

How to prepare a “perfect” (?) SAXS beamtime application

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Structure-function relations of flavoenzymes

BioSAXS User since 2002
in Priorities Evaluation Committee (PEC)

EMBL Hamburg P12 Virtual User Meeting
November 17—19, 2020

Before you start writing your application for beamtime @EMBL-HH:

- read carefully the notes from this user meeting and the BioSAXS group pages
- remember that the complete application will be subjected to evaluation with respect to:
 - Scientific quality of the proposal
 - Biological relevance and expected impact
 - Track record with respect to the proposed project
 - Successful publication record of previous EMBL proposals (if applicable)
 - Importance for instrument development (if applicable)
- and also
 - Technical feasibility
 - Estimate of actual beamtime needed to carry out experiments

If needed: contact EMBL-Hamburg staff before you start for advice

The application consists of two main parts

-Application form:

-«Proposal Summary»

- Heading (Title)

- Concise information on type of proposal, proponents, expertise, experimental plan (9 tabs!!!)

- «Main Text» of the proposal

-«Detailed Sample information» (3 tabs + Save!!!)

Please do balance information in different parts and sections keeping in mind that:

«Application» will be available to the Priority Evaluation Committee and EMBL Technical Staff

«Detailed Sample information» will be available to EMBL Staff only for evaluation of technical feasibility and advice on shifts allocation

Your contact at EMBL will read the complete application to prepare for your visit and to assist you during measurements

START @: <https://smis.embl-hamburg.de>



- Login to my EMBL User Portal (SMIS) account

You can now login through the [Umbrella](#) !

Account name : Password : [Login](#)

Please note: If you are an EMBL staff member you should use your site login and password!

I have lost my login or password: [Recover your login and reset your password](#)

I have lost my password and my email has changed: Please [contact us](#).

I am a new User [Create a new EMBL User Portal \(SMIS\) account](#)

Note: if you are already registered in the EMBL User Portal (SMIS) database, please do not create a new account: you will no longer be able to access details such as proposals submitted previously, A forms, reports or events.

Register as new user; get login and password
or login with your (known) password

Select **New Proposal** and the Type of proposal

You can go back and edit «Proposal in progress»,

You can also check «Previous proposals»

You will need to access the proposal to file the experimental report after measurements

The screenshot shows the EMBL User Portal interface. At the top, there is a navigation bar with the EMBL logo and the text "User Portal - v3.16.24.2". Below this, there are several menu items: "Accounts", "Proposals/Experiments", "Reception", "Travel", "Safety", "Administration", and "Review Process". The "Proposals/Experiments" menu is currently selected.

Below the navigation bar, there is a welcome message: "Welcome to the Electronic Utilities Application for EMBL Users".

Underneath the welcome message, there are four buttons: "New Proposal", "Proposals In progress", "Proposals with Final Number/Previous Proposals", and "In progress, as Co-Proposer". The "New Proposal" button is circled in red.

Below the buttons, there is a section titled "Information for users" with the following text:

- Before starting, make sure that each co-proposer has created an account and the scientist submitting the proposal (main proposer) **holds a PhD**.
- **BAG or single proposal?** Individual users applying for several projects and groups of users (e.g. local, regional, national or thematic research consortia) are requested to submit a **BAG proposal**.
- **Continuation of a previous proposal?** Please ensure that the **Experiment Report** for your previous proposal has been completed (under the tab "Proposals with Final Number/Previous Proposals").

Below the information section, there is a section titled "Submit New Proposal" with the following text:

To create your Beamtime Application Form, select the appropriate Proposal by clicking on the corresponding button.

- MX Single Proposal ?
- MX BAG Proposal
- Industrial Experiment (EMBL MX and BioSAXS) ?
- SAXS Single Proposal ?
- SAXS BAG Proposal
- SAXS iNEXT-Discovery Proposal ?

The list of proposal types is circled in red.

