Giovanna Fragneto(Rachel Morrison)

Raba)Tamim DarwishPeter Holden

Peixun LiKun Ma

Jürgen Allgaier(Andreas

Krishna Batchu

Marek Jura

John Webster

WP5 DEUNET

European chemical deuteration platform

JÜLICH FORSCHUNGSZENTRUM

Australian Government
Department of Education, Science and Training

DEUNET Platform

- Benefit from **methods/expertise/manpower** at all facilities
  - **Cost effective platform** to share materials
- **Include University, international and industrial partners**

Goals:

1. **User access** to existing products and services of the labs
2. **Development** of new methods and products
3. **Innovative materials** synthesized in collaboration between labs
4. **Coordinated access** for all European neutron users by 2019

- **ISIS:** Chemical deuteration by catalytic H-D exchange and synthesis of surfactants
- **ILL:** Extraction and purification of molecules from deuterated cell cultures
- **FZJ:** Polymer synthesis
- **ESS:** Synthesis of complex deuterated molecules

Network coordination

Survey of European deuteration needs

Sustainability plan by 2019

D	Name	Lead	Type	Diss	Month
5.1	Webpage and user portal	ESS	DEC	PU	9
5.2	Synthesis of deuterated precursors	STFC	R	CO	12
5.3	Novel route for isoprene synthesis	FZJ	R	PU	15
5.4	Synthesis of L- and D-lactic acid	ESS	DEM,R	PU	18
5.5	Synthesis of deuterated polythiophenes	FZJ	R	PU	20

5.6	**Report on DEUNET requirements (workshop)**	**ESS**	**R**	**PU**	**24**
5.7	Synthesis of surfactants for non-UK users	STFC	R, DEM	PU	28
5.8	Synthesis of deuterated polylactic acid	FZJ	R, DEM	PU	30
5.9	Optimisation of purification methods	ILL	R	PU	36
5.10	Physico-chemical characterisation	ILL	R	PU	42
5.11	Synthesis of deuterated lipids/surfactants	ESS	R	PU	42
5.12	Report on DEUNET management and access	ESS	R	PU	48

- Establishment of a new chemical deuteration laboratory at ESS
  - European User Survey (2017) on deuteration use and needs:

Top requests: Lipids, surfactants and polymers ■ Access to STFC deuteration facility to European users ■ Development of methods for lipid deuteration, and separation from cell cultures at ILL

- Joint R&D and new collaborations in e.g. enzymatic + chemical synthesis of chiral biopolymers at FZJ and ESS.
- DEUNET webpages
- New members of DEUNET – worldwide deuteration network

Objectives ■ **Chemical deuteration by catalytic H-D exchange and synthesis of surfactants:**

Kun Ma (open end contract), >40 d-chemicals, involved actively in 4 research projects(one of them is industrial parter)

- ***Provision of starting materials***:

  Successfully synthesis starting materials for user community and DEUNET parters

- ***Expanding access*** to the existing compounds for ***European (non-UK) researchers*** (D5.7)

  More than 15 Non-UK researchers have been supported by STFC under DEUNET

- Improved syntheses for the production of deuterated ***unsaturated fatty acids*** *(D5.7, D5.11)*

  The large quantities of per-deuterated and half-deuterated Oleic acid has been synthesized, and has been used for user's NR experiment at ISIS.

- ***Development of routes to novel bio-surfactants*** in collaboration with ILL and ESS (D5.11).

  Supplied deuterated precursors and strategy discussion for the novel surfactant development

Other activies:

- Strong collaboration with DEUNET Partner FZJ

  Synthesized d- and h- Triton-100, Jurgen Allgaier(JA), KM, PL, 10-15 June 2018

  Synthesized d-PDMS, d-PEG(10) and d-PEG(50), 18-JA, PL, Jian LU, 28 September 2018 ■ Organized 3 DEUNET and STFC Deuteration conferences/workshops ■ International conferences, such ACS spring meeting, 2019, PL, JW.

Continuation (sustainability):

- STFC WILL carry on the collaboration with DEUNET's partners, and share knowledge of Deuteration.
- Particularly interested in working on any science driven project with DEUNET partners, academia and industry.

