Current Status & Ideas for the evolution of ID29 & ID23

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ESRF Upgrade (MX)

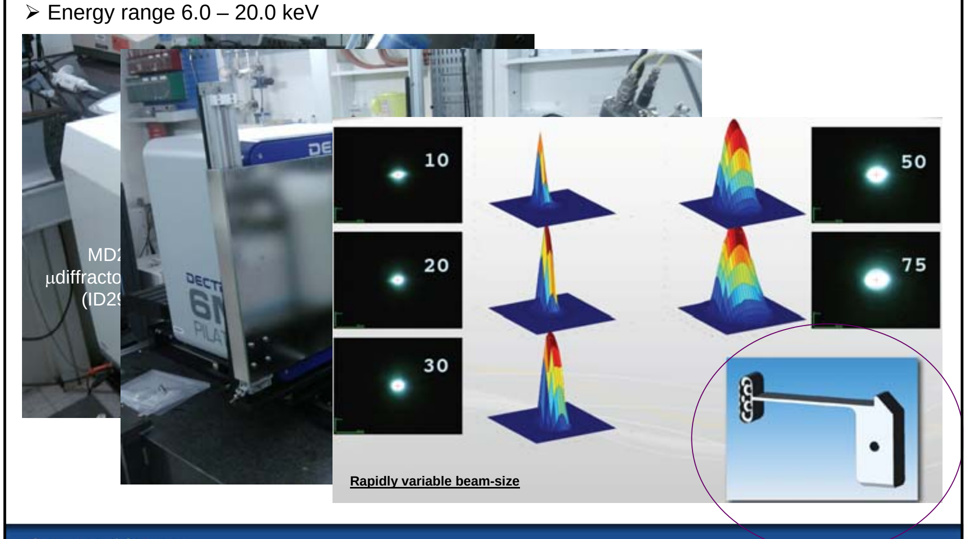
European Synchrotron Radiation Facility

- Phase I
  - Replacement of ID14 by UPBL10 beamlines
    - MASSIF - not just screening. Pipelines for fragment-based drug design etc.
    - BM29 - enhanced SAXS BL. Smaller sample volumes, HPLC-coupled SAXS
    - ID30B – replacement for ID14-4
    - 'Incremental' improvements of ID23-1, ID23-2, ID29
- Phase II
  - Much smaller beam sizes, massively increased flux densities
  - 4 Phase II Upgrade BLs

	Structural Biology Group Beamlines 2013-2014				
		Beamsize [µm² H x V]	**Energy [keV]**	**Flux [ph/sec]**	**Detector**
ID14-1,2→	***MASSIF-1***	100	≈12.8	$>10^{13}$	Pilatus3 2M (250 Hz)
	MASSIF-3	≤10		$2x10^{13}$	Eiger 4M (750 Hz)
ID14-3 →	**BM29**	700 x 700 [100 x 100]	7-15	$3x10^{12}$	Pilatus 1M
ID14-4 →	**ID30B**	200-20	5-20	$>10^{13}$	Pilatus3 6M (100 Hz)
	ID23-1	30 x 20 [10x10]	6-20	$>10^{12}$	Pilatus 6M (25 Hz)
	ID23-2	5 x 7	14.2	$4 x 10^{11}$	Pilatus3 2M (250 Hz)
	ID29	60x30 [10x10]	6-20	10^{13}	Pilatus 6M (25 Hz)

