Scientific Support Division update

Hanna Wacklin-Knecht

Reorganisation 2025

Science Directorate

Research Coordination Office

intrument divisions

Diffraction and Imaging

Large Scale Structures

Spectroscopy

Data Management and Software Center

Hanna Wacklin-Knecht

Scientific Support

Neutron Scattering Systems

NMX instrument

Macromolecular crystallisation (Zöe Fisher)

Support Laboratories

Sample environment

Deuteration

Hall Coordinators

Recruitments

Scientific Support Division
Hanna Wacklin-Knecht

Support Laboratories
Ryan Oliver (9/3)

Katrin Michel
Nicholas Weisend
Ghazaleh Roostai (PL)

Vacancy: RML Scientist – interviews held

Sample Environment

Alex Holmes
Oleksiy Zhadorosko
Damian Paliwoda
Lauritz Saxtrup
Andreas Hagelberg
Niklas Ekström
Alice Corani
Harald Schneider
Oskar Summerton (technician)

Vacancies:
Group Leader – interviews held
2 SE technicians
SE engineer HT/gas
(VR Early science (UU)

Deuteration

Jia-Fei Poon
Oleksandr Kovalenko
Naomi Elstone (AMBER PD)

Vacancies:
Group Leader
Biodeuteration Scientist
Postdoc – nanodisc deuteration/SEC-SANS

Hall Coordinators
Dana McKenzie (1/1)

Vacancies:
7 Hall Coordinators

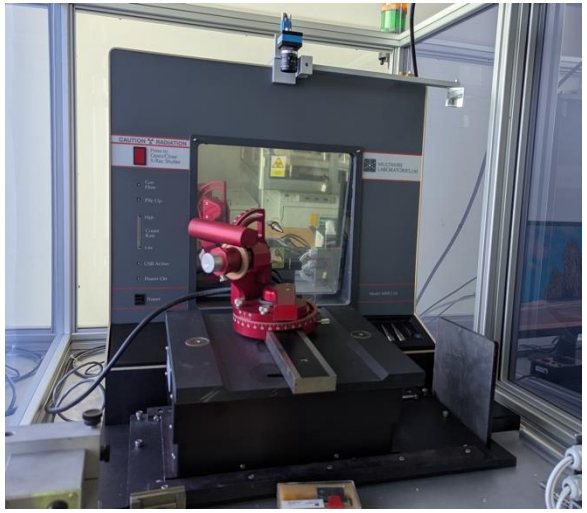
Support Laboratories

Update

- New X-ray capabilities acquired and commissioned
- Scientific responsibles from instrument divisions agreed for X-ray instruments
- E04 Soft/Biolab: NMX crystallisation activities

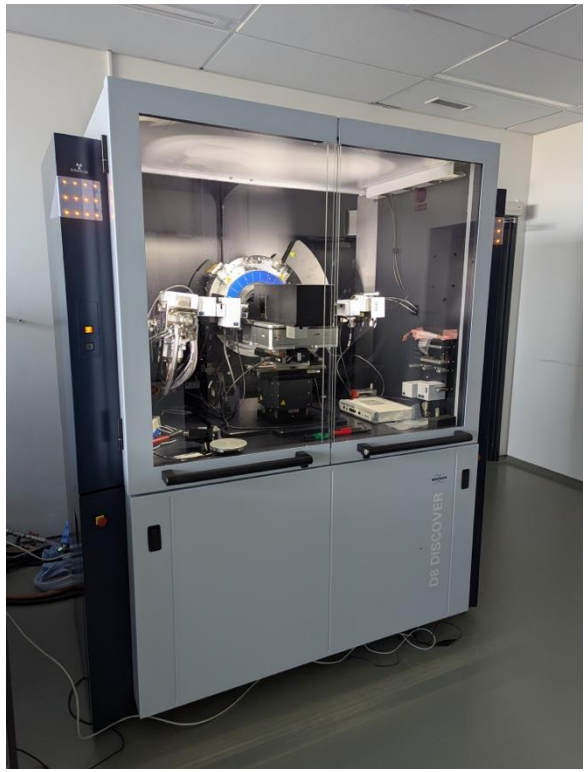
-> GMM1 permit application sent for growth of BSL1 test cultures.

- Final steps of installation by in D08 laboratories started – access by 1 Sep
- Handover of lab infrastucture maintenance agreed with facility management



Laue diffractometer
for crystal alighment

X-ray reflectometer for soli
and liquid interfaces



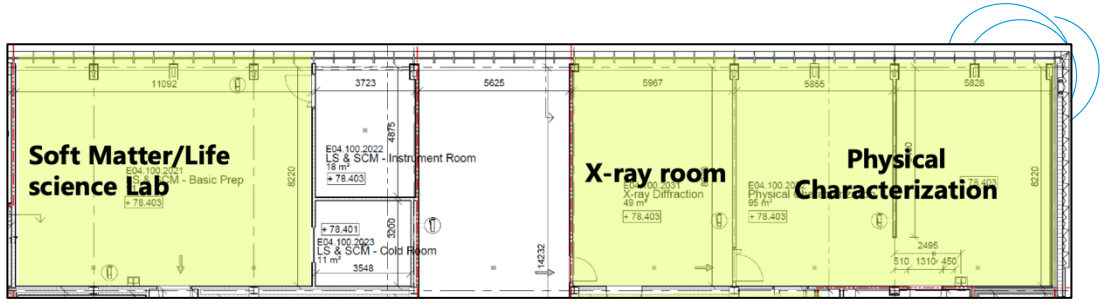
Support Laboratories:

