

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

**J-L Ferrer  
IBS/Synchrotron Group (Grenoble, France)**

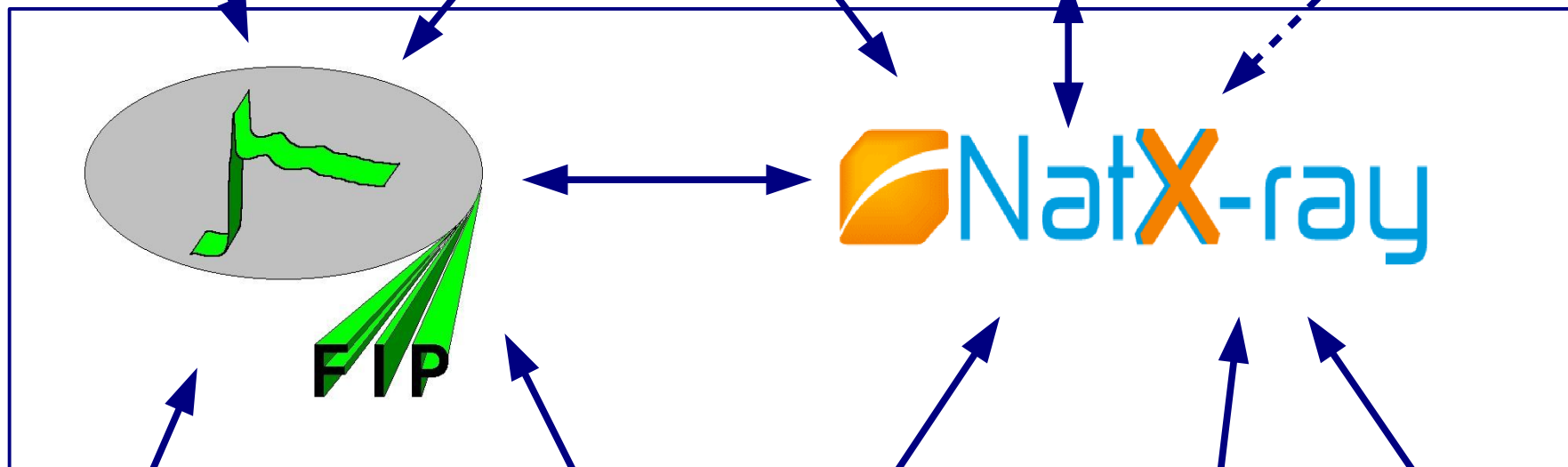
**UT Southwest, October 2013**

**1 – Generalities about G-Rob**

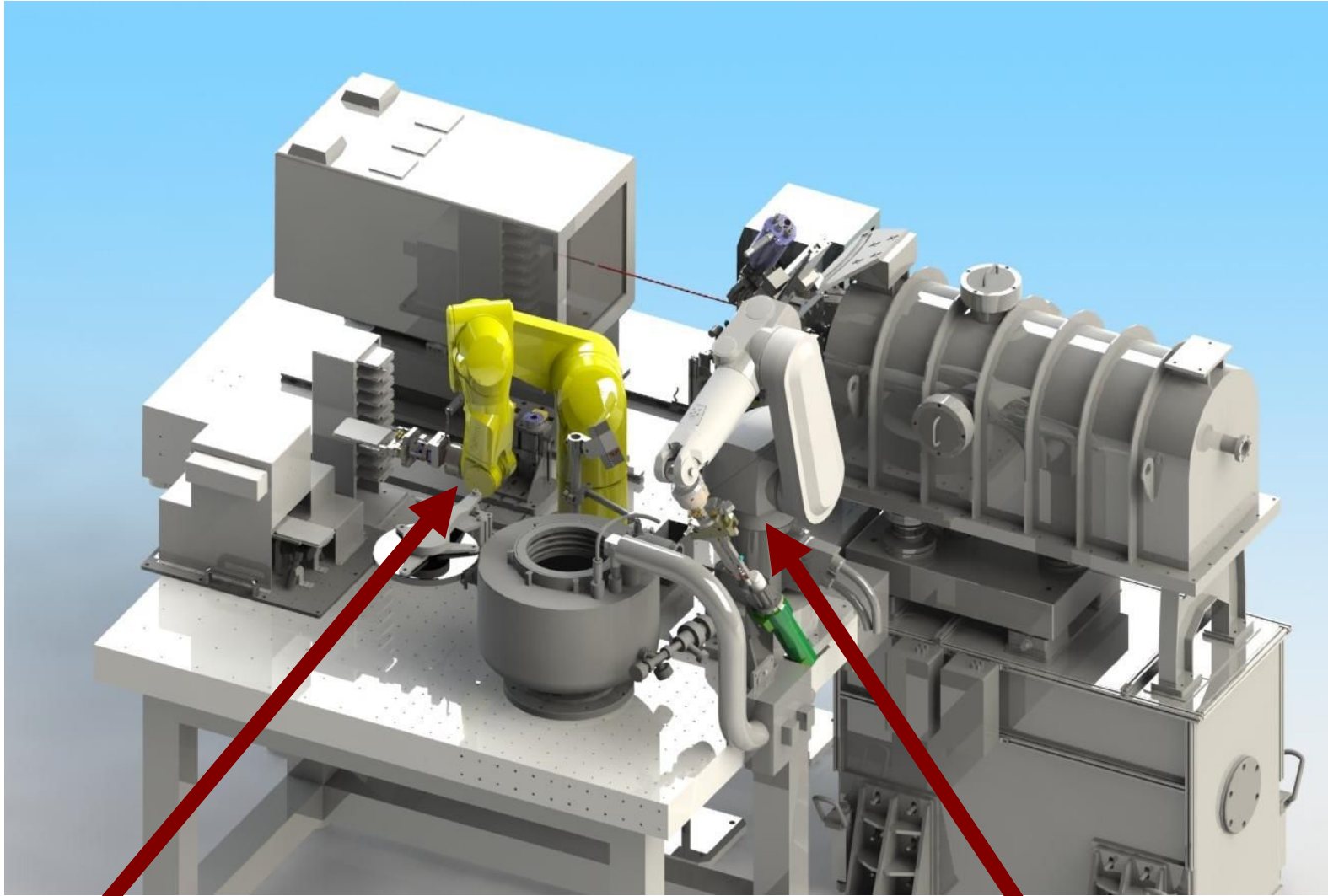
**2 – G-Rob functionalities**

**3 – Peripheral equipments**

**4 – Consumables for PX**



# 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

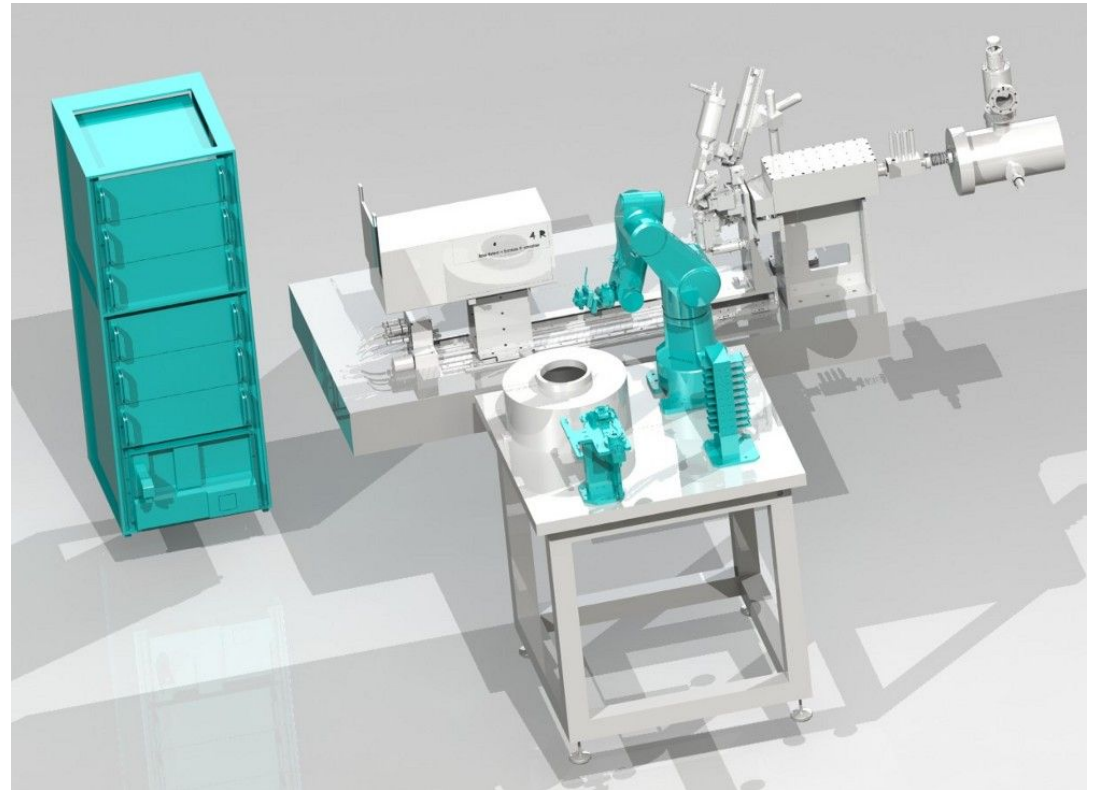
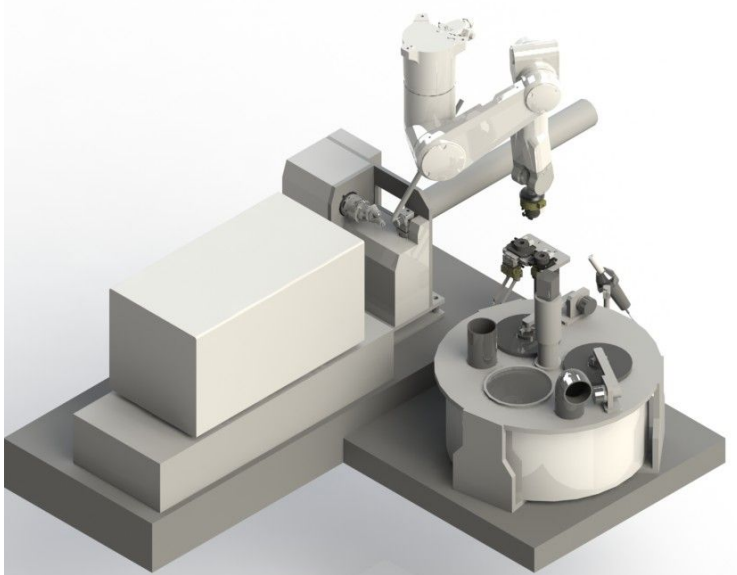
- **automation**: setup reconfiguration, remote control
- **flexibility**: multi-task, evolution, upgrading
- **reliability**: simple, compact, industrial standard
- **new possibilities**: phi data collection, *in situ*, HP...
- **open architecture** (published mechanical interface)

Main limitation: mechanical accuracy

# G-Rob for beamlines

## Usually including

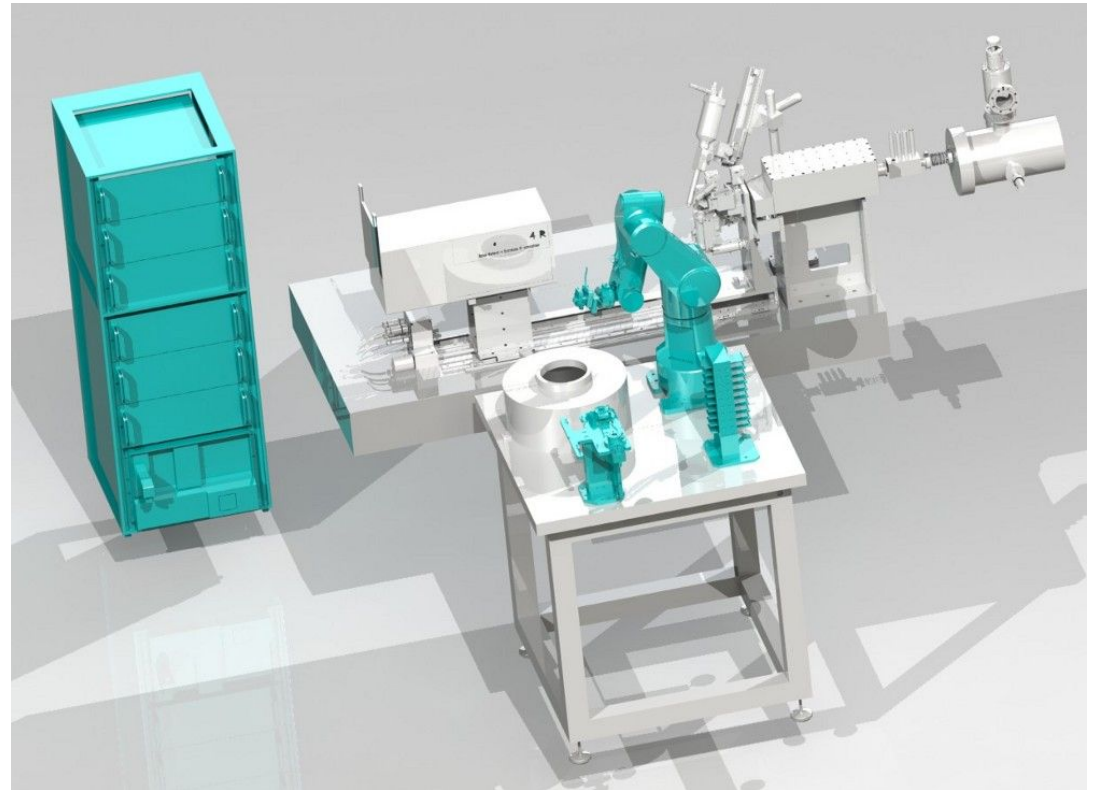
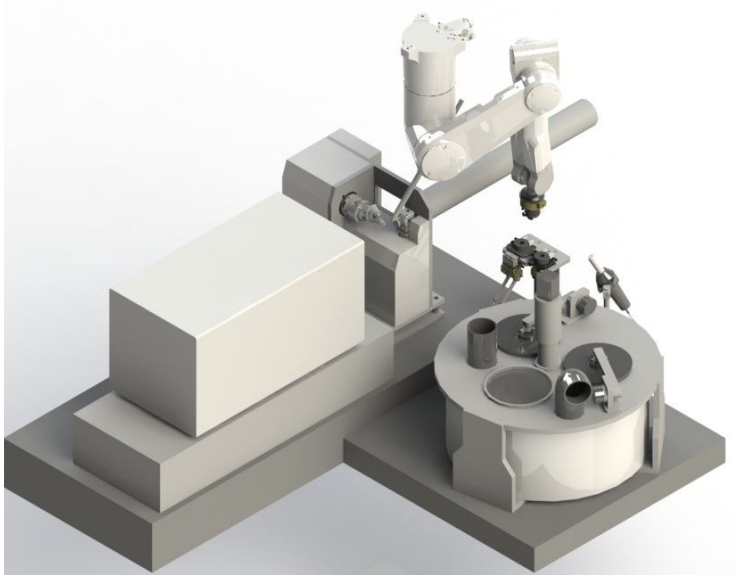
- G-Rob functionalities
- (Sample environment)
- Supporting frame



# G-Rob for beamlines

## Usually including

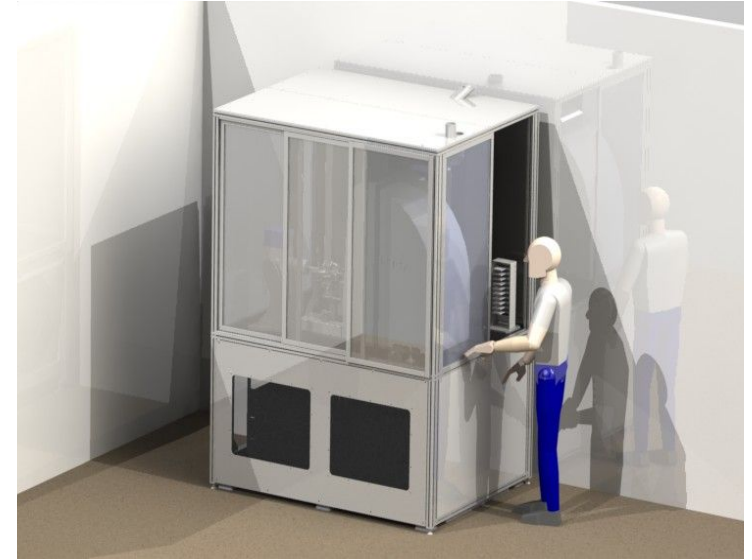
- G-Rob functionalities
- (Sample environment)
- Supporting frame



# G-Rob lab systems

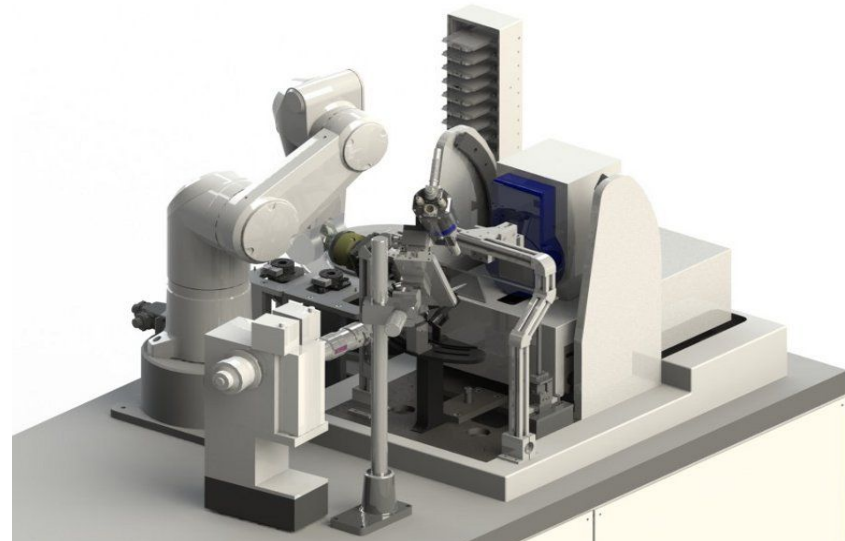
## All-in-One laboratory solution, with

- 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

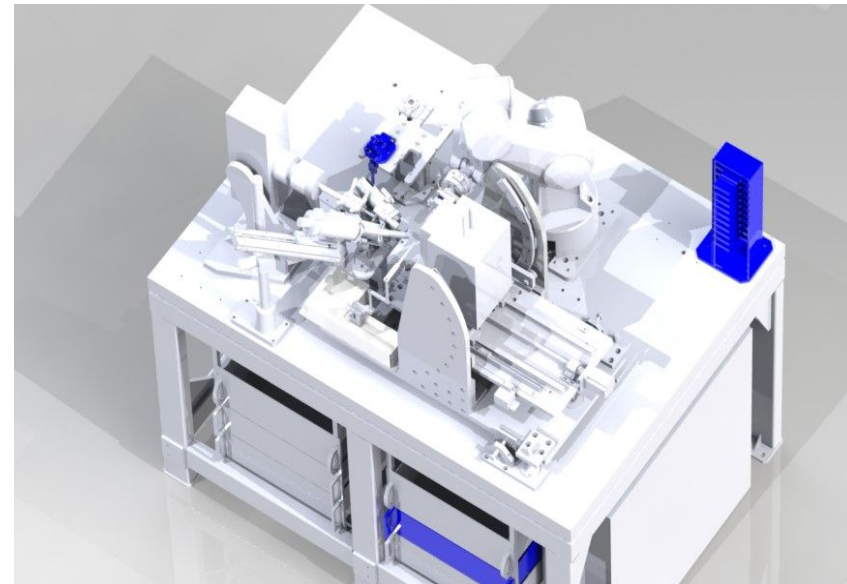
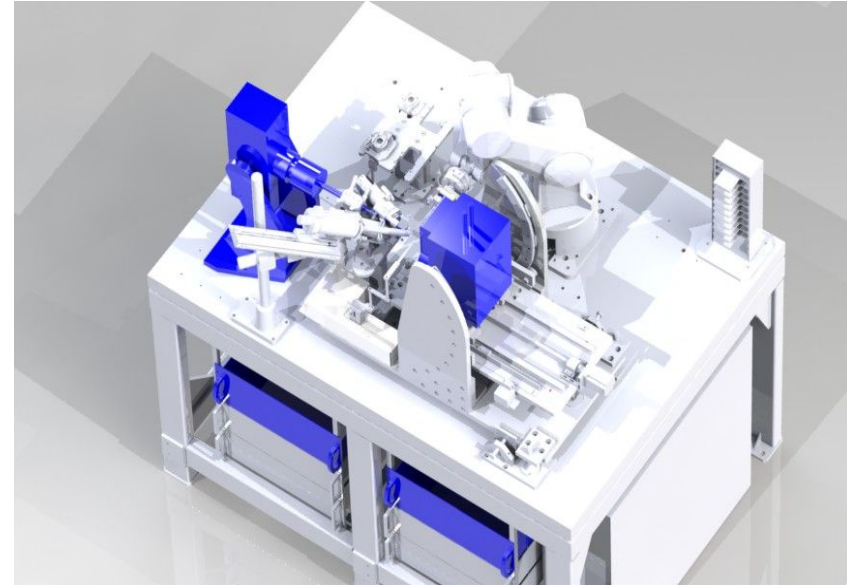
IP, CCD, Solid-State detectors

## A large choice of options

- cryo-cane
- Etc.

