



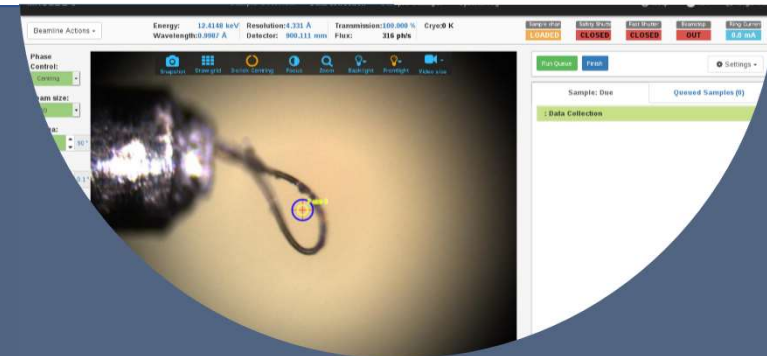
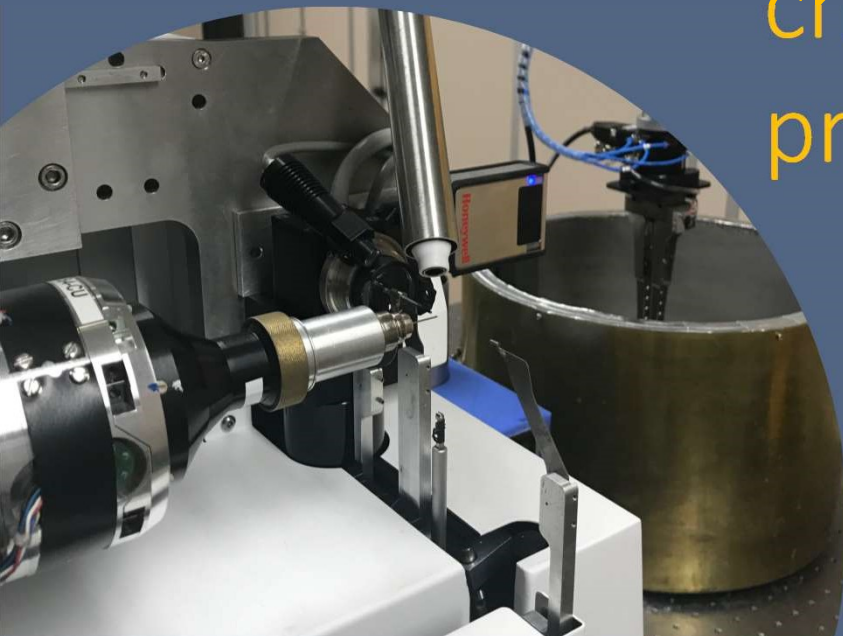
Protein Production and Purification
Partnership in Europe



One step further
on the protein
characterization
process :

XRD2 dedicated MX beamline at Elettra

presented By Annie Héroux
May 22-23, 2023



Synergy in between facilities

Most synchrotron facilities in the world have ancillary labs nearby

"Biologists" Structural Biology
Crystallographers ????

Elettra

Protein expression, productions proprietary, formation, user
Crystallisation facility easy access flexible schedule



Protein Production and Purification
Partnership in Europe



XRD2 is a
dedicated MX
beamline
operated and
managed by
Elettra and
Indian
Partners IISc

- Super Conduction Wiggler
(insertion device)
- Tunable energy (0.6- 15 Å)
- MD2S (Arinax diffractometer)
- Pilatus 6M (Dectris detector)
- Automounter (Stäubli)





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Partnership in Europe



Capabilities....

