

Life Science at the First Ultimate Storage Ring MAX IV, Lund, Sweden



Uwe Mueller

MAX IV – A dream for a long time came true



Architects 3D model

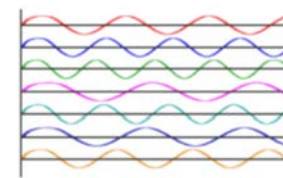
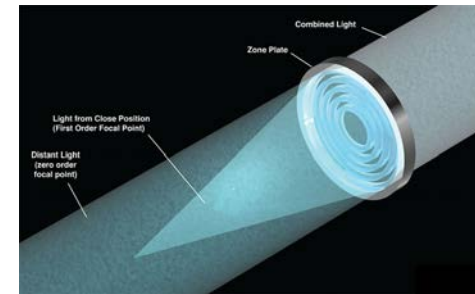
MAX IV



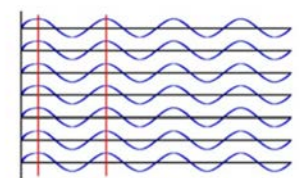
Why do we need novel photon sources ?

Source parameter

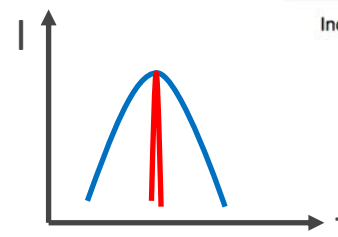
- Reduced X-ray beam size at low divergence and high photon flux:
 - To match smaller samples
 - To increase the spacial resolution (spectroscopic nanoprobes)
 - Advantageous for almost every experiment
- More symmetrical horizontal and vertical emittances (round beam)
 - H-V symmetric optics (zoneplates, CRL-focusing))
 - More flexibility in optics design
- Coherent x-rays
 - Better imaging possibilities (creating a uniform wavefront)
 - Nanofocussing
 - Ultra high flux
- Fs-pulses
 - Sampling of fast dynamics
 - Radiation damage free observations



Incoherent light waves



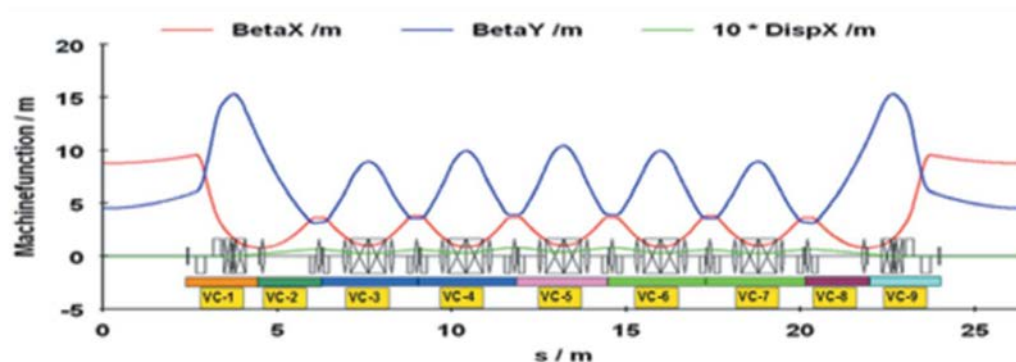
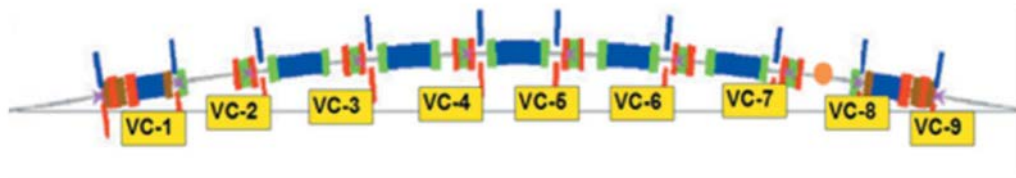
Coherent light waves



How to build a low emittance ring ?

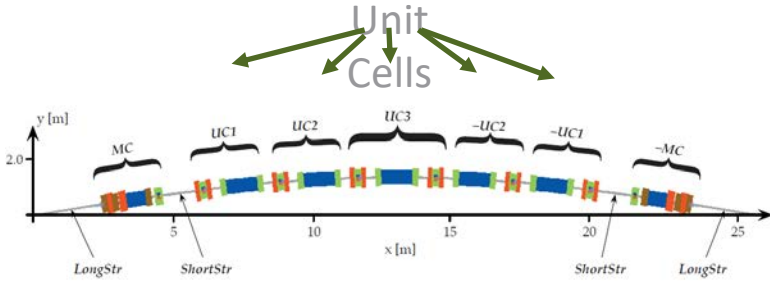
How to minimize emittance?

- Reduce dispersion and beta function in bend magnets, achieved by refocusing beam 'inside' bending magnets -> need space -> too expensive
- 'Split' bending magnets -> multi bend achromats → how?

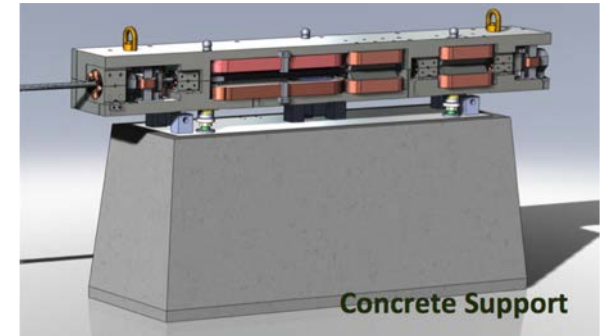
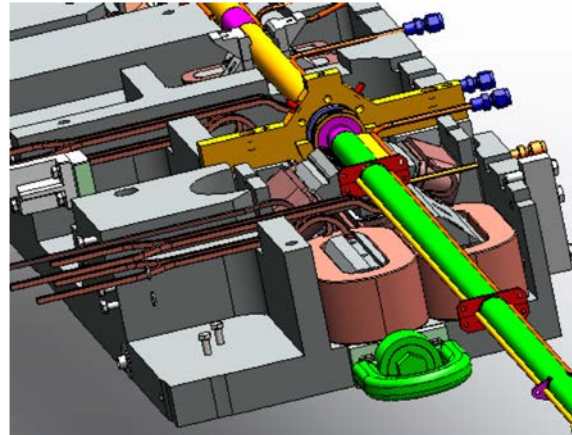


7-bend achromat magnet lattice of MAX IV

Novel magnet lattice technologies



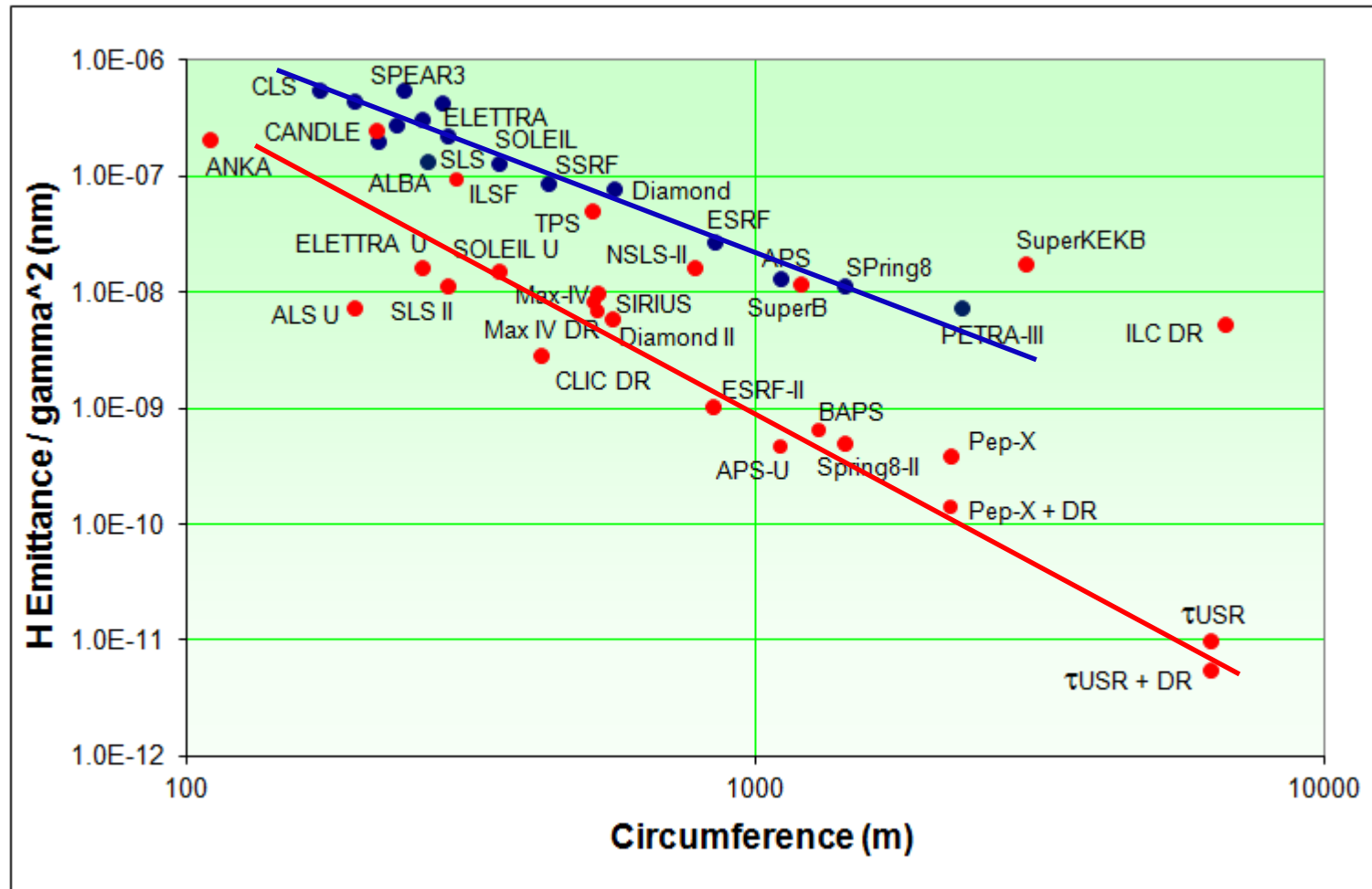
- Emittance: 200 -330 pmrad
- Max. current: 500 mA



Compact magnet and vacuum technology

Courtesy S. Leemans

New storage rings in the future



R. Bartolini

The MAX IV Photon Sources

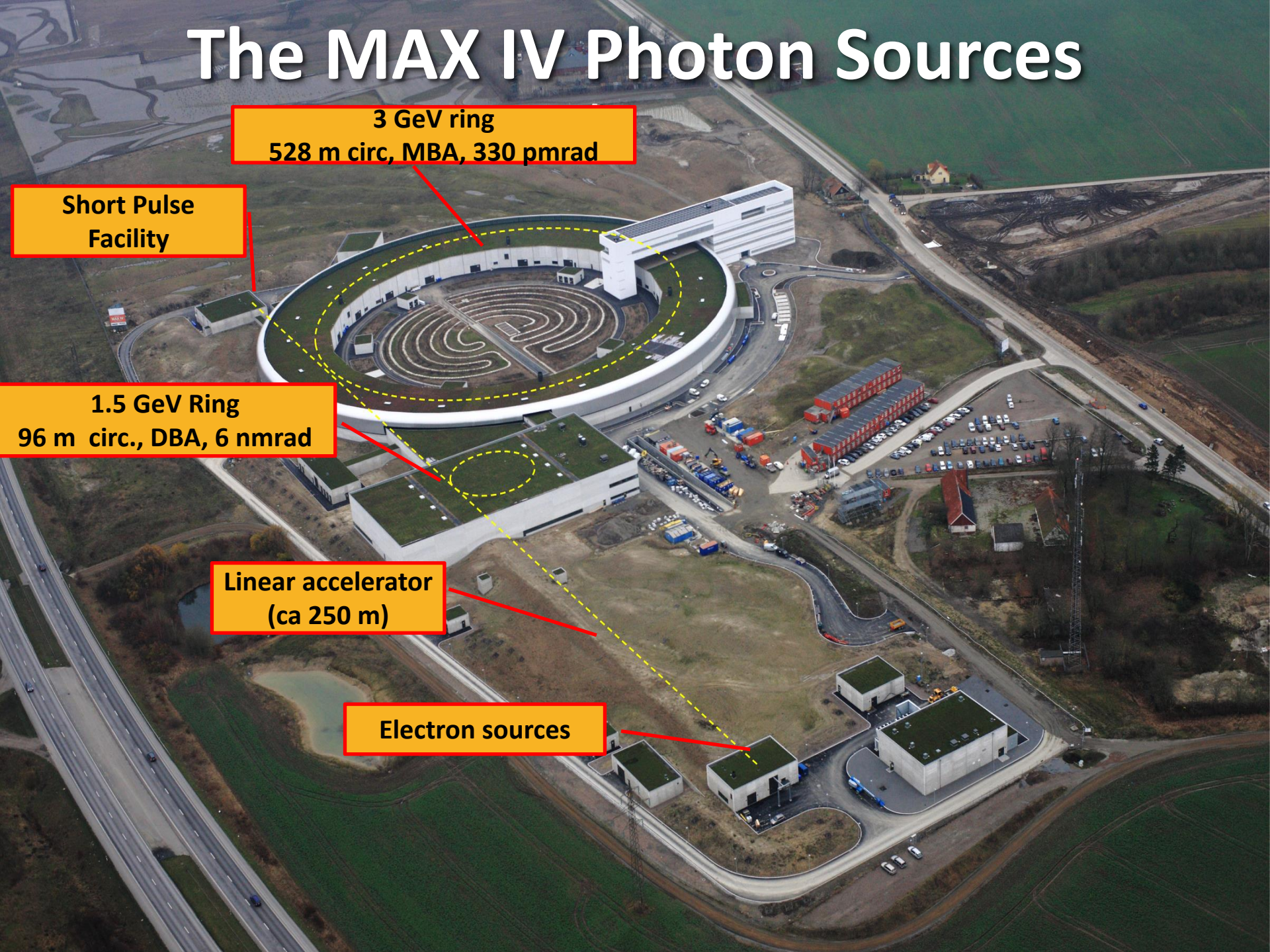
3 GeV ring
528 m circ, MBA, 330 pmrad

Short Pulse
Facility

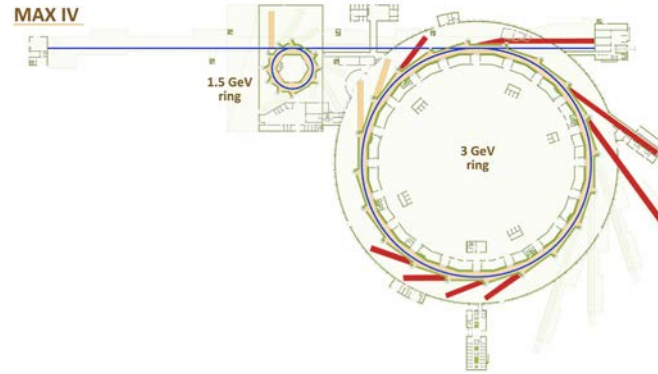
1.5 GeV Ring
96 m circ., DBA, 6 nmrad

Linear accelerator
(ca 250 m)

Electron sources



Life science at different length scales



Imaging

MedMAX II

MedMAX I

NanoMAX
SoftiMAX

Diffraction

coSAXS

BioMAX

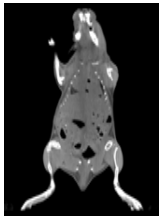
MicroMAX

Spectroscopy
FemtoMAX
Balder

10^{-6} m

10^{-9} m

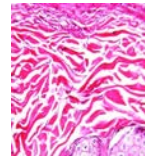
10^{-10} m



Animals



Organs



Tissues



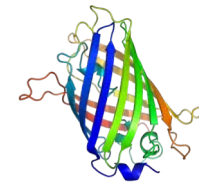
Cells



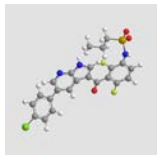
Micro-
structures



Molecular
complexes



Biomolecules



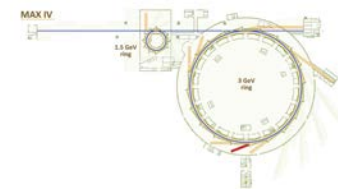
Atoms

Disease
models

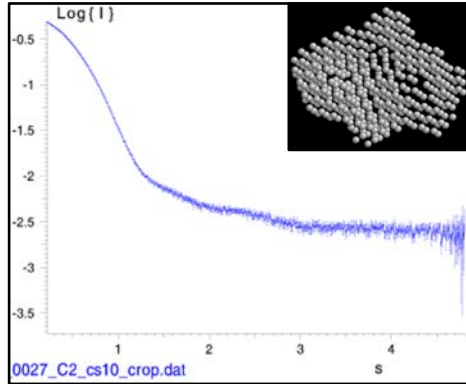
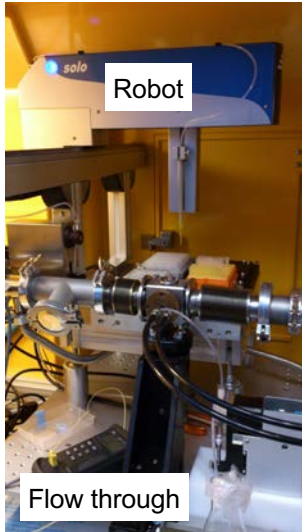
Histopathology

