



Australian Government

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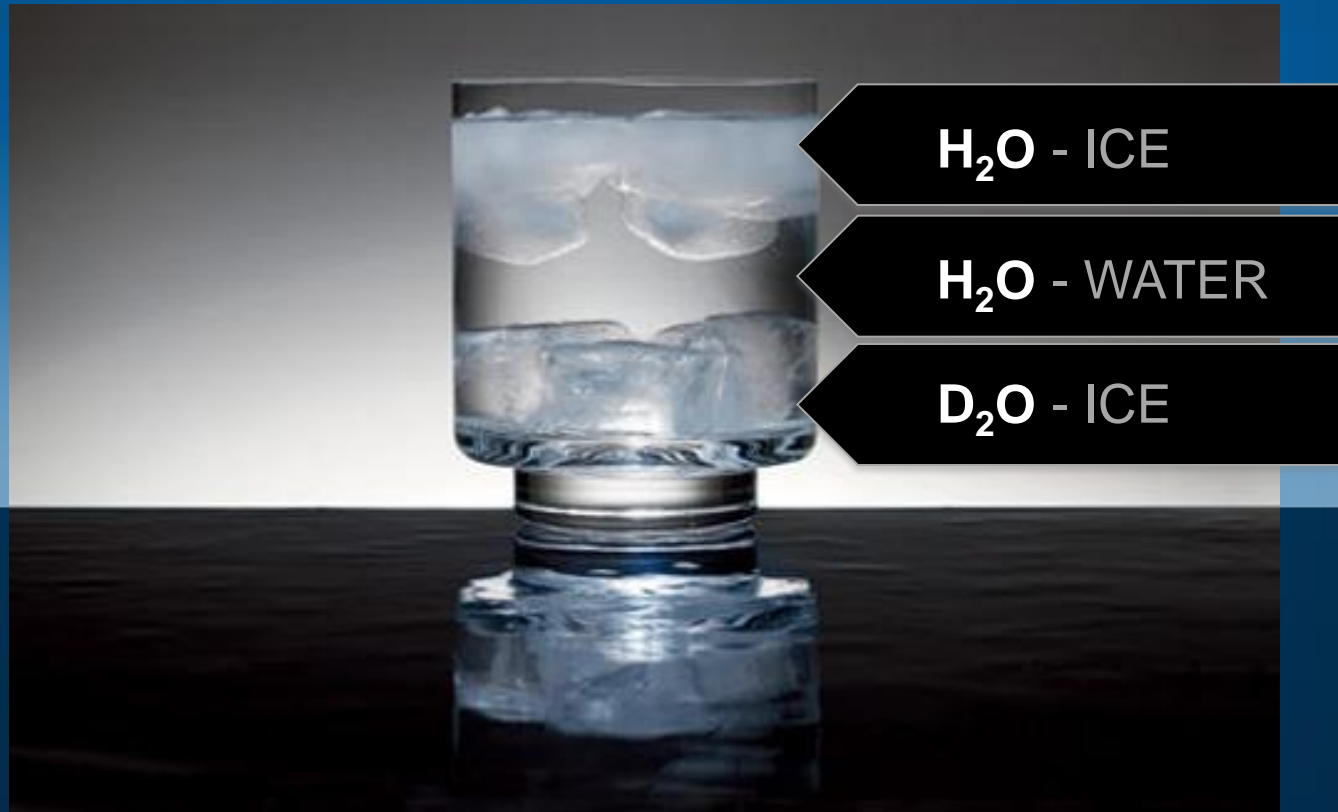
# National Deuteration Facility

