

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.

The chemical deuteration facility at the NDF consists of four labs that are fully equipped for the synthesis, purification and characterisation of deuterated molecules. Two wet chemistry laboratories accommodate eight hydrothermal Parr reactors for H/D exchange to generate perdeuterated precursors for the synthesis of target molecules.

The Parr reactors are of different sizes ranging from 50 mL vessels for method development, to 1200 mL vessels for large scale synthesis of deuterated materials. Two additional laboratories contain all of the instruments that are required for analysis, purification and characterisation of the deuterated products.

Deuterated molecules

The chemical deuteration laboratories offer a variety of classes of deuterated molecules. Please refer to our document on sample deuterated molecule. All enquiries should be directed to **Tamim Darwish** or **Peter Holden**.

Certificate of analysis

All of the deuterated compounds produced by the chemical deuteration facility will be analysed and characterised using the facility's analytical instruments. This includes multi-nuclear NMR spectroscopy; 1H , 2H , ^{13}C and ^{31}P (for phospholipids) to confirm purity and to calculate the deuteration level at the different molecular sites.

In addition, MS will be used to calculate the isotopic abundances of the different isotopologues which provides a measure of the overall deuteration level of the product. The NDF has a polarimeter for sugars and other optically active compounds, TLC, HPLC and other analytical and chromatographic methods will also be used when appropriate.

The NDF will provide a **Certificate of analysis** for each deuterated product produced by the facility.



Capabilities

- Synthesis laboratories
- Parr reactors (50 ml – 1200 mL)
- GPC
- HPLC
- Flash chromatography
- IR spectroscopy
- Polarimetry
- LC-MS
- NMR spectroscopy

Proposals for molecular deuteration should be submitted at <http://neutron.ansto.gov.au>.

You can also contact **Professor Peter Holden** on + 61 (2) 9717 3991 or other NDF staff at any time.