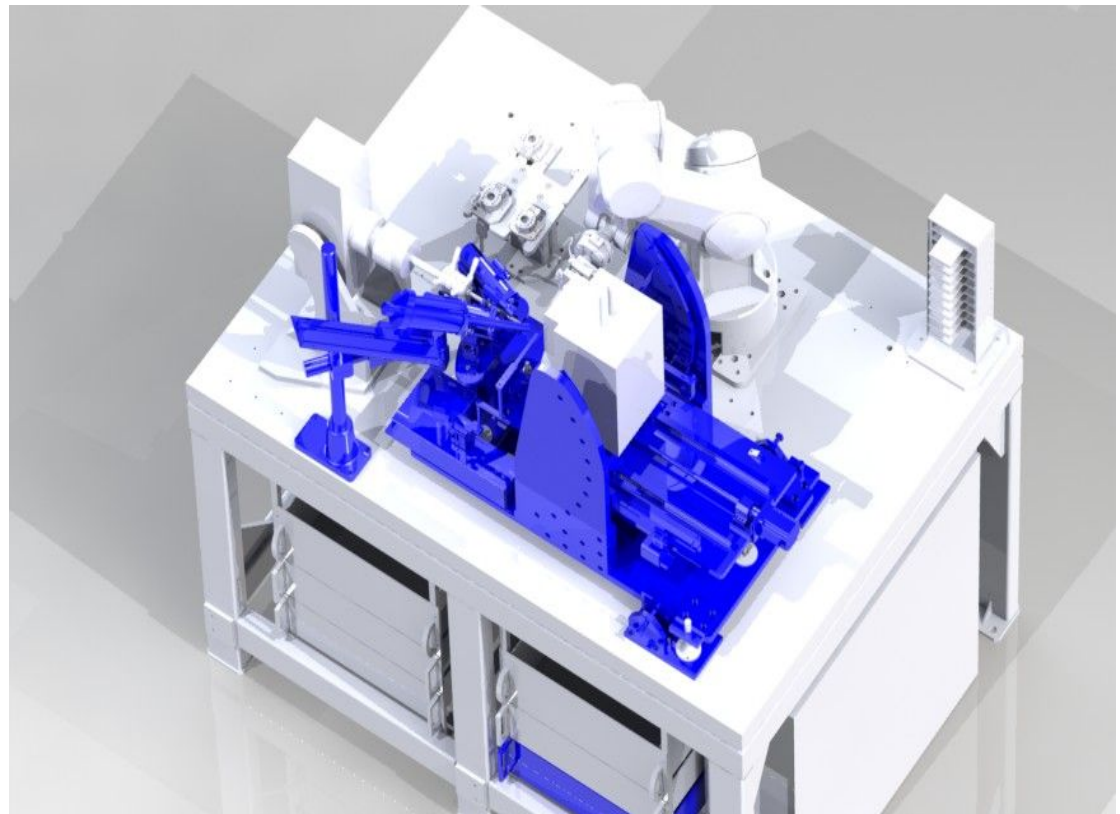
## A choice of G-Rob functionalities

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

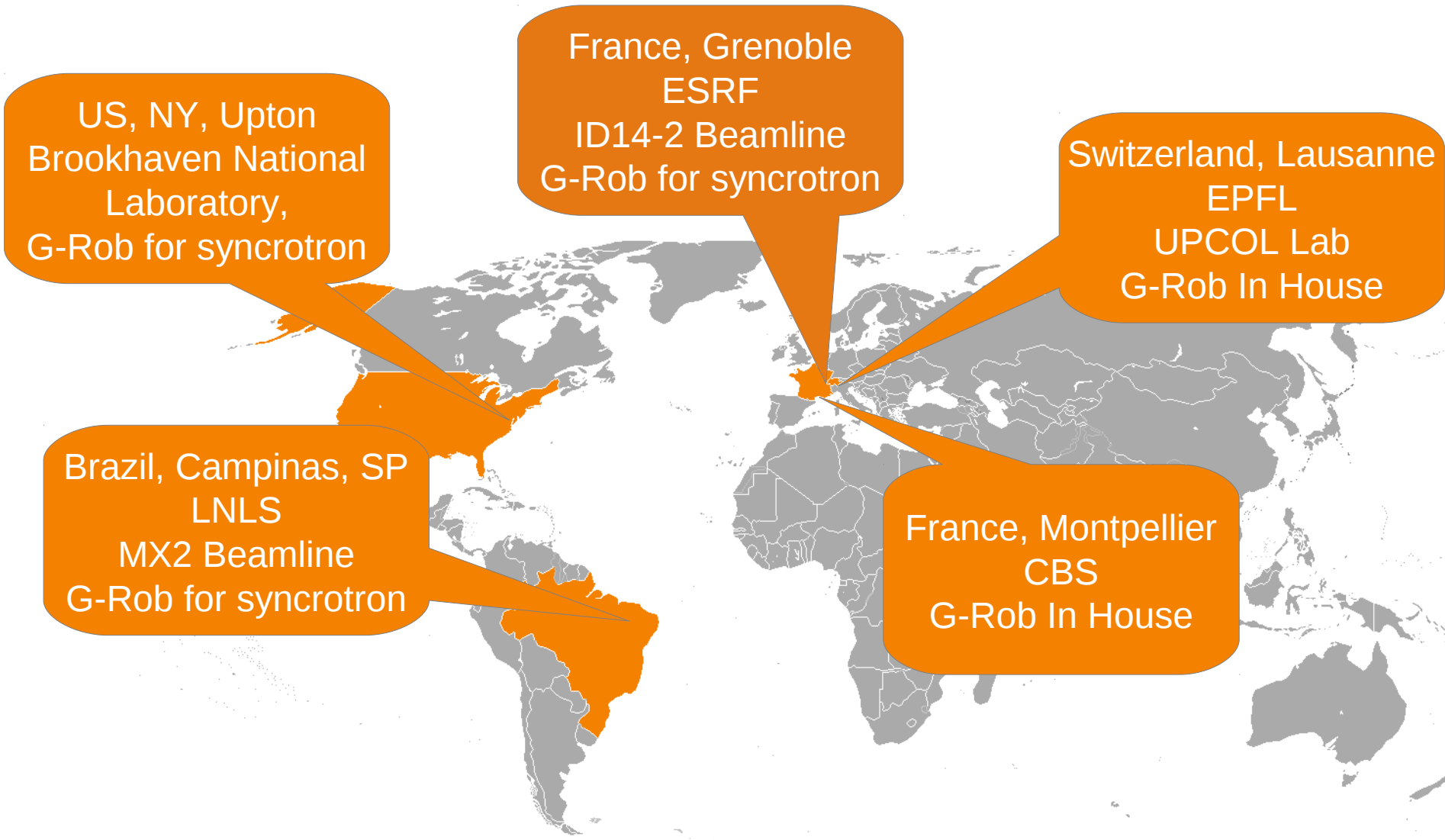


# Sample environment

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

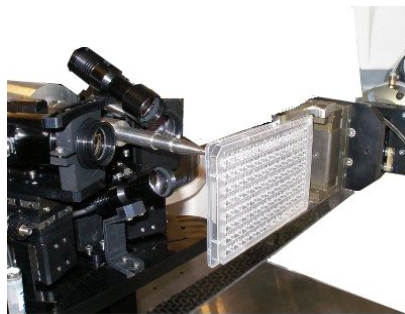


# 5 G-Rob systems in operation

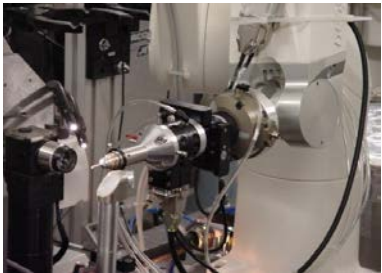




Cryo-sample transfer



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



Frozen crystals,  
capillaries, powder



Beam monitoring,  
quick-realign

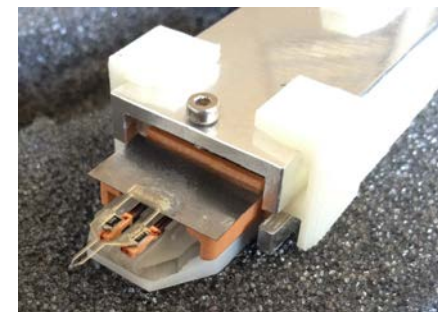
# G-Rob Sample Changer



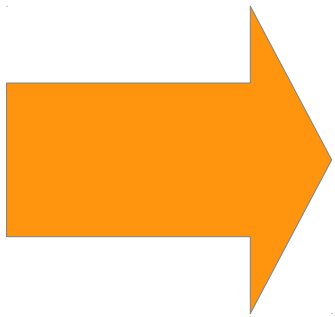
Sample changer

## Cryo-frozen samples transfer

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



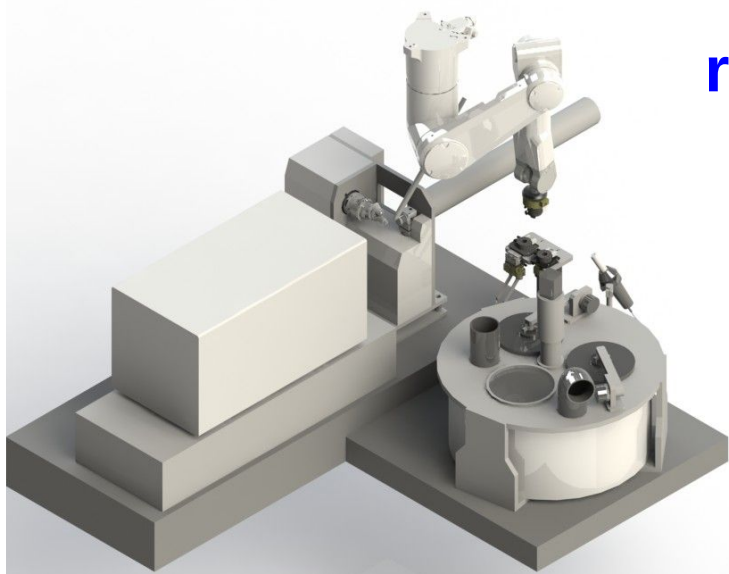
Sample harvesting



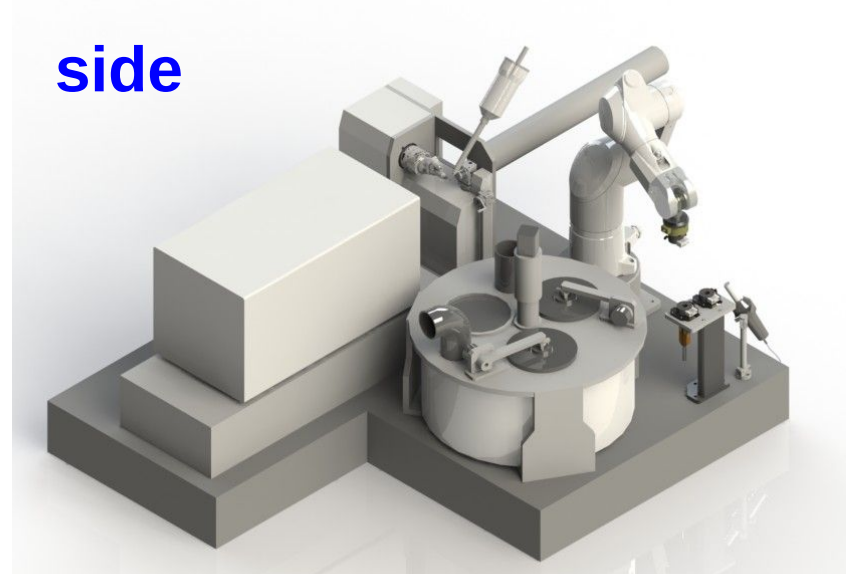
## Applications

- high throughput screening of frozen crystals
- remote controlled experiments

# G-Rob Sample Changer: 2 configurations

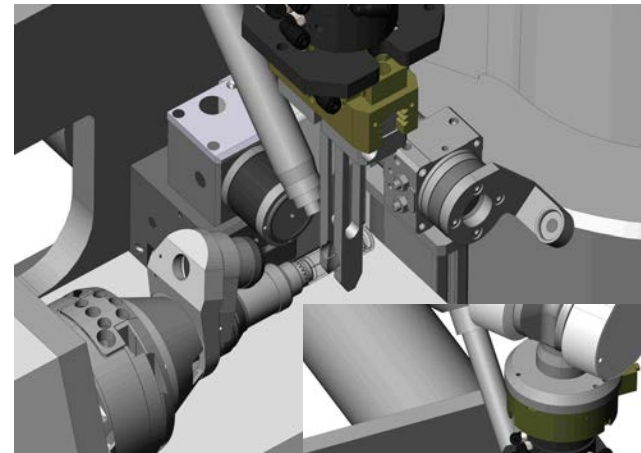
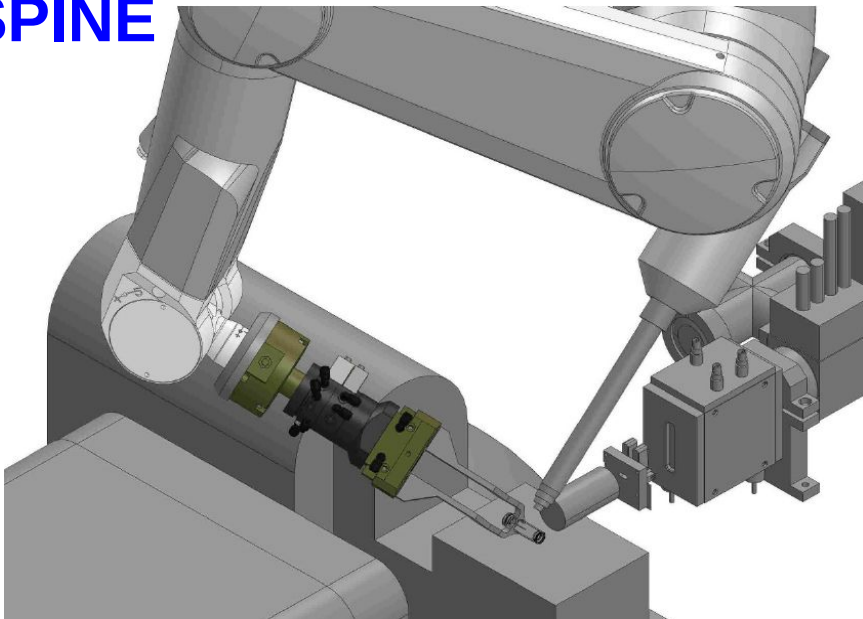


roof



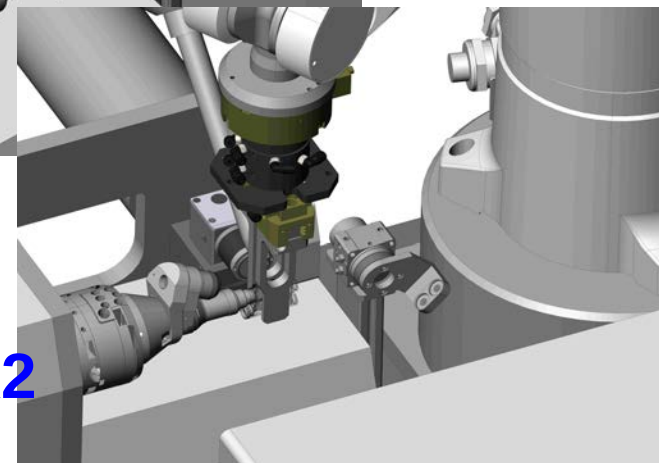
side

SPINE

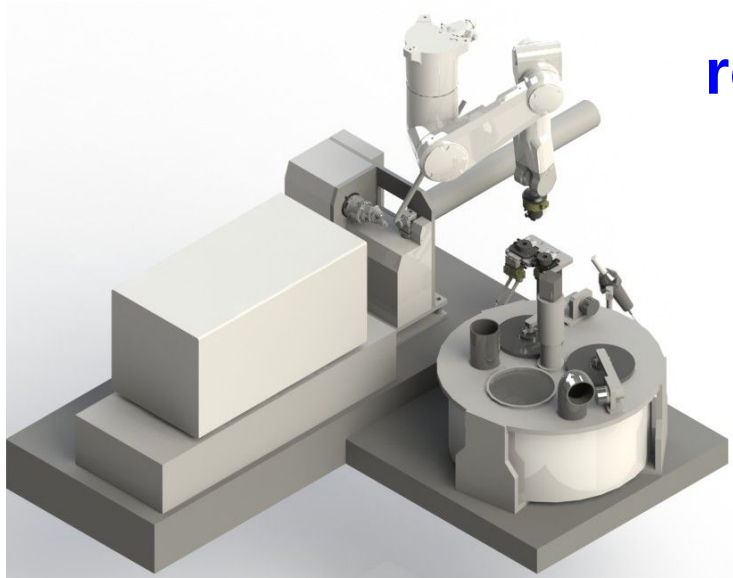


SPINE

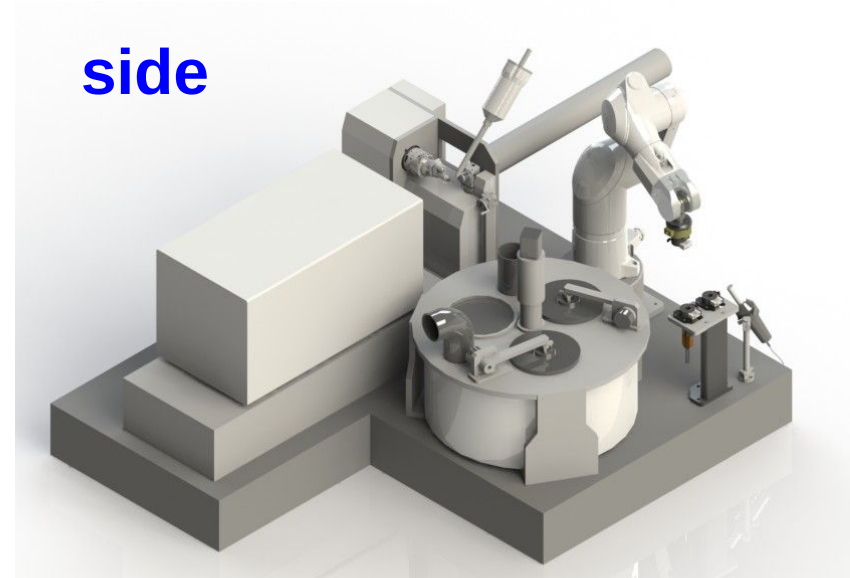
SPINE x2



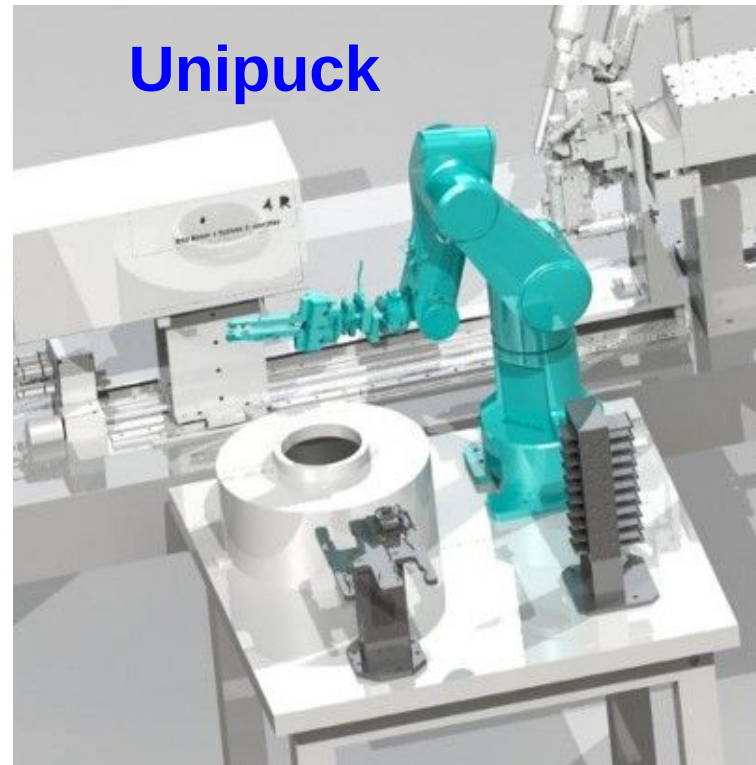
# G-Rob Sample Changer: 2 configurations



roof



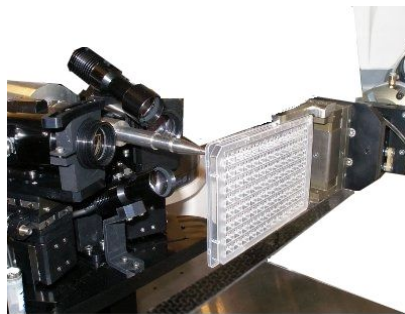
side



Unipuck



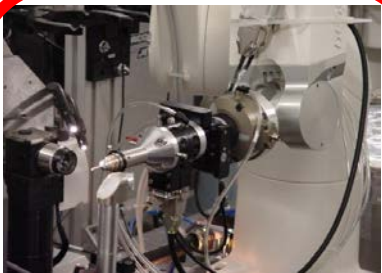
Cryo-sample transfer



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



Beam monitoring,  
quick-realign



Frozen crystals,  
capillaries, powder

# G-Rob 1D/1D+

**a goniometer for single sample**

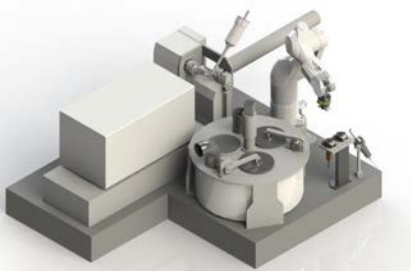
- frozen crystal, capillary

## Applications

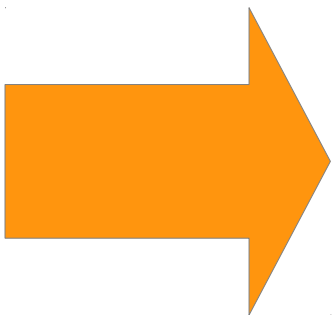
- classical data collection
- shutter-less data collection
- Phi data collection
- powder diffraction