Chemical

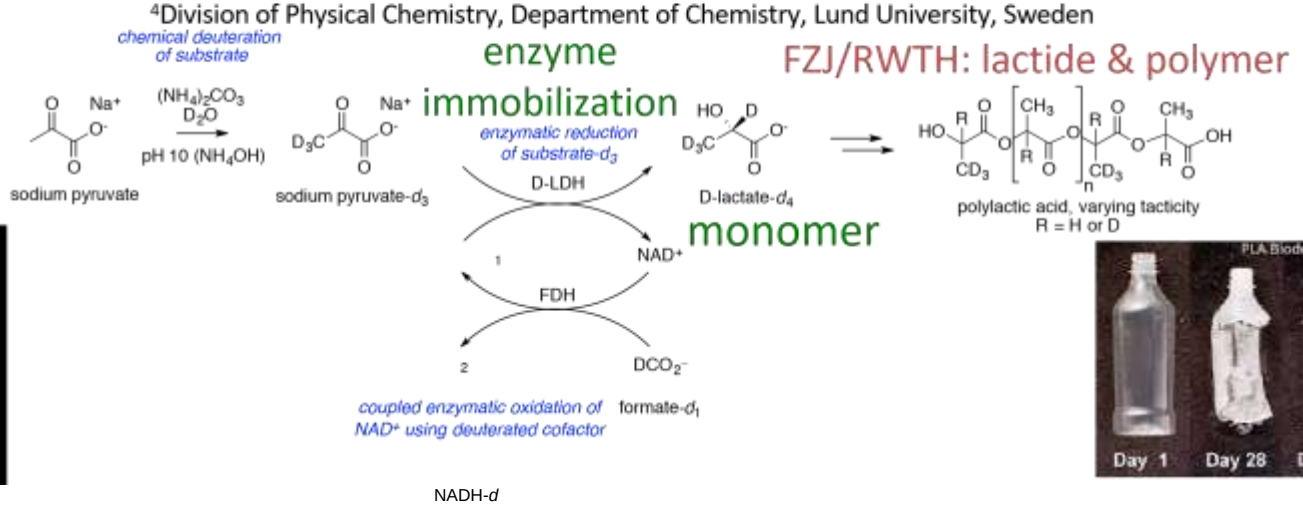
Deuteration

SINE2020 WP5: Immobilised enzyme catalysis for biopolymer synthesis

The enzymatic synthesis of perdeuterated D- and L-lactic acid-d4 and polymerisation of their lactides to polylactic acid.

Anna E. Leung[1], Andreas Raba[2#], Klaus Beckerle[3], Jürgen Allgaier[2*], Hanna P. Wacklin-Knecht[1,4*]

[1]European Spallation Source ERIC, PO Box 176, Lund, Sweden
[2]Jülich Research Centrer, Jülich, Germany
[3]Institute for Inorganic Chemistry, RWTH Aachen University, Germany
[4]Division of Physical Chemistry, Department of Chemistry, Lund University, Sweden



Immobilised enzymes for lipid synthesis Combined enzymatic/chemical approach for facile POPC synthesis (100mg):