Cell Biology

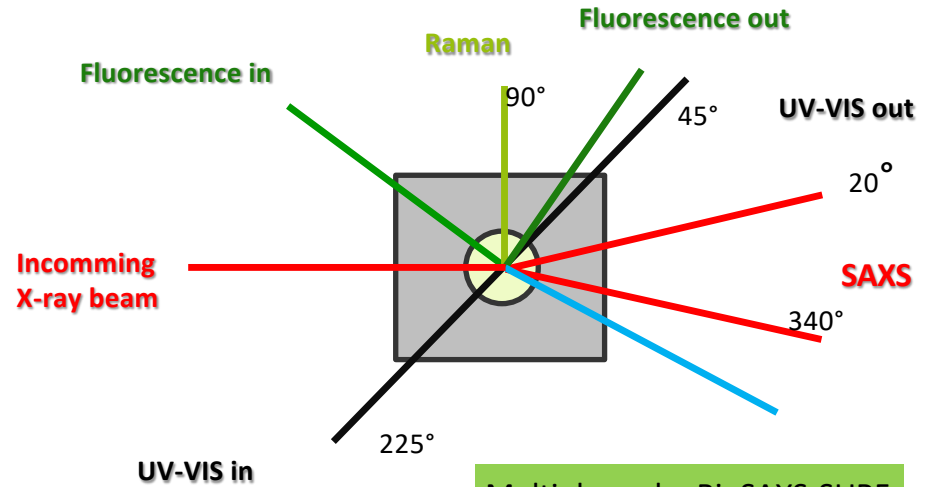
Molecular Medicine/Chemical Biology



coSAXS-BioSAXS

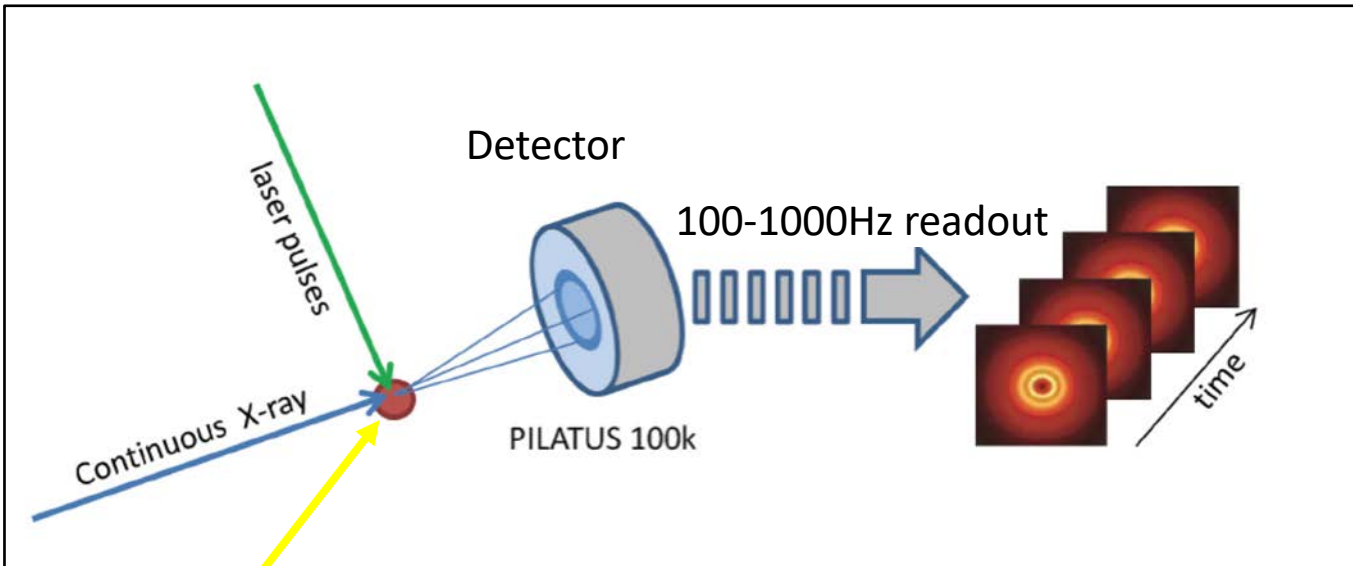


Static BioSAXS



Multiple probe BioSAXS-SURF

CoSAXS-LU-SWING (Soleil)

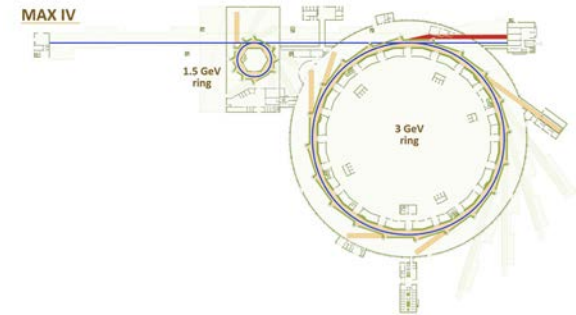


Dynamic BioSAXS
Conformational changes

CoSAXS-FemtoMAX
Lübeck University-EMBL/Ham.

FemtoMAX

Jörgen Larsson, email: Jorgen.Larsson@fysik.lth.se



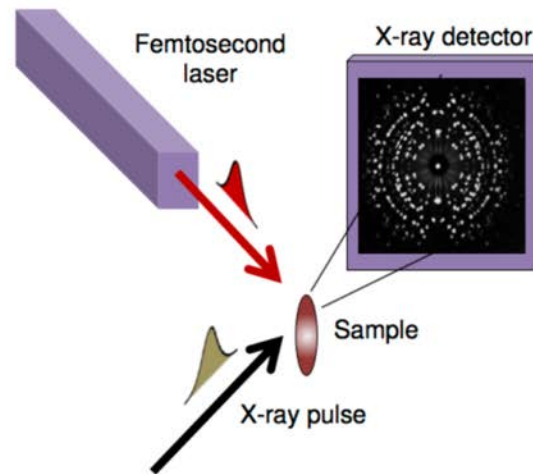
Aim:

Study of ultrafast chemical reaction, dynamics of biomolecules

Probes:

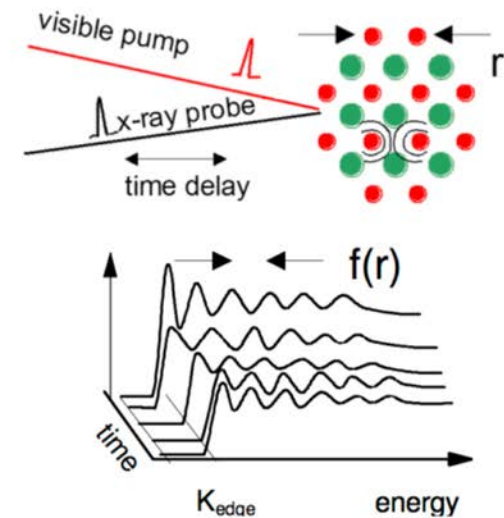
- Fs –Laser
- X-ray
- Ps –THz probe

Time-resolved x-ray diffraction



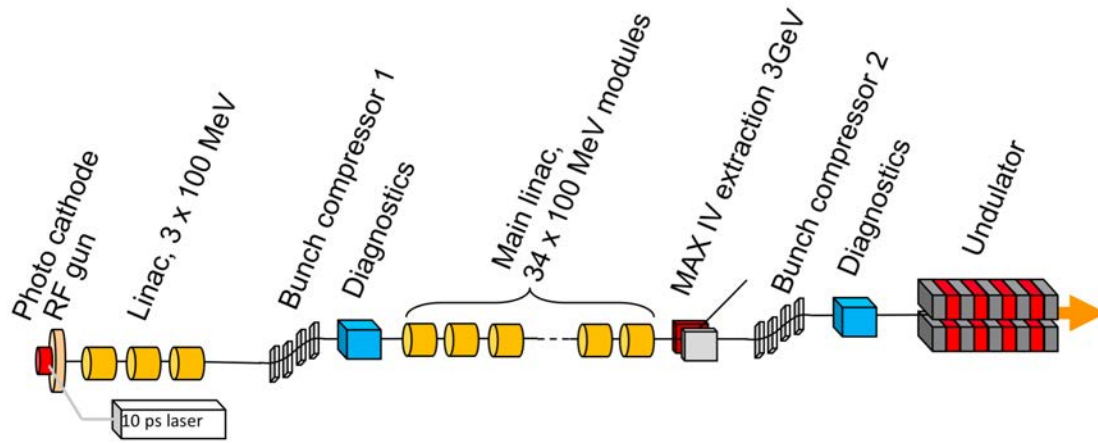
Phase-transitions, phonons in ordered systems

Time-resolved EXAFS

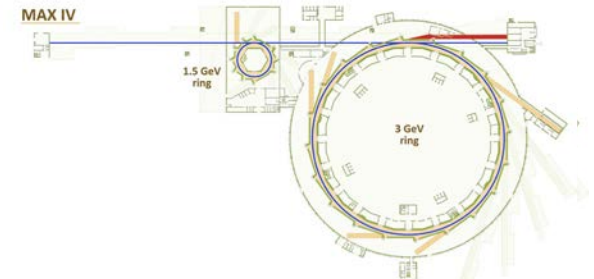


Complex disordered materials

FemtoMAX



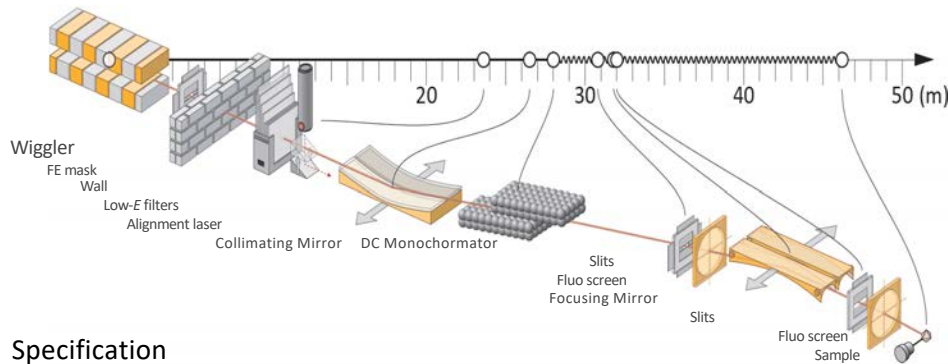
Beamline schematics



10m long FemtoMAX ivu

	Electrons	Photons
Energy	3 GeV	2-20 keV
Emittance	$e_N \sim 2.5$ mmRad	
Beam size in undulator	100 μ m FWHM	100 μ m FWHM
Pulse duration	100 fs FWHM	100 fs FWHM
Energy spread/Bandwidth	1.5%	1% with multilayer mono
Charge/Flux	100 pC/pulse	10^7 ph/pulse at 6 keV

Balder



Specification

Energy range: 2.4 - 40 keV (S to La K-edges)

Flux: 10^{12} - 10^{13} photons/s

Beam spot size: focused $\sim 100 \times 100 \mu\text{m}^2$ or defocused $V \sim 0.1\text{-}2\text{mm} \times H \sim 2\text{-}9\text{mm}$

Suitable for time resolved studies (sub-sec) and dilute, radiation sensitive samples.

2.4 – 40 keV = sample with elements

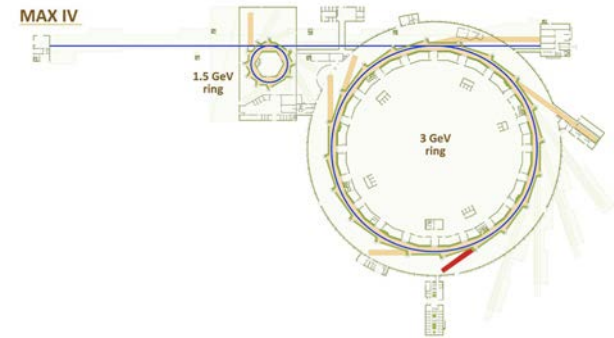
X-ray Excitation Energies of the Elements

Based on tables of McMaster et al.

Energies are in KeV

Symbol	Z	E_K	E_L	E_{LII}	E_{LIII}
Li	3	0.054			
Be	4	0.112			
B	5	0.188	0.284	0.302	0.327
C	6	0.284	0.302	0.327	0.352
N	7	0.409	0.438	0.463	0.488
O	8	0.532	0.561	0.586	0.611
F	9	0.677	0.706	0.731	0.756
Ne	10	0.839	0.868	0.893	0.918
Na	11	1.072	1.101	1.126	1.151
Mg	12	1.305	1.334	1.359	1.384
Al	13	1.551	1.580	1.605	1.630
Si	14	1.815	1.844	1.869	1.894
P	15	2.139	2.168	2.193	2.218
S	16	2.523	2.552	2.577	2.602
Cl	17	2.969	2.998	3.023	3.048
Ar	18	3.472	3.501	3.526	3.551
K	19	4.132	4.161	4.186	4.211
Ca	20	4.940	4.969	4.994	5.019
Sc	21	5.894	5.923	5.948	5.973
Ti	22	6.991	7.020	7.045	7.070
V	23	8.241	8.270	8.295	8.320
Cr	24	9.745	9.774	9.799	9.824
Mn	25	11.463	11.492	11.517	11.542
Fe	26	13.408	13.437	13.462	13.487
Co	27	15.613	15.642	15.667	15.692
Ni	28	18.087	18.116	18.141	18.166
Cu	29	20.843	20.872	20.897	20.922
Zn	30	23.867	23.896	23.921	23.946
Ga	31	27.141	27.170	27.195	27.220
Ge	32	30.665	30.694	30.719	30.744
As	33	34.419	34.448	34.473	34.498
Se	34	38.393	38.422	38.447	38.472
Br	35	42.647	42.676	42.701	42.726
Kr	36	47.161	47.190	47.215	47.240
Rb	37	51.925	51.954	51.979	52.004
Sr	38	56.949	56.978	57.003	57.028
Y	39	62.223	62.252	62.277	62.302
Zr	40	67.747	67.776	67.801	67.826
Nb	41	73.521	73.550	73.575	73.600
Mo	42	79.545	79.574	79.599	79.624
Tc	43	85.819	85.848	85.873	85.898
Ru	44	92.343	92.372	92.397	92.422
Rh	45	99.117	99.146	99.171	99.196
Pd	46	106.141	106.170	106.195	106.220
Ag	47	113.415	113.444	113.469	113.494
Cd	48	120.939	120.968	120.993	121.018
In	49	128.713	128.742	128.767	128.792
Sn	50	136.737	136.766	136.791	136.816
Sb	51	144.991	145.020	145.045	145.070
Te	52	153.475	153.504	153.529	153.554
I	53	162.189	162.218	162.243	162.268
Xe	54	171.123	171.152	171.177	171.202
Ba	56	187.721	187.750	187.775	187.800
La	57	195.986	196.015	196.040	196.065
Ce	58	204.910	204.939	204.964	204.989
Pr	59	214.494	214.523	214.548	214.573
Nd	60	224.738	224.767	224.792	224.817
Pm	61	235.642	235.671	235.696	235.721
Sm	62	247.306	247.335	247.360	247.385
Eu	63	259.730	259.759	259.784	259.809
Gd	64	272.914	272.943	272.968	272.993
Tb	65	286.858	286.887	286.912	286.937
Dy	66	301.562	301.591	301.616	301.641
Ho	67	317.026	317.055	317.080	317.105
Er	68	333.250	333.279	333.304	333.329
Tm	69	350.234	350.263	350.288	350.313
Yb	70	367.968	367.997	368.022	368.047
Lu	71	386.452	386.481	386.506	386.531
Hf	72	405.706	405.735	405.760	405.785
Ta	73	425.730	425.759	425.784	425.809
W	74	446.534	446.563	446.588	446.613
Re	75	468.118	468.147	468.172	468.197
Os	76	490.482	490.511	490.536	490.561
Ir	77	513.626	513.655	513.680	513.705
Pt	78	537.550	537.579	537.604	537.629
Au	79	562.264	562.293	562.318	562.343
Hg	80	587.768	587.797	587.822	587.847
Tl	81	614.052	614.081	614.106	614.131
Pb	82	641.126	641.155	641.180	641.205
Bi	83	668.990	669.019	669.044	669.069
Po	84	697.634	697.663	697.688	697.713
At	85	727.058	727.087	727.112	727.137
Rn	86	757.262	757.291	757.316	757.341
Ac	89	804.516	804.545	804.570	804.595
Th	90	833.000	833.029	833.054	833.079
Pa	91	862.714	862.743	862.768	862.793
U	92	892.648	892.677	892.702	892.727
Np	93	922.802	922.831	922.856	922.881
Pu	94	953.176	953.205	953.230	953.255
Am	95	983.770	983.800	983.825	983.850
Cm	96	1014.584	1014.613	1014.638	1014.663
Bk	97	1045.618	1045.647	1045.672	1045.697
Cf	98	1076.872	1076.901	1076.926	1076.951
Es	99	1108.346	1108.375	1108.400	1108.425
Fm	100	1140.040	1140.069	1140.094	1140.119
Md	101	1171.954	1171.983	1172.008	1172.033
No	102	1204.088	1204.117	1204.142	1204.167
Lr	103	1236.442	1236.471	1236.496	1236.521

Important in biology: S, Ca, V, Mn, Fe, Co, Ni, Cu, Zn, Se, Mo



XAS/XES

- Elegant probe for element speciation in biological and environmental samples.
- Element-specific structural information.
- Detailed information on metal centers in proteins.

Sample environment for bio

4-300 K closed cycle cryostat: multiple samples, variable volume 10-200 μl , mapping inside -MAX IV design
Liquid flow cell
Electrochemistry cell

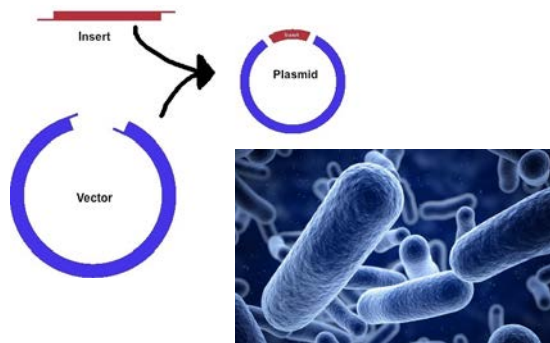
BioXAS/XES goals

- To measure XAS and XES on small dilute samples of metalloproteins without X-ray damage.
- To measure real-time changes in the metal coordination during biocatalysis (*in situ* BioXAS).
- To have high throughput data acquisition on multiple samples.

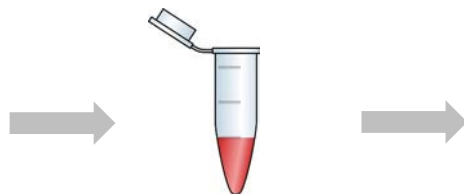
Timeline

First X-rays autumn 2016 – commissioning
First users during 2017

Macromolecular crystallography -Principle

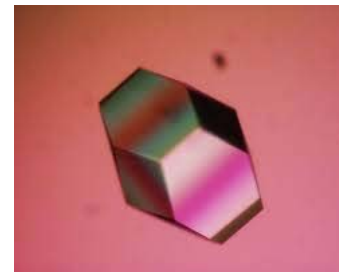


Heterologous or native expression in host cells (E.Coli, insect cells, etc.)

