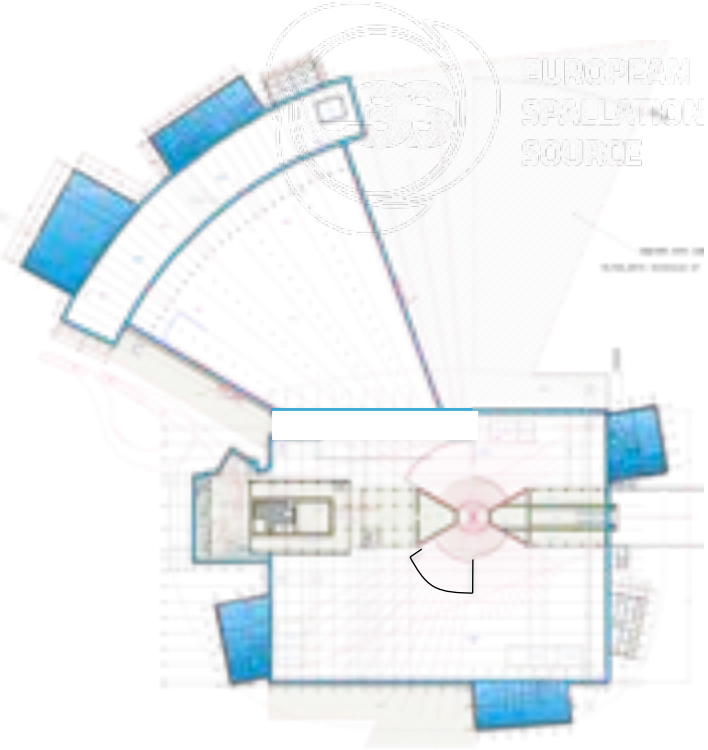
Science Support Systems: general user support labs, support labs for deuteration & crystallization



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Outline

EUROPEAN SPALLATION SOURCE

Summary of general user labs planned for ESS site.

- Current status of lab fit-out plans
- In-kind update

Summary of DEuteration MAcromolecular Xtallization user support labs

- Current status, future plans
- In-kind update

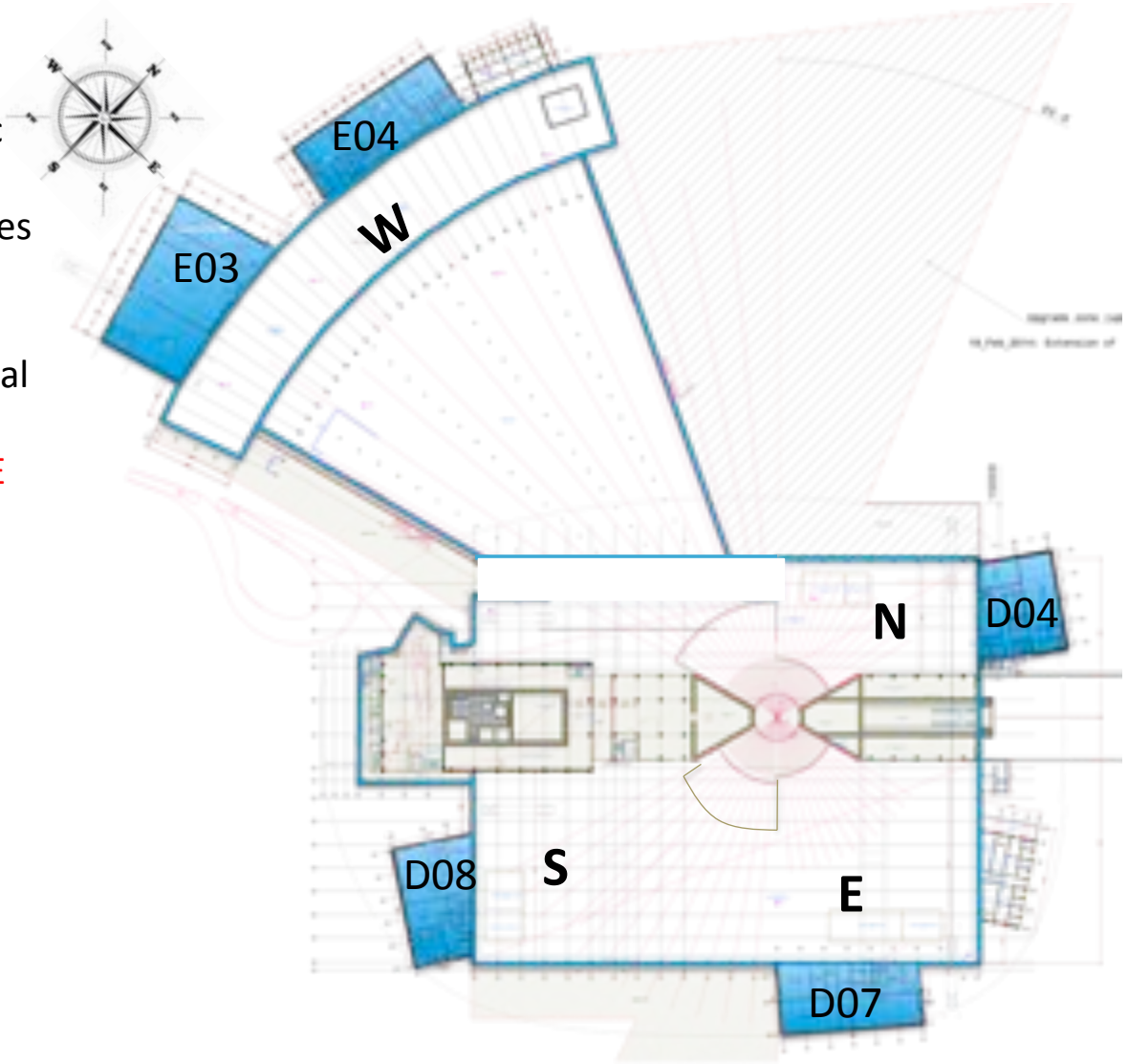
Instrument layout & user lab availability