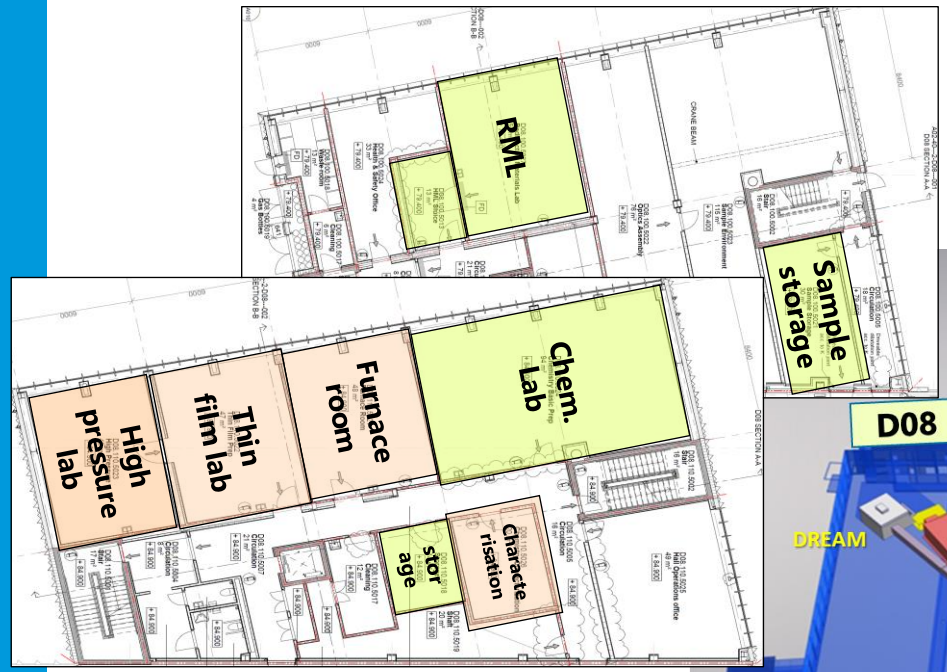
In the pipeline

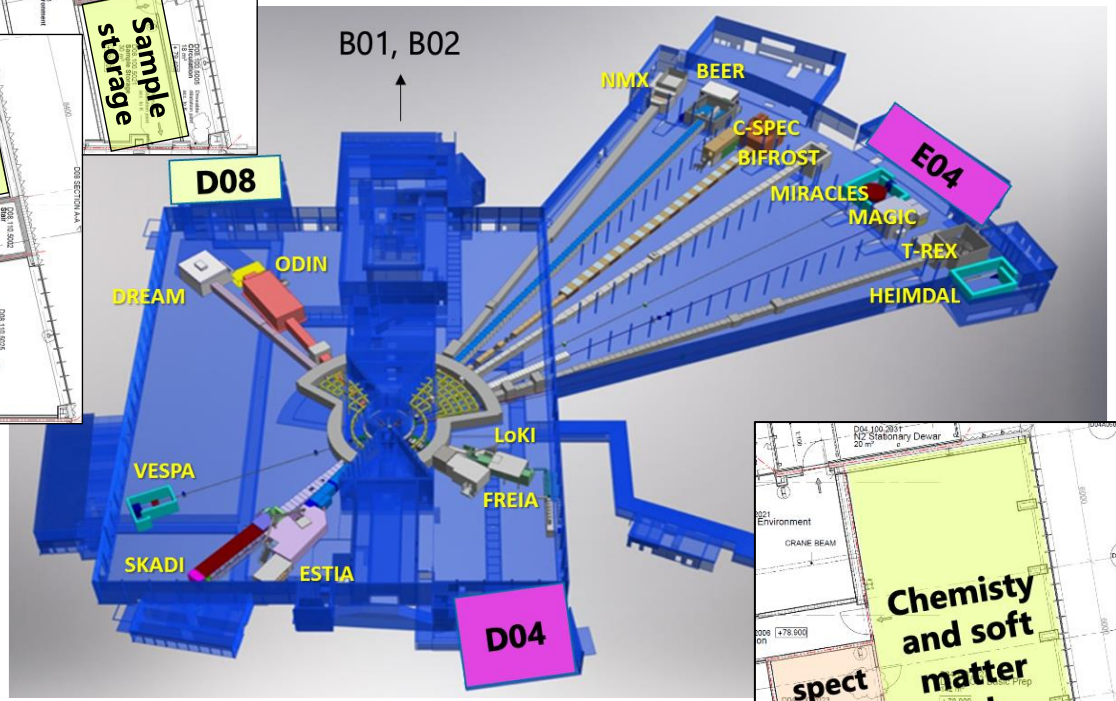
- material analysis for ESS machine and instruments
- training new instrument staff
- finalising RML for first users
- planning user training and access for operations
- planning lab equipment and organisation for user program
- electronic request systems for laboratory chemicals procurement, equipment booking and lab support
- non-activated sample storage

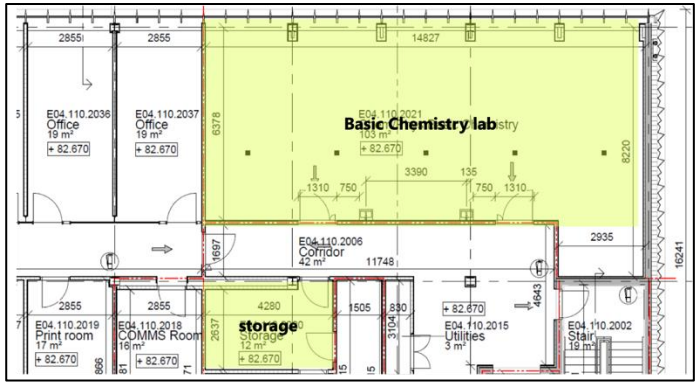
Support Laboratories

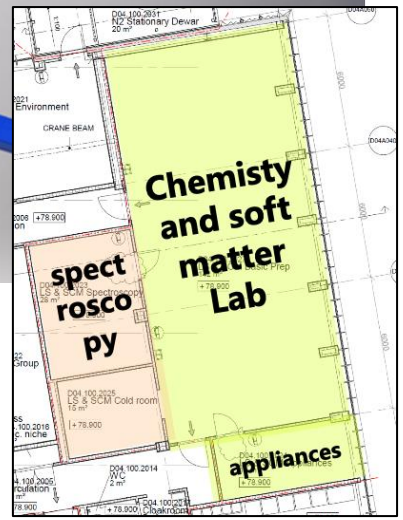
Readiness for BOT and SOUP











For BOT:

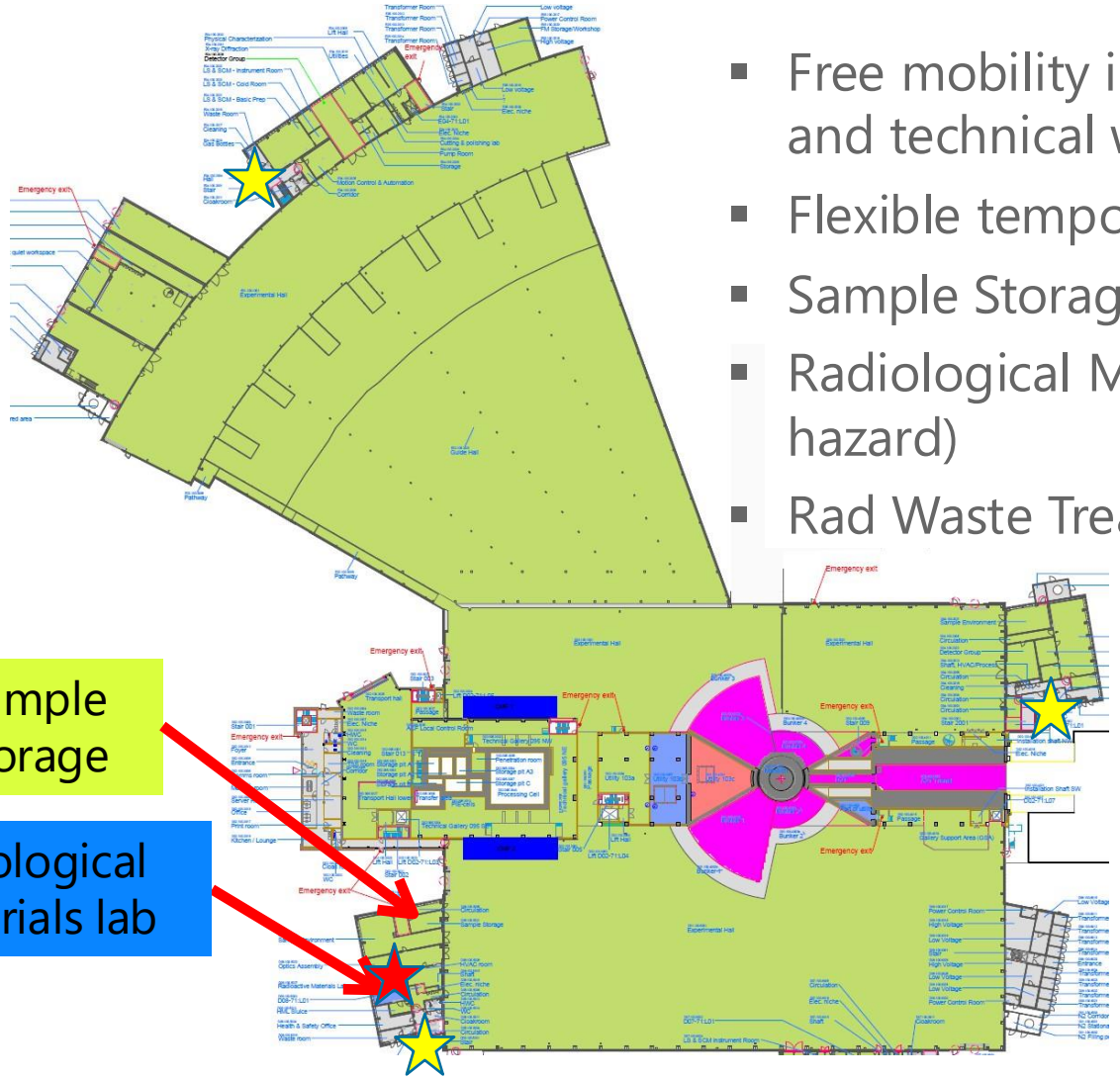
- finish installation of laboratory gas/water utilities in D08
- completion of basic D08/D04 chemistry labs for hot commissioning

For SOUP:

- completion of speclialised D08/D04 labs
- further equipment and capabilities for user program

Sample Management - zoning

Radiation zoning and sample relevant areas



- Free mobility in the green area between instrument, labs and technical workshops
- Flexible temporary zoning changes in the areas
- Sample Storage room in D08 (for samples retained at ESS)
- Radiological Materials lab in D08 (high contamination hazard)
- Rad Waste Treatment Facility in H09 (long decay time)

★ Entrances to supervised area for users

★ Entrance to controlled areas for users.

Storage of active samples

Update – preliminary process and RP guidelines

ESS staff (IOE/IS or RP depending on activity level) is responsible for user samples at ESS

Before removing a sample from sample position, its activity must be checked every time:

- Experiment Risk Assessment ERA will contain who should do this (user, LC, HC, RP)
- Depending on the result, the sample can be stored at:

1. Instruments

- Each instrument will have active sample storage cupboard(s) appropriate for their samples.
- RP provides advice and instructions on storage solutions and shielding of stored samples to <3 µSv/h
- RP checks samples prior to removal from storage and gives instructions for transport if required.