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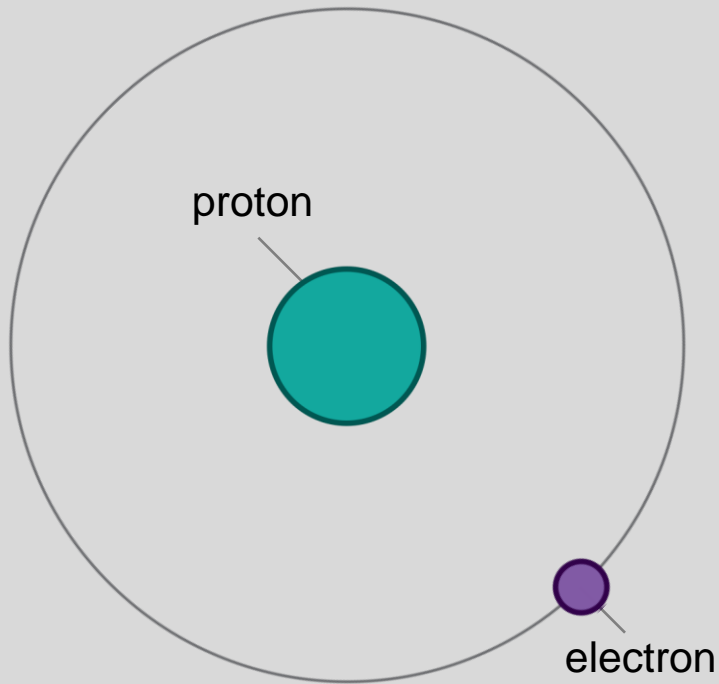
Tamim Darwish

New Users Symposium, September 2016

# Heavy ice from heavy water - $D_2O$

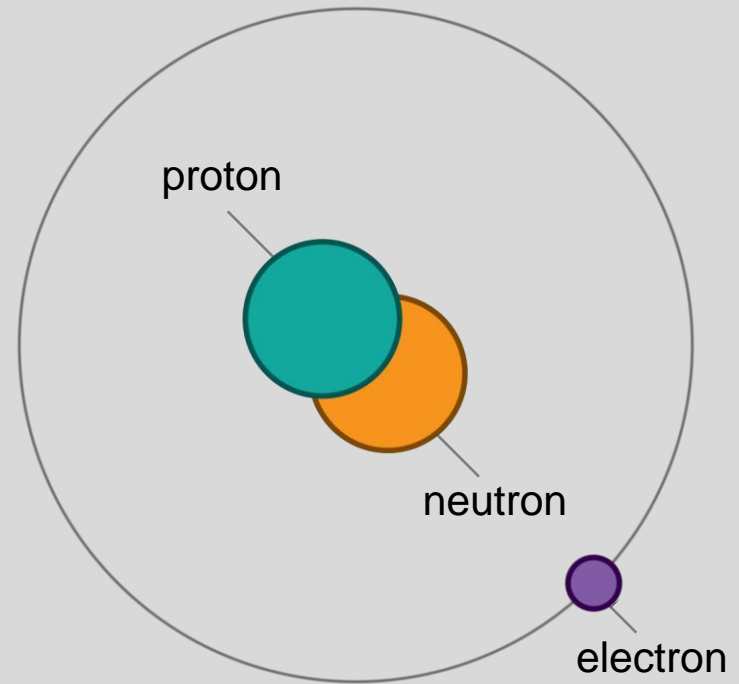


# Hydrogen isotopes



**Protium ( ${}^1\text{H}$ , H)**

6420



**Deuterium ( ${}^2\text{H}$ , D)**

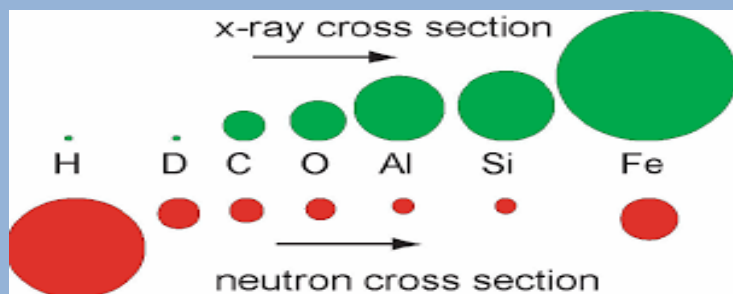
1

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# Why deuterate?