W1 NMX
W2 Beer
W3 C-Spec
W4 Bifrost
W5 Miracles
W6 Magic
W7 T-Rex
W8 Heimdal

N1 HR-NSE
N5 Freia
N7 Loki

E1 Estia
E7 Vespa
E8 Skadi

S2 Odin
S4 Dream
S11 Vor



D04
1 × LS/SCM
1 × cold room
2 × support room

D07
1 × LS/SCM
1 × cold room

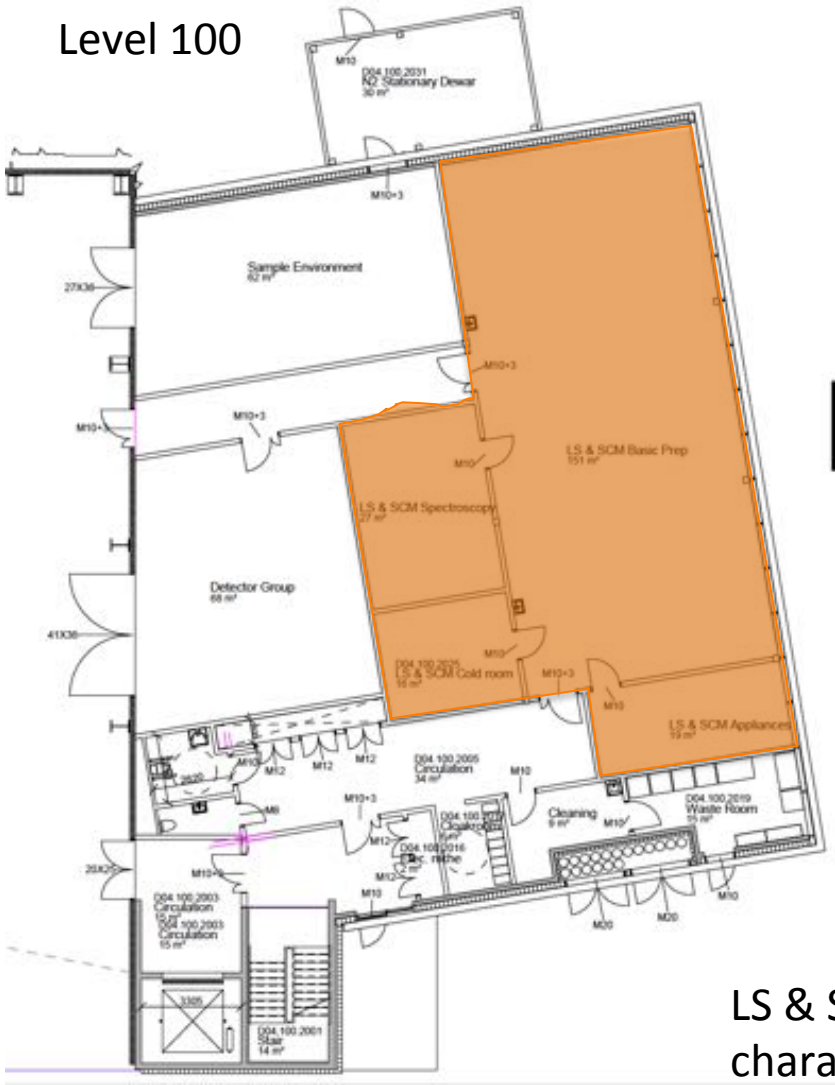
D08
1 × RML
1 × Basic chemistry
1 × Sample storage facility

