Australian Government

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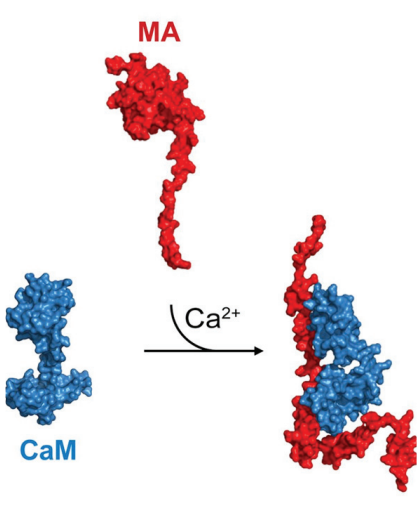
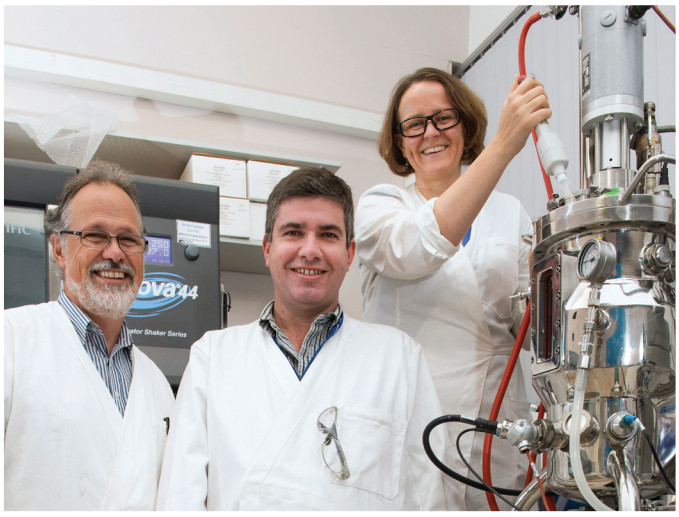
National Deuteration Facility





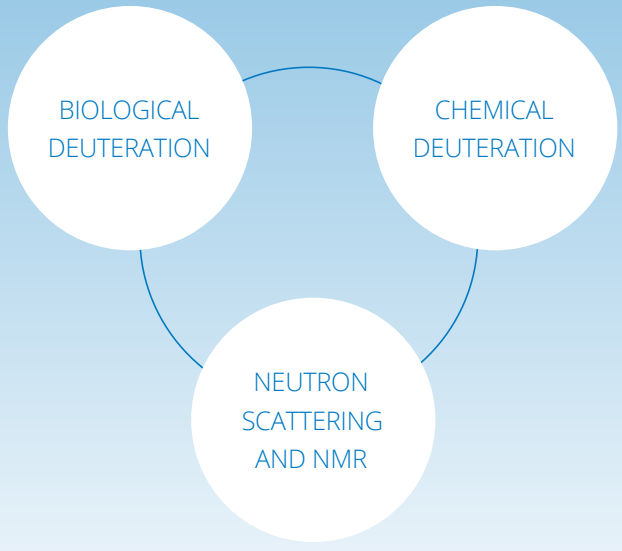
National Deuteration Facility

The Australian Nuclear Science and Technology Organisation's (ANSTO) 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 (^{2}H or D).

The facility produces deuterated proteins, biopolymers, nucleic acids and synthesised 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 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_2O) culture medium supplemented with either a deuterated or hydrogenated carbon substrate, depending on the level of deuteration required. The biomass is harvested and the deuterated molecule (e.g. protein) is purified and characterised.

