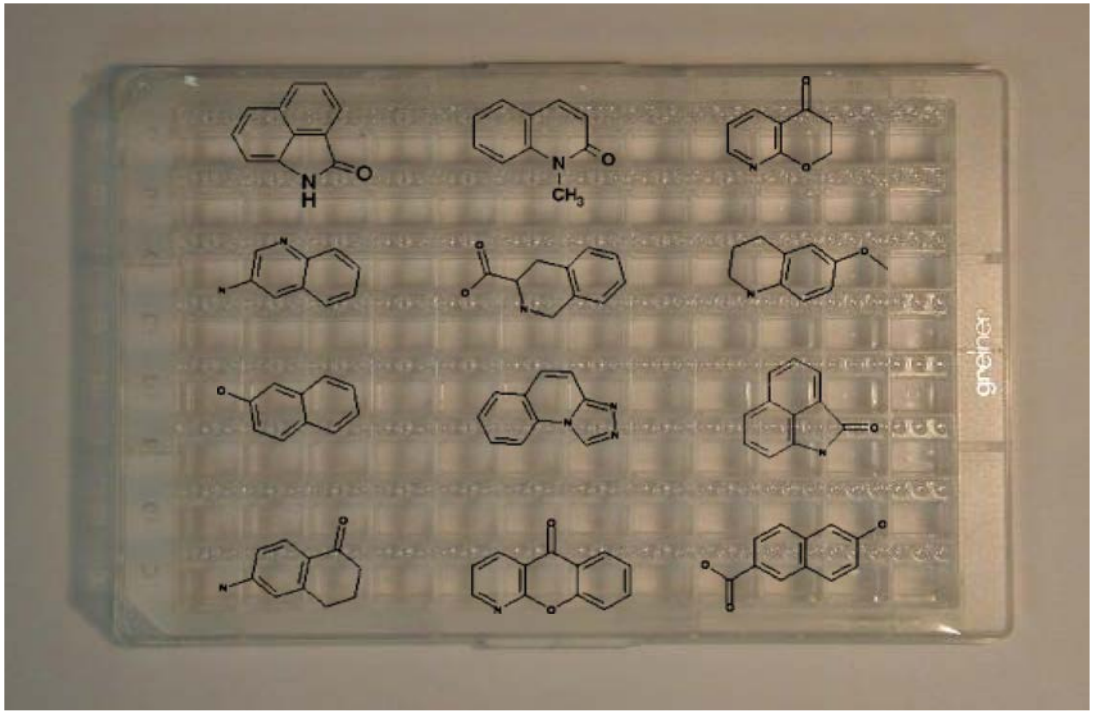
2fo-fc (blue) 0.9 sigma

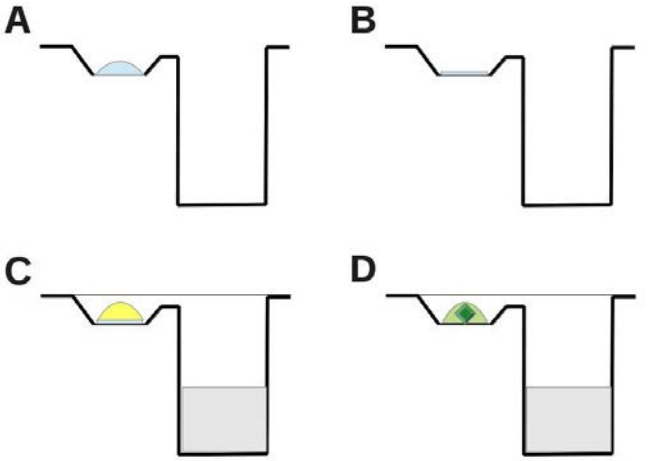
Collab. G. Labesse, CNRS/CBS (Montpellier)

In situ X-ray FBDD

- **Plates pre-coated with a fragment library (100-400 fragments)**
- **Same crystallization condition all over the plate**
- ***In situ* screening of crystals**

What will be the best fragment library?





Interest of *in situ* for protein dynamic

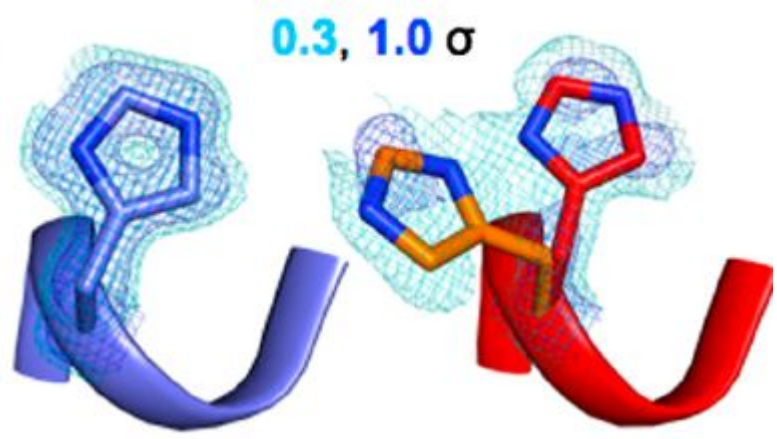
Flash cooling of protein crystals

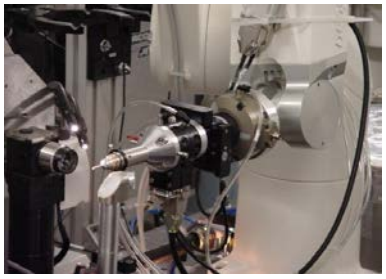
- biases structural collective motions in protein crystals;
- remodels the conformation of > 35% of side chains;
- eliminates packing defects necessary for functional motions;
- induces bias toward smaller, overpacked, and unrealistically unique models.

Instead, **room-temperature** X-ray crystallography experiments, such as the *in situ* experiments, helps in revealing

- motions crucial for catalysis,
- ligand binding,
- allosteric regulation.

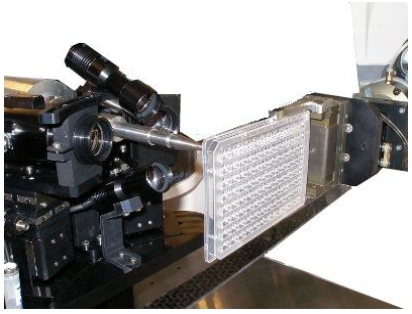
In the signaling switch protein, H-Ras, an allosteric network consistent with fluctuations detected in solution by NMR was uncovered in the room-temperature, but not the cryogenic, electron-density maps (Fraser *et al.*, PNAS, 2011 (108), 16247-52).





Frozen crystals, capillaries, powder

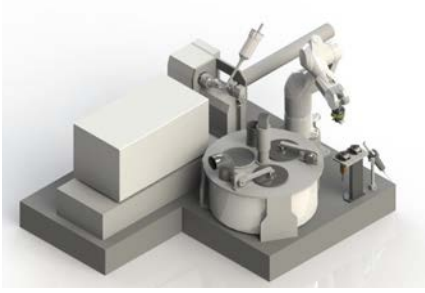
Cryo-sample transfer



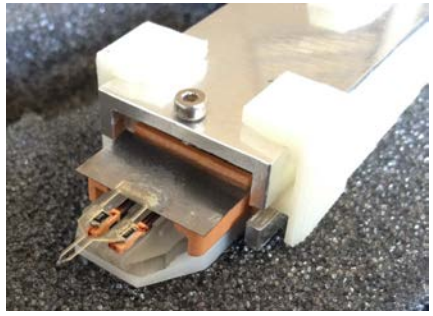
Plates, microchips (*in situ* screening & datacoll.)

