National Deuteration Facility
ANSTO’s National Deuteration Facility (NDF) offers the facilities, staff and expertise to produce molecules where all or part of the molecular hydrogen is in the form of deuterium (H or D).

The facility produces deuterated proteins, biopolymers, nucleic acids and synthesises small organic molecules such as lipids, phospholipids, sugars, surfactants, aliphatic hydrocarbons and aromatic, heterocyclic compounds. Double and triple labelling of proteins with both deuterium and the stable isotopes carbon-13 and/or nitrogen-15, are also available.

The NDF also produces deuterated molecules to enhance the properties of materials used in industry and health.

The NDF offers molecular deuteration using either in vivo biodeuteration or chemical deuteration techniques.

A unique facility

**Biological deuteration**

Biodeuteration involves the growth of microorganisms (commonly E. coli) in a heavy water (D,O) culture medium supplemented with either a deuterated or hydrogenated carbon compound, depending on the level of deuteration required. The biomass is harvested and the deuterated molecule (e.g. protein) is purified and characterised.

**Chemical deuteration**

Chemical deuteration involves deuterating whole molecules or building blocks for the synthesis of a desired molecule by exposing them to D,O 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.
Case studies

01 The morphology and structure of Organic Light Emitting Diodes (OLED)

Deuteration of the organic compounds provided the contrast, enabling detection of diffusion between two layers of an OLED when heated, using neutron reflectometry.

![Diagram of OLED structure](image)


02 Storage in solid Metal-Organic Frameworks (MOF)

Neutron diffraction experiments are used to unveil the site-specific binding properties of CO2 within MOF materials while systematically varying both the amount of CO2 and the temperature. A comprehensive study of carbon dioxide adsorption in the metal-organic frameworks M2 (dobdc).

![Diagram of MOF structure](image)

Queen et al., 2014. Chem. Sci., 5, 4569 (journal back cover).

03 Structural characterisation

Structural characterisation of the interaction between:

- HIV-1 structural matrix protein (MA)
- the intracellular mediator protein, calmodulin (CaM)

Binding of HIV-1 MA protein to deuterated calmodulin, modelled from small-angle neutron scattering (SANS) conducted at multiple solvent contrasts.

"Calmodulin binds a highly extended HIV-1 MA Protein that Refolds upon its release"


![Diagram of MA and CaM interaction](image)
### Types of deuterated molecules produced

| Saturated fatty acids, alcohols, bromides, amines, aldehydes, thiols, alkanes | Partial and perdeuterated recombinant proteins |
| Saturated diacids and bifunctional surface active molecules | Double and triple labelled recombinant proteins |
| Deuterated silanes | Unsaturated fatty acids (e.g. oleic acid) |
| Membrane protein detergents (e.g. DDM and OG) | Glyme and glycol ethers |
| Deuterated surfactants including ionic and non-ionic | Lipids including glycerides; phospholipids (e.g. DOPC and POPC); and selective deuteration of lipids (head deuterated, tail deuterated and fully deuterated) |
| Aromatics and heterocyclics for MOFs | Deuterated cholesterol and derivatives |
| Compounds for organic light emitting diodes and solar cells | Electrolytes for batteries |
| Selective deuteration of small drug molecules including radio-tracers | Sugars |
| Biopolymers – cellulose, chitosan, chitin, PHAs | DNA |
Applications of deuteration

- Drug delivery
- Thin film nanotech devices
- Food-lipid digestion
- Energy and gas storage materials
- Biopolymers and biotechnology
- Mechanistic studies
- Structural biology
- Thin film nanotech devices
- Food-lipid digestion
- Energy and gas storage materials
- Biopolymers and biotechnology
- Mechanistic studies
- Structural biology

Activities enabled

- New materials and applications
- NMR spectroscopy
- Neutron scattering
- Vibrational spectroscopy

NDF
National Deuteration Facility
Access

Access to the NDF is merit-based through a proposal program via the ACNS Customer Portal; however, in some cases, NDF can provide deuterated material with some cost recovery.

For enquiries please contact us on ndf-enquiries@ansto.gov.au

Locations

Lucas Heights | Camperdown | Clayton

www.ansto.gov.au