2. RML

- For handing samples with contamination hazard or exceeding 25µSv/h
- 4 fumehoods + 2 gloveboxes (wet/dry)
- 90 min. fire cabinets
- Access only during normal hours/weekdays
- Trained users supervised by RML scientist

2. Sample storage room

- Storage of active samples that can be shielded to <3 µSv/h
- Storage for active samples requiring fridge/freezer/inert atmosphere
- Waste hood for emptying sample containers
- Managed/supervised by RML scientist
- Access for trained ESS staff

Sample Management and Tracking

Update

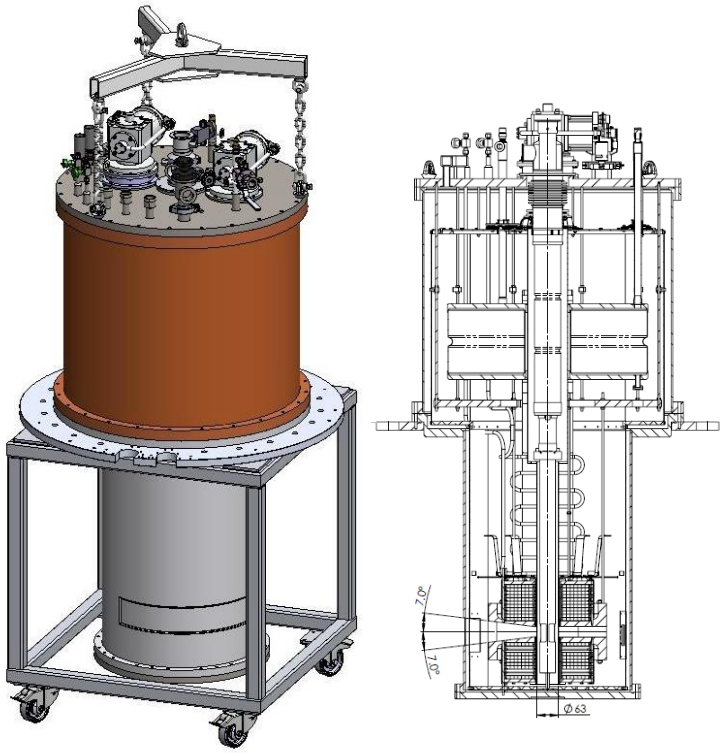
- All samples will be barcoded with labels produced by the User Office software from user proposal
- Samples shipped to ESS will be registered and delivered by Logistics to recipient (user laboratory or IOE) for barcoding/storage.
- Samples brought to ESS by user will be taken by the user/IOE to the support laboratories (day time), or Hall Coordination office (out-of-hours) for barcoding.
- Samples will be registered in/out of storage and supervised/controlled areas after appropriate RP checks
- IOE is responsible for arranging RP checks as well as sample return shipping

Sample Environment

Highlights

- Laser pump probe on loan to ILL for user experiments on IN16B
- Staff training at ILL and ISIS for laser and soft matter experiments

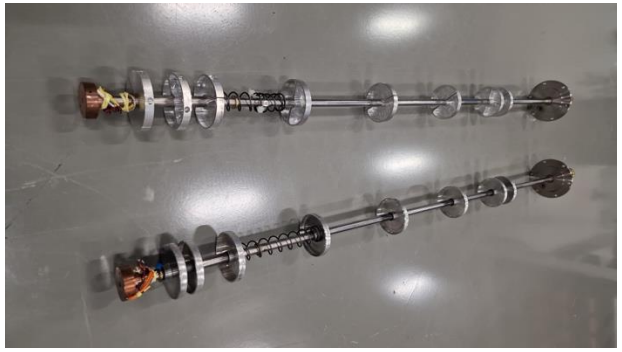
DREAM Electrochemistry Cryofurnace received



14T Spectroscopy HTS magnet preliminary design

new workshop technician Oskar

new baffle design for samplesticks (BIFROST)

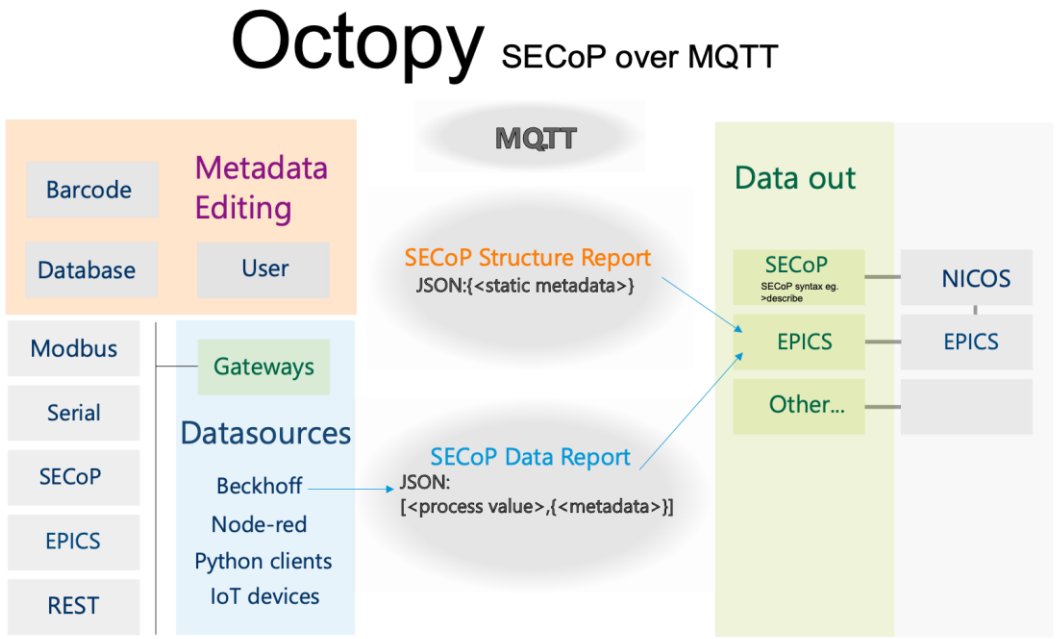


2 dilution inserts ICE Oxford in preliminary design

Sample Environment

Nicos/SeCop workshop 24 March

- "Should ECDC consider connecting NICOS directly to SECoP Sample Environment equipment instead of via EPICS?"



