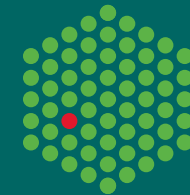


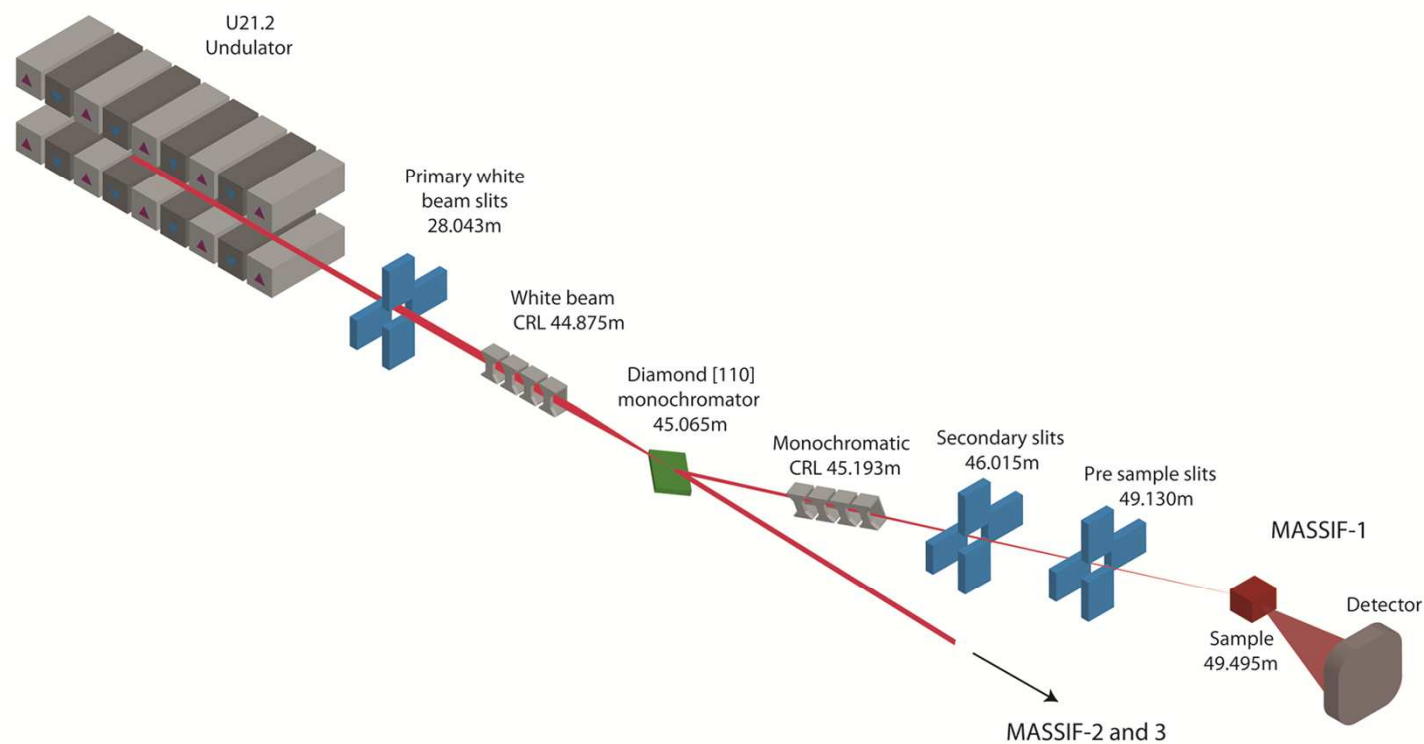
MASSIF-1: an autonomous intelligent beamline

Matthew W. Bowler and Didier Nurizzo



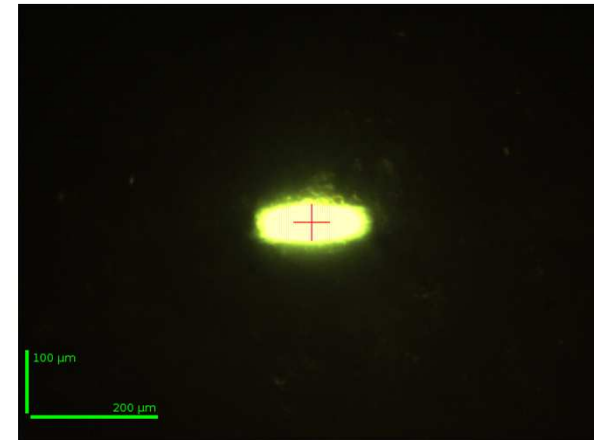
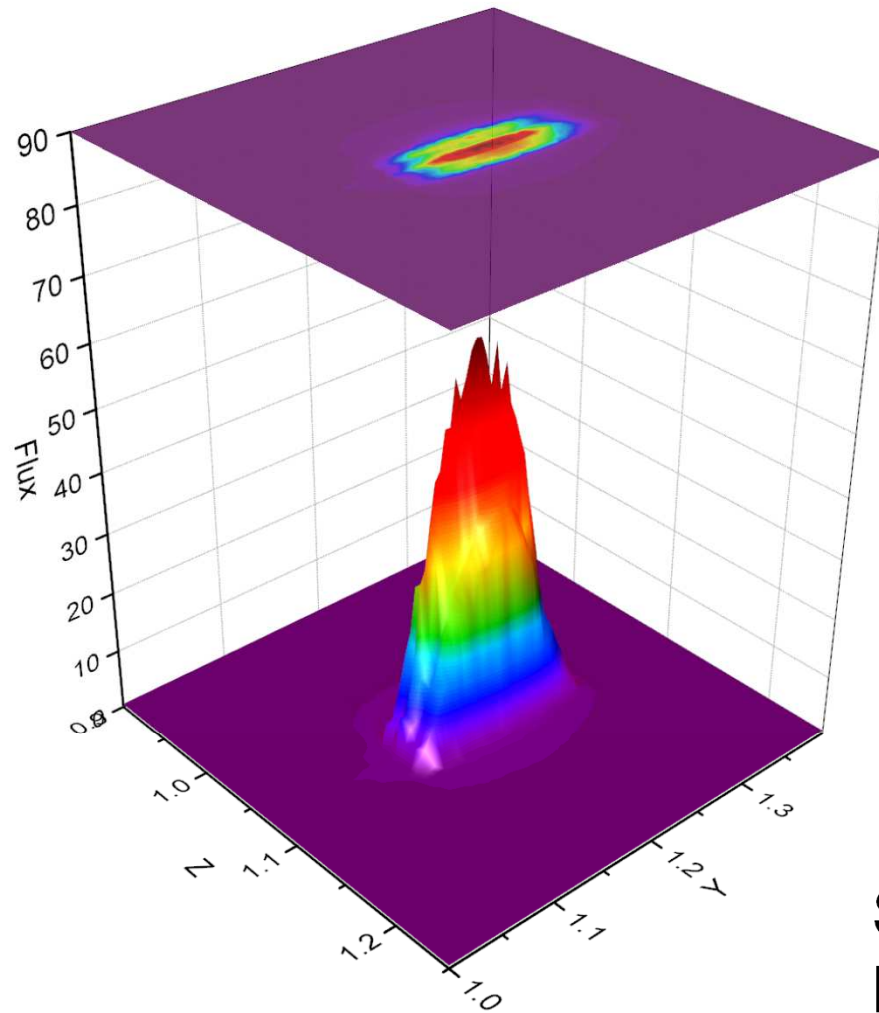
EMBL





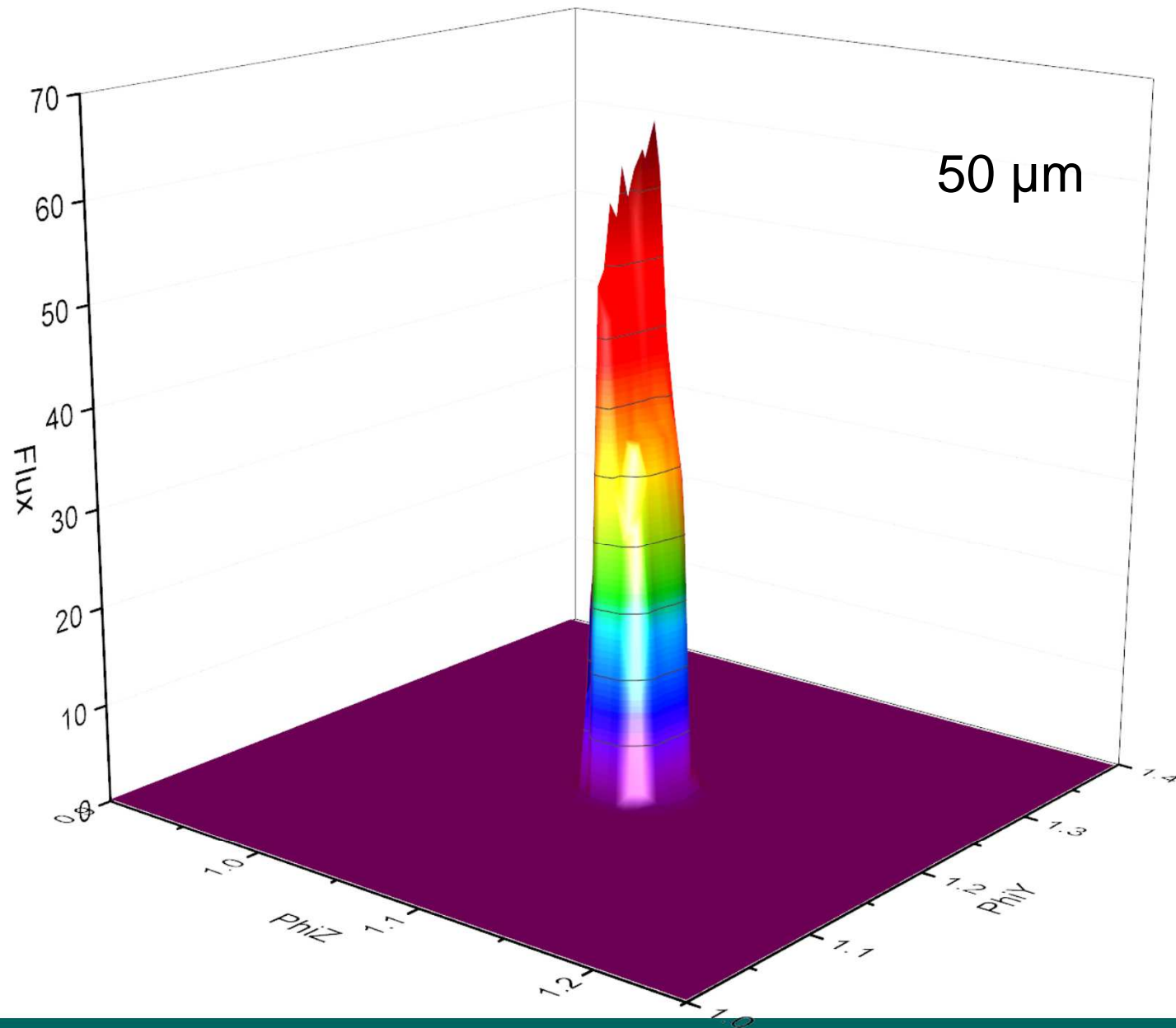
Bowler MW, Nurizzo D *et al.* (2015). MASSIF-1: A beamline dedicated to the fully automatic characterisation and data collection from crystals of biological macromolecules, *J. Synch. Rad.* **22**, 1540-1547

