

DEMAX project update

1. DEMAX – organization, facilities, budget
2. Proposal call (scope, materials, services offered)
3. Next steps

STAP meeting 2-3 April 2019

Lund, Sweden

What is DEMAX?

- DEMAX is the ESS user support lab that offers deuteration and crystallization service and support
- Our services and support are aligned to enable first science on the first instruments
- Techniques: small angle scattering, spectroscopy, diffraction, reflectometry
- Scientific community that needs our help: life science, soft matter, chemistry, materials

DEMAX offers 3 pillars of support



0.5 FTE
(LU)

ESS Deuteration and Macromolecular Crystallization (DEMAX) Platform

Chemical Deuteration

- Organic synthesis
- Enzymatic Synthesis
- Separate, analyze a range of molecules
- Biomass-derived lipid extraction, analysis and purification
- Future: optimize large scale separation/purification of lipids from biomass

Biological Deuteration

- Deuterated biomass production (algae, bacteria, yeast)
- Protein expression & purification
- Biophysical characterization (DLS, thermofluor, nanotemper, purity)
- D incorporation with ESI-MS
- Future: optimization of fermenters for large scale yeast biomass growth

Macromolecular Crystallization

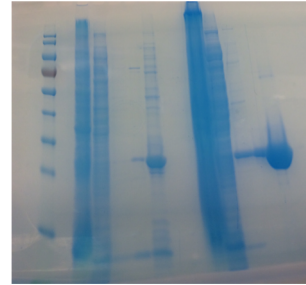
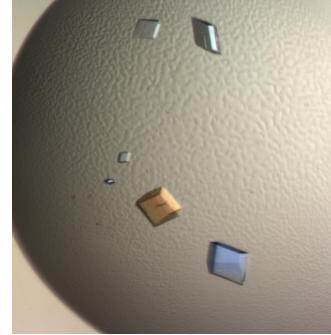
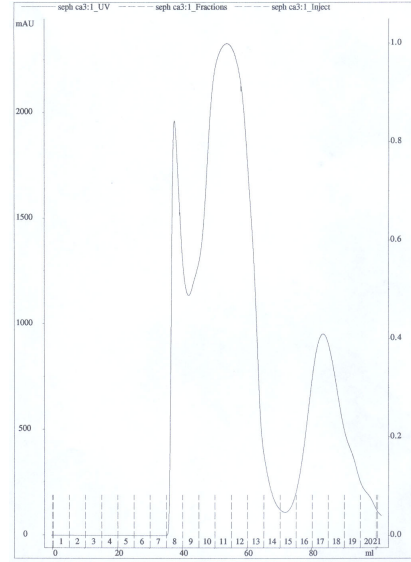
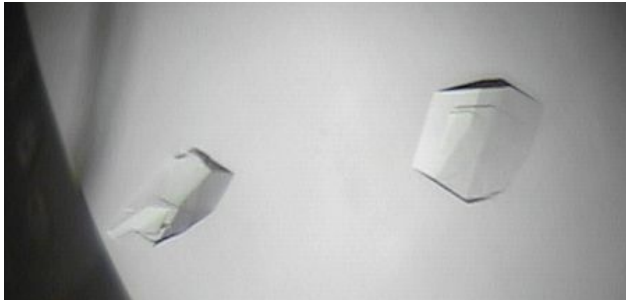
- High- and low-throughput screening
- Large volume crystallization
- Optimization (seeding, fine-screening, temperature)
- X-ray testing 100 K @ MAX lab (with LP3)
- Support for xtal mounting & H/D exchange for RT measurements

Chemistry lab lease



- SULF to move out in 2020
- DEMAX takes over payment of rent at that time (Admin is paying right now)
- The current lease runs from May 2018 – May 2023
- Cost: 600 000 SEK per year – incl H lab, office and lab
- Waste handling is set up with STENA
- Pay for NMR access (walk up fee with Red Glead), MS-service (LU)

Biological Deuteration & Crystallization



LUND
UNIVERSITY



- Co-located with LP3 in Biology Department (LU)
- Essential equipment in place to support both crystallization efforts and biodeuteration (equipment both ESS & LU)
- Crystal screening/data collection at Biomax through BAG with LP3

Biocryst lab lease



- DEMAX shares labs & office with LP3 in Biology Dept at LU
- The current service agreement runs until December 2020
- Cost: 180 000 SEK 2019, ramps up as we grow – incl lab, office, access to shared equipment
- Safety, waste, lab coats, dishes etc are handled centrally and are included
- Pay for ESI-MS service through collaboration with KI in Stockholm, MALDI-TOF at LU
- Research contract renewed for 24 months for 0.5 FTE from LP3 for Biodeuteration & Crystallization tasks (966 000 SEK for 2019 & 2020)

Council-approved initial operations budget – Covers DEMAX 2019 - 2020 (k€)

	2019	2020
Travel	10	10
Consumables	45	45
Premises (MV & LU)	35 & 44 (=79)	35 & 44 (=79)
Services (0.5 FTE LP3)	46	46
Equipment – BIOCRYST	20	20
Equipment - CHEM	20	30
Totals:	220	230

Labor costs not included here!

