



**EUROPEAN
SPALLATION
SOURCE**



Chemistry and Life Science Support

(ESS.120.03.01)

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Agenda



ESS 120.07.03: Chemistry and Life Science Support (structure & location distribution)

1. SULF- Sample Handling and User Laboratory Support

- a) Mission
 - b) Scope
 - c) Projected labor resources
 - d) Projected non-labor resources
 - e) Benchmarking
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2. DEMAX – Deuteration & Macromolecular Crystallization

- a) Mission
 - b) Scope
 - c) Projected labor resources
 - d) Projected non-labor resources
 - e) Benchmarking
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3. SCSE – Soft matter and Chemistry Sample Environment

- a) Mission
 - b) Scope
 - c) Projected labor resources
 - d) Projected non-labor resources
 - e) Benchmarking
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4. Neutron Optics

- a) Mission
 - b) Scope
 - c) Projected labor resources
 - d) Projected non-labor resources
 - e) Benchmarking
-

Summary



WBS 120.07.03 – structure

How do we work? Chemistry & Life Science Support (CLS)

The Chemistry and Life Science Support Group is responsible for delivering **user support** for world-class science in the areas of **chemistry (including soft matter) and life science**.

This includes the following work units/teams:

- ESS.120.07.03.01 Sample Handling and General User Lab Facilities (SULF)
- ESS.120.07.03.02 Deuteration and Crystallization (DEMAX)
- ESS.120.07.03.03 Soft matter and Chemistry Sample Environment (SCSE)
- ESS.120.07.03.04 Neutron Optics Support

ESS.120.07.03 – location distribution



Who do we support ? Chemistry & Life Science Support (CLS)

- CLS support the **ESS neutron scattering users** in the sample handling laboratories for sample preparation, modification and characterization before, during and after beamtime at ESS
- CLS provides the **ESS users** with deuteration of samples for ESS neutron scattering beamtime.
- CLS will support the **neutron scattering instruments and users** with (developing, providing, setting up & removing of) sample environment equipment.
- CLS will support material analysis for neutron optics as well as beam characterization for **ESS neutron scattering instruments** (Science)

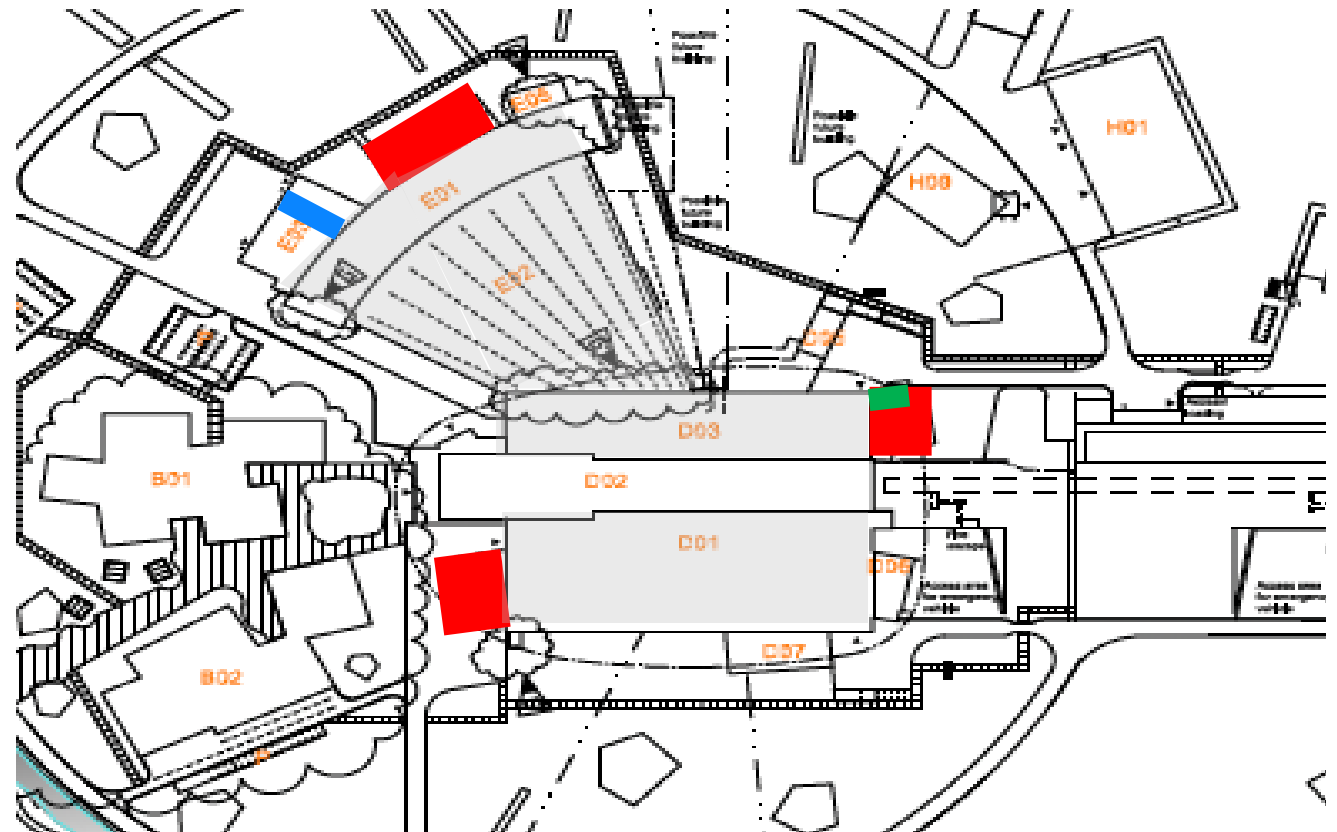
CLS will support all of ESS during maintenance periods with tasks expected to come from AD, Target, Science, & ES&H.