Beam monitoring, quick-realign

G-Rob Monitoring



Sample changer



Sample harvesting

Beam monitoring

- fluorescent screen
- diode monitor

Application

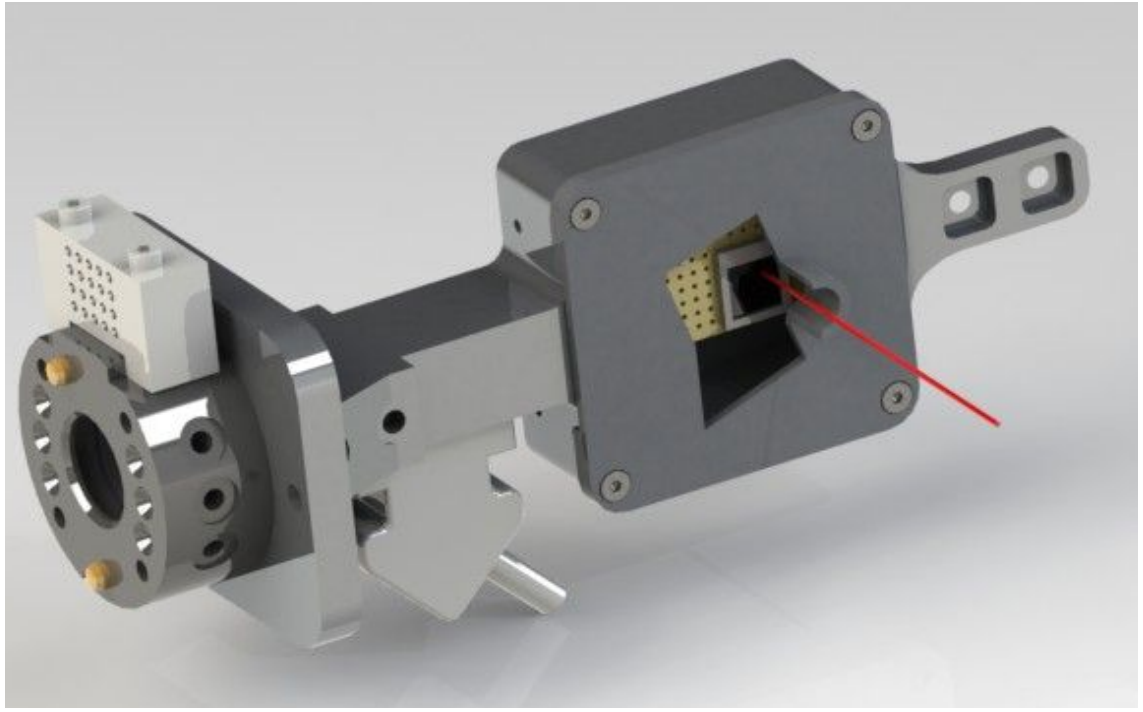
- Check the beam position
- Check the beam intensity
- automated beam optimization (~”Quick Realign”) by users

G-Rob function: Monitor

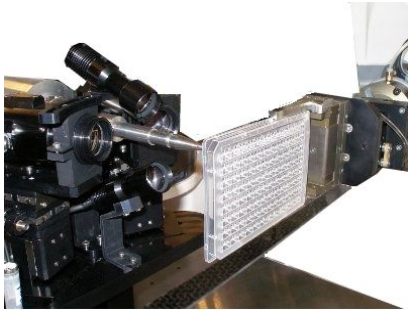
A robot tool for beam monitoring

- A diode for intensity measurement
- A fluorescence screen for beam imaging

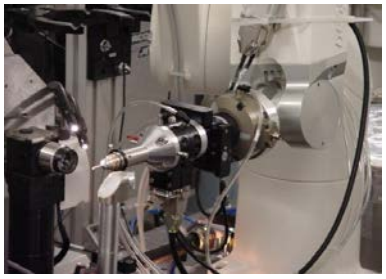
In association with motorized optics ➡ **automated beam alignment**



Cryo-sample transfer



Plates, microchips
(*in situ* screening & datacoll.)

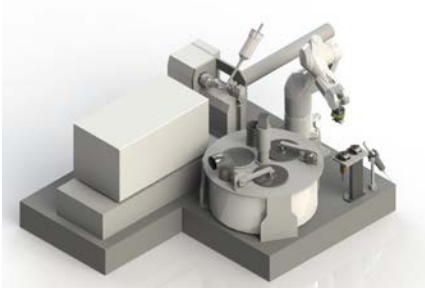


Frozen crystals,
capillaries, powder

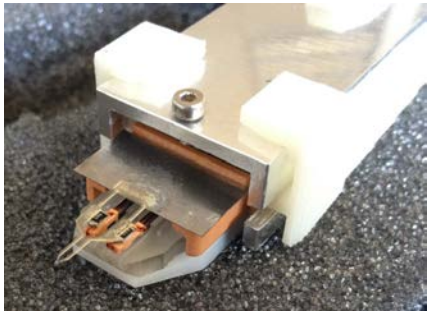
G-Rob Harvesting

(in development)

Beam monitoring,
quick-realign



Sample changer



Sample harvesting

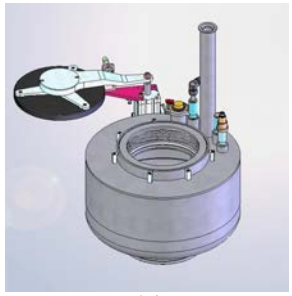
Sample Harvesting

- Semi-automated harvesting
- Remote controlled micro-gripper

Applications

- Remote harvesting
- Crystal freezing

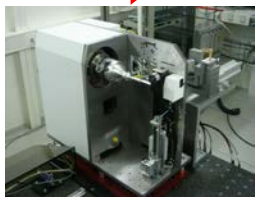
G-Rob Harvesting: a link between 2D and 1D

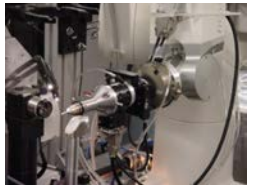


G-Rob SC

cryo-transfer

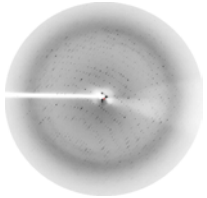
G-Rob 1DT





G-Rob 1D

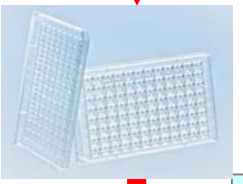
data coll.



G-Rob "Harvest"