E03
1 × Engineering

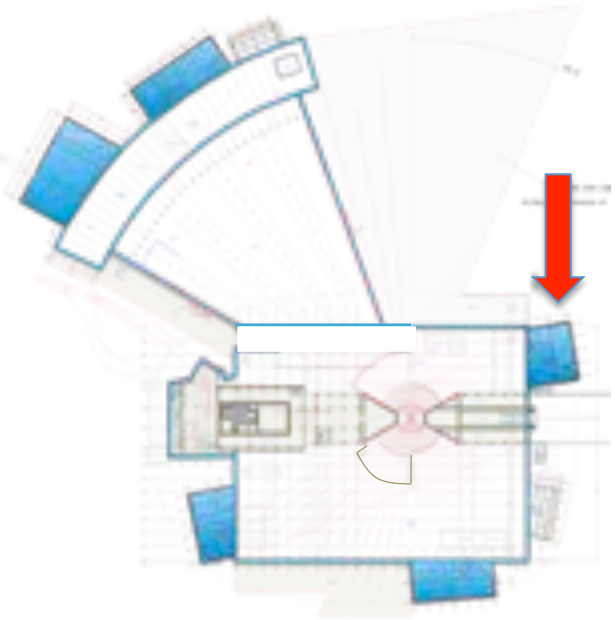
E04
1 × LS/SCM
1 × cold room
1 × support room
1 × Basic chemistry
1 × physical characterization

15 general user labs that will be outfitted during construction for hot commissioning (~2019)

