

A Light for Science



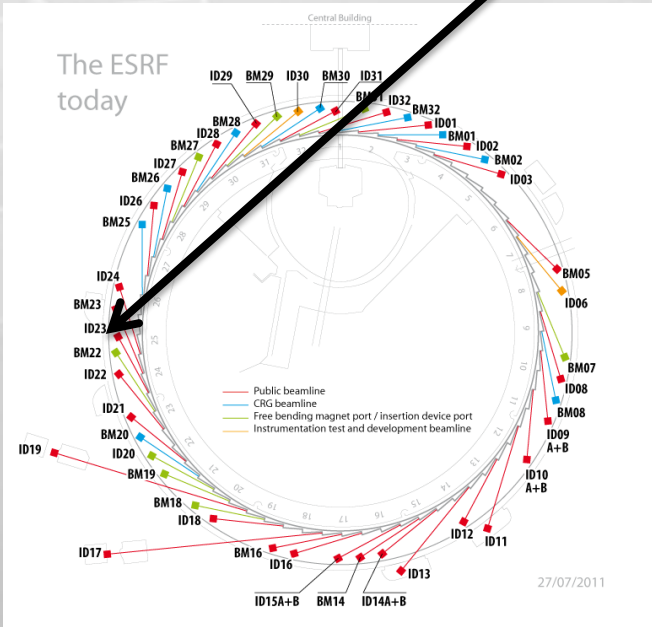
European Synchrotron Radiation Facility

ID23 MX beamline

Alexander Popov
ESRF, MX group

biosync.sbkb.org/beamlineprofile.do?synch_id=esrf®ion=European&bmln_name=ID23-1

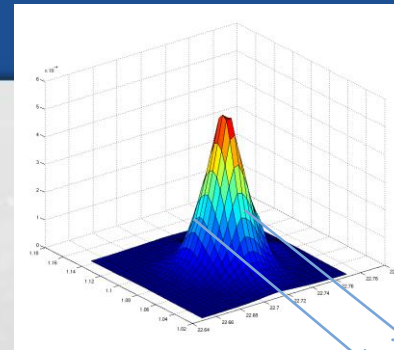
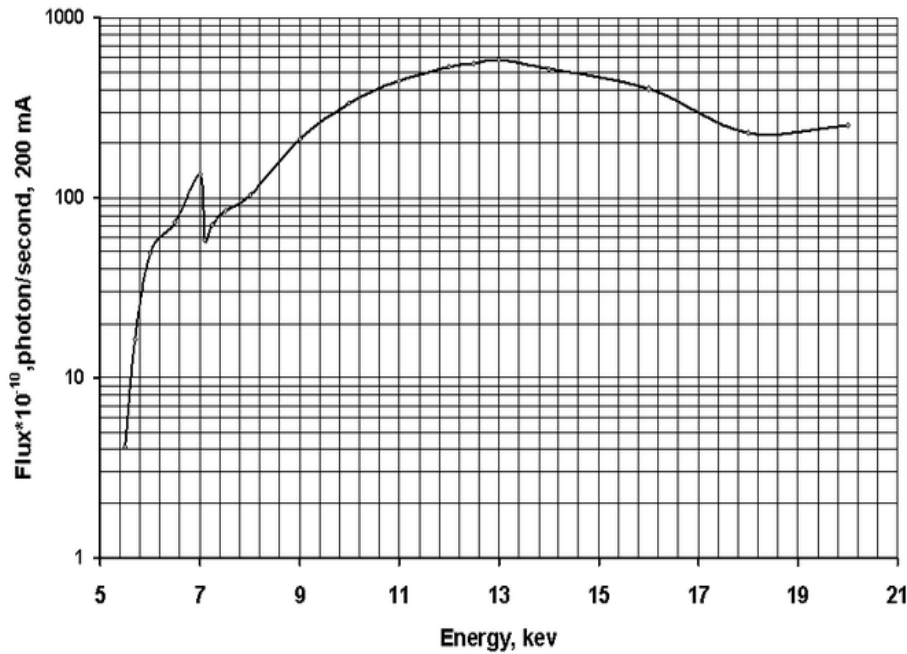
The ESRF today



Beamline Name	ID23-1
Primary Contact: Name	Alexander Popov
Owner/Operator	Gemini - Macromolecular Crystallography Group
Status	operational
Experiments	MAD
Services	Remote access
Source Type	insertion device
Spot Size (mm): Height	0.06
Spot Size (mm): Width	0.06
Monochromator	Single crystal
Crystal Type	Si(111)
Mirrors	bent cylindrical
Flux(PHOTONS/SEC)	$\times 10^6$
Flux Details	
Wavelength Range (Å)	0.62 - 2.48
Energy Range (keV)	5 - 20
Goniometer	Maatel Mini-diffractometer (MD2M)
Sample Handling: Robotics	EMBL Grenoble Sample Changer (SC3)
Robotics: More Info	The Sample Changer has been designed for use with SPINE standard sample holders and vials, which are loaded into the SC in baskets specifically designed for the SCs. The goniometer head that must be used in conjunction with the SCs is equipped with a SmartMagnet. This detects whether a sample is mounted on the goniometer head or not. Each individual SmartMagnet is tuned for operation on a particular beam-line and a goniometer head must NOT be taken from one beam-line for use on another.
Detector: Type	PIXEL
Detector: Model	DECTRIS PILATUS 6M
Detector: Activated for Service	info currently not available
Detector: Removed from Service	
Cryo Capability	Oxford cryosystems 700 series

