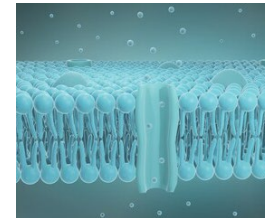
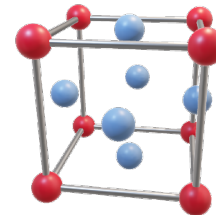
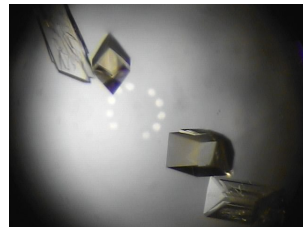


DEMAX

The Deuteration and Macromolecular Crystallization Platform



DEMAX overview

- DEMAX is the team at ESS that offers deuteration and crystallization service & support within the CLS group
- *Goal: Enable high impact science on ESS instruments in life science, soft matter, chemistry*
- We operate on a peer review proposal system, but also collaboratively for method development and scientific research



EUROPEAN SPALLATION SOURCE



DEMAX Platform



Users can collaborate with us, get advice + access to expertise (us and within DeuNet)



Chemical Deuteration

- Small organic molecules, monomers
- Lipids (e.g. POPC, SOPC, POPE)
- Surfactants (e.g. sugar-based)
- 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)

Extended team
(incl postdocs & tech support
From LP3/LU)