Staffing (as FTE) from 2019-2020

	2019	2020	2021
Chem + grants	3.0	2.0	2.0
Bio&Cryst + grants	1.5	1.5	2.5

- *Activities, collaborations and leveraged by external funding (see Hanna's talk for details)*
- *In reality – hands in the lab - we are ~ 1.6 FTE on DEMAX staffing budget for 2019. The rest (~2.9) of our staff costs are covered by external funds for R&D and collaborations (VR, SINE2020, B*2)*
- *Much of the activities overlap or complement DEMAX service*

SCIENCE SUPPORT
SYSTEMS

PREMP

FLUCO

TEFI

DEMAX

Call for Proposals Now Open

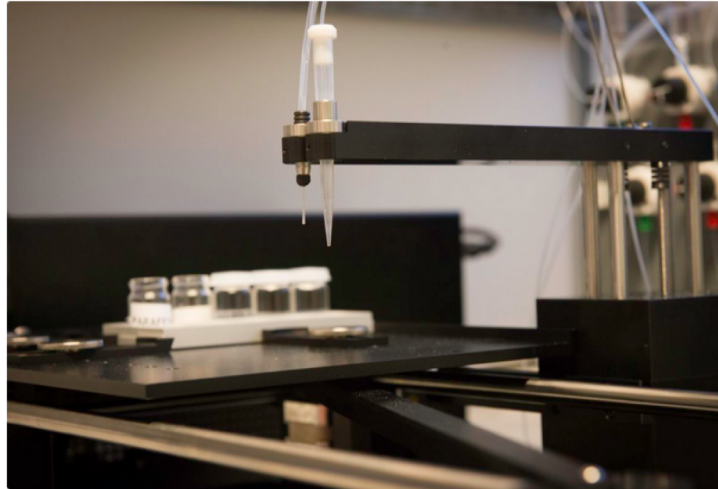
SULF

MESI

SCUO

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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 sciences and chemistry research areas. The relevant techniques that these communities use include: small angle scattering, reflectometry, single crystal diffraction, and spectroscopy. These classes of instruments are being built as part of the first eight instruments at ESS and have a science case that will benefit from DEMAX.

DEMAX offers three areas of support: Biological deuteration (e.g. cell paste, soluble proteins, lipids, membranes), Chemical deuteration (e.g. small organic molecules, surfactants, phospholipids), and Crystallisation (biological macromolecules e.g. proteins).

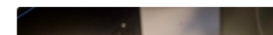
The hot commissioning of the first ESS instruments is planned for 2022, but DEMAX launches its initial operations for deuteration/crystallisation in 2019 in order to be ready to support first science at ESS. We kick-off with a pilot call for service requests with the ability to support a limited number of proposals. This will give us a chance to practice and refine our procedures while we are still establishing the labs and our methodological capabilities.

The deadline for proposal submission is **5 April 2019**

Delivery of materials/support will be between June and November 2019

More information, submission procedures, and registration is available after 24 February 2019 at: <https://demax.esss.se>

At this time, we offer a defined list of deuterated materials and services:



Anticipated service

- We should be able to to service 12-15 of the requests in first period
- Limited capabilities so we can't take all proposals and not too difficult
- Aim for a balance of easy and hard AND coverage across all three pillars

25 FEB – 5 APR	5 - 19 APR	19 APR – 6 MAY	06-19	07-19	08-19	09-19	10-19	11-19	12-19
PROPOSAL SUBMISSION OPEN	INTERNAL REVIEW	EXTERNAL REVIEW & NOTIFY	IN PROG	IN PROG	IN PROG	IN PROG	IN PROG	IN PROG	WRAP-UP, MAIL OUT, REPORT

As per STAP recommendation: Intend to send out user survey at the end to learn and improve

T&Cs for support:

- Free of charge (except S&H) to users during 3 pilot cycles ('19-'21)
- Access not limited to ESS-member states – all can apply
- Access granted on both Technical/Safety/Feasibility (internal) and Scientific Peer (external) review
- Customer should demonstrate awarded beam time, draft beamtime proposal, or demonstrate intention to apply for beamtime
- DEMAX has to be acknowledged in any resulting publications

Materials and services offered:

- Deuterated bacterial cell paste
- Purified recombinant proteins
- Yeast-derived total lipid extract
- Fatty alcohols/halides/thiols, lactic acid
- Saturated fatty acids and oleic acid
- Surfactants (e.g. sugar, amino acid)
- Support for large crystal growth (large volume optimization in vapour diffusion & dialysis, temperature control, fine-screening and optimization)

As per STAP recommendation: we encourage users to ask for things we don't advertise so we can track what the user community wants and respond to their evolving needs.

Next steps

- Proposal review – internal & external
- Notify users of acceptance or not
- Internal/ongoing planning of proposal execution
- Execute on grant deliverables, collaborations
- Aim to wrap up pilot run by end of November, ship out final materials
- Compile a report

KPI for DEMAX initial ops – and beyond?

- No. of users
- No. of proposals received in total
- No. of proposals received by "pillar"
- How many neutron experiments are done with materials we supplied
- Publications
- How much deuterated material we supplied (no. of unique small molecules, no. of proteins, no. of crystals)
- No. of proposals we execute
- Industrial interest (how to track?)

Short-term issues:

- Pilot call for proposal, initial ops process
- Survey (contents)
- SULF will move out – equipment, lab organization

Medium-long term issues

- How to best bridge bio & chem deuteration activities (with regards to yeast, algae, bacteria – beyond extracting proteins or providing biomass)
- Competence and timing requirements for next recruitment (less specific...)
- Cost of MV lab space higher than anticipated – we need to find a way to reduce the cost or find alternate space (beyond 2023)
- Please comment on future DEMAX location possibilities and implications