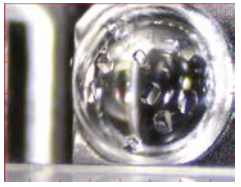
micro-plate transfer

G-Rob 2D



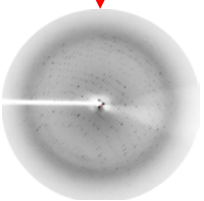
screening

G-Rob 2D

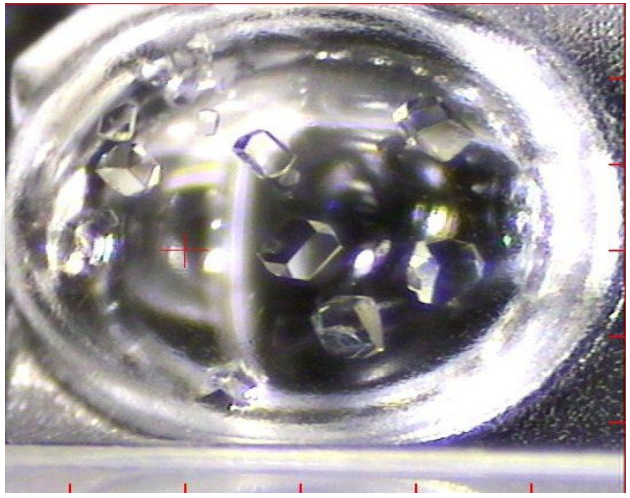


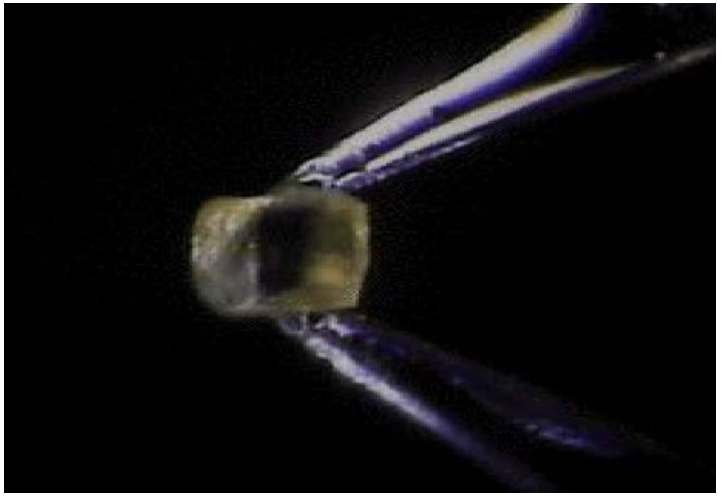
data collection

G-Rob 2D



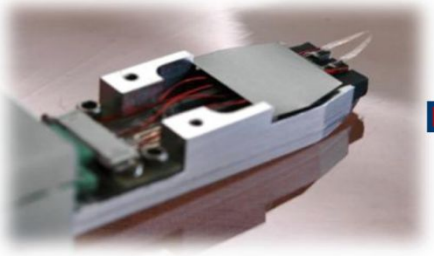
Crystal harvesting



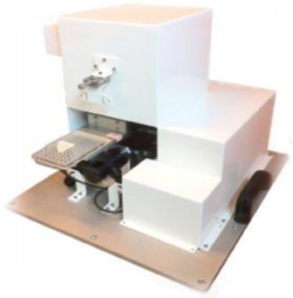


Harvesting…

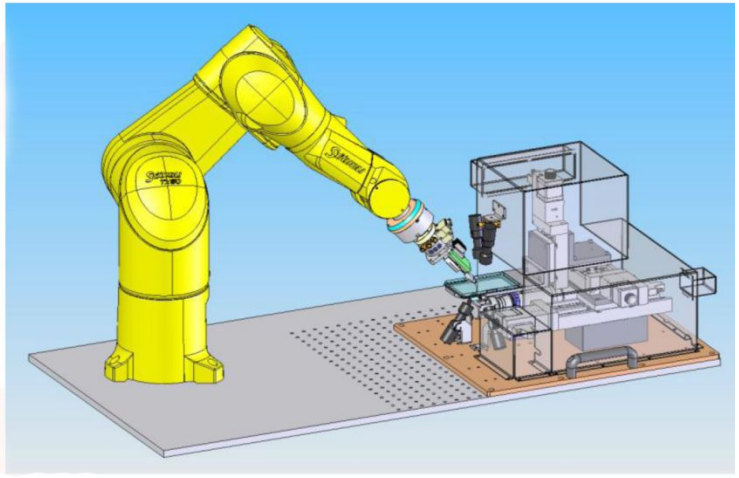
µTweezer



Inverted Microscope



6-Axis Robot

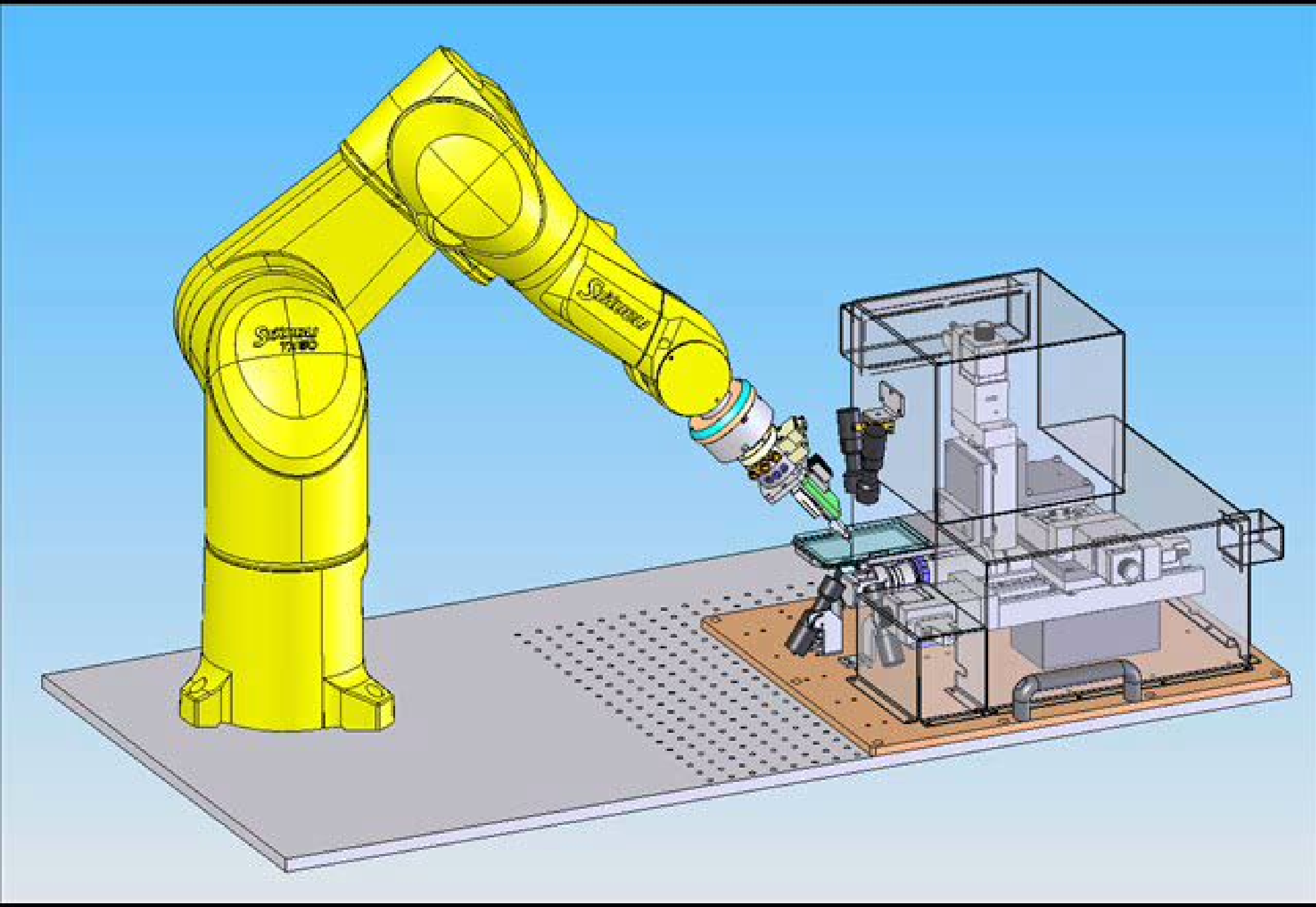


Harvesting

- *Transfer to a loop* → *Freezing* → *Sample storage*
- **Freezing** → **(Direct) data collection**

Manual vs robotic harvesting

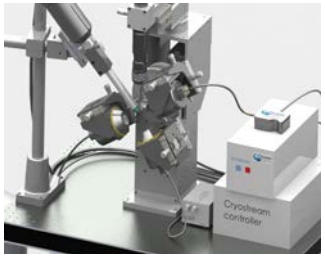
	lysozyme				NikA-FeEDTA			
Data set	**Manual 1**	**Manual 2**	**Robotic 1**	**Robotic 2**	**Manual 1**	**Manual 2**	**Robotic 1**	**Robotic 2**
Data reduction								
Resolution (last shell) (Å)	1.50	1.80	1.75	1.60	2.65	1.85	2.30	1.95
R_{sym} (last shell) (%)	4.9 (37.9)	5.5 (46.4)	8.8 (42.0)	5.8 (42.7)	12.4 (39.2)	4.7 (35.9)	5.6 (33.5)	5.3 (32.9)
I/σ (last shell)	17.2 (3.9)	21.5 (4.1)	10.8 (4.5)	17.7 (3.8)	7.34 (2.92)	19.23 (4.40)	16.68 (4.35)	16.45 (4.51)
Mosaicity	0.247	0.401	0.331	0.376	0.190	0.317	0.318	0.234
Refinement								
R_{work} (last shell) (%)	18.16 (22.45)	16.90 (21.34)	16.25 (20.0)	17.25 (21.72)	17.40 (22.95)	17.53 (27.20)	18.51 (25.34)	17.17 (25.63)
R_{free} (last shell) (%)	20.21 (25.77)	21.61 (26.09)	19.74 (27.11)	19.37 (22.08)	26.91 (33.81)	21.55 (32.57)	25.47 (35.85)	21.65 (31.81)



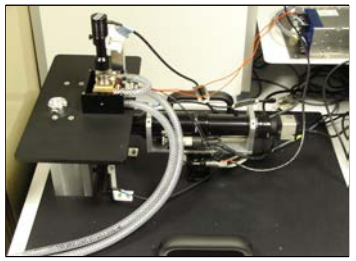

DELL

3 – Peripheral equipments

VisuBench & Crystal-Listing



Misc



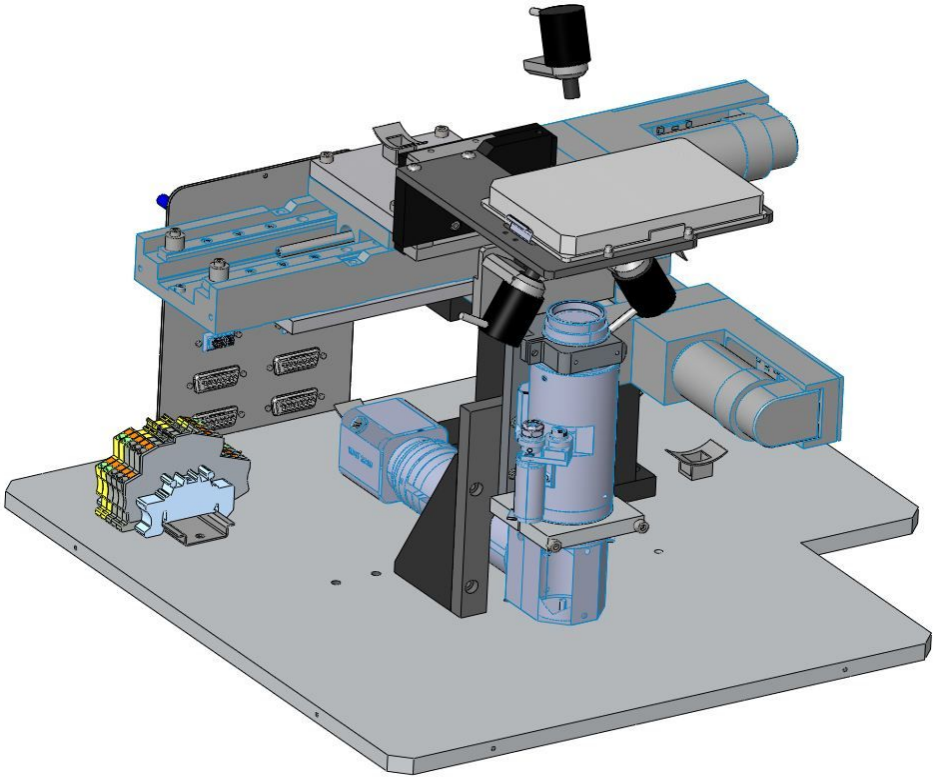
OptiCryst

The Visualization Bench

Beam monitoring
- Inverting microscope
- Crystal Listing

Applications
- Visual screening
- Crystal position recording
- On line: sample harvesting

