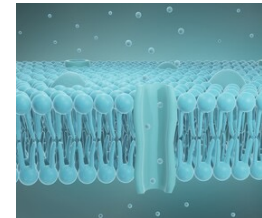
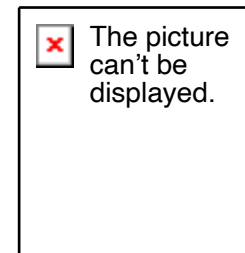
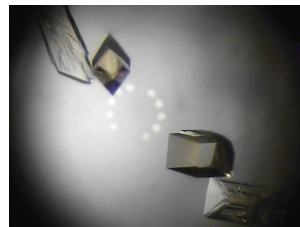


# The Deuteration & Macromolecular Crystallization platform at ESS

Dr. Zoë Fisher

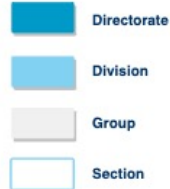
Team lead for the DEuteration & MACromolecular Xtallography Platform ([DEMEX](#)) at ESS

Snr. Adjunct lecturer at Biology Department, Lund University



# DEMAX overview

- Established in 2019, DEMAX is the ESS user support lab that offers deuteration and crystallization service & support
- We support the chemistry, life science, and soft matter community with access to deuterated materials and (large) protein crystals
- Goal is to help users get the appropriate samples to do meaningful & advanced neutron experiments



**EUROPEAN SPALLATION SOURCE ERIC**  
 Helmut Schober  
*Director General*

QUALITY & COMPLIANCE  
 DIVISION (81710)  
 Mattias Skafar

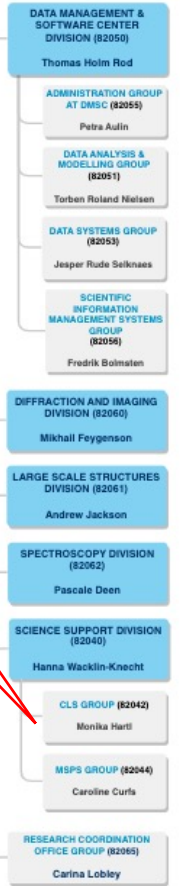
ESH & SECURITY DIVISION (81700)  
 Ola Dahlborg  
 OCCUPATIONAL HEALTH,  
 SAFETY & ENVIRONMENT  
 GROUP (81722)  
 Helen Boyer  
 RADIATION PROTECTION  
 GROUP (81723)  
 Per Roos

**SCIENCE DIRECTORATE**  
 (82000)  
 Giovanna Fragneto

**OPERATIONS AND  
 MACHINE DIRECTORATE**  
 (83000, 71000)  
 Kevin Jones

**PROJECT DIRECTORATE**  
 (8800091)  
 Andrew Kimber

**ADMINISTRATION DIRECTORATE**  
 (84000)  
 Anders Ihr



DEMAX is part of the CLS group

# DEMAX Platform



## Chemical Deuteration

- Small organic molecules, monomers
- Lipids (e.g. POPC), surfactants (e.g. sugar-based), detergents (DDM)
- Aldehydes, alcohols, acrylates etc.
- Novel organic molecules for various applications



## Biological Deuteration

- Deuterated biomass from *E. coli*, *B. braunii*, *P. pastoris*
- Recombinant soluble proteins, plasmid DNA, “other”
- Yeast-derived lipids (total, phospholipid)

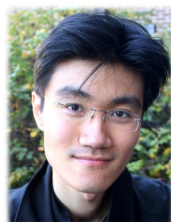


## Protein Crystallization

- High- and low-throughput screening
- Fine screening in large volumes
- Support for room temperature crystal mounting & data collection
- X-ray testing (LU BAG at MAX lab)



