

A European platform for advanced chemical deuteration

Leading beneficiary: ILL/ESS

Partners: Hanna Wacklin(ESS), Giovanna Fragneto(ILL), John Webster (ISIS).

Estimated budget (in person months, other direct cost) and tentative distribution per partner

Abstract of your innovative activity: *(please make sure that you mention the following points)*

With the recent and future advances in neutron sources and instrumentation, there is an increasing need for deuteration of complex molecular architectures for studying a range of advanced materials with neutron scattering. This is particularly true for novel materials developed for industrial applications which range from home and personal care products to (bio)nanotechnology, electronic devices and biomedicine.

Even though impressive advances have been made through macromolecular deuteration in cell cultures, pioneered at ILL, chemical deuteration by synthetic means remains an essential part of the toolkit for generating chemically pure, well-defined and specifically labeled molecules for structural characterization using neutron scattering.

The Oxford Isotope Unit has been providing the neutron user community with a selection of compounds based on simple hydrocarbons mainly for soft condensed matter studies for many years. More complex molecular architectures cannot however be obtained today from any of the existing deuteration facilities in Europe, except in those cases where they can be purified from cell cultures, e.g. nucleic and aminoacids. This is largely a matter of scope and resources of the individual facilities, and currently forms a bottle-neck for the scientific experiments that can be performed using neutron scattering.

We propose to establish a European platform for chemical deuteration, by adding advanced molecular deuteration capabilities at a node established at the ESS to complement the scope of the existing laboratories at ILL and ISIS. The platform will maximize the benefits for the user community arising from the expanded synthetic capabilities by enabling the most suitable and cost-effective routes to the desired compounds to be used, as well as sharing of the raw materials, manpower and competence. The platform will aim to provide all European neutron users access to its joint range of services, ideally through a common application process linked to the neutron facility access.

The ESS node will focus on the chemical synthesis of complex deuterated molecules based on both biological and non-biological starting materials, and on developing novel deuteration methods. Some of the key types of compounds that are urgently required include:

- heterocyclic, chiral and (poly)unsaturated compounds
- compounds based on natural components such as sugars, biomimetic polymers, lipids and aminoacids
- monomers for polymer synthesis
- synthetic polypeptides incorporating non-biological components

This 3-year grant is intended for setting up the platform (coordinated from Lund), establishing the node in Lund (we envisage 2 scientists + 1 technician), as well as supporting those activities of the existing facilities at ILL (1 scientist) and ISIS (1 scientist) required for the platform, such as purification and analysis of materials within their areas of expertise. This platform could also later serve as the ideal framework for an International Training Network for raising the impact of neutron scattering experiments through the use of advanced chemical labeling methods.

While it is proposed that the facilities will act as the core of the platform through which the activities are coordinated and carried out, we also plan to involve university groups through collaborations to enhance the knowledge base available for e.g. specialized applications such as peptide or polymer synthesis. In this respect, we expect interest for both synthesis and characterization methods from the universities in the ESS region (Lund, Copenhagen) as well as from the many small chemical and analytical service providers co-located on the Medicin Village site with ESS. It is thus foreseen that there is no need to purchase any major analysis equipment (e.g. NMR) from this grant.

Two of the proposers (HW and GF) have already carried out in the last three years pioneering work in lipid extraction and HPLC and fatty acid methyl ester (Fame) analysis from bio-mass provided by the D-Lab (one manuscript from this work has been just accepted, and a second is in preparation) and it is envisaged to continue with a similar scheme in the future for the part of this project carried out at the ILL with bio-mass obtained via proposals to the D-Lab, which will be purified, analysed and processed at ILL for use in synthesis of novel compounds via this platform. The simple hydrocarbon compounds synthesized at ISIS by the Oxford Isotope Unit can be used via this platform for building up more complex molecules. HW has previously experience of the synthesis of deuterated chiral compounds, lipids and unsaturated fatty acids, and the specification and in setting up the chemical deuteration laboratories at ANSTO. ESS currently rents approximately 100m² chemistry laboratory space in Medicin Village in Lund, and additional space will be available for the ESS node activities.