Standard Data collections

SAD.... Phasing

Ligands,

High Throughput

- Very reliable
- Optimised xtal swapping
- Accuracy ~ 20 um for remounting
- Automated data analysis pipelines

Data collection time is limited
to the flux at XRD2

6-12 min
before radiation
damage



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Energy: 10.000 keV
Wavelength: 1.0000 Å
Resolution: 2.074 Å
Detector: 400.044 mm
Transmission: 100.000 %
Flux: 189259 ph/s
Cryo: 100 K

Phase Control:
Centring
Beam size: 50
Omega: 330
Kappa: 0
Phi: 0
Y: -0.247
Z: -0.15
Focus: -0.107
Samp-X: 0.821
Samp-Y: 0.085

Box size is beam size

Name	V-Space (µm)	H-Space (µm)	Dim (µm)	#Cells
Grid-1	0.00	0.00	500 x 650 (130)	
*	0	0		

Overlay
*Normalised
Values

SHFT-DoubleClick at the position

What makes the difference?

Elettra Access Modes

- **in presence** is allowed but not encouraged
(we do like to see you though!)
- **Remote / Mailin**: preferred xrd2 is ready



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Proposals

No deadline for submitting a proposal

NO SEMESTRAL SUBMISSION

****We do not use BAG**

* proposal are kept *live* for a long time; concept of visits

* shifts mentioned are irrelevant to us

* Schedule by the hour, split time

* Schedule as fast as the dewar shows

up, within days

ALWAYS GO THROUGH ALL SAMPLES

<https://vuo.elettra.trieste.it>

VUO - Welcome to the Virtual Unified Office

Login

Username: Password: [\[Login\]](#)

Please note that in case you log in from a new location you will be asked to insert a validation code [captcha](#).

Indicate as username your identification code (USER ID) or your e-mail and the password (for Sincrotrone Trieste users it is valid also the password used for the e-mail system [Marconi](#)).

[Umbrella System](#)

Lost password

If you are already registered but you don't remember your password please don't try to register again but click [here](#) to reset your password.

[contact us](#)

Visits to the Elettra laboratory

If you are planning a visit to our laboratory just click [here](#) and fill the form. You will be contacted by our visitors office. Se intendi pianificare una visita al nostro laboratorio seleziona [questo link](#) ed inserisci i dati della tua richiesta. Sarai contattato dal nostro "Ufficio visite" quanto prima. Our visits [statistics](#)

Open Access Data Portal

The Elettra and CERIC [Open Access Data Portal](#) provides access to raw scientific data acquired during experiments. The data are published as Open upon explicit request by their Principal Investigator, in accordance to the facility's data policy or through other special agreements like for those regarding Covid-19. The Elettra scientific data policy is available [here](#).

Resource booking

Show here a [calendar](#) of the usage of the meeting rooms of the Elettra site. To book an event you must login in the VUO using username and password as indicated in the «Login» section.

Calendar

For details on Beamtime Allocation Calendar have a look to [Elettra](#) or [FERMI](#) Calendars.

Seminars

Forthcoming [seminars@Elettra](#)
Forthcoming [seminars@CNR-IOM](#)

Publication Search & Submission

Please note that all publications resulting from measurement runs or research done at Elettra must be entered into the Elettra Publication Database. Authors are invited to submit their publications through Elettra's Publication Submission page for each contribution - journal article, conference presentation, book or book chapter, thesis, contributed news articles, etc. Only published contributions should be submitted to Elettra's Publications Database. Publications can be searched for through [Elettra's Publication Search](#) page.

Elettra - Sincrotrone Trieste S.C.p.A.

S.S. 14 Km 163,5 in Area Science Park
34149 Basovizza, Trieste, Italy
T. +39 040 37581
F. +39 040 938 0903

P.IVA e C.F. IT00697920320
Cap. Soc. € 47.632.663,00 i.v.
PEC: sincrotrone.trieste.elettra@legalmail.it
www.elettra.eu

Iscritta al Registro delle Imprese di Trieste
Società di interesse nazionale
ai sensi dell'art. 10, comma 4,
L. 19 ottobre 1999 n. 370

**CENTRO
MANAGEMENT SYSTEM
CQY
CERTIFICAZIONE**

UNI EN ISO 9001:2015
UNI EN ISO 14001:2015
UNI CEI EN ISO 45001:2018

VUO contacts | [Disclaimer](#)

Operation: Remote Data collection

 User login NOT group/BAG

 Tested by Partners

Only need browsers opened
(we send links in advance)