Anna



Jia-Fei



LP3  
0.7 FTE



D-lab (lipids)  
0.2 FTE

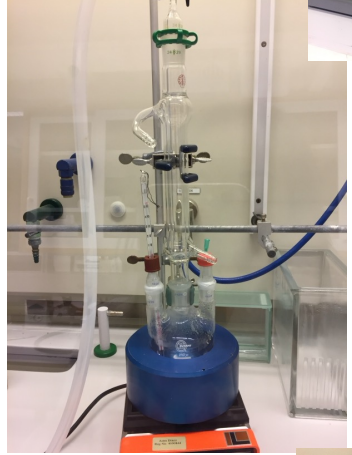
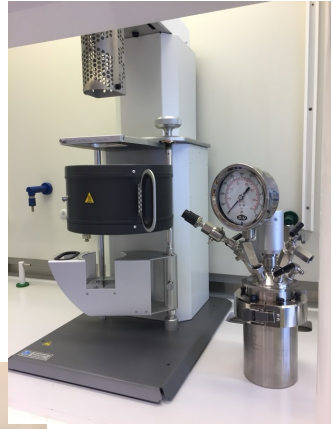
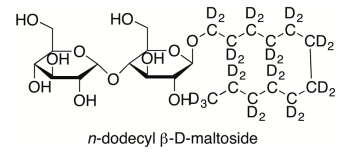
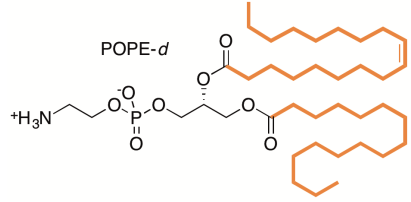
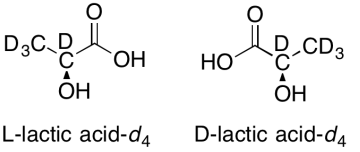


Zoë

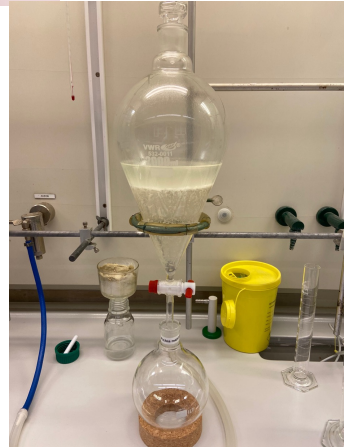
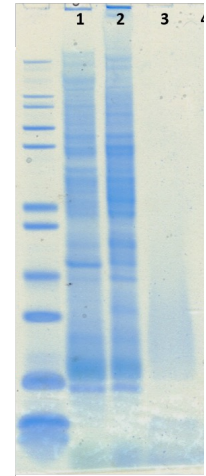


# Different kinds of deuteration: chem vs. bio

- Chemical deuteration:** organic synthesis of small molecules using either commercial deuterated precursors and deuterated solvents, or make the precursors/monomers in the lab using Parr reactor (pressure, temp, catalyzed H/D exchange).



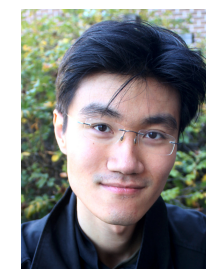
- Biological deuteration:** production of molecules under deuterated conditions in living cells (e.g. yeast for lipids, bacteria for protein/DNA, algae for cell extract preparation). Prepare cell culture media in D<sub>2</sub>O and feed cells d-labeled carbon source (e.g. glycerol)