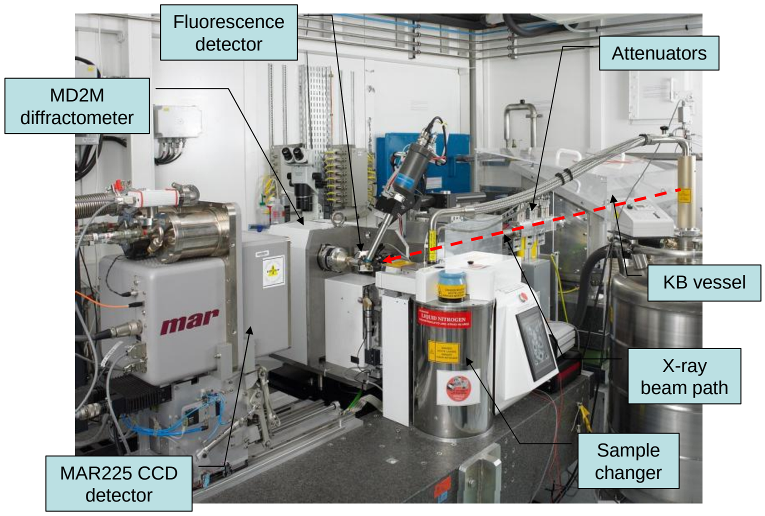
ID23-1 & ID29: current status

- Rapidly tunable facilities for MAD/SAD experiments in Structural Biology
- Energy range 6.0 – 20.0 keV

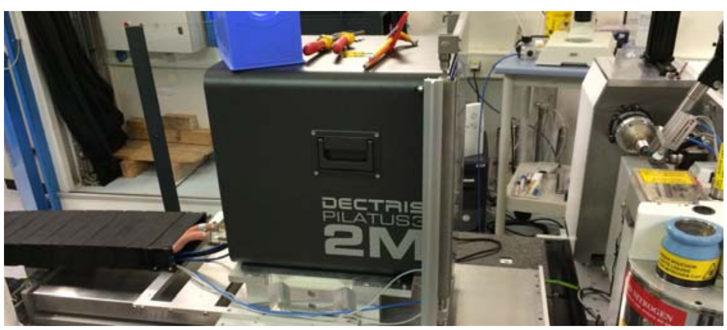


ID23-2: current status

- (first) μfocus beamline dedicated to MX
- beam size at sample: ~ 5 x 7 μm^2

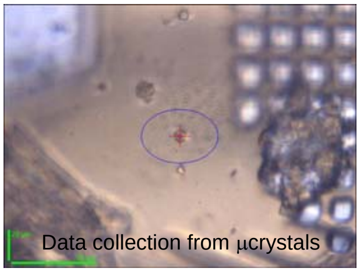


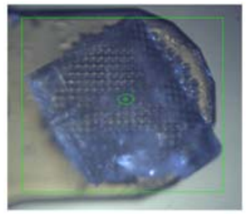
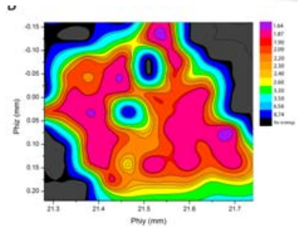
ID23-2: Data collection at 250 Hz frame-rate



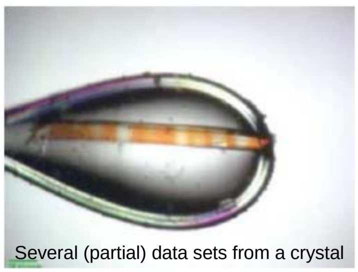
RESOLUTION LIMIT	NUMBER OF REFLECTIONS OBSERVED	UNIQUE	POSSIBLE	COMPLETENESS OF DATA	R-FACTOR observed	R-FACTOR expected	COMPARED	I/SIGMA	R-meas	CC(1/2)	Anomal Corr	SigAno	Nano
2.89	14344	5784	6462	89.5%	2.2%	2.3%	13101	35.20	2.8%	99.9*	2	0.845	1010
2.29	14191	5977	6294	95.0%	3.9%	3.8%	12896	20.52	5.0%	99.7*	-3	0.850	762
2.00	14702	5952	6188	96.2%	5.9%	5.5%	13599	15.24	7.4%	99.3*	3	0.910	951
1.82	14180	5810	6040	96.2%	8.9%	8.4%	13149	10.26	11.2%	98.7*	-1	0.894	745
1.69	13677	5810	6099	95.3%	13.9%	13.7%	12524	6.58	17.5%	96.9*	0	0.846	534
1.59	13030	5892	6103	96.5%	17.6%	17.4%	11811	4.85	22.7%	94.3*	2	0.817	330
1.51	13987	5940	6109	97.2%	25.2%	25.4%	12978	3.68	32.0%	89.5*	-2	0.794	626
1.44	15156	6306	6497	97.1%	32.6%	33.7%	14217	2.84	41.4%	83.1*	2	0.756	746
1.39	12956	5293	5473	96.7%	42.1%	43.6%	12254	2.23	53.3%	73.8*	-1	0.742	683
1.34	12690	5292	6331	83.6%	50.7%	53.3%	11883	1.80	64.4%	63.4*	0	0.719	623
total	138913	58056	61596	94.3%	5.2%	5.2%	128412	10.41	6.6%	99.9*	0	0.823	7010