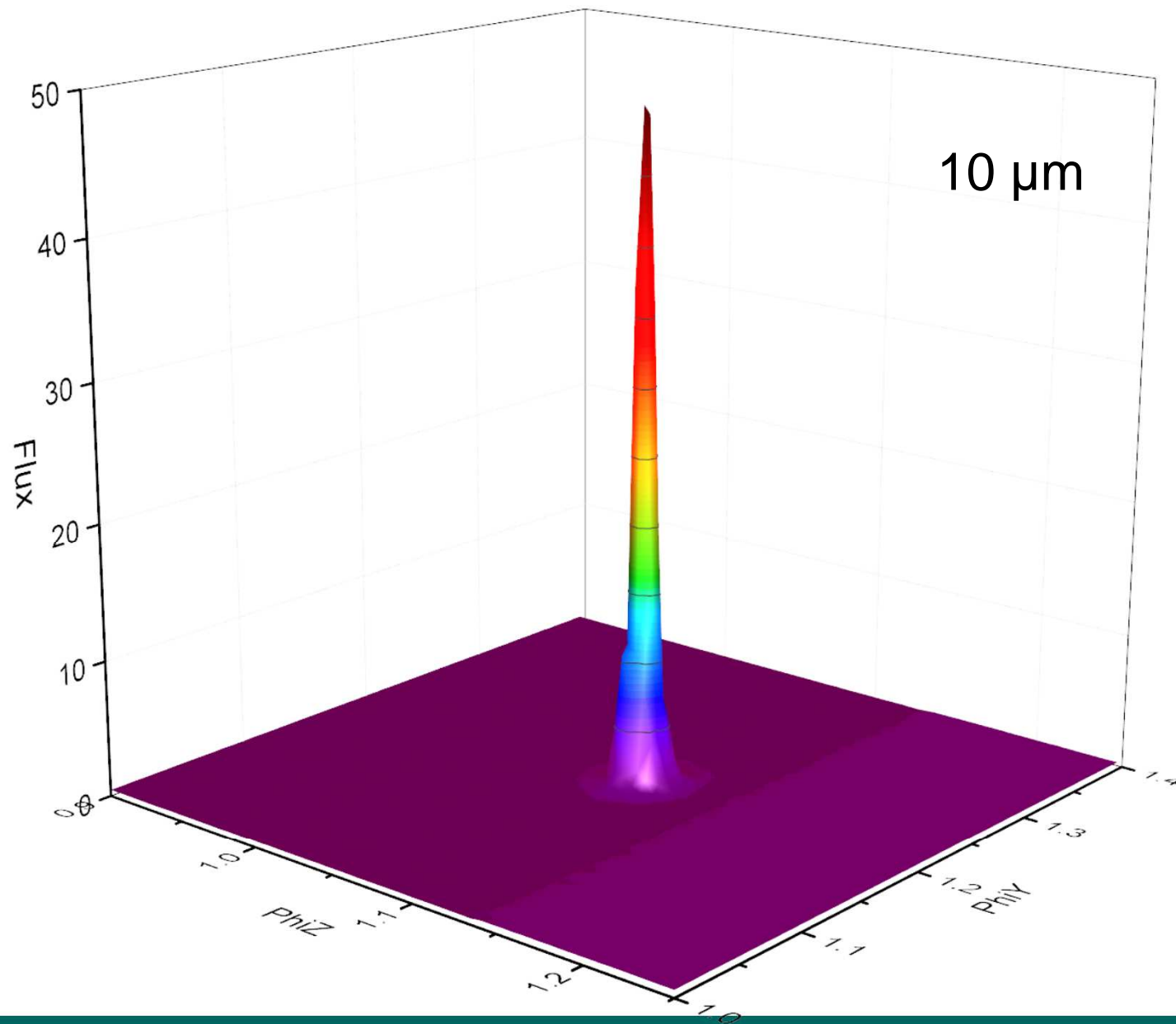
MASSIF1

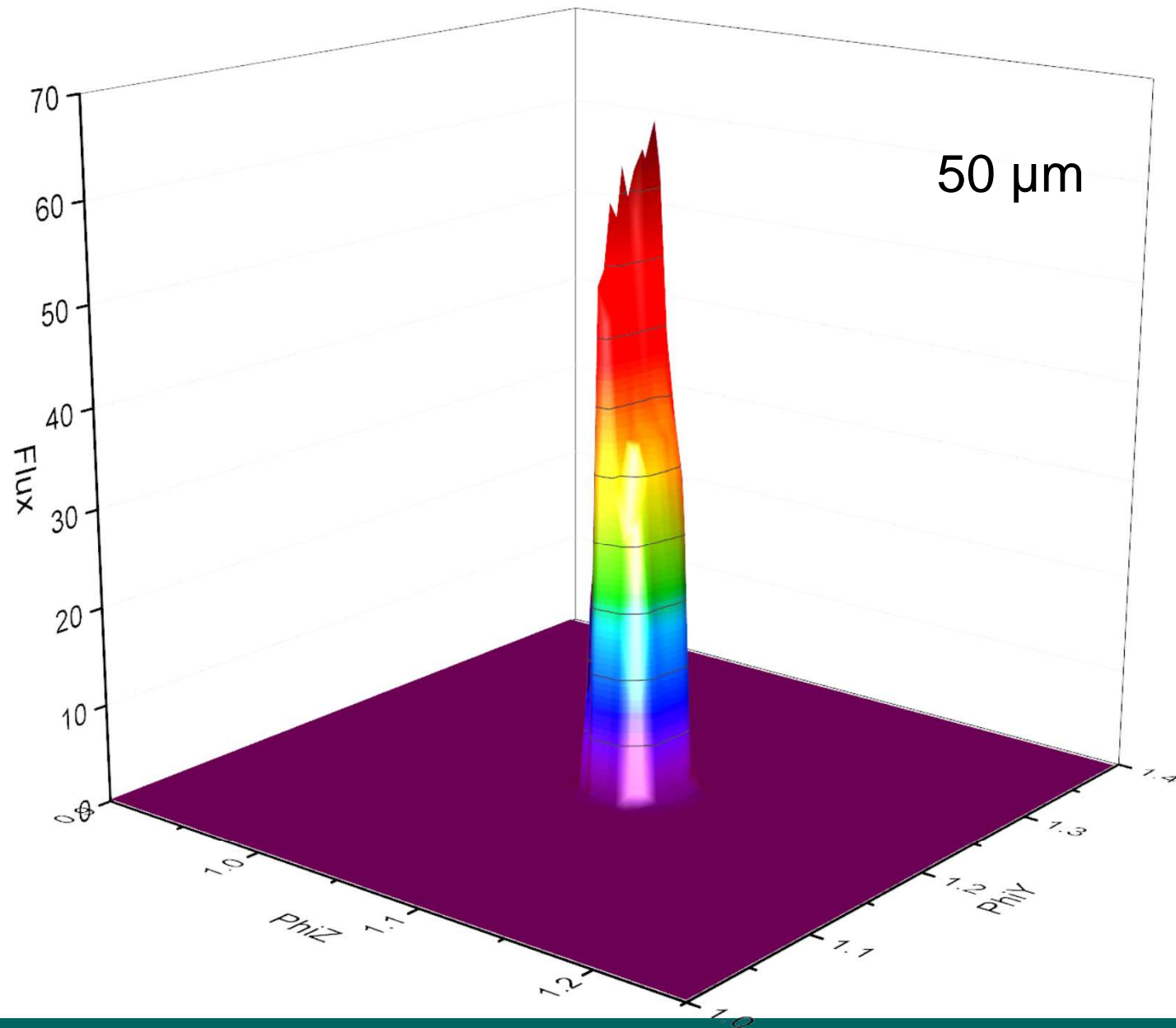


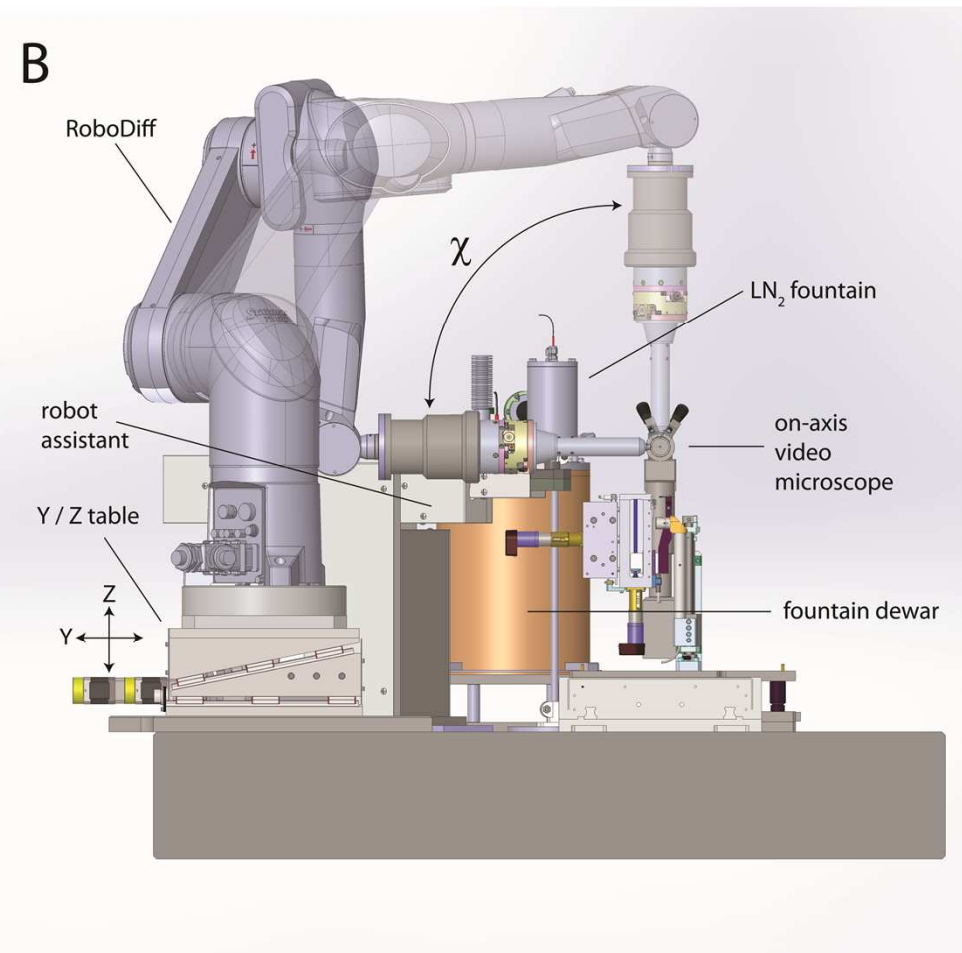
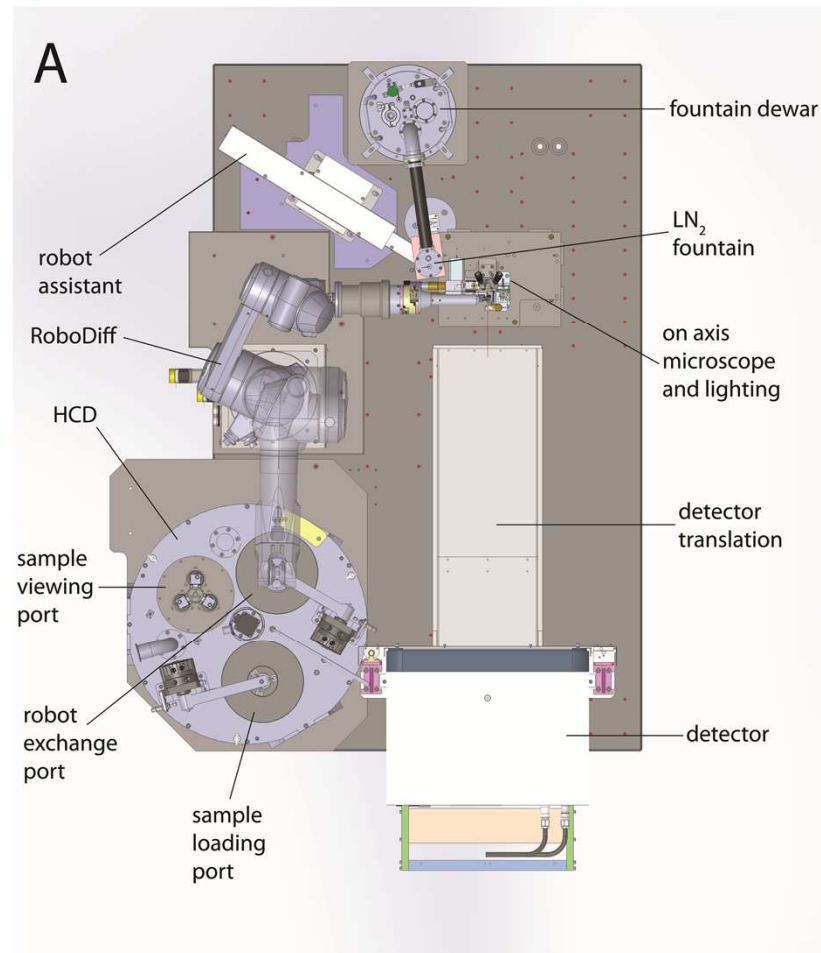
Size: 100 x 65 μm^2 FWHM

Flux: 3.1×10^{12} ph/s



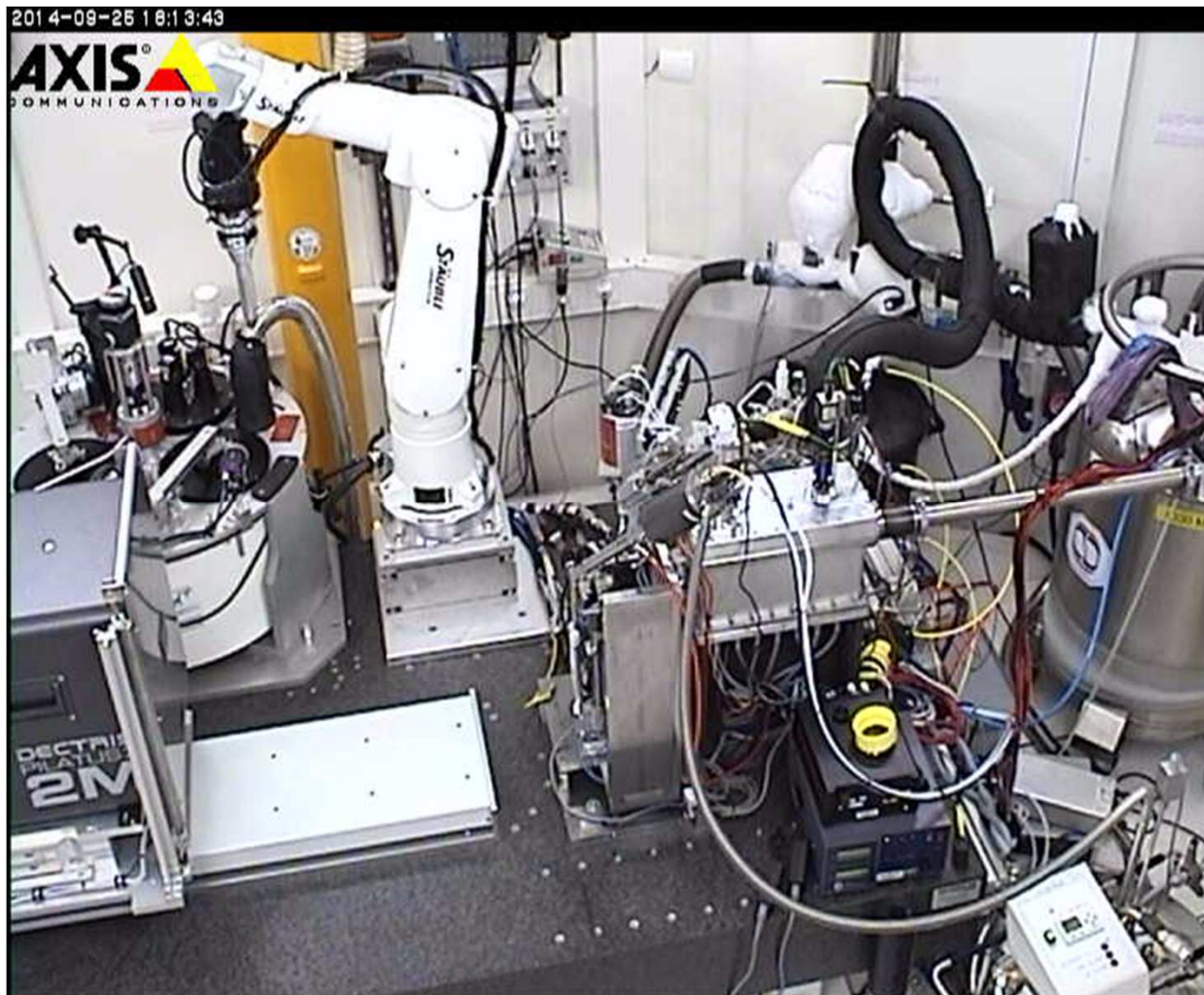




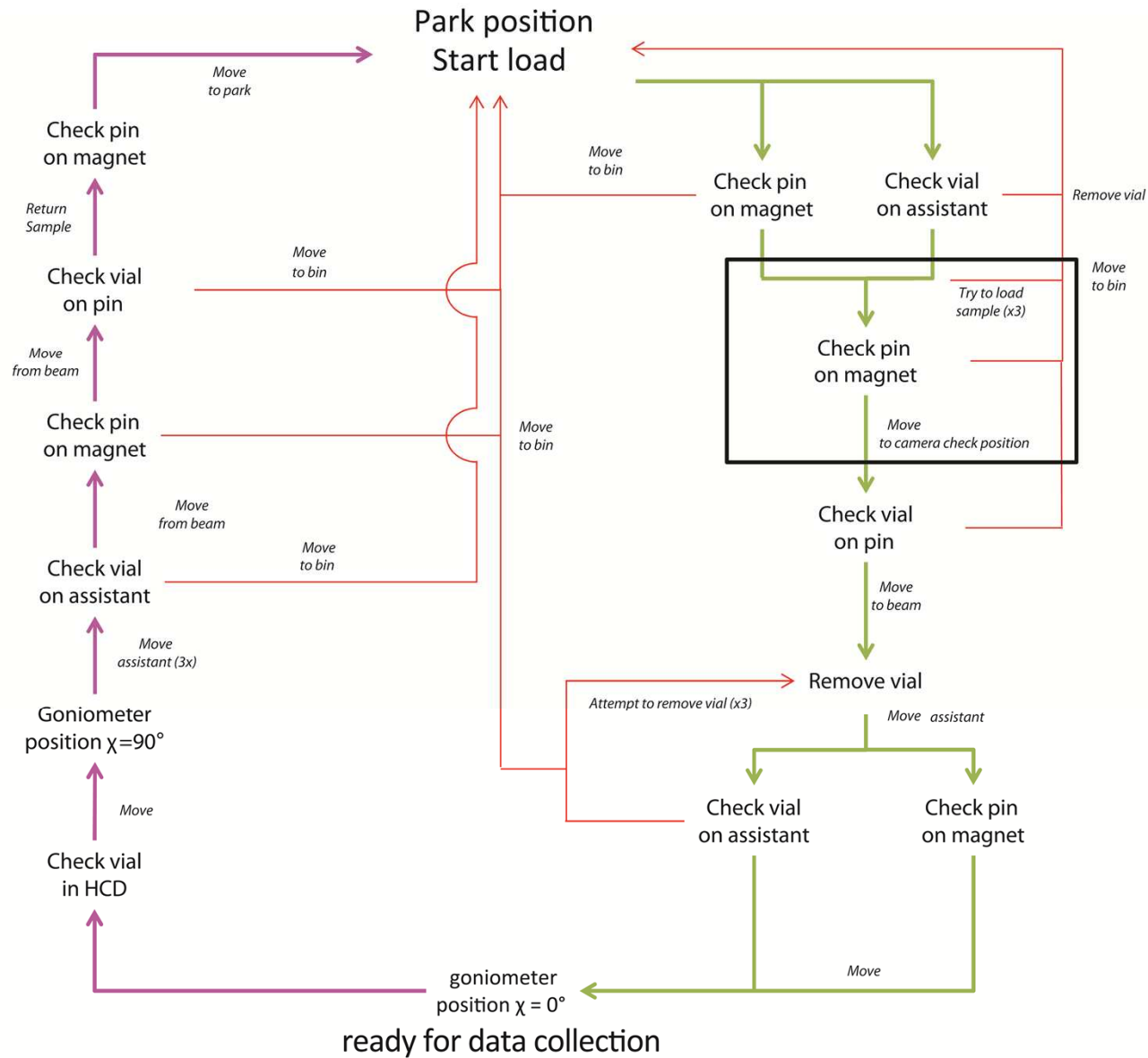


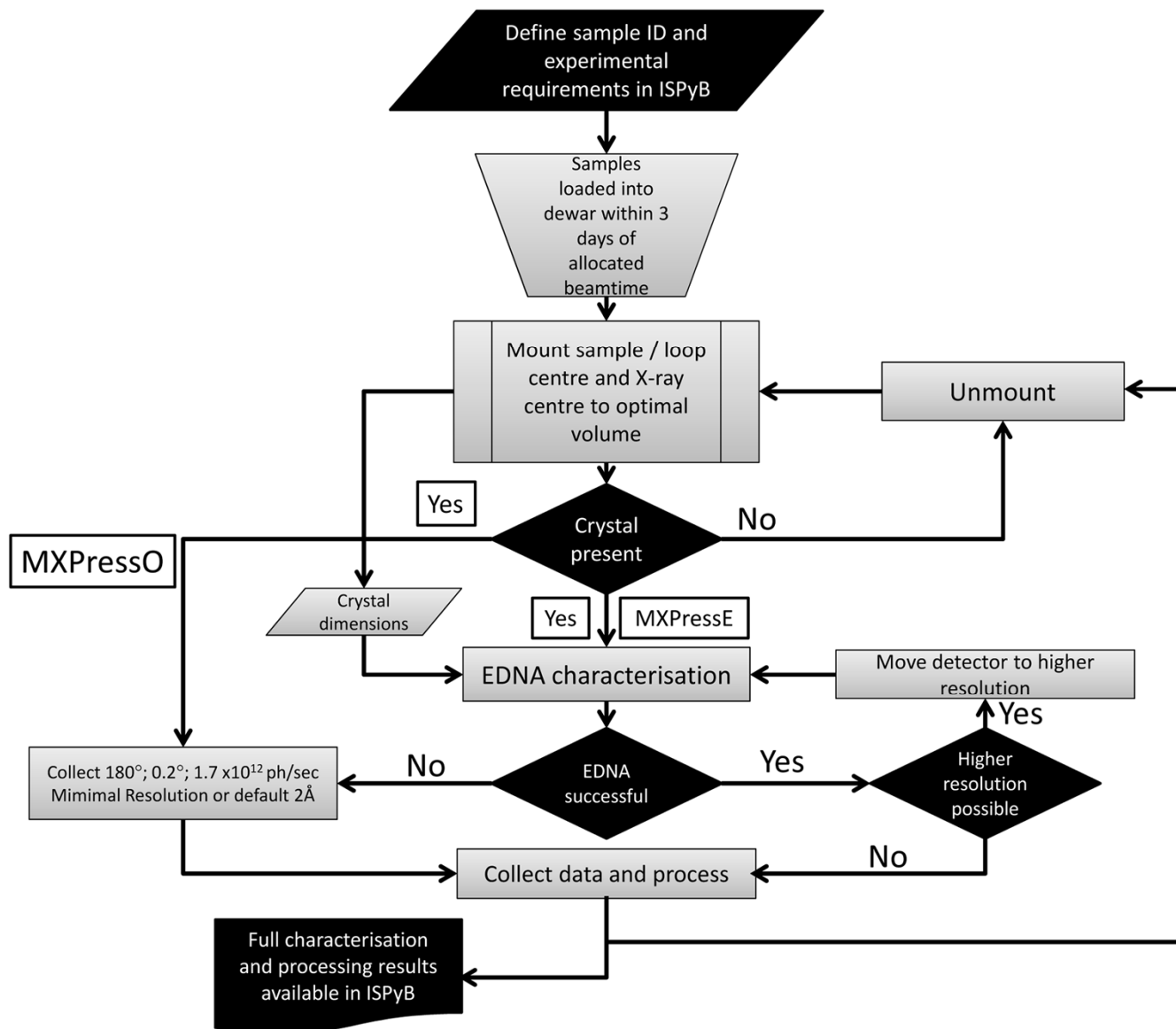
RoboDiff

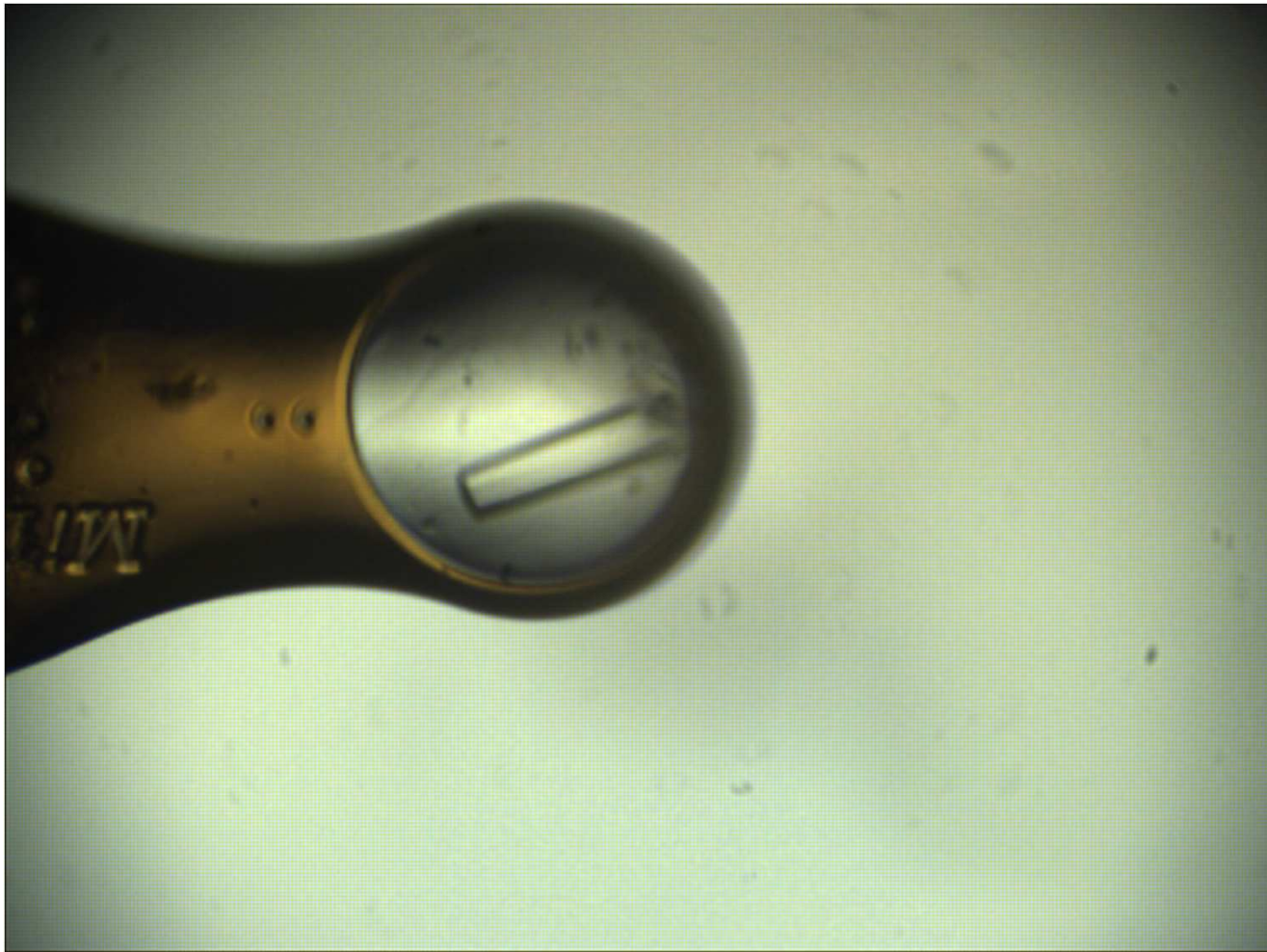
Nurizzo D, Bowler MW, *et al.* (2016), RoboDiff: combining a sample changer and goniometer for highly automated macromolecular crystallography experiments *Acta Cryst* **D72** 966-975



