

# ESS user office software and data handling

Zoë Fisher, Tobias Richter

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# Outline

- ESS policy on scientific data
- SciCat data catalogue
- DOI and publications
- DEMAX user portal
- ESS user office software – DMSC & SAD collaboraton

# ESS Policy for Scientific Data

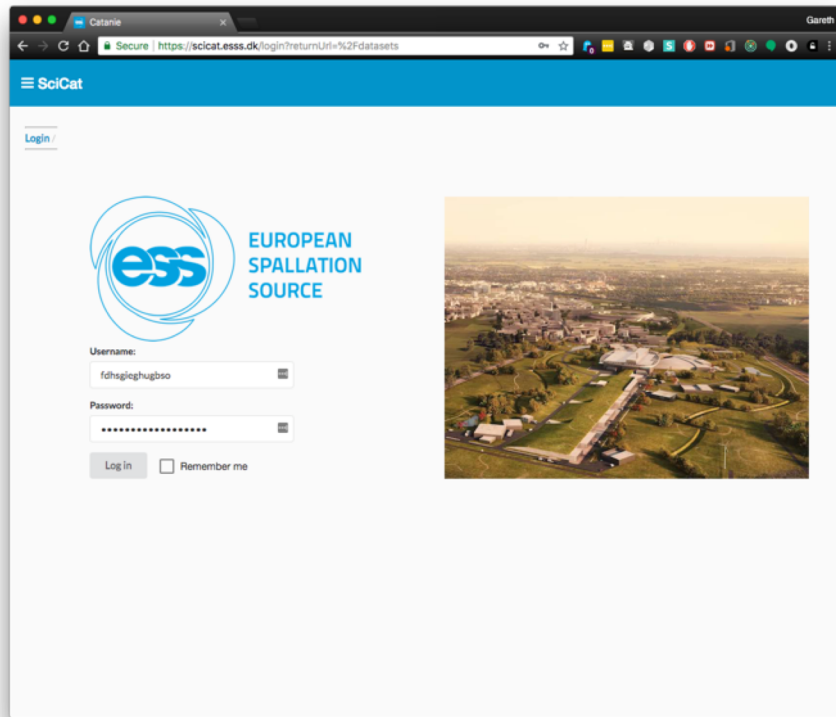
- Applies to non-proprietary use beam time only
- Defines actors & Data types
- A Data policy is essential
  - Open data
  - Requirement of citable data for certain journals
  - Existence of a curated data policy helps users submit papers
- Very similar to policies for ILL, ESRF, ISIS, DLS
- User acceptance of policy is a condition of facility access

# ESS Policy for Scientific Data – Terms

- ESS will store all raw and meta data for a minimum of 10 years after the restricted access period ends
- Raw and meta data will be catalogued
- ESS (DMSC) will act as custodian
- All raw data will be given a citable DOI
- Access to raw & metadata is restricted for 3 years (embargo period)
- Post-embargo access to catalogue and data will be open, consistent with ERIC statutes



# SciCat Data Catalogue Deployed at ESS, PSI and MAX IV



# Data Catalogue and Publications

- H2020 project BrightnESS published 250,000+ files in the ESS data catalogue (<https://scicat.esss.se>)
  - Each dataset linked to publicly accessible DOI and researcher ORCID (Findable).
  - Data can be downloaded (Accessible)
  - Catalogue is searchable and links to data use instructions (Interoperable, Reusable)
- Post-Embargo all ESS science access data will receive a DOI and publications shall cite these.
- Data can be published earlier by request to support journal articles.

ESS Public Data Repository

Sample Data from Multigrid

|                 |                  |
|-----------------|------------------|
| Creator         | Anton Khaplanov  |
| Publisher       | ESS              |
| Affiliation     | ESS              |
| Year            | 2018             |
| Resource Type   | raw binary files |
| No. of datasets | 1122             |
| Size            | 17095764         |

Access data | Data description

DOI: [10.17199/BRIGHTNESS/MG0001](https://doi.org/10.17199/BRIGHTNESS/MG0001)

Instructions: Login with brightness username and password

Abstract: This data was collected as part of BrightnESS, funded by the European Union Framework Programme for Research and Innovation Horizon 2020, under grant agreement 676548. It consists of test data for the detector.

**IN OPERATION**



kubernetes

F



A



I

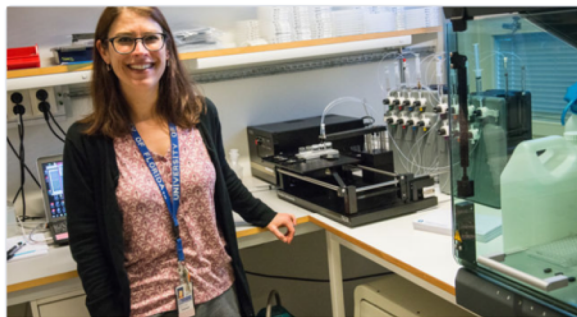


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# DEMAX proposal system for deuteration & crystallization lab

- Supported by DMSC under Tobias Richter: Jeremias Hillerberg & Gareth Murphy.
- Started end of September- protoype available mid-Feb with most functionality in place



ESS Support Laboratory Opens Pilot Call for Proposals in Preparation for First Science

FEB 25, 2019

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SCIENCE SUPPORT SYSTEMS

- PREMP
- FLUCO
- TEFI
- DEMAX
  - Call for Proposals Now Open
- SULF
- MESI
- SCUO

Home Science & Instruments Science Support Systems DEMAX Call for Proposals Now Open

## Call for Proposals Now Open

First pilot call for deuteration and/or crystallisation support from the DEMAX platform

The Deuteration and Macromolecular Crystallisation (DEMAX) platform at ESS supports neutron users from the soft matter, biology, life



<https://demax.esss.se>





EUROPEAN  
SPALLATION  
SOURCE

## DEMAX User portal

Deuteration and Macromolecular Crystallisation

register

login

First name \*

Last name \*

Email \*

Phone \*

Affiliation \*

Job title \*

Password \*



Please use password with min. 8 letter mixture of upper/lower case and numbers

**Receive updates about DEMAX and the proposal process through email.**

You can change this setting whenever you want.