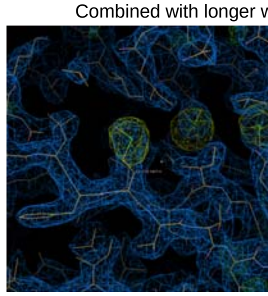
What a combination of microbeams & fast detectors allows


Data collection from μcrystals



Diffraction cartography

Combined with longer wavelength data collection


Several (partial) data sets from a crystal



Industrial client

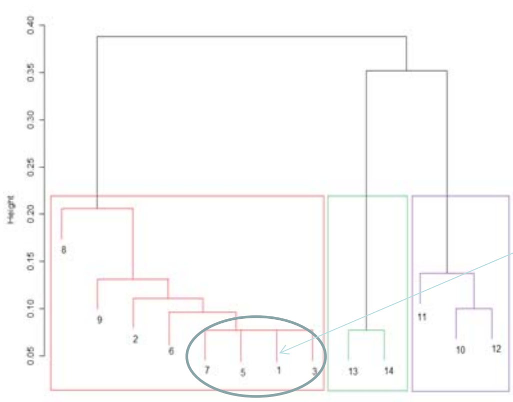
S-SAD phasing; E = 6 keV; S.G. = $P2_12_12_1$; d_{min} = 2.5 Å

Combined 2 data sets (2 x 3600 x 0.1º frames) from same crystal.

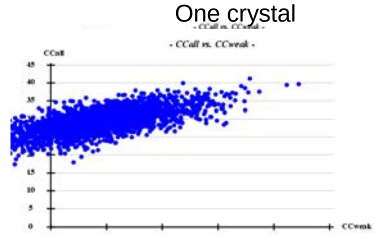
Beautiful electron density maps. No need to prepare derivative crystals

Multi-crystal data collection – choosing the best combination for *de novo* phasing using HCA

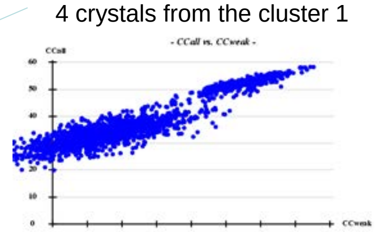
$$dist(i,j) = \sqrt{1 - cc_I^2(i,j)}$$



One crystal



4 crystals from the cluster 1



Multi-crystal data collection – choosing the best combination for *de novo* phasing using HCA

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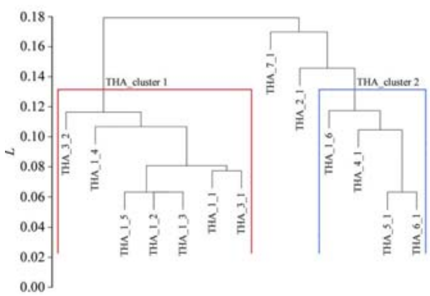
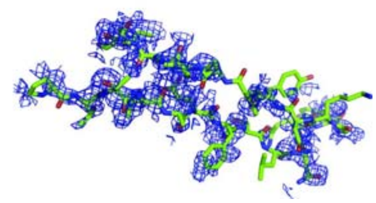
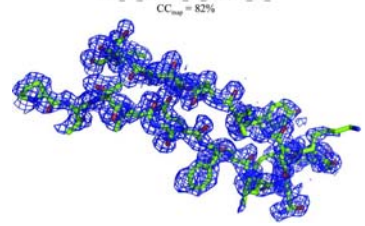
$$dist(i,j) = \sqrt{1 - cc_I^2(i,j)}$$



THA_L1_2 + THA_L2_1 + THA_L6_1
CC_{map} = 37%



THA_L1_2 + THA_L1_3 + THA_L1_5
CC_{map} = 82%



Giordano, R., Leal, R. M. F., Bourenkov, G. P., McSweeney, S. & Popov, A. N. (2012). *Acta Cryst.* D68, 649-658.