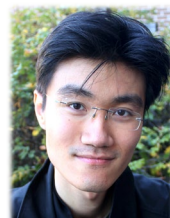
Zoë



Anna



Hanna



Jia-Fei



Jenny



Sophie

+



0.75 FTE

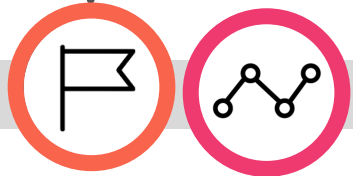
LU/LP3



LUND UNIVERSITY


**Formed a group
& initial ops**


2019Q2



2019Q1

Pilot call 1




**Pilot call 2a
(+ Covid call)**

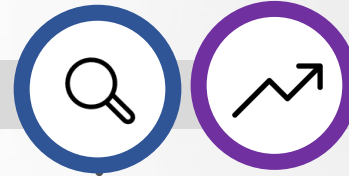


2020


Rolling access



2022Q2



2022Q4

Pilot call 2b



Lab move



2023Q1

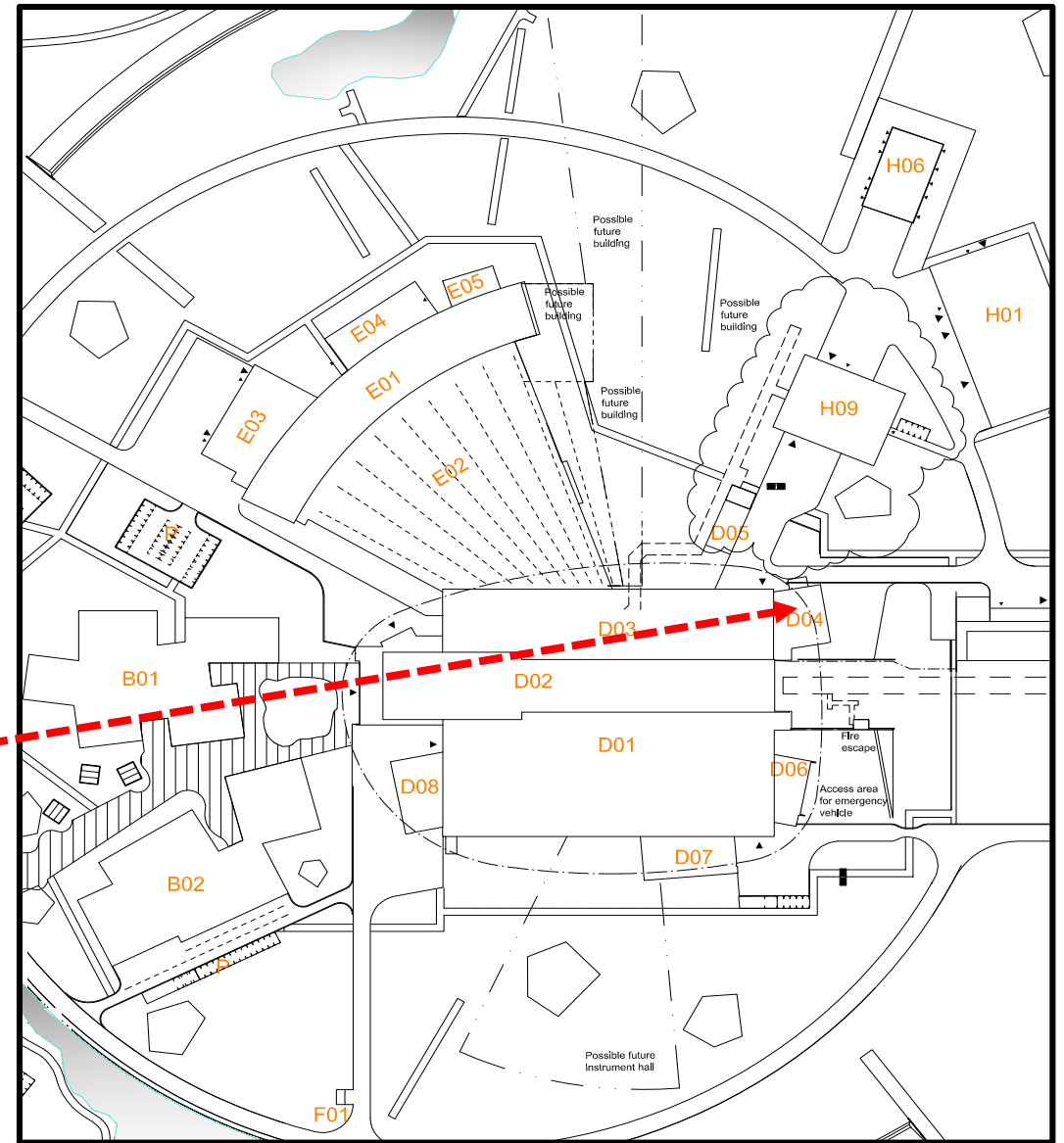
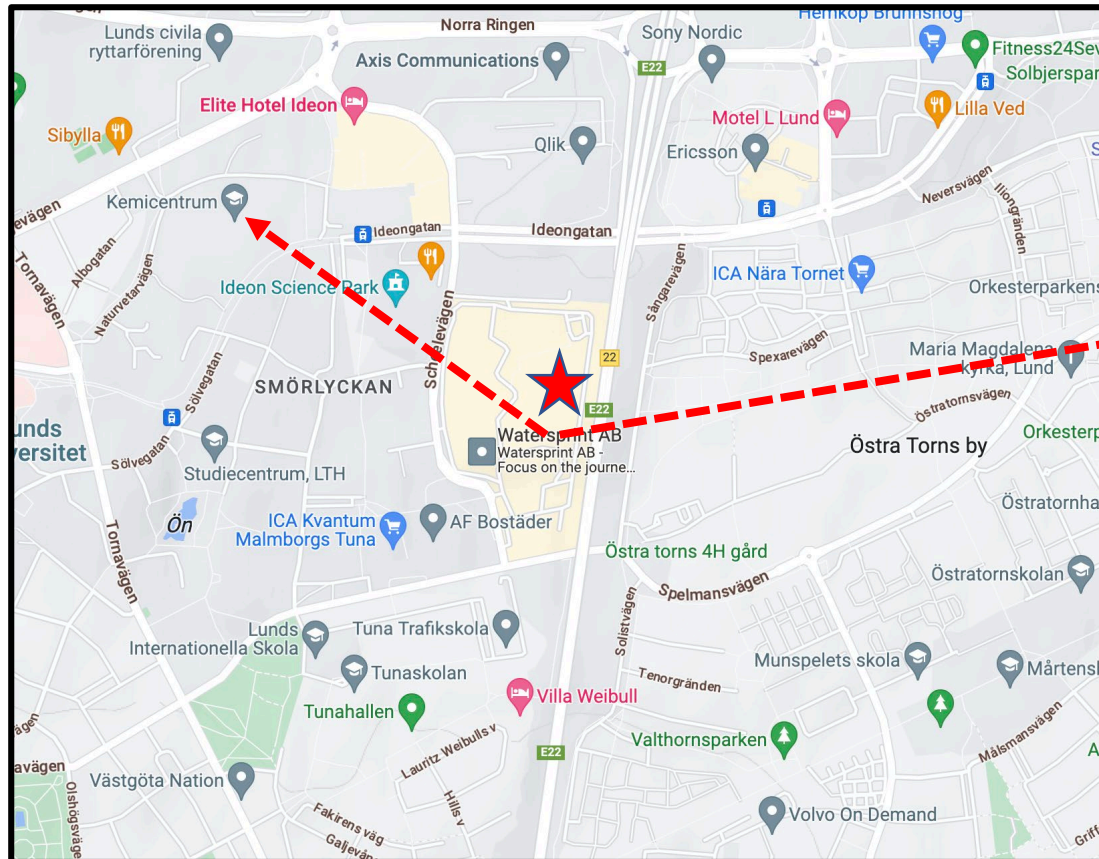