ID23eh1 FLUX

21/09/2009



0.045 mm

ID23-1 is equipped with the apertures
50, 30, 20 and 10 microns in diameter
at the end of the collimator.
ID23-1

E=12.75 KeV Curent =200 mA

Aperture	Beam_Flux (photon/s)
----------	----------------------

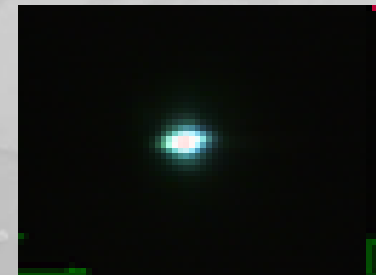
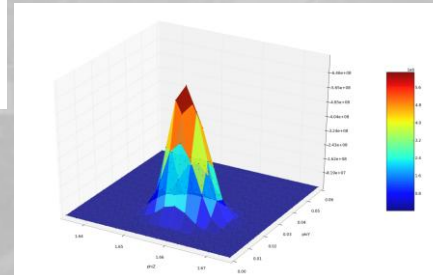
0.050 mm	3.5×10^{12}
----------	----------------------

0.030 mm	1.5×10^{12}
----------	----------------------

0.020 mm	6.0×10^{11}
----------	----------------------

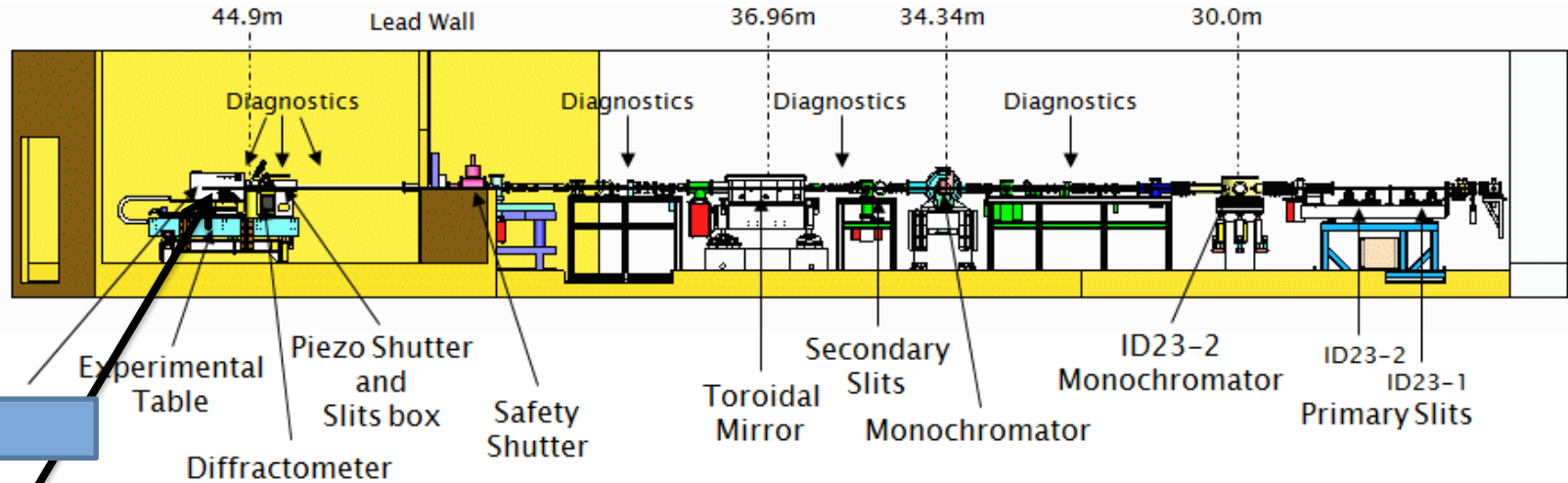
0.010 mm	2.0×10^{11}
----------	----------------------