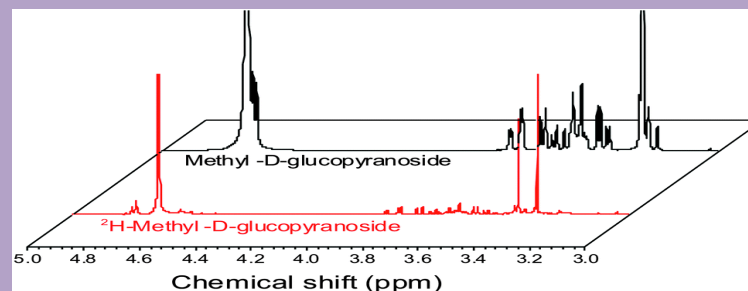
## Neutrons

Interact with the nucleus- Scattering length



## NMR

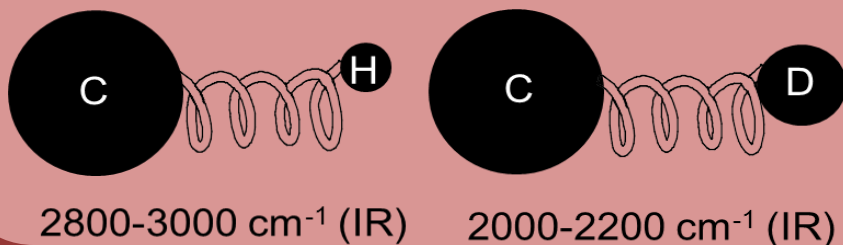
Nuclear spin properties



## Infra Red

Vibration frequencies

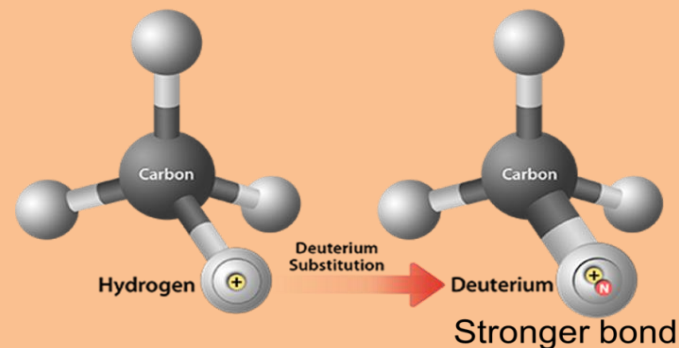
Vibrational modes



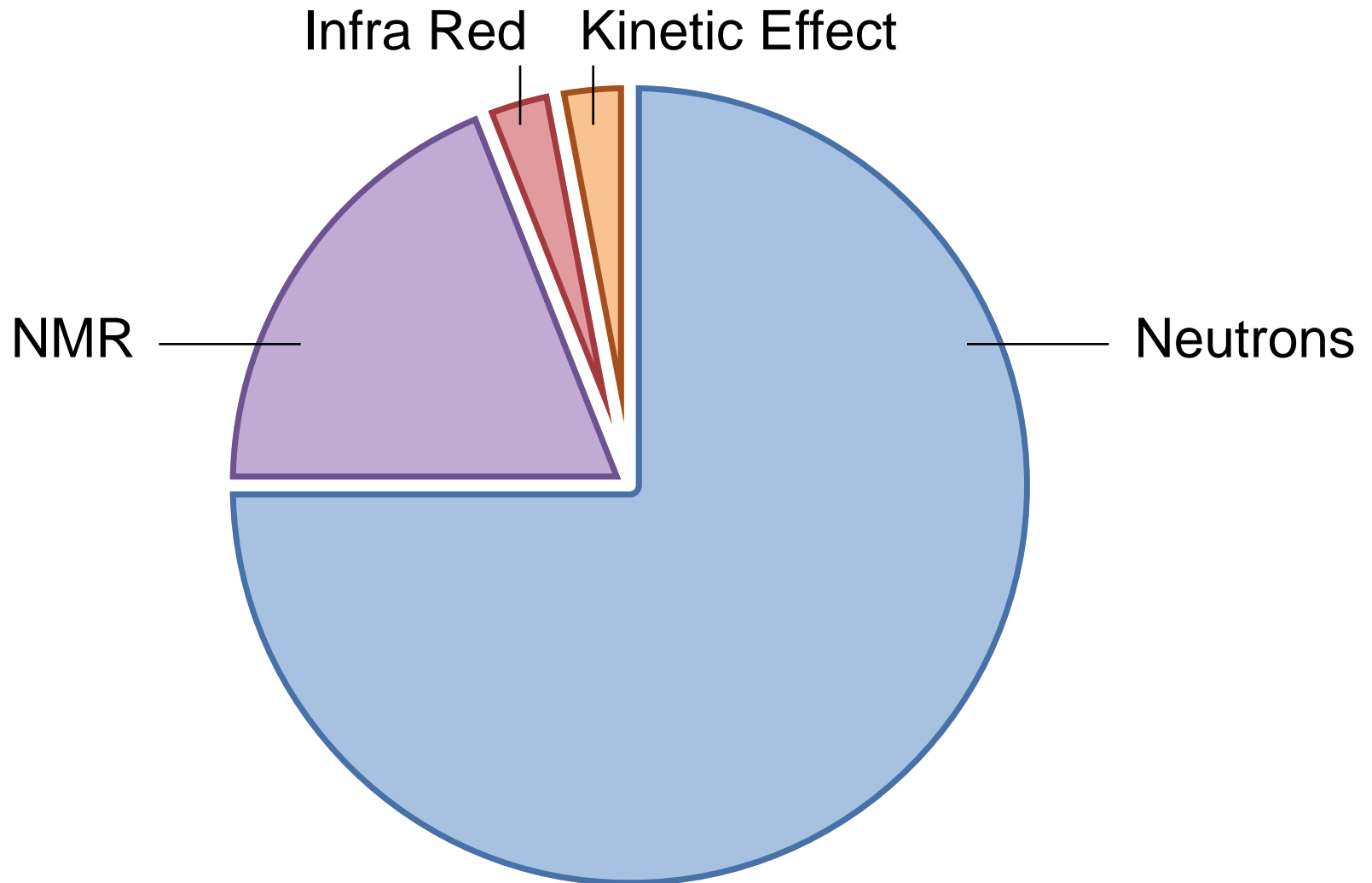
## Kinetic Effect

Non-Deuterated

Deuterated



# NDF usage breakdown



# What is the NDF?

- ANSTO/NCRIS funded facility
- Access via a merit based proposal system, two-rounds per year

**NCRIS**  
National Research  
Infrastructure for Australia  

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An Australian Government Initiative