Level 100

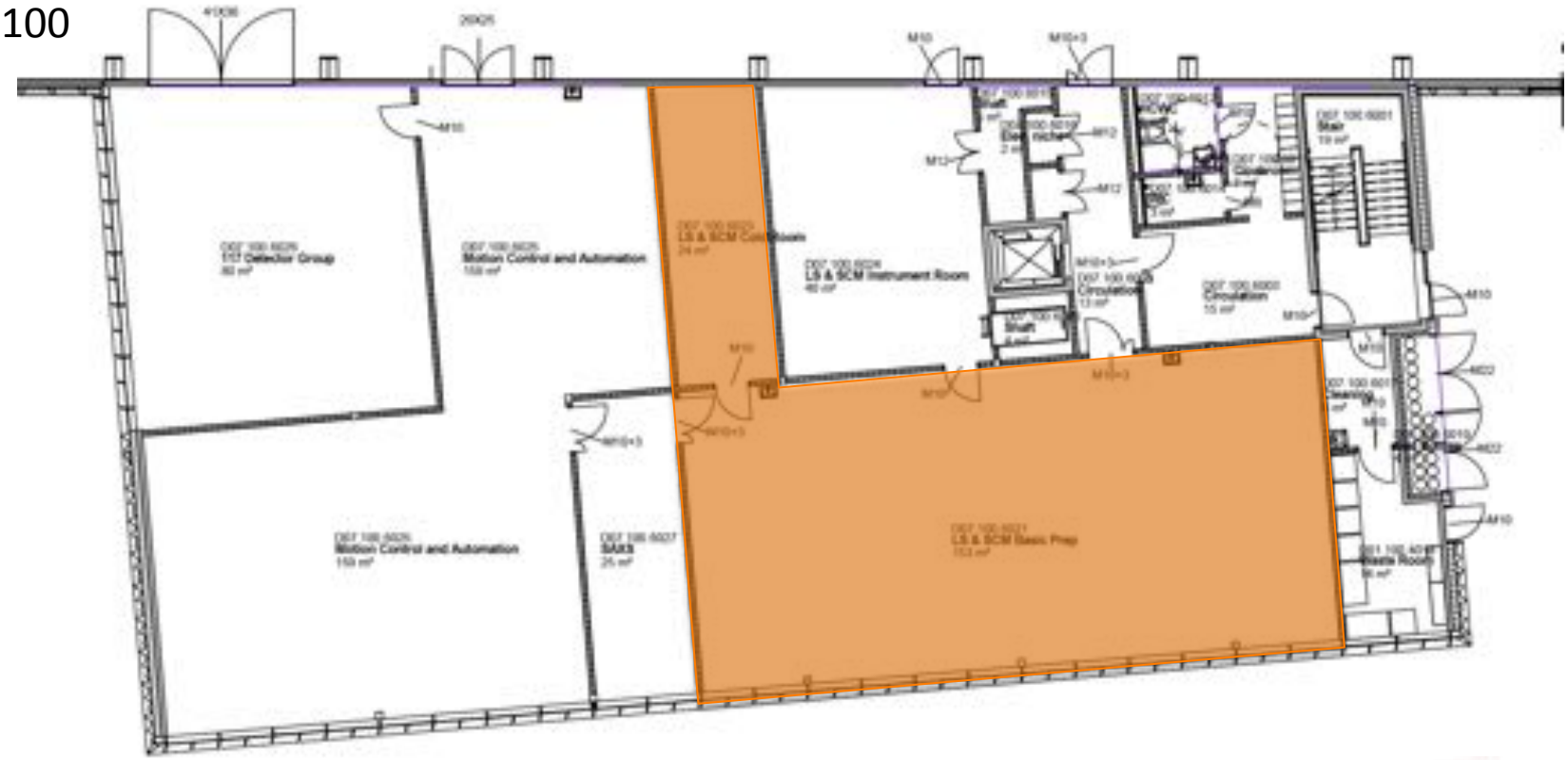


D04



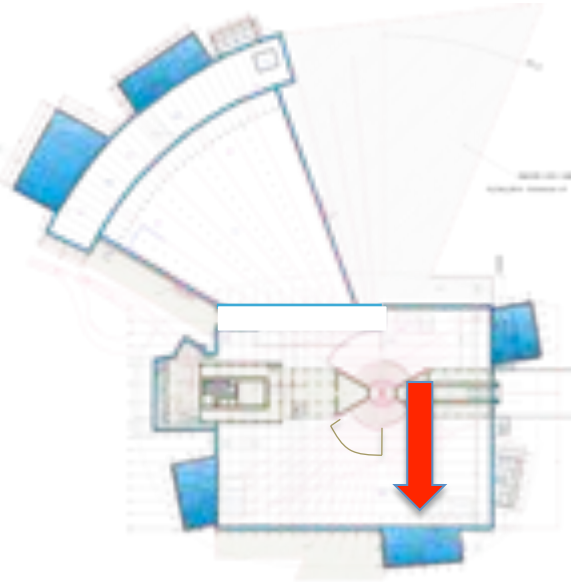
LS & SCM (basic prep, characterization), cold room