Visualization bench

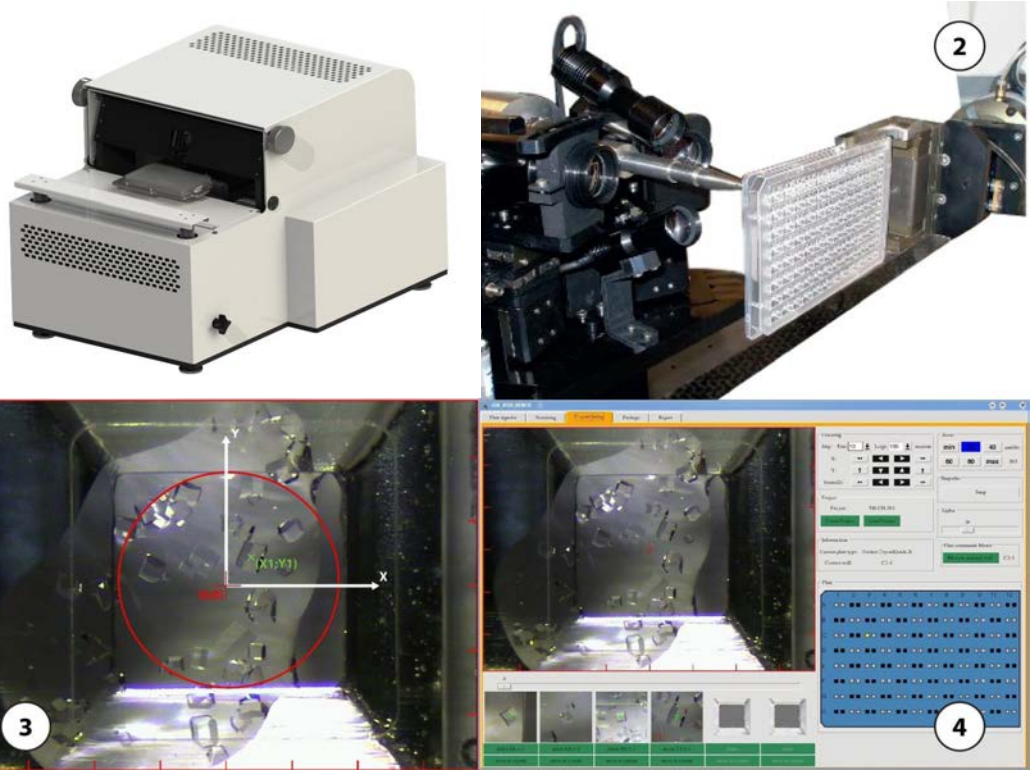


Fully motorized inverted miscroscope designed for the analysis of micro-plates.
Equipped with motorized zoom, front and back LEDs for sample lightening.
Controlled through a user friendly graphical interface.

Crystal Listing

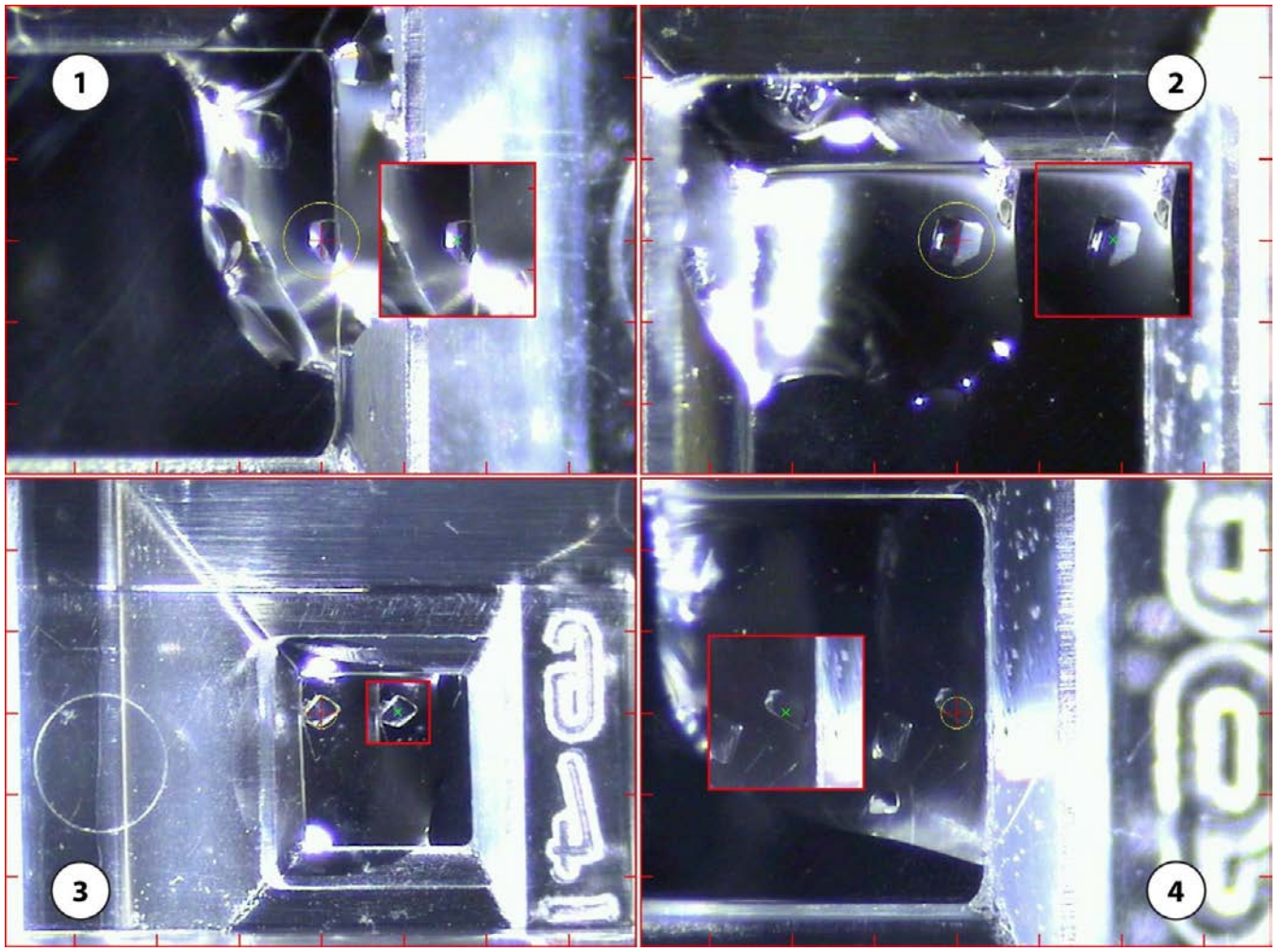
A dedicated microscope can be used off-line for
-Automated image recording
-Selection of crystals (one click)

→ Position of crystals recorded in a local coordinate reference
→ Data uploaded to the G-Rob database for automated screening



① Visualization Bench
② *In situ* X-ray diffraction with G-Rob
③ Automatically centered well with crystal coordinates in the local reference
④ Crystal Listing tab in Visualization Bench GUI

Crystal Listing

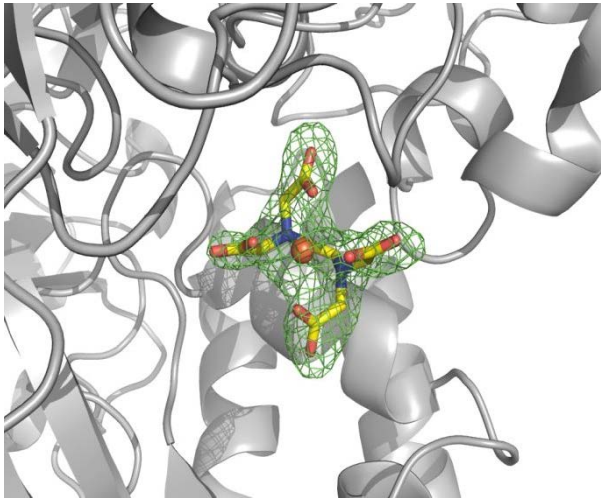


The four examples show small images of 500 µm x 500 µm
saved during the Crystal Listing procedure with G-Rob
and bigger images are taken after crystal centering with G-Rob.
① and ② correspond to NikA-FeEDTA crystals. ③ and ④ are lysozyme crystals.
These images correspond to crystals diffracted and used for structure resolutions.