Zoom

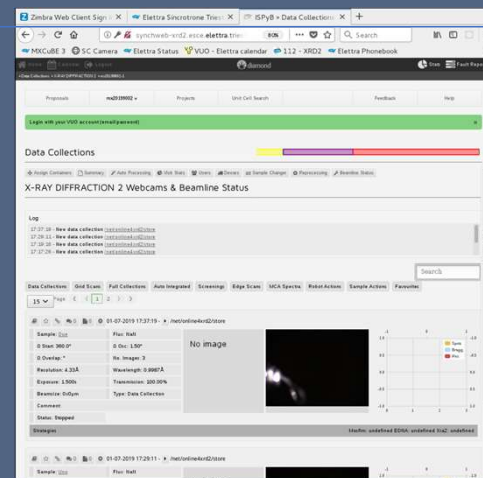
MXCube3

SynchWeb

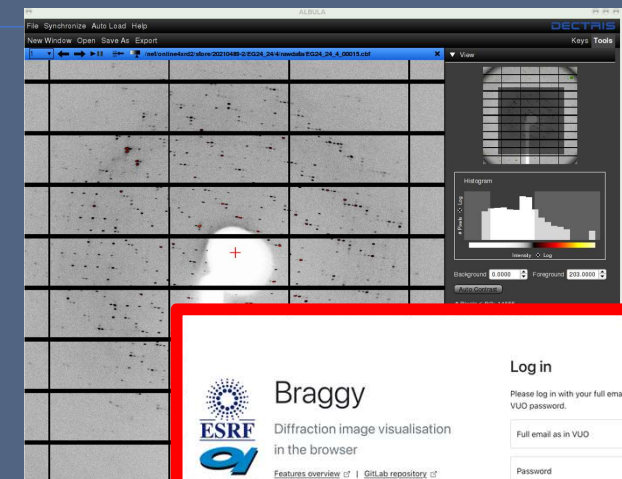
Rafec/Braggy



<https://140.105.207.47:8090>



<https://synchweb.elettra.eu>



<https://braggy.elettra.eu>

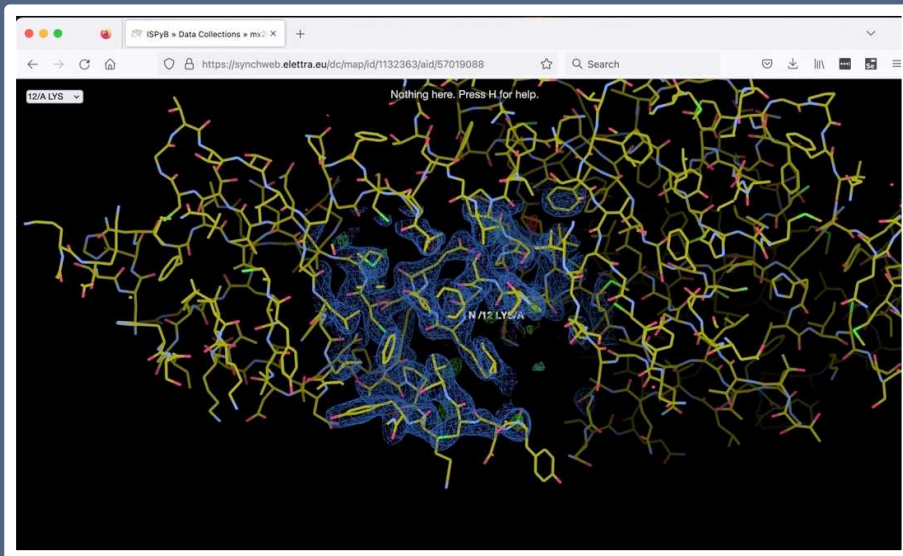


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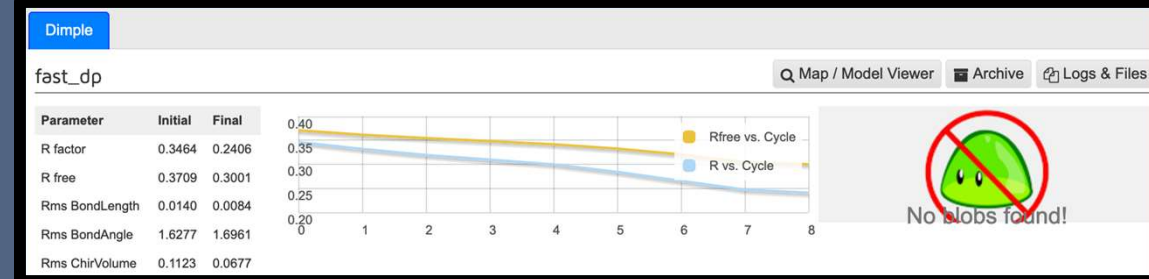
AREA
SCIENCE PARK

Elettra
Sincrotrone
Trieste

Automatic DIMPLE if there is a successful fast_dp / autoproc and a PDB code



Sample: mpro_5_11	Counts: 1.71e+5
Ω Start: 0.0°	Ω Osc Range: 150.00°
Ω Overlap: 0°	No. Images: 150
Det. Edge Resolution: 3.00Å	Wavelength: 1.0000Å
Transmission: 100.00%	Tot Exposure: 150.000s
Type: Data Collection	Beamsize: 100x100µm
Comment: updated - 22/10/22@23:30: Rfree=0.2658 on 7NG6.pdb+fast_dp.mtz in P212121(2.545A)	
Status: Stopped	
Auto Processing	fast_dp: ✓ autoPROC: ✓
Downstream Processing	dimple: ✓



New features in SynchWeb

Synergy in between facilities

Most synchrotron facilities in the world have ancillary labs nearby

"Biologists" structural biology

FOSTERING collaborations

Elettra

Protein expression, productions proprietary, formation, user access
crystallisation facility easy access flexible schedule

Synergy in between facilities

Most synchrotron facilities in the world have ancillary labs nearby

"Biologists" collaborations

FOSTERING

Elettra

Protein expression, purification, crystallisation facility

With facilities (software)

With Partners

With Users

Coordinate with other beam time

**** We are available experts ****

ess



Protein Production and Purification
Partnership in Europe



Duration: Apr. 2020 – Sep. 2021
18 partners from 7 countries

EXSCALATE
4COV