# Chemical Deuteration



Anna



Jia-Fei



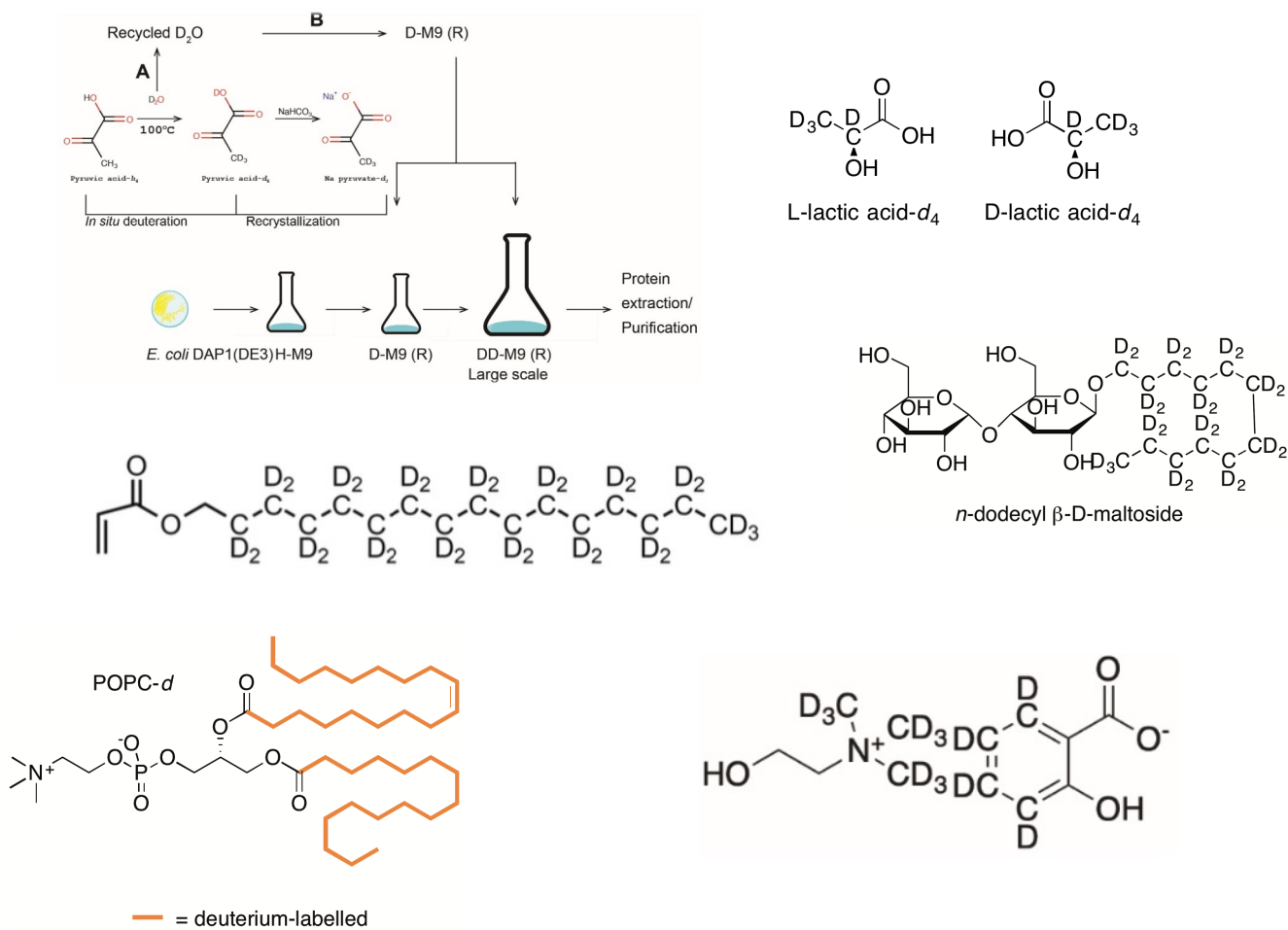
- Moved to ESS in June 2023
- Lab is up and running with essential equipment is in place for synthesis, separation, characterization.
- For some characterization needs (e.g. NMR) we have service arrangements with Red Glead & LU Chemistry.
- *In progress: Advion ESI-MS*