- The demonstration of NICOS using SECoP does not show any major showstoppers in regards to the experiment workflow.
- Emerging preferred path: Hybrid — OctoPy gateway with EPICS bridge, with a pilot project on Ymir.

Sample Environment

Events

- ISSE School January 2026 @ ESS/MAXIV:
- 16 lecturers, 21 students +26 on-line

Date	Sunday 18th Jan	Monday 19th Jan	Tuesday 20th Jan	Wednesday 21st Jan	Thursday 22nd Jan	Friday 23rd Jan
Time	Day 0	Day 1	Day 2	Day 3	Day 4	Day 5
		8:00-9 arrival/registration				
9:00 - 09:45		Welcome (10 mins) + Intro to ESS (25+25 mins)	Design considerations for SE I	Magnet use and design	Imaging, tomography	Automation/robotics
9:45 - 10:30		Intro to Max IV (30 mins)	Gas handling combined with HP incl. Hydrogen	High Temperatures	Cryogenics II	High Pressure II
10:30 - 11:00		*Break*	*Break*	*Break*	*Break*	*Break*
11:00 - 11:45		Electrochemistry/Batteries	Design considerations for SE II	Polarization & SE	Soft Matter II	Safety
11:45 - 12:30		XFEL SE challenges	Cryogenics I	Soft Matter I	High Pressure I	Experiences at a starting facility (online)
12:30 - 13:30		*Lunch*	*Lunch*	*Lunch*	*Lunch*	Lunch?/Departure
13:30 - 15:30		ESS tour	ESS Practicals	Practicals (MAX IV)	ESS Practicals	
15:30 -15:45		Break/transfer to MAX IV (15:30-16:00)	*Break*	*Break*	*Break*	
15:45 - 17:45		MAX IV tour (until 1800)	ESS Practicals	Practicals (MAX IV)	ESS Practicals	
18-21	Welcome			Social activity		

- Follow-up practicals 4-6 March for 22 ESS staff from istruments, cryogenics, vacuum, ECDC

– will be offered to new staff annually

Deuteration

Macromolecular Crystallisation activity -> LSS - NMX instrument/E04 Biolab

Oleksandr Kovalenko

Jia-Fe Poon

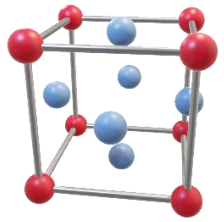
Chemical Deuteration

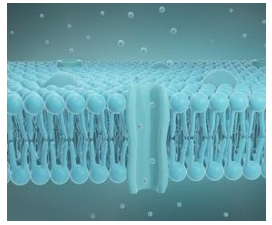
- Small organic molecules
- Synthetic Lipids
- Purification/analysis
- Surfactants
- Ionic liquids

Biological Deuteration
(@Lund University LP3)

- Deuterated biomass
- Recombinant proteins
- plasmid DNA
- Microbial lipid extracts

Naomi Elstone (natural lipids)

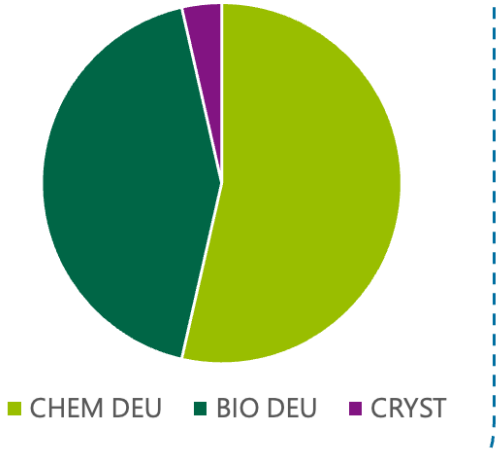


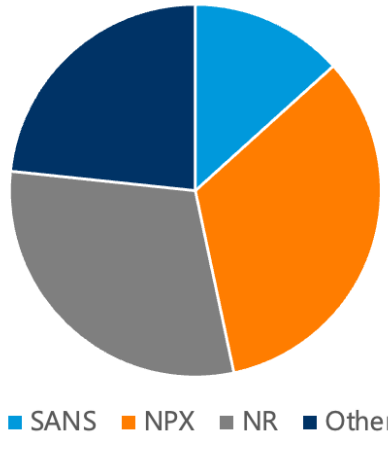


0.75->1 FTE LU in-kind + access agreement

0.2 FTE collaboration agreement with ILL 2023-2026

2025
3 proposal calls for external users and first science at ESS:

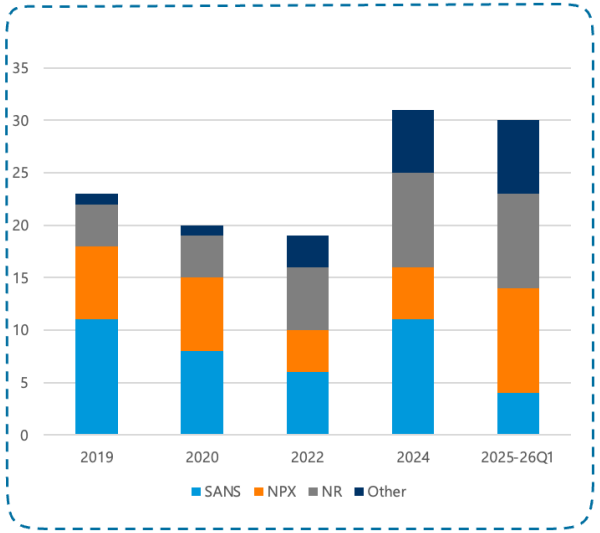


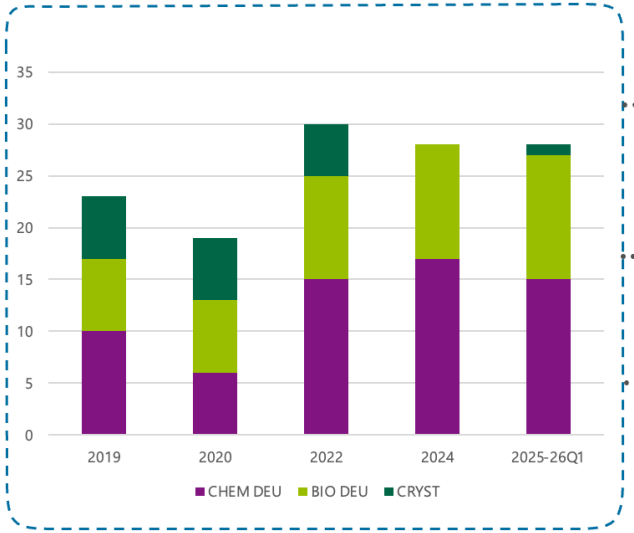


28 proposals received and assessed

38 materials/support requested

User access since 2019:
Statistics





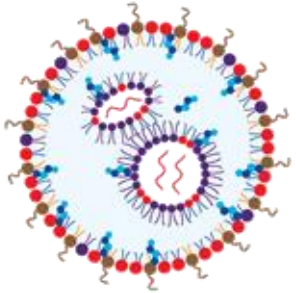
>100 Unique users

123 User proposals

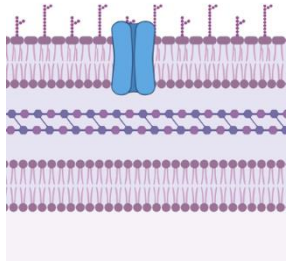
49 Publications

2025

New capabilities

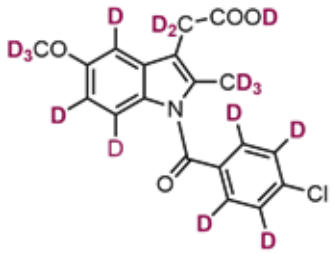


Drugs and delivery systems

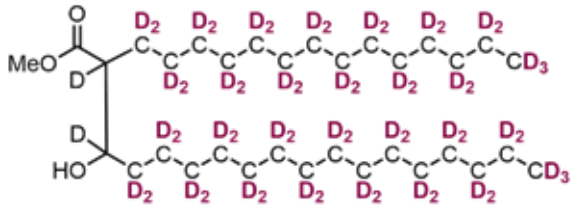


Antimicrobial resistance

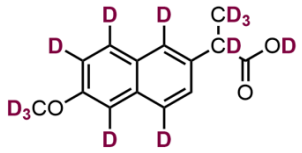
Chemical Deuteration



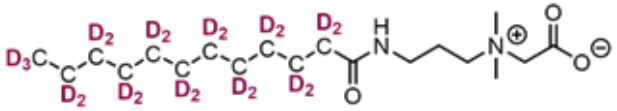
Indomethacin-d_{16}



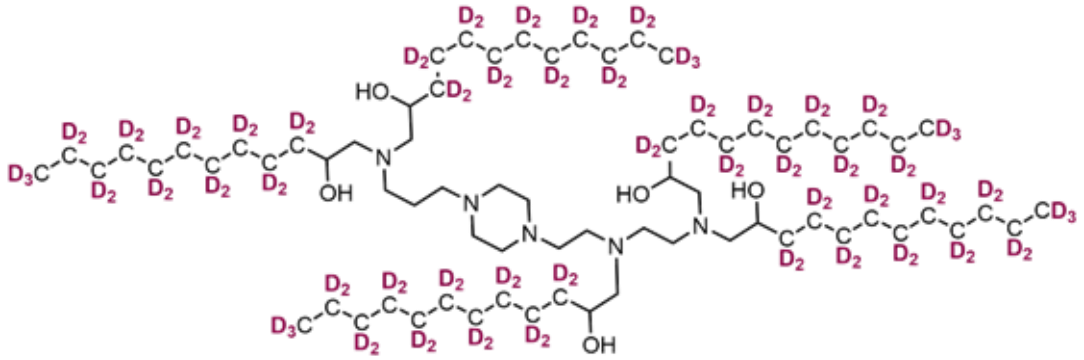
MMG1-d_{62}



Naproxen-d_{13}

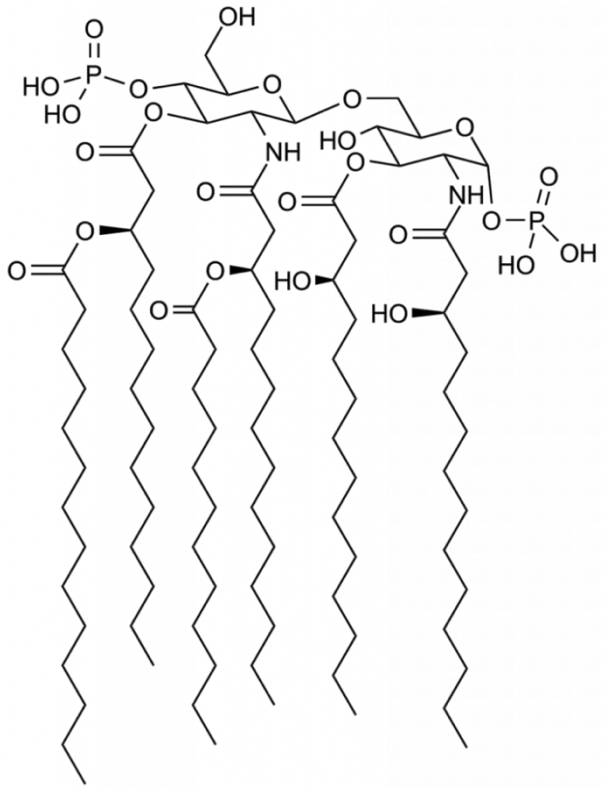


Cocamidopropyl betaine-d_{23}



C12-200-d_{105}

Biodeuteration



Deuterated LPS (extracted from E. Coli)