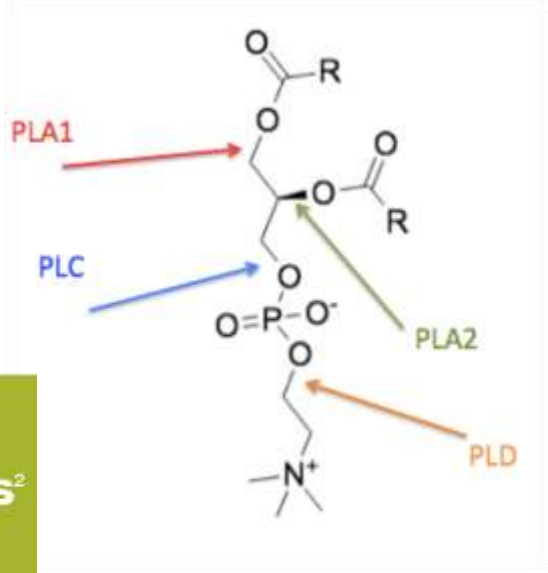

Oliver Bogojevic/Anna Leung

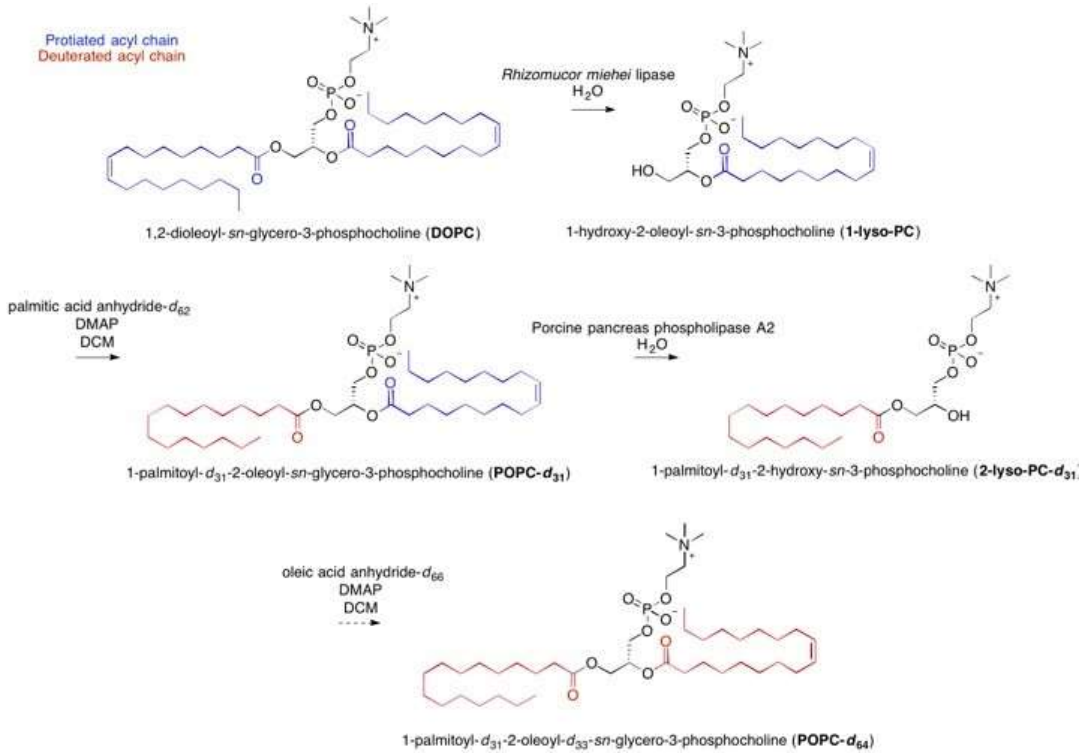
Enzymatic Synthesis

+ CLEAN and GREEN – few by products/no toxic chemicals
+ Highly specific – shortens reactions/purifications
+ Immobilised enzymes can be reused – cost effective

Application to lipid deuteration:

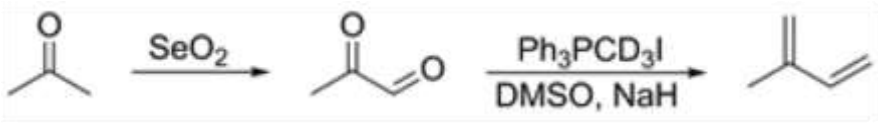
- different enzymes attack selectively in different positions
- Can be used to swap d-fatty acids h-fatty acids





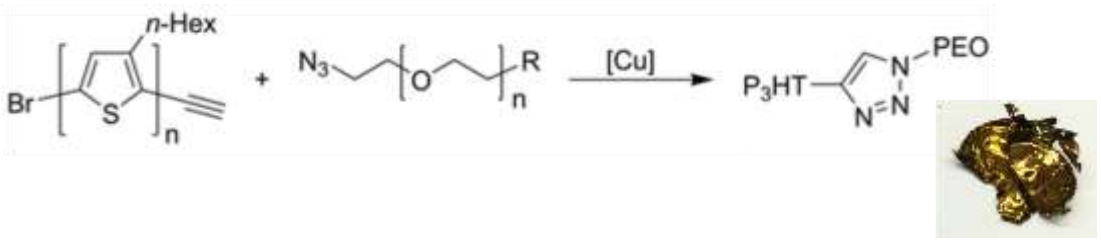
WP2 Task 2.3B: Deuteration For Soft Matter and Life Sciences ESS-STFC