10 microns



Experimental Hutch

Optic Hutch

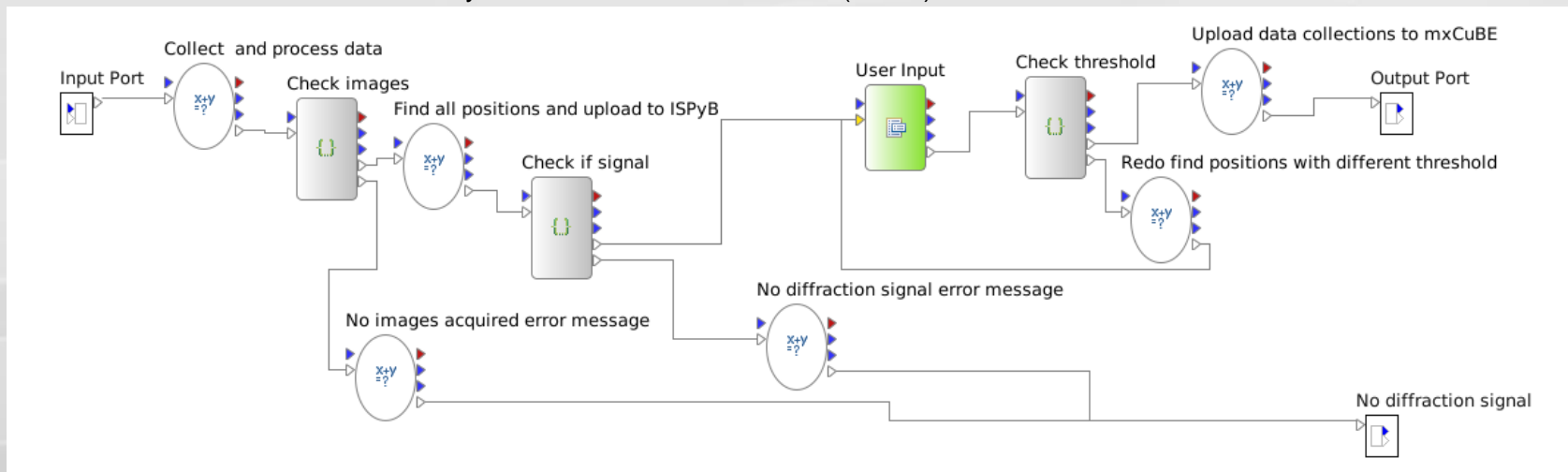


Application on the ID23-1 of the new PILATUS detector reduces the total time of data collection to 0.5-2 minutes

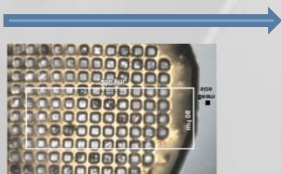
Diffuse scattering

Fast crystal best position screening
X-ray centering
Crystal cartography
Helical Data Collection
X-ray diffraction protein crystal detection

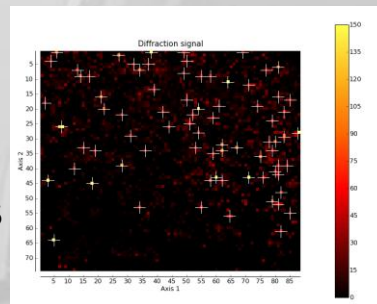
Mult-crystal data collection U. Zander (ESRF)