2025

New capabilities

Biodeuteratin

HABITAT Bioreactor system

- For high-density E.Coli/yeast cultures for:
- Lipid extracts, LPS, cholesterol
- Protein expression

-> 2 nd bioreactor planned

Chemical deuteratin

2026: 400MHz NMR

- structure determination in highly deuterated compounds (^{2}H-probe)
- reaction monitoring/method development
- deuterium incorporation

LUND UNIVERSITY

2025 Publications

bioengineering

MDPI

Article

The Enzymatic Synthesis of Perdeuterated D- and L-Lactic Acid-d_4 and Polymerization of Their Lactides to Polylactic Acid

Anna E. Leung [1,*], Andreas Raba [2], Klaus Beckerle [3], Jürgen Allgaier [2,*] and Hanna P. Wacklin-Knecht [1,4]

Chemical Science

ROYAL SOCIETY OF CHEMISTRY

EDGE ARTICLE

View Article Online
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Cite this: *Chem. Sci.*, 2025, **16**, 4048

All publication charges for this article have been paid for by the Royal Society of Chemistry

Exploiting spatial isomerism to modulate the assembled phase and rheological response of compositionally identical sugar-based surfactants†

Jia-Fei Poon, [a] Alfonso Cabezón, [b] Alessandro Gulotta, [c] Najet Mahmoudi, [d] Stefan Ulvenlund, [e] Rebeca Garcia-Fandiño [b] and Adrian Sanchez-Fernandez [*f]

communications chemistry

Article

A Nature Portfolio journal

https://doi.org/10.1038/s42004-025-01571-6

Unlocking the full compositional control of hydrophilic and hydrophobic deep eutectic solvents over protein structure and stability

Check for updates

Adrian Sanchez-Fernandez [1] ✉, Jake H. Nicholson [2], Susana M. Meza Huaman [2], Claudia Almuzara Romero [2], Jia-Fei Poon [3], Sylvain Prevost [4] & Alex P. S. Brogan [2] ✉

acs chemical biology

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pubs.acs.org/acschemicalbiology

Article

ess

Avoiding Mitochondrial Apoptosis by the Bcl-2-Driven Bax Oligomerization on Membrane Surfaces

Sophie E. Ayscough, Luke A. Clifton,* Jörgen Ådén, Sebastian Köhler, Nicolò Paracini, James Doutch, Éilís C. Bragginton, Anna E. Leung, Oliver Bogojevic, Jia-Fei Poon, Tamás Milán Nagy, Hanna P. Wacklin-Knecht, and Gerhard Gröbner*

Cite This: https://doi.org/10.1021/acschembio.5c00913

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Journal of Colloid And Interface Science

journal homepage: www.elsevier.com/locate/jcis

Regular Article

Check for updates

Encapsulation of single vesicles and single cells in a crosslinked microgel cage

Xiaoyan Liu [a,b,*,1], Shuwen Tan [a,1], Linda K. Månsson [c], Linnéa Gunnarsson [b], Jenny Marie Andersson [c,d], Hanna Wacklin-Knecht [b,d], Jérôme J. Crassous [e], Emma Sparr [b]