ESRF Upgrade Programmes

A Light for Science

Phase I
19 upgraded or refurbished BLs
Accelerator and source upgrade
Construction programme

more details at:
http://www.esrf.fr/news/general/whitepaperupgradephaseII

2009 — 2015

(2015) — (2020)

Phase II
New storage ring
4 new BLs
Enabling technoloy

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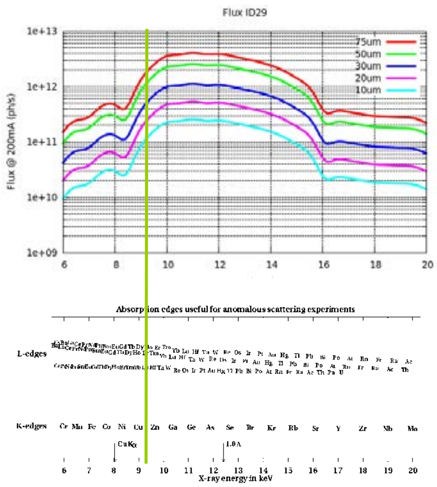
Evolution of ID29: softer energies & μfocus beam?



Softer Energies: MAD/SAD for metalloenzymes; lanthanide derivatives; L-absorption edges of Xe, I; S-SAD; identification of ions; etc.

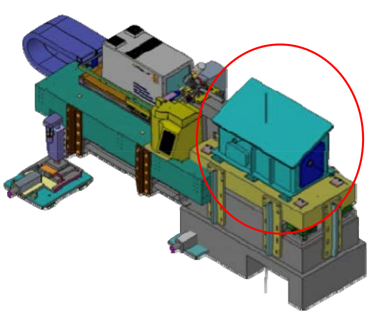
But, currently factor of 10-20 lower flux densities below 9 keV

Table 5. Potential flux densities (photons/sec/μm^2) ID29

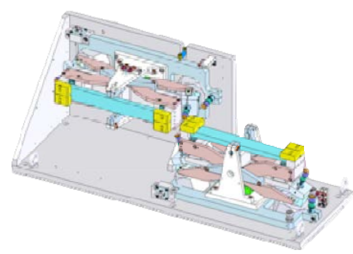
Beam size	10 x 10 μm	5μm x 5μm			
	Collimated Current	Collimated Current	+ Undulators	+ UHV	+ μfocus
6.0 keV	3.2×10^7	3.2×10^7	6.4×10^7	1.9×10^8	1.5×10^{10}
8.0 keV	6.4×10^7	6.4×10^7	1.3×10^8	2.1×10^8	2.0×10^{10}
10.0 keV	6.4×10^8	6.4×10^8	6.4×10^8	8.0×10^8	4.8×10^{10}
12.0 keV	6.4×10^8	6.4×10^8	6.4×10^8	7.3×10^8	4.3×10^{10}
14.0 keV	4.7×10^8	4.7×10^8	7.0×10^8	7.6×10^8	5.2×10^{10}
16.0 keV	6.4×10^7	6.4×10^7	1.3×10^8	1.4×10^8	9.4×10^9

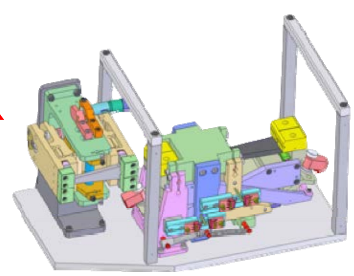
For comparison, the flux density available on the fixed-wavelength (E ~ 14.2 KeV; λ ~ 0.837 Å) ESRF micro-focus beam-line ID23-2 (focal spot 5 x 7 μm^2; V × H, FWHM) is ~2×10^9 ph/sec/μm^2 (Flot et al., 2010)