Listing on:	Visualisation bench	G-Rob
Number of samples	44	79
<|X|> error (µm)	33	3
<|Y|> error (µm)	21	3
<|radius|> error (µm)	41	5
X standard deviation (µm)	17	2
X standard deviation (µm)	14	2
radius standard deviation (µm)	17	3

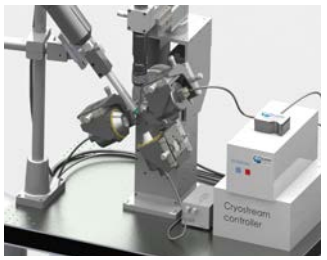
Experiments performed on the
in-house G-Rob system
of the the EPFL crystallography platform
(Prof. S. Cole laboratory, Lausanne).

	Lysozyme	NikA-FeEDTA
Data collection		
Resolution (last shell) (Å)	2.10	2.45
Completeness (last shell) (%)	71.6 (75.0)	68.4 (71.4)
R_{sym}[a] (last shell) (%)	13.9 (38.5)	13.8 (41.6)
I/σ (last shell) (I)	5.61 (2.75)	4.45 (2.20)
Refinement		
R_{work}[b] (%)	18.82	17.39
R_{free}[c] (%)	23.11	25.07

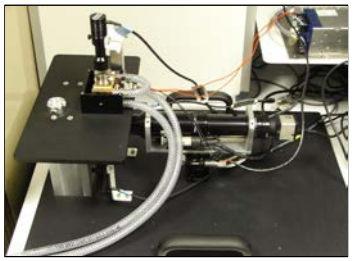


Fe(III)-EDTA binding site in NikA.
Omit Fourier electron density map
of Fe-EDTA contoured at 3 sigma

VisuBench & Crystal-Listing



Misc



OptiCryst

MiSC: a MicroSpectroPhotometer

MiSC

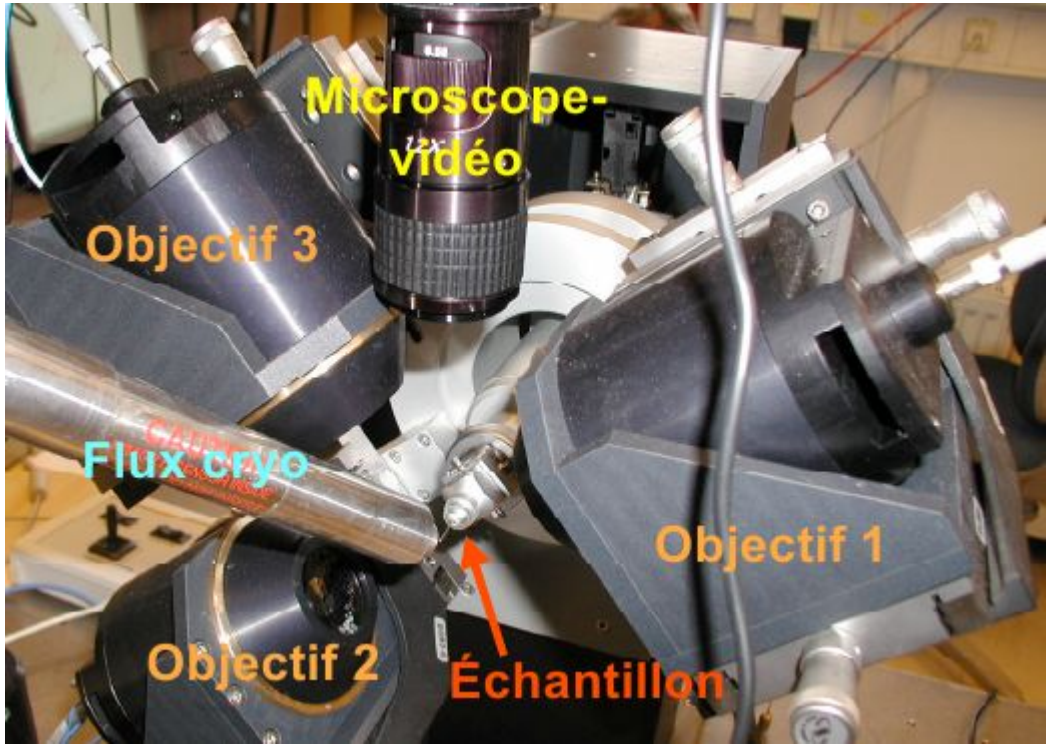
- Goniometer + microscope + cryo-cane
- Reflective optics
- Spectrometer

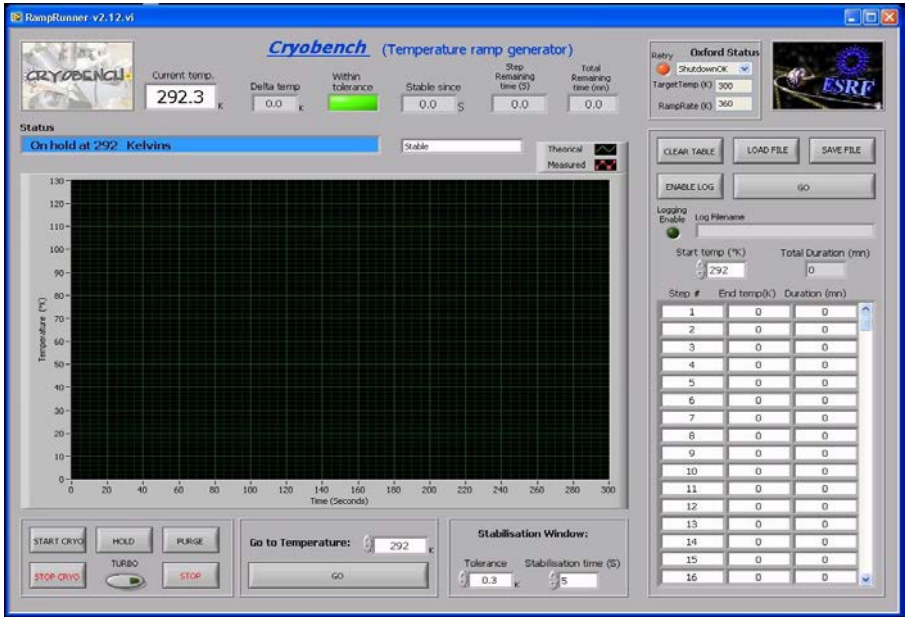
Applications

- Fluorescence measurements
- Absorption measurements
- Synchronized experiment

The CryoBench at the ESRF

(A. Royant team at IBS – ESRF/ID29)



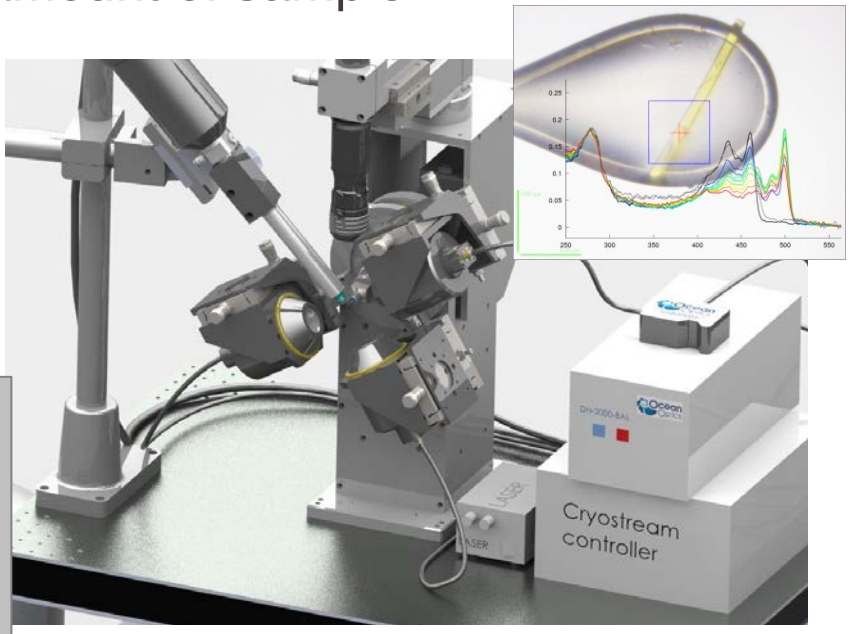


D. Bourgeois, X. Vernede, V. Adams, E. Fioravanti & T. Ursby (2002). "A microspectrophotometer for UV-visible absorption and fluorescence studies of protein crystals." J. Appl. Cryst. 35, 319-326.