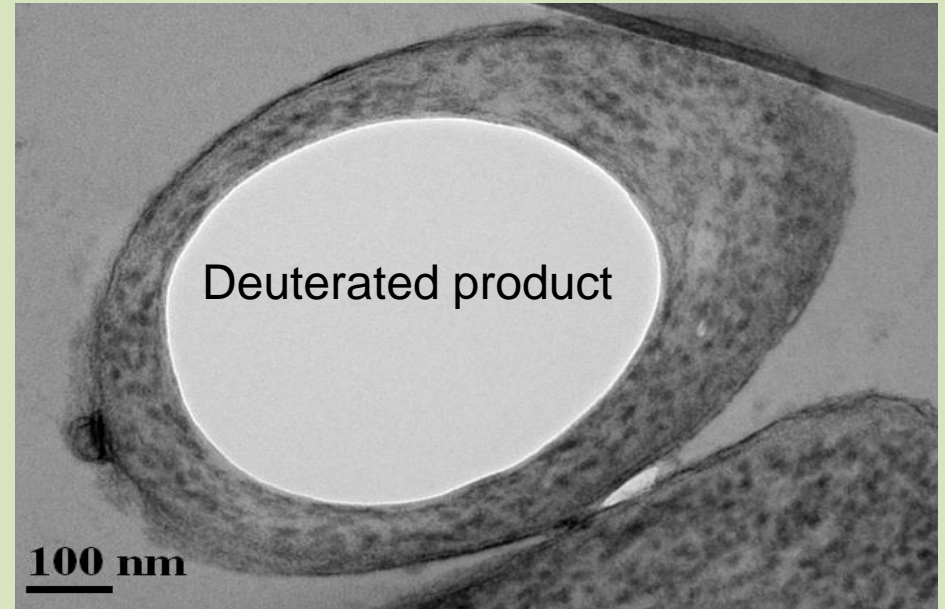
# Biological and Chemical Deuteration

## Chemical synthesis in D<sub>2</sub>O



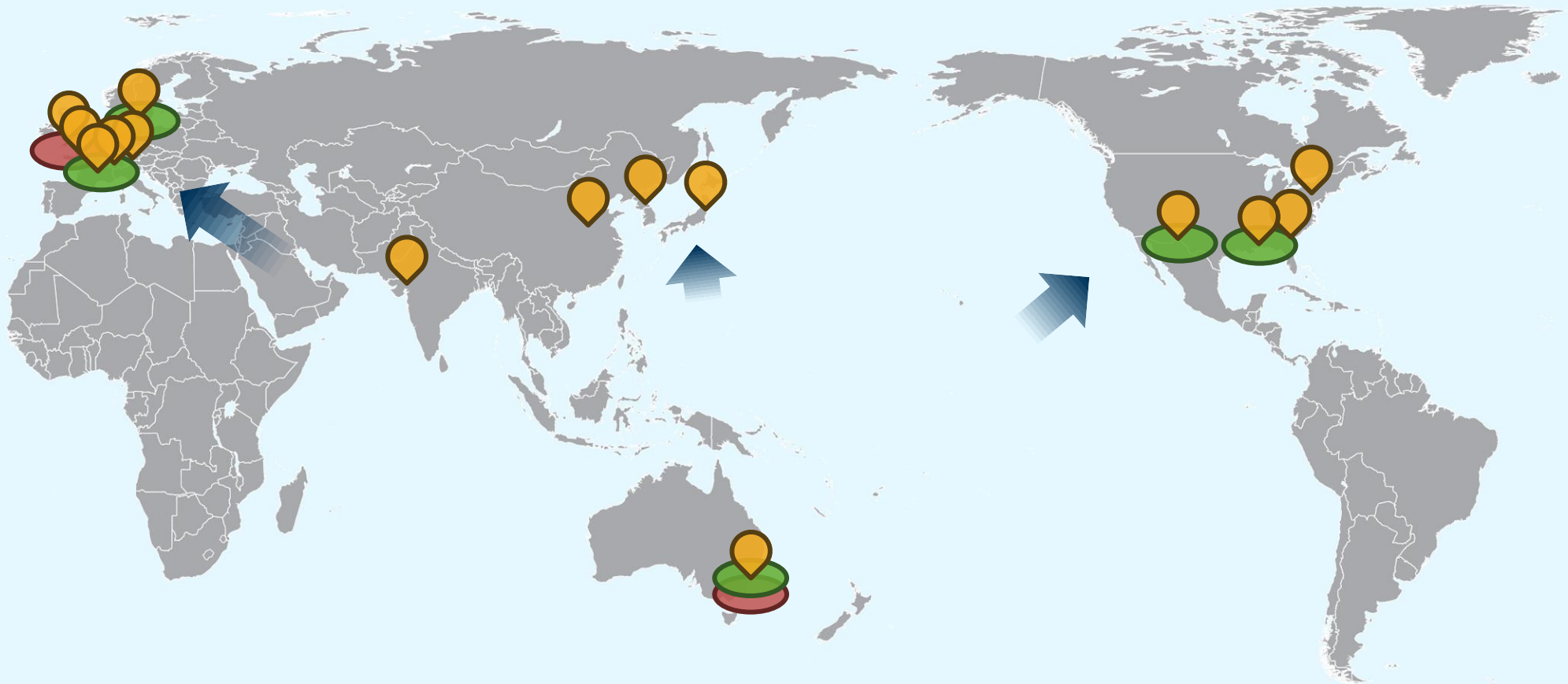
Chemical Deuteration  
(surfactants, lipids, small molecules)

## Growing bacteria in D<sub>2</sub>O



Biological Deuteration  
(proteins, DNA, RNA, carbohydrates)