Ideas for providing a μfocus beam on ID29



ID23-2-like; 5x5µm²
ESRF 300-300 KB

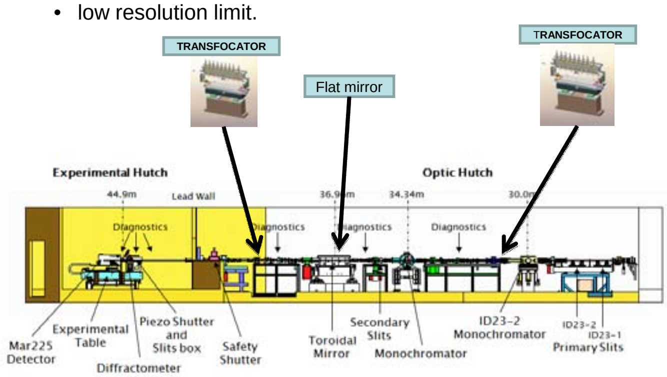




ID22-like, 1x1µm²
ESRF 170-92 KB

Evolution of ID23-1: variable focal spot size?

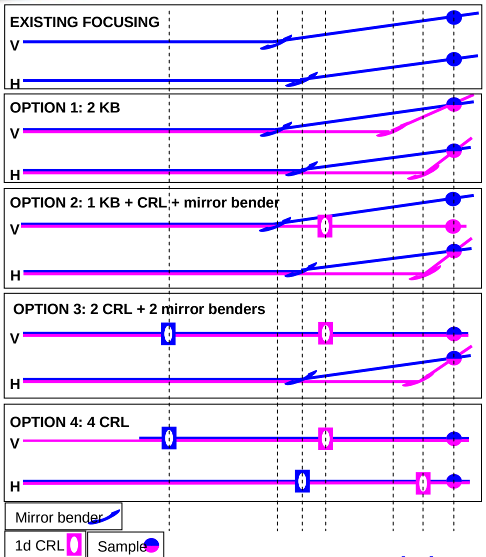
- Variable beam-size: Beam size 150μm^2 (max) to 5 μm^2 (min).
  - Match the X-ray beam and crystal sizes
    - improved S/N
    - reduced systematic errors to reduce
    - measurements to ultra-high resolution (d_{min} better then 0.8 Å)
    - reduced divergence
      - improved beamline resolution
      - low resolution limit.



Ideas for the evolution of ID23-2: Selectable beam size: "small" (current size) and "smaller" (~ 1x1 μm^2)

- Design Goals:
  - Easily selectable beamsize: either ~1x1 μm^2 or ~7x10 μm^2
  - Preserve stability of current layout
  - ~1x10^{11} ph/s
  - Mechanism to limit convergence for low resolution/large unit cells
- Resraints:
  - Cost – including human resources
  - Physical space limitations
  - Down time (beamtime currently at a premium)
  - Stability
  - Usability
  - Maintainability

Optical configurations for ID23-2 1x1 μm^2 beam

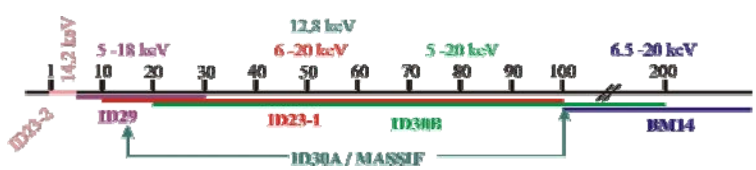


Large beam (~7x10 micron)			Small beam (~1.2x1 micron)		
V (mrad)	H (mrad)	Flux (x10^11 ph/s)	V (mrad)	H (mrad)	Flux (x10^11 ph/s)
0.55	0.36	2	-	-	-
0.55	0.36	2	2.42	2.1	2
0.55	0.36	2	0.39	2.1	1.4
0.1	0.36	2	0.39	2.1	1.4
0.1	0.18	1	0.39	0.07	0.28