MiSC

A Micro-Spectrophotometer for Crystals

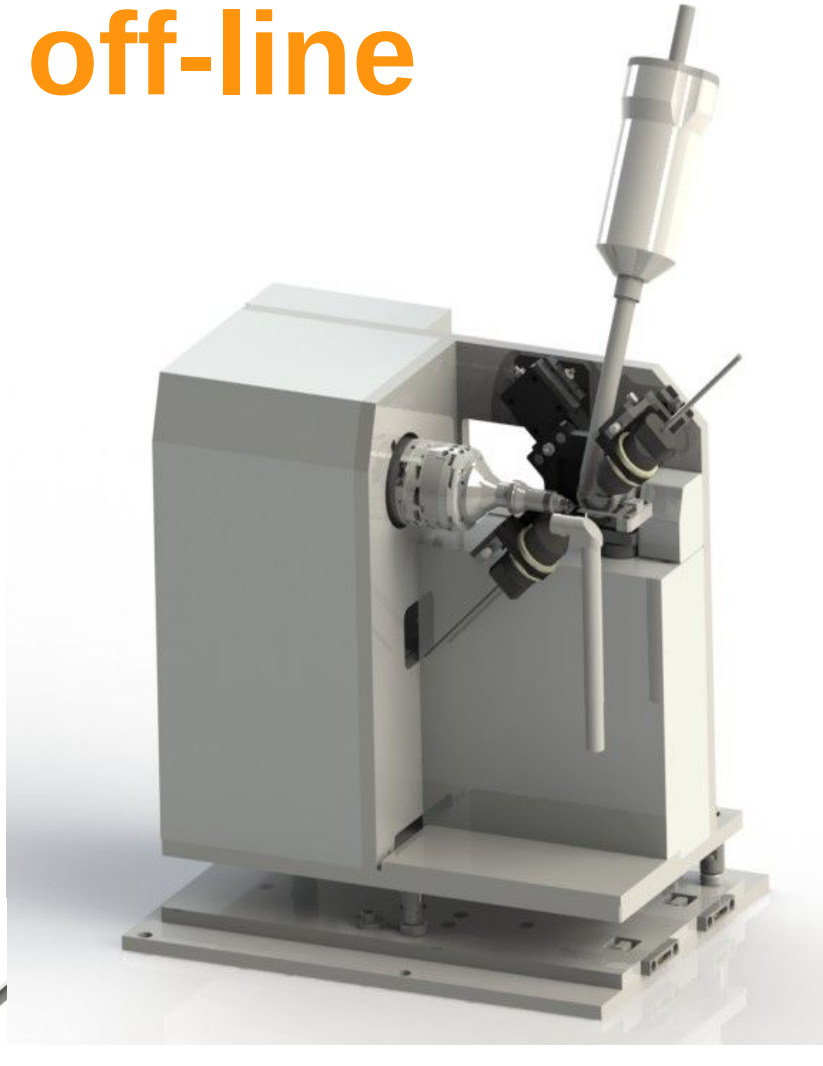
- **UV/Visible absoption**, measured on the 200-1100 nm range
- **Fluorescence measurements** at 90° on micro-amount of sample
- **Samples can be:**
  - Crystal down to 10 µm
  - Nanoliters solutions
- **Spectrometer :** 200-1025 nm range

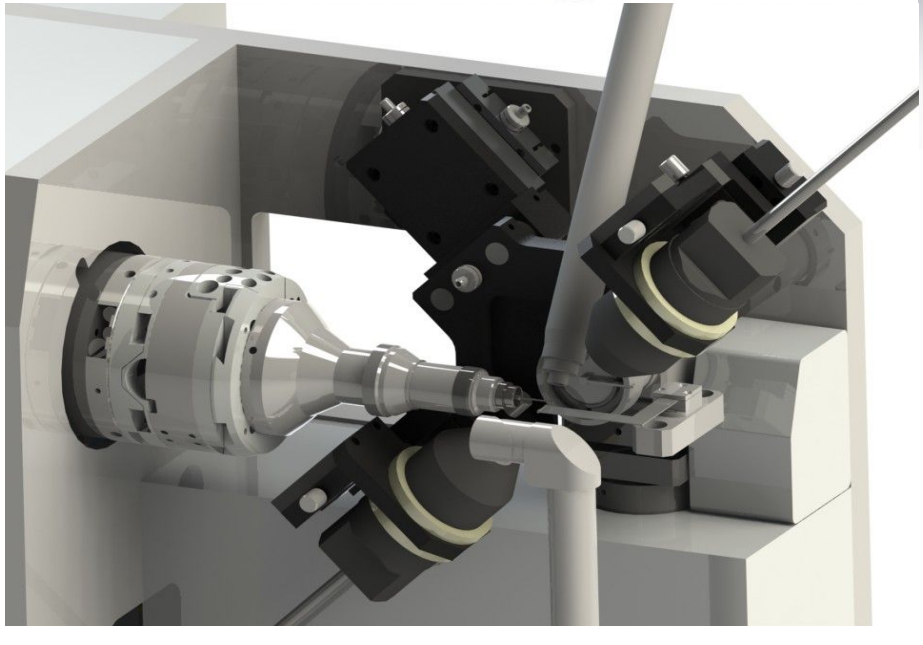


Based on the CryoBench (IBS & ESRF/ID29)
Stand alone version
commercialized by NatX-ray
As a G-Rob function
Under development

- **Absorption source**: 210-1700 nm UV-NIR deuterium/tungsten source
- **Fluorescence source**: 455 nm LED source or 473 nm SS laser
- **Source/measurement optics**: 4X Reflective objectives
- **Sample holder**: 2-axis gonio head (crystals), cuvette holder (solutions)
- **Sample visualization**: with video microscope
- **Polarizer, optical fibers**

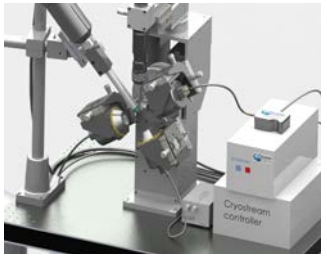
MiSC: on-live *vs* off-line



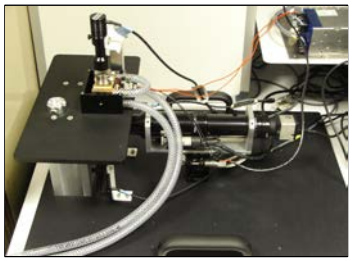


Detector as close as 40 mm
Access for sample changer

VisuBench & Crystal-Listing



Misc



OptiCryst

OptiCryst

OptiCryst: a crystal optimization bench

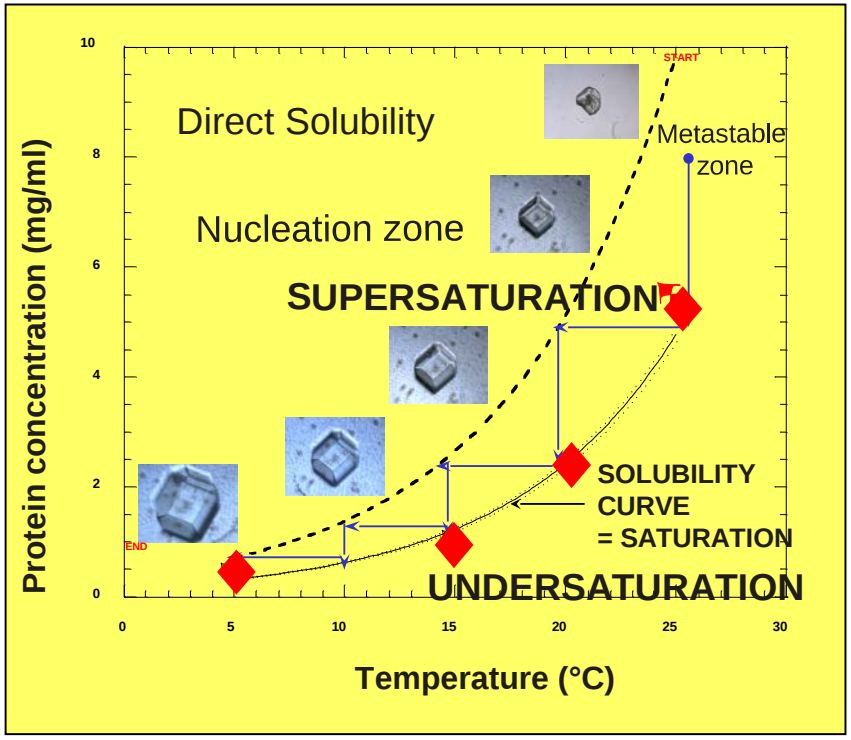
- Inverted microscope
- Temperature control
- Dialysis