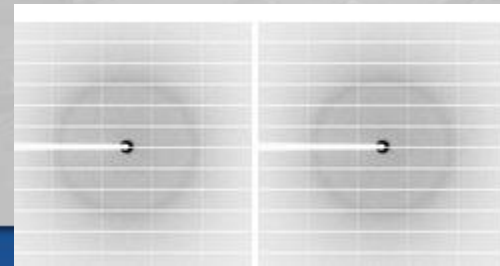
Fast Two-dimension mesh scan

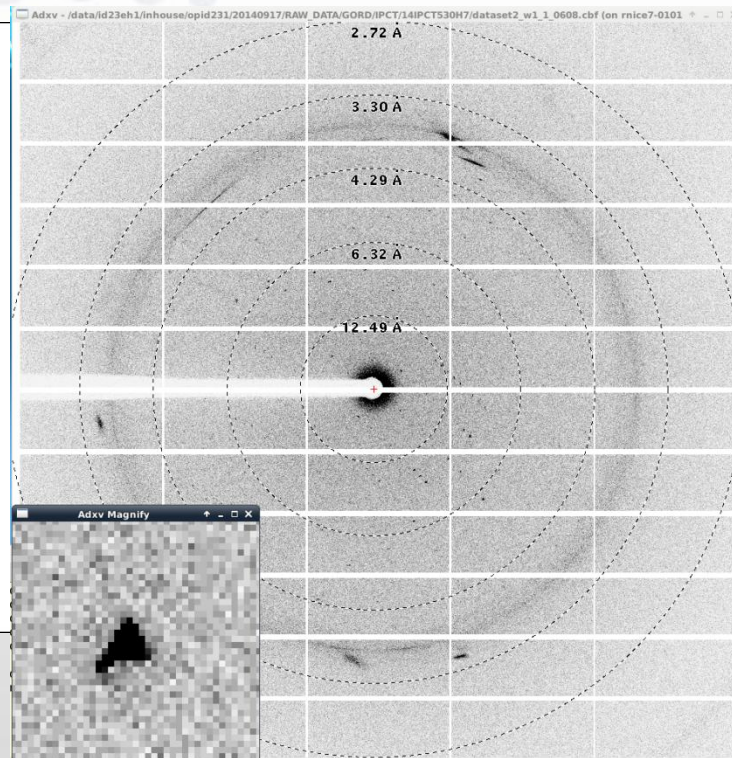
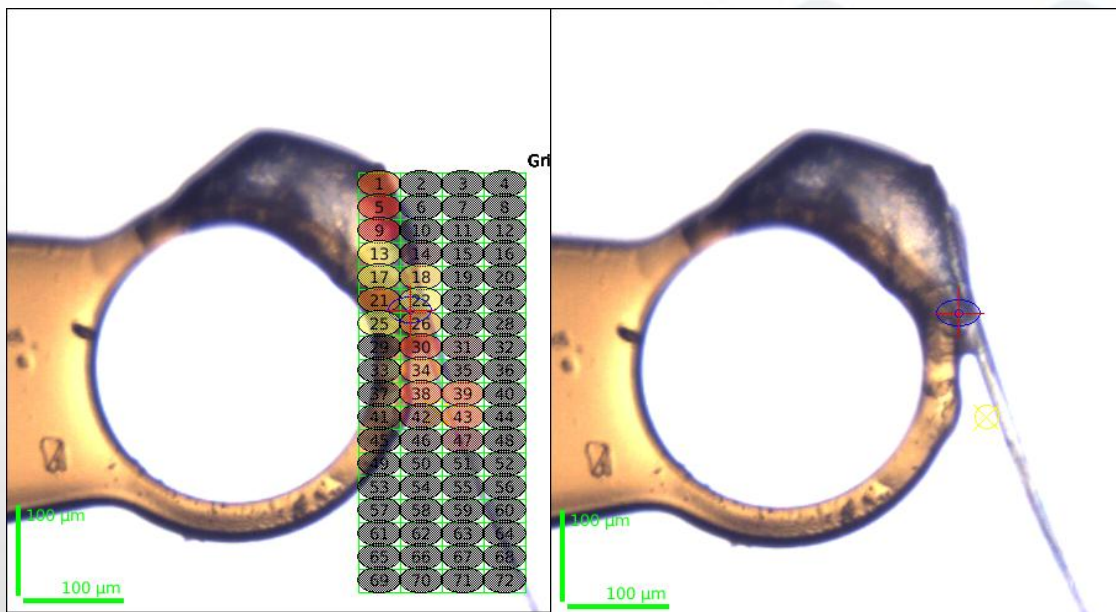


Recognition of crystals using diffraction images



Data collection

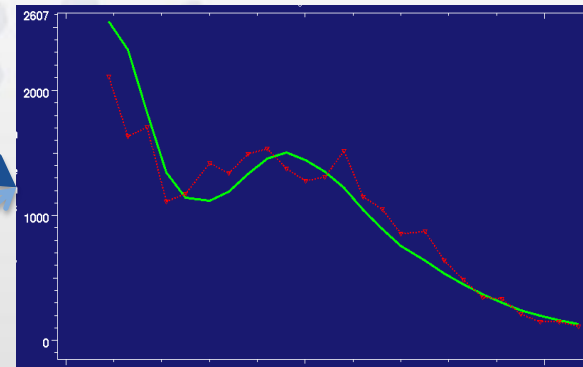
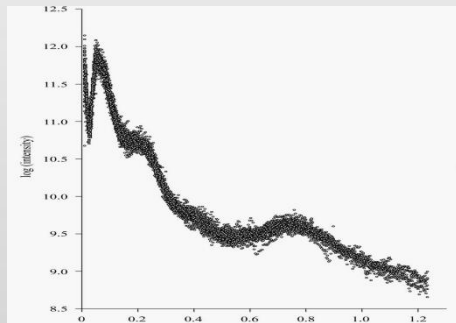
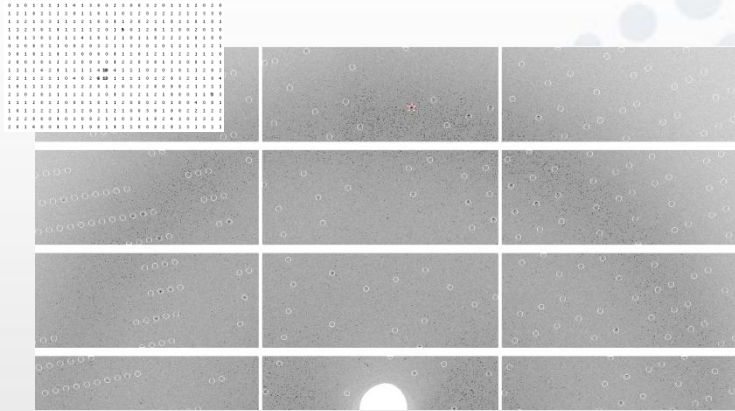