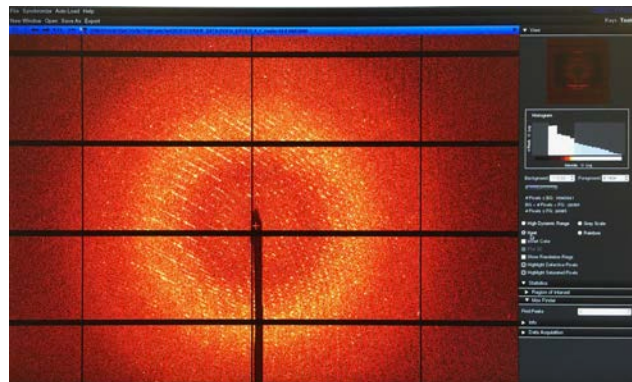


Highly purified protein in mg quantities

Protein crystallization

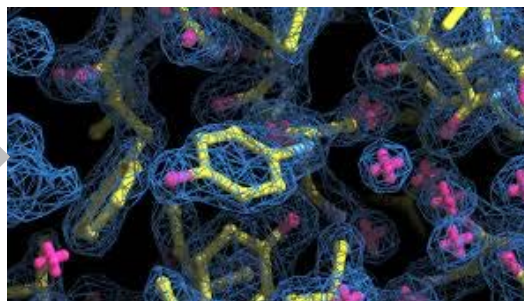


Single, diffracting protein crystal

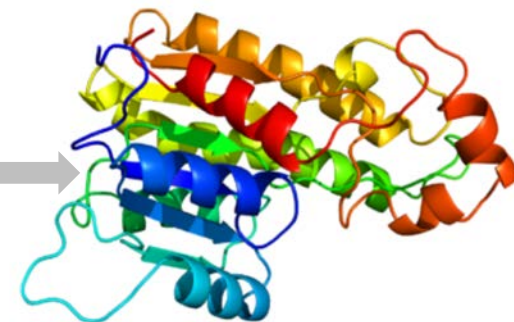


Complete diffraction experimental data-set at high resolution

Phase problem

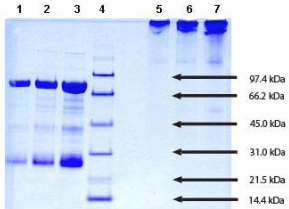


Interpretable electron density



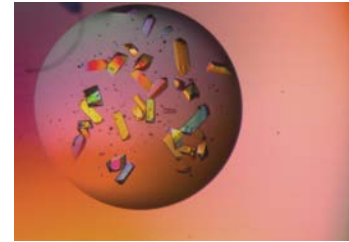
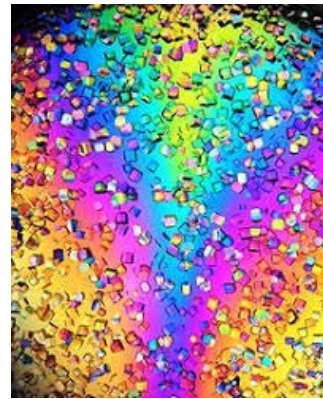
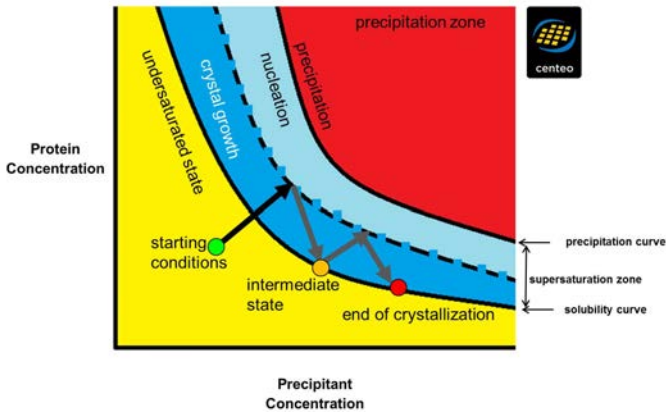
Final structure model

Macromolecular crystallography -Crystallization



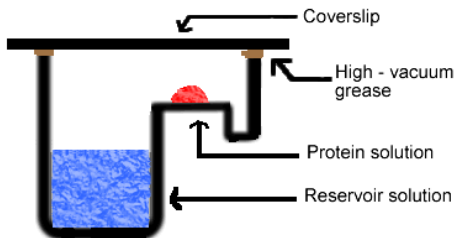
Requirements:

- Concentrated, highly pure and monodisperse sample

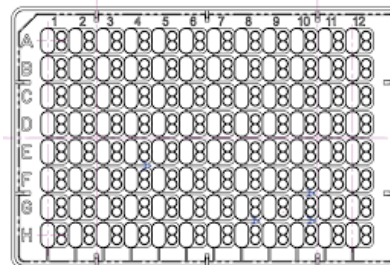


Protein crystals,
5-100 μm size

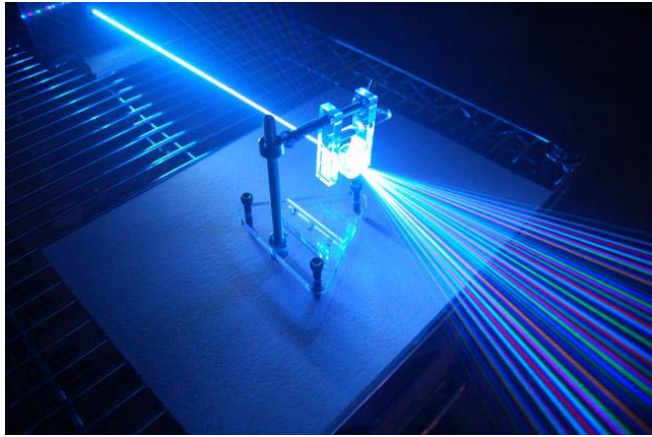
Vapor diffusion



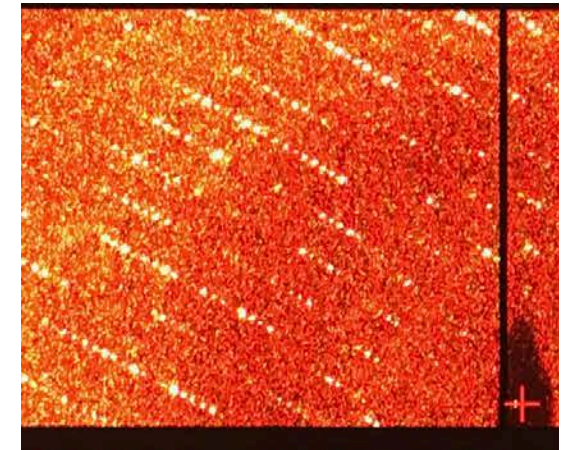
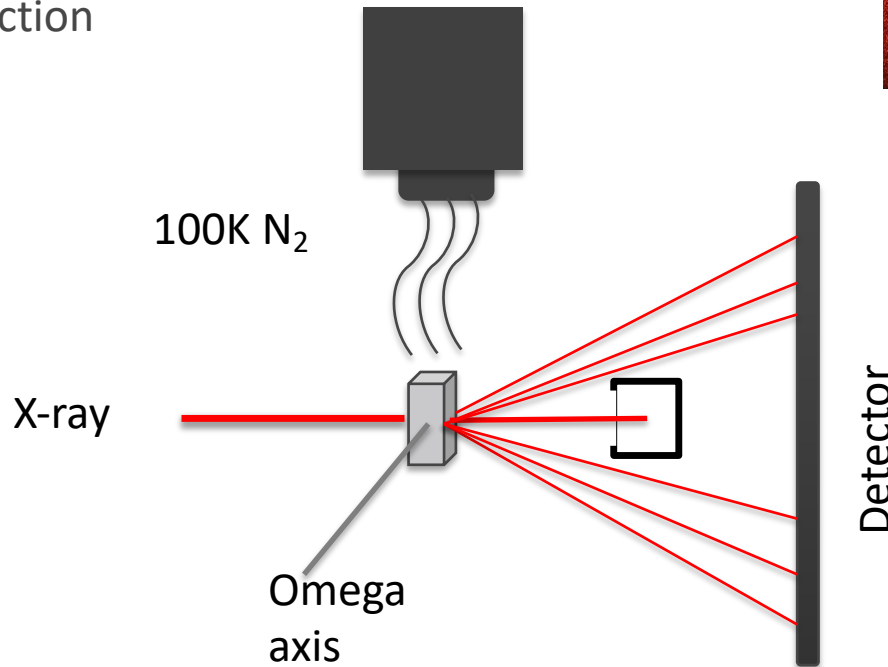
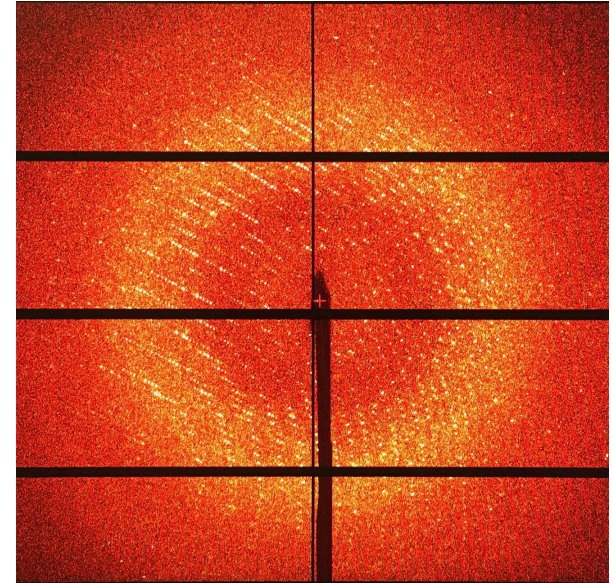
96 well crystallization plate



Macromolecular crystallography – Diffraction

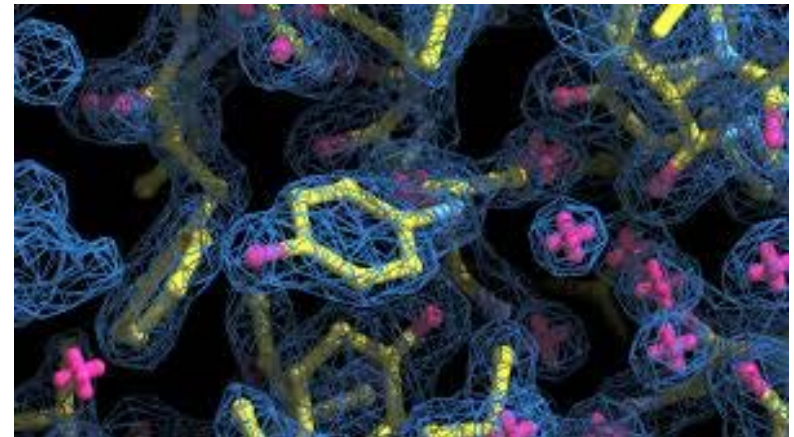
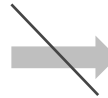
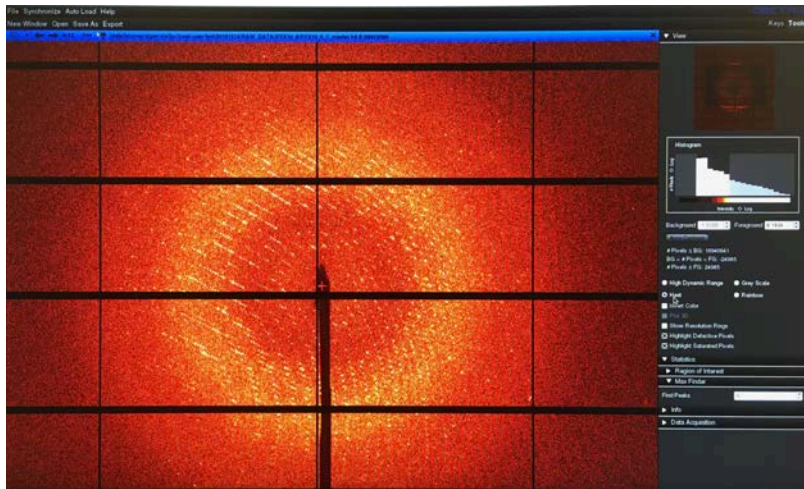


Visible light diffraction

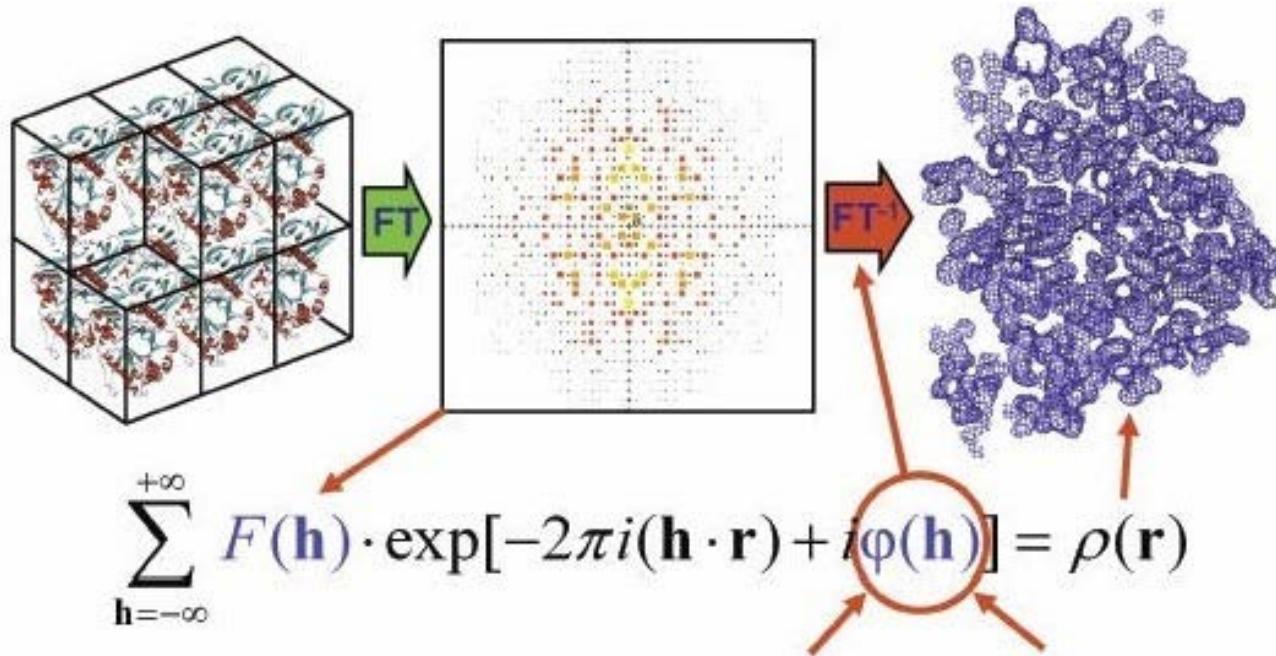


X-ray diffraction

Macromolecular crystallography –Phase problem



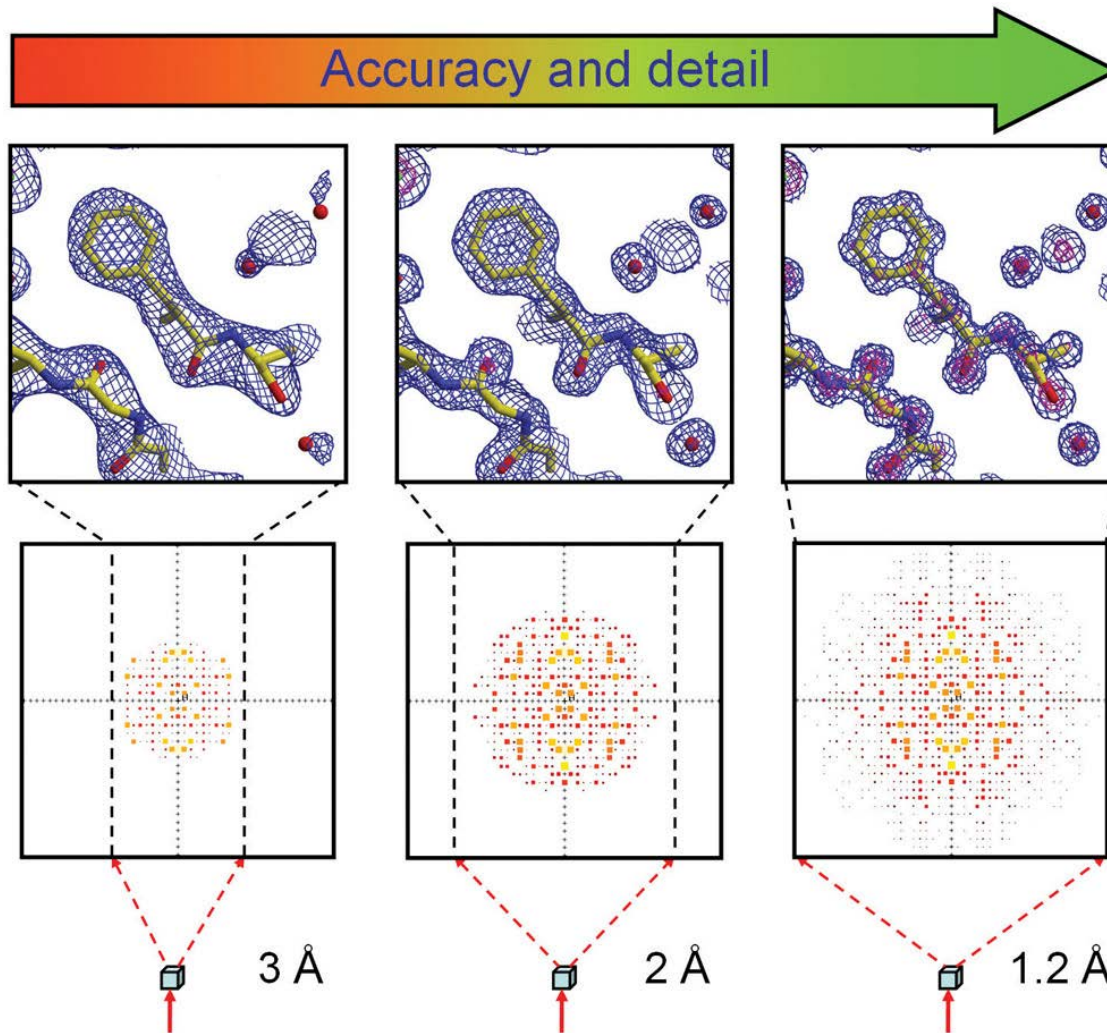
Macromolecular crystallography –Phase problem



Phasing methods:

- Molecular replacement
- Anomalous diffraction
- Isomorphous replacement
- *Ab initio* phasing