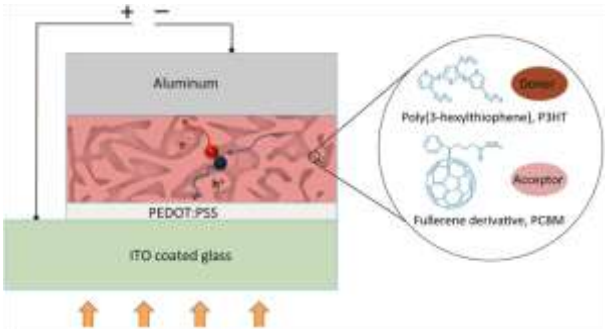
- Task 5.3 for



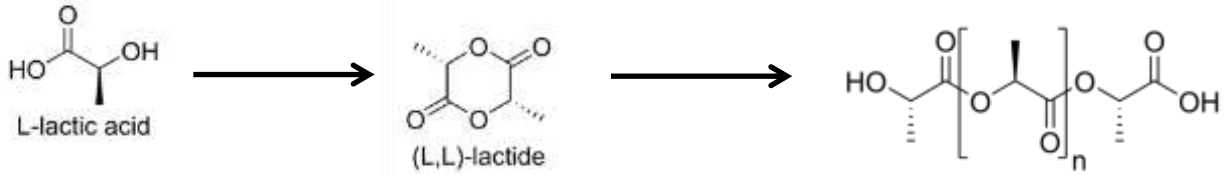
Novel route isoprene synthesis

- Task 5.5 D-labelled polythiophene



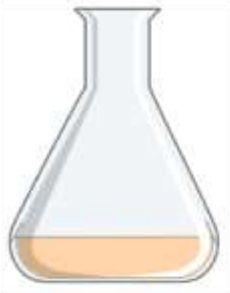


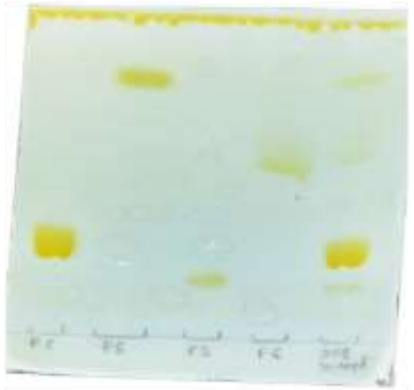
- Task 5.8 D-labelled polylactic acid

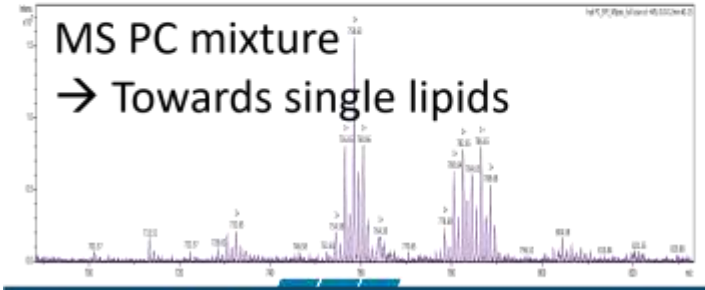


Collaborative work of ESS and JCNS

- Deuteration (polymers) support of users in Garching is in progress
- Planned collaboration with ESS on polymerlipid interactions






MS PC mixture
→ Towards single lipids

Extraction, Separation, Characterization of biodeuterated lipids

SINE 2020

DEUNET

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Deunet

Tweets 35 | Following 121 | Followers 103 | Likes 34

Deuteration Network

@deuteration_net

The Deuteration Network provides neutron scattering users with access to deuterated materials and crystallisation support.

deuteration.net

Joined December 2016

19 Photos and videos

Tweets | Tweets & replies | Media

Deuteration Network Retweeted

Institut Laue-Langevin @ILLGrenoble · May 20

"Here, small-angle #neutron scattering and tailored #deuteration have been used to follow the molecular lipid exchange between human lipoprotein particles and cellular #membrane mimics made of natural, "neutron invisible" phosphatidylcholines."

