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## Abstract

The ‘Deuteration for Neutron Scattering – DEUNET’ meeting held in May 2017 in Oxford, UK, provided an opportunity to demonstrate and discuss the scientific impact of deuterium-labelling for neutron scattering studies in Europe and throughout the world. Organised jointly by the STFC and the Deuteration Network (DEUNET), it included experienced and novice users of the combination of deuteration and neutron scattering. A wider survey about labelled molecules, experiments and facilities comprised part of registration. The results of this survey were presented at the meeting and are presented below.

*Introduction*

Task 5.6 (ESS) in WP5 focuses on surveying and understanding:

1. The impact deuterium-labelling can have and is having on neutron science in Europe;
2. The requirements for extending availability of deuterated molecules – and how this will increase the impact of scientific investigations with neutrons.

It was important that these topics were discussed in a coordinated fashion in order to be comprehensive. It was for this reason that the first DEUNET workshop was combined with the ISIS Deuteration Facility meeting (which was last held in November 2015). The organising committee aimed to include a broad range of research fields and institutions in order to accurately represent the deuteration landscape across Europe.

It was also important to discuss the second point in a consultative fashion in order to accurately represent the insufficiencies in the range of or access to deuterated molecules. A deuteration survey was prepared and advertised to the target audience in various ways. Importantly, this survey was included in the registration for the workshop. It surveyed the types of deuterated molecules currently used and the techniques they are used with, the sources of these molecules and the institutions where the experiments are performed. It additionally surveyed which deuterated molecules researchers would use if they were available, and what they would use them for. Importantly for the deuteration laboratories, it also examined the type of access researchers would be likely to require.

*The Impact of Deuterium-Labelling*

As a first step towards addressing a), the first ‘Deuteration for Neutron Scattering – DEUNET’ joint workshop was held in May 2017. Hosted jointly by the STFC and the DEUNET, it included 60 participants, 25 invited speakers, updates from each of the DEUNET laboratories and collaborators, and featured discussion and poster sessions. In addition to attendees from universities in the United Kingdom, Sweden, Denmark, Norway, Germany, France, Italy, Spain, Austria, Australia and Canada, there were also registrants from facilities other than those which are members of the DEUNET - from J-PARC, Japan and Oak Ridge National Laboratory, USA.

It was important that a broad range of sessions were included in the workshop, to represent the areas of science in which deuteration has long been making an impact on the field, and also areas which are less advanced in the use of the technique. The following scientific areas were represented: polymers, surfactants, small molecules including ionic liquids, lipids and membranes, protein structure and function, and soft matter including colloids. It was also of interest to include scientific projects with varying levels of maturity. Researchers such as Bob Thomas and Jeff Penfold presented some advanced research using deuterium labelling/neutron scattering, but others presented preliminary studies using deuterium labelling/neutron scattering, or the results of other techniques suggesting deuterium labelling/neutron scattering would be useful.

The scheduled breaks and discussion sessions were useful opportunities for researchers to discuss their research with one another. The topics raised during the discussion were varied and useful for the DEUNET to consider. The discussion acknowledged that the demand for deuterated materials is increasing. Suggestions to handle the increase in demand included: publicising the availability of deuterated materials at the various facilities (and indeed commercially); to include academic groups with expertise in specific relevant chemistry to the Network; and for the DEUNET to participate in more conferences in order to continue to identify how deuteration benefits neutron scattering and how it might in the future. The discussion also raised questions about how a unified proposal system might work, particularly in cases where more than one facility is required to synthesise a molecule; and how access to the facilities will be ensured after the grant period.

*Survey*

The survey was advertised via email, twitter, and on websites such as neutronsources.org. It was additionally incorporated into registration for the workshop.