2023Q2

**Team
expansion**



Chemistry lab move 2023



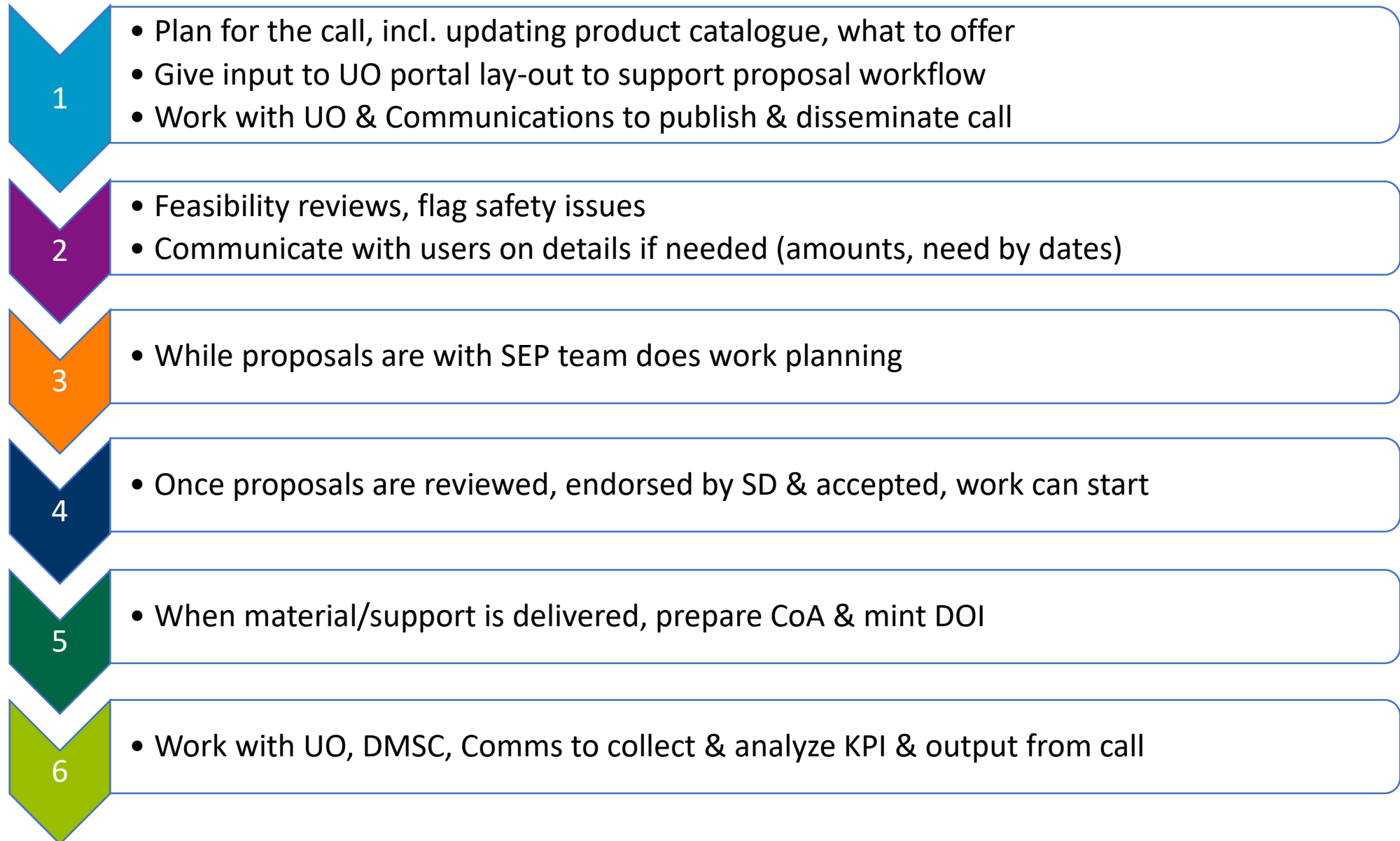
Chemistry lab move 2023

- MAY 2023: Yeast lipid activity will temporarily move to Chemistry Dept at LU (Sophie, Hanna, Jenny)
- JUNE 2023: The rest goes to D04 (Jia-Fei, Anna, Zoe helping)
- End of May: cease lab work to allow time for cleaning/sorting/packing
- Expected downtime: 5-6 months (incl. moving time, unpacking, setting up basic services)
- Goal: up and running smoothly by October