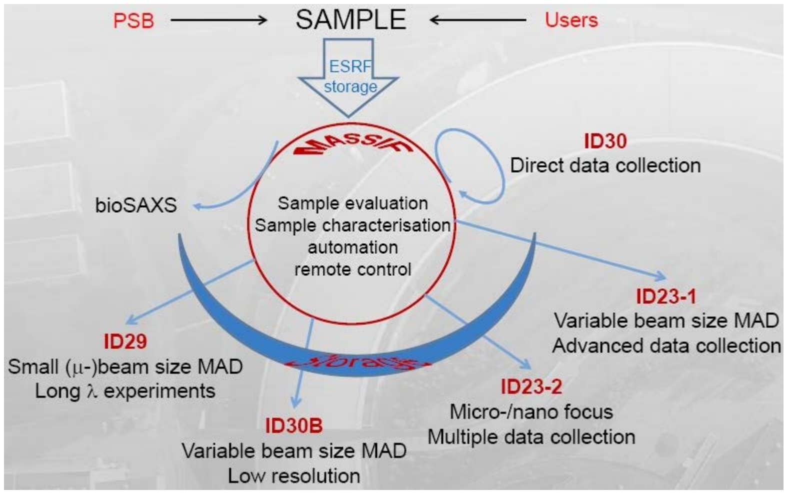
BLUE: Big beam PINK: Small beam

Structural Biology Group Beamlines 2016?

	Beamsize [μm^2 H x V]	Energy [keV]	Flux [ph/sec]	Detector
MASSIF-1	100	≈12.8	$>10^{13}$	Pilatus3 2M (250 Hz)
MASSIF-3	≤10		$2x10^{13}$	Eiger 4M (750 Hz)
BM29	700 x 700 [100 x 100]	7-15	$3x10^{12}$	Pilatus 1M
ID30B	200-20	5-20	$>10^{13}$	Pilatus3 6M (100 Hz)
ID23-1	Variable	6-20	$>10^{12}$	Pilatus 6M (25 Hz)
ID23-2	5 x 7 1 x 1	14.2	$2 x 10^{11}$	Pilatus3 2M (250 Hz)
ID29	60x30 [5 x 5]	6-20	10^{13}	Pilatus 6M (25 Hz)



A paradigm for Structural Biology at ESRF



ESRF – Phase II Source Properties

	Emittance		Beta [m]		λ [A]	L [m]	Rms size [µm]		Divergence [µrad]	
	H [nm]	V [pm]	H	V			H	V	H	V
High beta	4	5	37.2	3	6.2	3.2	409	10.8	14.5	10.3
					1	3.2	409	5.6	11.9	6.1
					0.2	4	409	4.7	11.3	4.7
Low beta	4	5	0.37	3	6.2	3.2	50	10.8	104	10.3
					1	3.2	49	5.6	104	6.1
					0.2	4	49	4.7	104	4.7
New lattice	0.13	2	4.7	2.7	6.2	3.2	26.7	10.3	11.4	10.2
					1	3.2	25	4.7	7.4	5.3
					0.2	4	25	3.5	6.8	4.4

Potential characteristics of a ESRF Phase II MX beamline

ID29 Beam characteristics with current and Phase-II lattices				
	Current	New Lattice (current optics)	New lattice (perfect optics)	**New Lattice (50:1)**
Source size (FWHM; H × V; μm²)	115 × 13.2	59 x 11	59 x 11	**59 x 11**
Divergence (r.m.s. H × V; μm²)	104 × 6.1	7.4 x 5.3	7.4 x 5.3	**7.4 x 5.3**
Demagnification ratio	3:1	3:1	3:1	**50:1**
Beamsize @ sample (μm²)	~60 x 30	30 x 25	20 x 4	**1.2 x 0.2**
Flux @ sample (ph/sec)	~1 x 10^{13}	~1 x 10^{14}	~1 x 10^{14}	**~1 x 10^{14}**
Flux density @ sample (ph/sec/μm²)	7.0 x 10^{9}	1.7 x 10^{11}	2.1 x 10^{12}	**2.4 x 10^{14}**
Absorbed dose rate (Gy/sec)	3.2 x 10^{6}	7.7 x 10^{7}	9.6 x 10^{8}	**1.2 x 10^{11}**
Time to Henderson Limit (sec)[c]	6.3	0.26	0.021	**0.0002**
Low res. data collection	?	Yes	Yes	**Yes**
μbeam MAD[e]	Yes	Yes	n/a	**n/a**
μfocus MAD	No	No	Yes	**Yes**
Serial μcrystallography	?	?	Yes	**Yes**

Thanks for your attention