Nurizzo D, Bowler MW, *et al.* (2016), RoboDiff: combining a sample changer and goniometer for highly automated macromolecular crystallography experiments *Acta Cryst D* **72** 966-975

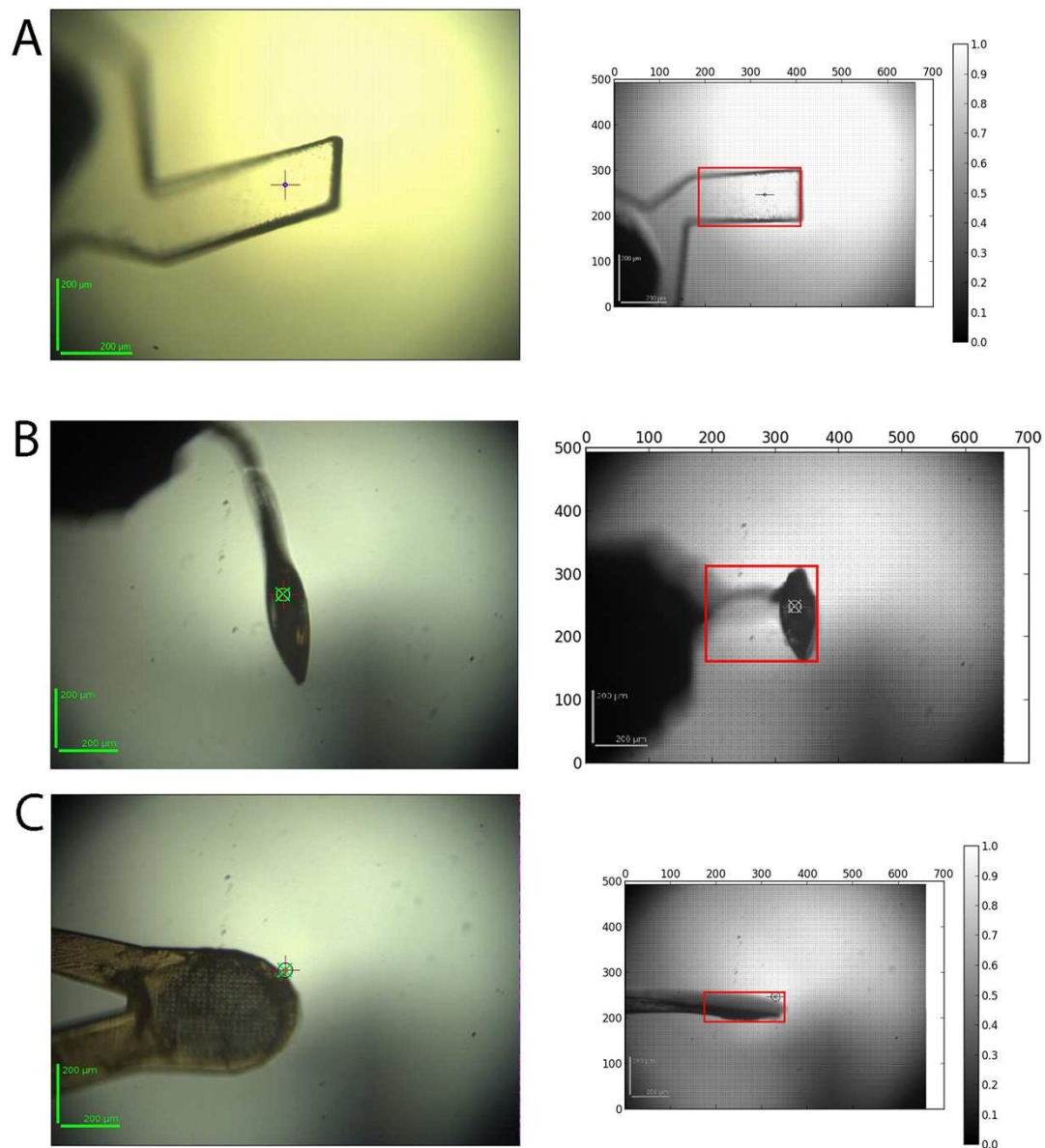


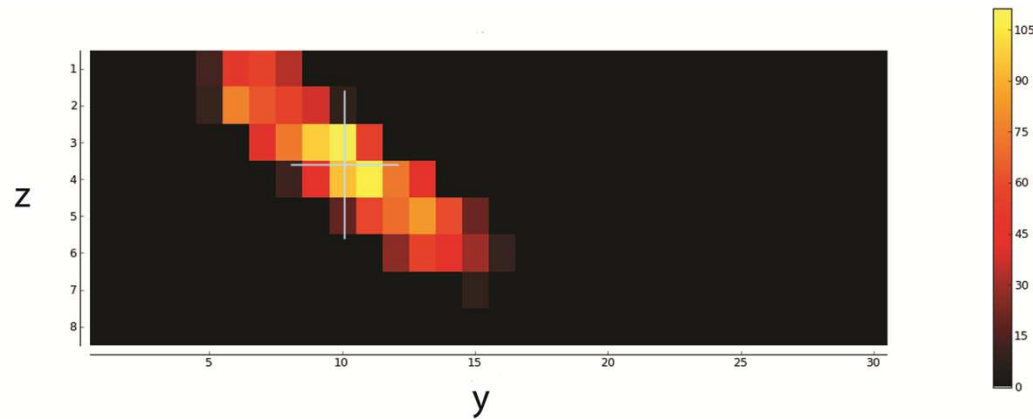






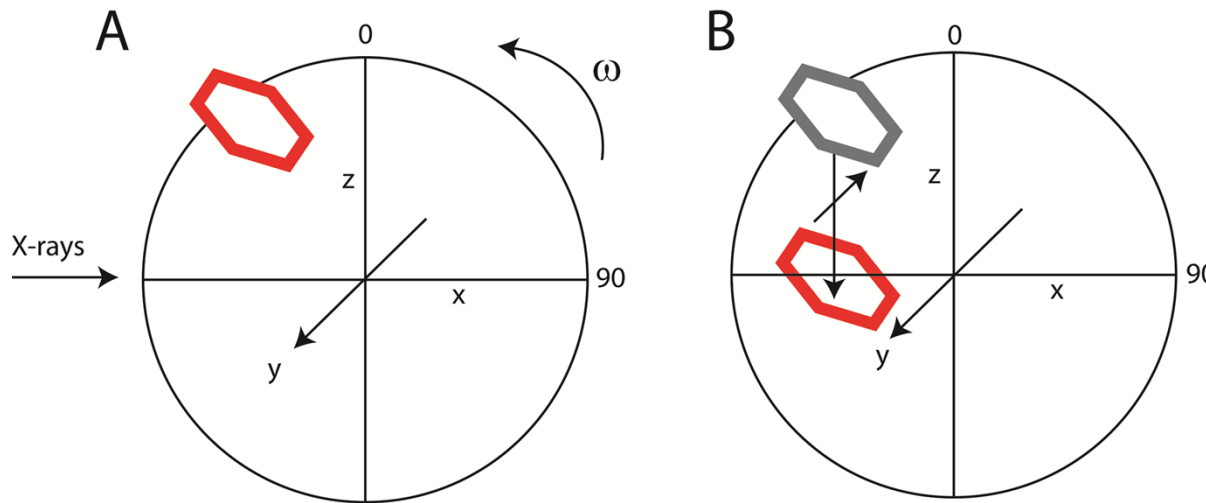
Svensson, O., Monaco, S., Popov, A., Nurizzo, D. and Bowler, M. W. (2015)., Fully automatic characterization and data collection from crystals of biological macromolecules. *Acta Cryst.* **D71**, 1757-1767

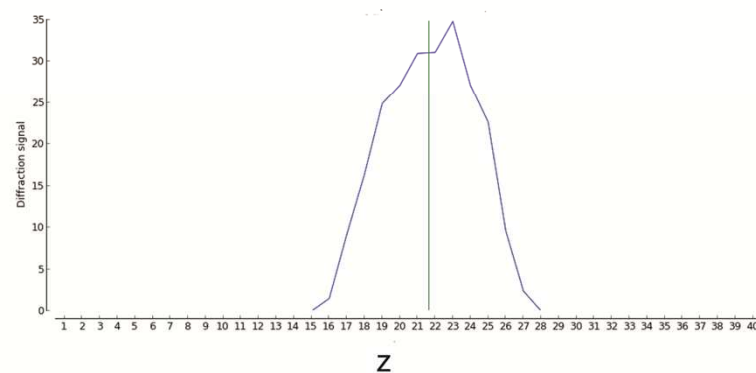
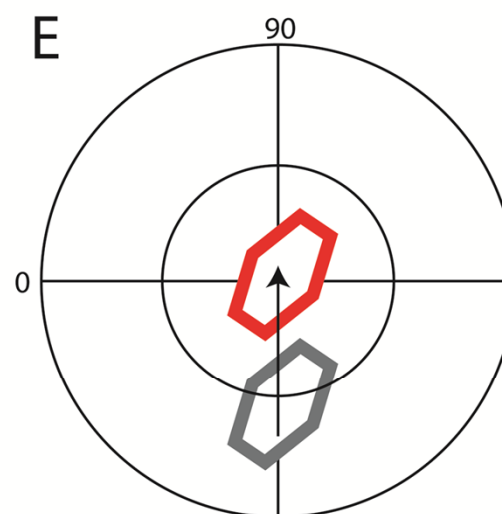
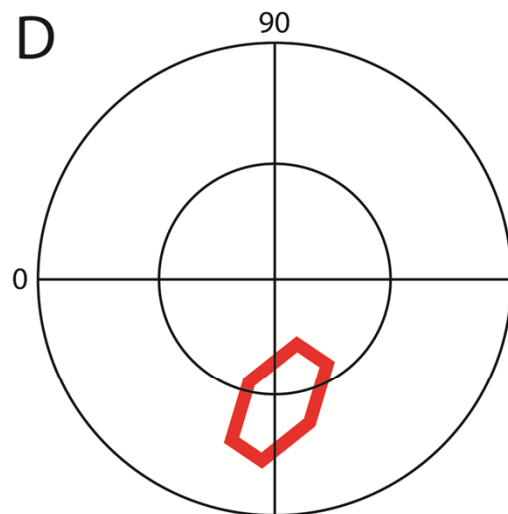




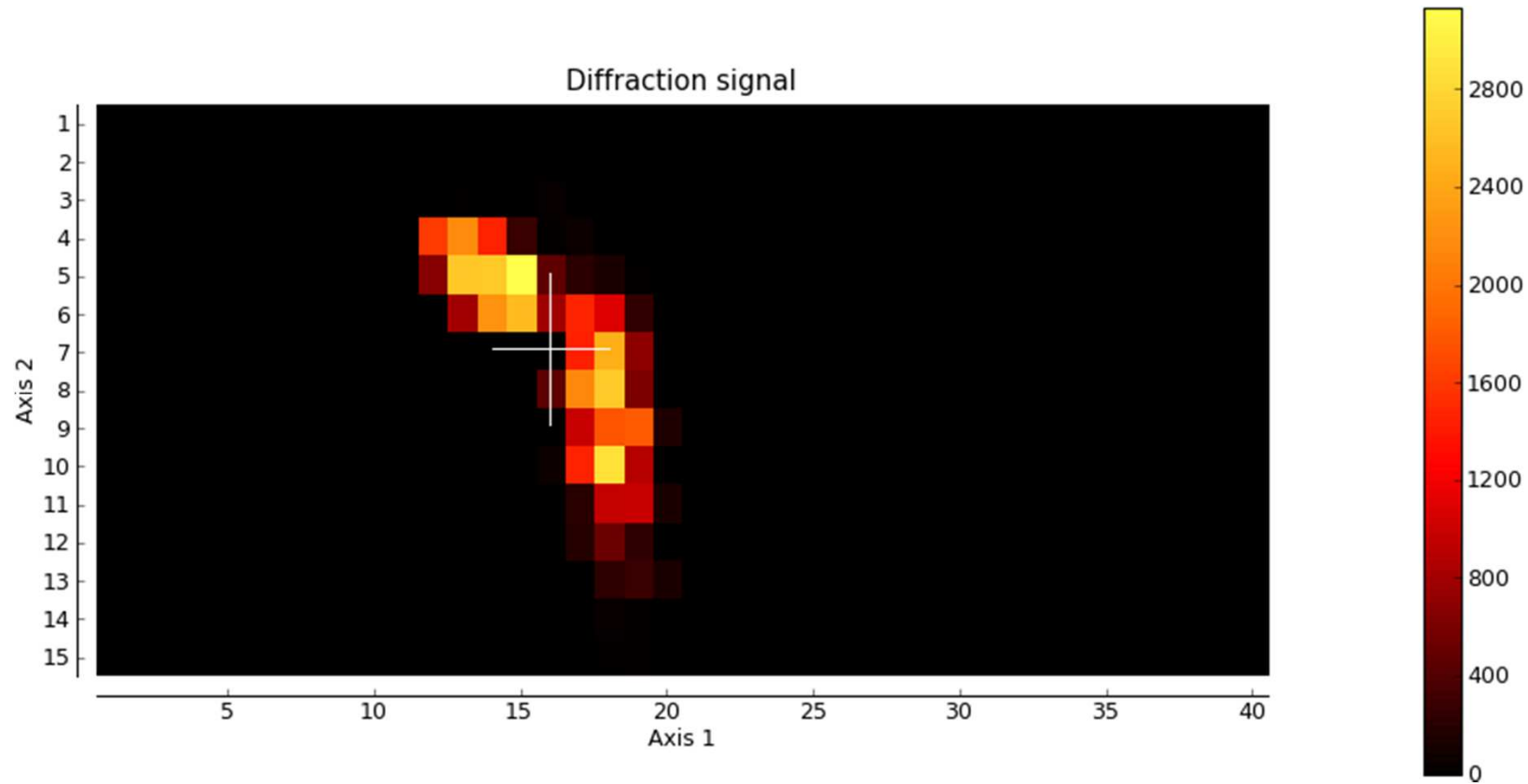
Software routines locate crystals and centre to best volume.

Characteristics such as beam size and flux as well as crystal volume lead to highly optimised data collection