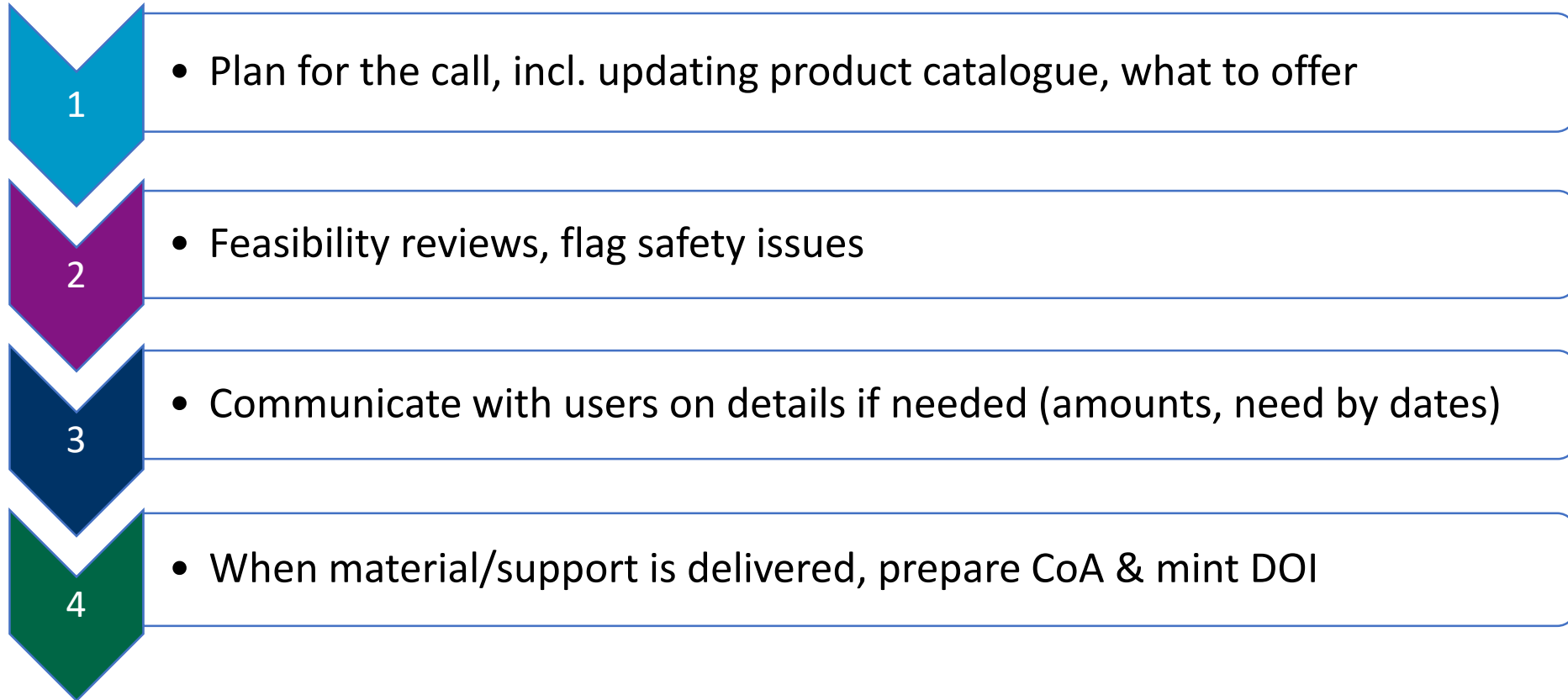
Bio & cryst lab activities

- Biodeuteration & crystallization activities are co-located at Biology dept at LU (specifically with the LP3 under Wolfgang Knecht)
- 2 contracts that underlie our collaboration: 1) Access agreement (2021-2025, ~ 23 kEuro/yr, grants us access to centralized services, LP3 or departmental equipment, and also space to put ESS equipment), 2) “DLS” (Swedish in-kind 2023-2025, ~77 kEuro/yr for deuteration lab services, effectively we get 0.75 research technician support towards general lab help, cell culture, and X-ray data collection at BioMAX)
- Both expire 2025 and we would like to continue. Many synergies and benefits but it is not cheap (100+ kEuro/yr)

NOW: Proposal workflow within DEMAX team



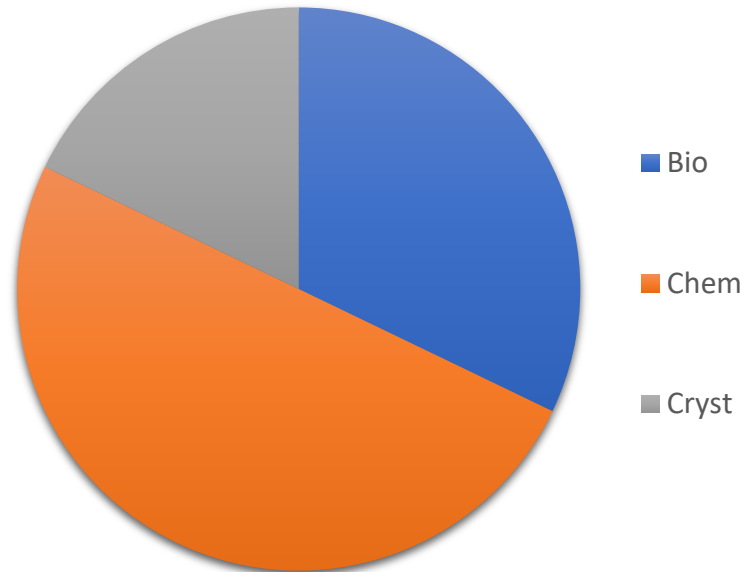
Future vision: simplify & integrate workflow