# Neutron and deuteration facilities



 Neutron facility

 Biological deuteration

 Chemical deuteration



# Bio-deuteration Capability

**Biopolyesters – Poly-Hydroxyalkanoates**

**Partially and perdeuterated proteins**

**DNA**

**$^2\text{H}$  /  $^{15}\text{N}$  /  $^{13}\text{C}$  proteins**

**Cellulose**

**Chitosan**

**Selectively labelled proteins**

# Chemical Deuteration Capability

## ➤ Deuterated Lipids, Phospholipids, Sugars, Fatty acids (saturated, branched, unsaturated)

### NR, SANS

- Digestion of lipids
- Bilayer lipid membrane models
- Organic gelators
- Lyotropic liquid-crystalline phases
- Cryoprotective membranes

## ➤ Deuterated Metal Organic Framework and battery electrolytes

### Neutron Diffraction

- Energy & gas storage materials
- Mechanism of their thermal dynamics (NTE)

## ➤ Deuterated Organic Light Emitting Diodes

### NR

- Morphology and diffusion of organic layers in OLED devices

## ➤ Deuterated Surfactants and Detergents

### SANS

- Match-out detergent for structural studies of integral membranes
- Nano-structures in ionic liquids

## ➤ Organometallic Ligands

### Inelastic NS

- Metal hydride- mechanism of catalytic processes

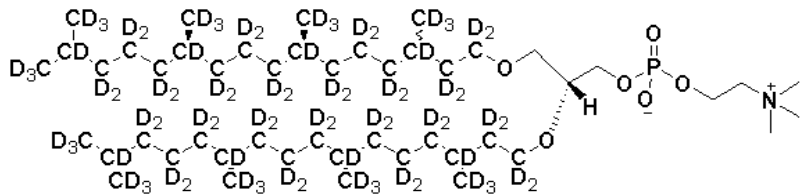
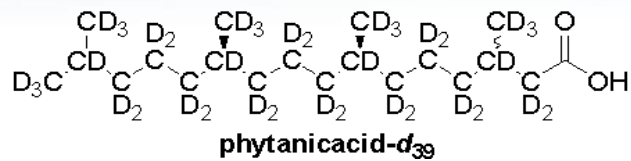
## ➤ Organic Liquids

### Quasielastic NS

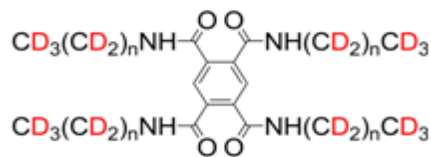
- Molecular dynamics within supercooled liquids.