Sample harvesting

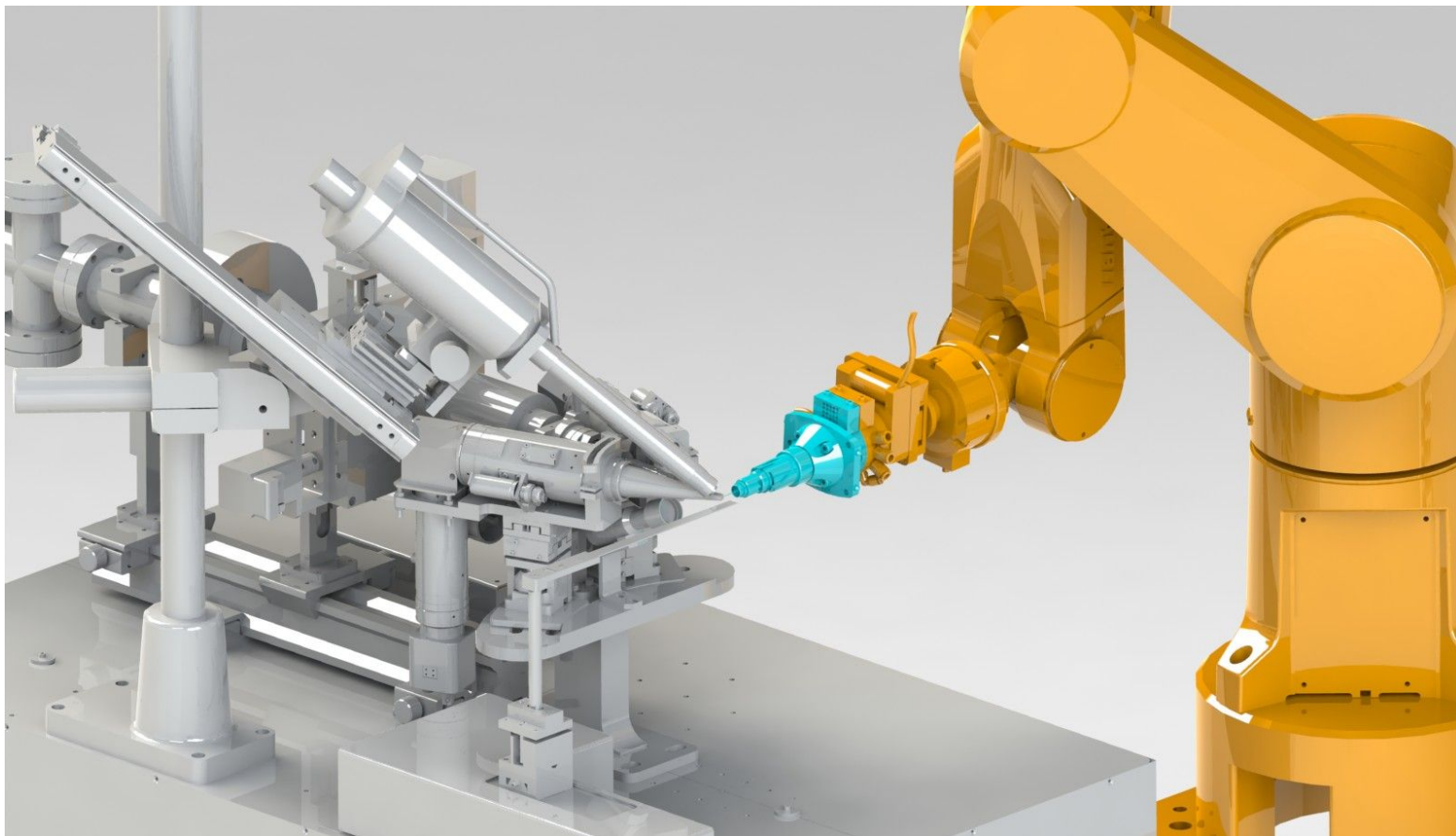


Sample changer



# G-Rob function: 1D

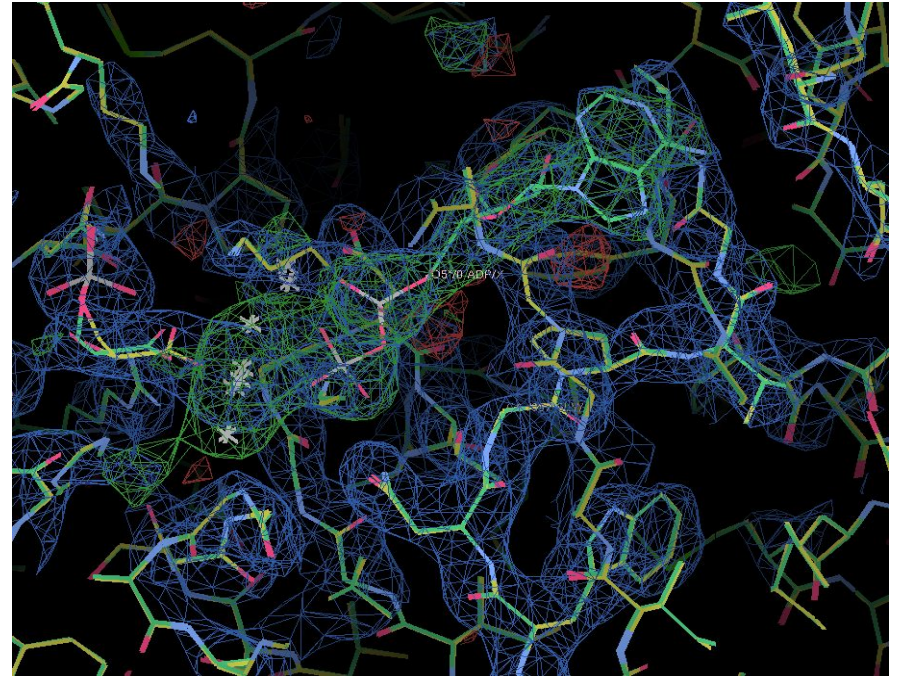
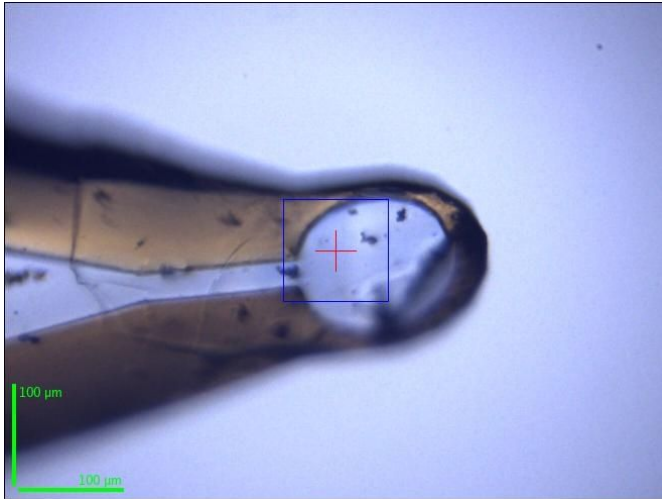
- Goniometer capability
- Validated with beam down to 90  $\mu\text{m}$
- Exposure time as short as 0.1s for 1° oscillation





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

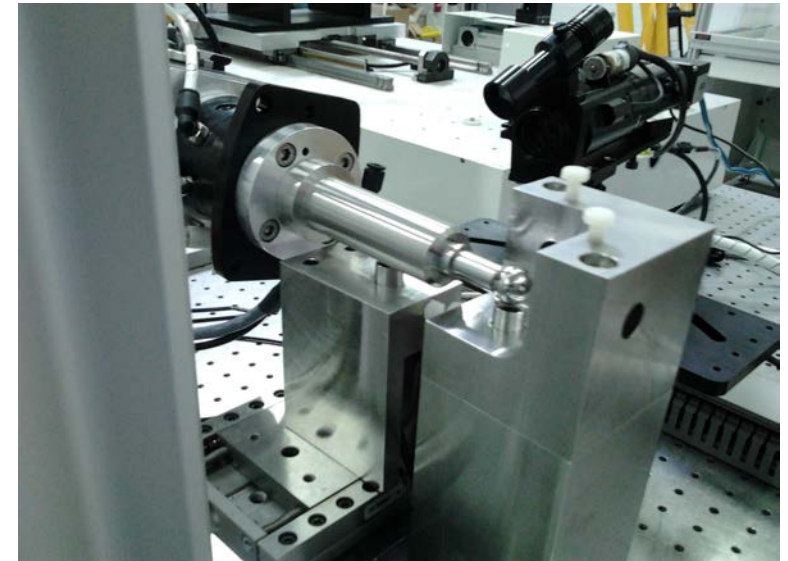
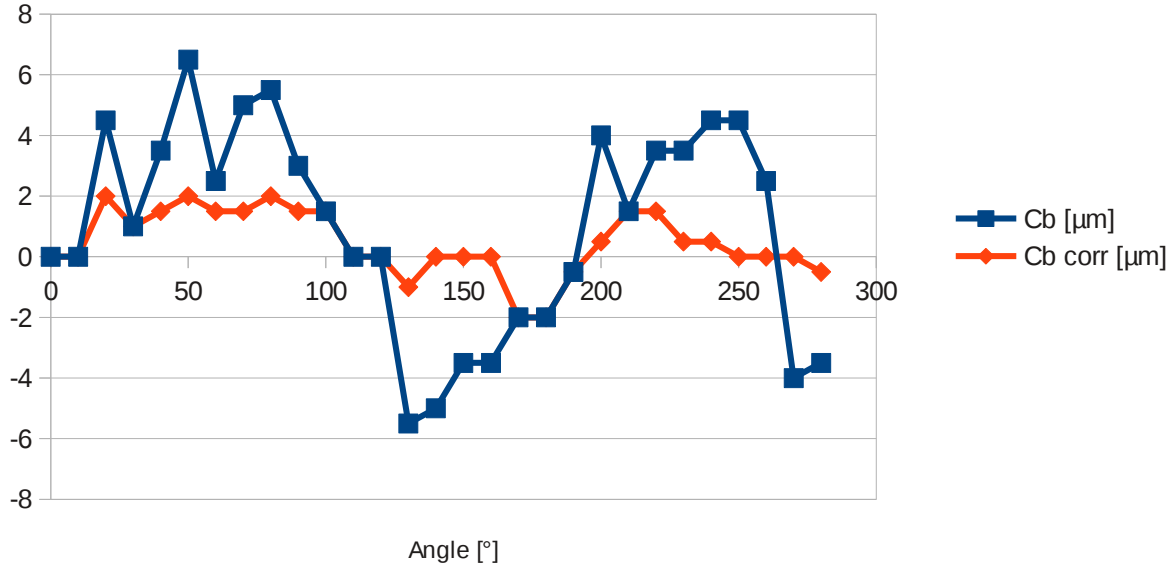
M. Bowler, ESRF (ID14-1 and ID14-2)



	<u>Overall</u>	<u>Inner shell</u>	<u>Outer shell</u>
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 $\langle I/s \rangle$	8.10	12.6	3.30

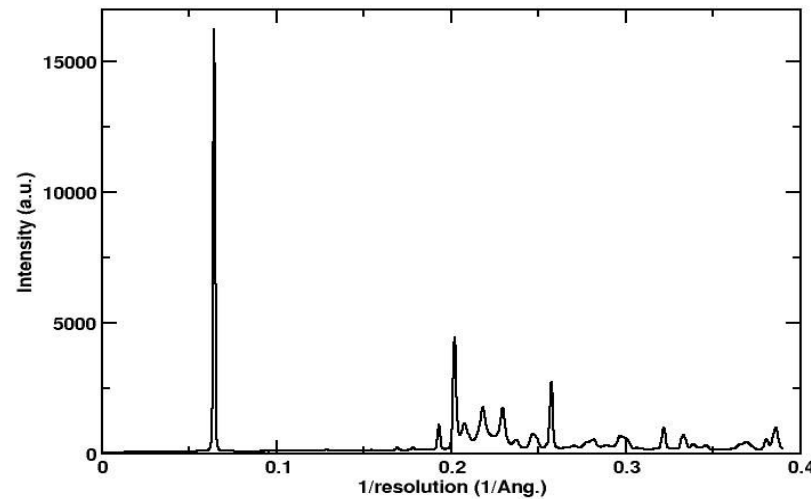
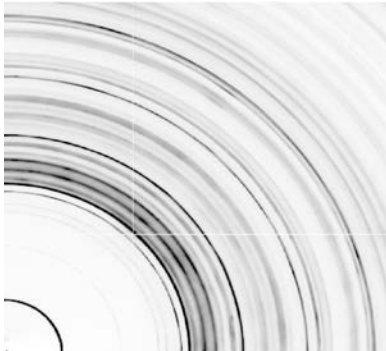
# G-Rob function: 1D+

- Improved goniometer capability
- Compatible with beam down to 40  $\mu\text{m}$  diameter !!!!

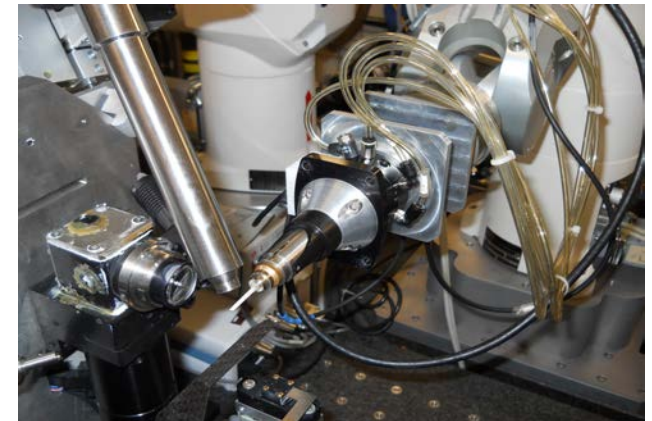


# G-Rob function: Powder diffraction

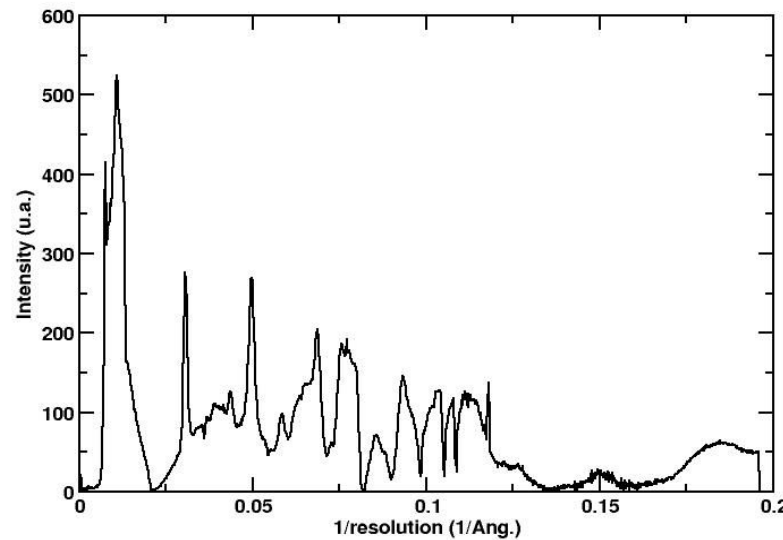
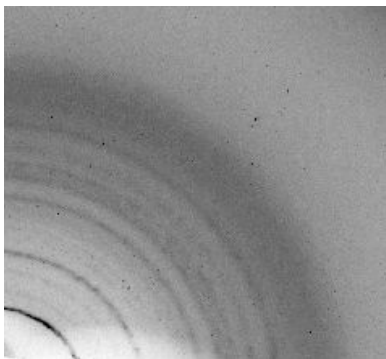
## Small molecule powder



2-4 rotation / sec  
Continuous translation

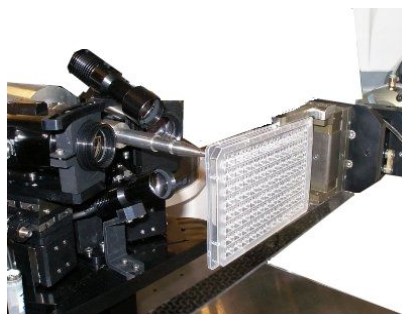


## Protein powder





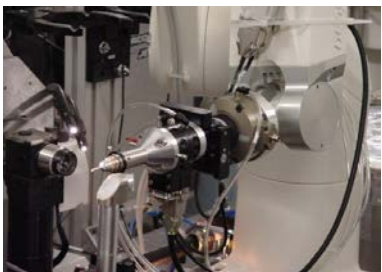
**Cryo-sample transfer**



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

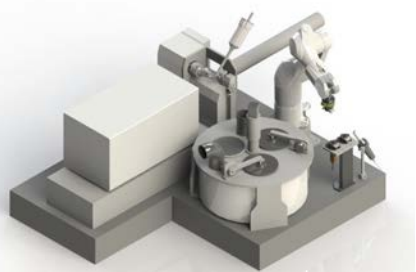


**Beam monitoring,  
quick-realign**



**Frozen crystals,  
capillaries, powder**

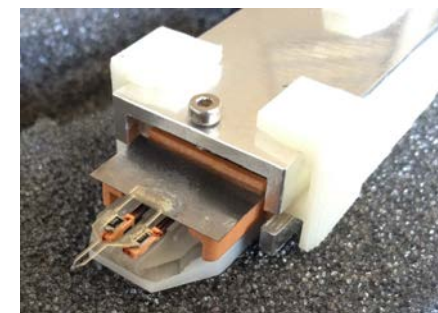
# G-Rob 1DT



**Sample changer**

## **Cryo-frozen samples transfer**

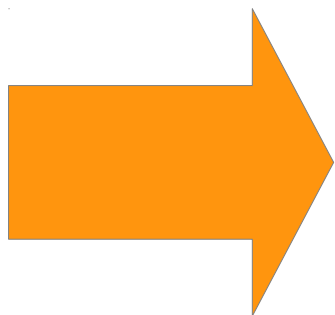
- Automated transfer of frozen samples
- 90 to 240 samples storage Dewar
- SPINE standard format



**Sample harvesting**

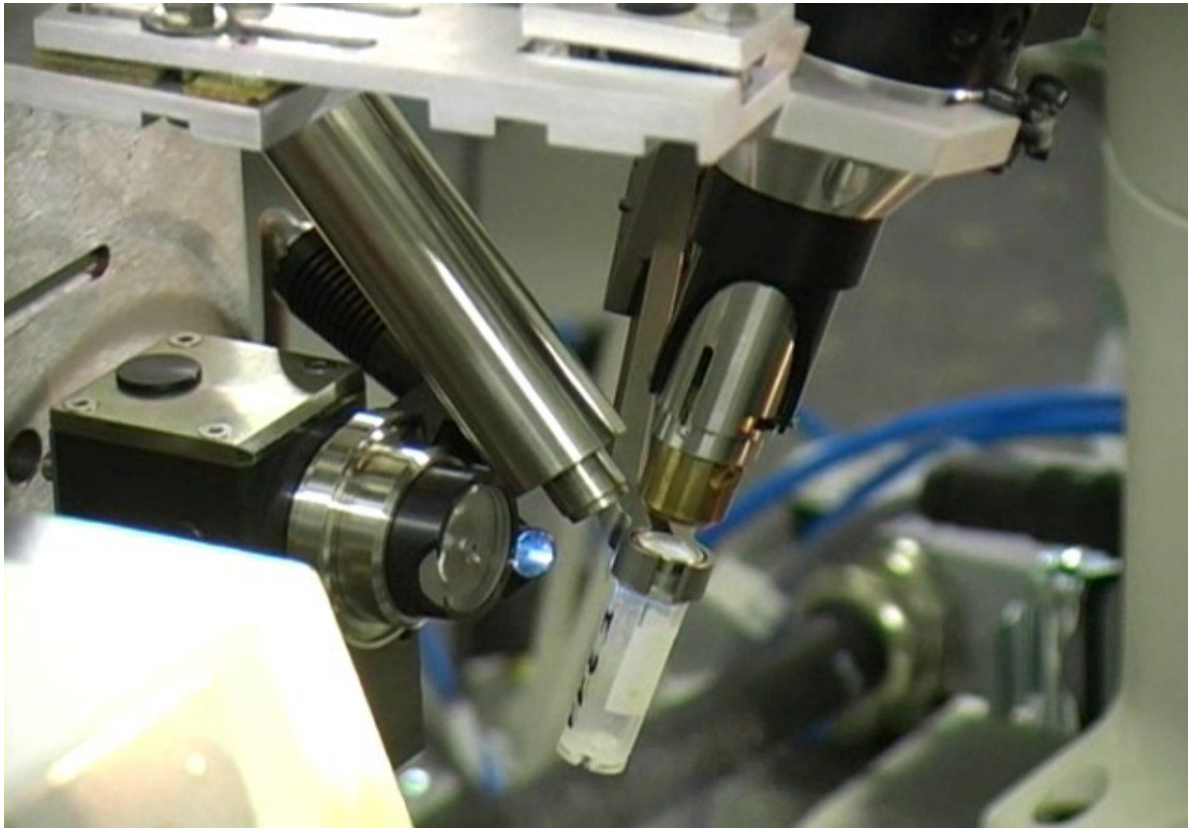
## **Applications**

- high throughput screening of frozen crystals
- remote controlled experiments



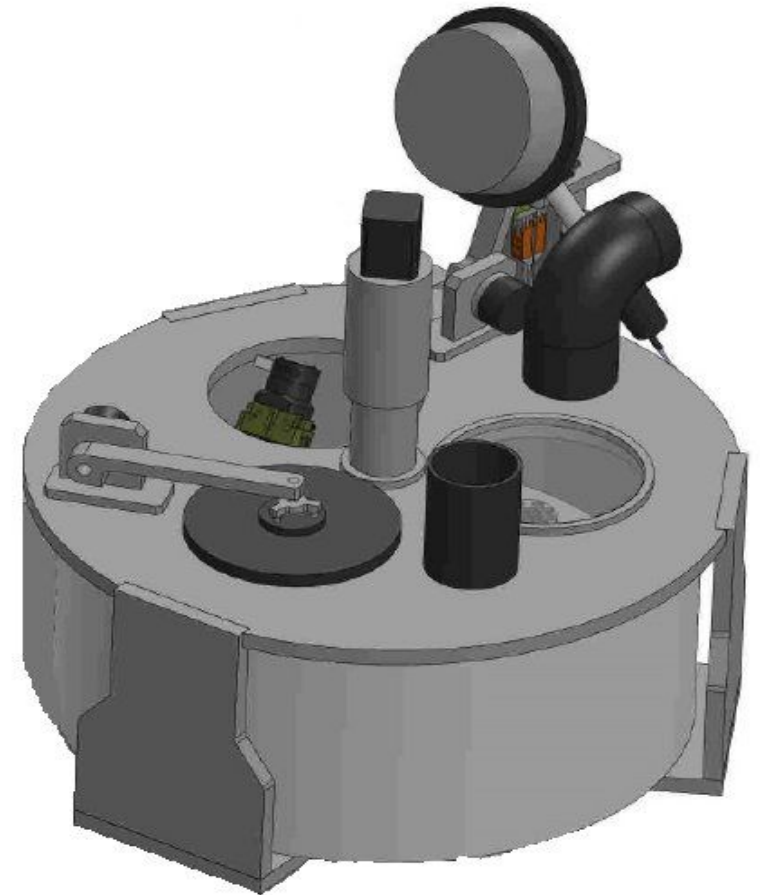
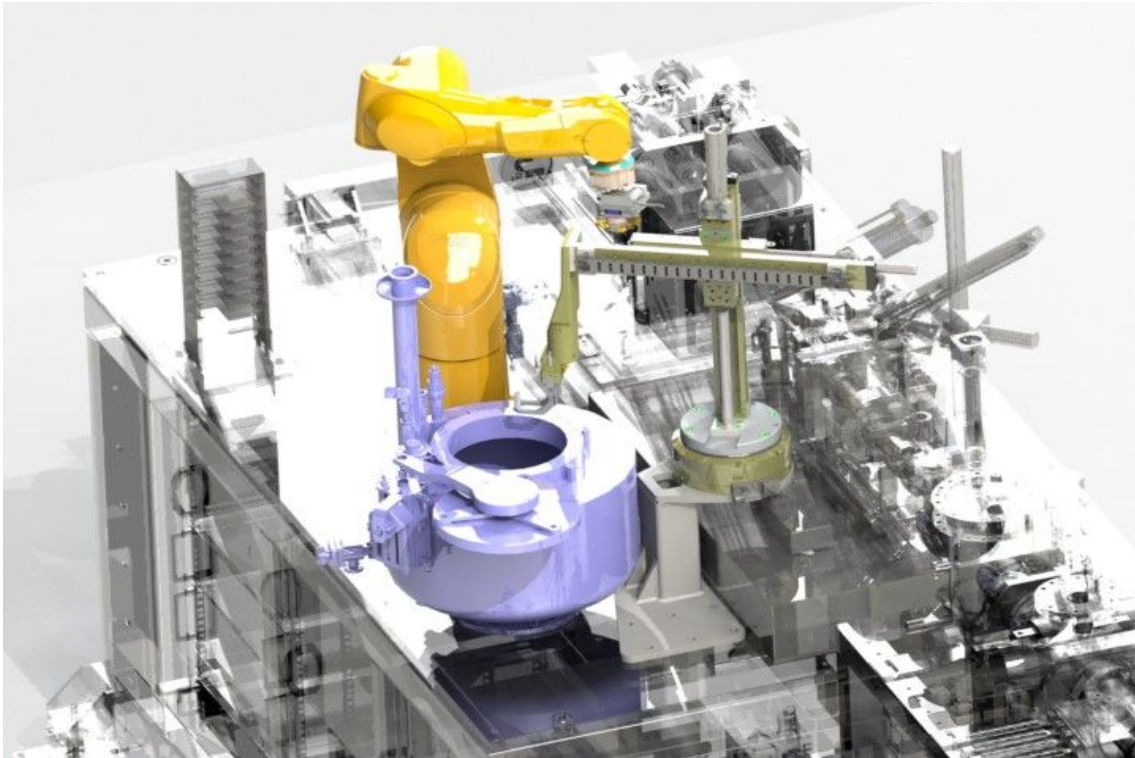
# G-Rob 1DT for in-house systems