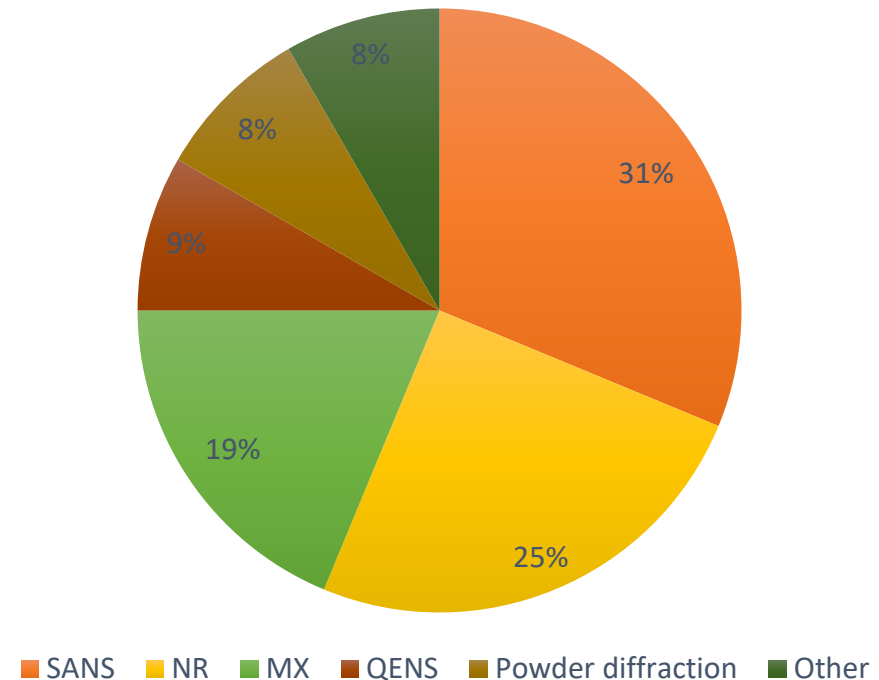
2022 3rd Proposal Round + Rolling Access

- 23 proposals received and assessed, asking for 43 materials/support
- A few are internal proposals for making stocks e.g. oleic acid & POPC
- In addition, weekly e-mail enquiries on various molecules (e.g sphingomyelin, cellulose)