«Proposal Summary»



EMBL User Portal - v3.16.24.2

Accounts ▾ Proposals/Experiments ▾ Safety ▾

Application for a Proposal at the EMBL - BioSAXS Beam Time

New proposal

General Information Societal Theme Beamlines Request Proposers Laboratory Support Facility Sample Environment Sample Description Experience Publications

- You will have to answer the questions in these 9 tabs

Once this is provided you will be asked to:


- Upload "Main text"
- Give "Detailed sample information"
- Save

DO balance information in different parts and sections

DON'T fill these fields in a hurry

The Application

- «**Proposal Summary**» : Information on proposal type, proponents, samples, etc (from the 9 tabs)
- «**Main text**» (to be uploaded as a pdf)

Ref. No 29246	EUROPEAN MOLECULAR BIOLOGY LABORATORY	EMBL 
Application for a Proposal at the EMBL - BioSAXS Beam Time		
Proposal Summary		
Title		
test proposal		
Keywords		
#1: <input type="text" value="test"/>	#2: <input type="text"/>	#3: <input type="text"/>
		#4: <input type="text"/>

General information

• This proposal is
A new proposal
A resubmission of
A continuation of :

• Is the project a Service project or a Collaborative project? :

Service
 Collaborative

• This proposal is directly linked to an MX proposal? Yes No If yes: EMBL MX Proposal Number

• This proposal is principally
Fundamental Science % Applied Science % Industrial Science %

- New **project**, resubmission or continuation of previous project at EMBL-HH
- If multiple proposals are to be submitted by one group (or closely collaborating lab from, e.g., same institution, network), better to apply as a single Block Allocation Group (BAG) for more efficient management of allocated time.
- **Service or collaborative:**
 - Service:
 - you will get training on the use of the beamline
 - you will be responsible for experimental design, data acquisition, data analysis;
 - there will be a scientist helping you with beamline-related technical issues
 - Collaborative:
 - Establish contact with collaborator at EMBL-HH before filing the application
 - Coordinate proposal with collaborator @ EMBL-HH (exchange drafts)
- Link to MX proposal.

The screenshot shows a web form titled "Proposal Type". It contains several sections:

- A section with a blue header "Proposal Type" and a red asterisk indicating a required field: "This proposal is * A new proposal ?" with an unchecked checkbox.
- A section highlighted with a red border: "This proposal was approved by iNEXT-Discovery? *" with radio buttons for "Yes" (selected) and "No", and a text input field for "If yes: ?" containing "Import proposal from iNEXT-Discovery". Below this is a text input field for "iNEXT-Discovery proposal ID ?".
- A section with "Is this proposal related to COVID-19? ?" and an unchecked checkbox.
- A section with "Do you need Rapid Access to the beamlines? ?" and an unchecked checkbox.
- A section with "Reason/s for applying for rapid access:" followed by a large text area.

- **iNEXT-D:**
- do apply under iNEXT-Discovery program
- if the proposal is approved by iNEXT:
 - (ltd) expense refund may be available (e.g.: sample shipping costs)
 - the proposal will be given high priority (unless serious problems are found with the proposal, which were missed by the iNEXT reviewers).
- may file application to both EMBL@HH and iNEXT, but do notify EMBL@HH if your proposal has been approved by iNEXT ASAP to avoid double allocation of beamtime

covered by: Th. Nov.19, 2020 Hello from the User Office - Sarah Marshall-Bensch

General information

• This proposal is directly linked to an MX proposal? Yes No If yes: EMBL MX Proposal Number

• This proposal is principally
Fundamental Science % Applied Science % Industrial Science %

• Is this proposal related to COVID-19?

• Do you need Rapid Access to the beamlines?

Reason/s for applying for rapid access:

If «COVID-19» box is checked, «Covid-19» will be appended to the proposal title. Still it will be evaluated thoroughly as all other proposals.