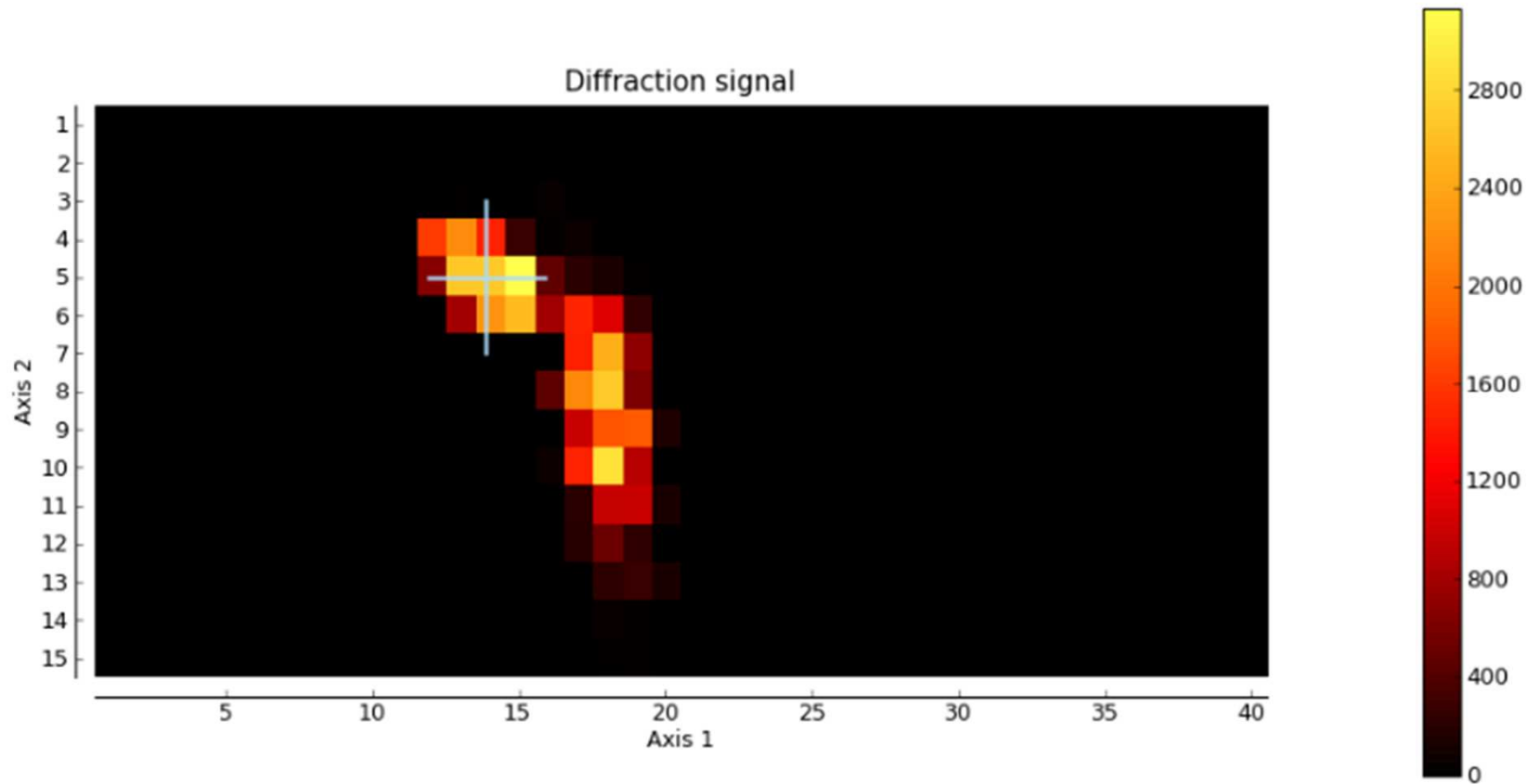


COG determination

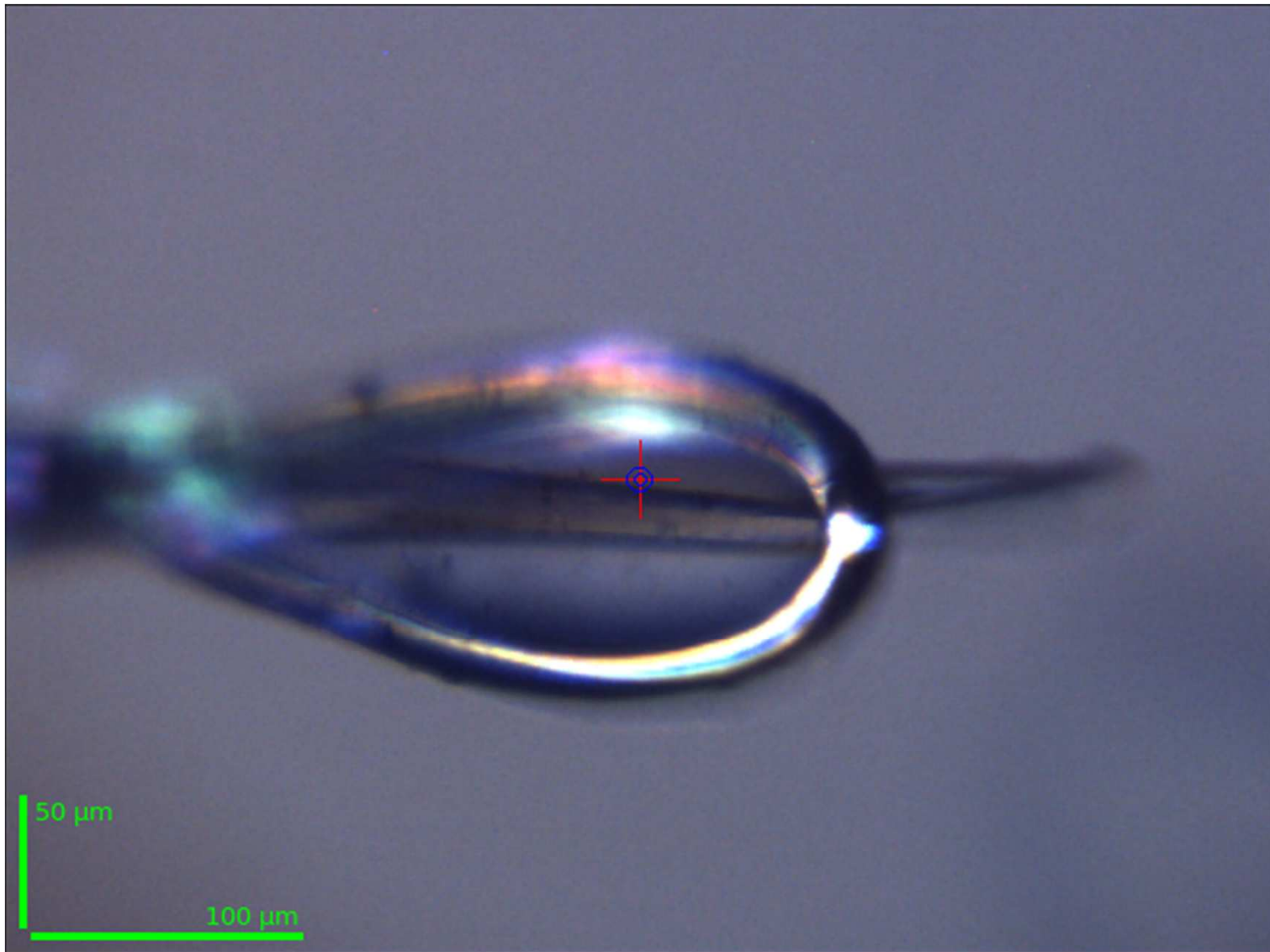


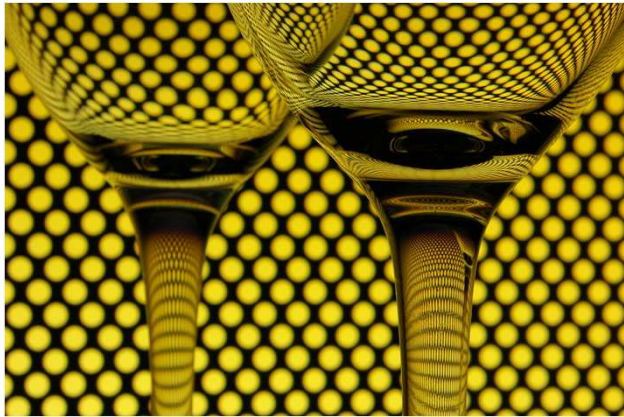
Svensson, O., Monaco, S., Popov, A., Nurizzo, D. and Bowler, M. W. (2015), The fully automatic characterization and data collection from crystals of biological macromolecules. *Acta Cryst.* **D71** 1757-1767

COG determination



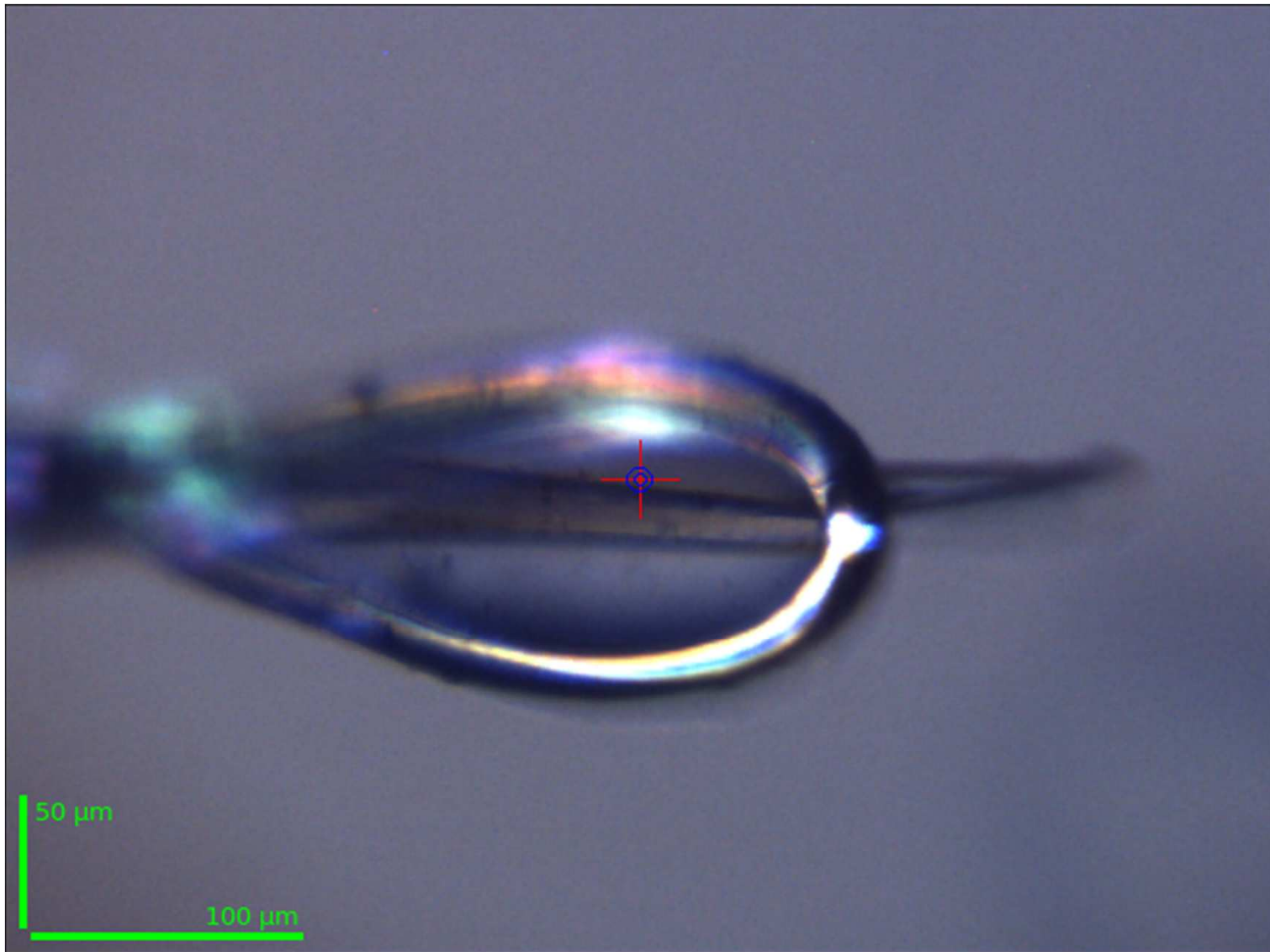
Svensson, O., Monaco, S., Popov, A., Nurizzo, D. and Bowler, M. W. (2015), The fully automatic characterization and data collection from crystals of biological macromolecules. *Acta Cryst.* **D71** 1757-1767

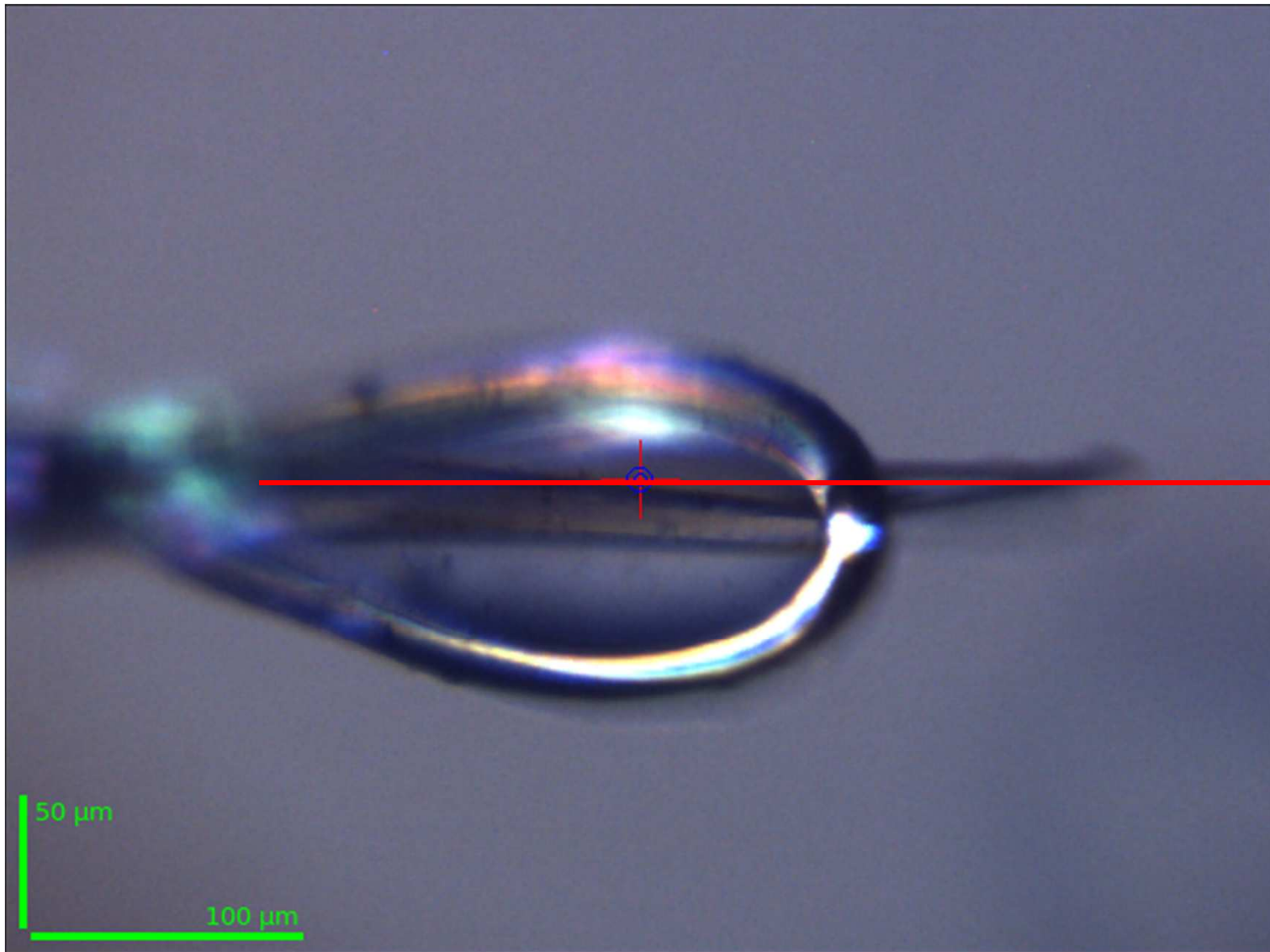






“Fata Morgana”



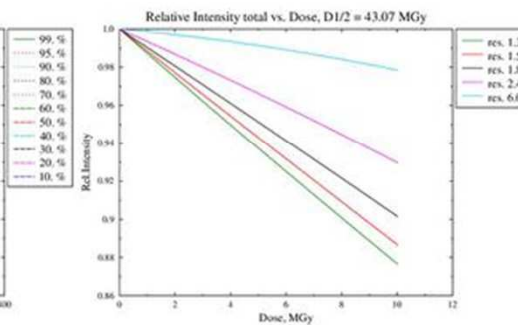
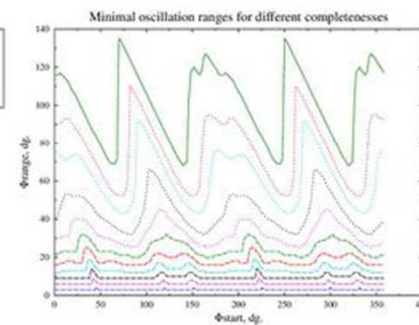
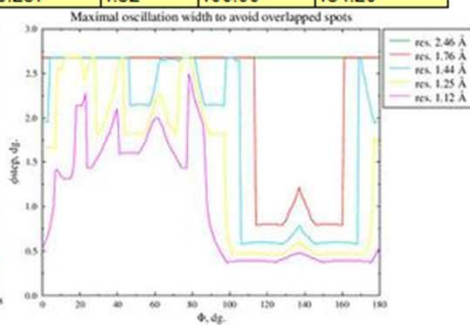
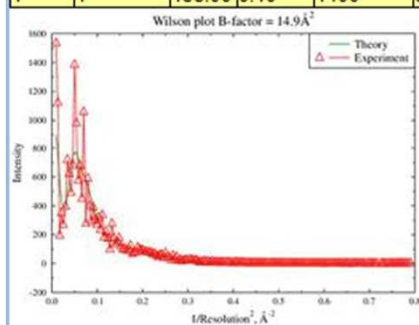


space group	data	multiplicity	completeness	at highest res.	resolution (Å)
None	False	Default (optimized)	Default (≥ 0.99)	BEST Default	Default (highest possible)

Collection plan strategy (**RADDOSE log file** , **BEST log file**)

Resolution limit is set by the radiation damage

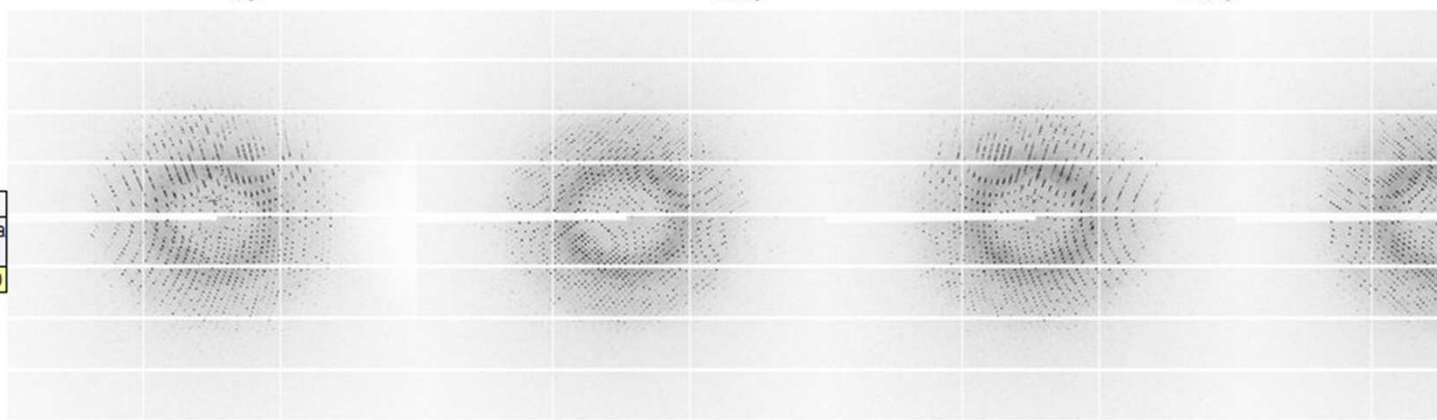
Wedge	Subwedge	Start (°)	Width (°)	No images	Exp time (s)	Max res (Å)	Rel trans (%)	Distance (mm)
1	1	158.00	0.10	1400	0.257	1.32	100.00	134.20



Indexing summary: Selected spacegroup: P222

Refined unit cell parameters (Å/degrees)					
a (Å)	b (Å)	c (Å)	alpha (°)	beta (°)	gamma (°)
43.460	64.160	86.180	90.000	90.000	90.000

[Indexing log file](#)



ref-S52P-T4-SC001_B6_5_0001.cbf

ref-S52P-T4-SC001_B6_5_0002.cbf

ref-S52P-T4-SC001_B6_5_0003.cbf

ref-S52P-T4-SC001_B6_5_0004.cbf

[Integration log file 1](#)

Services offered to users on MASSIF1:

- MXPressO - load/optical centre/X-ray centre/180°
- MXPressE - load/optical centre/X-ray centre/eEDNA strategy/collect
- MXScore - load/optical centre/X-ray centre/eEDNA strategy
- MXPressE_SAD - load/optical centre/X-ray centre/eEDNA SAD strategy/collect
- MXPressM – high exposure mesh scan
- No restrictions on sample size, mount or quality

ISPyB Information System for Protein Crystallography Beamlines

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Puck Information

Shipping: Test_shipment

Dewar: Dewar1

Puck: AAA1234A

Create Puck

Save Reset Change sample name automatically

Sample Position	Protein Acronym (*)	Sample Name (*)	Pin Barcode	Space Group	Pre-Observed resolution	Needed resolution	Pref. Diameter	Experiment Type	Number of positions	Radiation sensitivity	Required multiplicity	Required completeness	Unit Cell a	Unit Cell b	Unit Cell c	Unit Cell alpha	Unit Cell beta	Unit Cell gamma	SMILES	Comments	Action
1	TRIM24 - Undefined	X1		Undefined			20	MXPressO	2				0	0	0	0	0	0			
2	Eng - P64	X01		P64	1.6		100	MXPressE_SAD					212	212	53	90	90	120			
3	Eng - P64	X02		P64	1.6		100	MXPressE_SAD					212	212	53	90	90	120			
4	Eng - P64	X03		P64	1.6		100	MXPressE_SAD					212	212	53	90	90	120			
5	Eng - P64	X04		P64	1.6		100	MXPressE_SAD					212	212	53	90	90	120			
6	Eng - P64	X05		P64	1.6		100	MXPressE_SAD					212	212	53	90	90	120			
7	Eng - P64	X06		P64	1.6		100	MXPressE_SAD					212	212	53	90	90	120			
8	S52P-T4 - Undefined	X01		Undefined	3.0			MXPressE		2.0	6	0.9	0	0	0	0	0	0			
9	S52P-T4 - Undefined	X02		Undefined	3.0			MXPressE		2.0	6	0.9	0	0	0	0	0	0			
10	S52P-T4 - Undefined	X03		Undefined	3.0			MXPressE		2.0	6	0.9	0	0	0	0	0	0			

(*) mandatory field for each sample

Svensson, O., Monaco, S., Popov, A., Nurizzo, D. and Bowler, M. W. (2015), The fully automatic characterization and data collection from crystals of biological macromolecules. *Acta Cryst.* **D71** 1757-1767



ISPyB
Information System for Protein Crystallography Beamlines

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Select Dewars
 Last dewars
 All dewars
 Fill sample changer

Help

Puck Information
 Shipping: Test_shipment
 Dewar:

Save Reset Change sample name automatically

Sample Position	Protein Acronym (*)	Sample Name (*)	Pin Barcode	Space Group	Pre-Observed resolution	Needed resolution	Pref. Diameter	Experiment Type	Number of positions	Radiation sensitivity	Required multiplicity	Required completeness
1	TRIM24 - Undefined	X1		Undefined			20	MXPressO	2			
2	Eng - P64	X01		P64	1.6		100	MXPressE_SAD				
3	Eng - P64	X02		P64	1.6		100	MXPressE_SAD				
4	Eng - P64	X03		P64	1.6		100	MXPressE_SAD				
5	Eng - P64	X04		P64	1.6		100	MXPressE_SAD				
6	Eng - P64	X05		P64	1.6		100	MXPressE_SAD				
7	Eng - P64	X06		P64	1.6		100	MXPressE_SAD				
8	S52P-T4 - Undefined	X01		Undefined	3.0			MXPressE		2.0	6	0.9
9	S52P-T4 - Undefined	X02		Undefined	3.0			MXPressE		2.0	6	0.9
10	S52P-T4 - Undefined	X03		Undefined	3.0			MXPressE		2.0	6	0.9