# Samples of Deuterated Chemicals

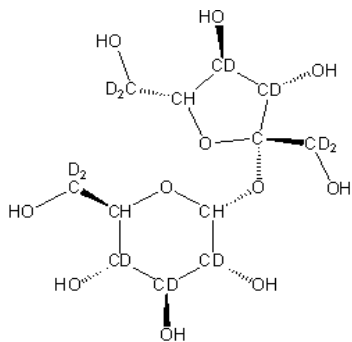
## Branched Fatty acids and Lipids



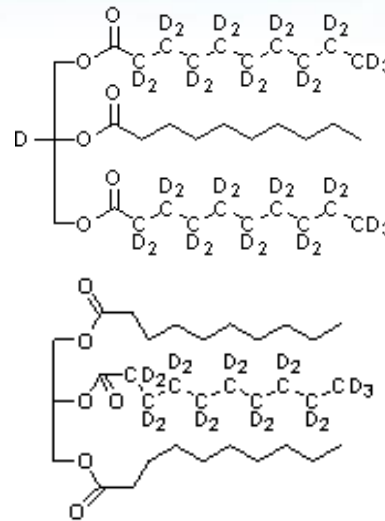
## Gelators



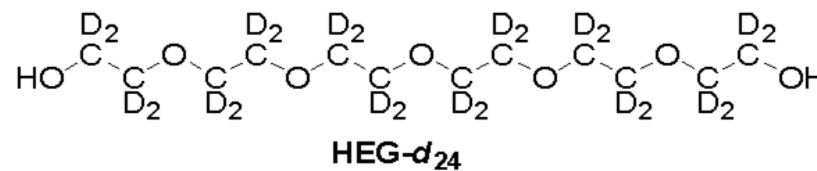
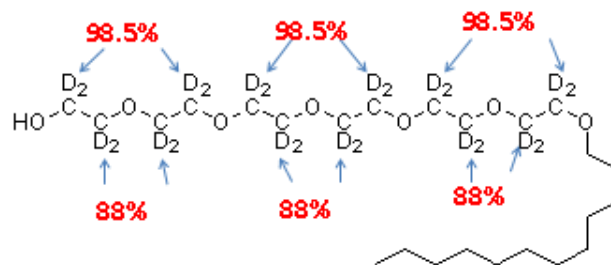
## Sugars



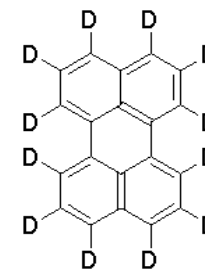
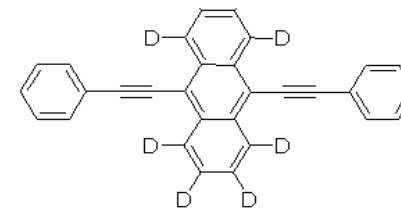
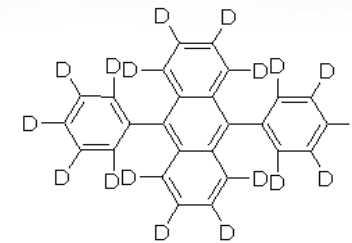
## Triglycerides