If «Rapid Access» box is checked , please fill in the box here and remember to insert a paragraph in the proposal main body explaining the special urgency of the SAXS measurements

For special cases do contact the EMBL@HH staff

E.g.: Industrial science: beamtime allocation and fees depend on the goal of the measurements.

Societal theme

Societal Theme

- Earth and Environment
- Fundamental Science
- Enabling technologies
- Health
- Energy
- Transport and Space
- Key technologies

The **Societal theme** does not influence scoring, but remember this is BioSAXS!!!

Beamline requested

Beamline(s) requested:

(See description of [P12](#) for details)

Principal

P12

Number of shifts requested

6

Total required shifts: 6

Mail in access

Yes

No

Preferred starting time: Please select the period

Unacceptable dates

- **P12** is the BioSAXS beamline

Shifts requested

- 1 shift = 8 h
- Normally, no more than 3 shifts are assigned to single projects, due to oversubscription, and one cannot split shifts in more than one visit.
- Take into account the measuring time, special setups, sample preparation time (measuring time may be much shorter than sample preparation!)
See specific presentations
- Applications within a BAG, may allow optimization of allocated beamtime.
- In the «Detailed Sample Description» form you will be able to further justify your beamtime request

Mail-in access: the beamline scientists will carry out the experiment for you.

Read carefully <https://www.embl-hamburg.de/biosaxs/mailin.html>

Main proposer (to whom correspondence will be addressed):

Laboratory University of Milano Dept. of Biomol. Sciences and Biotechnology Via Celoria 26 IT - 20133 Milano

Name Prof **VANONI Maria Antonietta** Phone +390250314901 Fax +390250314895 Email maria.vanoni@unimi.it

Co-Proposers (Laboratory if different from main proposer)

Laboratory EMBL EMBL Notkestrasse, 85 DE - 22603 HAMBURG

Name Dr **SVERGUN Dmitri** Email svergun@embl-hamburg.de

Main proposer:

«Senior scientist» (PI) that will take responsibility for the project (including on-site supervision of co-proposers)

Co-proposers:

- List the people that will participate in the experiments.
- See «Hello from the User Office - Sarah Marshall-Bensch” for registration with SMIS, safety courses for access to beamline, User lab; request DACHS card and accommodation.

If Collaborative:

include your EMBL-HH collaborator(s) after making specific arrangements with him/her and agreeing upon the collaboration and the experimental plan.

Laboratory support facilities

Laboratory Support Facility

- DLS
- FPLC
- Refractometer
- SLS

Equipment list and manuals are available at:

https://www.embl-hamburg.de/biosaxs/user_info.html

Additional equipment at the Sample purification and characterization facility (SPC) facility, but one needs to contact scientists at SPC in advance to make arrangements:

<http://www.embl-hamburg.de/services/spc/index.html>

*** See specific presentations***

Sample environment

Sample Environment

Items Supplied by EMBL

Solution scattering experiments

- BioSAXS with automated robotic sample changer. 25 ul sample; 0.2-10 mg/ml; 20 x 50 ms exposures (1 s total); 1 min turnover (loading, measurement, cleaning). Temperature 5-50C. Remote and mail-in measurement possible
- Standard size exclusion chromatography (SEC)-SAXS with or without UV. FPLC or HPLC SEC column connected directly to the beam line. Requires 45-80 min per experiment. Maximum 100 ul injection (recommend 50-100 ul sample at 5-10 mg/ml.). Room temperature only
- Size exclusion chromatography (SEC)-SAXS with with parallel MALLS, DLS, RI and UV detection for molecular weight validation and hydrodynamic radius measurements (Wyatt TREOS/QELS/T-rex system. Collaborative projects only. Please fill out section 4 of THIS FORM). Room temperature only

Non-standard ('in air') sample environments:

- No "Non-standard ('in air')" sample environment required
- Temperature controlled (5-95C) capillary holder
- Stopped flow, time resolved setup. temperature: 5-80C (on collaborative basis only)
- Other (specify, for example your own tailored sample environment):

- We plan to use lasers
- For scattering vectors outside the standard range, $s = 0.05\text{-}4\text{ nm}^{-1}$ (e.g., WAXS, please fill out section 5 of THIS FORM)
- Anomalous SAXS, ASAXS ((5)7-20 keV; Collaborative only)

Use of SEC – SAXS needs to be justified in the proposal.