SUBSET OF INTENSITY DATA WITH SIGNAL/NOISE ≥ -3.0 AS FUNCTION OF RESOLUTION

RESOLUTION LIMIT	NUMBER OF REFLECTIONS			COMPLETENESS OF DATA	R-FACTOR observed	R-FACTOR expected	I/SIGMA	R-meas	CC(1/2)	Anomal Corr	SigAno	Nano	
	OBSERVED	UNIQUE	POSSIBLE										
6.44	5119	1275	1319	96.7%	4.4%	4.3%	5001	24.35	5.0%	99.8*	-20	0.752	553
5.11	5259	1207	1217	99.2%	6.7%	7.0%	5185	16.66	7.6%	99.6*	-2	0.773	606
4.47	4928	1177	1187	99.2%	6.1%	6.6%	4857	16.96	7.0%	99.6*	-13	0.698	534
4.06	5286	1183	1198	98.7%	8.0%	8.1%	5227	14.41	9.0%	99.4*	-5	0.777	588
3.77	4560	1111	1141	97.4%	13.2%	12.6%	4502	9.32	15.1%	98.6*	-5	0.830	499
3.54	5117	1210	1242	97.4%	20.9%	19.6%	5053	6.41	23.8%	97.1*	-3	0.807	576
3.37	4851	1099	1119	98.2%	30.4%	30.0%	4792	4.63	34.4%	93.8*	-2	0.792	572
3.22	5325	1174	1190	98.7%	39.2%	40.8%	5264	3.37	44.2%	92.0*	-3	0.738	635
3.10	4683	1122	1136	98.8%	65.2%	66.8%	4621	2.03	74.6%	77.6*	-5	0.734	547
2.99	4789	1133	1170	96.8%	89.3%	90.2%	4730	1.50	102.1%	66.6*	-4	0.662	561
total	49917	11691	11919	98.1%	9.6%	9.7%	49232	10.20	10.9%	99.8*	-5	0.756	5671

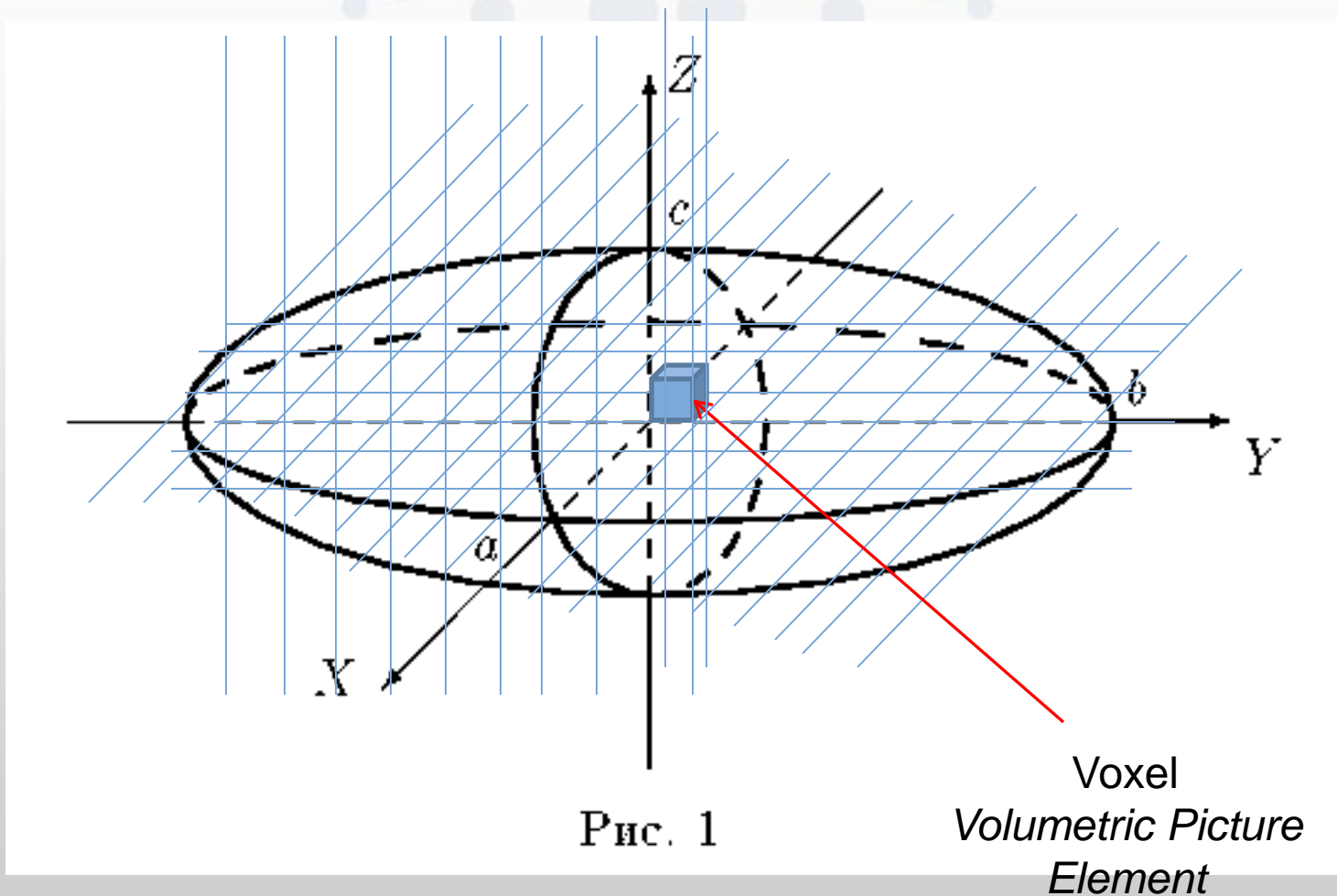
Evaluating diffraction signal with DOZOR