Macromolecular crystallography – Resolution

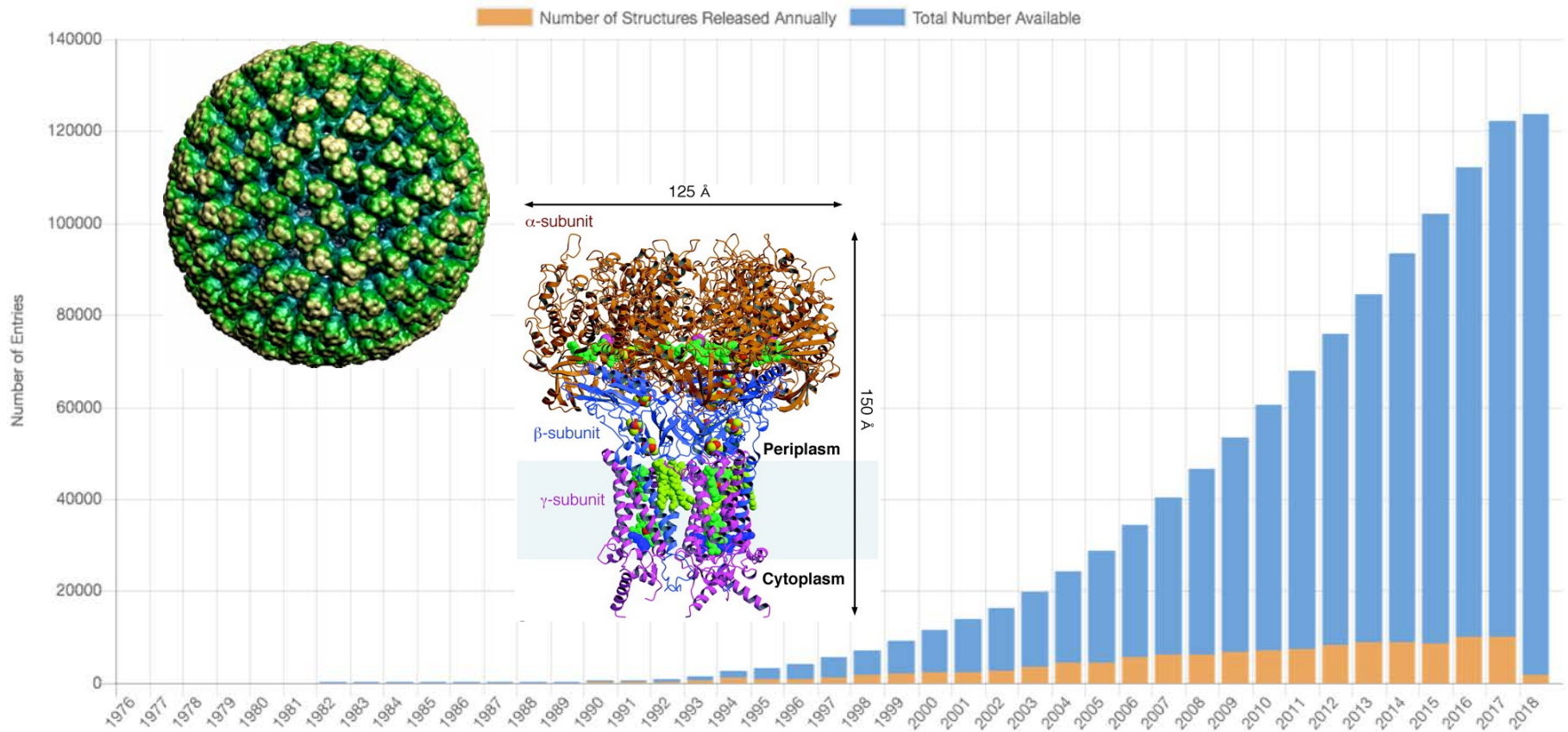


Bragg law

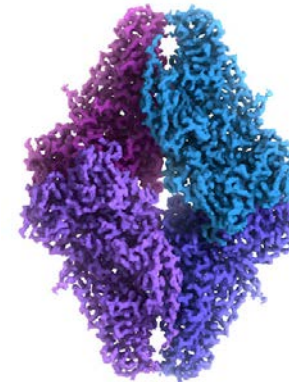
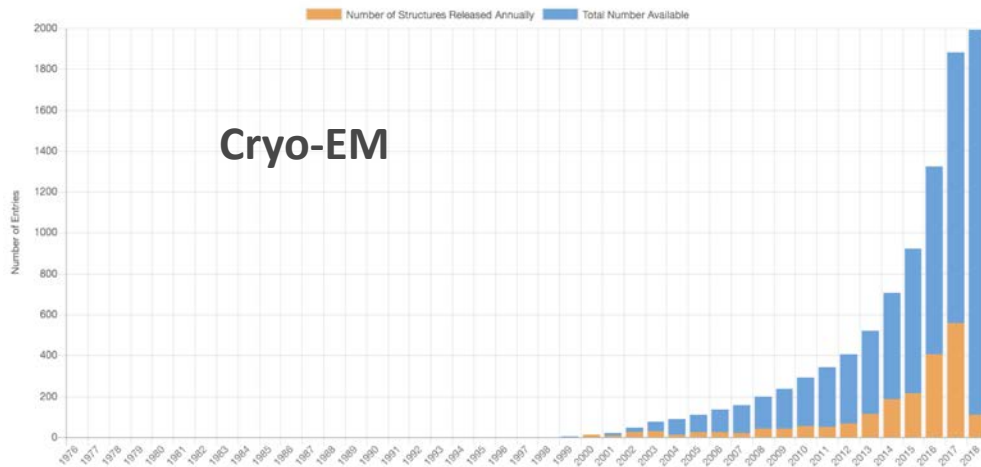
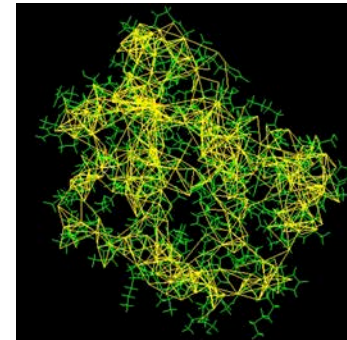
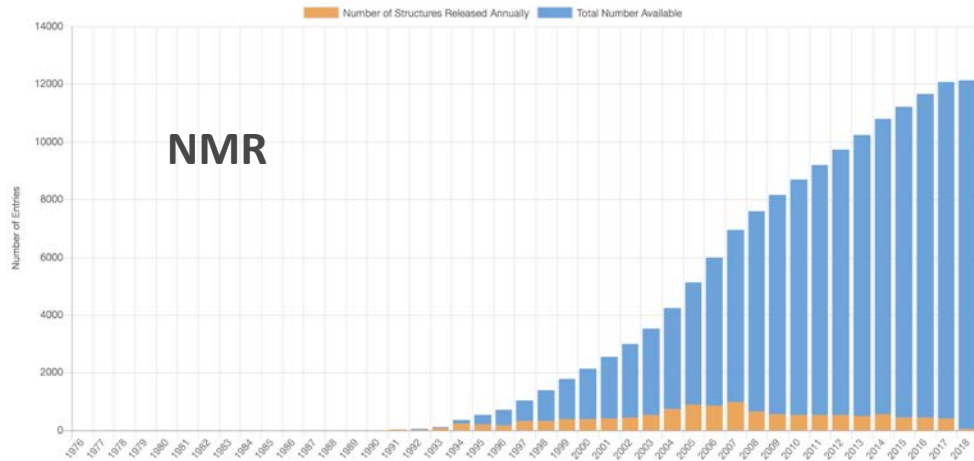
$$d = n\lambda / 2\sin\Theta$$

© Garland Science 2010

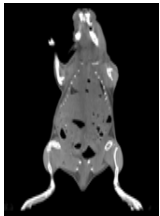
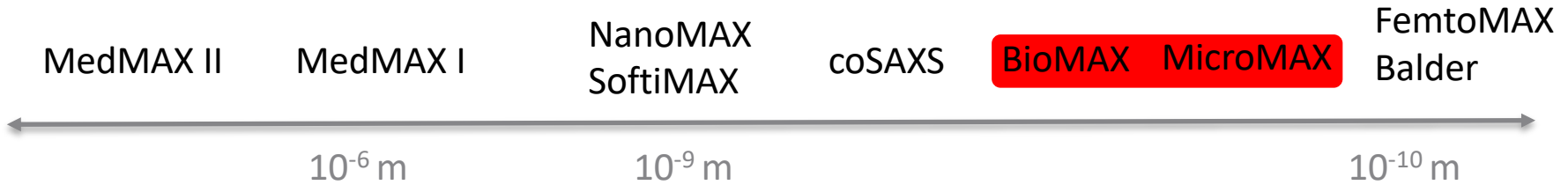
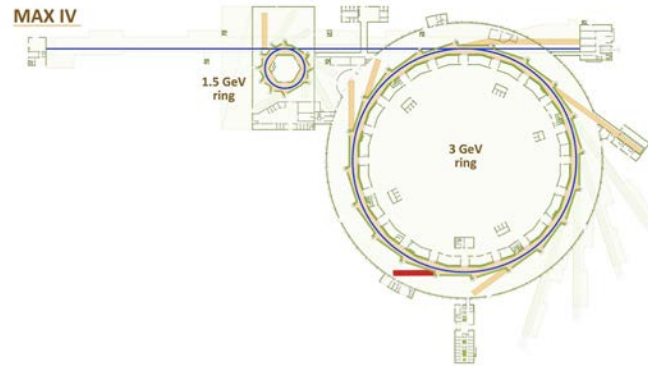
Macromolecular crystallography – Potential



Macromolecular crystallography –Potential



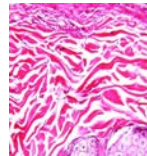
Macromolecular crystallography



Animals



Organs



Tissues



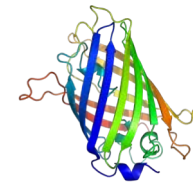
Cells



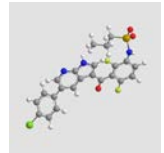
Micro-structures



Molecular complexes



Biomolecules



Atoms

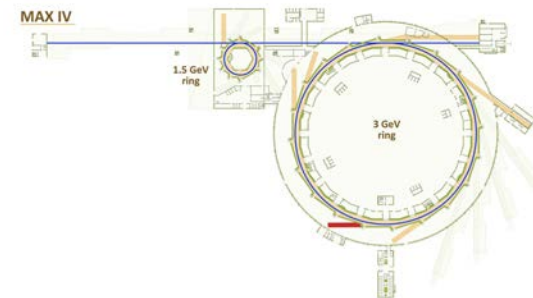
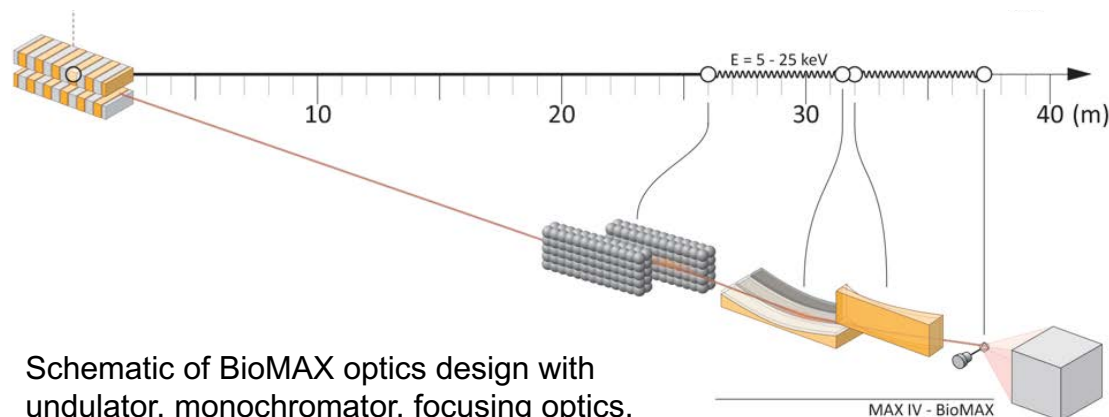
Disease models

Histopathology

Cell Biology

Molecular Medicine/Chemical Biology

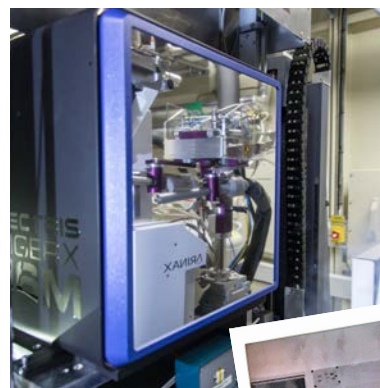
BioMAX Overview



Schematic of BioMAX optics design with undulator, monochromator, focusing optics, sample and detector.

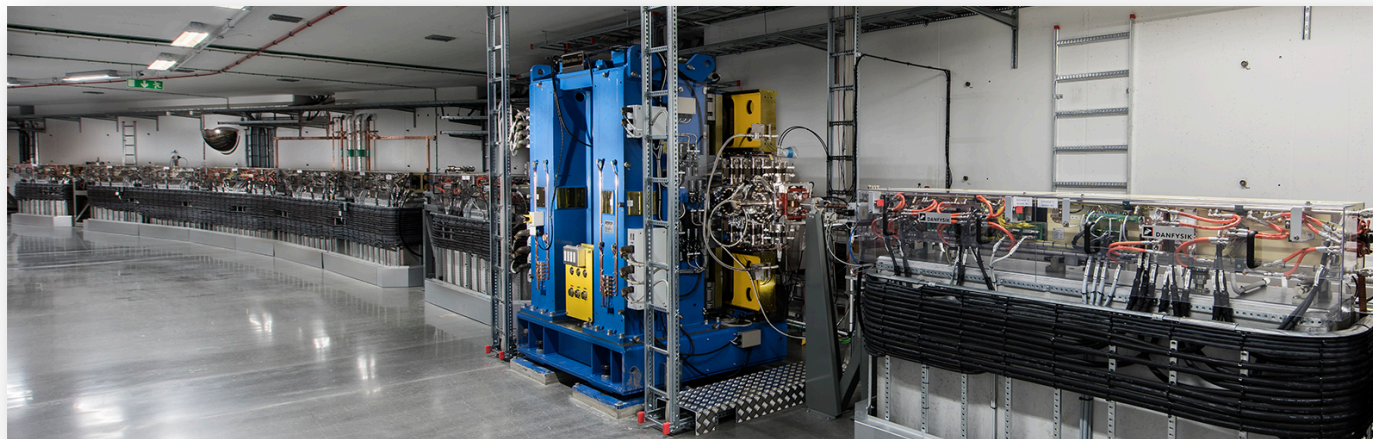
Beamline characteristics:

- **Support all relevant techniques for MX**
- Beam characteristics:
 - Small focus ($20 \times 5 \mu\text{m}^2$ h_v FWHM)
 - Low divergence ($0.1 \times 0.1 \text{ mrad}^2$)
 - High flux ($2 \times 10^{13} \text{ phot/s} \times 0.1\% \text{ bw}$)
- MD3 Microdiffractometer
- Large energy range (5-25 keV)
- Short data collection times (2-30 ms /frame)
- High throughput environment

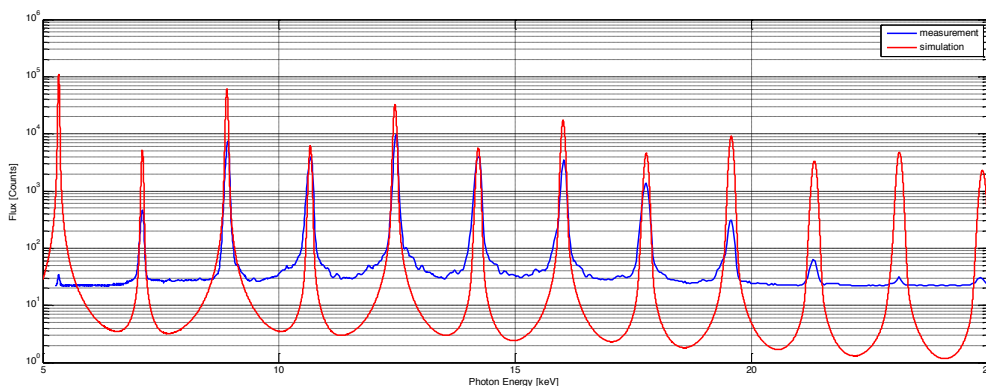
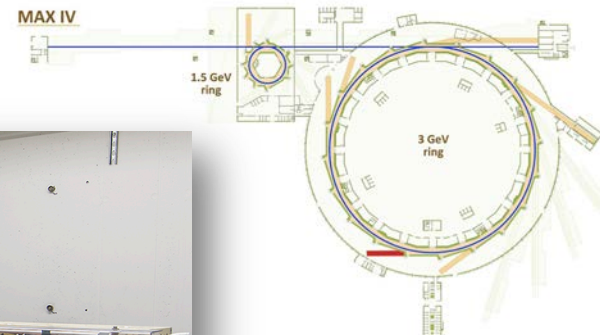


2017-2019: 71 proposals, 506 users, 5860 samples, 9495 datasets

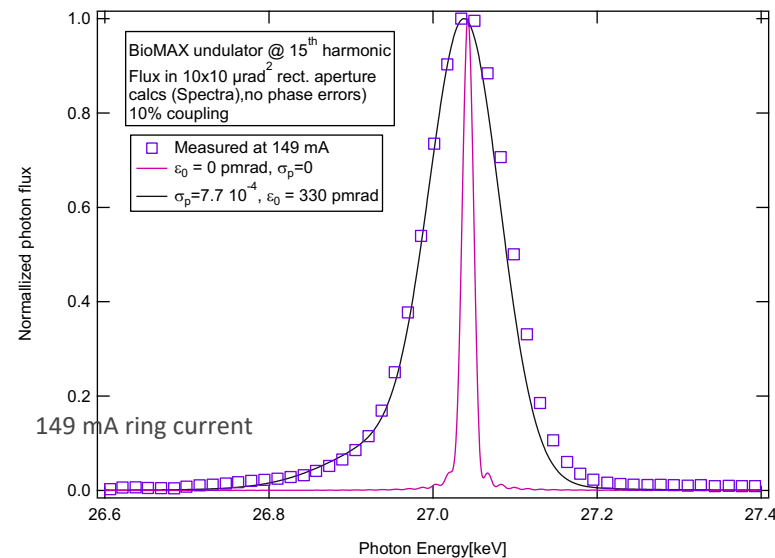
BioMAX Undulator



In-vacuum undulator



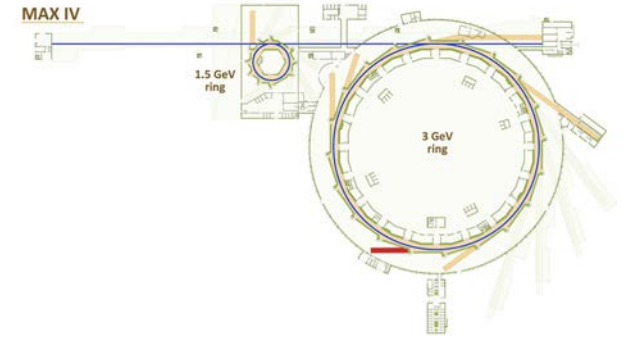
3 mA ring current, courtesy of H. Tarawneh



Data by T. Ursby and D. Olsson

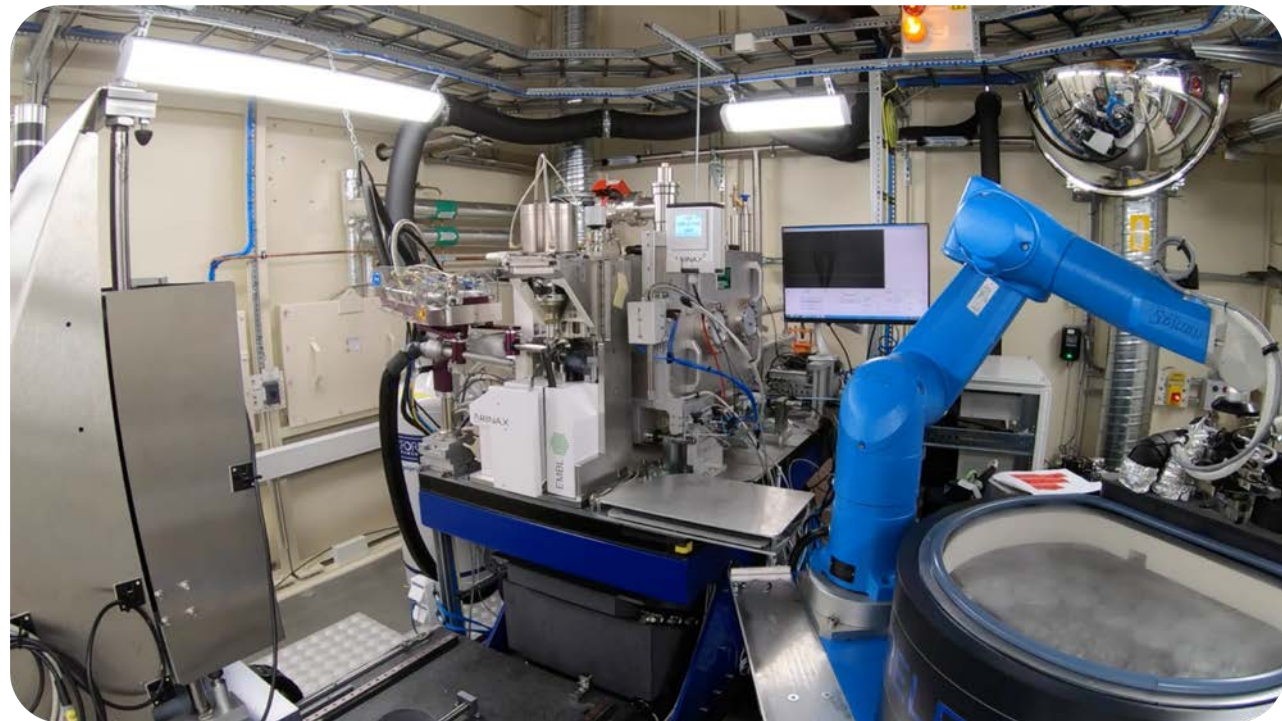


BioMAX experimental station



Experimental environment

- MD3 micro-diffractometer
- Eiger 16M hybrid pixel detector
- ISARA sample changer
- Operations center
- Sample preparation lab
- BioLab



