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Keywords: beta lactamase, neutron diffraction, toho-1

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Deuteration of oleic acid, lipids and other molecules for neutron studies

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In this paper, the synthesis and application of a range of deuterated organic molecules for the investigation of complex systems in the fields of structural biology, biotechnology and nanotechnology will be discussed. In chemical reactions, deuterium (^{2}H) behaves similarly to hydrogen (^{1}H); however, the different physical properties of the hydrogen and deuterium nuclei mean that they scatter neutrons quite differently. Techniques such as Small Angle Neutron Scattering, Neutron Reflectometry and Neutron Crystallography exploit this difference in scattering length densities to obtain data for properties such as: atomic and molecular structure, the precise location of hydrogen atoms in organometallic systems, and highlighting molecular components in complex nanostructured systems.

In studies where one may wish to observe the interaction between hydrocarbon-based chemicals or biological molecules with lipids or surfactants, there is often a lack of neutron scattering contrast in the system which can be overcome by deuteration of the tail component of these lipids or fatty acids. Oleic acid forms an unsaturated tail component in many phospholipid molecules that are fundamental to the structure and functioning of cellular membranes. We have recently produced deuterated oleic acid on a gram scale in our laboratories from deuterated fatty acid molecules with the appropriate mono- and bi-functional terminal groups; prepared using a multi-step reaction scheme. This involved hydrothermal heterogeneous catalytic H/D exchange reactions in D_2O followed by synthetic reactions. Conjugating the two deuterated alkyl chains using the Wittig reaction afforded purely a *cis*-conformation around the carbon-carbon double bond, essentially producing deuterated oleic acid. This facilitated the synthesis of deuterated glycerol monooleate through esterification of the prepared d-oleic acid with a glycerol fragment. Similar reactions were also used to prepare lipids with hydrophobic (different alkyl chain lengths) and hydrophilic (ethylene oxide) moieties where the head group is conjugated to a sulfur- or alkene-containing anchoring ligands for surface modification and self-assembly (i.e., on gold or silicon surfaces).

The strategies used for deuteration and synthesis of oleic acid, lipids, surfactants, sugars, bioactive small organic molecules, heterocyclic and aromatic compounds will be presented. We will also demonstrate how the availability of these deuterated compounds greatly increases the scope of some neutron scattering, reflectometry and diffraction experiments. For example, deuterated trehalose was used to determine the localisation of sugar molecules with respect to lipid head groups using neutron diffraction, to provide insight into the molecular mechanisms of cryoprotection by sugar molecules. Using neutron scattering, deuterated oleic acid and glycerol monooleate allowed investigation of surfactant interaction with cubosome and hexosome liquid crystal nanoparticles forming 3D structures with intertwining aqueous channels. Deuterated organic light emitting diode (OLED) molecules facilitated investigation of the morphology of thin-film multilayer organic light emitting devices using neutron reflectometry [1].

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Cyber-enabled learning and practice in crystallography: educating the next generation

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This talk will describe the current state of crystallographic science and new pedagogy made possible by Web 3.0. In the last fifteen years, academic crystallography has largely migrated from a research specialty to a technique employed by a broad user community. Yet, the knowledge gained from analysis of its structures is a key underpinning of modern science and technology. Crystallography has gained importance for researchers in disciplines where it has not previously appeared, such as engineering and solar energy technology. Technical advances, however, now enable users with little or no training, or deeper understanding, to often but not always produce quality results, as revealed by recent high profile and embarrassing retractions in the peer reviewed literature, many the result of pathological science or inadequate review. The absence of crystallography in many curricula has led to growth of and dependence on independently funded workshops and summer schools, as well as other, non-traditional curricular resources for crystallography instruction, such as Web pages and online courses, which allow crystallography to be self-taught. Implementing modern Web technologies with sound pedagogy requires skilful integration of relevant, often disparate resources into useful and usable frameworks, enabling learners to interact, explore new situations, and use scientific reasoning skills such as hypothesis testing and model-based reasoning. The evident disproportion in implementing contemporary technologies into our global crystallography education resources requires that we shift our focus from simply imparting content knowledge to empowering students with the fundamental processes and skills needed for on-demand learning and practice in crystallography.

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Promoting crystallography: using crystal structures in chemical education

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Crystallography is truly interdisciplinary. It has its roots in physics, mathematics and computer science, and has practitioners and beneficiaries from chemistry, biology, materials science and many other disciplines. Despite its pre-eminence as *the* preferred method for