Selma Maric @DrSelmaMaric

New science out using #neutrons to probe #dynamics of #fat #exchange. Great collaboration involving @MalmoUniversity @biofilms_mau @ILLGrenoble @isisneutronmuon @lunduniversity @unioslo @NUSingapore nature.com/articles/s4159…

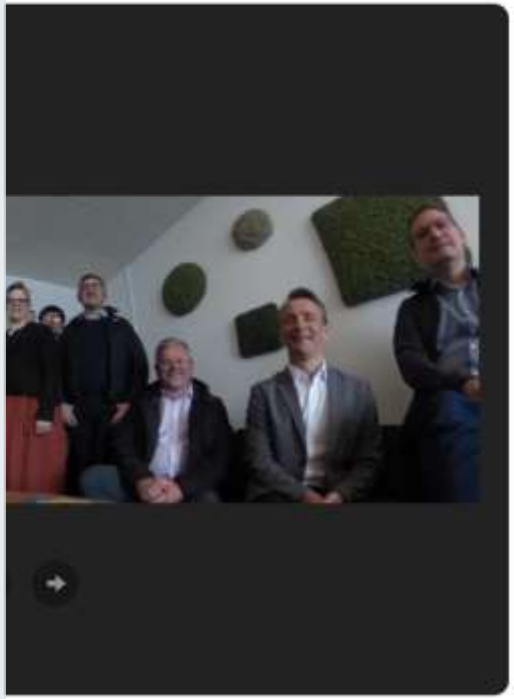
Show this thread

7 13

Deuteration Network Retweeted

EU Neutron @EUNeutron · May 9

Our next location on The Road to the ESS is Jülich. Here they are looking into deuterated polymers for #neutron techniques: sine2020.eu/about/the-road… #sine2020 #polymers #roadtoESS



The DEUNET is growing! Our most recent meeting was held in Lund last week and included several new members. The Lund Protein Production

New members: ANSTO NDF, JPARC-MLZ, LP3-LU

New possible collaborations with ORNL/NIST/UMD chemical and biodeuteration

Larodan Lipids first industrial partner interested in distributing deuterated (and nondeuterated) products

Each deuteration laboratory operates within the framework of its home facility
- Access provision to deuteration service varies from national/international to none

Coordinated user access requires facility agreement & support for cross-facility provision of materials/access

Minimum staffing identified for sustainable access to chemical deuteration in Europe:

ESS	FTE	STFC	FTE	ILL	FTE	FZJ	FTE
3 scientists	1	4 scientists	4	1 scientist	1	2 scientists	2
1 technician	1	1 technician	1	1 technician	1	1 Post-doc	1
1 Post-doc	1	2 Post-docs	1	1 Post-doc	1	1 PhD student	1
1 PhD student	1	2 PhD student	2	1 PhD student	1		
Currently funded	**FTE**		**FTE**		**FTE**		**FTE**
2 scientists	2	3 scientists	3	1 technician	0.2	-	-
		1 technician	1				
		2 Post-docs	2				
		3 PhD students	2				
SINE2020 Funded	PM				2		2
1 postdoc	48	1 postdoc	24	1 postdoc	36	1 postdoc	18

The continuation of DEUNET partner activities depends on facility investment in dedicated staff and agreement

Additional costs of consumables/chemicals also need to be considered

Conclusions and recommended actions:

1) **Continued staffing resources for a sustainable DEUNET**
2) Inclusion of biodeuteration/macromolecular crystallisation facilities in DEUNET
3) Continued R&D and international networking to facilitate innovation in neutron science
4) A cross-facility working group on inter-facility access to deuteration

Sample deuteration is as significant to soft matter & life science experiments as e.g. a cryogenics service or helium to other user groups.

LENS WG3 : Synergies in technological development and operation

- Task Deuteration Technologies (Chem, Bio, Xtal) ESS, ILL, STFC, FZJ

4 Pillars:

- chemical deuteration
- biological deuteration
- macromolecular crystallisation
- networking and synergies Priorities:

1. Identifying new R&D projects and collaborations aligned to future research themes and priorities in Europe
2. Networking with international deuteration facilities
3. Cross-facility working group on deuteration user access in Europe

WP2 Task 2.3B: Deuteration For Soft Matter and Life Sciences (ESS-STFC)

- i) chemical and/or microbial production of perdeuterated fatty acids and lipids
- ii) enzymatic synthesis of complex novel deuterated compounds.

Thank you for your attention

Questions?