bioengineering

MDPI

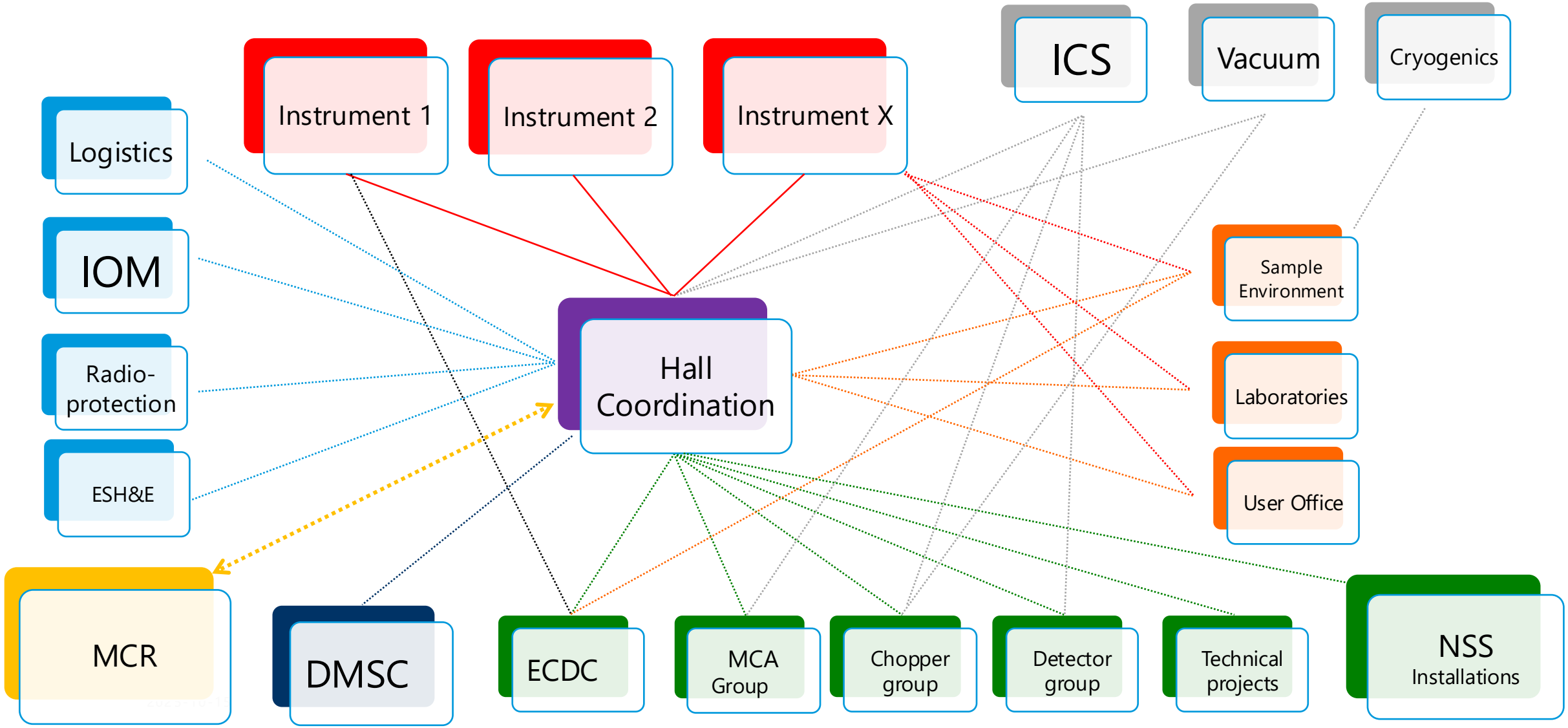
Article

Development of the Direct Deuteration Method for Amino Acids and Characterization of Deuterated Tryptophan

Chie Shibazaki [1,*], Haruki Sugiyama [2], Misaki Ueda [3], Takayuki Oku [1], Motoyasu Adachi [4], Zoë Fisher [5,6] and Kazuhiro Akutsu-Suyama [3,*]

Hall Coordination

Overview of stakeholders and interfaces



Hall Coordination Group

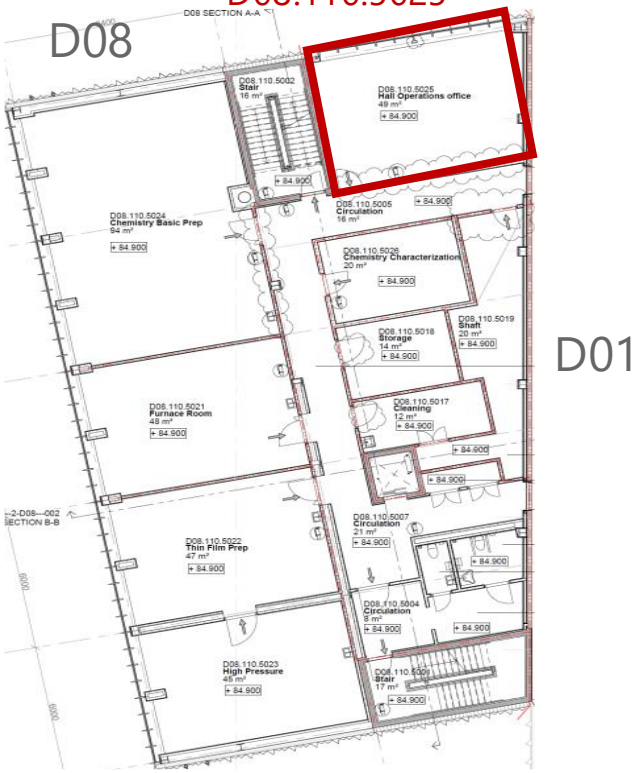
Roles

- Dana McKenzie: Group Leader
- 7 Hall Coordinators – senior technicians, 3-shift during neutron production days
  - 1 Hall Coordinator on duty per shift

Out of hours support:

- Primary information point-of-contact for users and staff working in experimental halls
- General technical support and first-line troubleshooting.
- Calling out-of-hours support from technical groups
- Basic radioprotection services (sample/equipment surveys, assessments, reporting)
- Experimental hall orientation and basic user training
- User and staff support for late laboratory access, consumables/spares/tools, sample management.
- Activities requiring authorization (e.g. operating cranes, filling dewars, changing gas bottles).
- Walk-throughs and monitoring activities in all experimental areas
- Respond to alarms and malfunctions in experimental halls and laboratory buildings
- Respond to incidents and emergencies in experimental halls and laboratory buildings, working with Emergency team lead (MCR).

Hall Coordination office
D08.110.5025



Hall Coordination Group

Responsibilities during normal working hours:

- Support all users and staff working in experimental halls and laboratory buildings
- Area responsibility in general experimental hall areas
- Act as main point of coordination between the experimental halls and MCR
- Coordinate all activities and monitor safety in experimental halls
- Support general maintenance and upgrade programs in experimental halls
- Participate in Emergency response team

Interaction with ongoing instrument construction:

- Coordinate hall operations activities with Installation teams
- Coordinate area transitions between construction and operations
- Communicate about hall operations activities with installation and instrument teams
- Provide coordination and assistance to installation teams during shutdowns, as appropriate

Future science

Current focus is on hot commissioing experiments/early science.

Support strategy for future science and new instruments needed to plan ahead.

-> participation in early science initiatives, instrumentn first science workshops etc. to understand needs.

Energy materials
Sustainable materials
Quantum Materials
Food/Health/Pharma
Adaptive materials
...?

Call for Input to the ESS Instrument Roadmap

FEBRUARY 3, 2025

ESS is pleased to invite the European scientific community to contribute input to a roadmap for instruments beyond the 15 currently under construction. This roadmap will guide future developments of the instrument suite, ensuring that ESS supports a versatile science portfolio in the decades to come. The call will be open for one year.

EUROPEAN
SPALLATION
SOURCE