(*) mandatory field for each sample

Svensson, O., Monaco, S., Popov, A., Nurizzo, D. and Bowler, M. W. (2015), The fully automatic characterization and data collection from crystals of biological macromolecules. *Acta Cryst.* **D71** 1757-1767



Diffraction Plan entry	Definition	Default value
Protein acronym	Defines the protein that is registered with the ESRF safety group	Required field
Sample name	User defined unique identifier	Required field
Pin barcode	Barcode identifier	none
Experiment type	Define MXPressE / O / SAD / Score	MXPressE
Space Group	If present used for strategy calculation and autoprocessing	none
Pre-observed resolution	Resolution that the detector will be set to for mesh scans, characterisation images and default data collection	2.0 Å
Required resolution	Threshold resolution, samples below cutoff will not be collected	none
Radiation sensitivity	BEST input in case of highly radiation sensitive crystals	1
Required completeness	-	99%
Required multiplicity	-	4
Number of positions	For multiple crystals	1
Preferred beamsize	Select appropriate beamsize for crystals	50 µm

Detailed reports in ISPyB display all sample analysis

Exp. Type	Acronym	Image Prefix	Run#	Parameters	Results	Image Thumbnail	Crystal snapshot	Graph	Second Graph	Comments
22-05-2015 (1 Item)										
MXPressE	S52P-T4-SC001_B6_2	S52P-T4-SC001_B6_2	1	Nb tot images: 1220 Nb images: 1220 Exp. time: 0.679 s Phi range: 0.15 ° Flux: 1.83E11 ph/sec Detector resolution: 1.37 Å Transmission: 100.00 Wavelength: 0.965 Å Total expo time: 570.36 s	MXPressE EDNA dp GrenADES fp GrenADES pp Space Group: P 21 21 2 Completeness:					EDNA dp: pseudo-translation detected.
Start time: 22:25:37 22-05-2015 (1 Item)										
MXPressE	S52P-T4-SC001_B6_1	S52P-T4-SC001_B6_1	1	Nb tot images: 1111 Nb images: 1111 Exp. time: 0.487 s Phi range: 0.15 ° Flux: 1.9E11 ph/sec Detector resolution: 1.28 Å Transmission: 100.00 Wavelength: 0.965 Å Total expo time: 383.27 s	MXPressE EDNA dp GrenADES fp GrenADES pp Space Group: P 21 21 2 Completeness:					EDNA dp: pseudo-translation detected.
Start time: 22:07:30 22-05-2015 (1 Item)										
MXPressE	S52P-T4-SC001_B6	S52P-T4-SC001_B6	1	Nb tot images: 1647 Nb images: 1647 Exp. time: 0.257 s Phi range: 0.10 ° Flux: 1.9E11 ph/sec Detector resolution: 1.32 Å Transmission: 100.00 Wavelength: 0.965 Å Total expo time: 355.80 s	MXPressE EDNA dp GrenADES fp GrenADES pp Space Group: P 21 21 2 Completeness:					EDNA dp: pseudo-translation detected.
Start time: 21:52:07 22-05-2015 (1 Item)										
MXPressE	TRIM24-T2_CS	TRIM24-T2_CS	1	Nb tot images: 1264 Nb images: 1264 Exp. time: 0.200 s Phi range: 0.20 ° Flux: 1.95E11 ph/sec Detector resolution: 2.00 Å Transmission: 100.00 Wavelength: 0.965 Å Total expo time: 180.00 s	MXPressE No autoproccessing results found					No characterisation results, default 180.0 degree data collection.
Start time: 21:37:32 22-05-2015 (1 Item)										
MXPressE	TRIM24-T3_B6	TRIM24-T3_B6	1	Nb tot images: 1211 Nb images: 1211 Exp. time: 0.200 s Phi range: 0.20 ° Flux: 2.0E11 ph/sec Detector resolution: 2.00 Å Transmission: 100.00 Wavelength: 0.965 Å Total expo time: 180.00 s	MXPressE No autoproccessing results found					Very weak diffraction. No characterisation results, default 180.0 degree data collection.
Page 5 of 5										



Move to...



Mail



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Set

Subject **MX-1682: Data collection for PenFab started on beamline MASSIF1**

From massif1@esrf.fr

To F.Forneris@uu.nl

Date Fri 12:34

Dear MASSIF1 User,

Automatic data collection for protein PenFab has started on beamline MASSIF1, the first sample is PenFab-C269A_1. Data collection can be followed in ISPyB.

Best wishes,

The MASSIF1 team.

If results based on diffraction data from MASSIF1 are used in publications, please cite the following papers:

Svensson, O., Monaco, S., Popov, A. N., Nurizzo, D. & Bowler, M. W. (2015). The fully automatic characterization and data collection from crystals of biological macromolecules, *Acta Cryst. D* 71, 1757-1767, <http://dx.doi.org/10.1107/S1399004715011918>

Bowler, M.W., Nurizzo, D., et al. (2015). MASSIF-1: A beamline dedicated to the fully automatic characterisation and data collection from crystals of biological macromolecules, *J. Synchrotron Rad.* 22, 1540-1547, <http://dx.doi.org/10.1107/S1600577515016604>.

Web: <http://www.esrf.eu/MASSIF1>

FAQ: http://www.esrf.eu/MASSIF_FAQ

Twitter: https://twitter.com/ID30_MASSIF1





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Agenda

Aujourd'hui



juillet 2016

Jour

Semaine

Mois

4 jours

Planning

Plus



CRÉER

juillet 2016

L	M	M	J	V	S	D
27	28	29	30	1	2	3
4	5	6	7	8	9	10
11	12	13	14	15	16	17
18	19	20	21	22	23	24
25	26	27	28	29	30	31
1	2	3	4	5	6	7

Mes agendas

- Matthew Bowler
- Anniversaires
- ESRF Scheduling
- HC1 calendar
- Local Contacting
- Rappels
- Vacance Scholaires

Autres agendas

- Ajouter l'agenda d'un ami
- Jours fériés en France
- Météo
- Numéros de semaine

Conditions - Confidentialité

lun.	mar.	mer.	jeu.	ven.	sam.	dim.
27 10:00 Set up remoteESF	28 Machine Dedicated Tin	29 MX1728 (50 samples) MX1738 (50 Samples)	30 MX1728 (50 Samples) MX1779 (50 Samples)	1 juil. Not available	2 MX1743 (50 Samples) MX1784 100 samples	3 MX1794 Forneris (40 X)
4	5 Not available Machine Dedicated Tin Vacances d'été - Zone	6 FX-29	7 MX-1792 (150 crystals)	8 Not available	9 MX1743 (100 samples) 17:00 MX1743 (100 san	10
11 IHR BOWLER 50 sam MX1736 (50 Samples)	12 Not available Machine Dedicated Tin	13 MX1782 (50 samples)	14 MX-1787 150 La fête nationale	15 Not available	16 MX1777 (150 crystals)	17 MX1743 (90 samples)
18 MX1788 (98 crystals)	19 Not available Machine Dedicated Tin	20 100 samples only MX-1752 Mark J van R	21 MX-1735 MATIAS (80)	22 Not available	23 MX-1738 (50 samples) MX1794 Forneris (30 X) 14:00 MX1743 (100 San	24 MX-1752 Daniel Lietha
25 MX-1792 (100 crystals)	26 Not available Machine Dedicated Tin	27 MX-1794 - 50 MX1748 - 100	28 FX-48 30 MX-1789 Thunnisse	29 Not available	30 Not available	31

Tâches

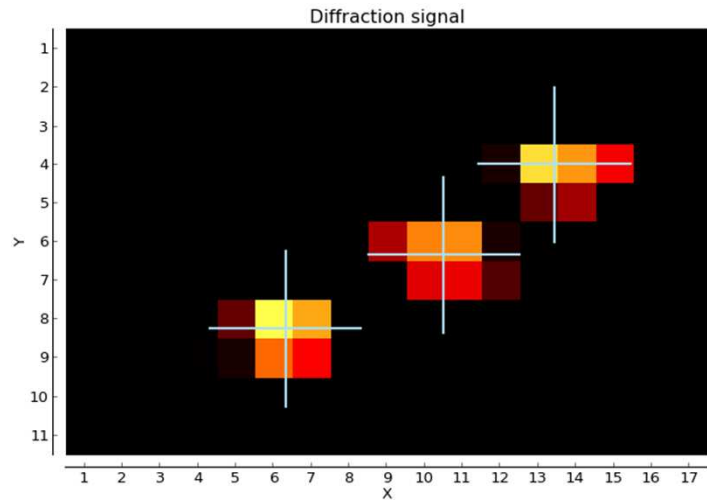
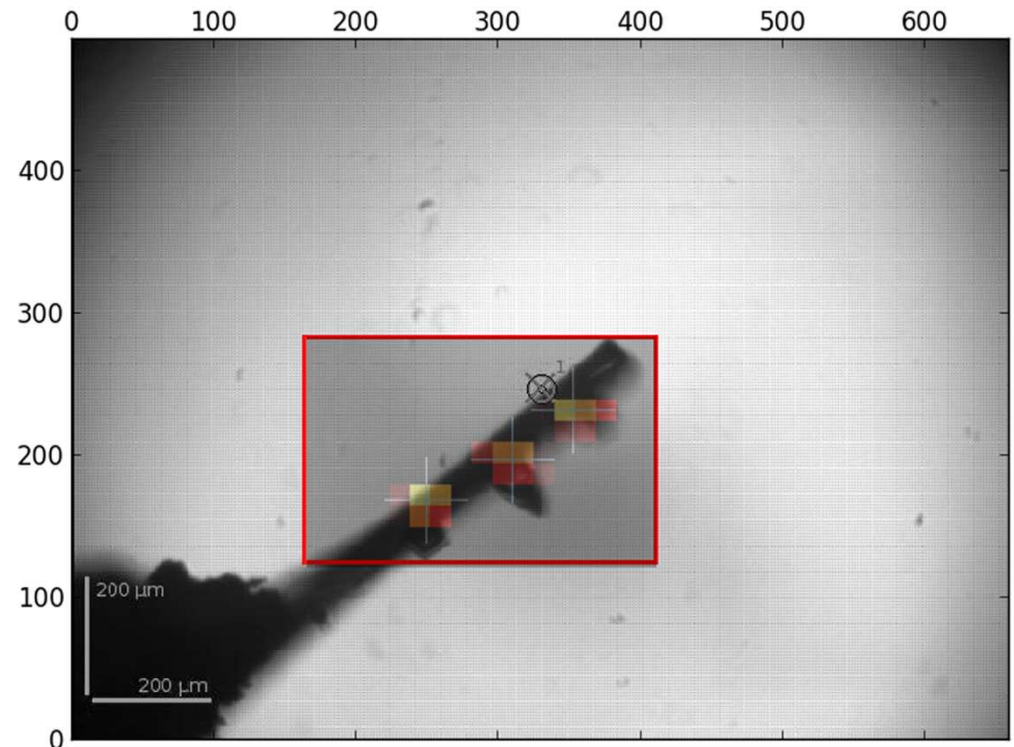
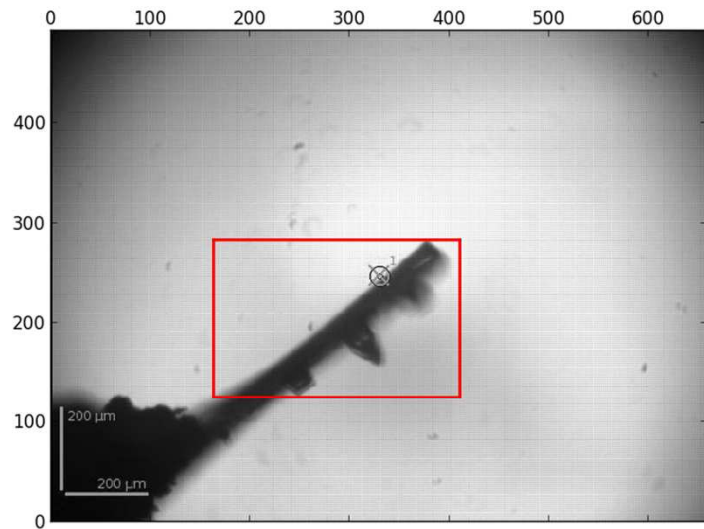
Liste par défaut

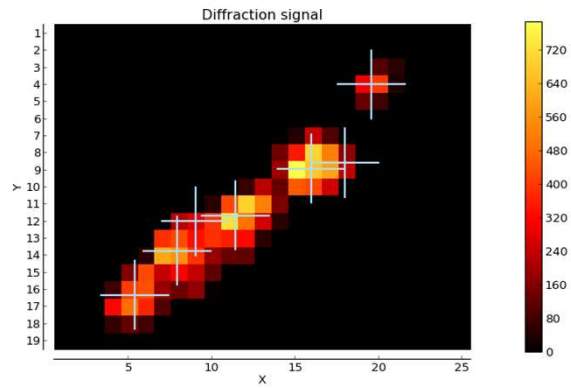
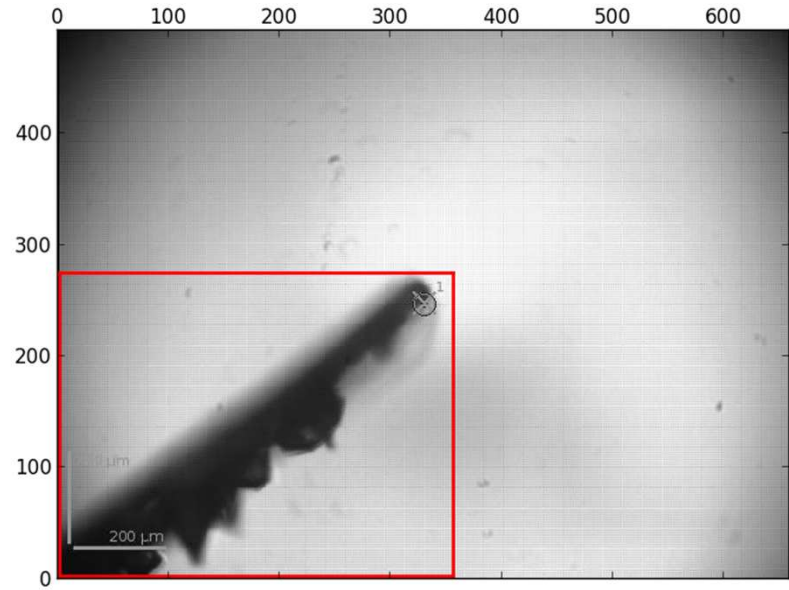
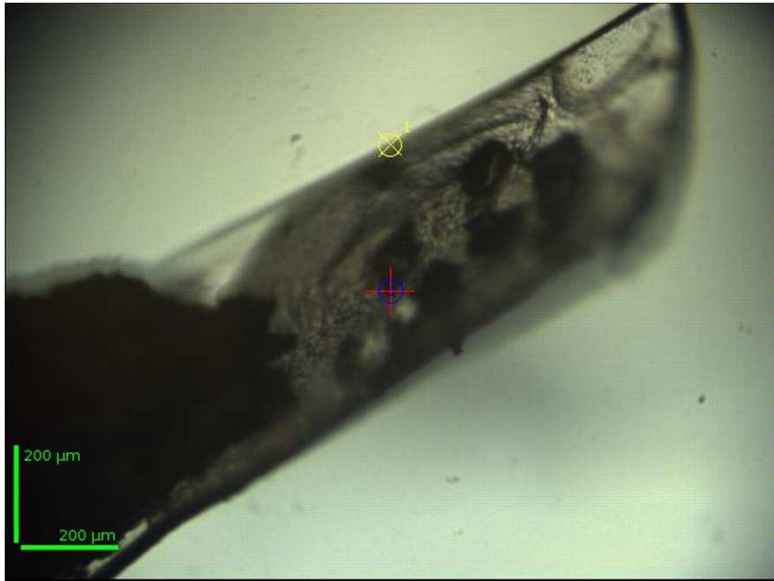


Actions +

EMBL







Crystal mapping

determine regions of crystal homogeneity and size

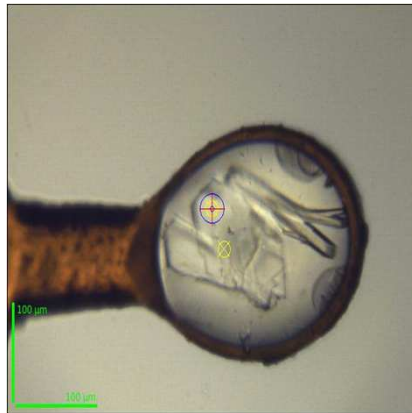
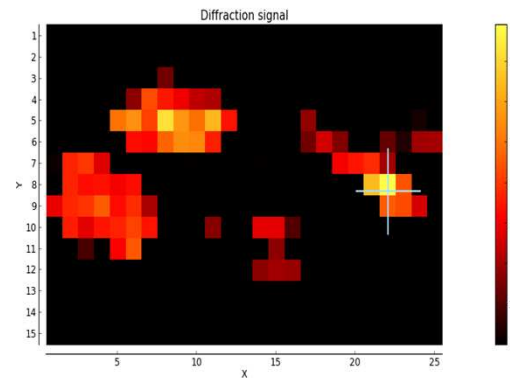
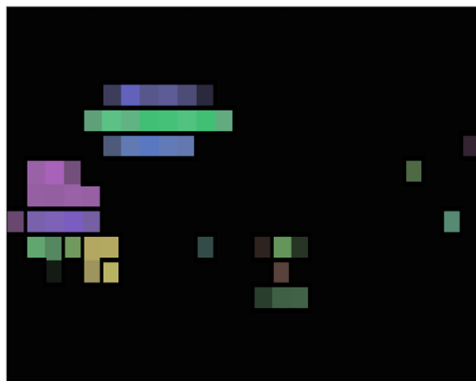