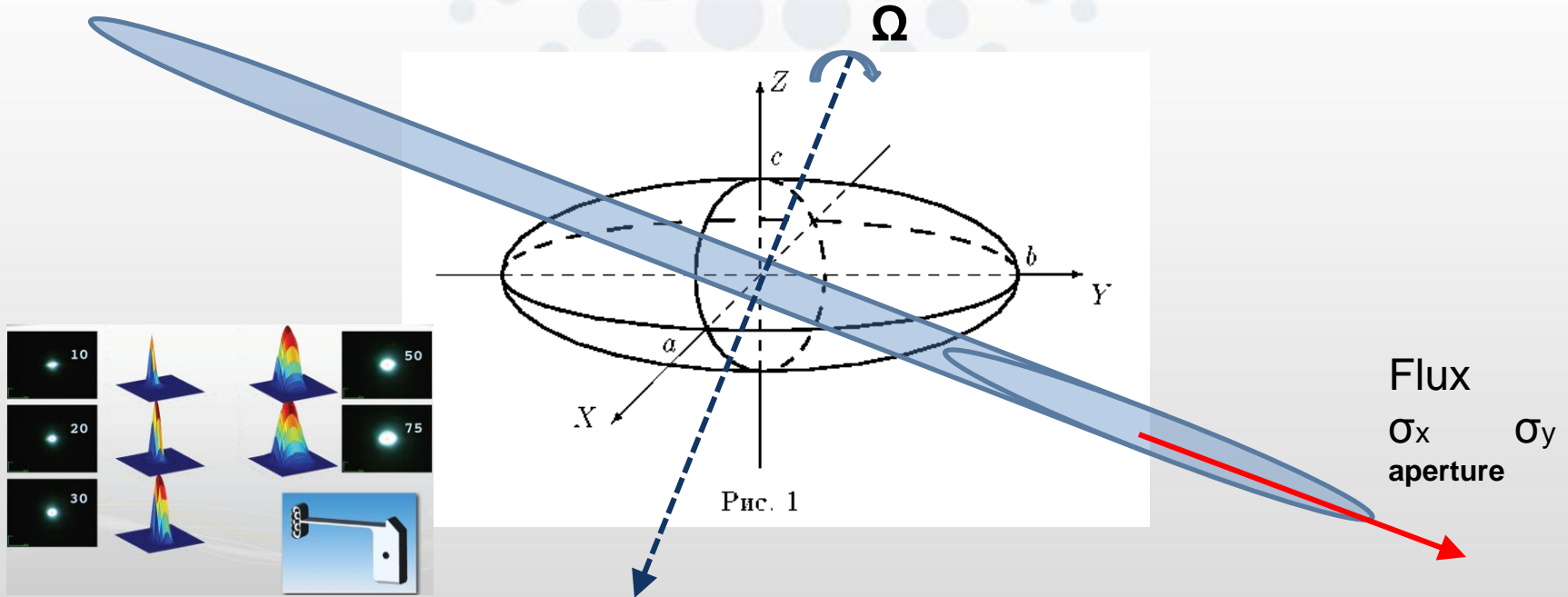
score =

$$\text{total scattered intensity} \times \text{radial shape similarity}$$

- Use Wilson plot as a prior
- Use all pixels, not just the local maxima



$$Scale(\Omega) = Scale(voxel) \times NumberVoxel(\Omega)$$

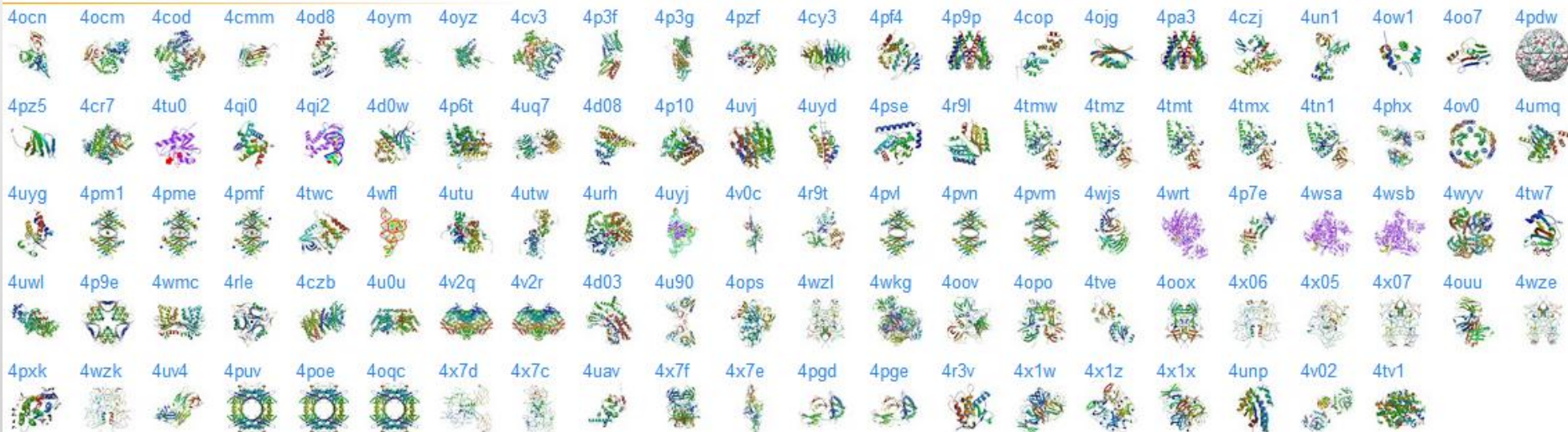


$$\hat{J}(\mathbf{h}, D) = \hat{J}_o(h) \sum_{voxel} \sum_{x,y} I_{x,y}(beam) \times scale(voxel, D_{voxel}) \exp(-\mathbf{h} \cdot \mathbf{B}(D_{voxel}) \cdot \mathbf{h}^T / 2)$$

Year	2004-2007	2008	2009	2010	2011	2012	2013	2014
n. of structures	192	126	153	158	135	181	170	112