ESS.120.07.03 – location distribution



Where do we work? Chemistry & Life Science Support (CLS)

- **ESS.120.07.03.01** (SULF user labs) will operate 20 laboratories + 5 smaller spaces (approx. 1120 m²) in three buildings (E03, D04, D08) including the Radioactive Materials Laboratory (RML)
- ESS.120.07.03.02 (DEMAX deuterated materials) operates in one laboratory (100m²)
- **ESS.120.07.03.03** (SCSE sample environment) operates one workshop in D04 (57m²)
- **ESS.120.07.03.04** (Neutron Optics) operates in one workshop in E03 (94 m²)



1

Sample Handling and User Lab Facilities (SULF)

(ESS.120.07.03.01)

Mission for reliable operation (ESS.120.07.03.01)



SULF - sample handling and user laboratory facilities

This work unit is responsible for the operation, maintenance and upgrades of the Sample and User Laboratory Facilities (SULF): 1120 m², 25 rooms

ESS neutron scattering users will use the laboratories to prepare, modify and characterize their samples before, during and after the beam time. SULF is responsible for providing a facility for users to handle their sample in a way that supports world-class science on the ESS neutron scattering instruments.

Lab operation will take place year-round:

- during the run cycle, we will focus on user support (incl. 1 person on call)
- during down times, we will restock, refurbish, repair and perform maintenance

The facilities will serve both the user program and internal science projects. **During run cycles users will have the priority. During down times, internal science and maintenance projects will come first.**

Scope for reliable operations (ESS.120.07.03.01)



SULF sample handling and user laboratory facilities

- **Operations of laboratory spaces** & provision of PPE, consumables, common chemicals, gases and appropriate chemical waste removal.
- Assure **appropriate maintenance of lab instrumentation** and safety-related equipment/ furniture (fume hoods, ventilated cabinets, specialized fire extinguishers..)
- **Cradle-to-grave sample handling** together with ESS instruments, ESH and Logistics.
 - participation in experimental safety reviews for user proposals prior to beam time
 - ability to register, tag, temporarily store samples
 - user safety orientation in labs, user support in safe handling of samples, safety walk downs
- **Operation of the Radiological Materials Laboratory (RML)** in the controlled zone including presence of SULF personnel when users are present/working in the RML: risk analysis for the work, administrative and engineering controls

Scientific user support, e.g. user education on lab instrumentation, support with sample preparation and characterization to optimize user beamtime on the neutron scattering instruments and to facilitate high impact publications by the users.