**I confirm that I have read, consent and agree to the [DEMAX Privacy Statement](#)**

**I consent to the [DEMAX Cookie policy](#)**

Register

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# Welcome

to the DEMAX user portal for deuteration & crystallization support!

Users are strongly encouraged to contact DEMAX staff prior to preparing and submitting a deuteration/crystallization proposal.

General enquiries can be sent to: [demax@ess.se](mailto:demax@ess.se) or to one of the [subject matter experts](#).

- Proposals should be written in English, properly referenced, and prepared in the [Word template](#). Please keep to the 2 page limit, including Summary, Background (Science Case, Practical Consideration, References, Figures/Tables).
- Access to DEMAX is granted on the basis of both a technical and a peer-review process.
- Proposals awarded during initial operations (2019-2022) will be free of charge. During formal user operations (beyond 2023) we reserve the right to ask for partial financial contributions towards consumables & shipping costs.
- During initial operations, we will not limit access to DEMAX based on ESS-membership. Beyond this period, we will respect the user access policy that will be applicable ESS-wide.
- Biological and chemical deuteration proposals are run as a service but users for protein crystallization are welcome to come in person as well.
- *Users should note that the contributions by DEMAX should be acknowledged in any publications containing materials obtained from us. For particularly challenging projects that require above average involvement from DEMAX, relevant DEMAX staff should be acknowledged through co-authorship of any subsequent publications.*

[Download proposal template](#)

## Important dates

Proposal submission: 25 February - 5 April

Review: 5 April - 6 May

Notify users: 6 - 31 May

Run cycle: June - November

Wrap-up & user survey: December

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# Create a new proposal

[Next](#)[1. General information](#)[2. Crystallization](#)[3. Biological deuteration](#)[4. Chemical deuteration](#)[5. Review & submit](#)

## Proposal ID: 2NKU4UX5

Proposal title \*

Brief summary \*

Max 500 characters

0/500

## Main proposer

First name

Zoe

Last name

Fisher

Email

zoe.fisher@esss.se

Phone

0721792250

Employer

ESS

Job title

Scientist

## Co-proposers

First name \*

Last name \*

[Delete](#)

Affiliation \*

Email \*

[+ Click to add](#)

## Indicators

Links with industry?

Yes

No

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## Create a new proposal

[Back](#)[Next](#)[1. General information](#)[2. Crystallization](#)[3. Biological deuteration](#)[4. Chemical deuteration](#)[5. Review & submit](#)

### Check to select: Crystallization

Required information to include in the "Practical Considerations" section of your proposal:

- SDS-PAGE
- Chromatogram of protein purification to indicate yield & purity
- Photo of crystal

Name of molecule to be crystallized:

*(e.g. superoxide dismutase)*

---

FASTA sequence or Uniprot number:

---

Molecular weight (kDA) :

---

Oligomerization state:

*(e.g. homodimer, tetramer etc.)*

---

PDB ID of crystal structure:

---

If the reference is publicly available, please provide the DOI or an accessible link:

---

If the reference isn't publicly available, please upload a copy:

---

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1. General information
2. Crystallization
3. Biological deuteration
4. Chemical deuteration
- 5. Upload proposal & review**

## Attachments

Required documents to upload

DEMAX Proposal

Upload your DEMAX proposal here

Proposals should be written in English, properly referenced, and prepared in the [Word template](#).  
Please keep to the 2 page limit, including Summary, Background (Science Case, Practical Consideration, References, Figures/Tables)

### Upload file

Accepted formats: PDF

Choose file

Upload

Beamtime proposal

## Uploaded files

| Document type | Filename | Size | Filetype |
|---------------|----------|------|----------|
|---------------|----------|------|----------|

Generate PDF for review

## Review & submit

Generate and review a merged PDF of the form data and all attached documents.

Submit proposal



- All the basic functionality is in place in the "user" view: users can register, generate a new proposal, fill in all required information, attach references/images/proposals and then save & generate an integrated PDF of everything that can we review and send out for review.
- Admin view allows us to see if proposals are submitted, download the PDF, see a list of registered users & their permissions, reset passwords (!! also ability to "delete" users and their proposals !!)

Still needed:

- We need a way to assign proposals to internal and external reviewers, they must be able to log in and "see" only their proposals, and enter a score & comments or attach a PDF review.

# DEMAX, SAD, and SCUO

- DEMAX prototype gave us the impetus to collaborate across the organisation regarding authentication, GDPR, security, permissions, etc.
- Also established working relationship with the Scientific Activities Division that hosts both DEMAX and the User Office
- Officer for the Scientific User Office has been recruited and starts in May (person with a very high level of relevant experience)



# ESS & MAX IV User Office

## Collaboration with MAX IV:

- Plan: Component-wise migration away from DUO, while leaving database and workflows intact
- A little more effort than development from scratch in an ideal scenario
- But we gain valuable input on workflows, testing with real users and share the development effort

# User Office Software

- Web Section Lead to start in early May  
(hire has high level of relevant domain experience)
  - Web Developer positions as first UO team member is currently advertised
  - DEMAX Contractor (Junior Developer) contract expires end of May –  
working now on documentation, smooth hand-over
- \* SciCat scope will migrate into UO section as well

Questions?      Comments?