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



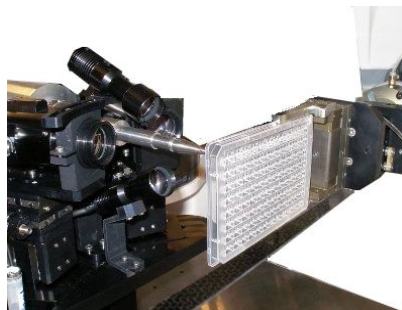
# G-Rob 1DT for beamlines

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

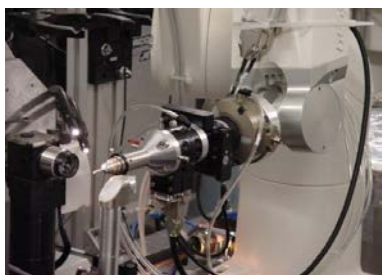




Cryo-sample transfer



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



Frozen crystals,  
capillaries, powder

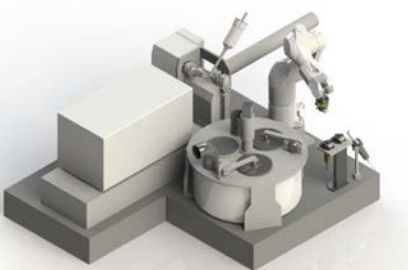


Beam monitoring,  
quick-realign

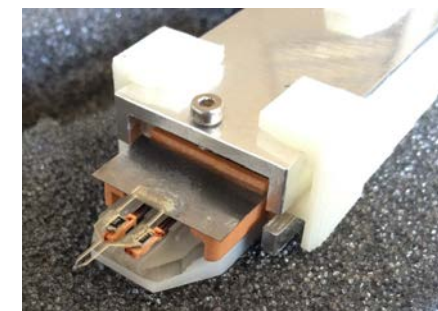
# G-Rob 2D

## *in situ* screening & data collection

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



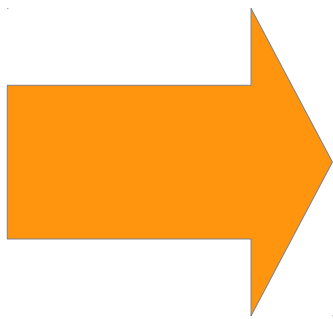
Sample changer



Sample harvesting

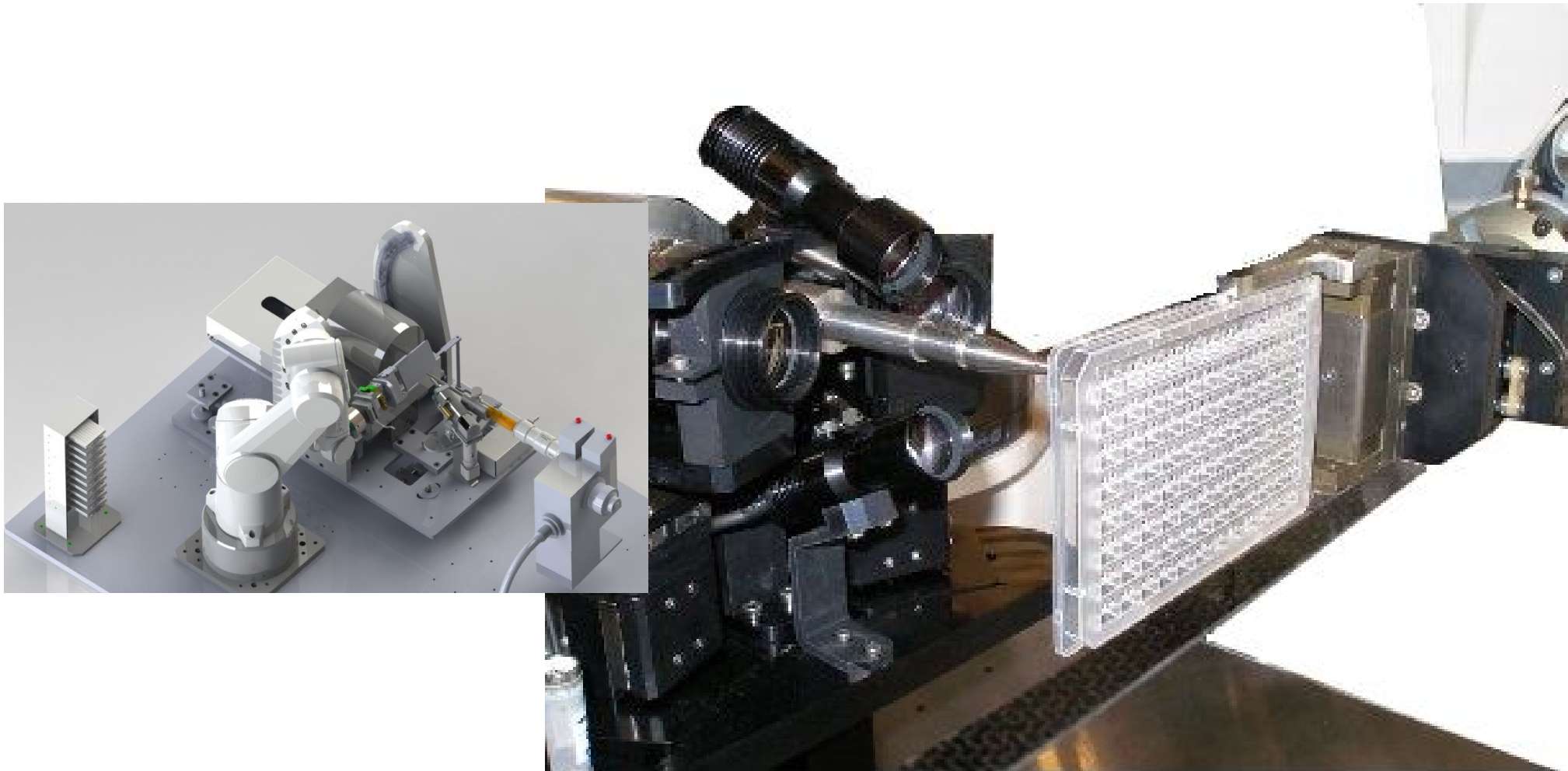
## Applications

- 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



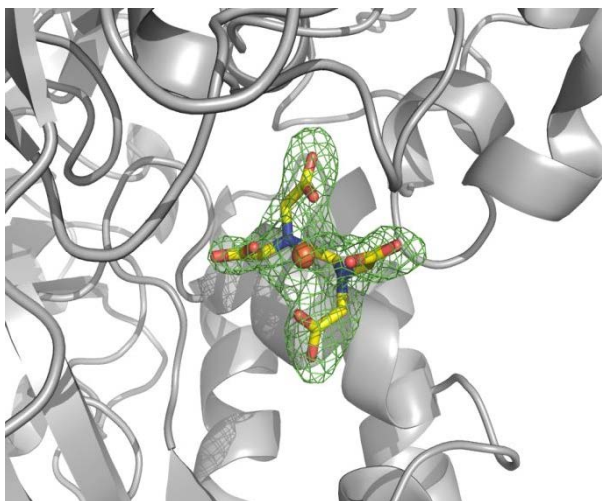


# Crystal Listing

Position of 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 ( $\mu\text{m}$ )	3
< Y > error ( $\mu\text{m}$ )	3
< radius > error ( $\mu\text{m}$ )	5
X standard deviation ( $\mu\text{m}$ )	2
Y standard deviation ( $\mu\text{m}$ )	2
radius standard deviation ( $\mu\text{m}$ )	3

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



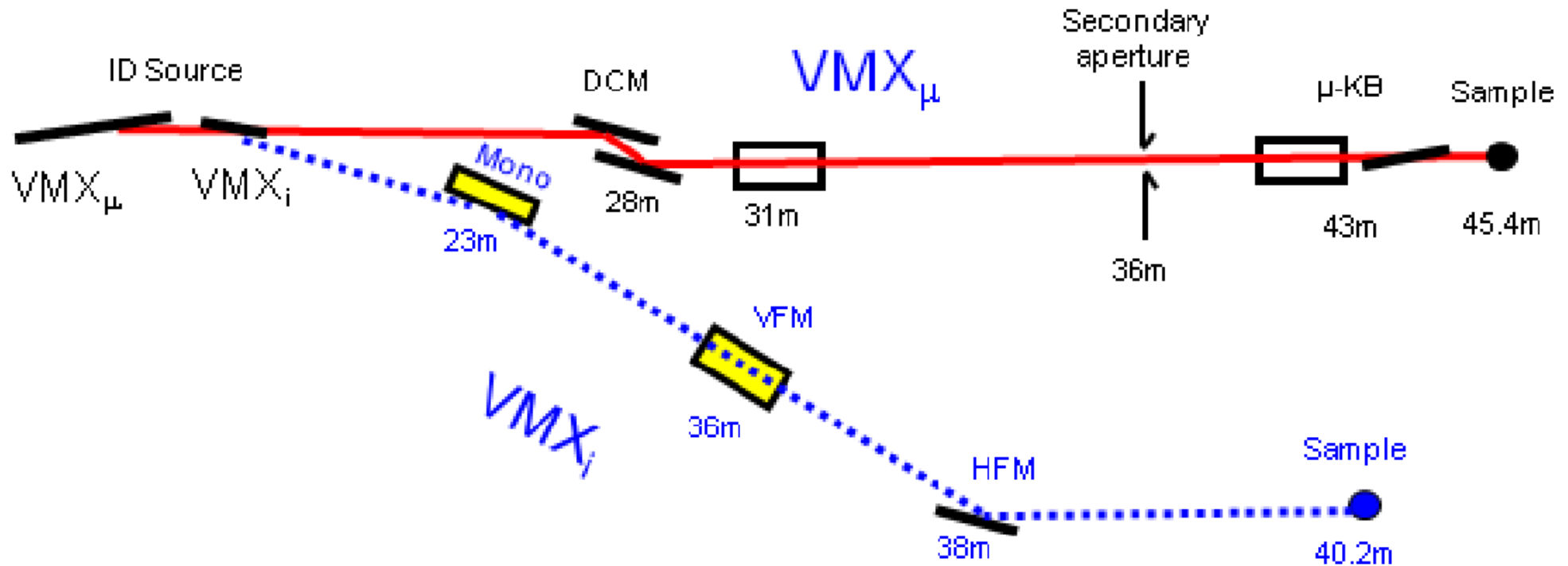
	Lysozyme	NikA-FeEDTA
<b>Data collection</b>		
Resolution (last shell) ( $\text{\AA}$ )	2.10	2.45
Completeness (last shell) (%)	71.6 (75.0)	68.4 (71.4)
$R_{\text{sym}}^{\text{a}}$ (last shell) (%)	13.9 (38.5)	13.8 (41.6)
$I/\sigma$ (last shell) (I)	5.61 (2.75)	4.45 (2.20)
<b>Refinement</b>		
$R_{\text{work}}^{\text{b}}$ (%)	18.82	17.39
$R_{\text{free}}^{\text{c}}$ (%)	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

<b>Synchrotron</b>	<b>Beamline</b>	<b>Equipment</b>	<b>Availability</b>
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



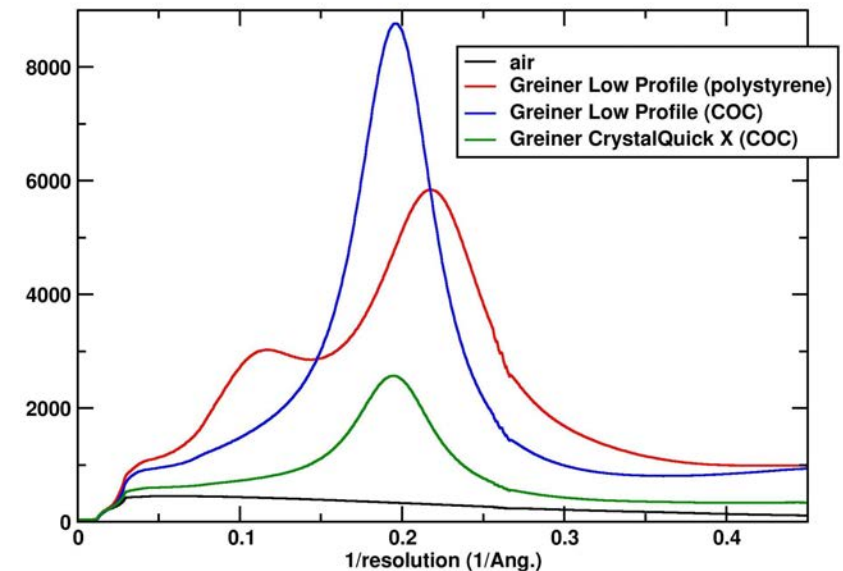
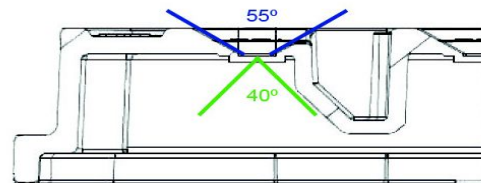
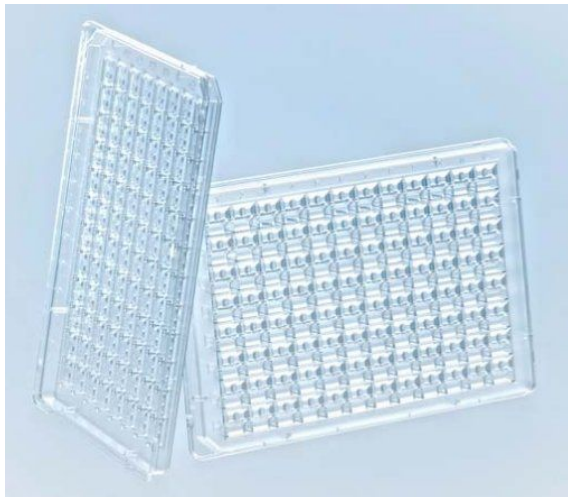
<u>Endstation</u>	<u>Sub microfocus (<math>VMX_{\mu}</math>)</u>	<u>In situ (<math>VMX_i</math>)</u>
Energy range (keV)	5 – 30	Nominally ~14 keV
Beamsize ( $\mu\text{m}$ )	0.5 – 5 (300)	5 – 50
Flux (phs/s)	~ $1e12$ at 20 keV	> $1e12$

# 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	Landscape	High	~30
Greiner BioOne	609120	Landscape	High	~30
Greiner BioOne	609171	Landscape	High	~50
<b>Greiner BioOne</b>	<b>609890/895</b>	<b>Landscape</b>	<b>Low</b>	<b>~80</b>
<b>Mitegen</b>	<b>InSitu-01CL</b>	<b>Both</b>	<b>Low</b>	<b>~90</b>
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	CrystalEX, 1-well	(Both)	High	~30
Corning	CrystalEX, 3-well	(Both)	High	~30

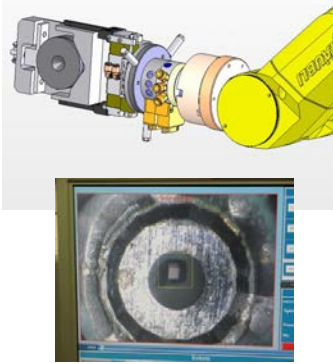
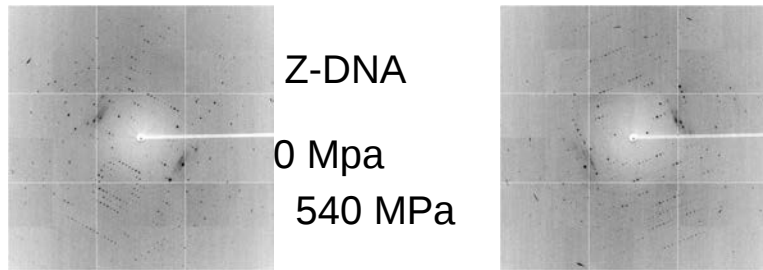
# CrystalQuick™ X plate

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

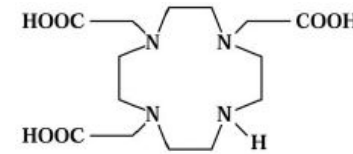


greiner bio-one

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

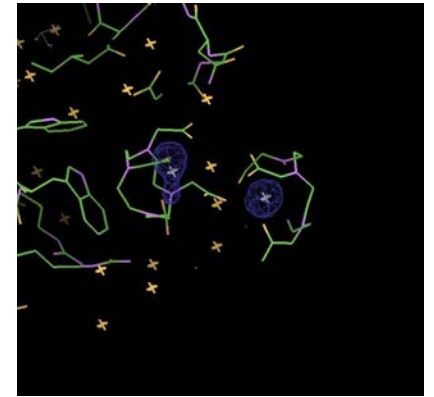


## Anomalous data of Yb-DO3A / lysozyme complex solved “in the drop”



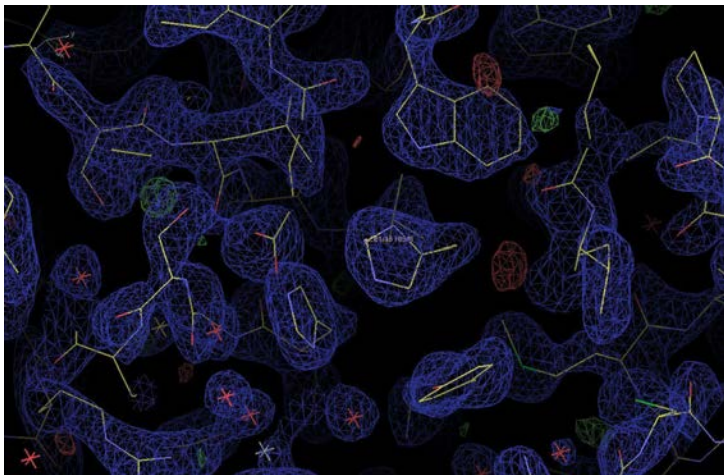
Anomalous diff. map  
(threshold:  $6\sigma$ )

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

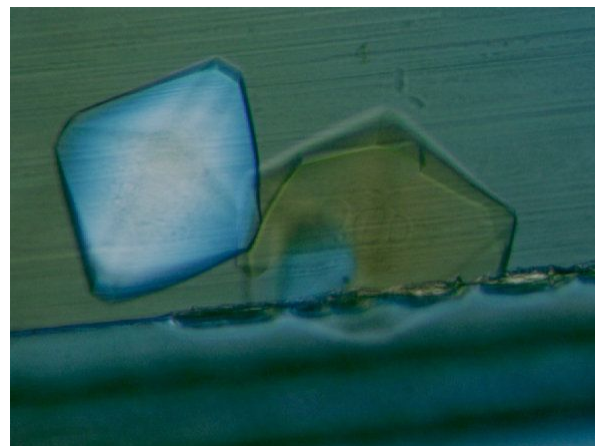


## Structure of NDK from *A. Polyphaga* Mimivirus solved “in the drop” (C. Abergel, CNRS)

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

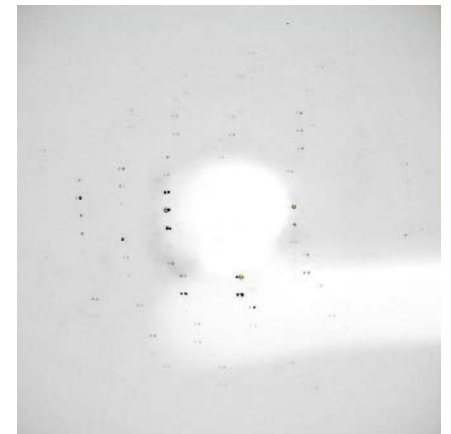


## Extra-cellular domain of a membrane protein (A. Haouz, Inst. Pasteur, Paris)



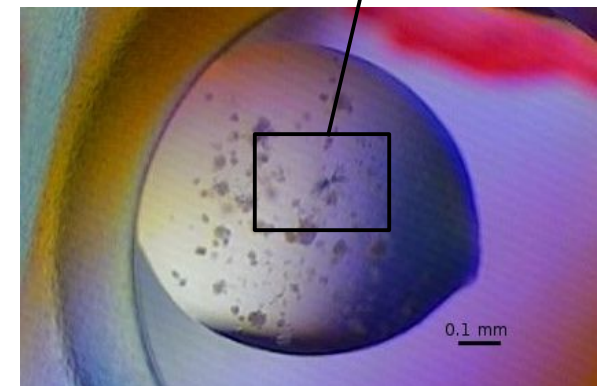
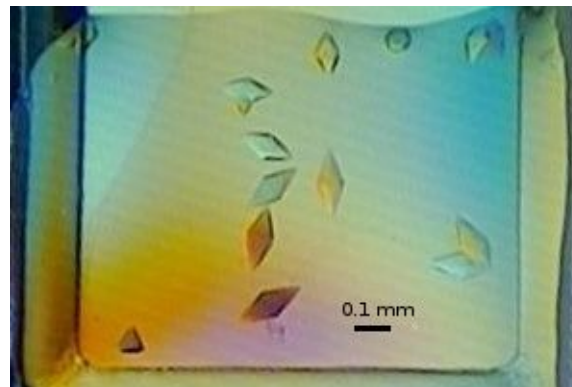
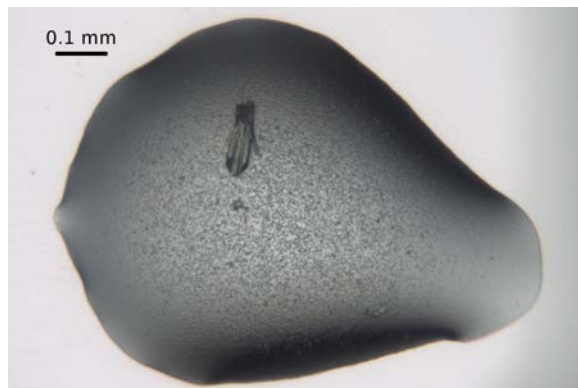
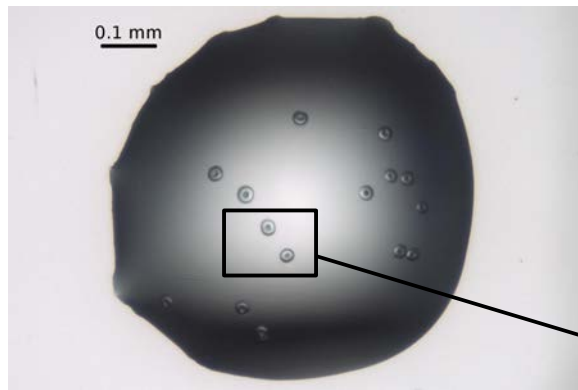
>300 μm crystals  
No diffraction when frozen