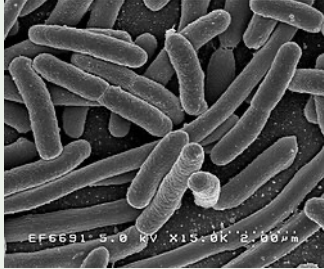
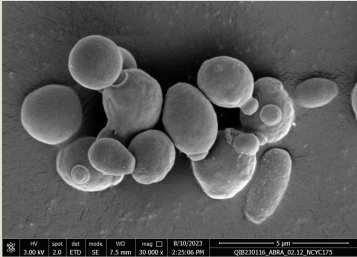
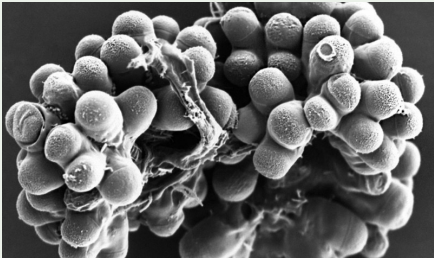


# Deuterated organic molecules

H/D exchange, chemical & enzymatic synthesis of a range of small molecules  
(surfactants, monomers, alcohols, aldehydes, lipids, fatty acids etc.)

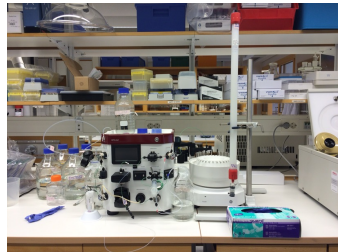
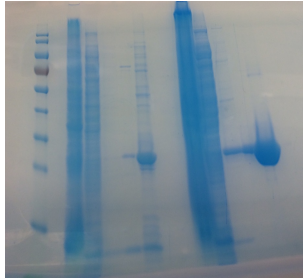


# DEMAX offers biodeuteration from following:

<p><b>Bacteria</b> Escherichia coli (E. coli)</p>	<p>prokaryote</p> 	<p><b>Recombinant proteins</b> <b>Plasmid DNA</b> <i>(cellulose)</i></p>
<p><b>Yeast</b> Pichia pastoris (P. pastoris)</p>	<p>eukaryote</p> 	<p><b>Lipids (total, phospholipid)</b> <i>(membranes, ergosterol, cholesterol)</i></p>
<p><b>Algae</b> Botryococcus braunii (B. braunii)</p>	<p>eukaryote</p> 	<p><b>Total cell extract</b> <i>(lipids, oil, exopolysaccharides)</i></p>

\*All of these can tolerate up to ~99% D

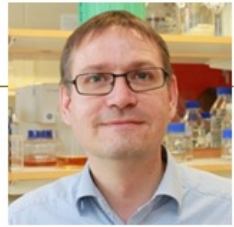
# Deuterated biomolecules



Zoë



LP3 0.7 FTE



Wolfgang

- Essential ESS equipment in place, access agreement to be able to use LP3 labs & equipment
- LP3 research engineer supports some tasks related to biodeu (Swedish in-kind)
- Produce full or partially d-labeled biomass, proteins & DNA
- Yeast-derived lipids



Hanna



Sophie

- Check protein purity, yield (SDS-PAGE, UV/Vis), biophysical characterization tools for proteins (SEC-MALS, NanoDSF)

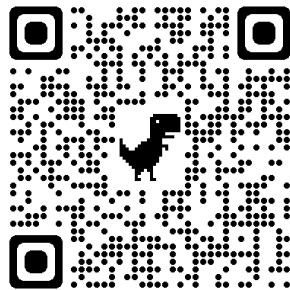
# DEMAX product catalogue

[demax@ess.eu](mailto:demax@ess.eu)

- Updated product catalogue is available on the DeuNet website

<https://deuteration.org/demax/>

- Also includes instructions for the dry shipper we use for sending perishables



## Deuteration and Macromolecular Crystallisation Platform

### Product List & Sample Shipping

August 2023

Biological: proteins, biomass, nucleic acids.....	2
Biological: purified lipid mixtures .....	2
Chemical: carboxylic acids, aldehydes, alcohols, alkyl halides.....	3
Chemical: surfactants .....	4
Chemical: phospholipids.....	6
Chemical: aromatic & heterocyclic aromatic molecules .....	7
Chemical: miscellaneous .....	9
Crystallisation support: .....	10
About DEMAX: .....	10
Shipping of perishable sample to/from DEMAX.....	11



# DEMAX Access

- Users have to submit a proposal.
- Proposal are subject to internal feasibility review and scientific (peer) review by a DEMAX panel.
- Access is free (for now) and granted upon acceptance of the proposal.
- In addition to user service, we also participate in collaborative projects & support other groups at ESS if needed.