Objectives: **Operation during Pandemic: high throughput**

Identify molecules
capable of targeting
SARS-CoV-2

Develop effective
tools to counter
future pandemics
Exploit European
supercomputer
capabilities

Elettra contributes by determining the crystallographic structure of the 2 SARS-Cov-2 druggable proteases in complex with selected hit compounds.

Elettra performs the production and crystallization of viral proteins by the Protein Facility and the diffraction, data collection and reduction by XRD2 beamline.



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4COV

Objectives: **Operation during Pandemic:** high throughput

Identify molecules
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SARS-CoV-2
Develop effective
tools to counter
future pandemics
Exploit European
supercomputer
capabilities

More 1000 data sets collected

29 structures deposited in PDB

3 papers published; 1 accepted; 5 in preparation



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What is coming up....

Elettra 2.0

CryoEM facility



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What is coming up....

July 3rd, 2023
Hybrid Mode

AREA Science Park Elettra 2.0: New Structural Biology Opportunities

3 July 2023
AREA Science Park
Europe/Rome timezone

OVERVIEW

TIMETABLE

CONTRIBUTION LIST

MY CONFERENCE

MY CONTRIBUTIONS

REGISTRATION

Org.

✉ annie.heroux@elettra...



Elettra Sincrotrone Trieste

With the future Elettra 2.0 upgrade, several new facilities will be available to the *Structural Biology Community* either at Elettra Sincrotrone or at the CNR center.

We will share with you our vision for the future MX beamline uXRD and unveil our plans concerning the new CryoEM center.