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



# *In situ* screening

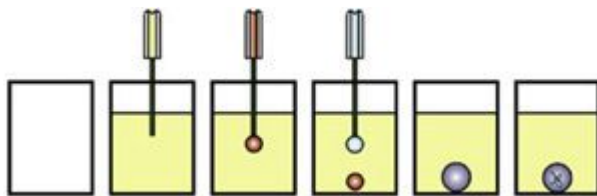
Samples recently proved to be diffracting protein crystals using G-Rob 2D (*in situ*) screening



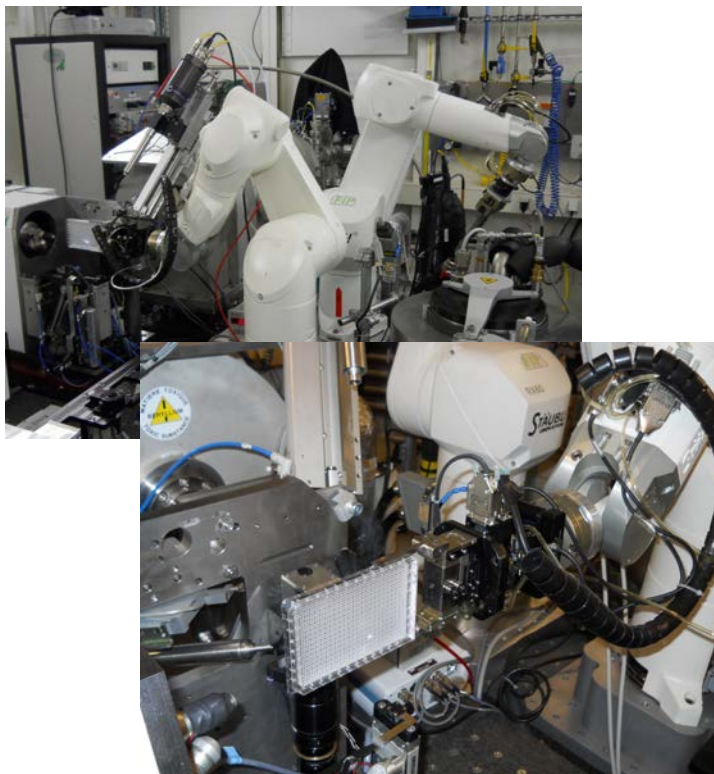
# Adenovirus surface protein in complex with its receptor

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)



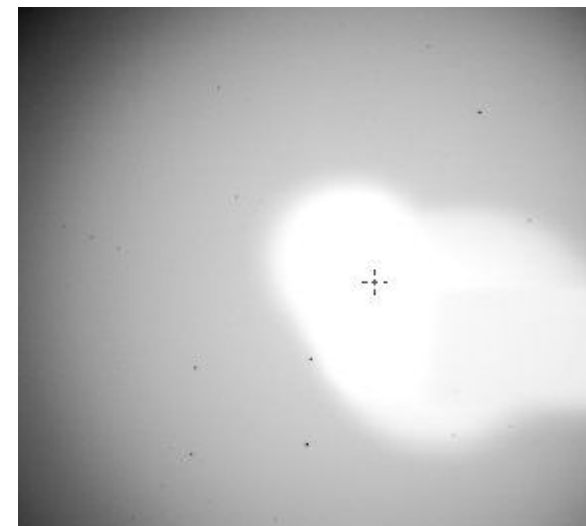
*situ* screening in 1536-well plate  
with G-Rob on FIP-BM30A



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.



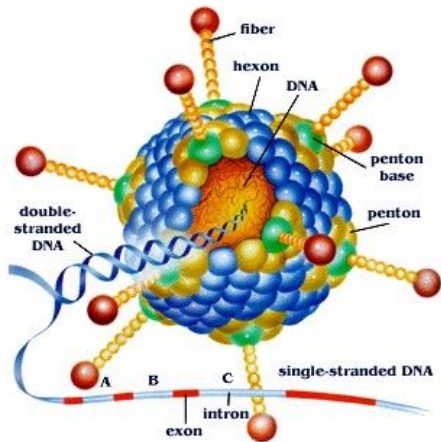
Diffraction at 6.3 Ang on  
30x10  $\mu\text{m}^2$  crystals



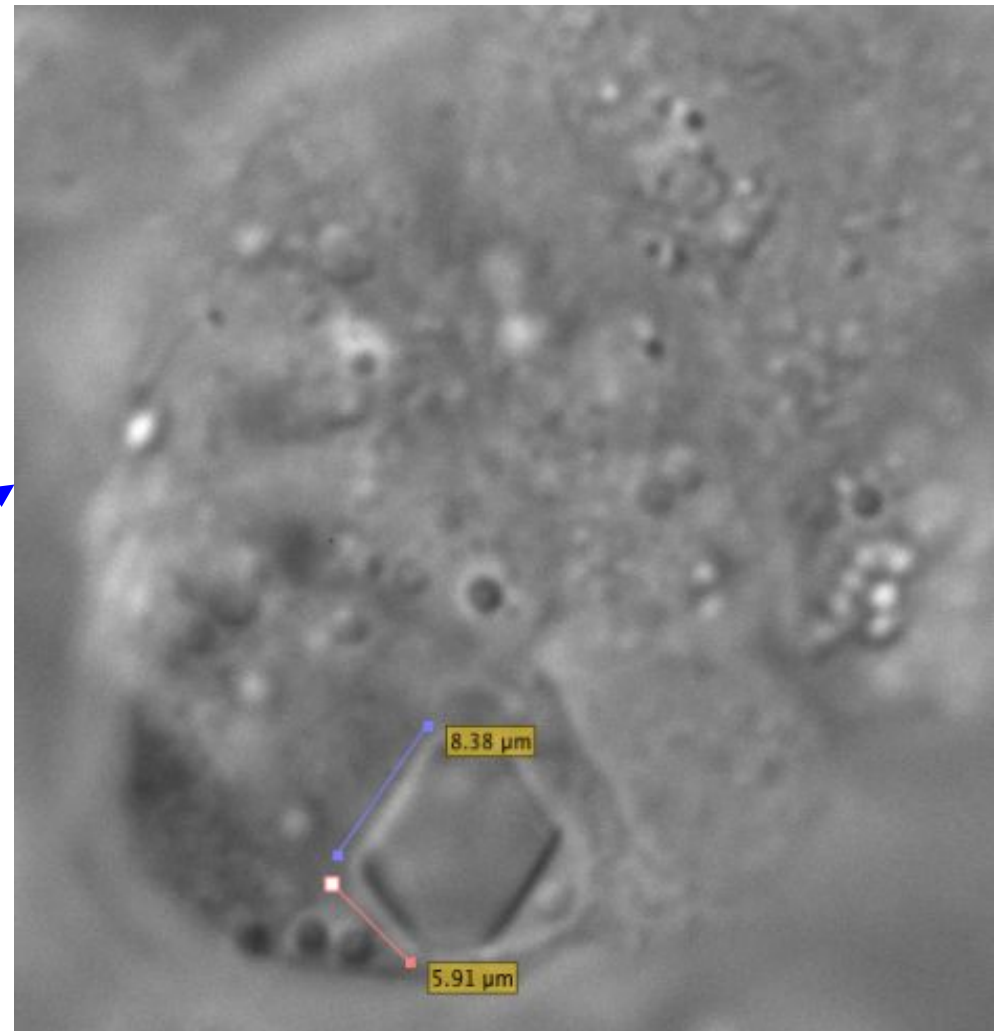
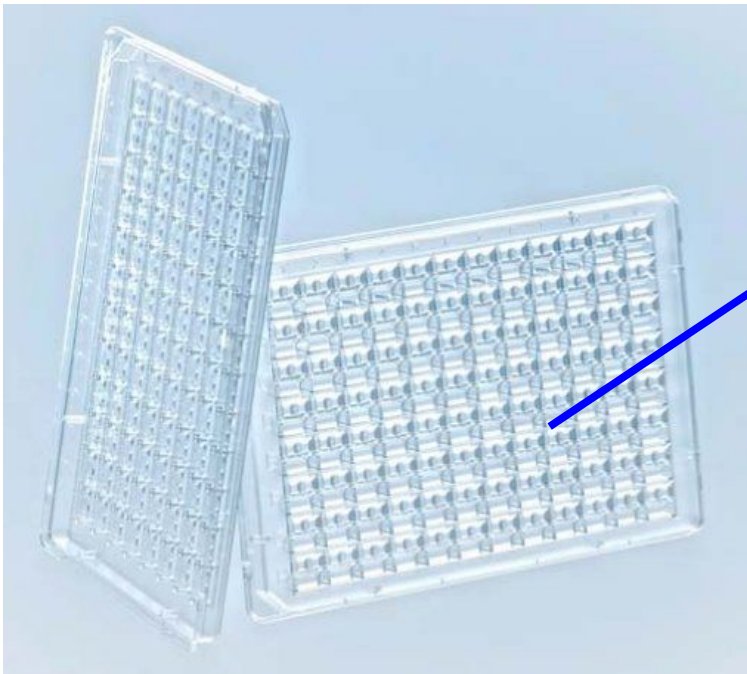


# Intranuclear Adenovirus crystals

P. Fender *et al.*, EMBL

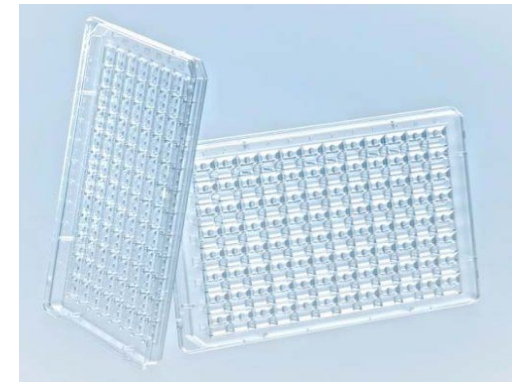
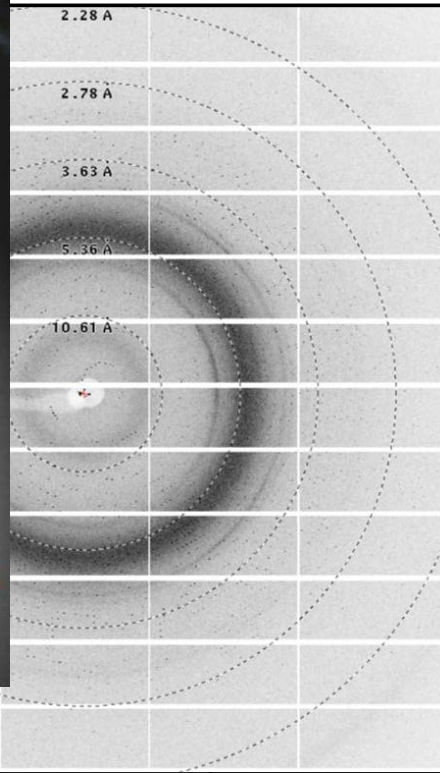
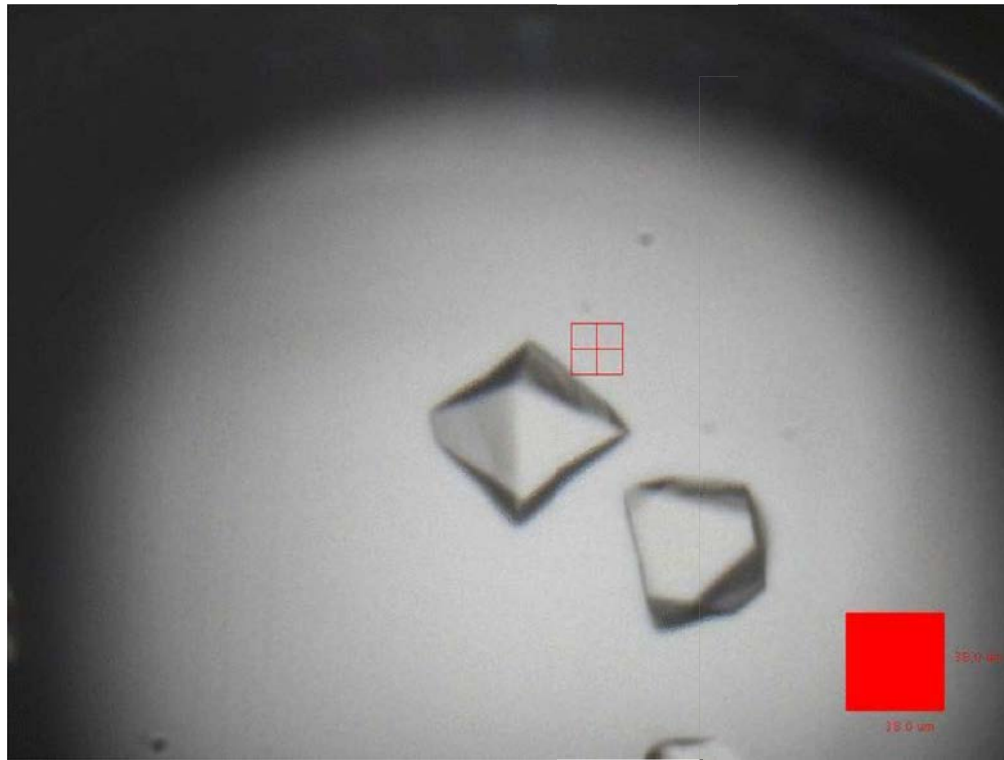


*In situ* analysis of crystals appeared in the insect cells used for expression.

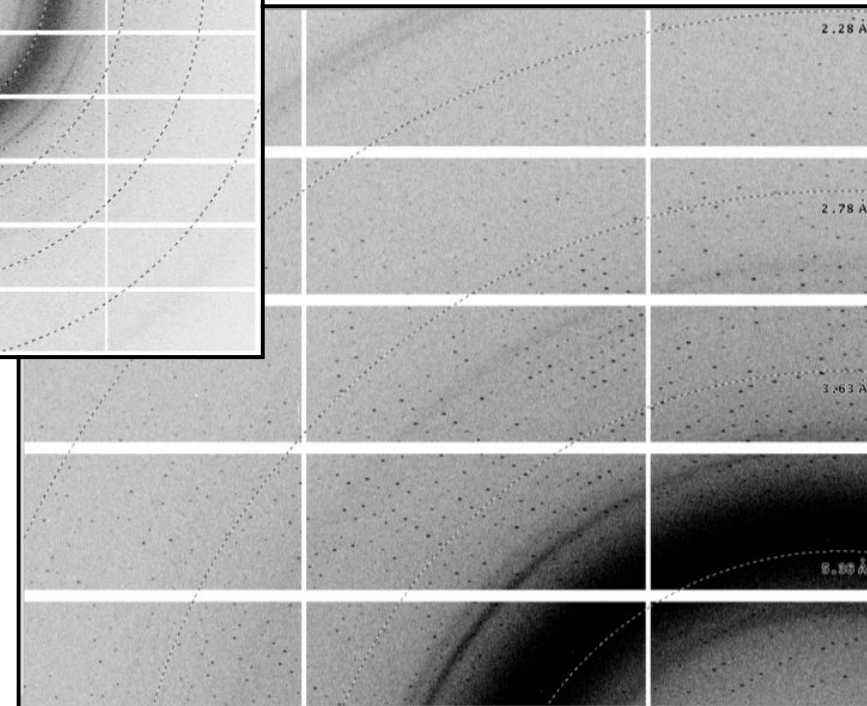


# A new virus structure: Bovine enterovirus 2

## Crystallization plate screening on I24



**CrystalQuick X plate**

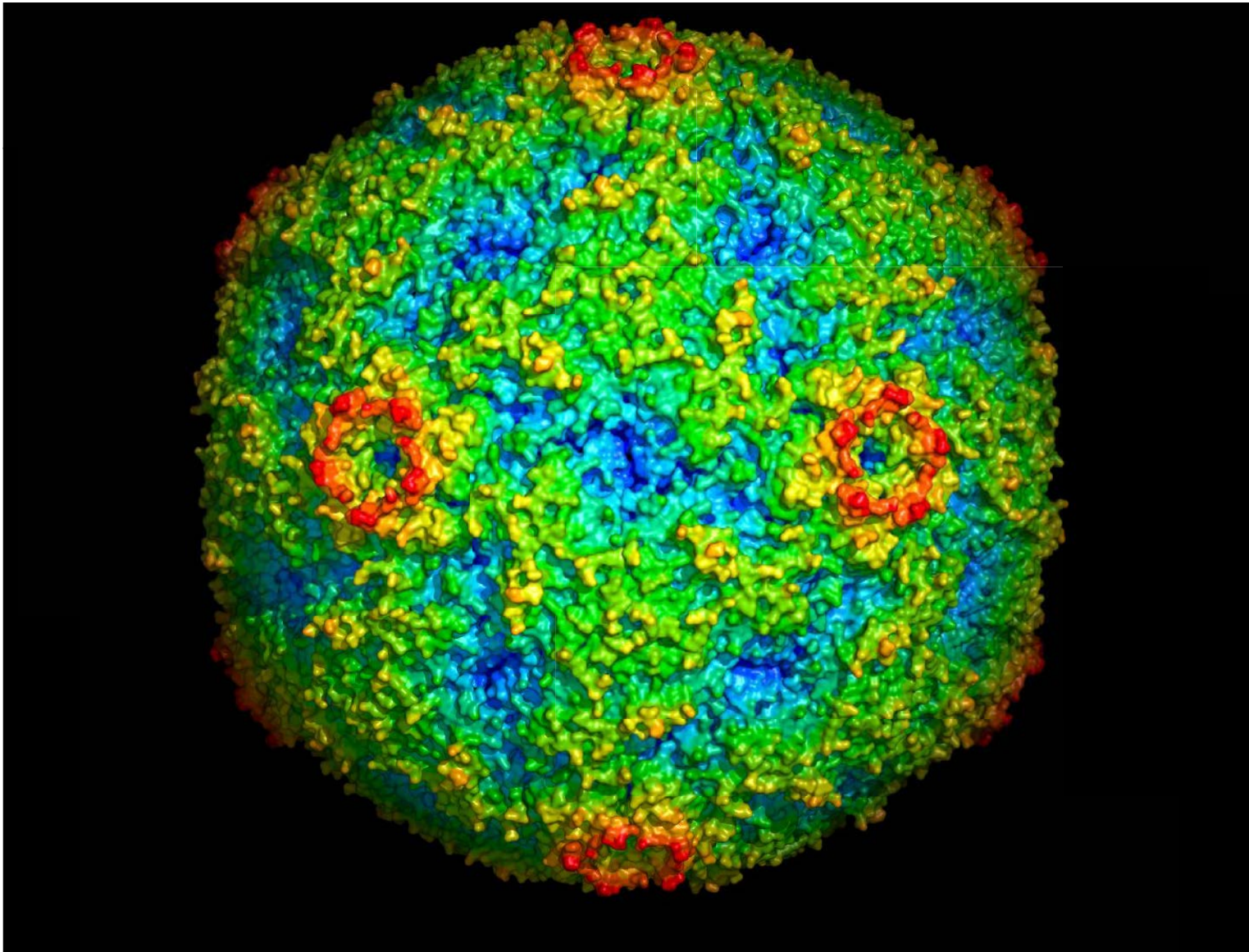


Data collected at DLS, I24  
Beam size 20 microns, focus at detector (P6M)  
exposure time 0.1 sec, 0.1° oscillation,  
detector distance = 480 & 645 mm,  
resolution at edge of detector 2.28 & 2.97 Å

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



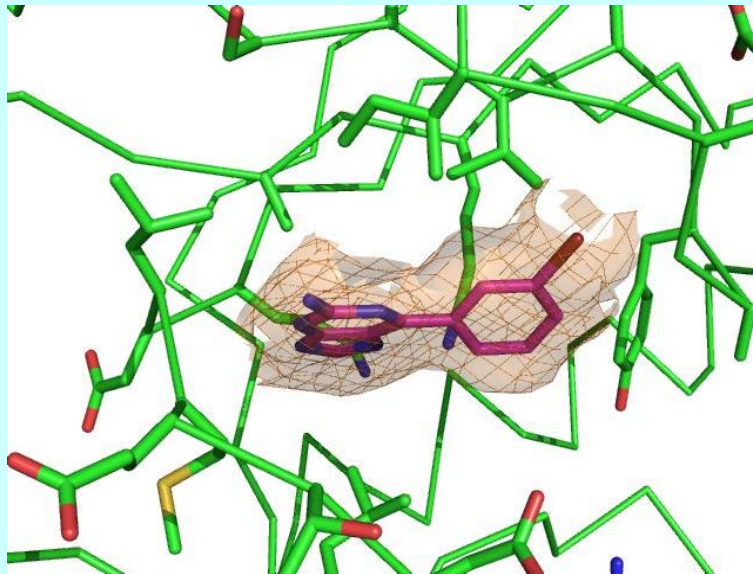
E.E. Fry, J.S. Ren, A. Kotecha, T.S. Walter, C. Porta, D.I. Stuart,  
The Wellcome Trust Centre for Human Genetics, University of Oxford (UK),  
D.J. Rowlands, Institute of Molecular and Cellular Biology, University of Leeds (UK) and  
Gwyndaf Evans, Robin Owen, Danny Axford, Jun Ashima, I24, Diamond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

# Test of ERK-2 in P21 with bromated ligand

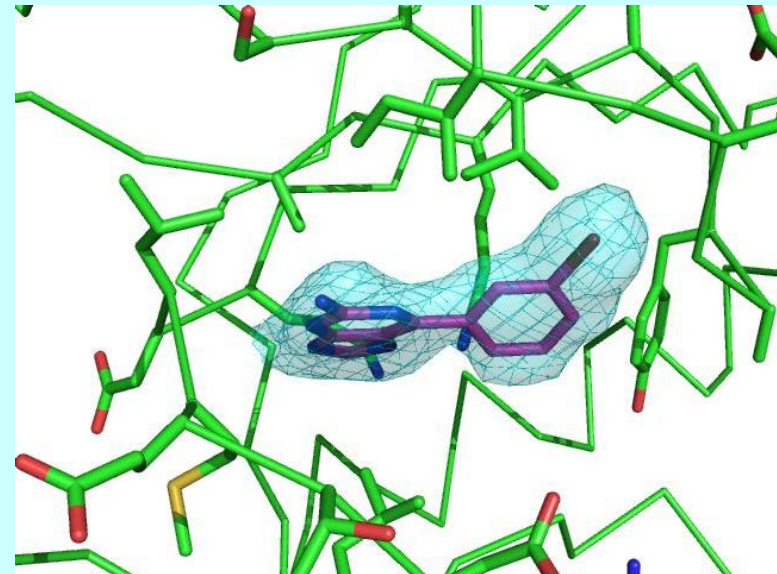
Completeness of 83%  
by merging 3 dataset (50+50+41 frames)  
Rsym ~5.4 at 2.15 Å.