SEC-SAXS if MALLS is required, and all other «Non standard set-ups» available on a collaborative basis only

*** See specific presentations***

Application for a Proposal at the EMBL - BioSAXS Beam Time

New proposal

General Information Societal Theme Beamlines Request Proposers Laboratory Support Facility Sample Environment **Sample Description** Experience Publications

Sample Description

A detailed description of the sample will be requested in the sample sheets

Advance notice period * [?](#)
...

The sample(s) will be available from * [?](#)
... (dd/mm/yyyy)

Macromolecules and other compounds * 0

Full-length **IMORC1** and truncated foms (0.1-10 mg/ml) in 20-50 mM phosphate or Hepes buffer, pH 5-8, 0-100 mM NaCl, 1 mM EDTA, 1 mM DTT, 0-10% glycerol

A «detailed sample description» is required in a separate section (see later)

Here, give sufficient **information on the samples** (quantities and quality) (and in the main text) to allow PEC to evaluate (also) feasibility.

- Make sure you have enough sample*** (also in case you need to repeat measurements if something goes wrong)!

Experience with synchrotron radiation

Experience with Synchrotron Radiation

Do you have a specific reason for using the EMBL beamlines? If yes, please state here.

Have you used synchrotron radiation at the EMBL? No Yes

Have you used synchrotron radiation at other sources? No Yes, at:

Have you already used synchrotron radiation for this project? No Yes

Publications

	Description	
[1]	<input type="text"/>	

Here highlight:

- **Technical reasons** for applying to this beamline
- **Previous experience** with this and other SAXS beamlines

for proposal evaluation and also to help evaluating the level of assistance you will need from the EMBL staff.

New users are welcome!

Expertize of the proponents

Publications	
	Description
[1]	

- Here list a representative selection of **your publications** and/or those of co-proponents (not of the EMBL staff that will assist you or you will be collaborating with, but it is OK to include publications in collaboration with BioSAXS group) to show the relevant expertise with respect to:
 - use of synchrotron radiation, especially SAXS (hands-on)
 - the specific projectand your publication record
- Limit the list to **~5 references**
- Include **full reference**: authors' list, full title, year, Journal, volume, pages

«Main text» of the proposal (to be uploaded as a separate file)

It will be appended to the Project summary (9 tabs) for evaluation and later use.

In the allowed space, justify your application for beamtime and propose your experiments in order to allow the proposal to be evaluated for the scientific relevance and technical feasibility by the Project Evaluation Committee and the Technical Staff

Application for beam time at EMBL – Experimental Method

The activating conformational changes of human MICAL1: the multidomain flavoenzyme participating in actin cytoskeleton dynamics

Aims of the experiment and scientific background

Experimental method

Results expected

References

Your contact at EMBL will later read and use the proposal to prepare for your visit and assist you during the visit

Aims of the experiment and scientific background

Remember to clarify:

- The **biological relevance** of the project.
- The **specific question** you will ask:
 - which relevant information you are looking for
 - **why SAXS measurements will provide key information and how urgent they are** (e.g.: The SAXS data are needed to complete an on-going project/paper *vs.* preliminary/ exploratory work).
- If Rapid Access box was checked, please make sure to include a paragraph that explains the extreme urgency

Experimental method and Results expected.