Level 100



LS & SCM (basic prep), cold room

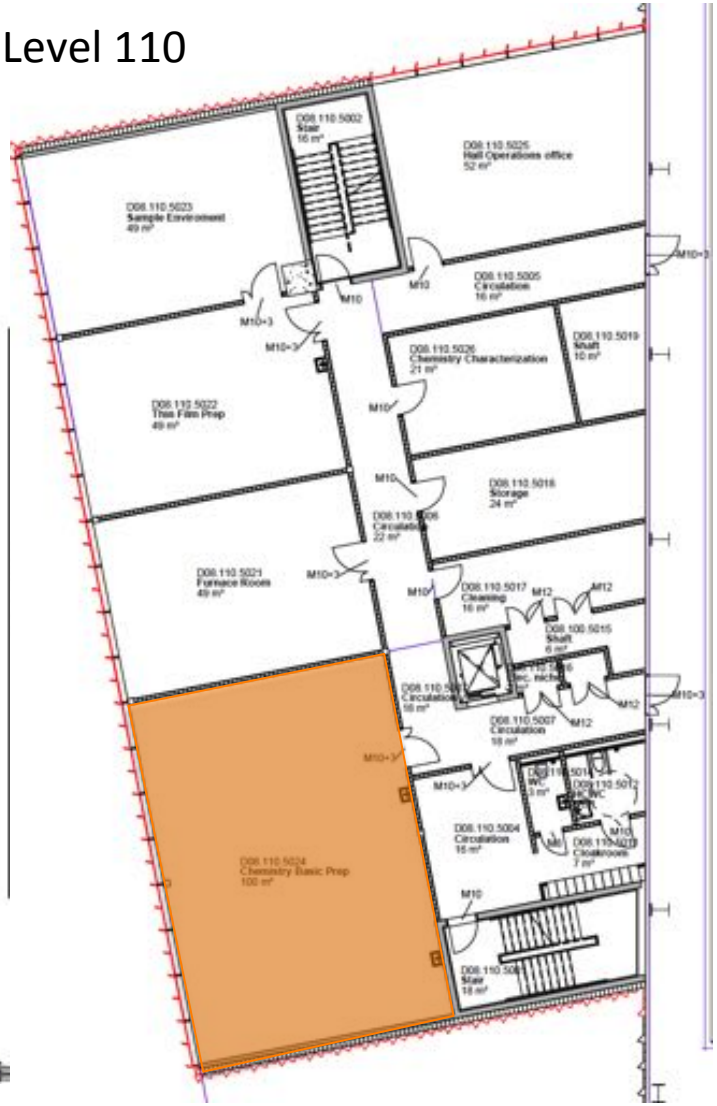
D07

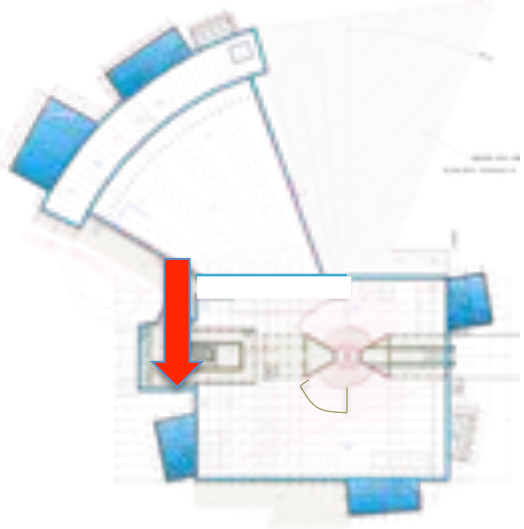


Level 100

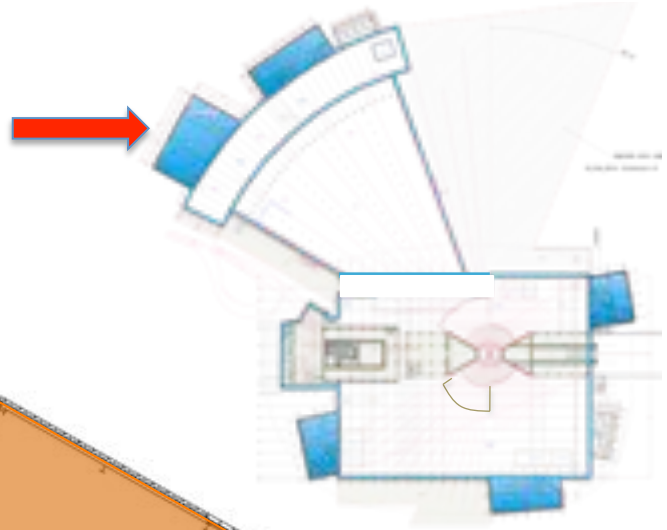
Level 110

D08





Radioactive Materials Lab, sample storage, chemistry basic prep



Engineering lab

Level 100

E03

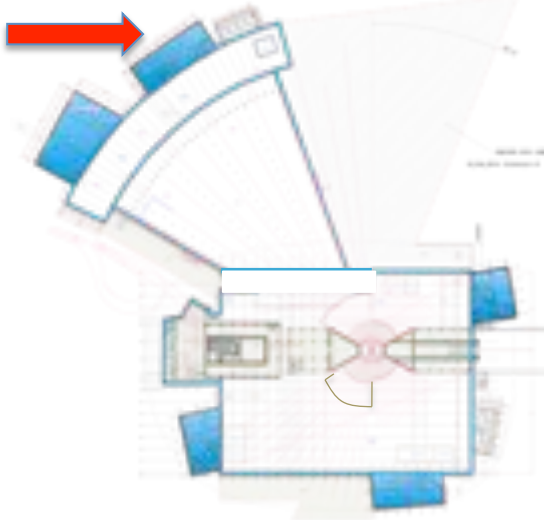
Level 110

E03

Level 100

LS & SCM labs, chemistry, basic prep, physical characterization

Level 110



Labs UK IK contribution

EUROPEAN SPALLATION SOURCE

- **Background:** SAD is charged with *delivering functional user labs* for Sample Handling and General Use Labs and Facilities.
- **Purpose:** To *outfit user labs* in the areas of chemistry, physics, soft matter and life sciences in D & E building (RML and Engineering excepted)
- **Scope:**
  - Determine the needs of ESS users for laboratory facilities, space, equipment and consumables.
  - Review the detailed design and layout of the laboratories (including utility needs)
  - Engage a lab contractor to design labs, purchase materials, and install lab furniture (incl. fumehoods, extraction, storage, benches)
  - Includes basic laboratory equipment

Labs for deuteration & macromolecular xtallization (DEMAX)

EUROPEAN SPALLATION SOURCE

- Core mission: to deliver user support labs, access, expertise for chem/bio deuteration and protein crystallization for users in the fields of soft matter & life science research (MX, NR, SANS etc.).