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



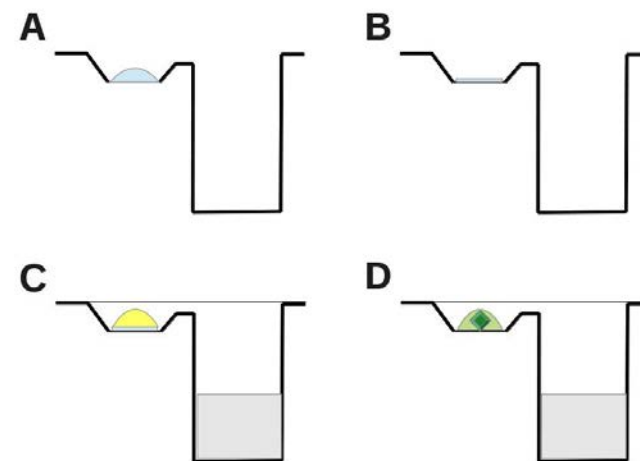
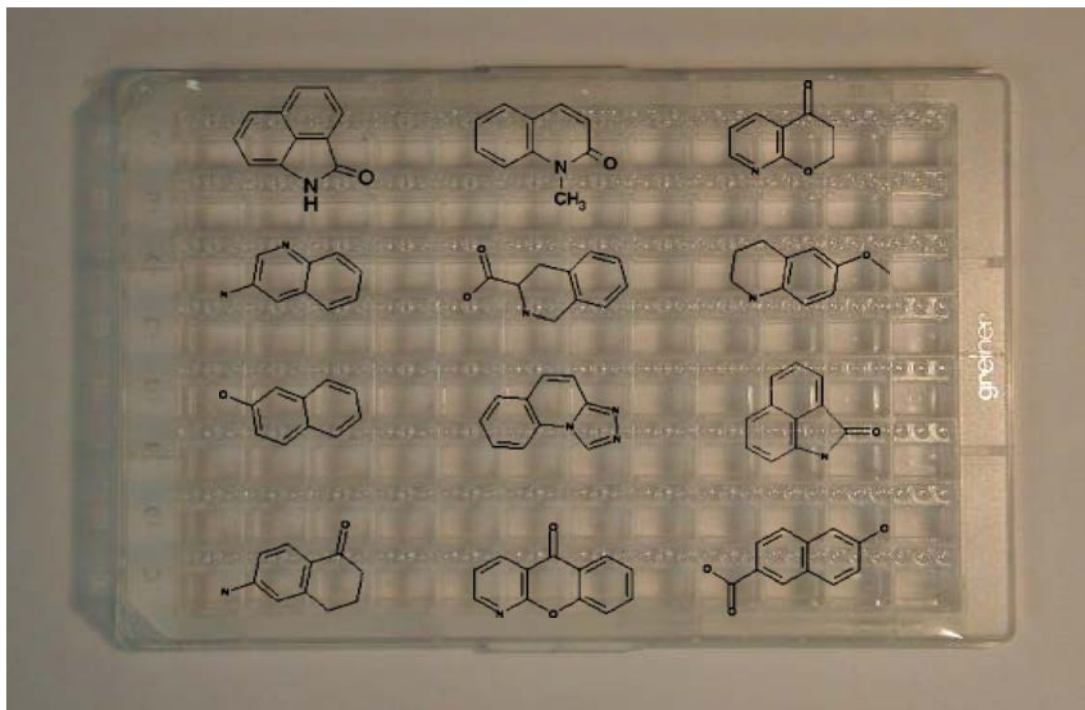
2fo-fc (blue) 0.9 sigma

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

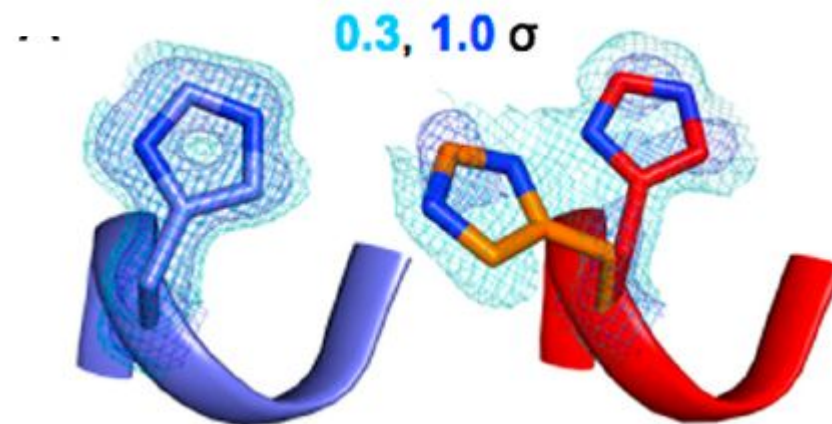
## Flash cooling of protein crystals

- 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

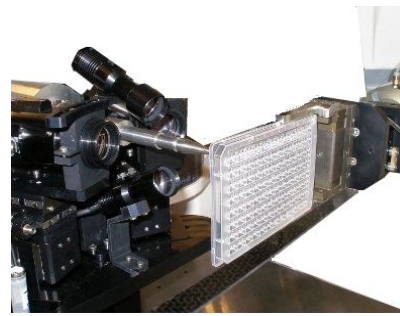
- motions crucial for catalysis,
- ligand binding,
- allosteric regulation.

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).

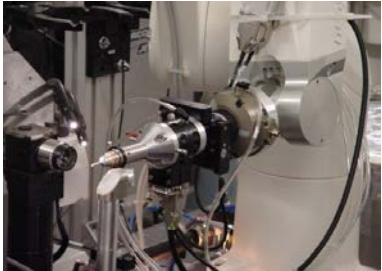




Cryo-sample transfer



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

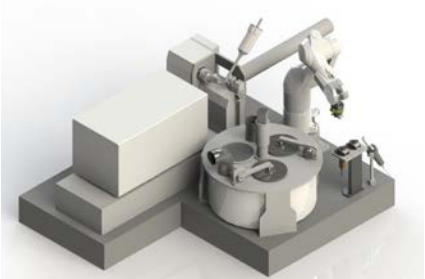


Frozen crystals,  
capillaries, powder



Beam monitoring,  
quick-realign

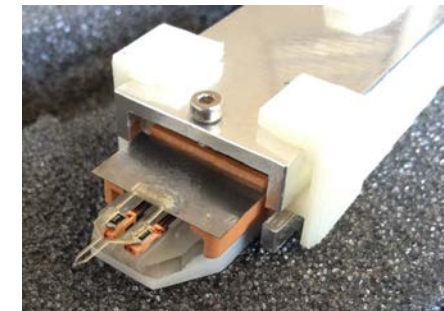
# G-Rob Monitoring



Sample changer

## Beam monitoring

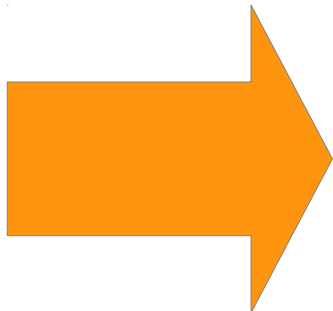
- fluorescent screen
- diode monitor



Sample harvesting

## Application

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

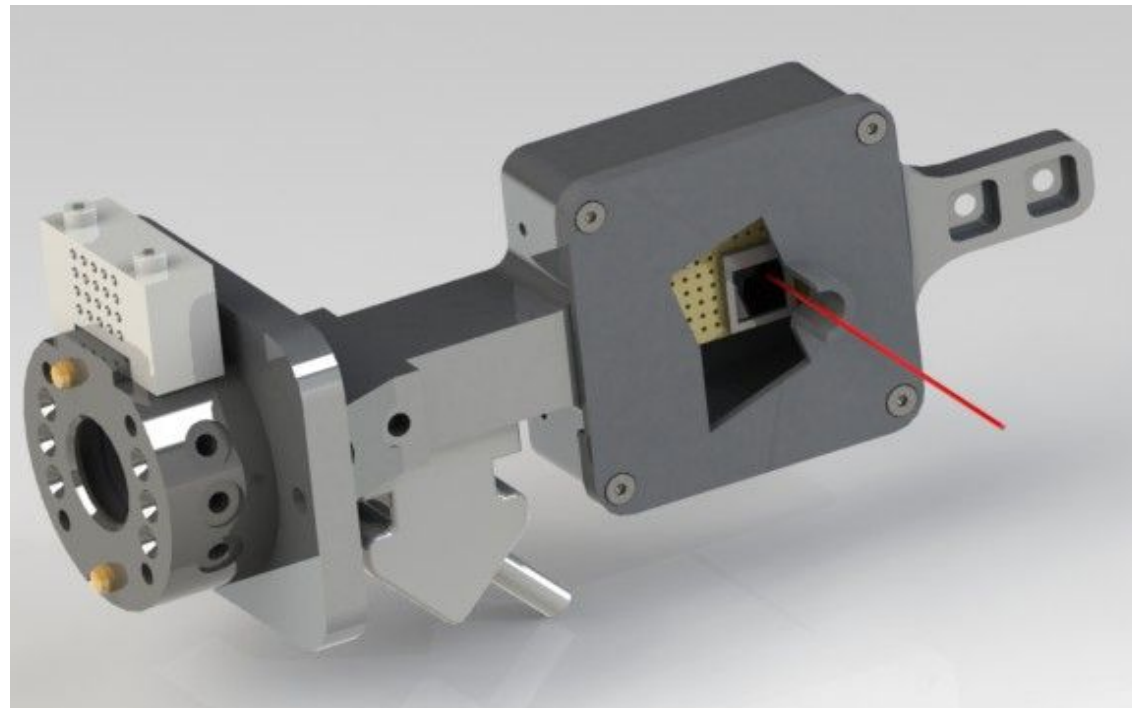


# G-Rob function: Monitor

## A robot tool for beam monitoring

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

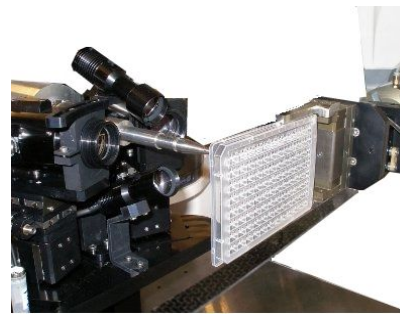
In association with motorized optics → **automated beam alignment**



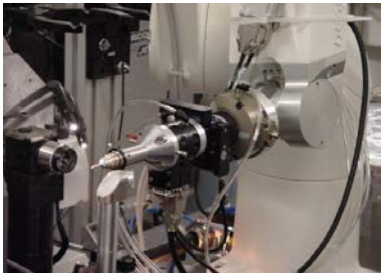




Cryo-sample transfer



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

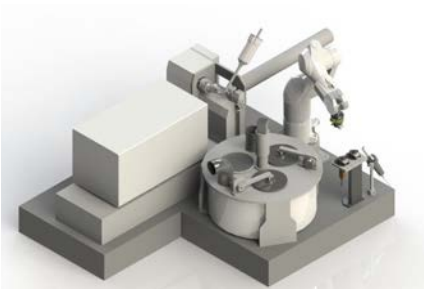


Frozen crystals,  
capillaries, powder



Beam monitoring,  
quick-realign

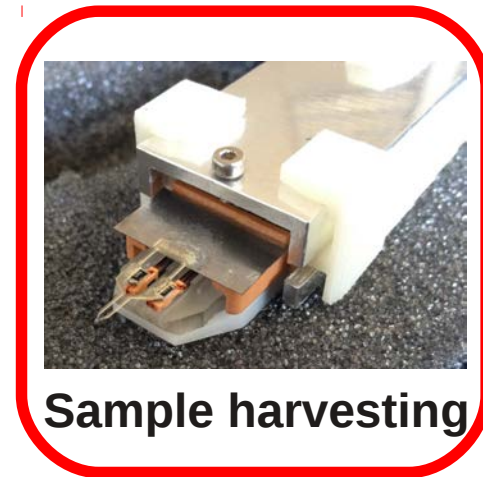
# G-Rob Harvesting (in development)



Sample changer

## Sample Harvesting

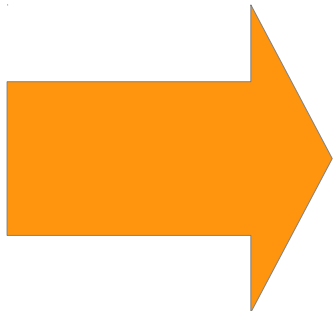
- Semi-automated harvesting
- Remote controlled micro-gripper



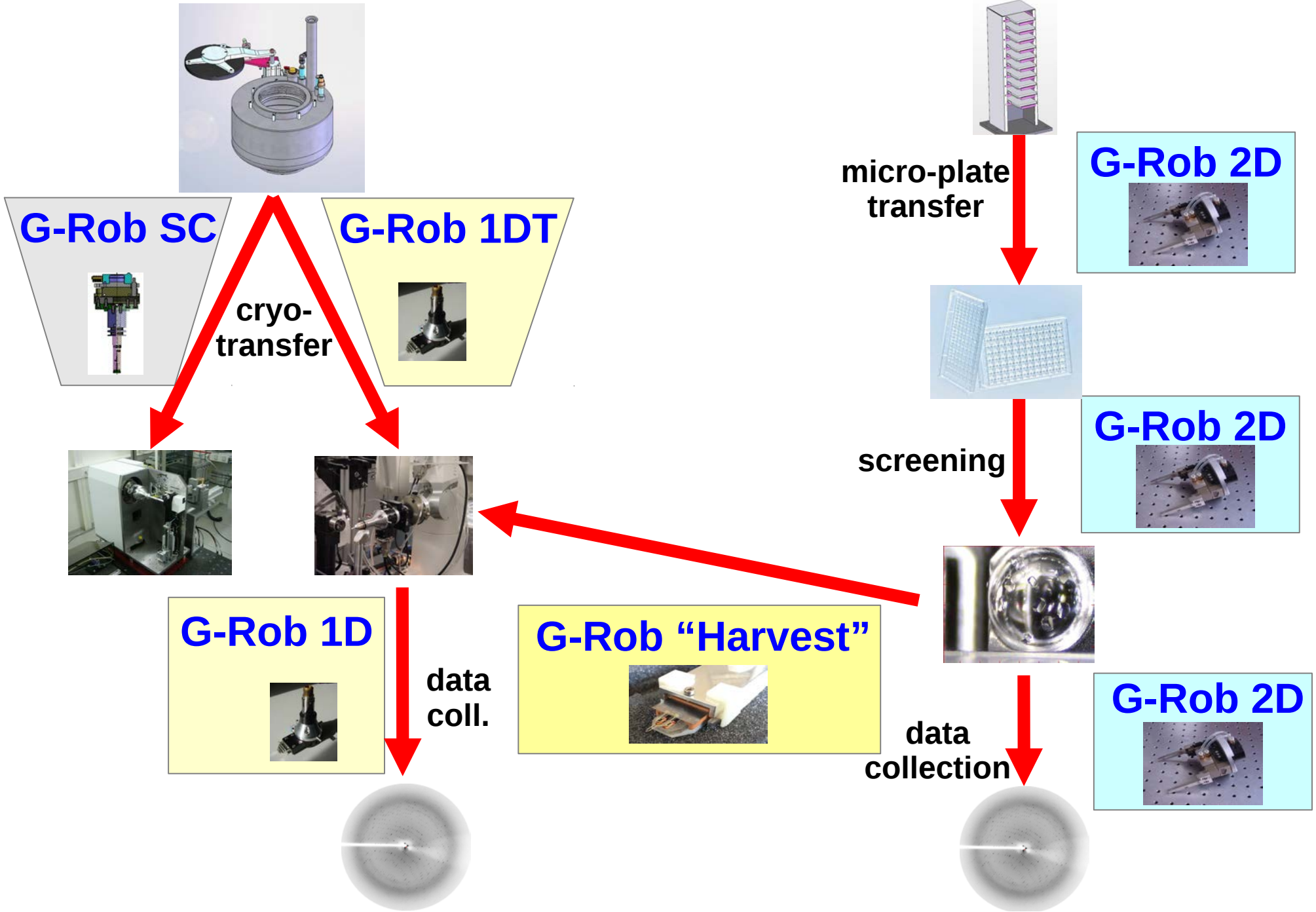
Sample harvesting

## Applications

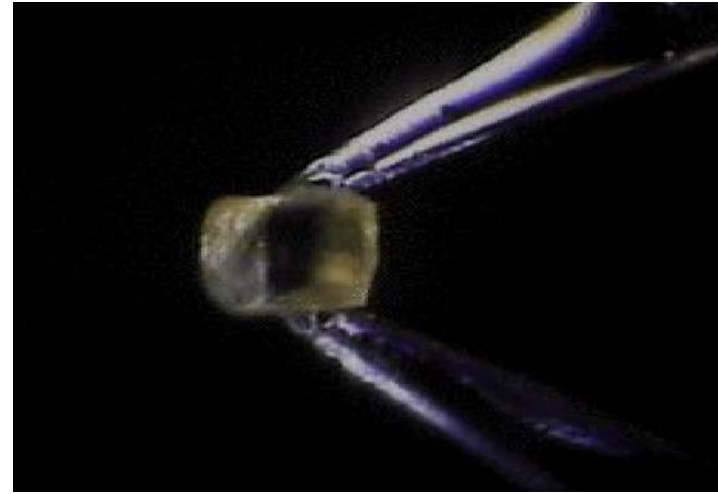
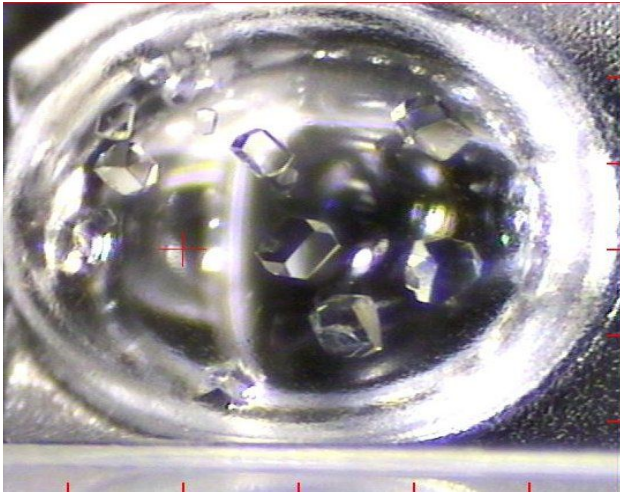
- Remote harvesting
- Crystal freezing



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

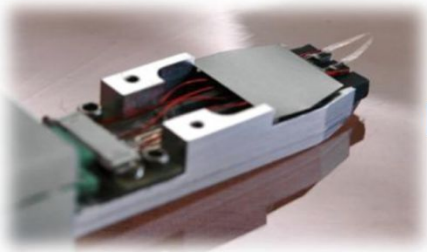


# Crystal harvesting

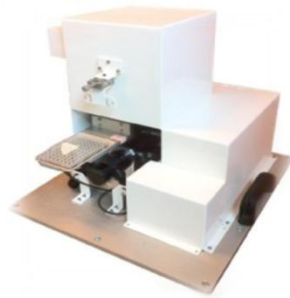


# Harvesting...

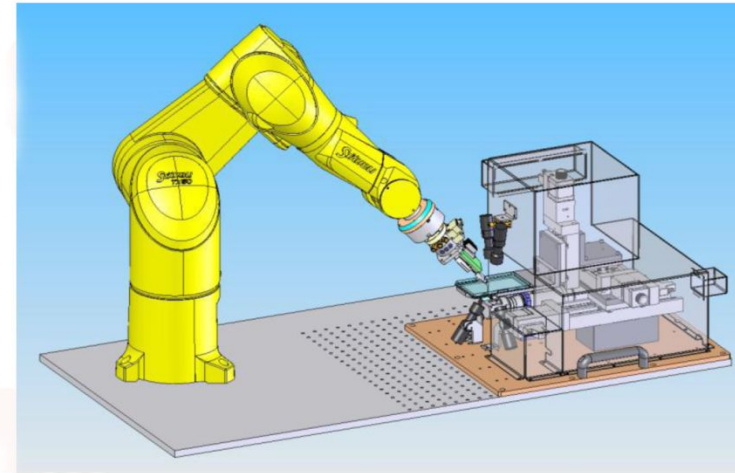
$\mu$ Tweezer



Inverted Microscope



6-Axis Robot

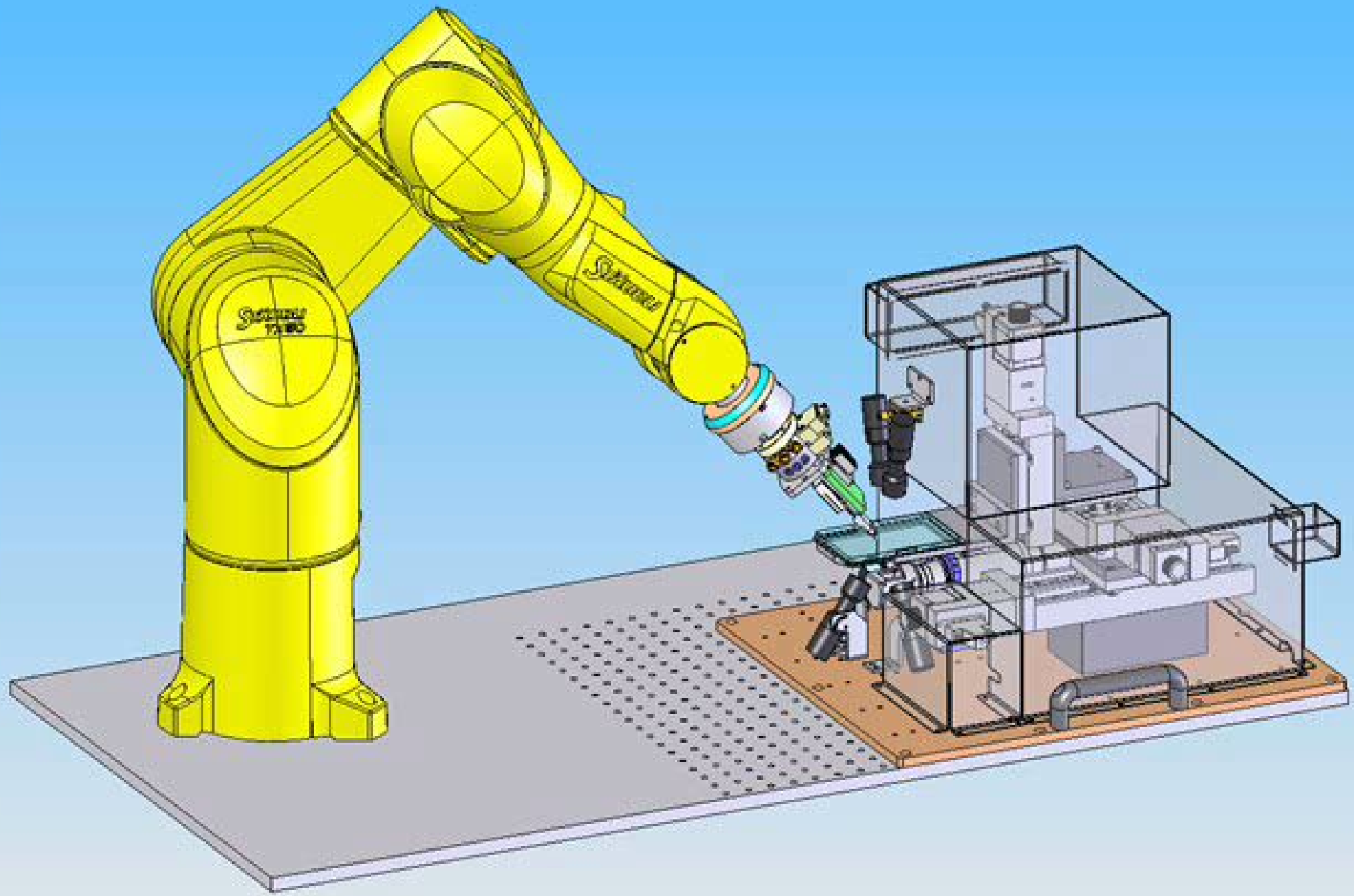


## Harvesting



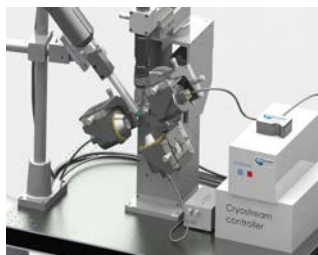
# Manual vs robotic harvesting

Data set	lysozyme				Nika-FeEDTA			
	Manual 1	Manual 2	Robotic 1	Robotic 2	Manual 1	Manual 2	Robotic 1	Robotic 2
<b>Data reduction</b>								
Resolution (last shell) (Å)	1.50	1.80	1.75	1.60	2.65	1.85	2.30	1.95
R <sub>sym</sub> (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
<b>Refinement</b>								
R <sub>work</sub> (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 <sub>free</sub> (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)