Projected labour resources (ESS.120.07.03.01)



SULF sample handling and user laboratory facilities

12 FTE:

- 1 group leader for CLS
- 5 scientists (chemistry + life science + physical chemistry + materials chemistry + radiation chemistry)
- 6 technicians (4 chemistry, 2 life science)

Justification:

- *1 scientist and 2 technicians per lab building (E04: chemistry, D04: soft matter/life science, D08: physical chemistry)*
- *2 scientists for the Radiological Materials Laboratory (radiation chemistry, materials chemistry) – one lab responsible needs to be present when users work (controlled zone).*
- *1 person on call during run cycle*

Projected non-labour resources (ESS.120.07.03.01)



SULF sample handling and user laboratory facilities

Operations Cost Estimate: 600 k€ (based on experience with current lab running since '21)

Justification: PPE and consumables for lab operations to **support approx. 3000 user visits per year** + internal researchers + machine support. Includes e.g. lab coats, gloves, goggles, wipes, glassware, spill kits, compressed gases, common chemicals, sample holders and others.

- 100 k€ per lab building: **300 k€** (this is based on experience with current labs operated since '21)
- Service, service contracts and repair of lab equipment: **200 k€**
- Replacement of small lab equipment, i.e. temp. probes, pH electrodes, UV lamps, sensors : **100 k€**

Capital Cost Estimate: 600 k€ (based on ISIS input)

- Renewal of large equipment and additional new equipment : 500 k€
- Investment budget to renew/update laboratories every 5-10 years: 100k€

Benchmarking (ESS.120.07.03.01)



SULF sample handling and user laboratory facilities

User labs are strongly impacting the quality of the scientific publications resulting from beamtime at the neutron sources. This unit best compares to the ISIS user laboratories.

- ISIS (8 FTE): 1 group leader, 4 Lab manager/scientist (2 Chemistry, 1 Bio/Life science, 1 Material), 3 FTE techs (1 materials, 2 chemistry); in addition 2 junior scientists (placement students). **No sample tracking** but safety reviews.
- ILL (4 FTE) provides chemistry and soft matter **support primarily in partnerships** and **sample handling is not included** (performed by ESH).
- SNS (7 FTE): 1 group leader, 1 technician sample handling& shipping, 2x technicians for receiving/bar coding/delivering samples, general user support, 2x technicians for bio lab, 1x scientist for X-ray lab; **Approx. 300 m² = 1/3rd of the ESS space**; other specialized support labs available (X-ray lab, bio X-ray lab, bio crystallization/protein lab, Raman lab, thin film lab, soft matter lab, synthesis lab, hot lab (no users!)) provided by scientists from SNS instruments and biology...

2

Deuteration and Crystallisation (DEMAX)

(ESS.120.07.03.02)



Mission for reliable operation (ESS.120.07.03.02)

DEMAX - Deuteration and Crystallization

This work unit provides deuterated compounds necessary for world-leading neutron scattering experiments at ESS in the areas of

- Chemical Deuteration (soft matter chemistry, organic chemistry, hybrid materials)
- Biological Deuteration (biomass, protein expression, yeast-derived lipids, DNA)
- Macromolecular crystallization facilities (protein crystal growth)

DEMAX will support ESS neutron scattering users with deuterated materials for their beamtime at ESS as part of the proposal system.

DEMAX operation will take place year-round independent from the run cycle as the synthesis of deuterated compounds needs to take place ahead of time.

Scope for reliable operations (ESS.120.07.03.02)



DEMAX - Deuteration and Crystallization

- Feasibility review of user proposals for deuteration once the scientific review panel has approved the ESS user proposal. Communication with the user groups about the sample and the experiment
- **DEMAX will provide in full service mode**
 - sample will be provided with supporting characterization data ready to be included in the user publication
 - service includes procurement of deuterated pre-cursor materials, specialized glass ware, characterization services if not available within ESS.
- DEMAX is cultivating host organisms in heavy water to achieve deuterated protein and yeasts as source for biodeuterated molecules (proteins, lipids)
- **DEMAX will develop new synthesis strategies according to the change in research interests of the ESS neutron scattering user community.**
- DEMAX will operate the owned or rented chemistry laboratory.