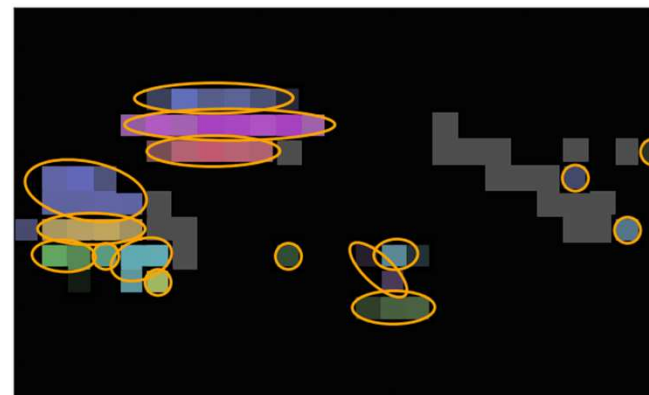
Photo snapshot of the sample



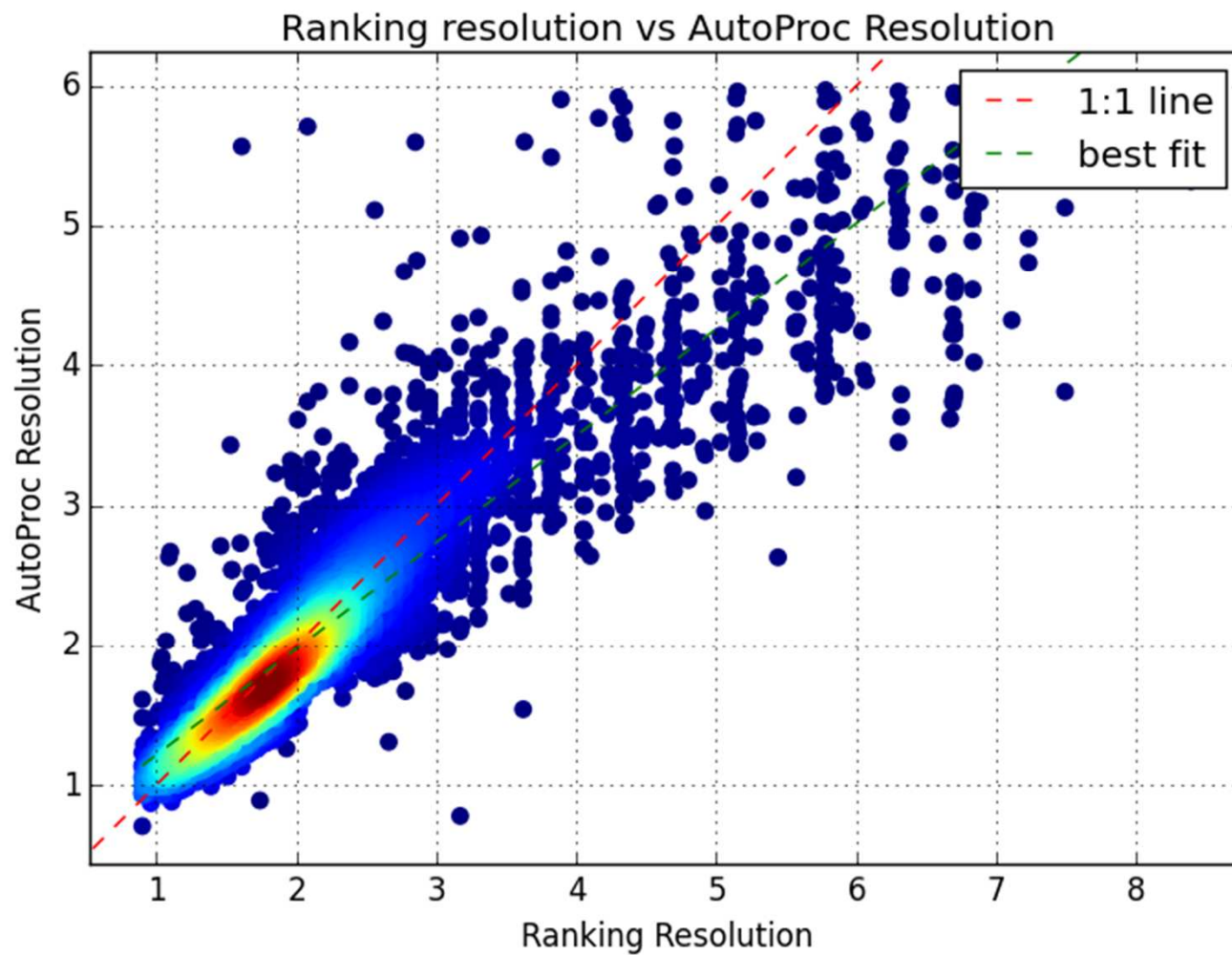
Initial diffraction map, showing regions with better protein crystal diffraction quality

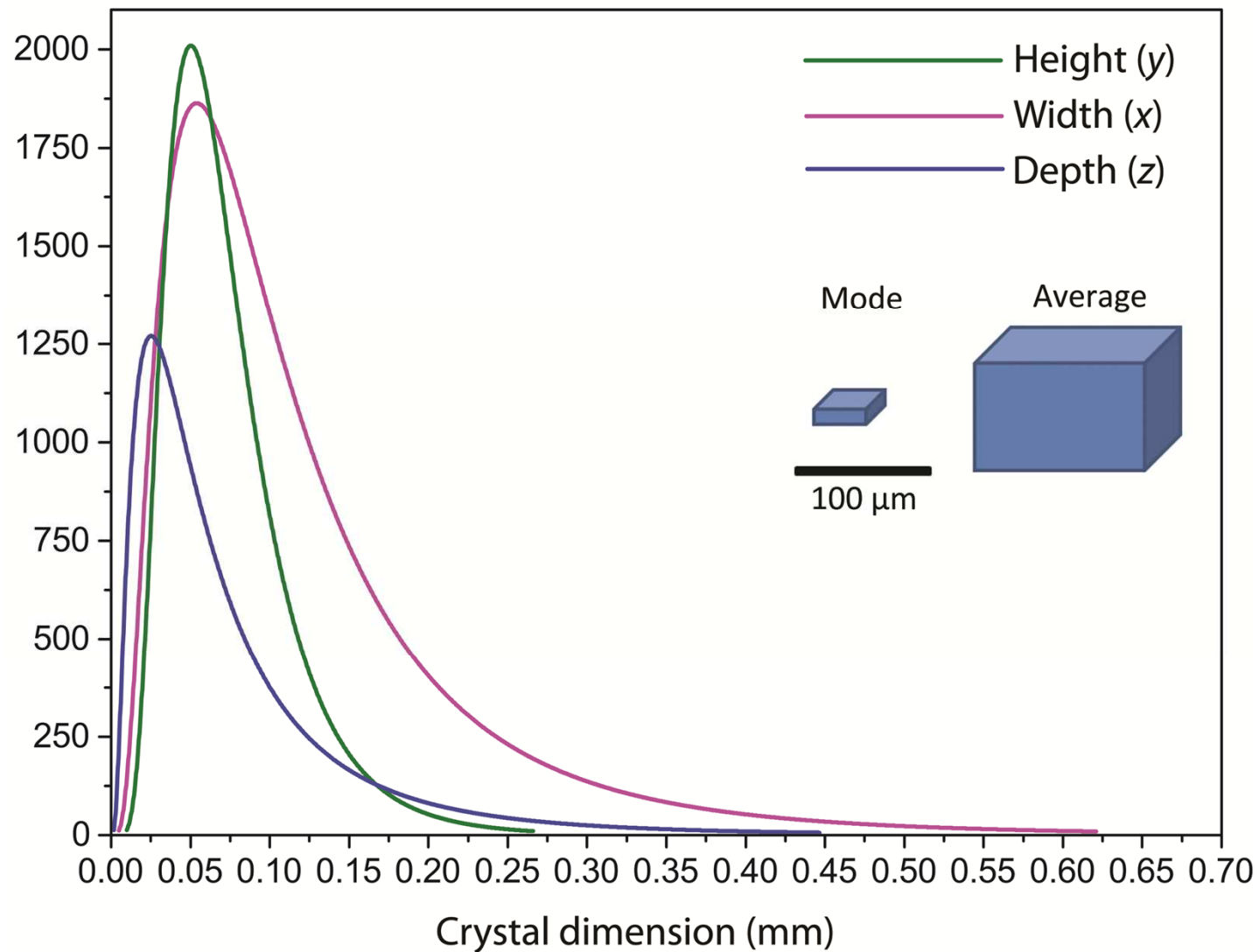


Crystal map omitting regions of overlapping



fit crystal shapes, corresponding to regions of crystal integrity.

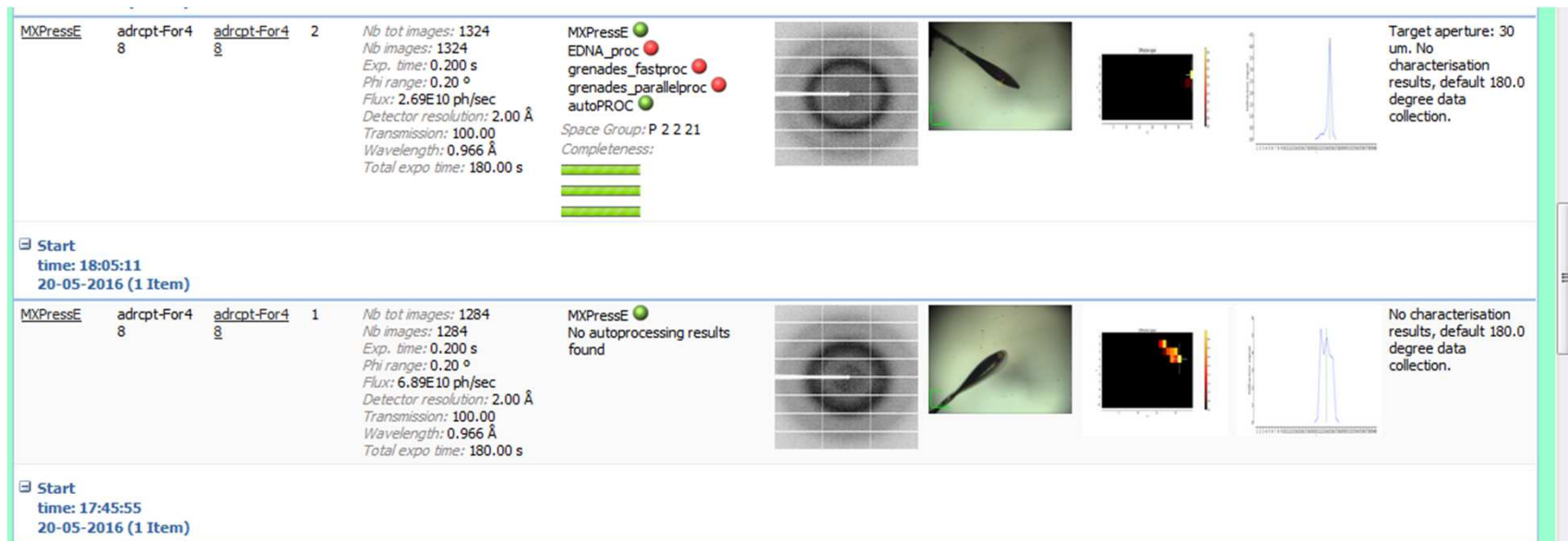




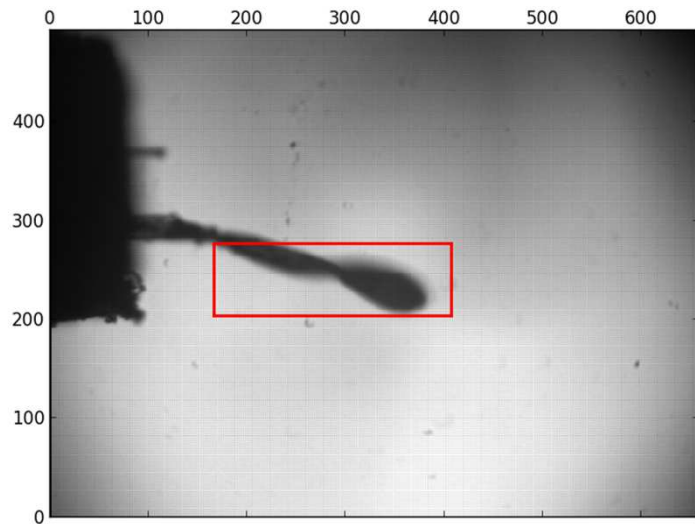
Dynamic beamsizing

GPCR crystals: default 50 um aperture changed to 30 um after mesh with crystals determined to be 60 x 30 x 30 um³

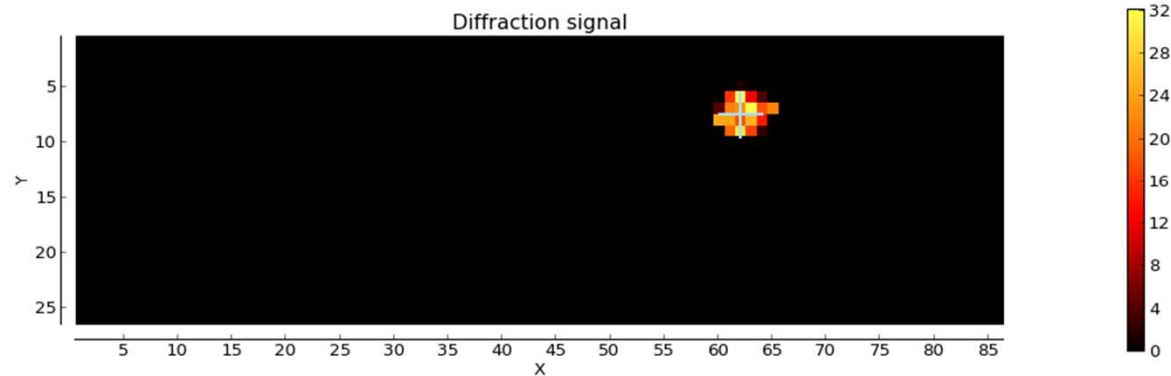
Difference between processable data set or not for difficult cases



Dynamic beamsizing



Users selected 10 μm aperture
but crystal determined to be 30 x
30 x 30 μm^3

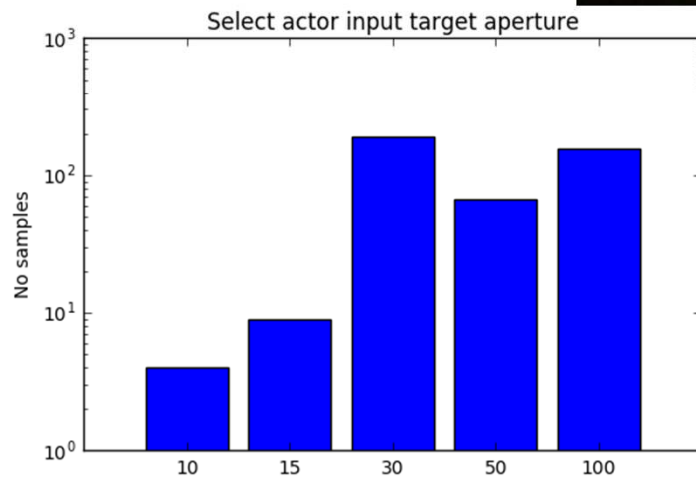
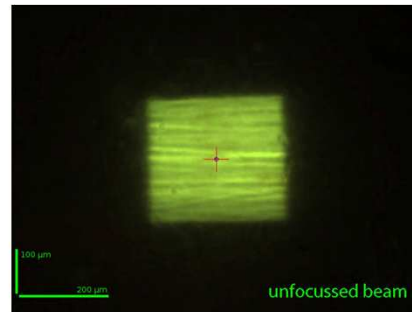


Dynamic beamsizing

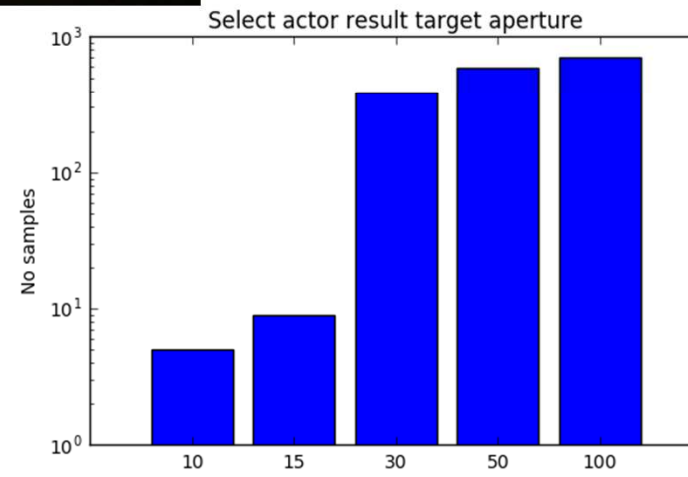
				Wavelength: 0.966 Å Total expo time: 391.98 s						
<p>Start time: 19:56:11 04-10-2016 (1 Item)</p>										
MXPRESS	CBCA-9-A-06	ref-CBCA-9-A-06	4	<p>Nb tot images: 264 Nb images: 264 Exp. time: 0.200 s Phi range: 1.00 ° Flux: 1.75E11 ph/sec Detector resolution: 2.00 Å Transmission: 100.00 Wavelength: 0.966 Å Total expo time: 0.80 s</p>	<p>MXPRESS ● No autoproccessing results found</p>					Dynamic aperture set to 30 um New exposure time 0.2 s The average Dozor score after characterisation is below the threshold of 0.2, therefore no data collection.
<p>Start time: 19:44:11 04-10-2016 (1 Item)</p>										
MXPRESS	CBCA-9-A-05	CBCA-9-A-05	1	<p>Nb tot images: 749 Nb images: 749 Exp. time: 0.143 s Phi range: 0.15 ° Flux: 1.1E12 ph/sec Detector resolution: 3.65 Å Transmission: 100.00 Wavelength: 0.966 Å Total expo time: 65.92 s</p>	<p>MXPRESS ● EDNA_proc ● grenades_fastproc ● grenades_parallelproc ● autoPROC ● XIA2_DIALS ● Space Group: P 31 2 1 Completeness: ----- ----- -----</p>					Dynamic aperture set to 100 um New exposure time 0.1 s
<p>Start time: 19:38:52 04-10-2016 (1 Item)</p>										
MXPRESS	CBCA-9-A-04	mesh-CBCA-9-A-04	1	<p>Nb tot images: 76 Nb images: 76 Exp. time: 0.100 s Phi range: 0.05 ° Flux: 3.97E11 ph/sec Detector resolution: 2.00 Å Transmission: 100.00 Wavelength: 0.966 Å Total expo time: 1.90 s</p>	<p>MXPRESS ● No autoproccessing results found</p>					No diffraction.
<p>Start time: 19:34:00 04-10-2016 (1 Item)</p>										
MXPRESS	CBCA-9-A-03	mesh-CBCA-9-A-03	1	<p>Nb tot images: 54 Nb images: 54 Exp. time: 0.100 s Phi range: 0.06 ° Flux: 3.97E11 ph/sec Detector resolution: 2.00 Å Transmission: 100.00 Wavelength: 0.966 Å Total expo time: 1.80 s</p>	<p>MXPRESS ● No autoproccessing results found</p>					No diffraction.
<p>Start time: 19:20:41 04-10-2016 (1 Item)</p>										
MXPRESS	CBCA-9-A-02	CBCA-9-A-02	1	<p>Nb tot images: 686 Nb images: 686 Exp. time: 0.139 s Phi range: 0.30 °</p>	<p>MXPRESS ● EDNA_proc ● grenades_fastproc ● grenades_parallelproc ● autoPROC ●</p>					Very weak diffraction. Dynamic aperture set to 50 um New exposure time 0.1 s

MASSIF-1: smart beamsizing

- Beamline will automatically collect data, new feature selects beam diameter
- Beamline automatically adjusts beamsize to best volume within crystal
- Leads to higher signal to noise in data



User selected beam size



Auto selected beam size

Dynamic beamsizing

Wavelength: 0.966 Å
Total expo time: 391.98 s

Start
time: 19:56:11
04-10-2016 (1 Item)