Applications

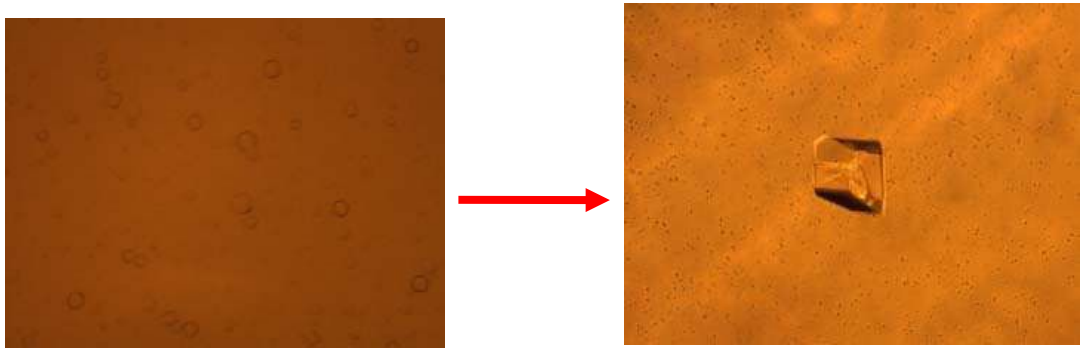
- Crystallization
- Crystal quality improvement
- Size optimization

OptiCryst

A bench for crystals optimization



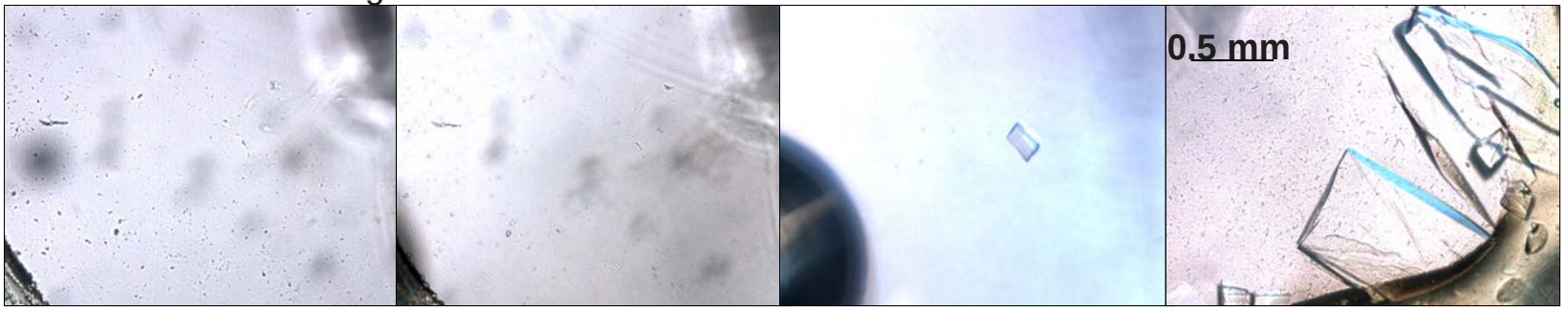
25Pl of protein, prot. Conc. 18 mg/ml
(NH4)2SO4 2M, Bicine 100 mM, pD 8.0, Tinit = 20°C
Crystal nucleation & Growth at 22.5°C



Budayova-Spano et al., Acta Cryst. D63, 2007, 339-347
Oksanen et al., J. Royal Society Interface 6(S5), 2009, S599-S610.

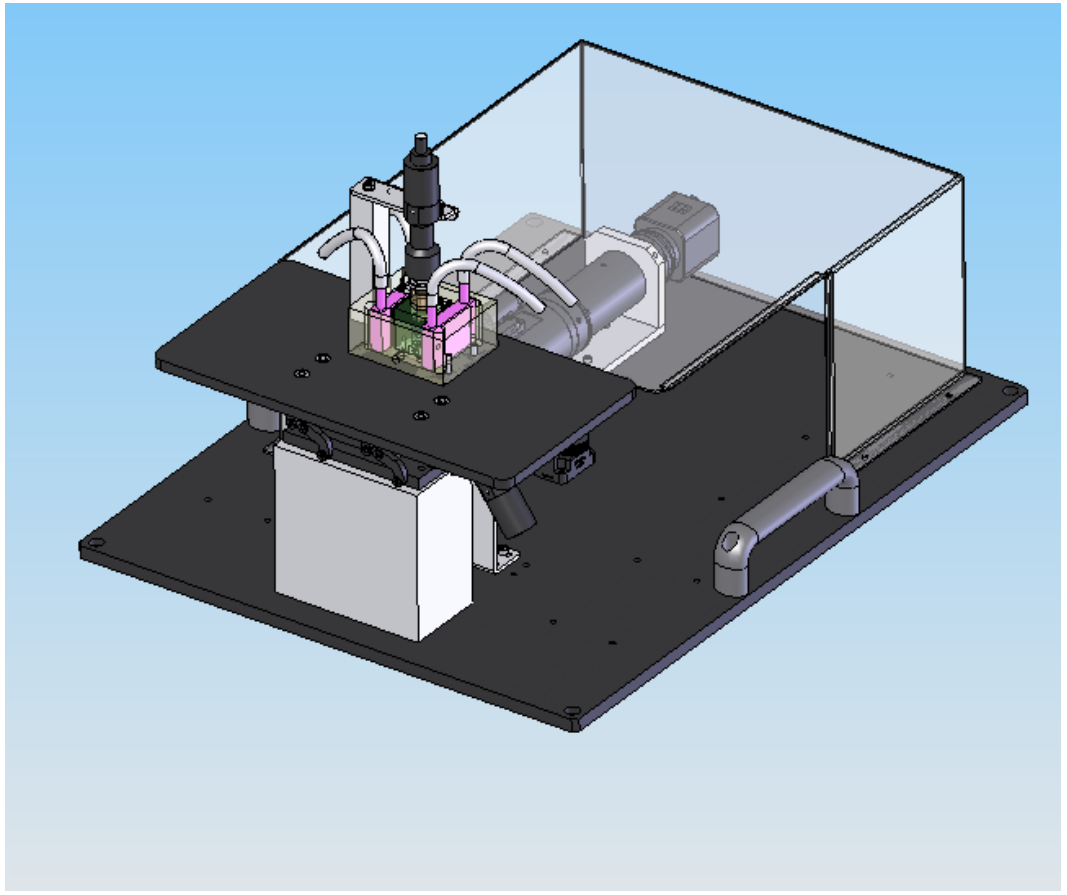
Case of hyperthermophile lactate dehydrogenase

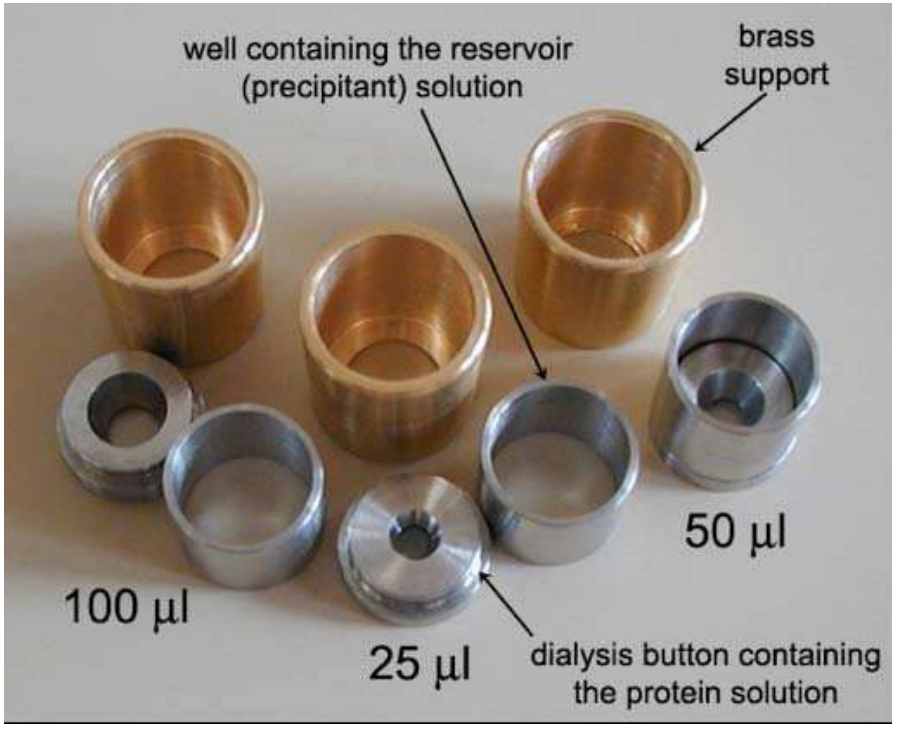
2.5% PEG 6k | gradient: 2.5% to 5% PEG 6k | 5% PEG 6k | 5% PEG 6