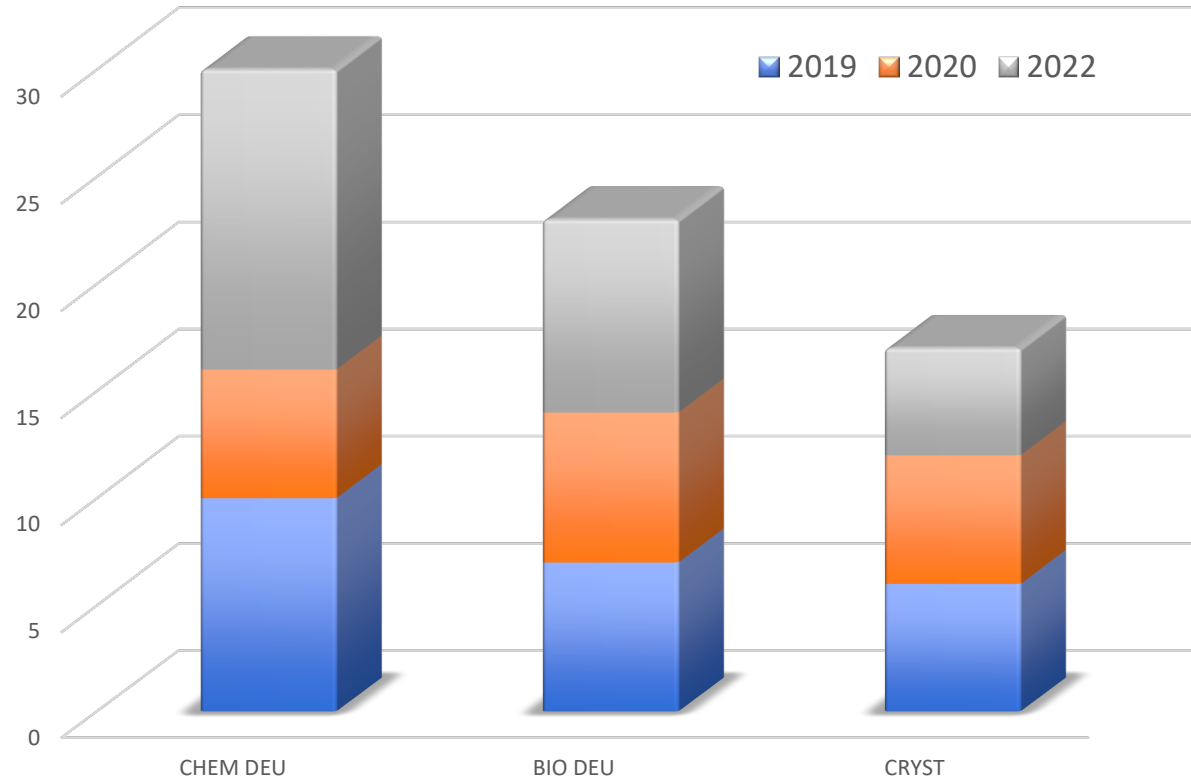
DEMAX support requested



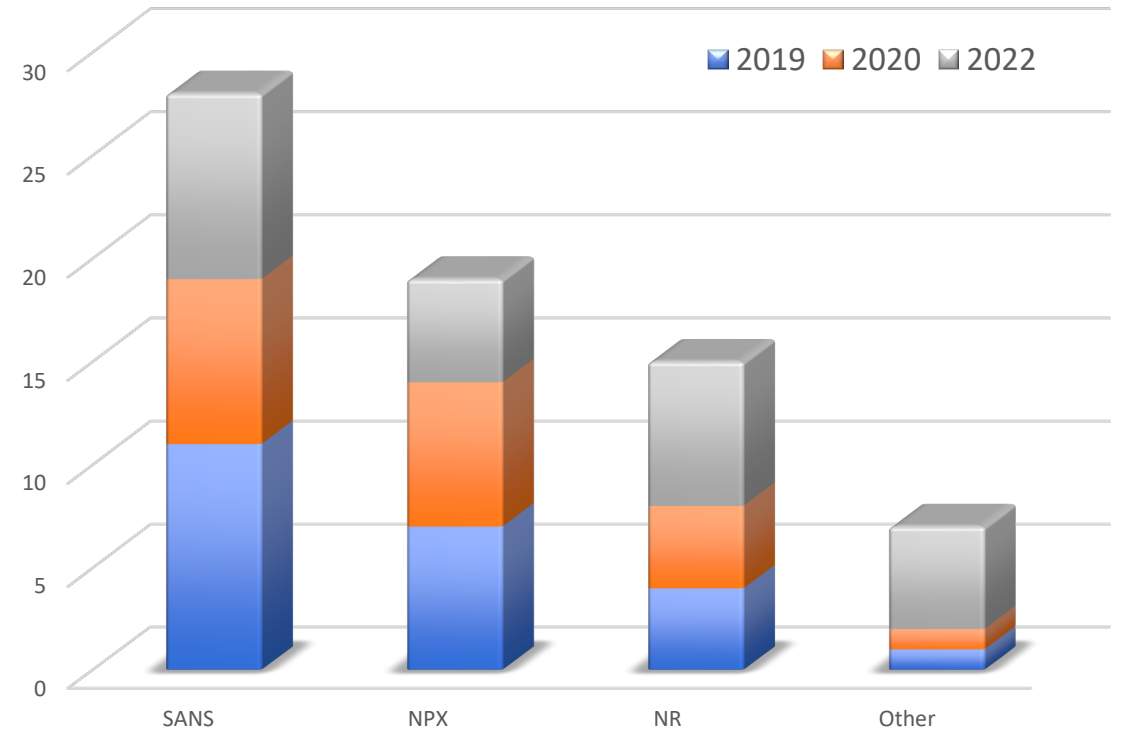
Intended neutron method 2022 + RA



Proposals by DEMAX area



Intended neutron method



- 59 proposals, 60 unique users, 9 molecules requested
- 28 papers in print (3 under review) since entering ops in 2019