The survey asked variations of the following questions (some as multiple-choice questions):

1. Do you currently use deuterated molecules in your research?
2. Which molecules do you use and where do you obtain them from (compound, supplier, quantity)?
3. Which techniques do you currently use with deuterated molecules?
4. Which deuterated molecules could your research benefit from that are currently not readily available?
5. Which techniques would you use if you had access to these deuterated molecules?
6. What kind of access would you need to a chemical deuteration service?
7. At which neutron facilities do you carry out experiments?

Though all of these questions are pertinent, the most pressing question for the Deuteration Network was about the types of molecules that are currently used, and those which would be useful to neutron scattering users but which are unavailable. The responses to the latter question are summarised in Figure 1. Lipids and monomers and polymers comprised the most desired molecules. (The ‘Other’ category is broad, and includes classes such as amino acids, peptides, ionic liquids, metal-organic frameworks, drugs, carboxylic acids and alkylamines). The types of molecules used already mirror almost exactly those represented in this chart, suggesting that the range of deuterated molecules available *in these classes* is not broad enough.

Figure 1. The molecules requested by the user community as part of the deuterated materials survey.

The survey otherwise noted that:

1. The vast majority of researchers would continue to use the same experimental techniques, but that the impact and scope would greatly increase and that their experiments would be better designed;
2. The kinds of molecules researches would like changes constantly and that often research questions are dismissed because the molecules required to perform experiments are not available;
3. That often researchers do not know which deuterated molecules are available;
4. That there can be an element of commercial sensitivity that should be considered by any facility producing deuterated materials for research groups.

Some additional analysis from the survey is included as an appendix to this report.

From the results of this survey, in addition to an analysis of the discussion that occurred at the workshop, the challenges facing European researchers seeking to use deuterated molecules can be summarised as follows:

1. The suite of deuterated molecules available commercially is limited. This results in neutron scattering experiments being performed on model systems which may not be optimal for the research question, or not being performed at all.
2. The range of deuterated molecules available from dedicated deuteration laboratories for neutron users in Europe, at ISIS (UK) and ILL (FR) currently, is limited – mainly by a lack of staffing resources. Staff at these facilities are generally occupied producing standard molecules or analogues of these.
3. Those molecules that *are* available from existing deuteration laboratories are often available only to researchers from the same country, or those who will perform their experiments at the home institutions.

Pleasingly, the DEUNET under SINE2020 is well placed to address these challenges, since it provides additional resources to the four laboratories in the network, but also facilitates the sharing of protocols, information and research results and also provides a mechanism for researchers to access deuteration facilities outside of their home country or outside of where their research takes place. The projects selected under the SINE2020 project are well-aligned with the research areas which are currently lacking in the deuteration community in Europe: particularly the projects related to novel monomers and polymers (lactic acid and polylactic acid; isoprene and polythiophene-based polymers), lipids (extraction of deuterated lipids from cell cultures). The third point is also addressed, with the ISIS deuteration facility expanding access to surfactants to non-UK users under SINE2020.

*Conclusions and Future work*

The work we have completed for D5.6 has provided a good understanding of the impact deuterium labelling has on the application of neutron scattering in Europe and around the world. It has further demonstrated the areas in which deuteration science must improve in order to continue serving the neutron scattering community. Pleasingly, this work has reinforced that the projects that have and will be undertaken by the Deuteration Network are well placed to improve the application of deuterium labelling in neutron scattering experiments. The Network recognises that the scientific landscape changes rapidly and so plans to continue surveying the community about how best to respond to needs for deuterated materials. While the survey is currently not accepting responses, it will be re-opened and advertised again in the future. The next Deuteration for Neutron Scattering – DEUNET workshop is tentatively scheduled for Q4 2018. Regular workshops such as this will help the DEUNET monitor and identify trends in deuterium-labelling neutron scattering applications.

*Appendix*

Figure 2. Classes of molecules currently used by the survey respondents and their proportions.

Figure 3. Techniques currently used by the survey respondents and their proportions.

Figure 4. Types of access that survey respondents anticipate requiring for chemical deuteration.

Figure 5. Neutron facilities that survey respondents use for experiments (with deuterated materials).