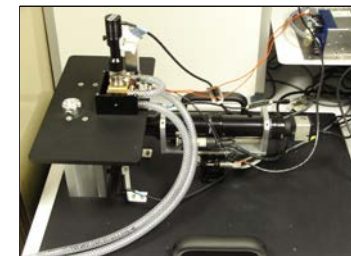




**VisuBench &  
Crystal-Listing**



**Misc**



**OptiCryst**

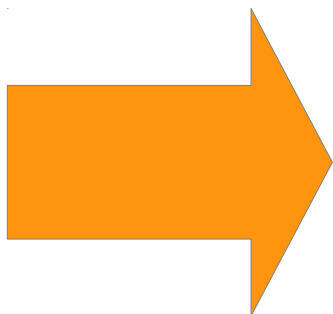
# The Visualization Bench

## **Beam monitoring**

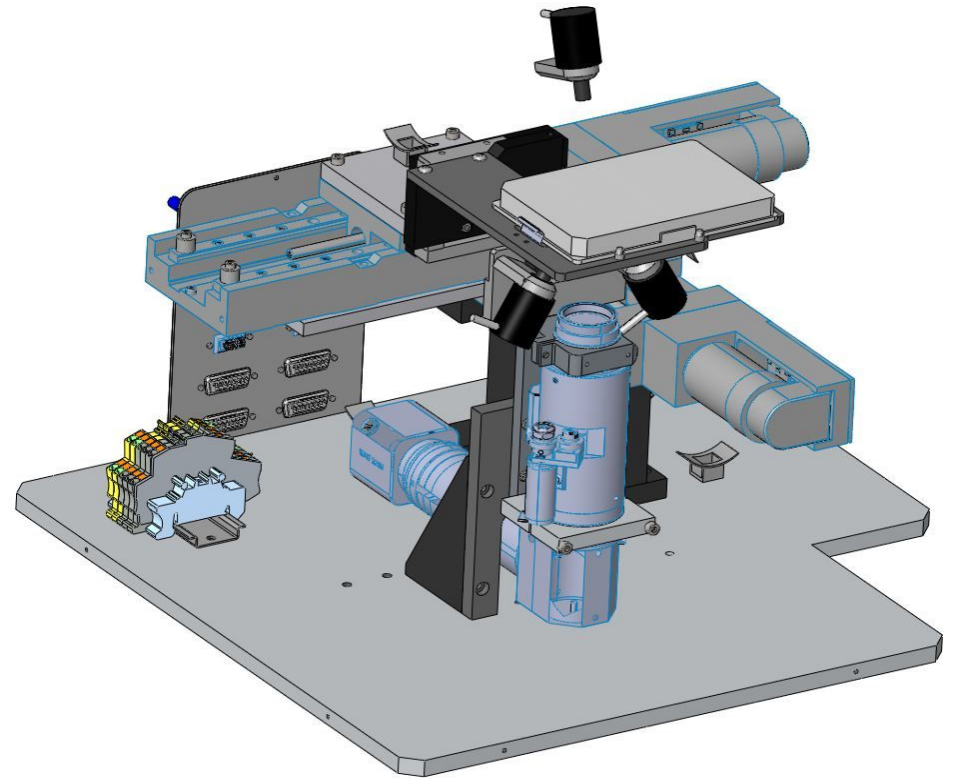
- Inverting microscope
- Crystal Listing

## **Applications**

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



# Visualization bench



Fully motorized inverted microscope 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.

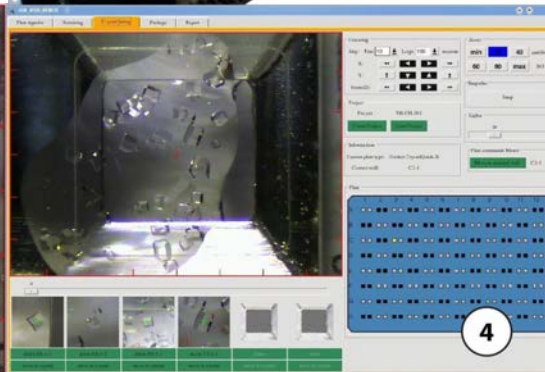
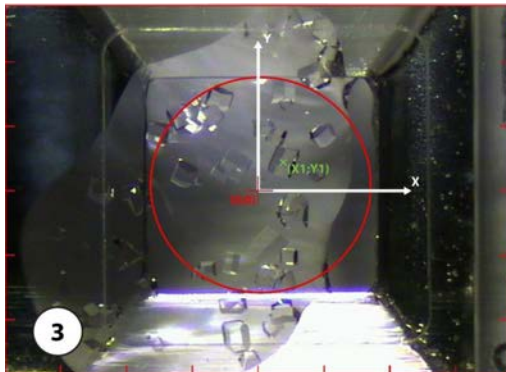
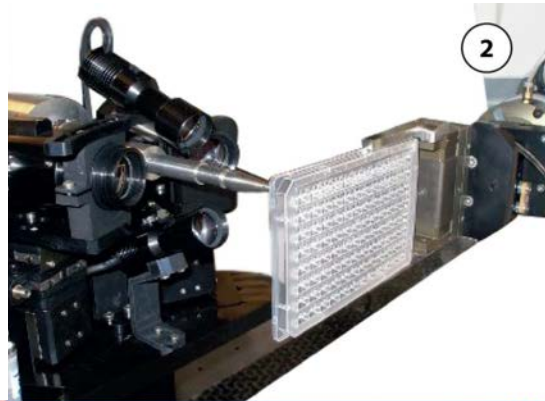


# Crystal Listing

A dedicated microscope can be used off-line for

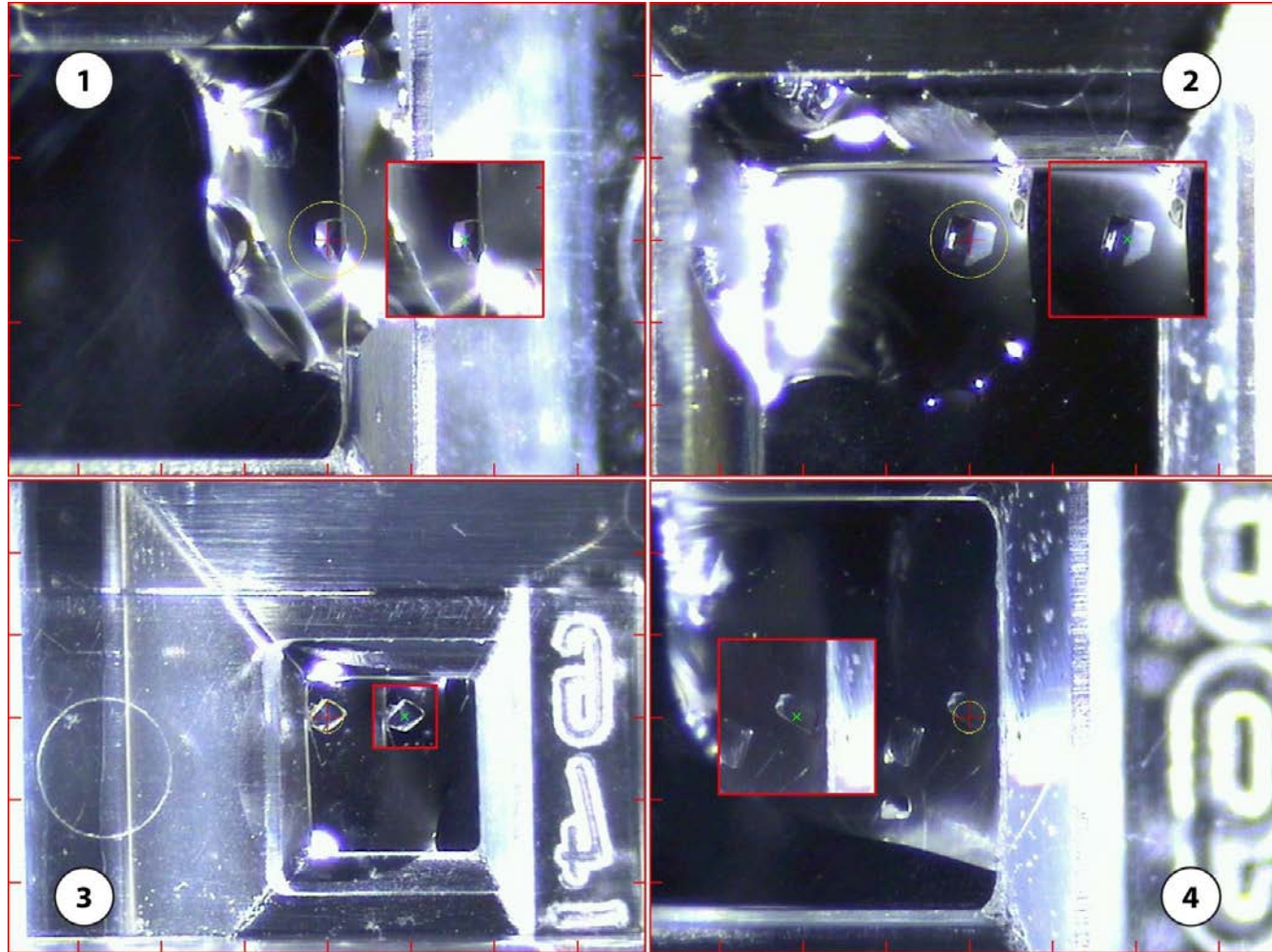
- Automated image recording
- Selection of crystals (one click)

- 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  $500\ \mu\text{m} \times 500\ \mu\text{m}$  saved during the Crystal Listing procedure with G-Rob and bigger images are taken after crystal centering with G-Rob.

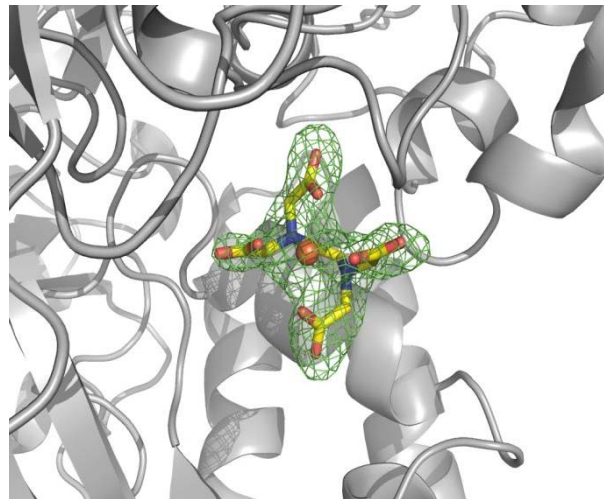
① and ② correspond to Nika-FeEDTA crystals. ③ and ④ are lysozyme crystals. These images correspond to crystals diffracted and used for structure resolutions.



Listing on:	Visualisation bench	G-Rob
Number of samples	44	79
< X > error ( $\mu\text{m}$ )	33	3
< Y > error ( $\mu\text{m}$ )	21	3
< radius > error ( $\mu\text{m}$ )	41	5
X standard deviation ( $\mu\text{m}$ )	17	2
Y standard deviation ( $\mu\text{m}$ )	14	2
radius standard deviation ( $\mu\text{m}$ )	17	3

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

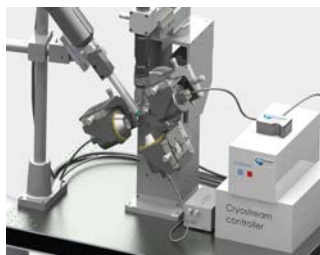
	Lysozyme	NikA-FeEDTA
<b>Data collection</b>		
Resolution (last shell) ( $\text{\AA}$ )	2.10	2.45
Completeness (last shell) (%)	71.6 (75.0)	68.4 (71.4)
$R_{\text{sym}}^{\text{a}}$ (last shell) (%)	13.9 (38.5)	13.8 (41.6)
$I/\sigma$ (last shell) (I)	5.61 (2.75)	4.45 (2.20)
<b>Refinement</b>		
$R_{\text{work}}^{\text{b}}$ (%)	18.82	17.39
$R_{\text{free}}^{\text{c}}$ (%)	23.11	25.07



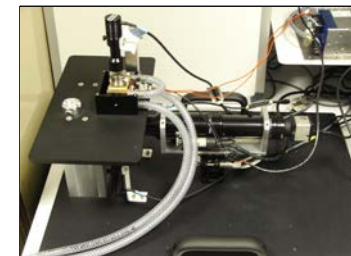
Fe(III)-EDTA binding site in NikA. Omit Fourier electron density map of Fe-EDTA contoured at 3 sigma



**VisuBench &  
Crystal-Listing**



**Misc**



**OptiCryst**

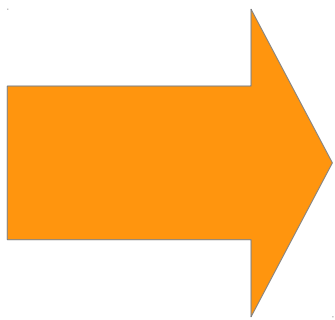
# MiSC: a MicroSpectroPhotometer

## **MiSC**

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

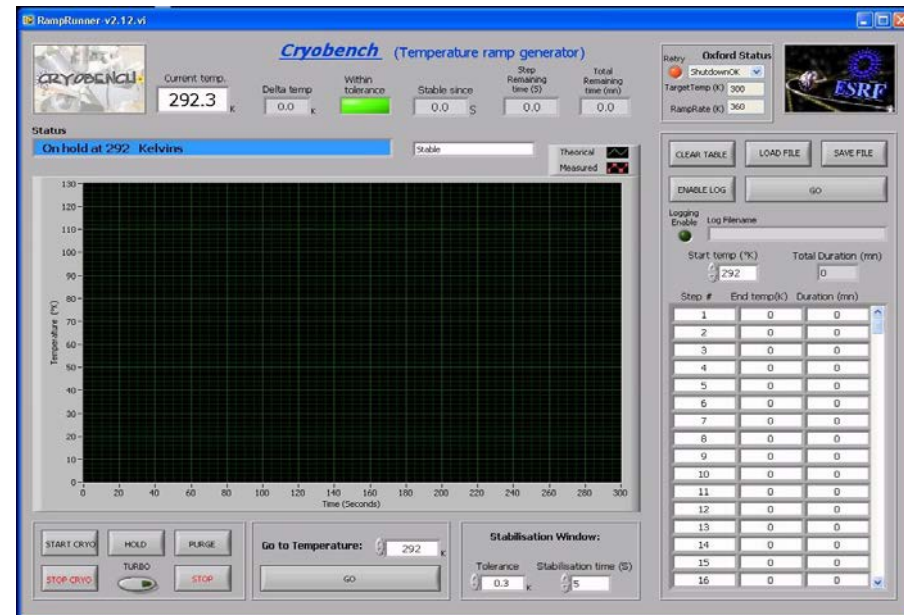
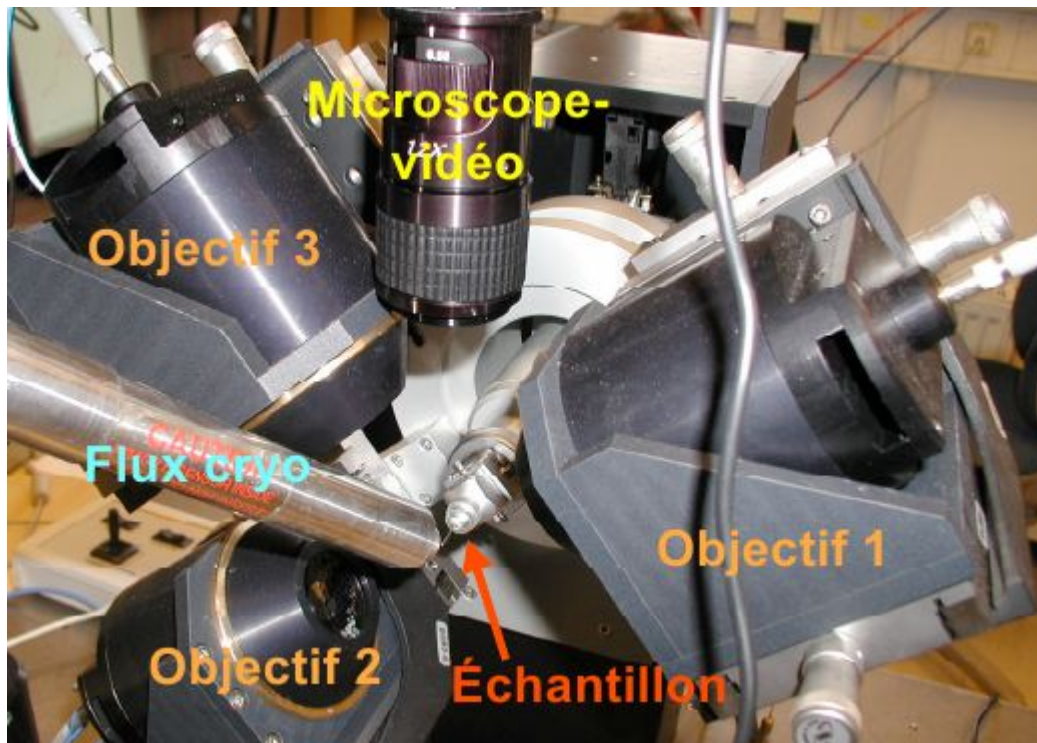
## **Applications**

- Fluorescence measurements
- Absorption measurements
- Synchronized experiment



# The CryoBench at the ESRF

(A. Royant team at IBS – ESRF/ID29)

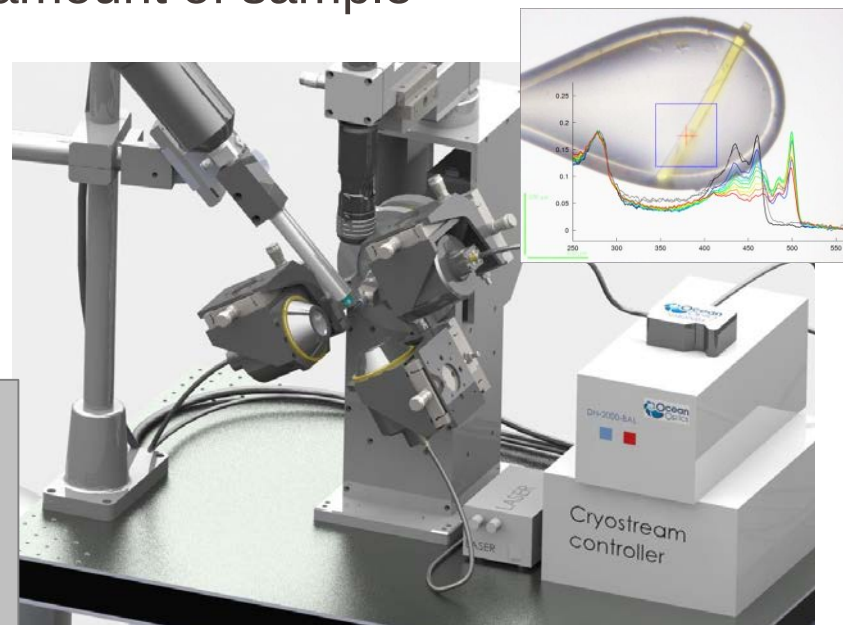


D. Bourgeois, X. Vernede, V. Adams, E. Fioravanti & T. Ursby (2002).  
"A microspectrophotometer for UV-visible absorption and fluorescence studies of protein crystals." *J. Appl. Cryst.* 35, 319-326.