MXPressE	CBCA-9-A-06	ref-CBCA-9-A-06	4	<p>Nb tot images: 264 Nb images: 264 Exp. time: 0.200 s Phi range: 1.00 ° Flux: 1.75E11 ph/sec Detector resolution: 2.00 Å Transmission: 100.00 Wavelength: 0.966 Å Total expo time: 0.80 s</p>	<p>MXPressE No autoprocessing results found</p>				Dynamic aperture set to 30 um New exposure time 0.2 s The average Dozor score after characterisation is below the threshold of 0.2, therefore no data collection.
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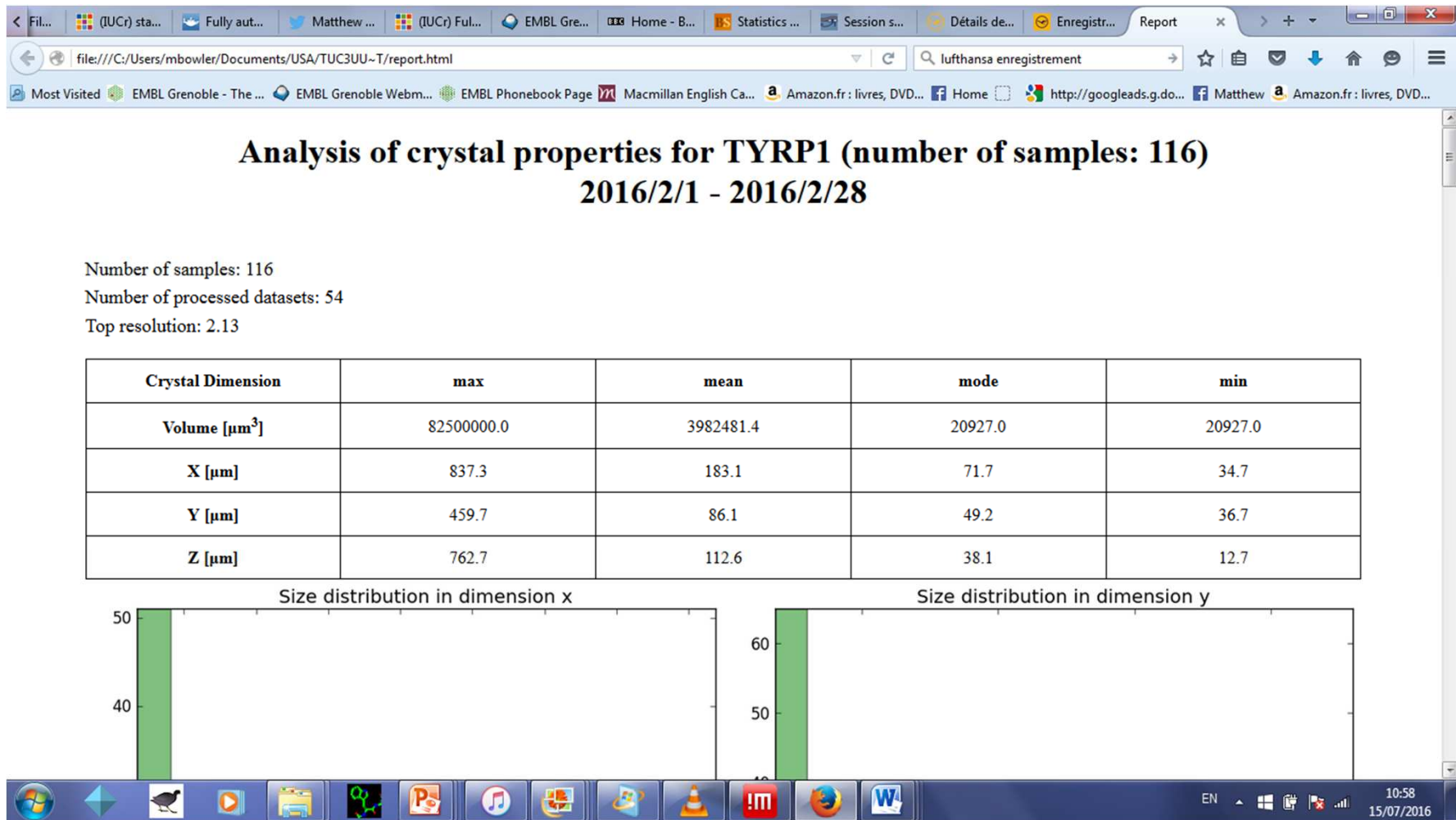
Start
time: 19:44:11
04-10-2016 (1 Item)

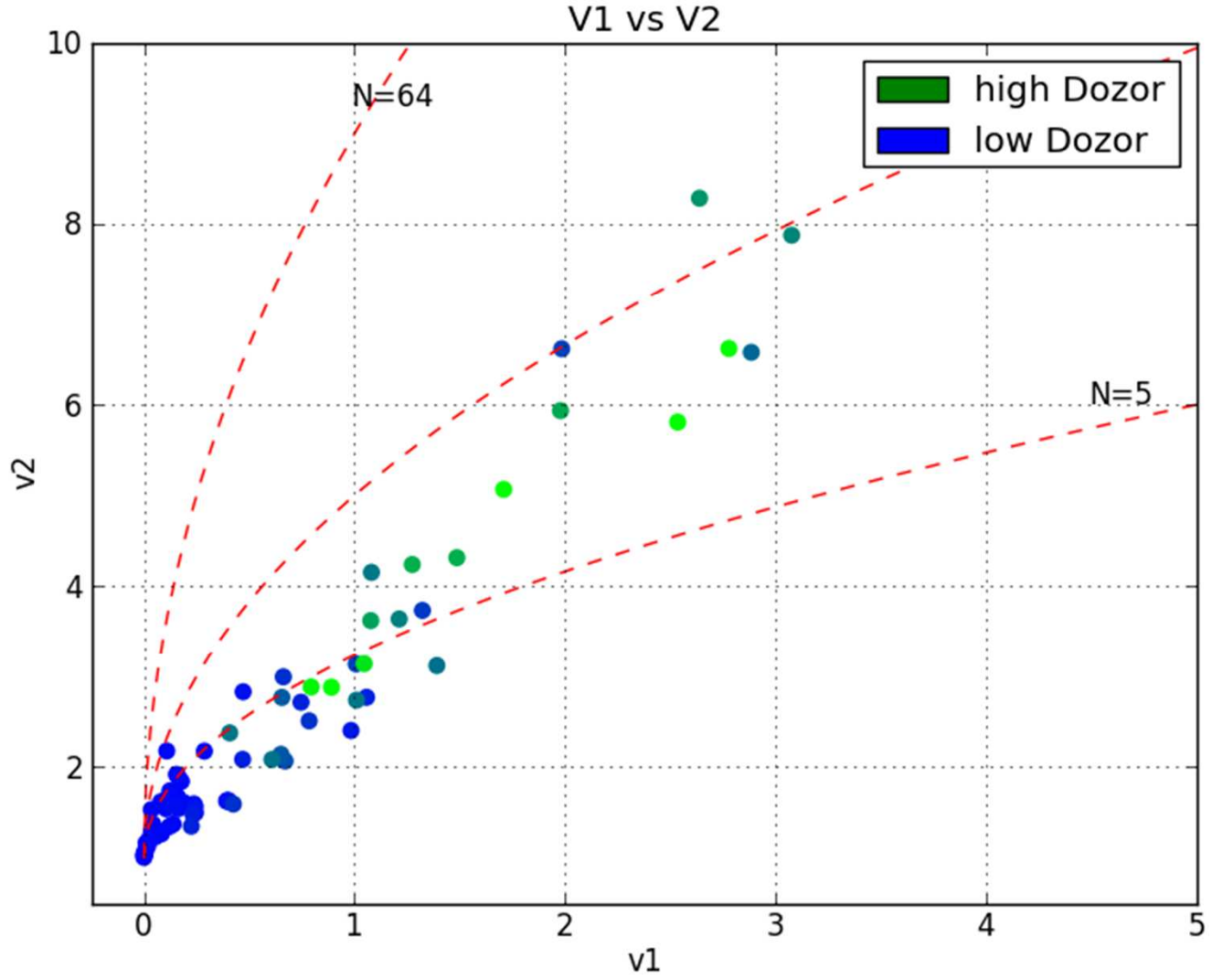
MXPressE	CBCA-9-A-05	CBCA-9-A-05	1	<p>Nb tot images: 749 Nb images: 749 Exp. time: 0.143 s Phi range: 0.15 ° Flux: 1.1E12 ph/sec Detector resolution: 3.65 Å Transmission: 100.00 Wavelength: 0.966 Å Total expo time: 65.92 s</p>	<p>MXPressE EDNA_proc grenades_fastproc grenades_paralleproc autoPROC Space Group: P 31 2 1 Completeness:</p>				Dynamic aperture set to 100 um New exposure time 0.1 s
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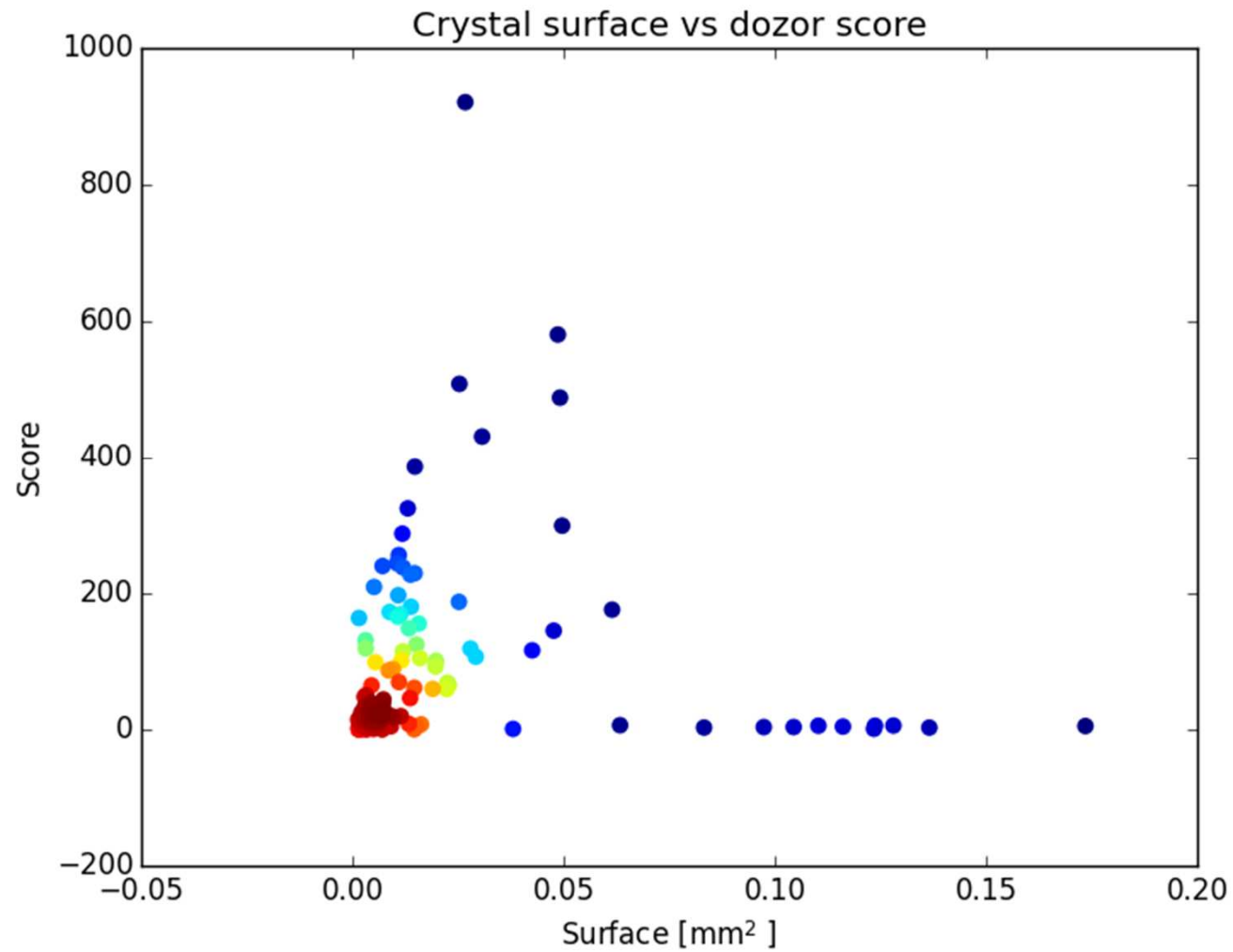
Start
time: 19:38:52
04-10-2016 (1 Item)

MXPressE	CBCA-9-A-04	ref-CBCA-9-A-04	1	<p>Nb tot images: 75</p>	MXPressE				No effective
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				Dynamic aperture set to 100 um New exposure time 0.1 s
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A new service on MASSIF-1

Dehydration workflow in MXCuBE

mxCuBE (opid-144)

File Instrumentation Help Expert mode

Collect XRF spectrum System Feedback Chat

User: opid-144

Sample list: Mode: Manually mounted, Centring: Automatic loop centring

- manually-mounted
 - Dehydration - 1
 - sample-centring
 - Lys0_1 - 0
 - Dehydration - 3
 - hc1-Lys0_1_1 Collection done
 - hc1-Lys0_1_2 Collection done
 - hc1-Lys0_1_3 Collection done
 - hc1-Lys0_1_4 Collection done
 - hc1-Lys0_1_5 Collection done
 - hc1-Lys0_1_6 Collection done
 - hc1-Lys0_1_7 Collection done
 - hc1-Lys0_1_8 Collection done
 - hc1-Lys0_1_9 Collection done
 - hc1-Lys0_1_10 Collection done
 - hc1-Lys0_1_11 Collection done
 - hc1-Lys0_1_12 Collection done
 - hc1-Lys0_1_13 Collection done
 - hc1-Lys0_1_14 Collection done
 - hc1-Lys0_1_15 Collection done

Sample centring Data collection

Dehydration Results

Effect of dehydration on crystal parameters: Relative humidity (%) vs Time (seconds). Parameters: a cell edge, b cell edge, c cell edge.

Effect of dehydration on crystal parameters: Unit cell axes (Å) vs Relative Humidity (%). Parameters: a cell edge, b cell edge, c cell edge, Total Integrated Signal.

Effect of dehydration on resolution: Number of Bragg peaks of spots vs Relative Humidity (%). Parameters: Number of Spots, Bragg peaks, Total integrated signal.

Effect of dehydration on crystal parameters: Relative humidity (%) vs Time (seconds). Parameters: Relative humidity, Labelit r1, Labelit r2, BEST RR.

Effect of dehydration on resolution: Resolution (Å) vs Time (seconds). Parameters: Resolution (Å).

Effect of dehydration on resolution: Relative Humidity (%) vs Number of Spots.

Effect of dehydration on resolution: Relative Humidity (%) vs Resolution (Å).

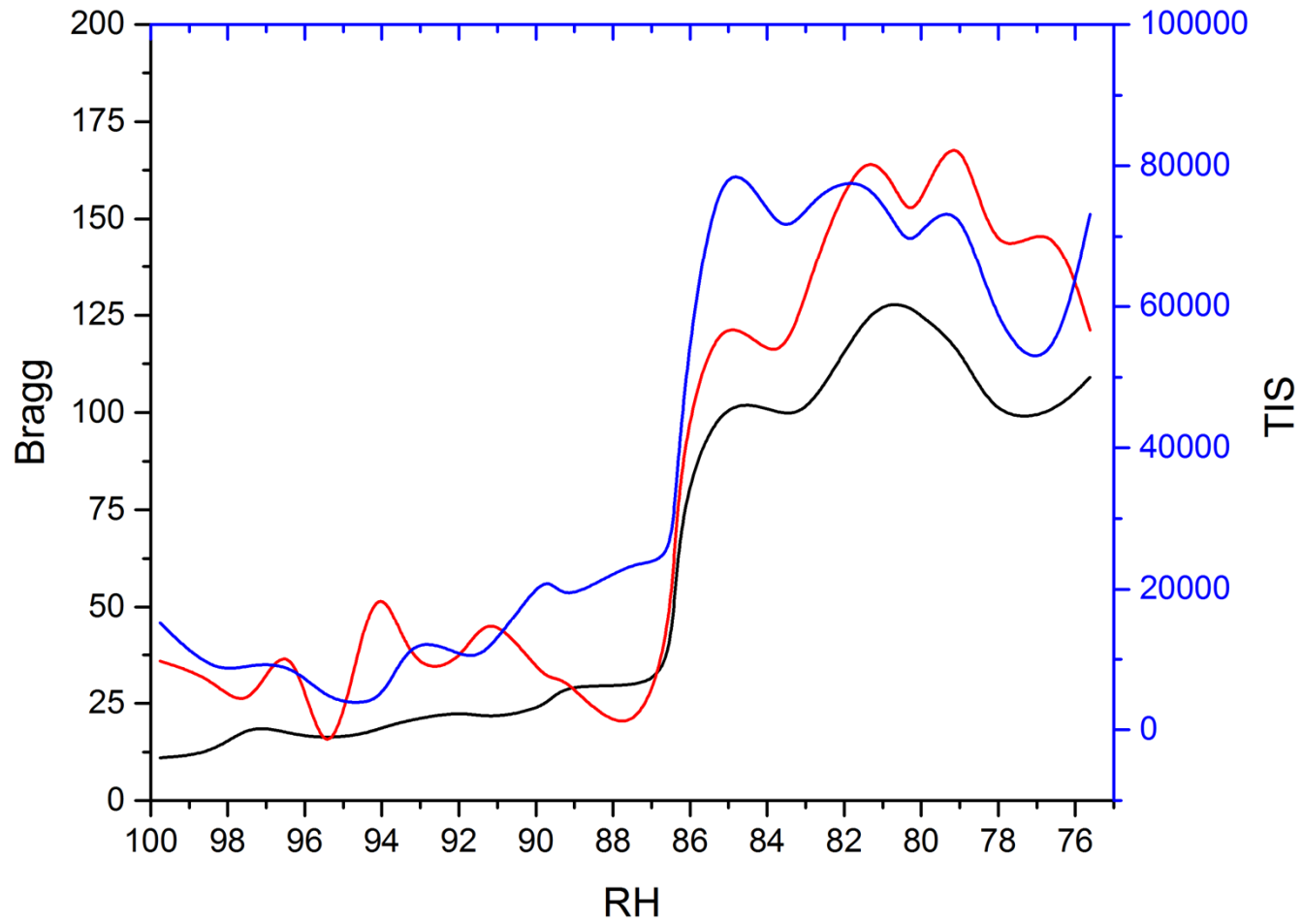
Machine current: 194.1 mA, 24°8+1bunch, Flux: 7.28e+10 ph/s, Energy: 13.3000 keV, 0.932, Current: 2.399 A, 365.26 mm, Transmission: 1.16%, Set to: Filters, Cryo: 99.9 K

Safety shutter: opened, Fast shutter: closed, Beamstop: in

Current users: Selecting gives control, Allow timeout control, Take control, My name: artemis2