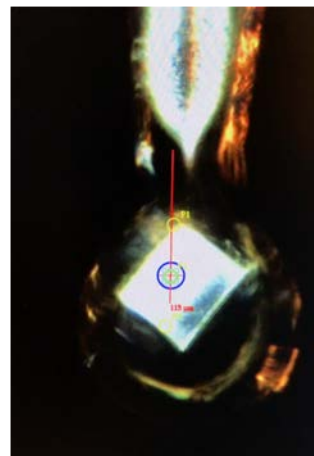
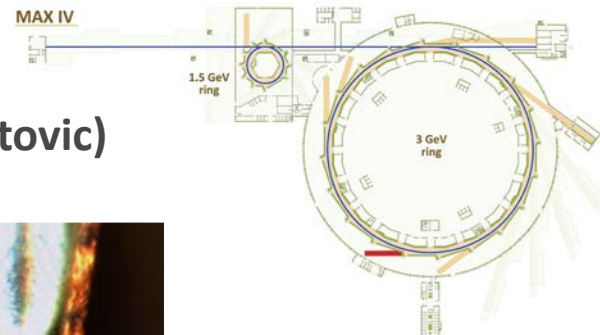
BioMAX experimental station

BioMAX Commissioning

Complete data collection within 4 sec., Cubic Insulin (R. Lizatovic)

Exp. Conditions:

- Exposure time: 10 msec
- Omega increment: 0.2 deg
- Omega range: 80 deg
- Images: 400
- Total time dc.: 4 sec



20 deg/sec frame rotation

RESOLUTION LIMIT	NUMBER OF REFLECTIONS			COMPLETENESS OF DATA	R-FACTOR observed	R-FACTOR expected	COMPARED	I/SIGMA	R-meas	CC(1/2)	Anomal Corr	SigAno	Nano
	OBSERVED	UNIQUE	POSSIBLE										
4.00	6270	1300	1310	99.2%	2.9%	3.0%	6256	45.08	3.2%	99.9*	29*	1.060	566
2.83	11197	2365	2366	100.0%	3.1%	3.3%	11191	38.25	3.5%	99.9*	7	0.878	1102
2.32	14470	3037	3039	99.9%	4.7%	4.6%	14465	26.92	5.3%	99.8*	8	0.961	1443
2.01	17158	3613	3617	99.9%	6.8%	6.4%	17146	19.05	7.7%	99.5*	8	0.916	1717
1.79	18415	4058	4061	99.9%	12.4%	11.7%	18402	10.67	14.1%	98.5*	8	0.895	1942
1.64	20452	4485	4489	99.9%	24.2%	23.0%	20438	5.83	27.4%	95.3*	9	0.910	2152
1.52	22549	4937	4945	99.8%	52.3%	50.5%	22527	2.80	59.4%	81.2*	12*	0.910	2374
1.42	23919	5220	5224	99.9%	123.2%	131.0%	23901	1.05	139.6%	49.3*	5	0.738	2525
1.34	25184	5663	5673	99.8%	366.2%	432.1%	25130	0.20	416.7%	7.5	1	0.573	2709
total	159614	34678	34724	99.9%	5.8%	5.9%	159456	11.23	6.6%	99.9*	8	0.835	16530

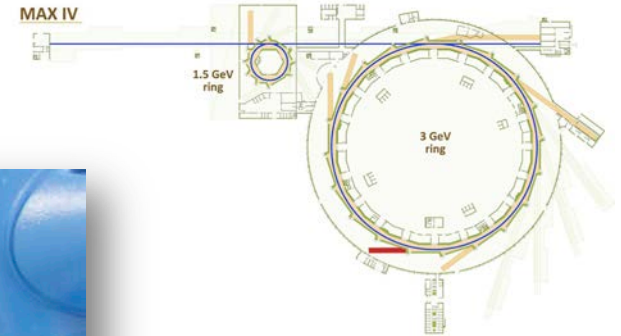
NUMBER OF REFLECTIONS IN SELECTED SUBSET OF IMAGES	160866
NUMBER OF REJECTED MISFITS	1252
NUMBER OF SYSTEMATIC ABSENT REFLECTIONS	0
NUMBER OF ACCEPTED OBSERVATIONS	159614
NUMBER OF UNIQUE ACCEPTED REFLECTIONS	34678

Final table from CORRECT.LP

Hclab – Room temperature



HClab facility operational



First Si chip operation at BioMAX,
(B. Vestergaard, UC)

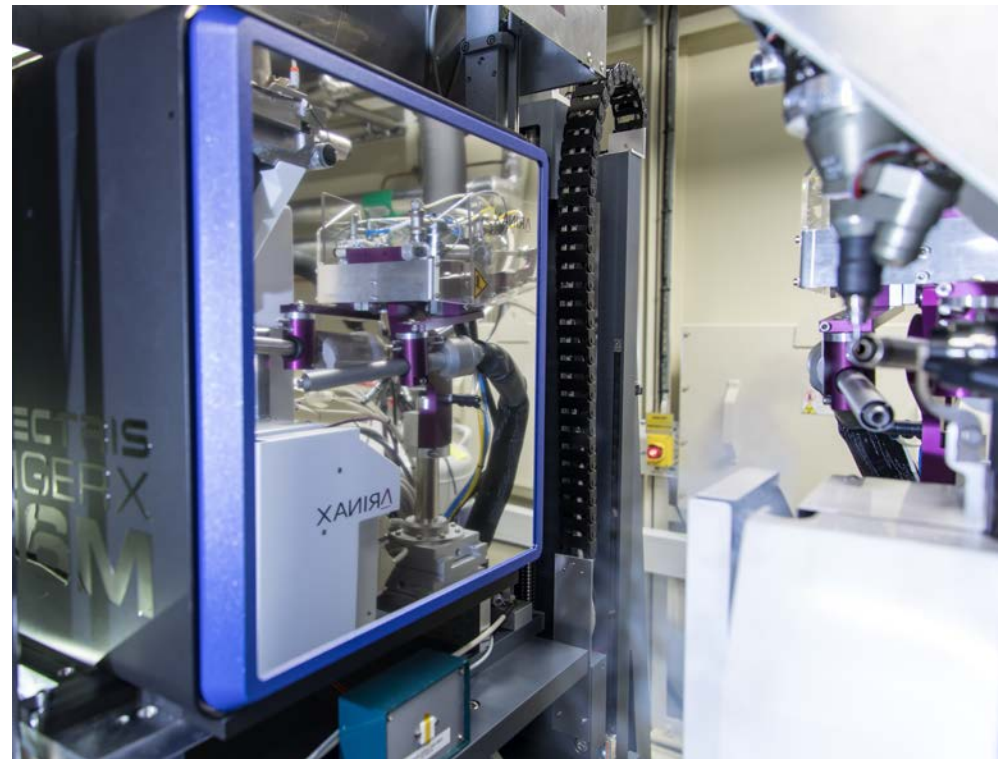
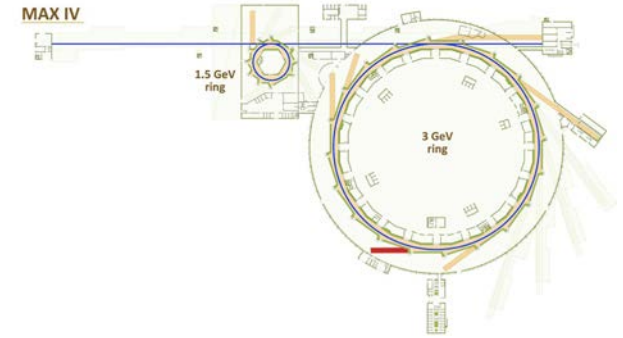
X-ray detector

Eiger 16M hybrid pixel detector:

- Sensitive area: $311.2 \times 327.8 \text{ mm}^2$
- $4150 \times 4371 = 18'139'650$ pixels
- Pixel size $75 \times 75 \text{ }\mu\text{m}^2$
- Scan speed:
 - 133 Hz (16M)
 - 750 (4M)

Challenges

- HDF5/Nexus file format
- Data streaming for real time analysis
- Large data volumes
 - Av. dataset size 10-20 Gb (15 sec)
- Data storage & processing for users



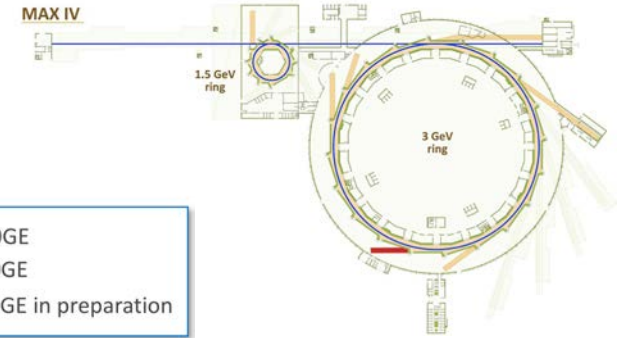
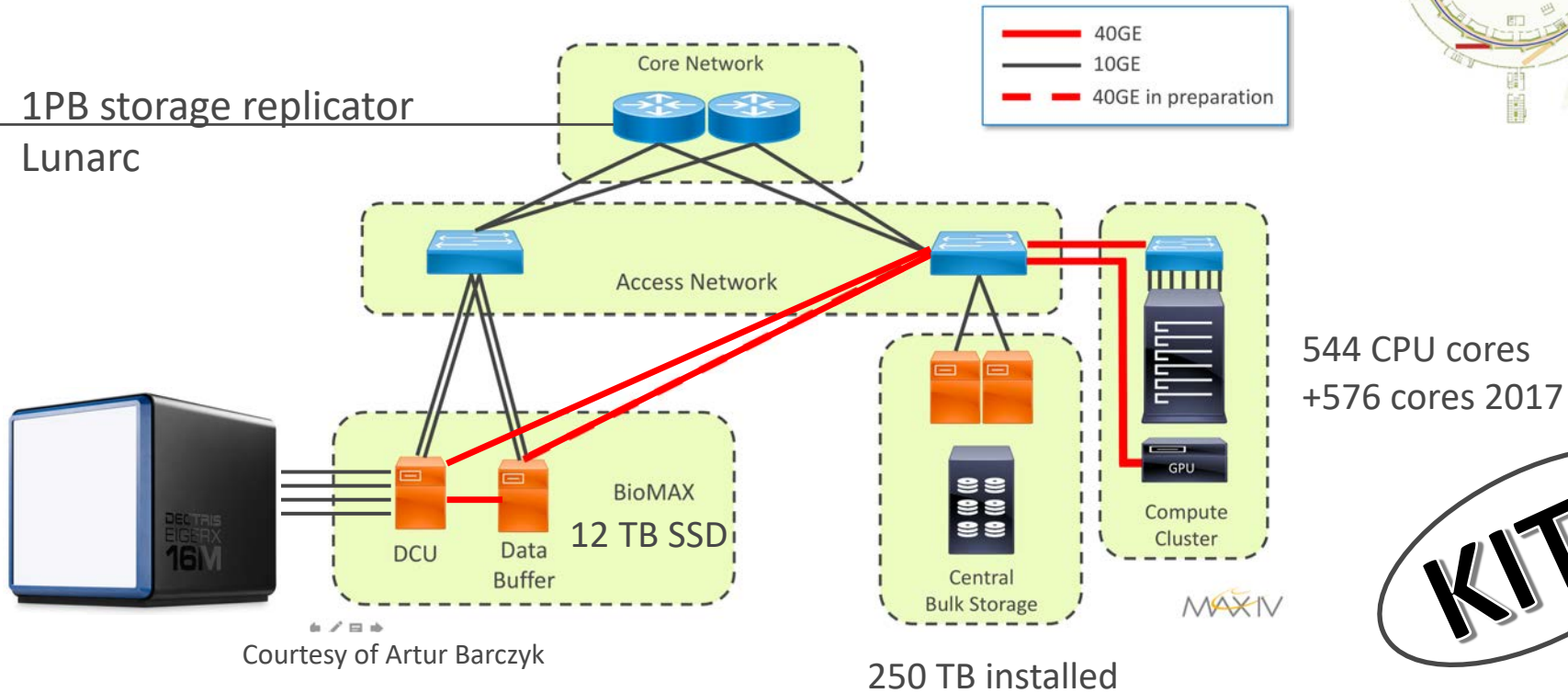
Eiger 16M hybrid pixel detector

IT environment

Eiger 16M IT-environment

1PB storage replicator

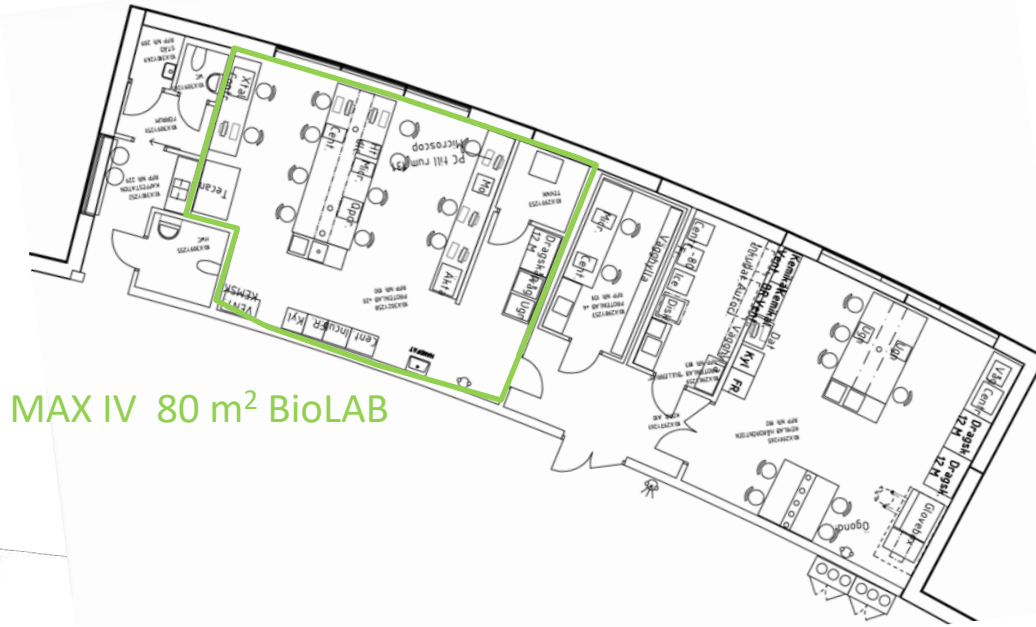
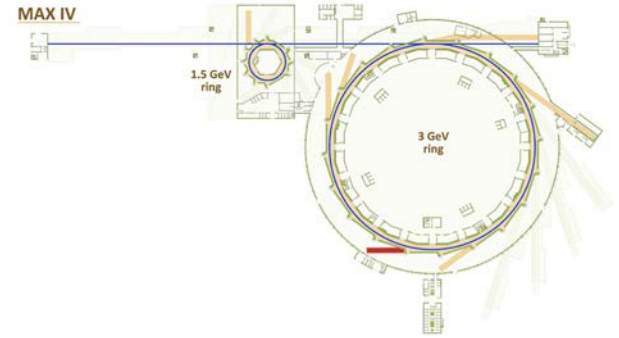
Lunarc



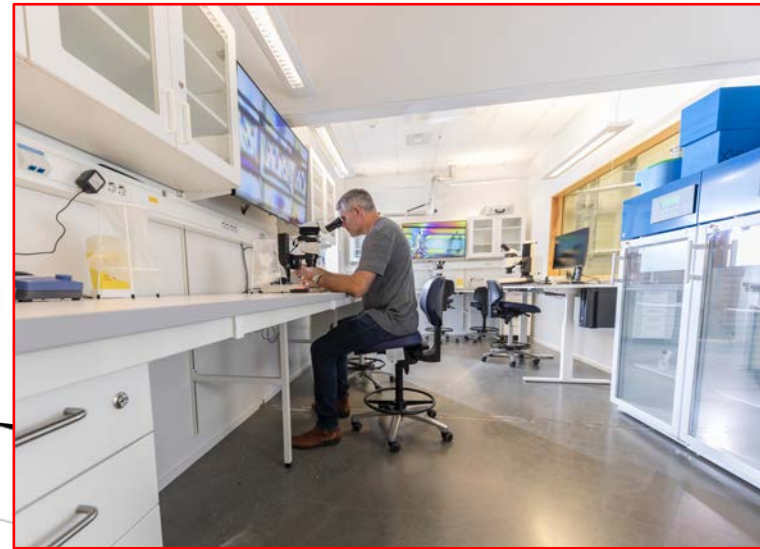
KITS

- Optimized data storage of all BioMAX data
- Automated data processing within minutes
- Alternative data retrieval via Globus (www.globus.org)