# MiSC

## A Micro-Spectrophotometer for Crystals

- **UV/Visible absorption**, measured on the 200-1100 nm range
- **Fluorescence measurements** at 90° on micro-amount of sample
- **Samples can be:**
  - Crystal down to 10  $\mu\text{m}$
  - Nanoliters solutions
- **Spectrometer** : 200-1025 nm range



**Based on the CryoBench (IBS & ESRF/ID29)**

**Stand alone version**

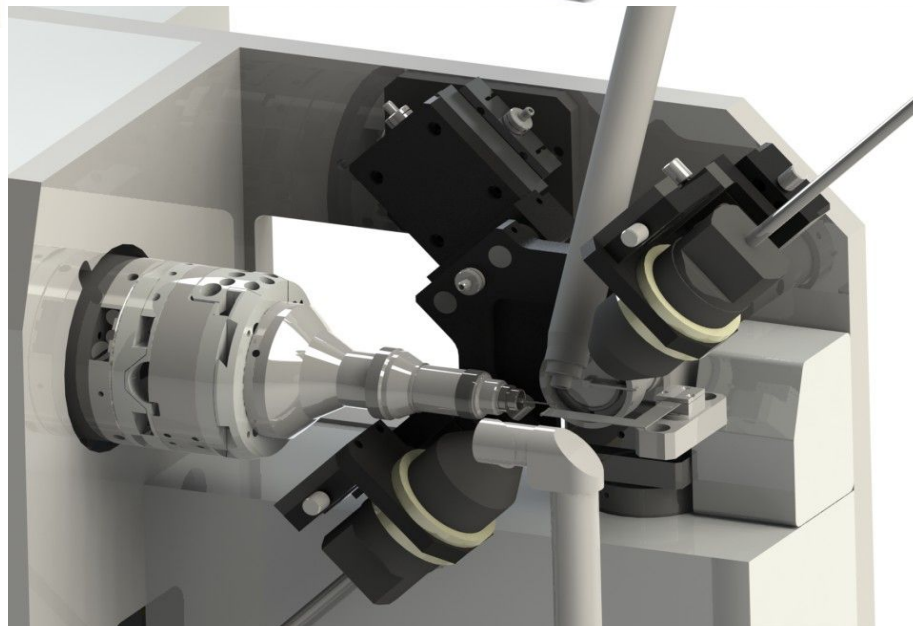
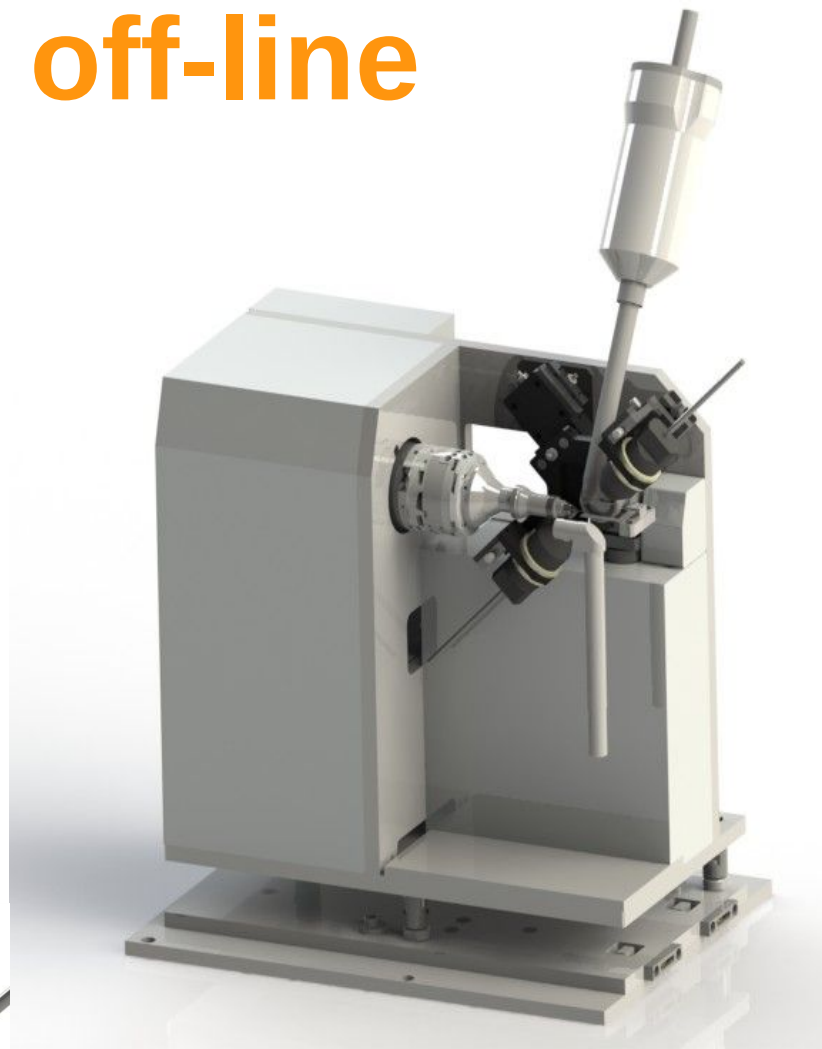
commercialized by NatX-ray

**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**

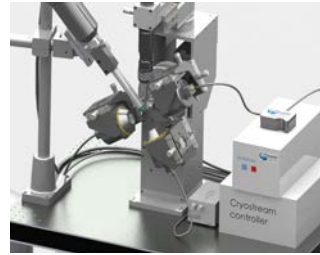
# MiSC: on-live vs off-line



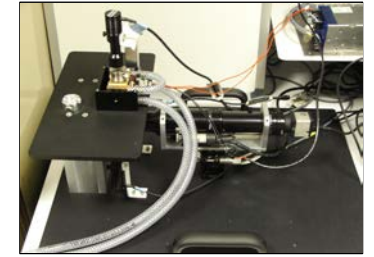
Detector as close as 40 mm  
Access for sample changer



**VisuBench &  
Crystal-Listing**



**Misc**



**OptiCryst**

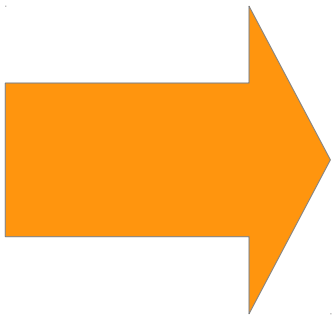
# OptiCryst

## **OptiCryst: a crystal optimization bench**

- Inverted microscope
- Temperature control
- Dialysis

## **Applications**

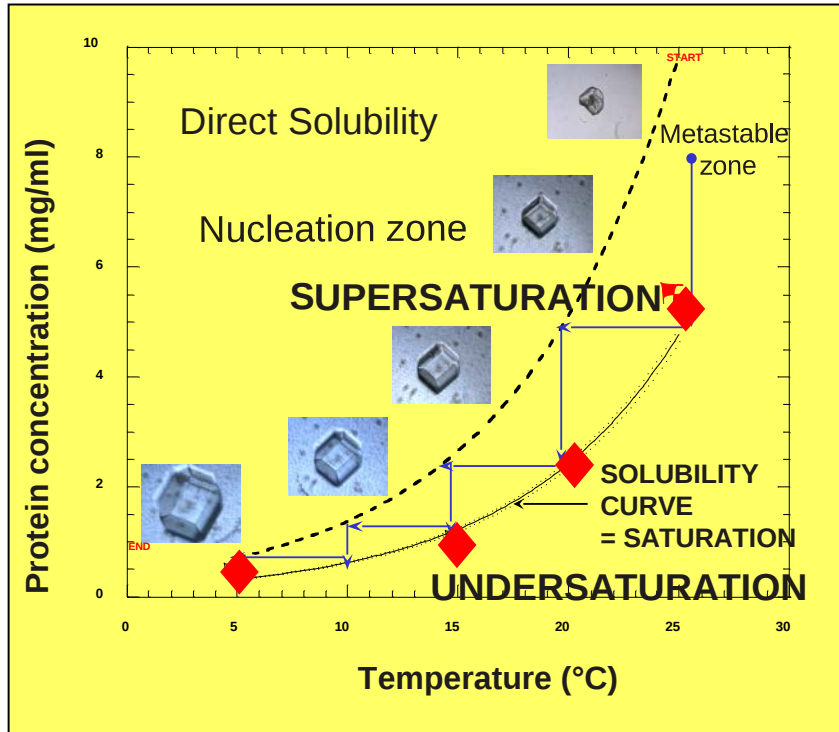
- Crystallization
- Crystal quality improvement
- Size optimization



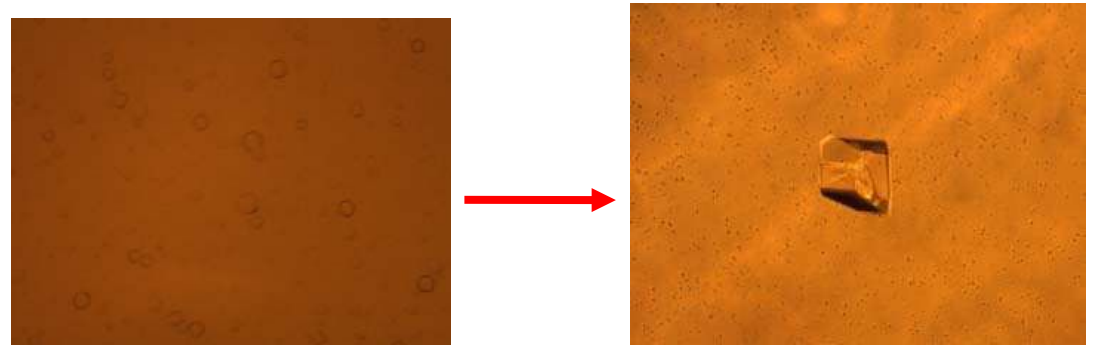


# OptiCryst

A bench for crystals optimization

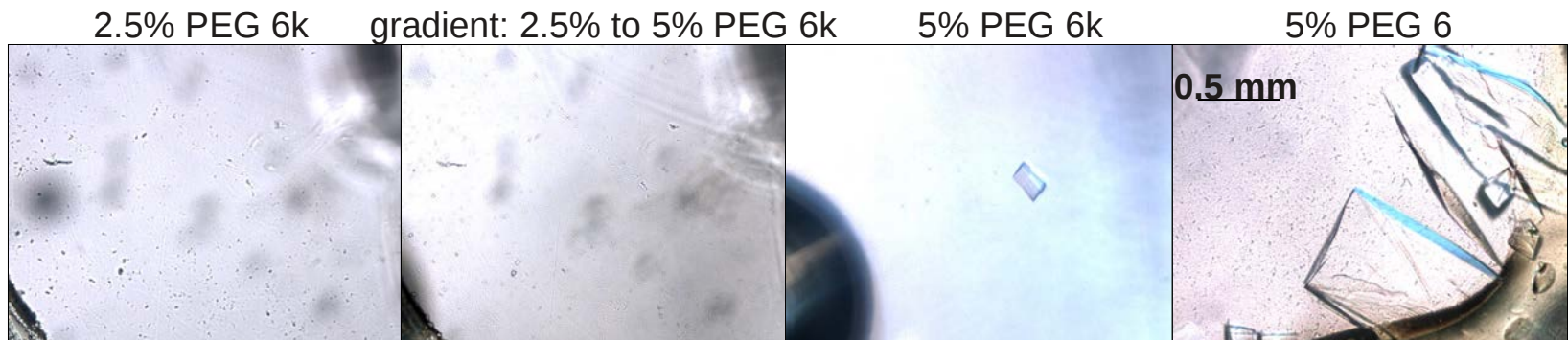


25PI of protein, prot. Conc. 18 mg/ml  
(NH<sub>4</sub>)<sub>2</sub>SO<sub>4</sub> 2M, Bicine 100 mM, pD 8.0, Tinit = 20°C  
Crystal nucleation & Growth at 22.5°C



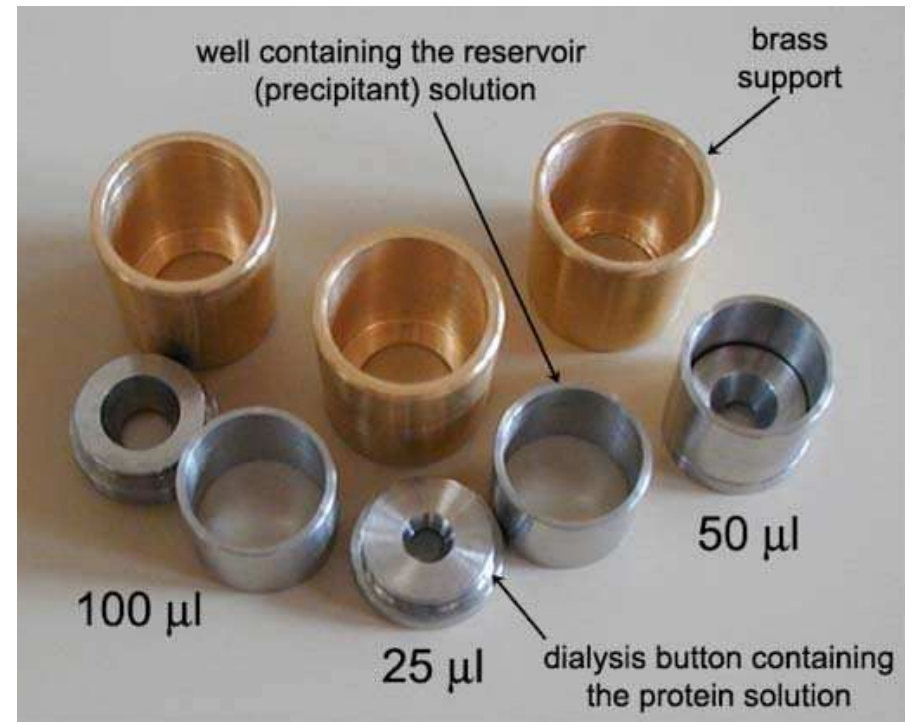
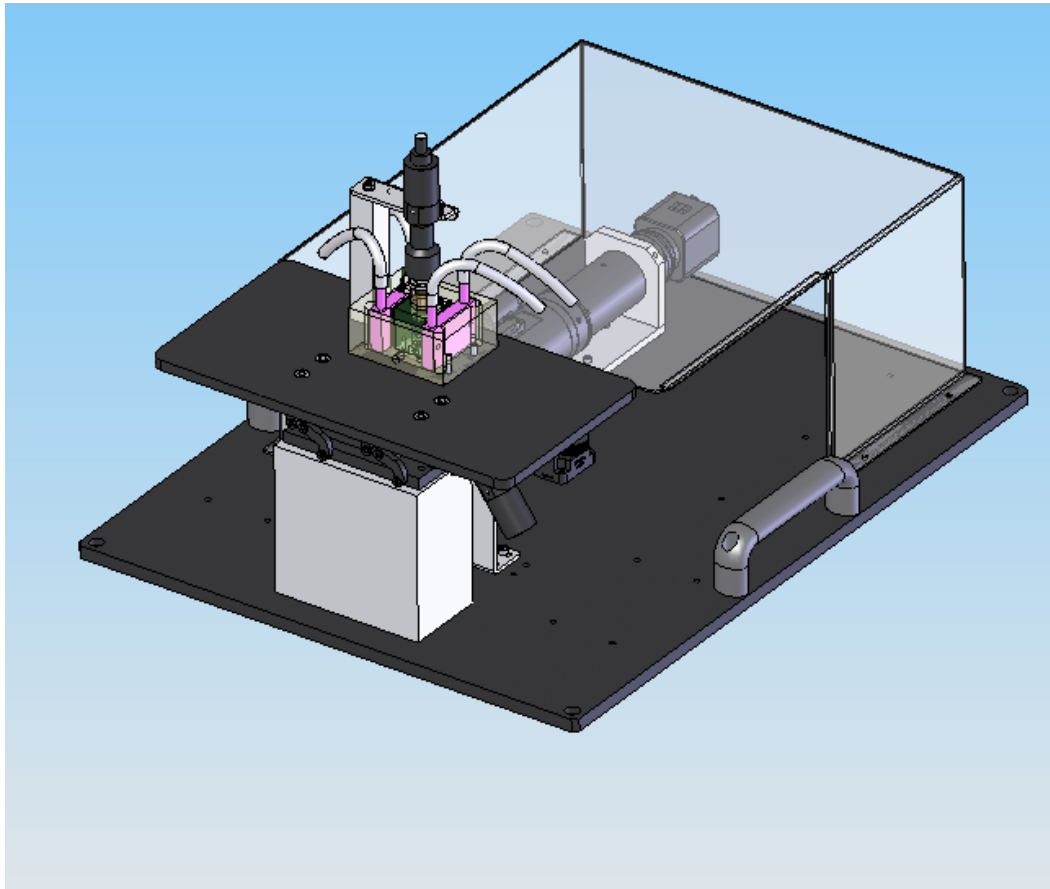
*Budayova-Spano et al., Acta Cryst. D63, 2007, 339-347*  
*Oksanen et al., J. Royal Society Interface 6(S5), 2009, S599-S610.*

## Case of hyperthermophile lactate dehydrogenase



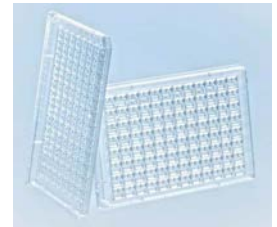
# OptiCryst

A bench for crystals optimization



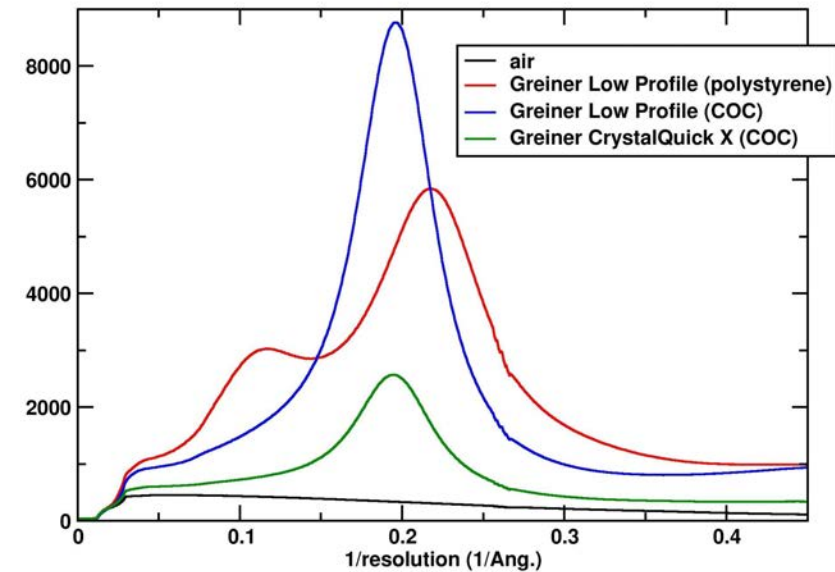
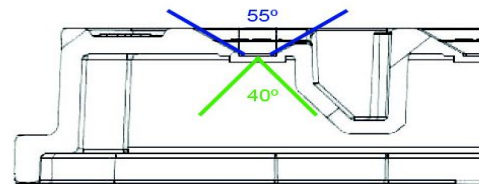
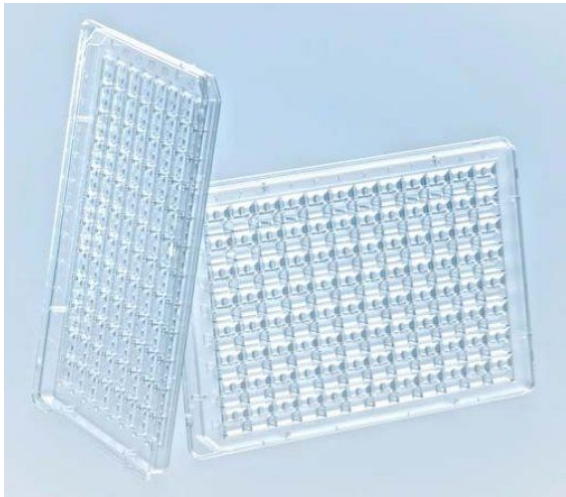
# Consumables & Accessories

- 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



## CrystalQuick™X plate

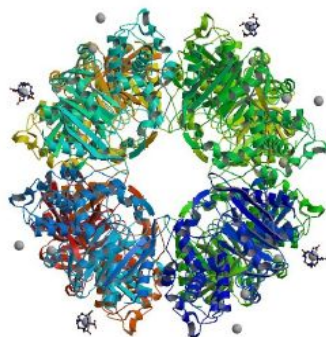
- Made with "low birefringence" COC
- 80 degrees of angular range
- Compatible with any crystallization robot
- Reduced bottom thickness
  - 250-300  $\mu\text{m}$  instead of 1000  $\mu\text{m}$  for other plates
  - Lower X or UV scattering
  - Higher brightness in visible range



# Phasing compounds



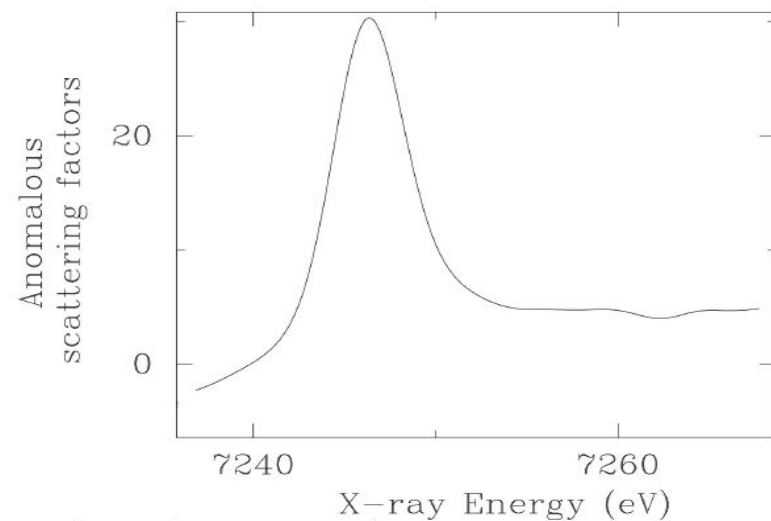
From R Kahn team  
at the IBS



(2qmi)

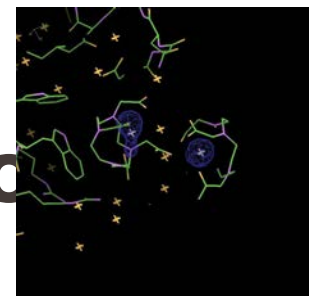


(2bh8)

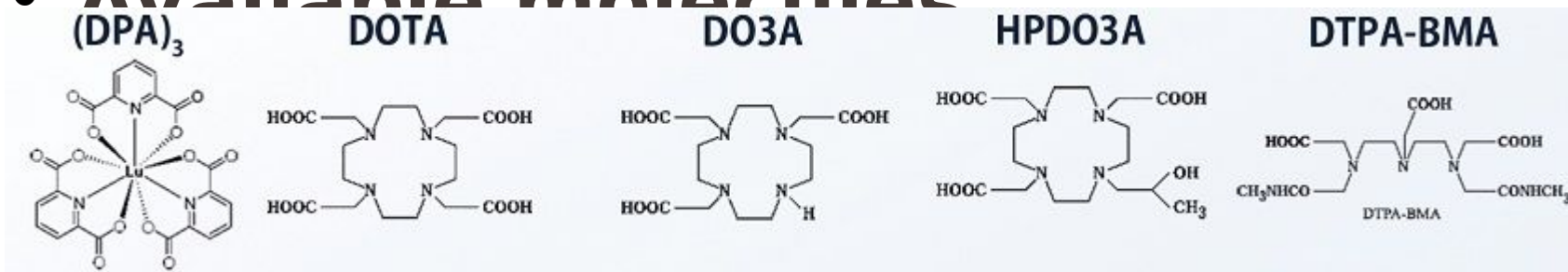


- **Lanthanide complex for anomalous phasing**

- HUGE anomalous signal
- Phasing, even at room temperature
- Successfully used to solve difficult structures



- **Available molecules**



X. Vernede  
Y. Sallaz-Damaz

N. Larive  
D. Mezel

For testing the in-house G-Rob system: EPFL, Switzerland

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

In both case contact: [jean-luc.ferrer@ibs.fr](mailto:jean-luc.ferrer@ibs.fr)

E. Girard  
A. Royant

M. Trivas  
R. Richaud

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

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