# User proposals

- Rolling access is currently open until end of September 2024
- Users should register and submit proposals online
- Access is merit based not restricted to member nation status (for now).
- Co-authorship vs acknowledgement

ESS European Spallation Source

User Office / Dashboard Logge

**Welcome to the ESS User Office Software**

**Now Open: Rolling access.**

DEMAX is now extending Rolling Access for proposals requesting support for chemical & biological deuteration as well as support for protein crystallisation

For a list of molecules/support, please see our product catalogue [here](#).

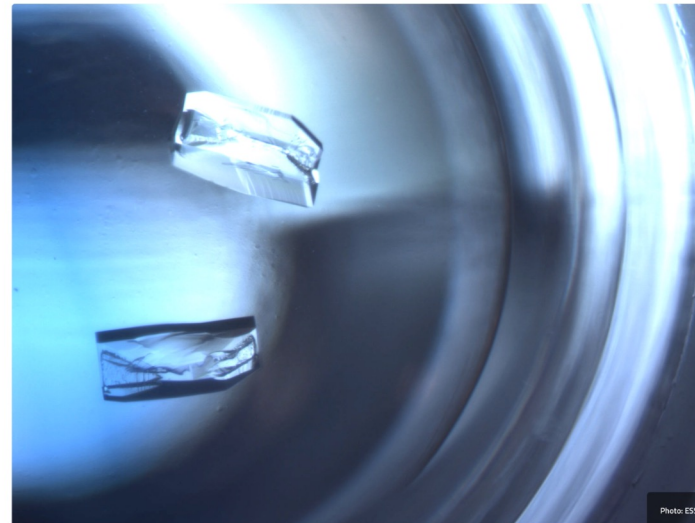
We strongly encourage users to reach out at [demax@ess.eu](mailto:demax@ess.eu) to discuss their project needs prior to submitting a proposal.

If you are interested in something that you don't see in the catalogue, please reach out to us at [demax@ess.eu](mailto:demax@ess.eu). We can do a feasibility review and see if it possible or we may be able to help through the Deuteration Network.

1st November 2022, 17:00 (CET): Rolling access opens  
 30th September 2024, 17:00 (CET): Rolling access closes  
 20th December 2024, 17:00 (CET): Final delivery of molecules

## Pilot call for chemical and biodeuteration support from the DEMAX platform

JANUARY 10, 2022



The Deuteration and Macromolecular Crystallisation (DEMAX) platform at ESS supports neutron users from the soft matter, biology, life sciences and chemistry research areas. The neutron techniques that these communities typically use include small angle scattering, reflectometry, single crystal diffraction, and spectroscopy. For steady state ESS operations, DEMAX is currently developing 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 (large protein crystal growth).

The following conditions apply to all DEMAX proposals:

Proposals must be submitted and fully completed online at ESS User Office portal: <https://useroffice.ess.eu>

Proposals will undergo technical and internal scientific review.

Users are responsible for the cost of charge.

Proposals may be submitted for materials at another neutron scattering facility (e.g. attach approved beamtime proposal).

