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National Deuteration Facility (NDF)

Chemical Deuteration

The National Deuteration Facility (NDF) is the only facility of its type in the Southern Hemisphere. It is partially funded by the National Research Infrastructure for Australia initiative.

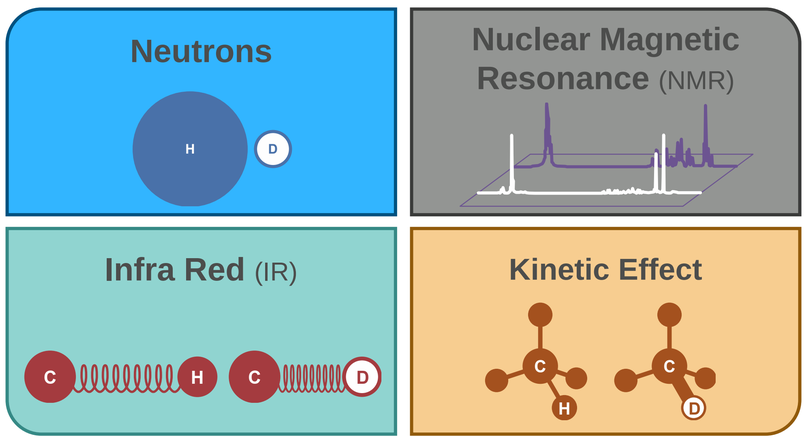
This unique facility offers molecular deuteration using both *in vivo* biodeuteration and chemical deuteration techniques.

Chemical deuteration

Chemical deuteration involves deuterating whole molecules or building blocks for the synthesis of a desired molecule by exposing them to D_2O at high temperatures and pressures in the presence of a catalyst. If required, compounds can then be synthesised from the deuterated building blocks using organic chemistry techniques.

Why is deuteration important?

Molecules synthesised via chemical deuteration are utilised for a number of different analysis techniques.



Capabilities

Some of the deuterated molecules able to be synthesised using chemical deuteration include:

- Saturated fatty acids (C4 – C20)
- Unsaturated fatty acids (e.g. oleic acid)
- Lipids and phospholipids
- Substituted aromatics
- Sugars (e.g. sucrose, trehalose)
- Surfactants
- Detergents
- Cholesterol
- Radiotracers/radiopharmaceuticals
- Ionic liquids
- Branched chain alcohols (e.g. phytantriol)
- Mineral oils
- Polyalkenes

Applications

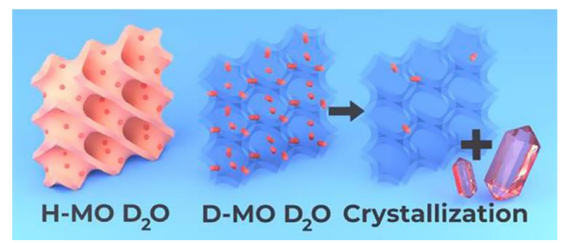
Chemical deuteration can provide information in a wide variety of scientific and technological disciplines including:

- Structural biology
- Thin film devices and molecular electronics
- Energy and gas adsorption materials
- Drug delivery
- Drug metabolism

Case studies

In meso crystallisation of membrane proteins

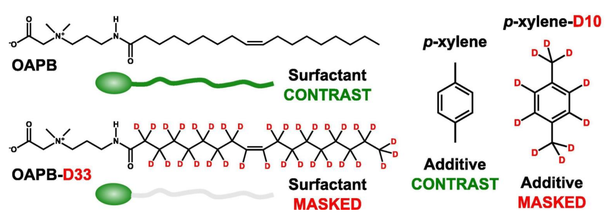
Deuterated monoolein (D-MO) has been used to provide contrast matching during small-angle neutron scattering experiments to observe the behaviour of integral membrane proteins during *in meso* crystallisation.

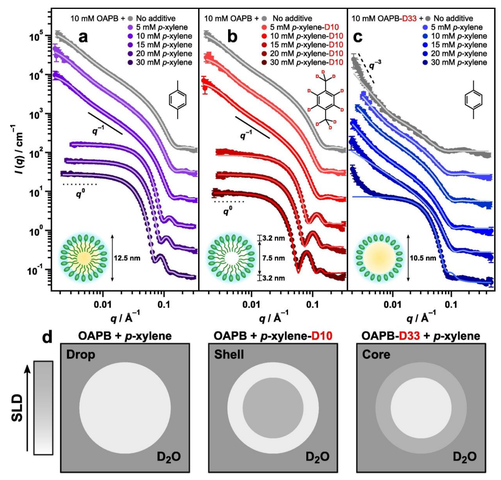


Langmuir 2019, 35, 8344−8356

Self-assembly of micellar fluids

The deuterated surfactant (oleyl amindopropyl betaine) spontaneously forms wormlike micelles in aqueous solutions. It has been mixed a variety of aromatic additives to study the effects of aromaticity and polarity of bulk assembly using small-angle neutron scattering.



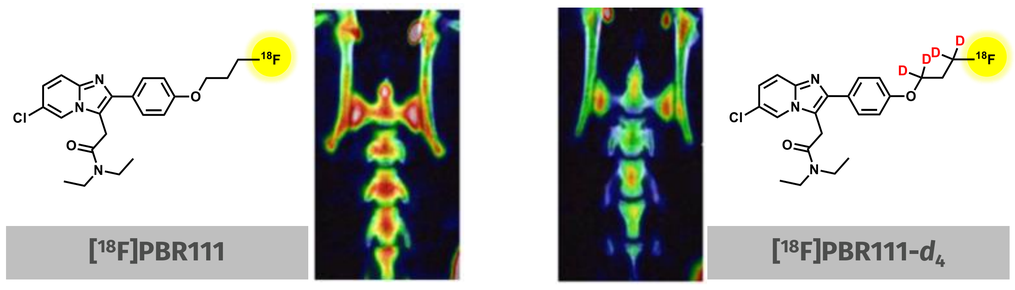


J. Colloid and Interface Sci. 2019, 534, 518-532.

Increasing metabolic stability of radiotracers with D incorporation

NDF and ANSTO colleagues have investigated the deuterium kinetic isotope effect (DKIE) on extending the metabolic lifetime of radiotracers.

A deuterated radiotracer, [^{18}F]D4-PBR111 was developed and evaluated *in vivo* in rats, showing it is more resistant to metabolic breakdown compared to non-deuterated [^{18}F]-PBR111 allowing better medical imaging.



Anal. Chim. Acta 2019, 1064, 65-70 / Nucl. Med. Biol. 2021, 96-97, 112-147

Access

NDF deuteration capabilities are offered through a merit-based proposal program. Accelerated or commercial access can be provided subject to service charges.

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