DEMAX product catalogue

- Product list updated in 2023, will soon be available on the DeuNet website

- Older version :

<https://deuteration.net/2021/11/24/deuteration-and-macromolecular-crystallisation-demax-at-ess/>

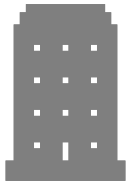
Talk to us!
demax@ess.eu

Deuteration and Macromolecular Crystallisation Platform

Product List

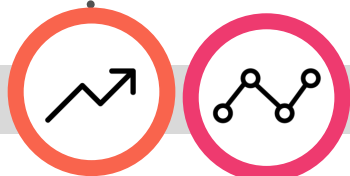
February 2023

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



D04 lab up and services running!

2023 Q3



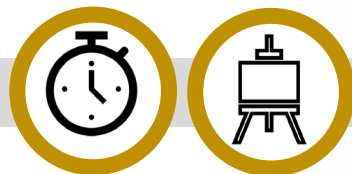
2023 Q4

Finalize current proposals from call 2'b'



Continue with rolling access, commission labs

2024



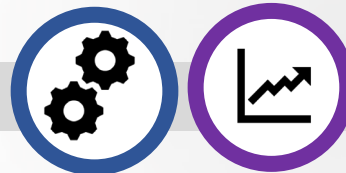
2024 Q4

Prepare call for FS



Team expansion - biodeu

2025



2025

Deliver on FS proposals

Friendly users

2026



User program!

2027



Expanding the team in 2025

- Staff ramp-up plan includes 1 FTE “biodeu” to join in 2025
- 1 FTE ESS biodeu specialist can focus on cell culture and protein & lipid purification, with emphasis on lipids (on-site)
- Complementary support from 0.75 FTE research engineer from LP3 to support the rest incl. cell culture, emphasis on protein/DNA purification, biophysical characterization, X-ray beamtime support (part of LP3 team at LU)

Questions:

- How do we balance “standard” request (things we have made before) vs. R&D type projects (that may be exciting and new, how do we meet expectations)
- E.g. organic cations, sphingomyelin, cellulose will all be new, development projects that will require a significant time commitment from DEMAX staff (12+ weeks) – but maybe it is important and exciting!?
- Our current contracts with LP3/LU only go until 2025 (both for DeuLabService & access agreement) – how do we continue with this mutually beneficial arrangement with increasing pressure to consolidate activities on-site and to save money?
- How do we establish DEMAX-biodeu support “in house” while also relying on LP3 for continued biodeuteration/protein biochemistry support?

Thanks to DEMAX, & LP3 & ESS



Hanna Wacklin-
Knecht



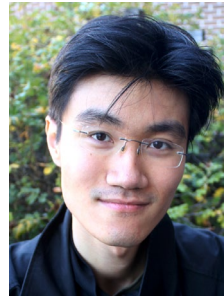
Anna Leung



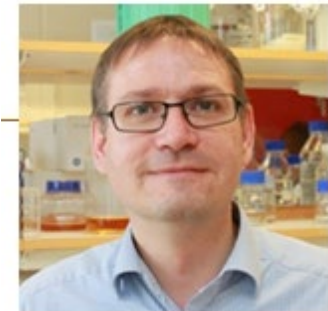
Zoë Fisher



Jenny
Andersson



Jia-Fei Poon



Wolfgang
Knecht



Vetenskapsrådet