Projected labour resources (ESS.120.07.03.02)



DEMAX - Deuteration and Crystallization

6 FTE:

- 4 scientists (chemistry 2x, life science, crystallography)
- 2 technicians (chemistry, life science)

Justification

- *Chemical deuteration: 2 scientists (chemistry) and 1 technician (chemistry) needed to cover the wide variety of different molecules needed for neutron scattering science at ESS.*
- *Biodeuteration: 1 scientist (chemistry/life science) and 1 technician needed to extract lipids and proteins from deuterated host organisms and purify them.*
- *Macromolecular crystallization: 1 scientist (crystallography) needed for crystal growth.*

Projected non-labour resources (ESS.120.07.03.02)



DEMAX - Deuteration and Crystallization

Operations Cost Estimate: 350 k€ (based on current experience)

Justification:

- Budget need to be sufficient to operate DEMAX activities in terms of deuterated chemicals (main cost), consumables, lab supplies and small equipment. Equipment repair and equipment service is included: **200 k€**
- Bench fee for hosting the activity on biological deuteration and crystallization at Lund Univ. jointly with MAX IV is included. **50 k€**
- Rent for the DEMAX laboratory (including utilities and waste disposal): **100 k€**

Capital Cost Estimate: 200 k€

Justification:

- new analytical equipment to provide synthetic and analytical capabilities

Benchmarking (ESS.120.07.03.02)



DEMAX - Deuteration and Crystallization

This unit is difficult to compare to the three large existing deuteration services at ILL, ISIS and ANSTO as these three facilities are deviating a bit in what they offer. ESS is splitting into half chemical deuteration and half biodeuteration/macromolecular crystallization.

- ILL PSB (6 FTE) for biological deuteration and crystallisation platform joint with ESRF PSB (4 FTE). 1FTE for lipid activities. No chemistry.
- ISIS (5 FTE) for chemical deuteration, no biological deuteration nor lipids.
- ANSTO (10 FTE) for chemical and biological deuteration. No lipids.

ESS is presenting 6 FTE and will rely on collaborations between the facilities e.g. through Deunet for special deuterated compounds. This effort scales with amount of instruments in operation and amount of science areas.

3

SCSE- soft matter and chemistry sample environment

(ESS.120.07.03.03)

Mission for reliable operation (ESS.120.07.03.03)



SCSE – Soft matter and Chemistry Sample Environment

CLS will provide sample environment equipment for the instruments in the areas of chemistry and soft matter/life science in collaboration with instrument scientists and associates (SCSE).

This includes operation, maintenance and upgrade of the equipment on the instrument and in the sample environment workshop.

Operation will take place year-round.

- During the run-cycle, the team will focus on user support (1 person on –call)
- During down-times, existing sample environment will be upgraded and new one developed

SCSE will support ESS neutron scattering users with setting up/removing of sample environment systems at the beamlines. SCSE will be on call during the beam on to assist with repair and replacement in case of issues.

Scope for reliable operations (ESS.120.07.03.03)



SCSE – Soft matter and Chemistry Sample Environment

- Operate, maintain, repair & re-new SCSE pool and instrument specific equipment & workshop
- Perform feasibility reviews and scheduling of the SCSE equipment as requested for approved ESS neutron scattering proposals.
- Install the SCSE equipment on the neutron scattering instrument in collaboration with the instrument teams. Train the users/instrument teams in the handling of the SE pool equipment as necessary. Remove the equipment after the experiment.
- **Perform rapid and reproducible equipment change-over at the beamline including quick repair or replacement of equipment in case of equipment failure to reduce beamtime loss.**
- Assure **reliability of SCSE equipment and validate** the calibration. Assure mechanical and software integration of SCSE equipment by interacting with the responsible teams.
- Develop new state-of-the-art SCSE equipment following input from the instrument teams and the user community.

Projected labour resources (ESS.120.07.03.03)



SCSE – Soft matter and Chemistry Sample Environment

5 FTE:

- 3 scientists/engineers
- 2 technicians

Justification:

- 1 scientist/engineer with focus on chemistry/spectroscopy
- 1 scientist/engineer with focus on soft matter/fluids
- 1 scientist/engineer with focus on gases/gas adsorption/reaction cells
- 2 technicians for equipment change-over on the instruments, workshop support, repair and assembly

(one person on call)

Projected non-labour resources (ESS.120.07.03.03)



SCSE – Soft matter and Chemistry Sample Environment

Operations Cost Estimate: 250 k€

Justification:

- Budget needed to operate SCSE sample environment equipment including procurement/replacement of small parts (sensors, optical sources, specialized tools, calibration samples, repair kits, accessories...)
- Operating the SE workshop including cleaning chemicals, gases, PPE
- Service and repair of equipment

Capital Cost Estimate: 300 k€

Justification:

- Providing state-of-the-art SE equipment and renewal of existing SCSE sample environment equipment.
- Procurement/development of new SE equipment.