Total 1228

2014

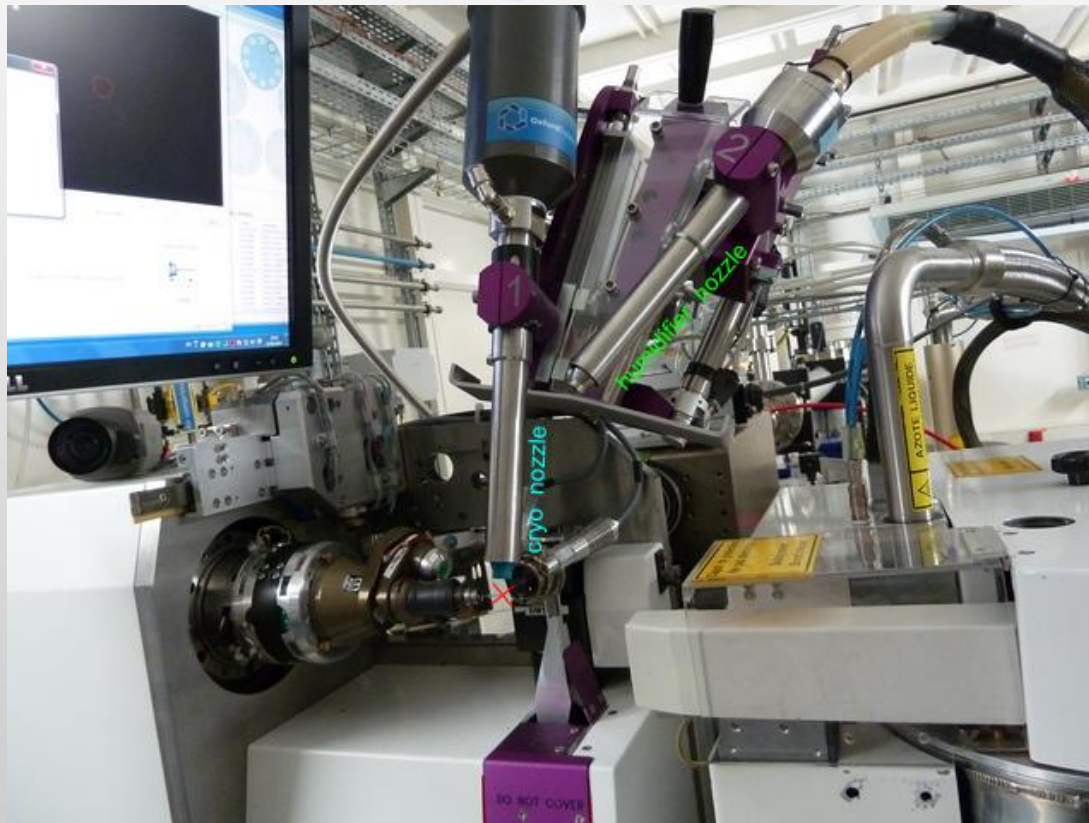


2015

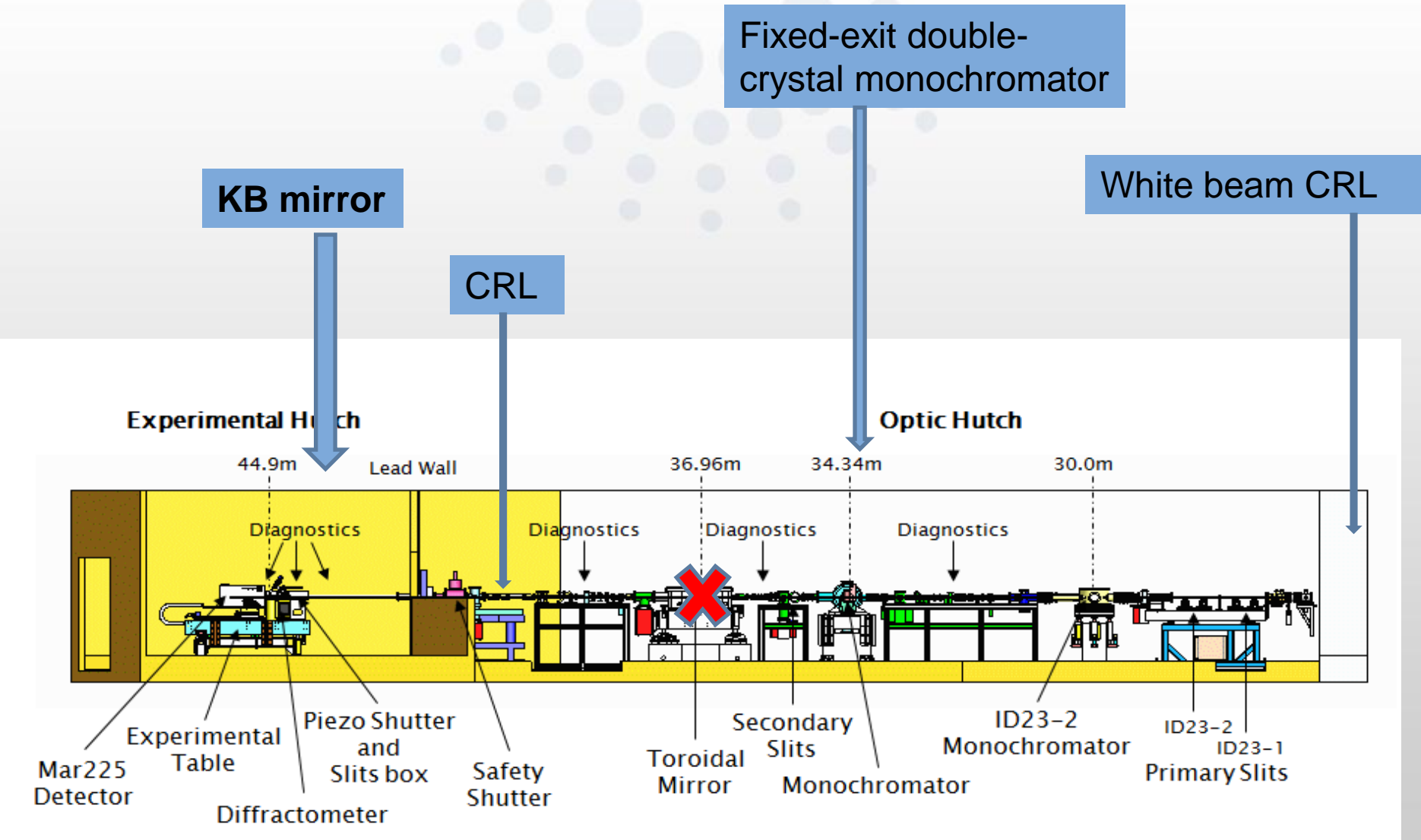
4xh9



1. Improvement / upgrade ID23-1 diffractometer – pop-up YAG screen
2. Rapid Exchanger (ReX) for automated exchange between HC1 humidifier nozzle and cryo-stream nozzle. Including mechanical support system with alignment axes



BM14 ESRF



	now	upgraded
Beam size [mm]	0.01 – 0.05	0.002 – 0.300
Flux [ph/s]	$2 \cdot 10^{11}$ - $3 \cdot 10^{12}$	10^{13} - 10^{14}
Flux density [ph/s/mm ²]	$2 \cdot 10^{13}$ - 10^{13}	$5 \cdot 10^{15}$ - $5 \cdot 10^{14}$
Crystal life-time [s]	20 -30	2 - 0.2

The background of the slide is a faded, aerial photograph of the ESRF facility. It shows several large, curved buildings, likely the synchrotron rings, and various smaller structures and parking areas. The overall tone is light and professional.

**Thanks for
your attention**