- Clarify the experimental plan with information that will allow to establish the feasibility vs. the stated aims including, e.g.:
- Amounts and quality of protein available (size, stability, tendency to aggregate, data from gel filtration, DLS, AUC, other spectroscopies, MX, kinetics...).
- Ancillary information (e.g.: X-ray, NMR structures available on this or homolog/similar systems). If dealing with complexes: K_d and stoichiometries (if known).

Balance information between here, «sample description» and the «Detailed sample description form»

References (relevant to the actual proposal):

- Include Title and full reference; if possible include the full list of authors;
- Make clear in the text which is the work from your lab and what comes from the literature.

Consider to include a figure and/or a table to clarify what you know, your questions, the expected outcomes.

«Manage your samples» will lead to
«Detailed sample information» = «Sample information & safety sheet»
= «Sample sheet»

EMBL User Portal - v3.16.24.2

Accounts ▾ Proposals/Experiments ▾ Reception ▾ Travel ▾ Safety ▾ Administration ▾ Review Process ▾

Welcome to the Electronic Utilities Application for EMBL Users

New Proposal Proposals In progress Proposals with Final Number/Previous Proposals In progress, as Co-Proposer

— Manage Previous Proposals (view details, submit reports) —

Click here to see the proposals existing in the EMBL database.

Change the number of proposals shown : 5 ▾ or Search proposal Ref. SAXS ▾ or Search proposals by type ... ▾ Search Clear filters

To carry out an action related to a proposal, click on the appropriate icon.

Code	Title	Type	Round	Report	Beam	Actions
SAXS	-Main proposer <input type="text"/> Structural and functional analysis of <input type="text"/>	EMBL SAXS BioSAXS	4/2016		Y	View proposal details Manage your Experiment Report Manage your samples : Duplicate this proposal

«Sample information and safety sheet» (3 tabs + Save) will be accessible to the EMBL scientists to establish technical feasibility, advice on shifts allocation and, later, to prepare for your visit and help you on site.

«Description» tab includes practical information on sample shipment and type of substance

EMBL User Portal - v3.16.24.2

Connected as: Sarah MARSHALL-BENSCH | Umbrella | Home | FAQ | Contact

Accounts | Proposals/Experiments | Reception | Travel | Safety | Administration | Review Process

SAMPLE INFORMATION & SAFETY SHEET

Sample #: Proposal / Experiment #: SAXS-525

* - Mandatory Field. ? - Tooltip. = Read-Only Field.

Complete all tabs prior to submission!

Description | **Handling** | Equipment | Data Collection | Certify And Save

Text Description of Sample and Protein*

Sample Description: Protein Acronym: * ?

Sample Type Isotropic Not Isotropic The Sample will be Brought by the User Sent by Courier

Molecular mass [kDa] * ?
Conc. Range [mg/ml] from ? to Buffer Composition ?

Classification of the Substance*

Tissue Crystal Powder In Solution Other Amount of substance, mg: ?
If Tissue or Other, please specify: ?

Classification Of The Sample*

Biological ? Synthetic ? Radioactive Contaminant Toxic Flammable Explosive Corrosive
 Oxidizing Derivatized Carcinogenic Infectious Live Virus Amyloids Narcotic
 Other (give a short explanation): ?

Synthetic Or Biological Sample *

Source Organism* : ?

Class Of Risk * ? ?
Group 1: no risk to human health and/or environment if standard hygiene is maintained according to current knowledge
Group 2: little risk to human health and/or environment
Group 3: moderate risk to human health and/or environment
Group 4: high risk to human health and/or environment

Is the sample recombinant? * (If yes: "Expression Host" and "Class Of Risk", below must be provided)

«Handling and Equipment » tab

- includes more practical information on samples ;
- details will be given here if special equipment is going to be used.

Handling / Equipment

Sample Storage*

4°C Cooler Room Temperature -80°C Cooler Other

Danger linked to the handling of the sample or the use of special equipment*

There is a risk
No risk
I'm not sure

If there is a risk or if you are not sure, please give some details.