- Aim to be ready by 2019 to start hot commissioning and pre-operations activities.

LU & DEMAX collaboration

- To realize our mission we are pursuing a collaborative partnership with LU (spec. the LU Protein Production Platform, LP3). ESS & LU have a signed MoU and we are now negotiating bench fees & services for a formal partnering starting in 2016.

LP3
Lund Protein-Production Platform

http://www.biology.lu.se/services/lp3-lund-protein-production-platform

LUND UNIVERSITY

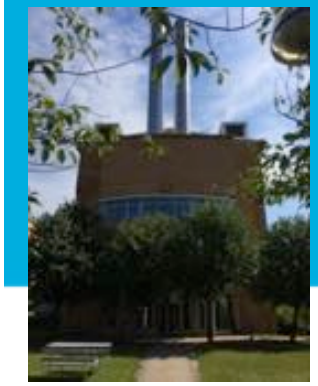
MAX IV LABORATORY

http://www.biology.lu.se/services/crystallization-facility

Partnership with LP3 and CF at LU

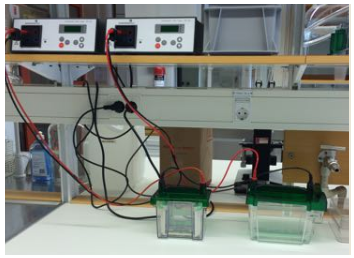
- DEMAX will be co-located with LP3 & (former MAX lab) CF in Biology Department @ LU.
- Easily accessible to ESS site by bus (~7 min).

- Staffing: currently 1 + 0.3 scientists. By 2023 we are planning for 2 FTE research engineers and 2 FTE scientists.



Current: DEMAX

- Housed in a shared ~100 m^2 rented lab in Medicon Village.
- Run a basic lab for protein characterization and crystallization.
- We are planning to expand and offer a full range of screening and optimization tools – with the focus on large crystals (SINE2020 & IK).
- Deuteration efforts currently being set up at LP3.



SINE2020 involvement: WP DEUNET (Hanna Wacklin)

- European Chemical Deuteration Platform (ESS, ISIS, ILL, FZJ, ANSTO).
- Establish a *deuteration network* to make deuterated molecules for neutron users (eg. chemical deuteration by H/D exchange, synthesis of smaller molecules, and precursors to complex biological materials).

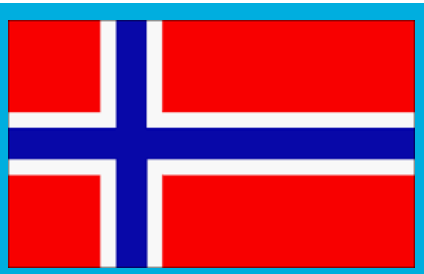
- <u>ESS role:</u>
- Synthesis of complex deuterated molecules/development of enzyme catalysis
- Network coordination, survey of European deuteration needs
- Business plan to secure further funding by 2019

SINE2020 involvement: WP XTALGEN (Zoë Fisher)

EUROPEAN SPALLATION SOURCE

- Goal: macromolecular crystallogenesis, phase diagram characterization for proteins (to consistently obtain large, single crystals).
- Investigate parameters that affect large crystal growth in two crystallization formats: dialysis and vapor diffusion (sitting drop).
- Parameters to be varied: *pH, temperature, precipitant concentration*.

DEMAX Norway IK contribution discussion



EUROPEAN SPALLATION SOURCE

- A variety of tools in one package for both deuteration and crystallization.
- Opticrys crystallization device developed by IBS (NatX-ray) - € 170 000
- Package of incubators for biodeuteration and crystallogenesis - € 67 000
- Crystallization/liquid handling robot Oryx8 (Douglas Instruments) - € 68 000
- [Perhaps: High Pressure cooler @ LN2 temps (ADC) - € 110 000]
- **Cost book** ~€ 415 000

- Thank you for your attention!
- Questions?