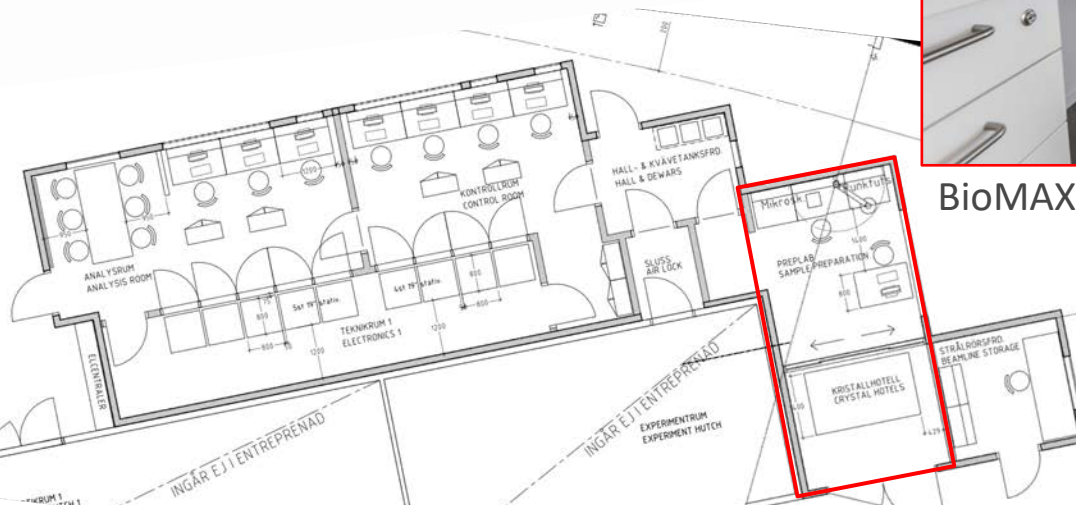
Lab facilities



MAX IV 80 m² BioLAB



BioMAX operations and sample lab



BioMAX operations and sample lab

ARTICLE

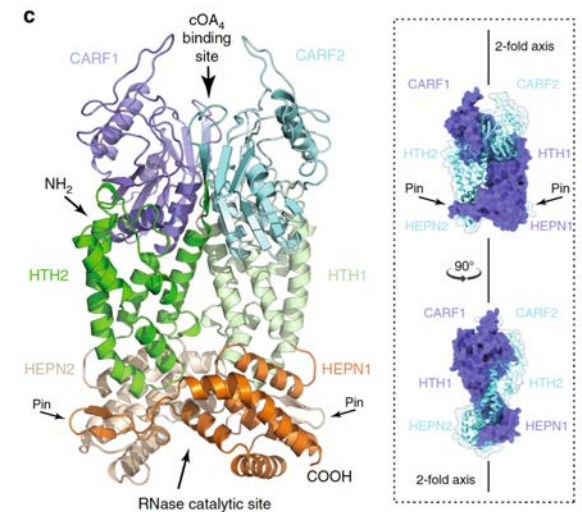
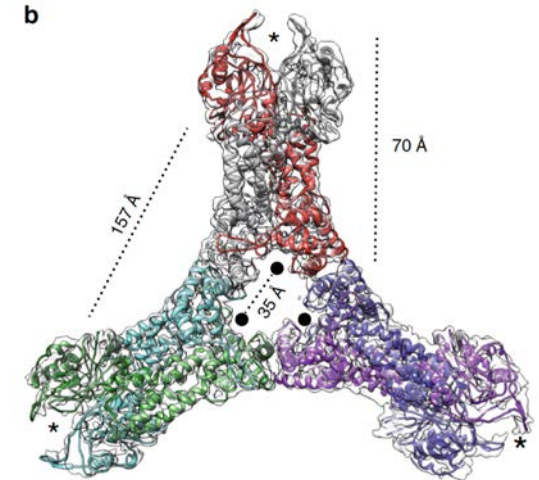
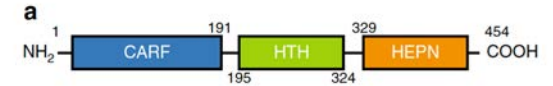
<https://doi.org/10.1038/s41467-019-12244-z>

OPEN

Structure of Csx1-cOA₄ complex reveals the basis of RNA decay in Type III-B CRISPR-Cas

Rafael Molina^{1,6}, Stefano Stella^{1,6}, Mingxia Feng^{2,3,6}, Nicholas Sofos¹, Vyktintas Jauniskis¹, Irina Pozdnyakova⁴, Blanca López-Méndez⁴, Qunxin She^{2,3,5} & Guillermo Montoya^{1,4}

Type III CRISPR-Cas multisubunit complexes cleave ssRNA and ssDNA. These activities promote the generation of cyclic oligoadenylate (cOA), which activates associated CRISPR-Cas RNases from the Csm/Csx families, triggering a massive RNA decay to provide immunity from genetic invaders. Here we present the structure of *Sulfolobus islandicus* (Sis) Csx1-cOA₄ complex revealing the allosteric activation of its RNase activity. SisCsx1 is a hexamer built by a trimer of dimers. Each dimer forms a cOA₄ binding site and a ssRNA catalytic pocket. cOA₄ undergoes a conformational change upon binding in the second messenger binding site activating ssRNA degradation in the catalytic pockets. Activation is transmitted in an allosteric manner through an intermediate HTH domain, which joins the cOA₄ and catalytic sites. The RNase functions in a sequential cooperative fashion, hydrolyzing phosphodiester bonds in 5'-C-C-3'. The degradation of cOA₄ by Ring nucleases deactivates SisCsx1, suggesting that this enzyme could be employed in biotechnological applications.



CHEMISTRY

Multiplicity conversion based on intramolecular triplet-to-singlet energy transfer

A. Cravcenco¹, M. Hertzog¹, C. Ye¹, M. N. Iqbal², U. Mueller³, L. Eriksson², K. Börjesson^{1*}

The ability to convert between molecular spin states is of utmost importance in materials chemistry. Förster-type energy transfer is based on dipole-dipole interactions and can therefore theoretically be used to convert between molecular spin states. Here, a molecular dyad that is capable of transferring energy from an excited triplet state to an excited singlet state is presented. The rate of conversion between these states was shown to be 36 times faster than the rate of emission from the isolated triplet state. This dyad provides the first solid proof that Förster-type triplet-to-singlet energy transfer is possible, revealing a method to increase the rate of light extraction from excited triplet states.

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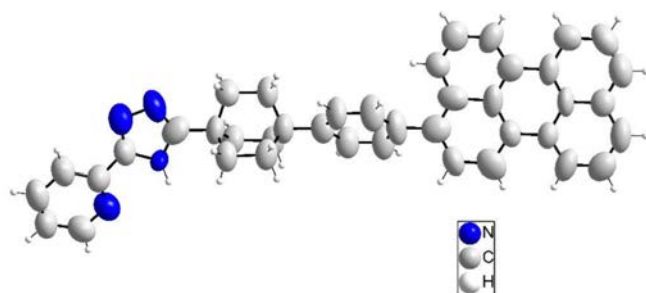


Fig. S7. Structure of the ligand (19), as solved by x-ray diffraction.

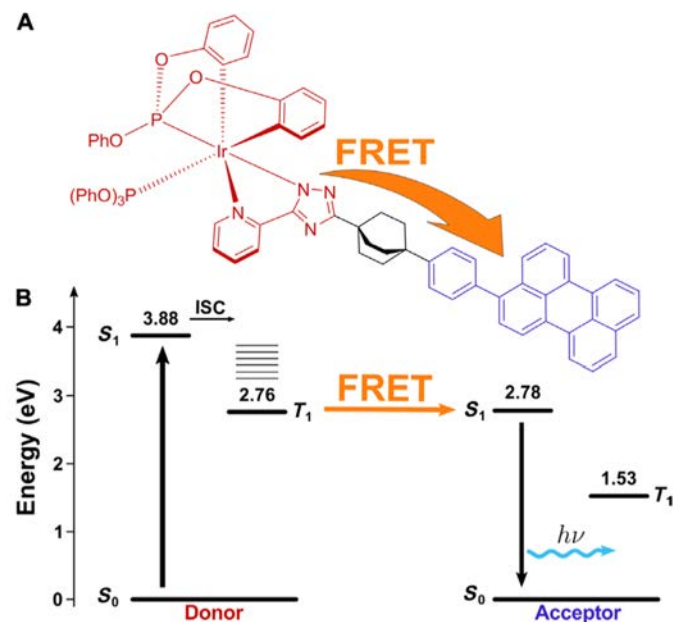


Fig. 1. Structure and energy levels of the dyad. (A) The DBA molecule used in this study. (B) Jablonski diagram showing triplet-to-singlet energy transfer via dipole-dipole interactions, i.e., the Förster-type resonance energy transfer (FRET) mechanism.

Enhancing Action of Positive Allosteric Modulators through the Design of Dimeric Compounds

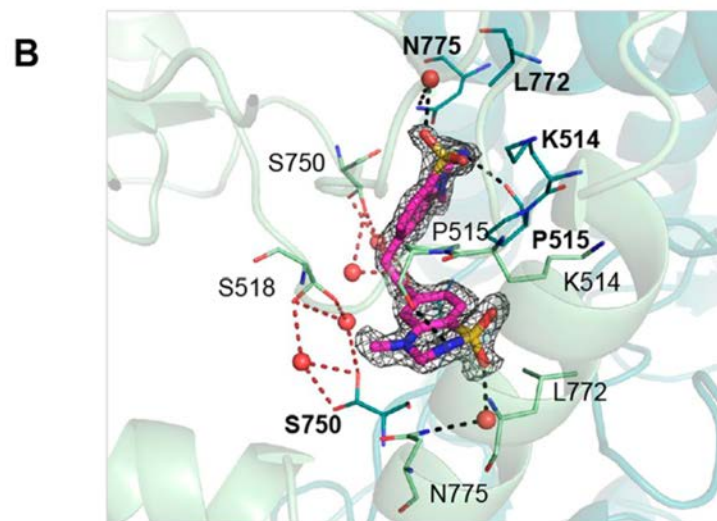
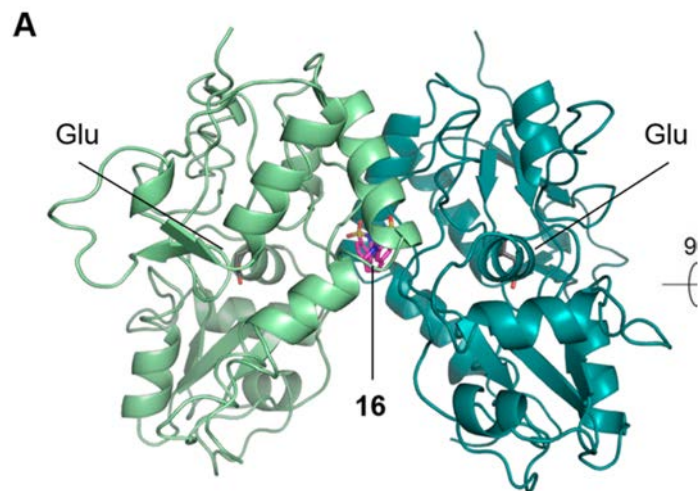
Thomas Drapier,[†] Pierre Geubelle,^{†,‡} Charlotte Bouckaert,[§] Lise Nielsen,^{||} Saara Laulumaa,^{||} Eric Goffin,[†] Sébastien Dilly,[†] Pierre Francotte,^{†,Ⓞ} Julien Hanson,^{*,†,‡} Lionel Pochet,^{*,§} Jette Sandholm Kastrup,^{*,||,Ⓞ} and Bernard Pirotte^{*,†,Ⓞ}

[†]Laboratory of Medicinal Chemistry, Center for Interdisciplinary Research on Medicines (CIRM), ULiège, Quartier Hôpital, Avenue Hippocrate, 15, B36, B-4000 Liège, Belgium

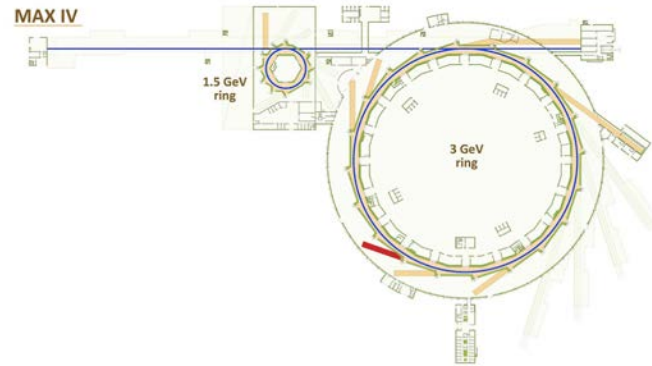
[‡]Laboratory of Molecular Pharmacology, GIGA-Molecular Biology of Diseases, ULiège, B34, Quartier Hôpital, Avenue de l'hôpital, 11, B-4000 Liège, Belgium

[§]NAmur Medicine & Drug Innovation Center (NAMEDIC), NARILIS, UNamur, rue de Bruxelles 61, B-5000 Namur, Belgium

^{||}Biostructural Research, Department of Drug Design and Pharmacology, Faculty of Health and Medical Sciences, University of Copenhagen, Universitetsparken 2, DK-2100 Copenhagen, Denmark



Life science at different length scales



MedMAX II

MedMAX I

NanoMAX
SoftiMAX

coSAXS

BioMAX

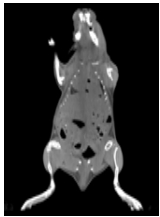
MicroMAX

FemtoMAX
Balder

10^{-6} m

10^{-9} m

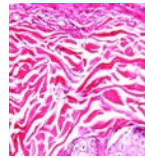
10^{-10} m



Animals



Organs



Tissues



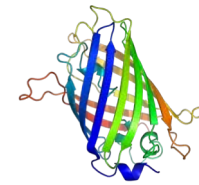
Cells



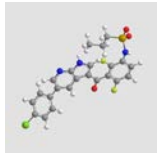
Micro-
structures



Molecular
complexes



Biomolecules



Atoms

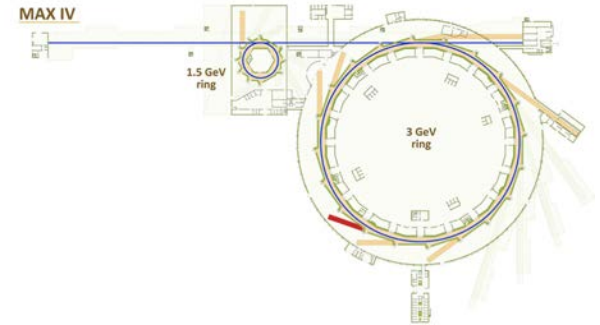
Disease
models

Histopathology

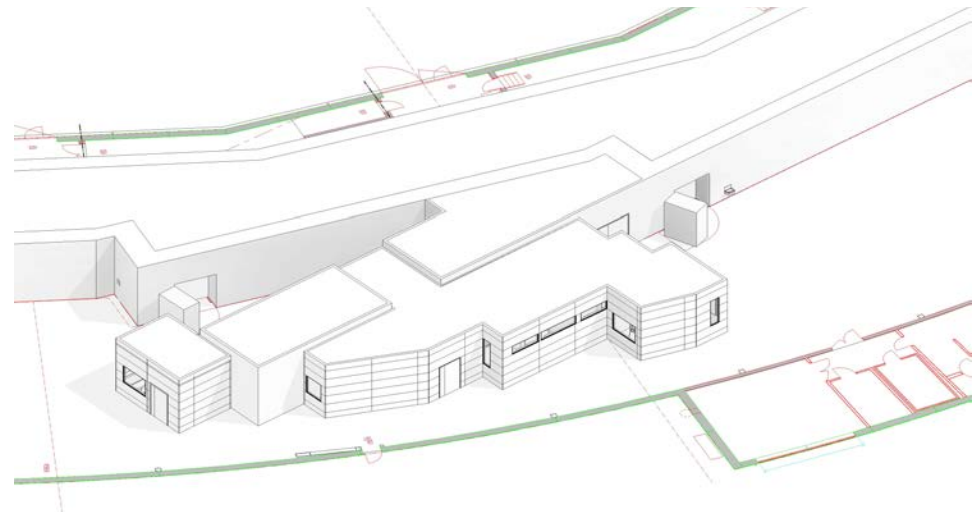
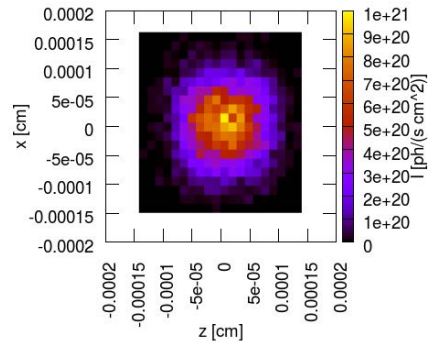
Cell Biology

Molecular Medicine/Chemical Biology

MicroMAX



Thomas Ursby: email: thomas.ursby@maxiv.lu.se

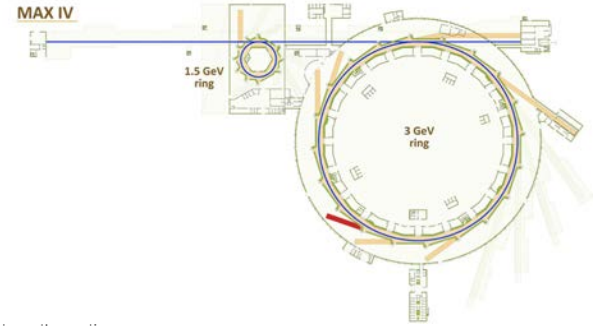


Plans for the second MX beamline

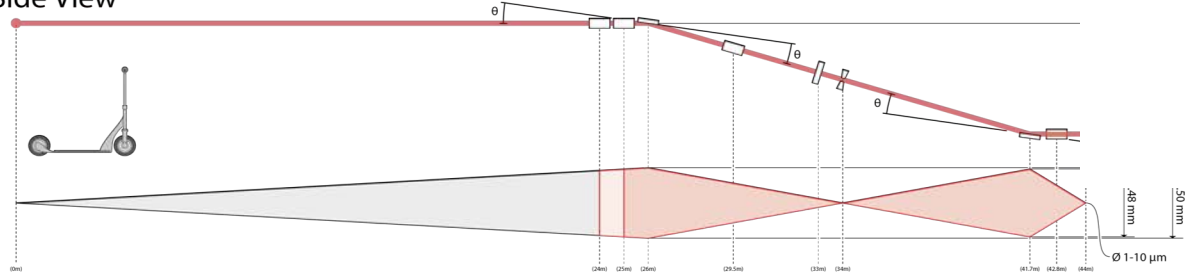
- Microfocus beamline
- **1 x 0.7 μm^2** beam at sample
- Photon flux **10^{13} - 10^{15}** phot/sec
- Traditional setup (goniometry, sample environment)
- Exploratory setup (serial crystallography, fixed target single shot)
- Optimal source for most demanding projects (large complexes, membrane proteins)