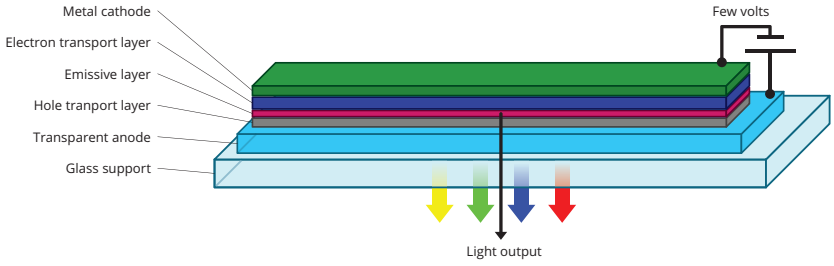
Chemical deuteration

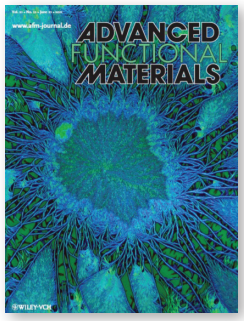
Chemical deuteration involves deuterating whole molecules or building blocks for the synthesis of a desired molecule by exposing them to D_2O at high temperatures and pressures in the presence of a catalyst. If required, compounds can then be synthesised from the deuterated building blocks using organic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

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.

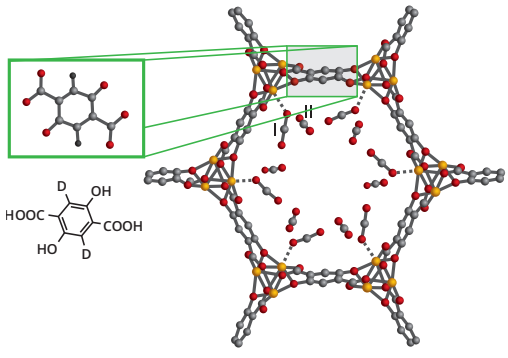


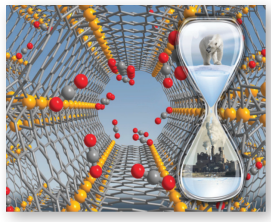


Smith et al., Adv. *Funct. Mater*. 2011, 21 (12), 2225-2231 (journal front cover).

02 Storage in solid Metal-Organic Frameworks (MOF)

Neutron diffraction experiments are used to unveil the site-specific binding properties of CO_2 within MOF materials while systematically varying both the amount of CO_2 and the temperature. Deuterated materials enabled a comprehensive study of carbon dioxide adsorption in the metal-organic frameworks M2 (dobdc) (M = Mg, Mn, Fe, Co, Ni, Cu, Zn).





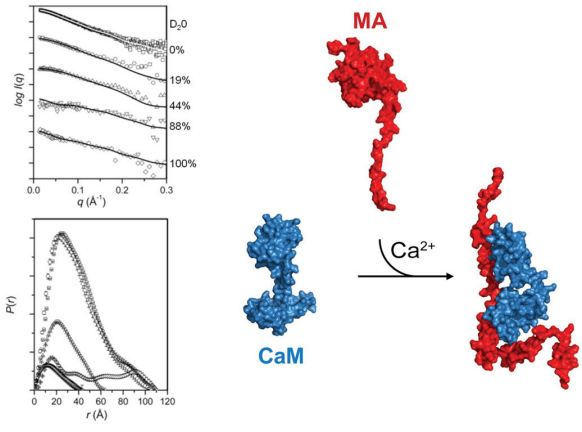
Queen et al., *Chem. Sci.* 2014, 5 (12), 4569-4581 (journal back cover).

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" Taylor et al., *Biophys*. J. 2012, 103 (3), 541-549.

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	Compounds for organic light emitting diodes
Compounds for solar cells	Electrolytes for batteries
Selective deuteration of small molecules	Sugars
Biopolymers – cellulose, chitosan, chitin, PHAs	DNA

Applications of deuteration

Drug delivery	Thin film nanotech devices	Food-lipid digestion
Energy and gas storage materials	**NDF** National Deuteration Facility	Molecular electronics
Biopolymers and biotechnology	Mechanistic studies	Structural biology

Complementary techniques

Neutron scattering

NMR spectroscopy

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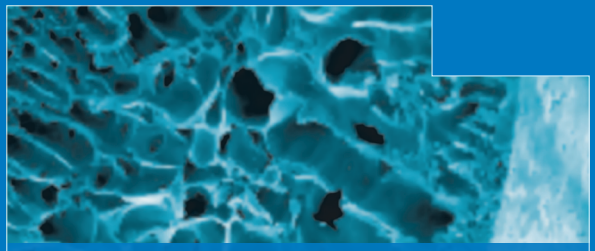

New materials and applications

Vibrational spectroscopy

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www.ansto.gov.au/ndf

Access

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

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

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