Specify special measures to be taken or equipment to be used/provided (gloves, goggles, ...):

After the experiment the sample will be*

Removed by the user
Disposed on site

«Data Collection» tab:

EMBL User Portal - v3.16.24.2

Accounts ▾ Proposals/Experiments ▾ Reception ▾ Travel ▾ Safety ▾ Administration ▾ Review Process ▾

SAMPLE INFORMATION & SAFETY SHEET

Sample #: Proposal / Experiment #: SAXS-525

* = Mandatory Field. ⓘ = Tooltip. [] = Read-Only Field.

Complete all tabs prior to submission!

Description Handling / Equipment **Data Collection** Certify And Save

— Scientific Justification* (Explain clearly the interest in and the status of this sample):

For this sample, please indicate:

- Number of sub-project to which the sample belongs
- Relevance
- Crystal availability (if yes, please provide diffraction limit)
- Any special requirements (e.g. microfocus, microspec, unusual wavelengths, extensive screening).

For bio-SAXS samples, following information must be entered in "Scientific justification":

1. How many constructs do you intend to study?
2. Please provide the length and molecular mass of each construct if known
3. Do the samples contain detergent?
4. What conditions do you want to measure at (range of pH, temp, addition of ligand XX)?

— Anomalous Scatterers

DON'T cut-and-paste from the Proposal form.


DO complete with technical/practical information (see questions in red as a guide, but add what is relevant to your system/planned experiments)

Remember to save!

Certify And Save

I certify that the sample information is complete and correct*

Extract data from the EMBL scientist database:
Type the first letters (2 at least) of a **surname** in the text field and wait a few seconds.
A list of possible names will appear.

- If the records found include your personal details, select the correct one in the displayed list. The fields below will then be automatically filled.
- If **no existing** record is found to match your personal details, click on  anyway so that the surname typed is transferred below and fill in the remaining fields manually.

Name:

Phone:

E-mail:

Further Information

«TO DO THINGS» after your application is approved: just follow the instructions!

The screenshot shows a web browser window with the URL https://www.embl-hamburg.de/services/access_infrastructures/preparing-your-visit/index.html. The page features the EMBL Hamburg logo and navigation menu. The main content area is titled "Preparing your visit" and includes a sidebar with a table of contents and a main text area with instructions.

EMBL Hamburg
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Preparing your visit

PRINT SHARE

Feedback

◀ SERVICES

ACCESS TO INFRASTRUCTURES

PREPARING YOUR VISIT

- Checklist and accommodation
- A Form
- DACHS cards
- Safety training
- Sample shipments
- Your experiment
- Contact

BAG PROPOSALS

Following positive evaluation of your proposal, you will receive an invitation for a scheduled beamtime session which has been allocated to your project.

Please make sure that you accept the scheduled beamtime before the deadline stated in the invitation.

In order to avoid any unnecessary delay to your beamtime, please consult the instructions under the section [Preparing for your visit](#) and carry out the required actions as far in advance of your beamtime as possible.

Not submitted your proposal yet?

To apply for beamtime, submit a proposal via the [EMBL user portal](#).

See: Th. Nov 19, 2020 - Hello from the User Office - Sarah Marshall-Bensch

What if?

- What if my proposal was well received , but could not be granted beamtime?
- What if I find out that I badly need to perform SAXS experiments after the deadline for presentation of «regular proposals»?

Can (re)apply as «Rolling proposal» throughout the year, depending on beamtime availability. Check the EMBL website.

- What if I have been awarded beamtime, but my experimental plans change because of novel results? (e.g.: no longer need beamtime, need to change experiment design, a novel/better protein form is available, can't produce (enough) protein, ...)
- Adjustments/refinements to the original experimental plan are expected (update «sample sheet» prior to actual visit)
- Major changes: Contact SAXS people ASAP to discuss novel scenario

Good luck!



... and thanks to the Svergun Group!