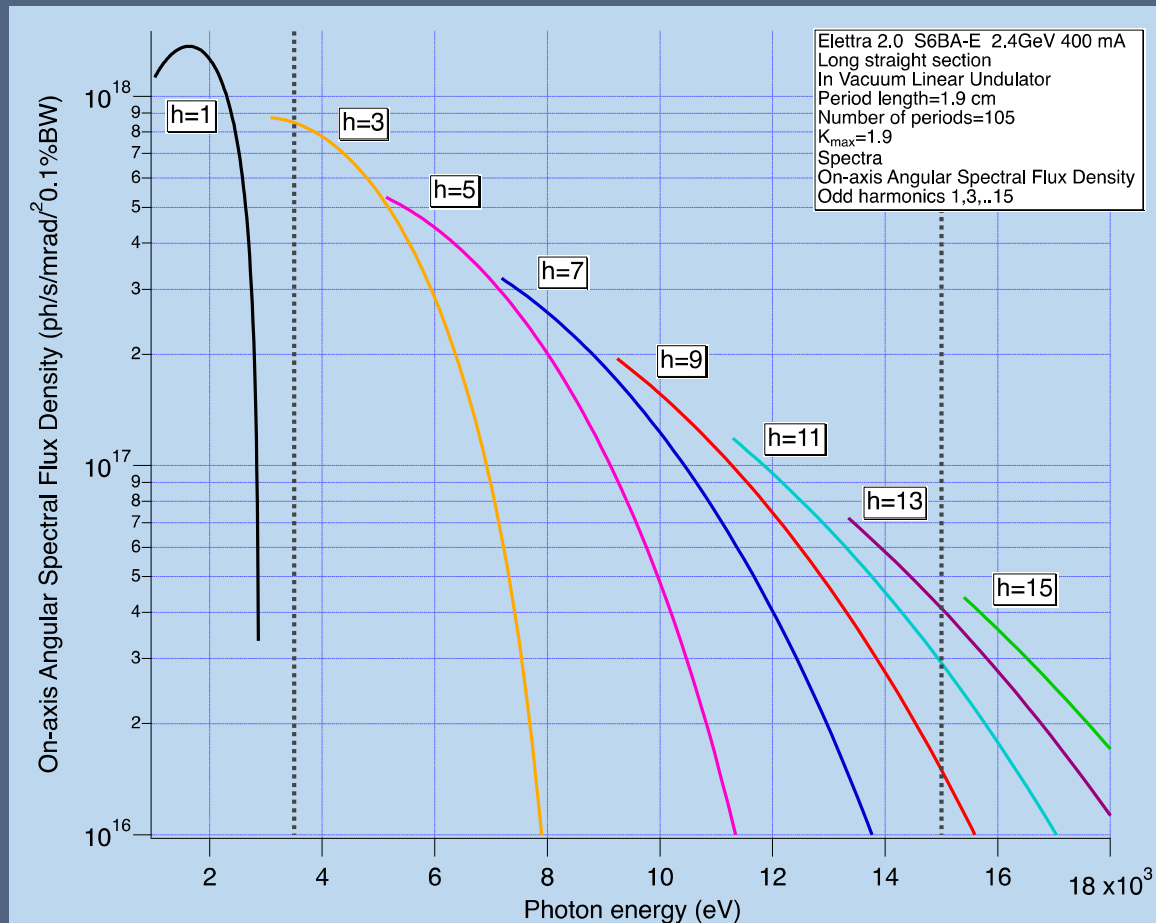
We hope this will provide a platform to share but also gather feedback on aspects and requirements from our scientific community in order to leverage our future state-of-the-art facilities.

We will discuss about the needs for sample preparation provided by the ancillary laboratories and protein facilities associated with the beamlines or CryoEM center: from protein expression, purification, characterisation.

We look forward to your participation either in person or via Virtual mode.



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Beamline moving on the other
side of the ring

Goal $5 \times 5 \mu\text{m}^2$ to $50 \times 50 \mu\text{m}^2$
 $\sim 10^{23}$ photons

Data collection
6 minutes to less than 0ne

First component
In Vacuum Undulator
No gap in the wavelength