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Molecular Deuteration at the National Deuteration Facility: Diversity of Molecules and Application

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The National Deuteration Facility (NDF) at the Australian Nuclear Science and Technology Organisation (ANSTO) provides deuteration for a diversity of molecules and applications. Molecular deuteration of organic compounds and biomolecules significantly increases the options in complex structure function investigations using neutron scattering and reflectometry, nuclear magnetic resonance (NMR), mass spectrometry (MS) and other techniques. Deuterium (2H or D) is a naturally occurring stable isotope of hydrogen (1H or H). Deuteration can provide contrast and improved resolution to assist investigations into the relationship between molecular structure and function of molecules of both biological and synthetic origin.

The NDF at ANSTO is the only facility of its type in the Southern Hemisphere, having the specialised expertise and infrastructure for both biological and chemical molecular deuteration. Access is available via a merit-based user program. Since the open access user program began in 2010 we have delivered over 280 different labelled molecules to collaborators.

The NDF has developed a suite of capabilities in both *in vivo* deuteration of biomolecules and chemical deuteration of small organic molecules providing access to a broad range of deuterated molecules for research and industry. Variably deuterated proteins can be produced via simple defined yet robust NDF-developed methods of high-yield recombinant expression in *Escherichia coli*. Multiply-labelled (2H, 13C, 15N) proteins are also produced via these protocols for NMR applications. The development of chemical deuteration protocols for a broader range of molecular classes unavailable commercially and a tailoring of deuteration approach has increased the range of systems that can be investigated using deuterated molecules. Lipids, phospholipids (including head or tail or head/tail deuterated mono-unsaturated lipids such as POPC and DOPC), heterocyclics, aromatics, surfactants, ionic liquids, sugars and match-out detergents have been deuterated. Common neutron applications include partially deuterated proteins for SANS experiments investigating multi-protein systems, neutron crystallography of perdeuterated proteins, neutron reflectometry of lipid bilayers systems and SANS using saturated lipid vesicles, or detergents amongst others. Microbial systems have also been recently utilised to produce deuterated cellulose and cholesterol, expanding the range of biosynthesised molecules available.

Recent advancements and the impact of deuteration on the research outcomes achieved by using deuterated molecules produced by the NDF will be presented through case studies [1-3] highlighting the diverse applications that benefit from availability of custom deuterated molecules.

[1]. Disulfide isomerase activity of the dynamic, trimeric Proteus mirabilis ScsC protein is primed by the tandem immunoglobulin-fold domain of ScsB. Furlong, E. J., Choudhury, H. G., Kurth, F., Duff, A. P., Whitten, A. E. & Martin, J. L. Journal of Biological Chemistry, 293, 5793-5805. (2018)
[2]. Transient antibody-antigen interactions mediate the strain-specific recognition of a conserved malaria epitope. Krishnarjuna, B., Sugiki, T., Morales, R. A. V., Seow, J., Fujiwara, T., Wilde, K. L., Norton, R. S. & MacRaild, C. A. Communications Biology, 1, 58. (2018)
[3]. Controlled deuterium labelling of imidazolium ionic liquids to probe the fine structure of the electrical double layer using neutron reflectometry. Akutsu-Suyama, K., Cagnes, M., Tamura, K., Kanaya, T. & Darwish, T. A. Physical Chemistry Chemical Physics, 21, 17512-17516. (2019)

Speakers Gender

Female

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Do yo wish to take part in the poster slam

No

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