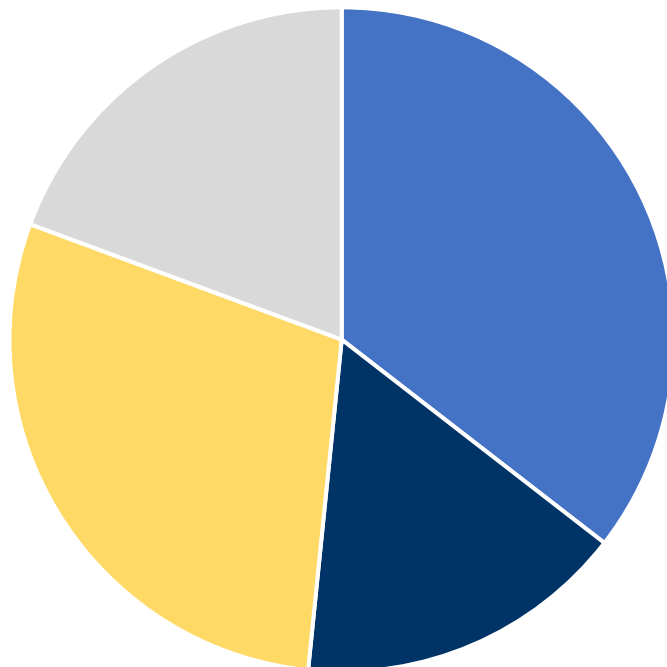
Users are responsible for the cost of charge, but we may ask that users pay for shipping & handling for dangerous good (e.g. dry

ice) if not acknowledged in any publications. Please read the publication guidelines [here](#)

The pilot call runs from 1st November 2022 to 30th September 2024 and has no specific deadline for proposal submission. We will aim to deliver all approved proposals by 20th December 2024 and inform users if we can support their work as soon as possible after review.

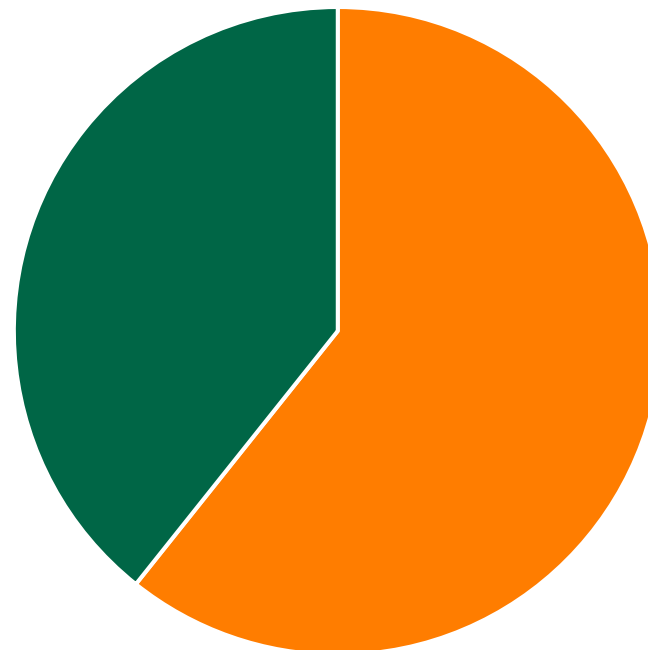
- Since starting (2019) we have now over **100 unique users**
- DEMAX has published or has under review **40 papers in peer-reviewed journals**
- In call 2b + Rolling Access we have received **31 proposals requesting 54 molecules/services** (accepted 28 proposals to deliver 48 molecules)

Intended neutron scattering technique



■ SANS ■ NPX ■ NR ■ Other

Type of deuteration required



■ Chemical deuteration ■ Biological deuteration





# Thanks to DEMAX, & LP3 & ESS



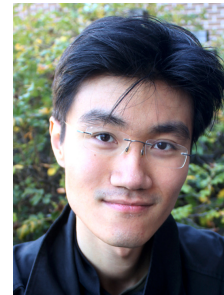
Anna Leung



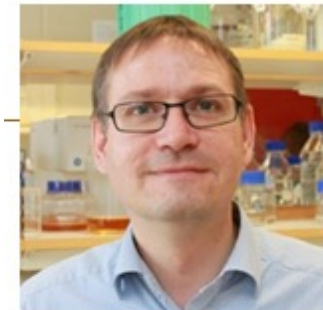
Zoë Fisher



Hanna Wacklin-Knecht



Jia-Fei Poon



LUND UNIVERSITY

Wolfgang Knecht



Vetenskapsrådet



LP3 research engineers