Status: funded by Novo Nordisk Foundation

MicroMAX

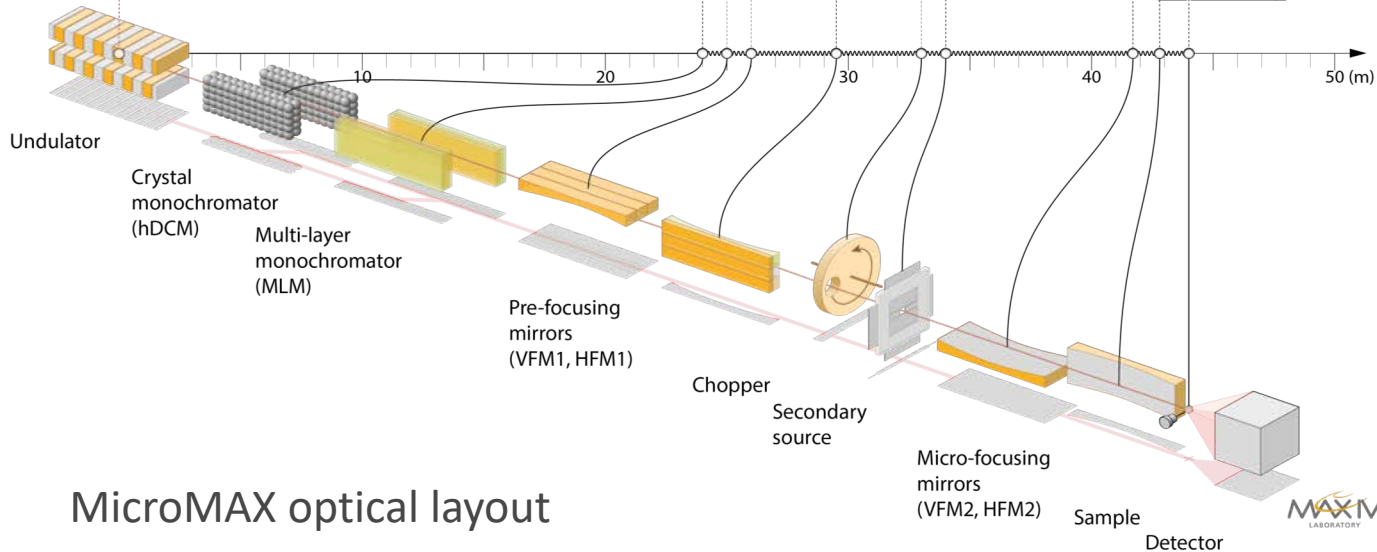
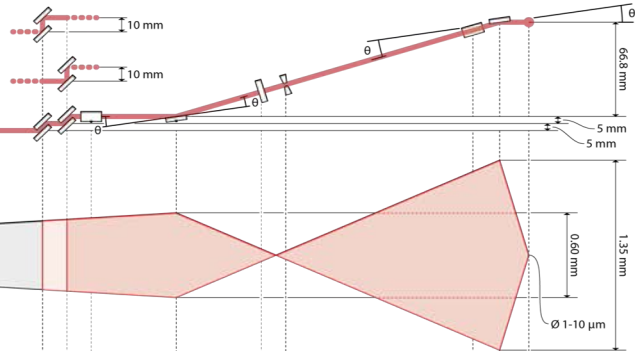


Side View



Top View

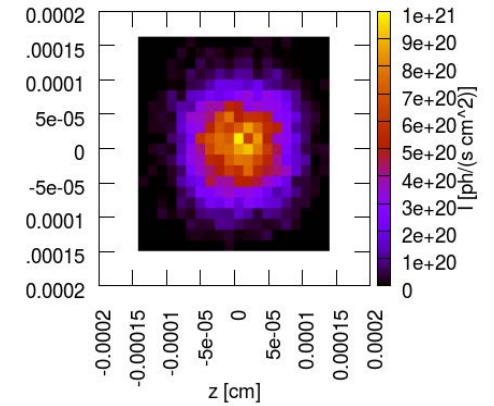
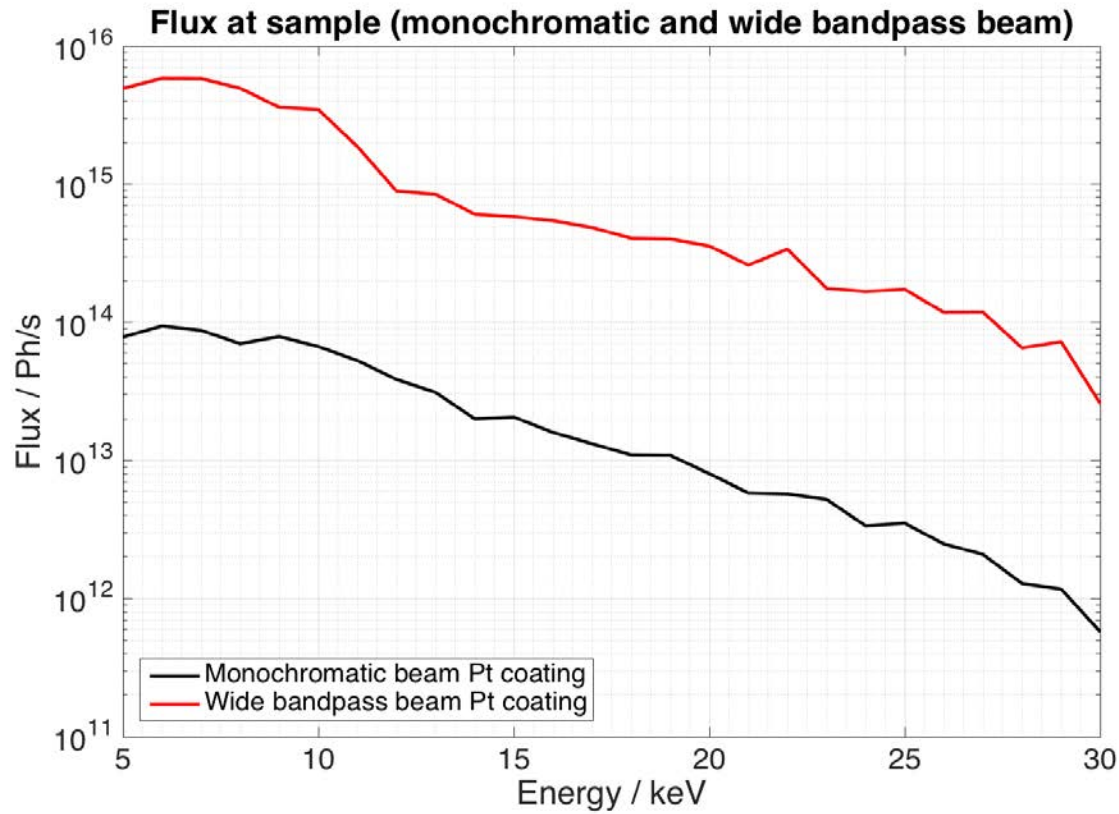
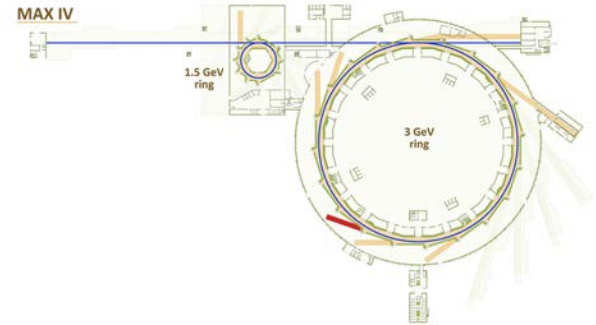
mirror incidence angles
 $\theta = 2.5 \text{ mrad}$



MicroMAX optical layout

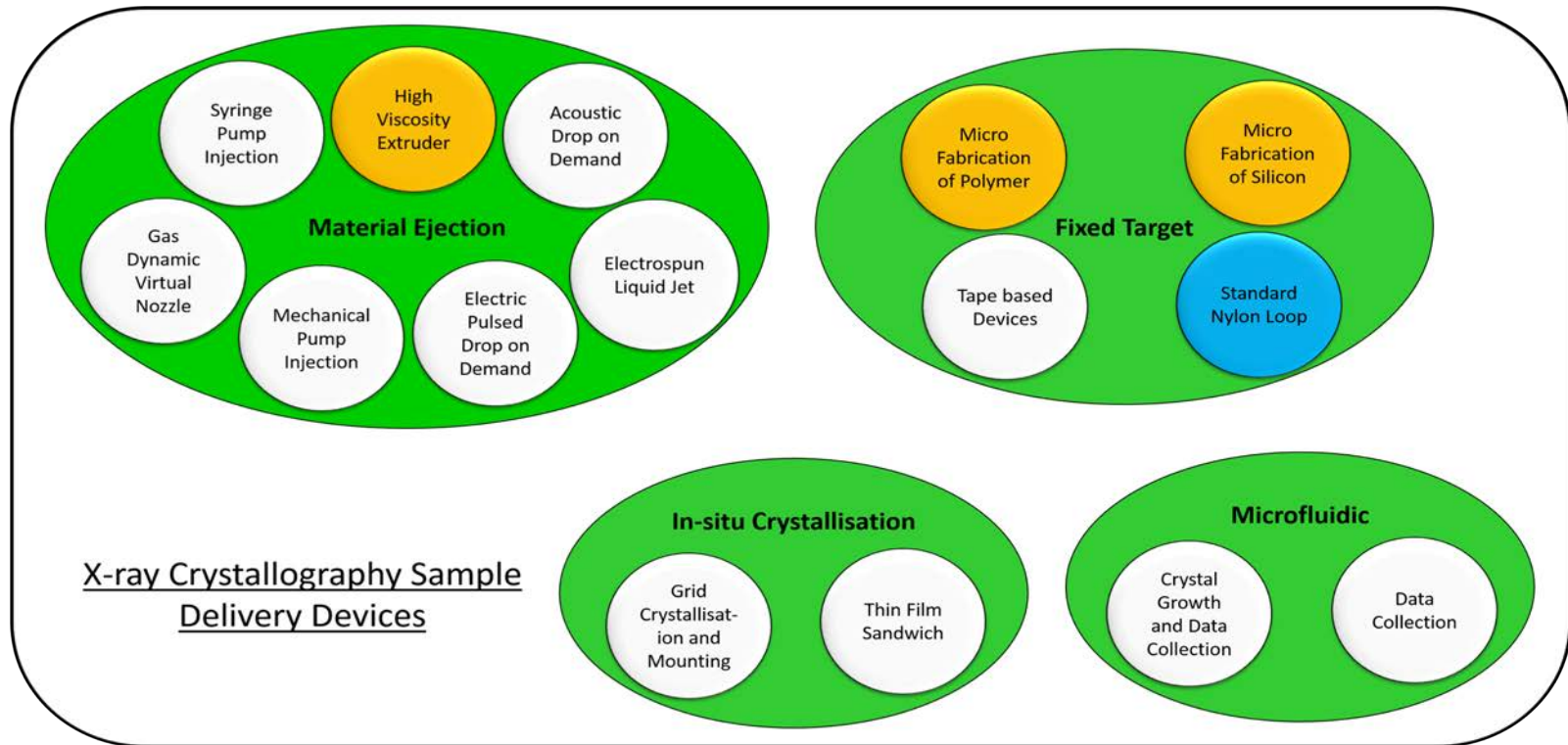
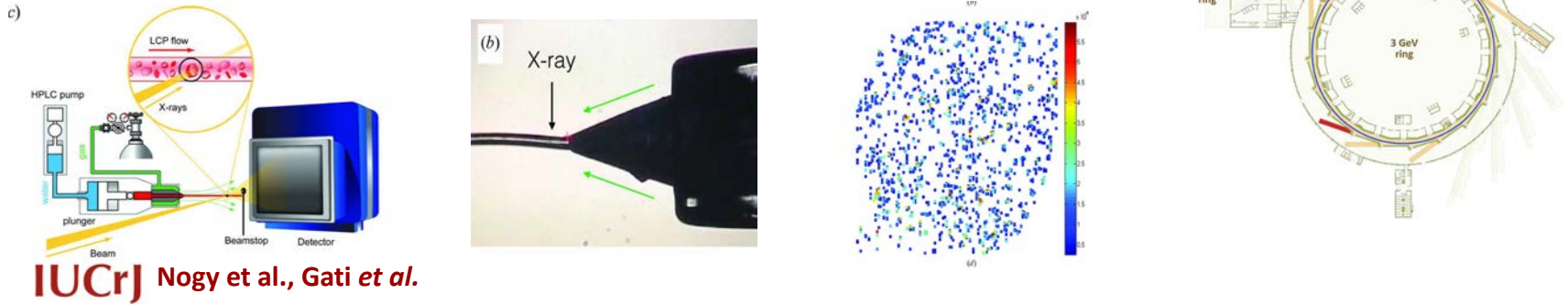


MicroMAX



Status: Preparation of funding application

MicroMAX

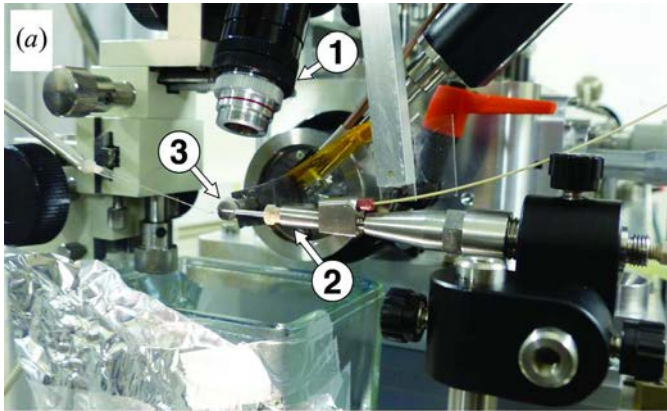


Novel sample delivery for micro-crystallography

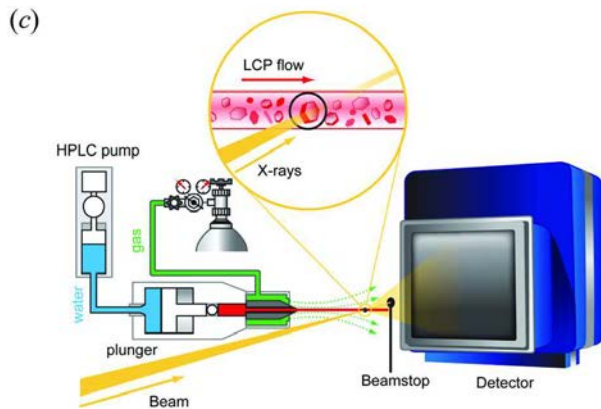
HVE-Injector project

Collaboration with MPI-Heidelberg

The experimental setup at the ID13 microfocus beamline. (a) (1) Microscope focused on the jet. (2) LCP injector with (3) nozzle close to the beamstop. (b) A view of the LCP nozzle as seen through the ...



HVE injector to mount on MAX IV Arinax goniometer
130 μ L sample reservoir (2.75 mm ID bore, 1/8" PTFE ball, 22 mm stroke)
8.46X amplification factor
Material: Stainless steel apart from Upchurch fittings, Festo push-fit connectors, and nozzle
Overall mass, including fittings: 380 g
All rights reserved.
Bruce Doak, Max-Planck-Institut für medizinische Forschung, Heidelberg, Germany
bruce.doak@mpimf-heidelberg.mpg.de, +49-6221 486-615

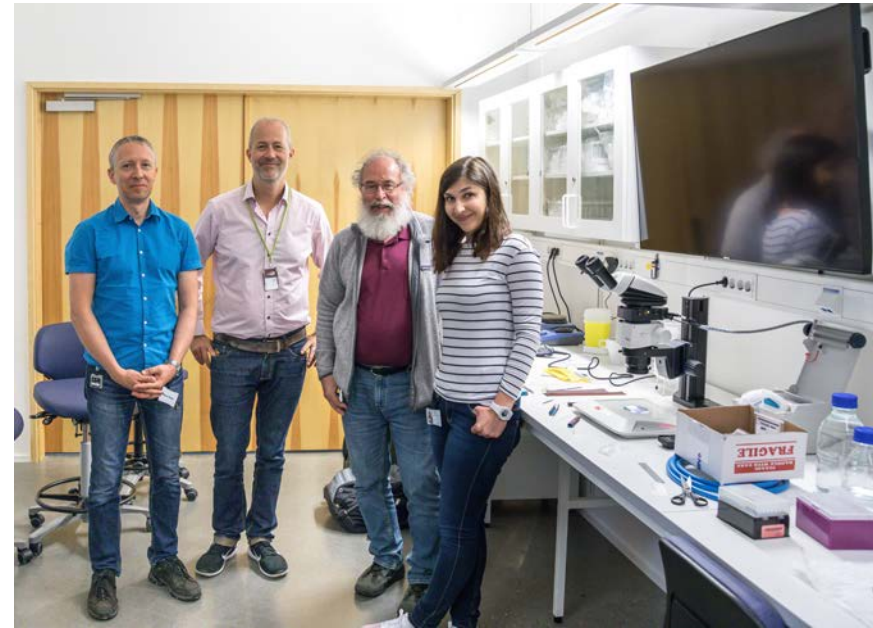
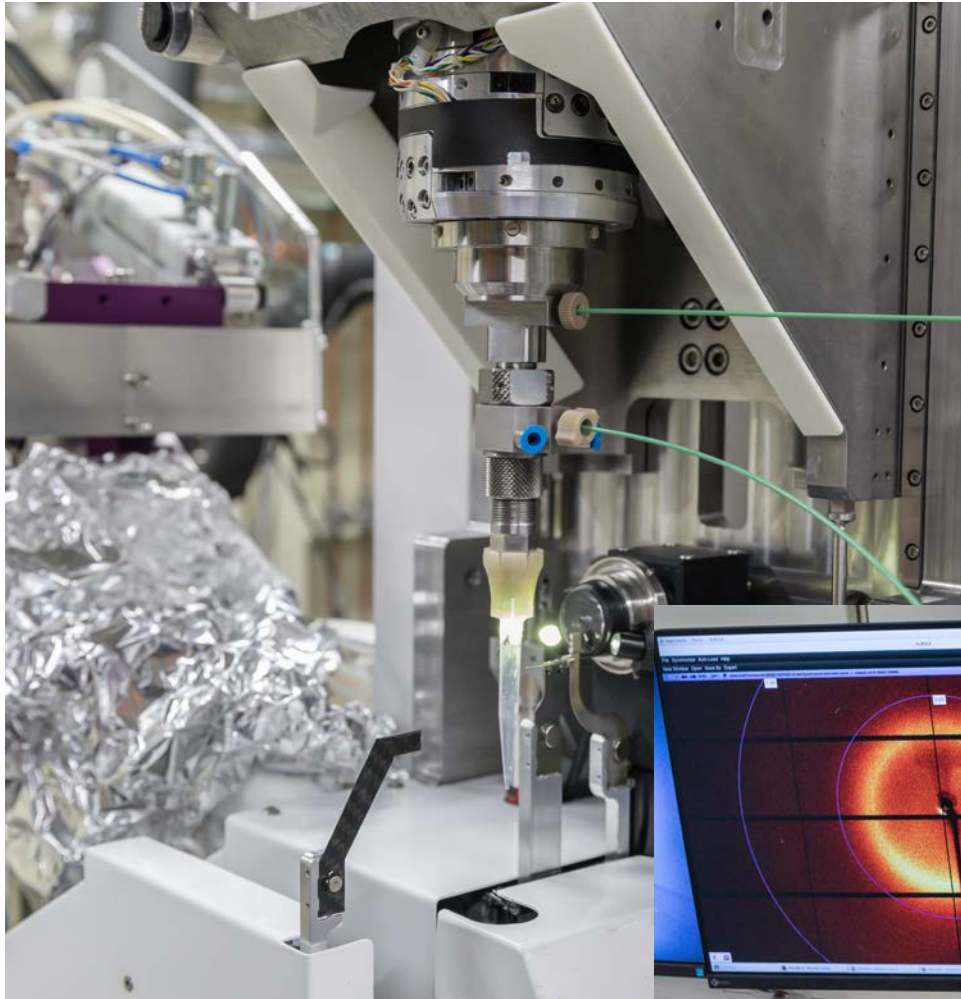