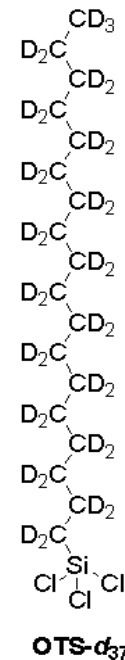
## Non-ionic surfactant



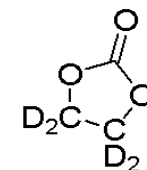
## Solar Dyes



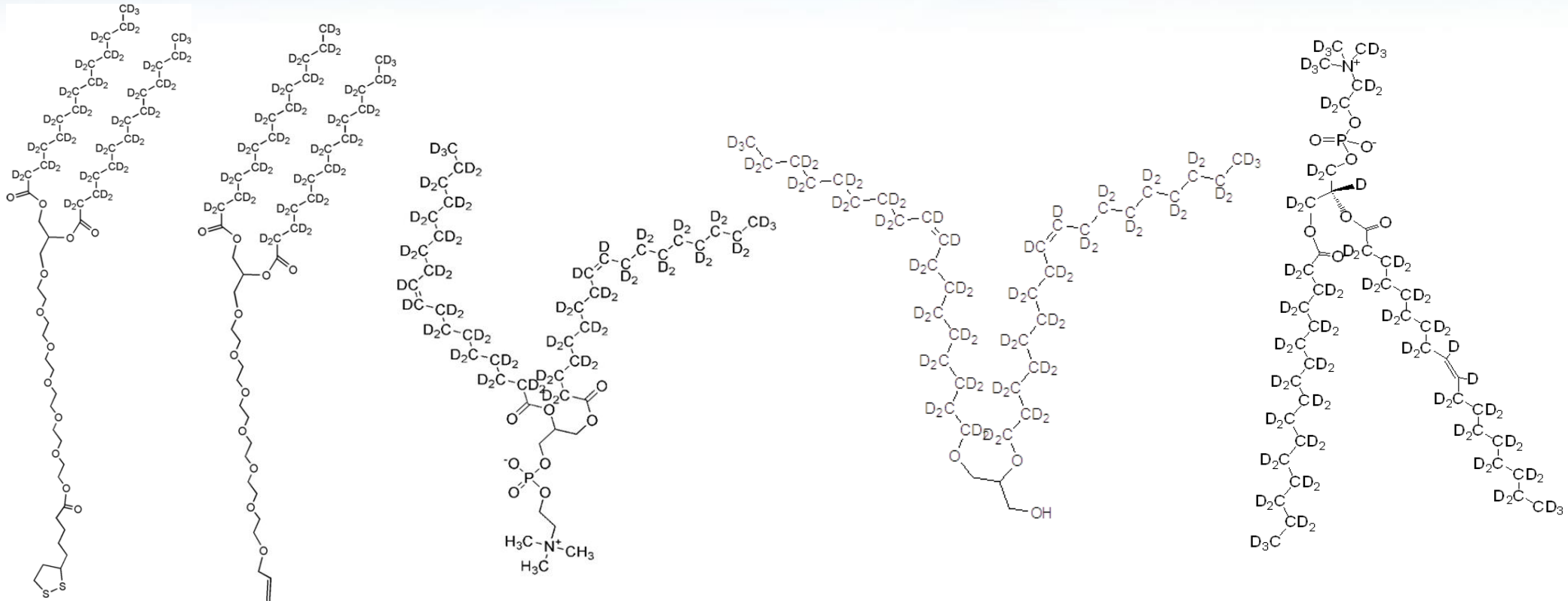
## Silyl compounds



## Electrolytes



# Samples of Lipid



Tethered Lipids

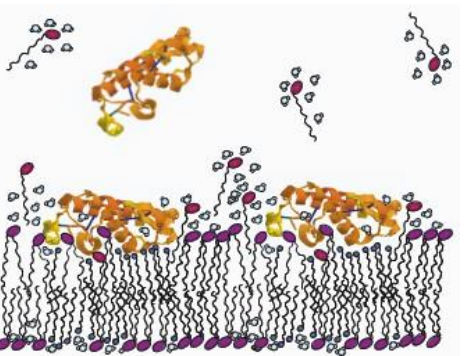
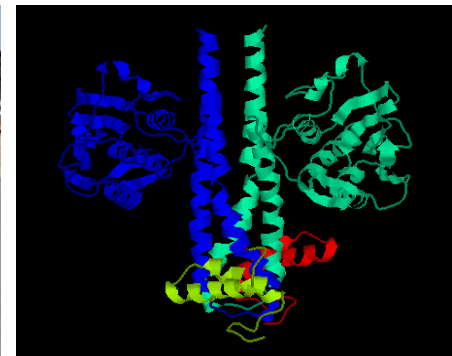
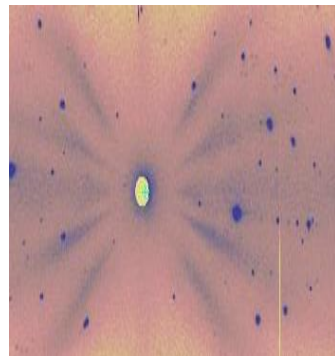
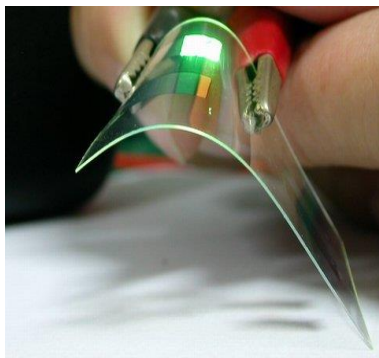
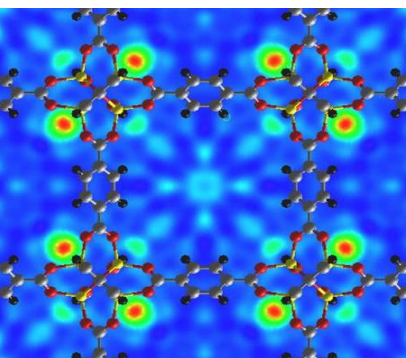
DOPC-deuterated tail  
gram scale!

GMO, GDO

POPC

➤ Deuterated head groups e.g., DOPC, POPC, DOPI, DOPE ...etc

# National Deuteration Facility applications



**For more: Visit our page**

<http://www.ansto.gov.au/ResearchHub/Bragg/Facilities/NationalDeuterationFacility/>

# The NDF team





Australian Government

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**ansto**

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**Thank you**

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