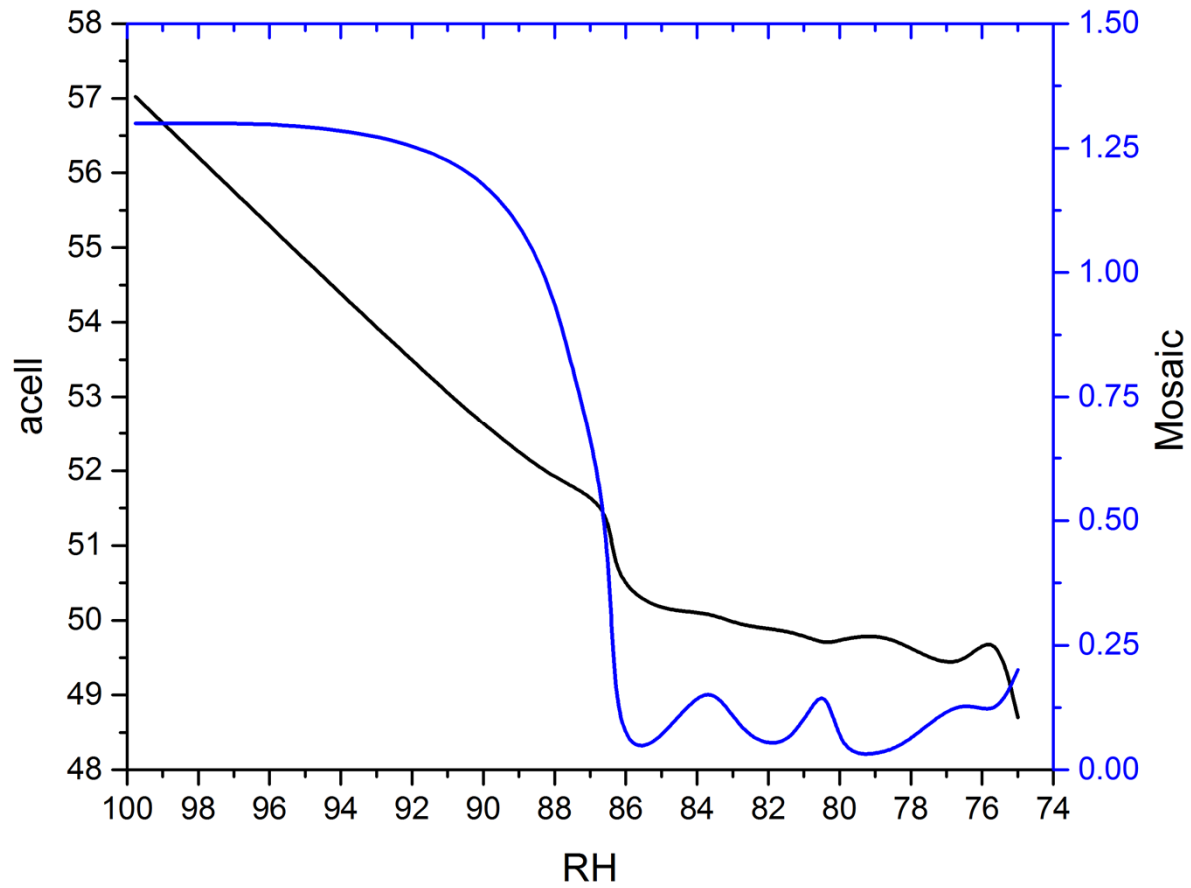
[2013-12-02 10:10:32] Integrated counts for image : 2.60716e+09

[2013-12-02 10:10:33] Collection completed



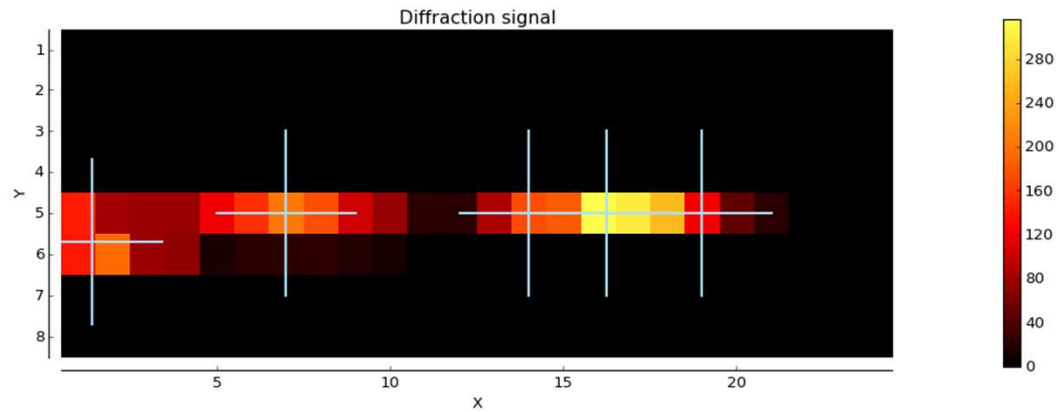
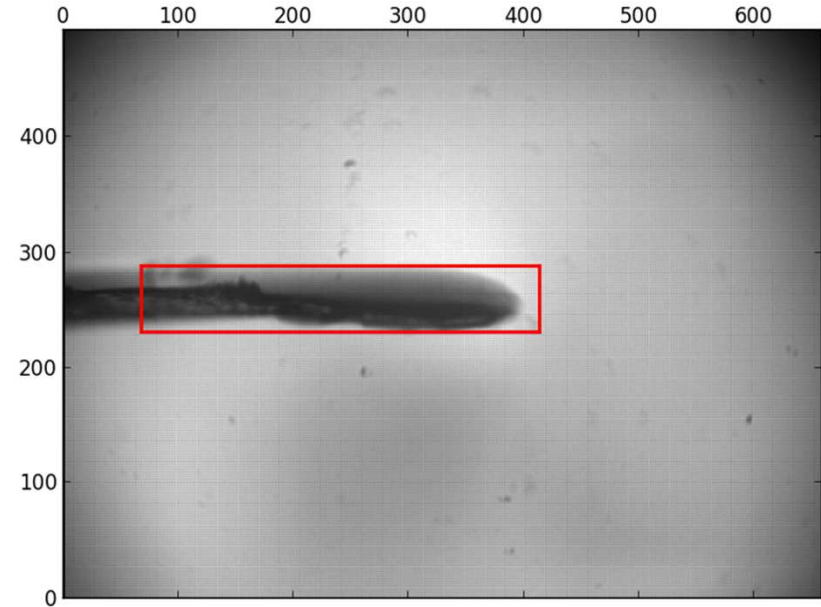
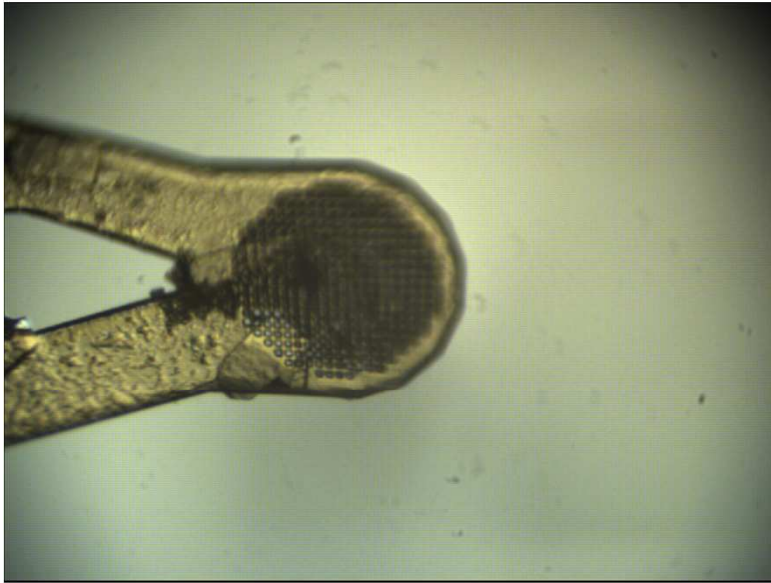
Bowler, M.W., and Rupp, B (2016) *unpublished*



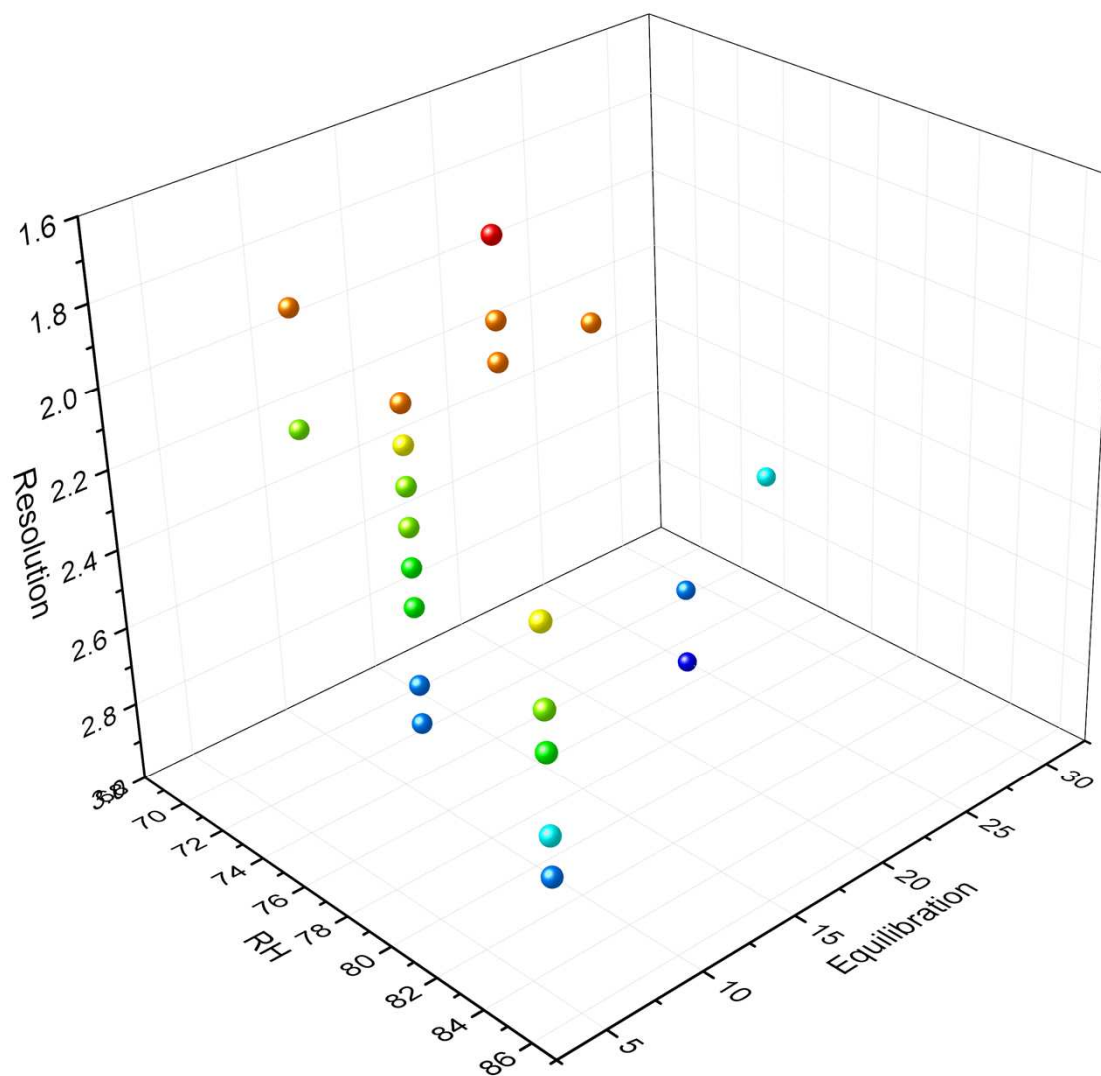


Bowler, M.W., and Rupp, B (2016) *unpublished*



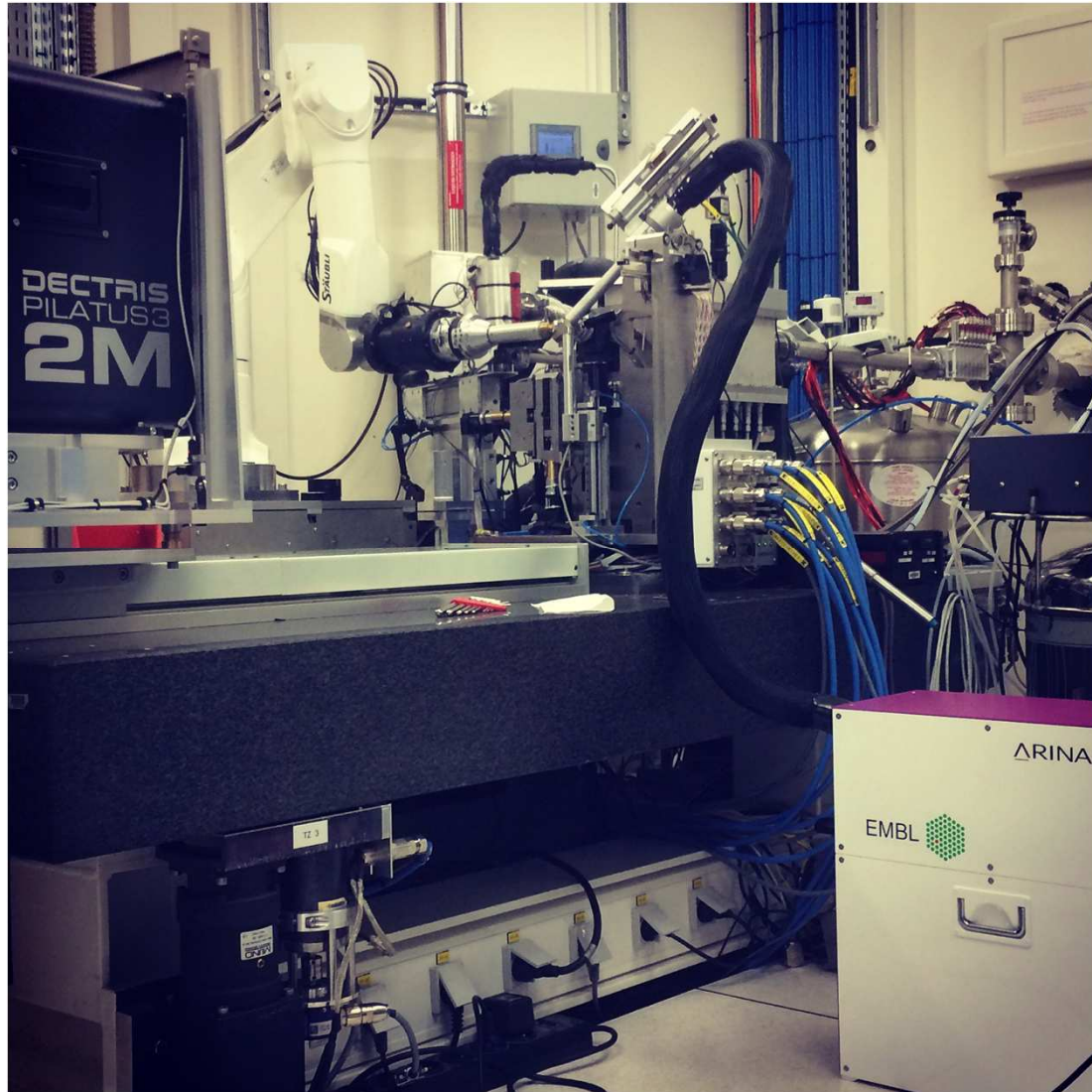


Bowler, M.W., and Rupp, B (2016) *unpublished*

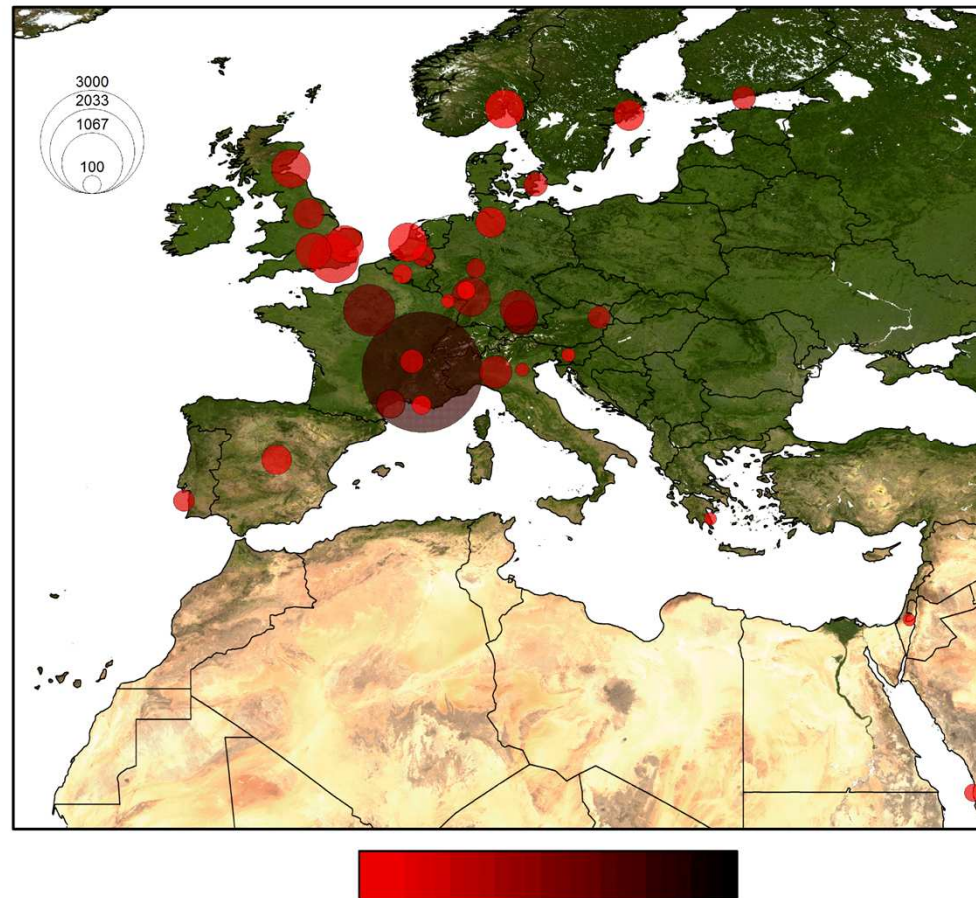


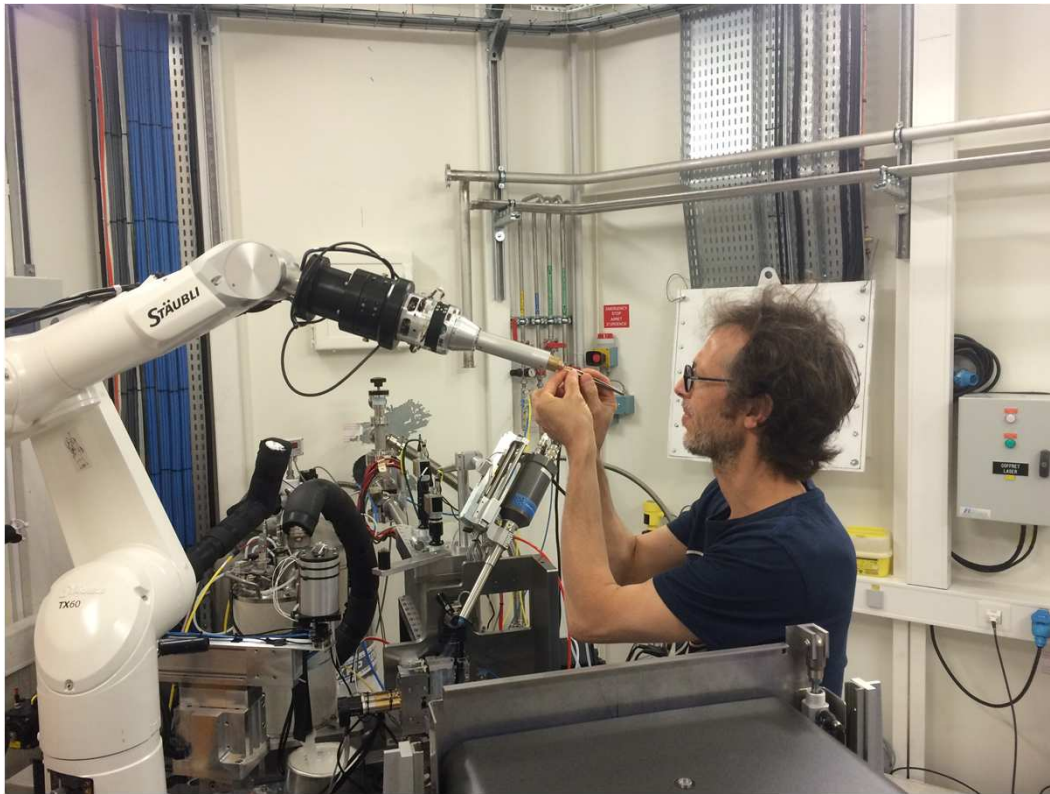
Bowler, M.W., and Rupp, B (2016) *unpublished*





- 26,357 crystals automatically processed since opening in Sept. 2014





Didier Nurizzo



Matias Guijarro



Olof Svensson