OptiCryst

A bench for crystals optimization





4 – Consumables for PX

Consumables & Accessories

- Sample holders, tools, ...
- Phasing compounds
- **Greiner BioOne** products
- **Mitegen** products
- **Crystal Positioning Systems** products
- **Jena Bioscience** products
- **Torrey Pines Scientific** products
- **Taylor-Wharton** and **Air Liquide** products
- **Spearlab** products

greiner bio-one

Taylor-Wharton

Jena Bioscience

MiTeGen

TORREY PINES SCIENTIFIC

Crystal Positioning Systems
A division of Elk Valley Enterprises

Spearlab

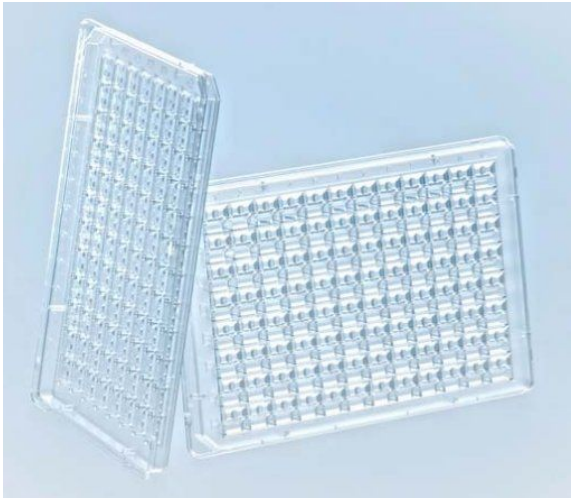
Greiner products

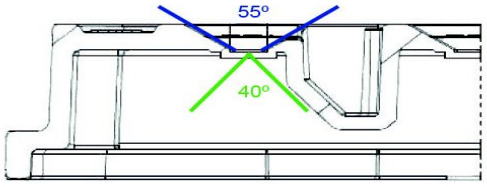
CSM001

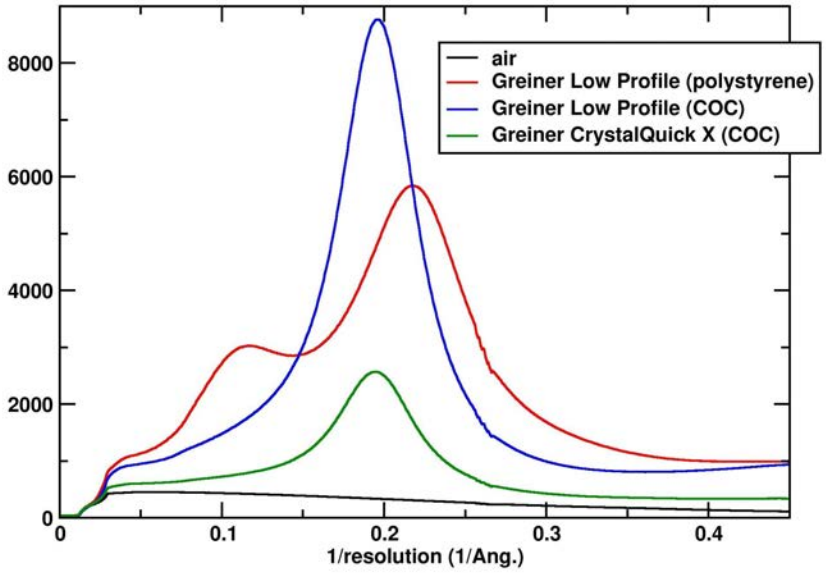
greiner bio-one

CrystalQuick™X plate

- Made with "low birefringence" COC
- 80 degrees of angular range
- Compatible with any crystallization robot
- Reduced bottom thickness
  - 250-300 µm instead of 1000 µm for other plates
  - Lower X or UV scattering
  - Higher brigtness in visible range

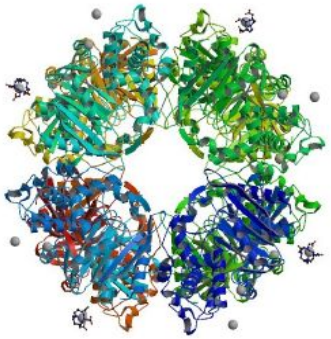




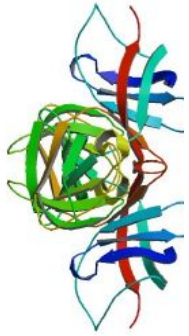


Phasing compounds

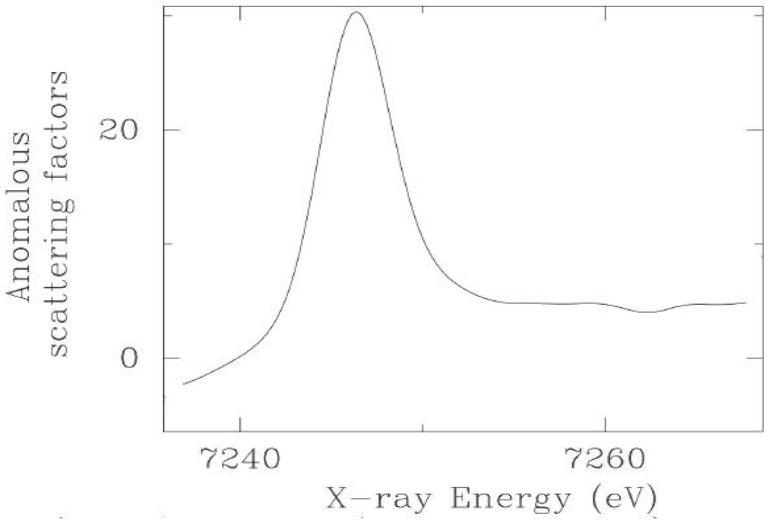
From R Kahn team at the IBS

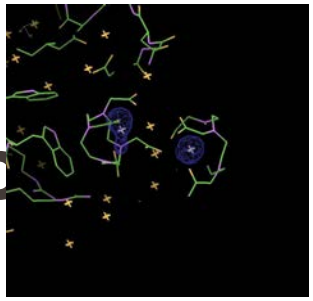


(2qmi)

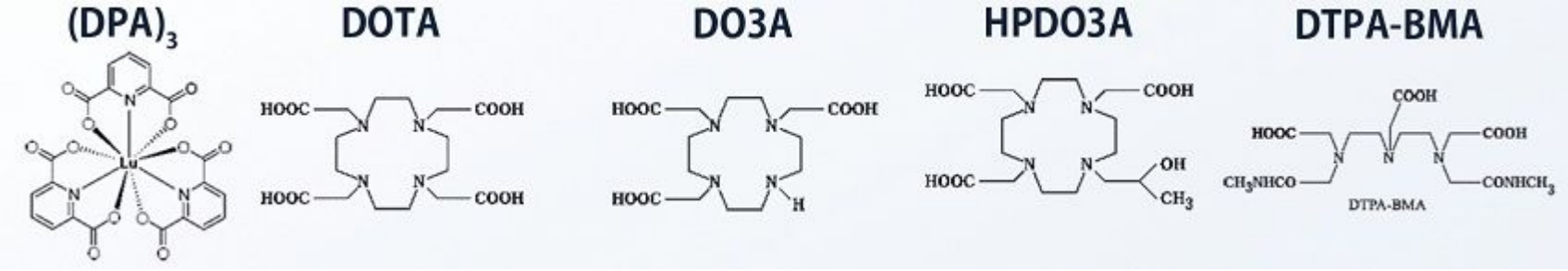


(2bh8)





- **Lanthanide complex for anomalo phasing**
  - HUGE anomalous signal
  - Phasing, even at room temperature
  - Successfully used to solve difficult structures
- **Available molecules**



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Girard E, Stelter M, Vicat J, Kahn R, Acta Cryst. D59 (2003), 1914-1922

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For testing the synchrotron G-Rob system: FIP-BM30A at ESRF, France

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…and the crystallography platform at the EPFL: F. Pojer, S. Cole

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