- Integration into BioMAX
- Future user facility for BioMAX users

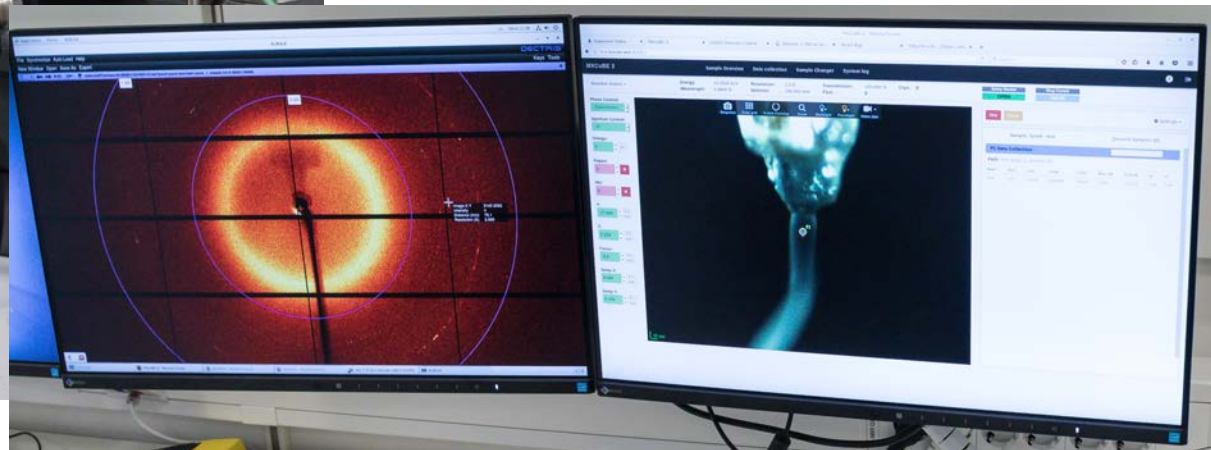
1. HVE-Injector experiment

A. Shilova, Jie Nan & Uwe Mueller
Robert Shoeman & Marco Kloos

May 2018



HVE experimental team (MPI-Heidelberg, MAX IV)



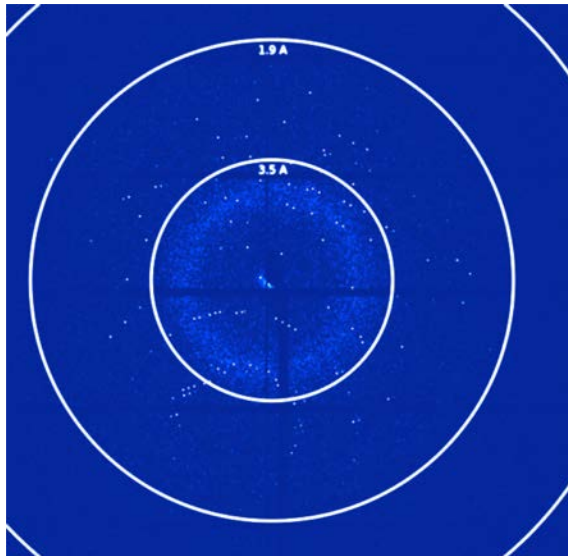
Data and extrusion viewer during experiment

Extruder mounted at MD3

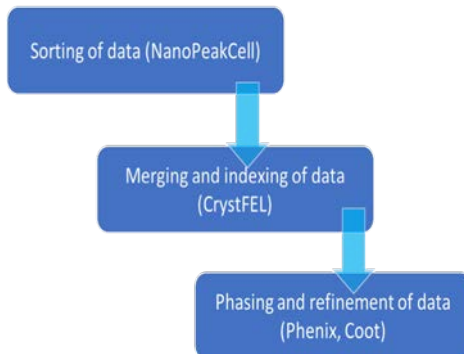
1. HVE-Injector experiment

A. Shilova

HEW Lysozyme



Diffraction image



Parameters	Lysozyme 10 μm
Wavelength, \AA	0.98
Beam size, μm^2	20*5
Beam flux, photons/sec	$1 \cdot 10^{13}$
Space group	P 4 ₃ 2 ₁ 2
Unit cell, \AA	a=b=79.2, c=38.36, $\alpha=\beta=\gamma=90^\circ$
Exposure per crystal, ms	2.8
No. collected frames	122000
Average hit rate (NanoPeakCell), %	22.3
No. of indexed patterns (CrystFEL)	19511
Indexing rate (CrystFEL), %	73
No. of total/unique reflections	15774/8668
Resolution range, \AA	56-1.9
Completeness, %	100
SNR ($I/\sigma(I)$) overall	6.4
B factor from Wilson Plot. \AA^2	41
Rsplit, %	8.53 (50)
CC*	0.99 (0.90)
Rwork/Rfree, %	18/20

2. HVE experiment

4.-7. June 2018

A. Shilova, J. Nan & U. Mueller
Bränden & Neutze group



Bränden, Neutze team at BioMAX

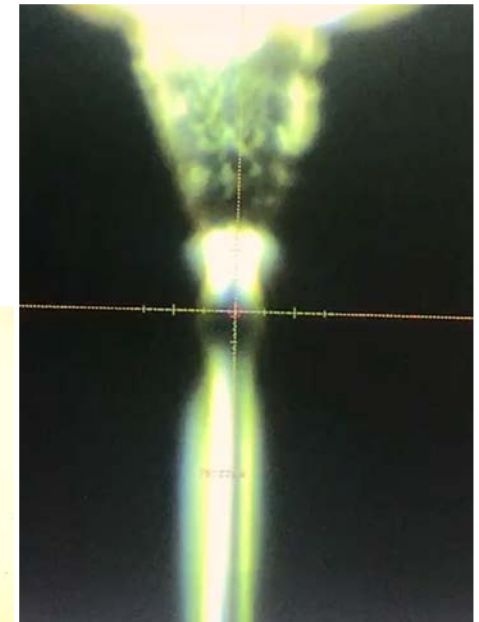
- 3 proteins injected
- 10 TB+ of data
- Data processing on-going



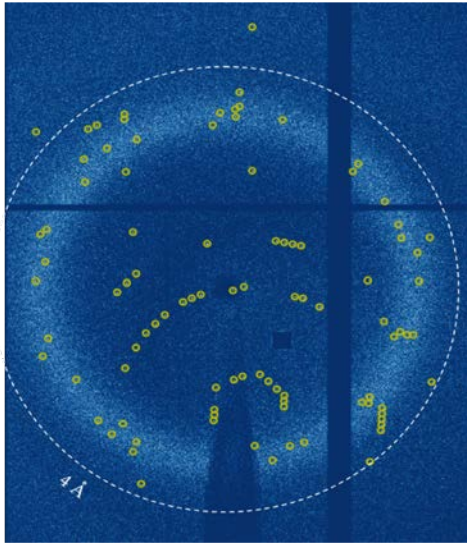
MPI HVE injector



ASU – LCP injector



A. Shilova



Cytochrome c oxidase



Parameters	BCO
Wavelength, Å	0.98
Beam size, μm^2	20*5
Beam flux, photons/sec	$1 \cdot 10^{13}$
Space group	C2
Unit cell, Å	$a=145.17$ $b=100.15$, $c=96.64$, $\alpha=\gamma=90^\circ$, $\beta=126.64$
Exposure per crystal, ms	2.8
No. collected frames	253766
Average hit rate (NanoPeakCell), %	3.5
No. of indexed patterns (CrystFEL)	6513
Indexing rate (CrystFEL), %	68
No. of total/unique reflections	27514/18454
Resolution range, Å	75.94-3.5
Completeness, %	100
SNR ($I/\sigma(I)$) overall	2.7
B factor from Wilson Plot. Å^2	68
Rsplit, %	34.02 (50)
CC*	0.90 (0.88)
Rwork/Rfree, %	32/36

Experiment was performed with user groups from Gothenburg University (Richard Neutze group and Gisela Branden)

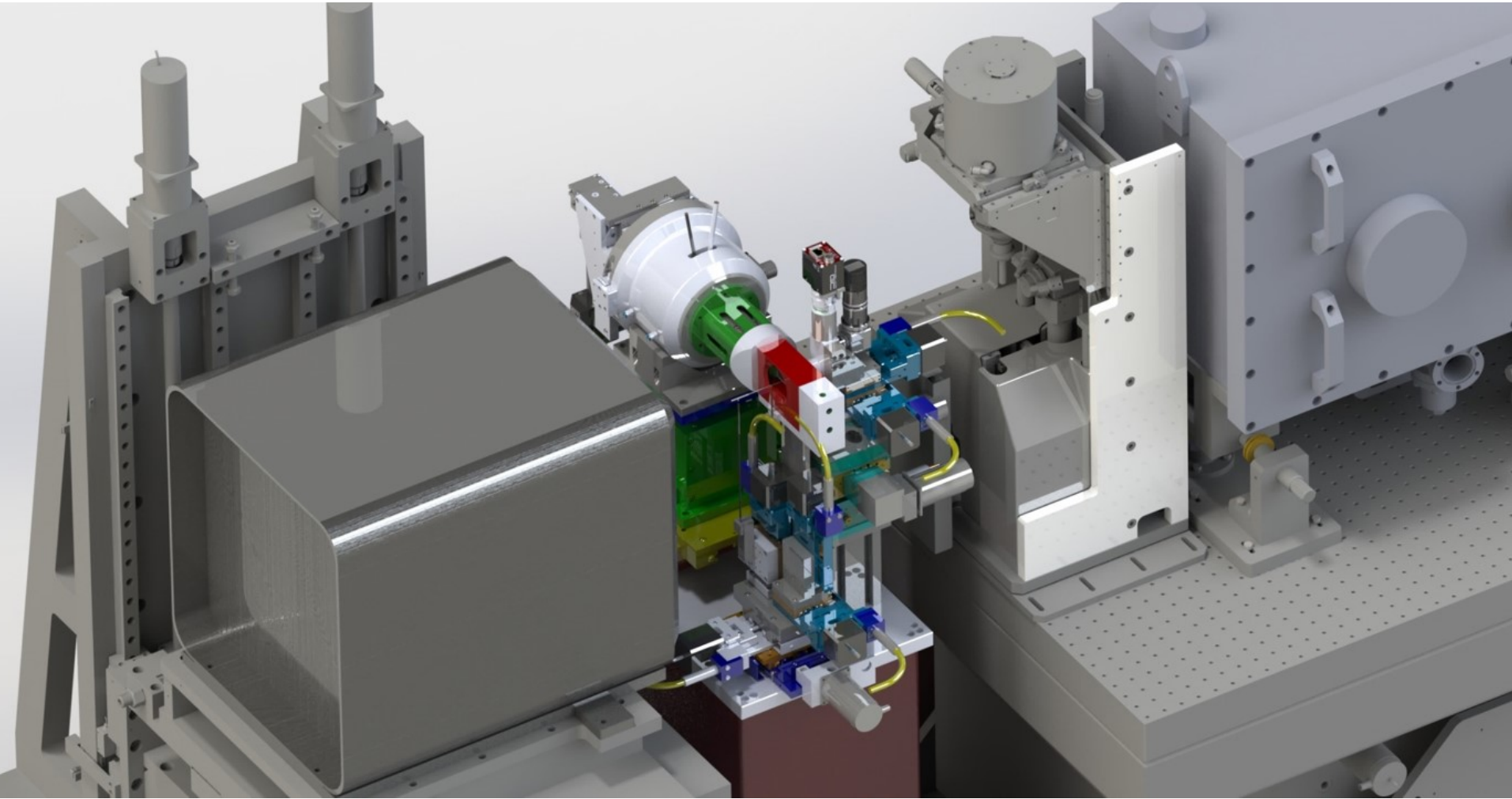
Raster-scan using MXCuBE3

J. Nan & M. Eguiraun
D. De Sanctis, M. Oskarson

The screenshot shows the MXCuBE3 web interface. At the top, there are navigation tabs for 'Sample Overview', 'Data collection', 'Sample Changer', and 'System log'. Below this, a status bar displays key parameters: Energy: 12.0000 keV, Wavelength: 1.0332 Å, Resolution: 5.400 Å, Detector: 793.480 mm, Transmission: 100.000 %, Flux: 0 ph/s, and Cryo: 0 K. There are also buttons for 'Sample chan' (DISABLED), 'Safety Shutte' (CLOSED), and 'Ring Current' (192.67). The main control area includes a 'Phase Control' section with a 'Centring' dropdown, a 'Beam size' dropdown (set to 5), 'Omega' (360), 'Kappa' (0), 'Phi' (0), and X, Y, Z coordinates. A 'Samp-X' and 'Samp-Y' section is also present. The central image shows a sample with a green grid overlay. A context menu is open over the grid, with 'Mesh Scan' selected. A red arrow points from this menu to a 'Mesh Scan' configuration dialog box on the right. The dialog box contains the following fields:

- Data location**
 - Path: /data/staff/biomax/commissioning/20180924/raw/undefined
 - Subdirectory: test/test-mesh/
 - Prefix: mesh-test
 - Filename: undefined_[RUN#]_[IMG#]
- Acquisition**
 - Oscillation range per image: 0.01
 - First image: 1
 - Oscillation start: 0
 - Total number of images: 400
 - Exposure time per image(ms): 0.01
 - Transmission: 100
 - Energy: 12
 - Resolution: 5.4
- Processing**
 - Buttons: Default Parameters, Reset Form, Run Now, Add to Queue

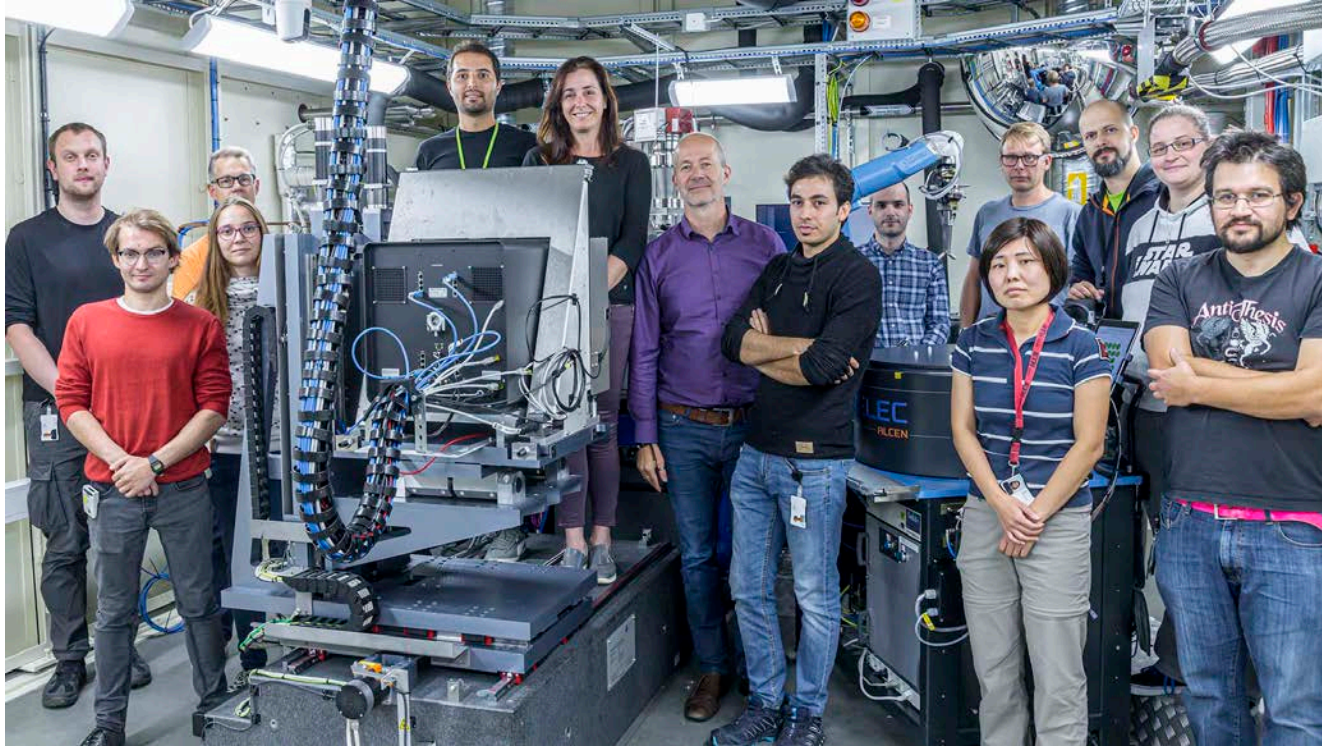
Fixed target scanning station: Roadrunner 3



Project in collaboration with
Alke Meents CFEL/DESY

Acknowledgement

The MX group



- From left to right:
- Oskar Aurelius
 - Vladimir Talibov
 - Laila Benz
 - Thomas Ursby
 - Gustavo Lima
 - Ana Gonzalez
 - Uwe Mueller
 - Vahid Haghghat
 - Mikel Eguraun (KITS)
 - Jie Nan
 - Johan Unge
 - Mirko Milas
 - Monika Bjelcic
 - Elmir Jagudin
- All BioMAX users

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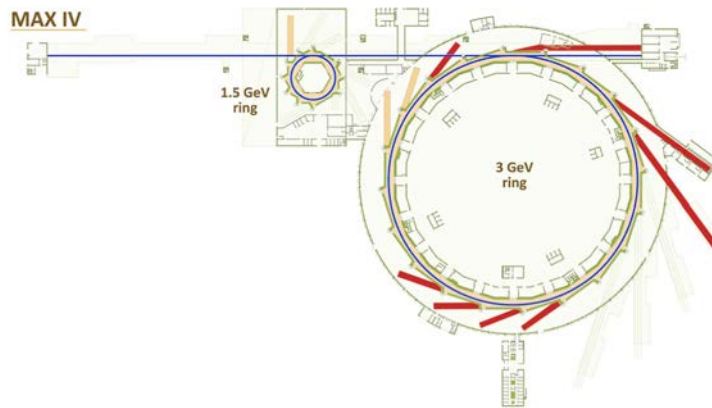
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KTH Royal Institute of Technology
Linköping University
Luleå University of Technology
Stockholm University

Swedish University of
Agricultural Sciences
Umeå University
University of Gothenburg
Uppsala University



Life science at different length scales



MedMAX II

MedMAX I

NanoMAX
SoftiMAX

coSAXS

BioMAX

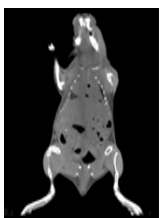
MicroMAX

FemtoMAX
Balder

10^{-6} m

10^{-9} m

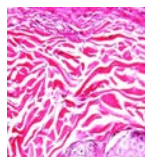
10^{-10} m



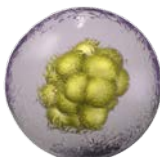
Animals



Organs



Tissues



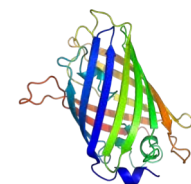
Cells



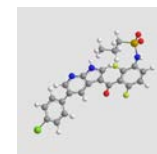
Micro-
structures



Molecular
complexes



Biomolecules



Atoms

Disease
models

Histopathology

Cell Biology

Molecular Medicine/Chemical Biology