Benchmarking (ESS.120.07.03.03)



SCSE – Soft matter and Chemistry Sample Environment

SCSE is setup very similar to ISIS except that we also cover chemistry. Some support is expected from the scientific associates from the instruments.

- ISIS (5 FTE): soft matter sample environment (does not contain gas adsorption, reaction cells)
- SNS / HFIR (5 FTE) but 6 FTE Technical and R&D support not included
- ILL LSS (3 FTE): resources provided as part of the LSS group not sample environment.

4

OPTICS – Neutron optics support

(ESS.120.07.03.04)



Mission for reliable operation (ESS.120.07.03.04)

Neutron Optics support (moved to SAD/CLS in Jan. 23)

CLS is responsible to provide “neutron optics” and material characterization support to ESS instruments. The work unit is covering the following areas:

- Neutron guide simulation and radiation damage assessment for neutron guides
- Beam characterization of the ESS instruments.
- Materials characterization of optical components, shutters and instrument shielding (mainly trace analysis).

Operation will take place year-round independently from beam status.

Neutron Optics will support and further develop these capabilities guided by the needs of the ESS neutron scattering instruments.

Scope for reliable operations (ESS.120.07.03.04)



Neutron Optics support

- Operational instrument support:
 - Maintain geometry models of guides for the instruments; support guide simulation if requested
 - Support installation & commissioning of new optics as requested by instrument teams.
 - Support elemental analysis of materials close to the beam using XRF/LIBS
 - Perform beam characterization measurements using metal foils and gamma spectroscopy (together with test beamline and ESS SP Group). Develop method to evaluate background levels in the instruments.
- Development/upgrades of neutron guides:
 - Identify causes of degradation of guides (floor movement, alignment, chemical effects such as corrosion)
 - Propose new solutions/designs where existing concepts are failing to meet expectations.

Projected labour resources (ESS.120.07.03.04)



Neutron Optics support

2 FTE:

1 scientist (physics, computational physics)

1 technician (physics, material science)

Justification:

- 1 scientist for guide simulation, radiation damage assessment, operation of optical bench
- 1 technician (physics, material science) for XRF/LIBS measurements, gamma spectroscopy and operation of Optics workshop

Projected non-labour resources (ESS.120.07.03.04)



Neutron Optics support

Operations Cost Estimate: 80 k€

Justification:

- Consumables for measurements (metal foils, standards), service& repair for XRF/LIBS/gamma spectrometer
- Optical bench maintenance and service.

Capital Cost Estimate: 40 k€

Justification:

- Development/upgrade of capabilities (optical bench, beam diagnostics) in optics lab.

Benchmarking (ESS.120.07.03.04)



Neutron Optics support

- PSI has 3 staff dedicated to operating the optics lab.
- ILL has 5 staff, 1 scientist and 4 technicians, but this was to cover large scale manufacture of wide angle spin echo analysers.

ESS is presenting 2 FTE, and will rely on the collaboration with ESS Spallation Physics and the instrument teams for some of the tasks. ESS will collaborate with partner facilities on some tasks (e.g. background investigations? PSI?).



Summary - WBS 120.07.03

Chemistry and Life Science Support

- **ESS.120.07.03.01 Sample Handling and General User Lab Facilities (SULF):**
 - 12 FTE: 1 group leader (CLS) + 5 scientists + 6 technicians
- **ESS.120.07.03.02 Deuteration and Crystallisation (DEMAX)**
 - 6 FTE: 4 scientists + 2 technicians
- **ESS.120.07.03.03 Soft matter and Chemistry Sample Environment (SCSE)**
 - 5 FTE: 3 scientists/engineers + 2 technicians
- **ESS.120.07.03.04 Neutron Optics Support**
 - 2 FTE: 1 scientist + 1 technician

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|--------------------------|-----------------|
| ▪ TOTAL cost: | 5,670 k€ |
| <hr/> | |
| ▪ <i>Labor (25 FTE):</i> | <i>3,250 k€</i> |
| ▪ <i>Operations:</i> | <i>1,280 k€</i> |
| ▪ <i>Capital</i> | <i>1,140 k€</i> |



Finish presentation