

Work package WP5 Chemical Deuteration

Work package leader: Hanna Wacklin

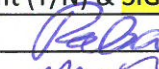
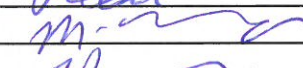
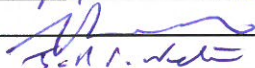
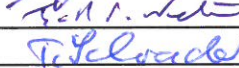
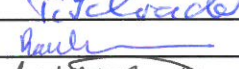
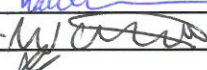


Venue : LIP Coimbra, Department of Physics, University of Coimbra, Rua Larga, P-3004 516 Coimb

Date : 7th of September

Agenda : Room E10A

- 14:00 Welcome and introduction
- 14:15 – 14:30 Update ESS – Hanna Wacklin/Anna Leung
- 14:30 – 14:45 Update ILL – Rachel Morrison
- 14:45 – 15:00 Update STFC
- 15:00 – 15:15 Update FZJ – Andreas Raba
- 15:15 – 15:30 Discussion – collaborations
- 15:30 – 15:45 Discussion – deliverables and reporting
- 15:45 – 16:00 WP meeting/User workshop 2017
- 16:00 – 16h30 Coffee/Tea break

List of participants

Name	email	Present (Y/N) & SIGNATURE
Raba, Andreas	a.raba@fz-juelich.de	Y 
MAREK JURA	maret.jura@stfc.ac.uk	Y 
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ANNA LEUNG	anna.leung@esss.se	Y 

(evtl Photo)

Collect all power point presentations and make them available on the intranet (contact info@sine2020.eu)

Detailed points incl discussion and outcome

- Agenda item 1
- Agenda Item 2



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Detailed points incl discussion and outcome

General information:

The meeting was opened with a welcome to new members Rachel Morrison at ILL and Anna Leung at ESS, followed by a recap of previous meetings (kick-off UCPH Oct 2015, WP5 kick-off at STFC Deuteration Facility workshop Oxford 27 Nov 2015) - where the goals and aims of the project were discussed - and information about the reporting procedures for SINE2020. There is need for 6 monthly internal reporting from ESS to the ILL coordinators on progress and expenditure, each deliverable needs to be reported with a separate template (available on the project homepage in the log in section) by the end of the month it is due in. In order to claim costs for the project, signed time sheets and original receipts are required.

The WP budget and expenditure until July 2016 was discussed – the recruitments took some time, not much has yet been spent except by FZJ, where Andreas has already been working for 9 months. The message in general was that there is a significant amount of funding within the project for travel and collaborations, so these should be used!

Recruitments are complete with Dr. Kun Ma to join STFC in a couple of months.

The first deliverable (D5.1 – Website and user portal) was met in M9 = June 2016 with the excellent help of Ines Crespo, the SINE2020 communication officer. The website has a description of the project and partners, with a calendar updated by Ines with events and a news page. Material to the website should be sent to the WP leader or Ines Crespo. There are some interviews on the SINE2020 homepage about the WP as well as the ILL lipid deuteration project – if other partners have highlights to advertise here, they should contact Ines.

Update ESS – Hanna Wacklin/Anna Leung

ESS recruited Anna Leung from the Australian National Deuteration Facility in June 2016. She is an experienced deuterated chemist. At ESS the effort so far has been aimed at establishing the DEULAB laboratory (based in Medicon Village, Lund) by procuring equipment (GC-FID for small molecule analysis, automated flash chromatograph for purification, new rotary evaporator) and setting up methods (methanolysis of lipid fatty acid chains, TLC analysis of lipid mixtures, GC protocols for Fame and sterol analysis). Access to NMR and mass spectrometers is currently being negotiated with Lund University and other local partners. Anna Leung has started working on the first SINE2020 project deliverable, D 5.4. Synthesis of L- and D-lactic acids using an immobilised enzyme catalyst system. The goal of this project is to explore deuteration of chiral molecules using enzymes, and to produce deuterated lactic acid monomers for the FZJ partner, who will synthesize polylactic acid polymers (D5.8) for a collaboration partner at Aachen University studying the microstructure and properties of these biodegradable plastics. We have so far established the needed starting materials and their preparation routes and are on track to meet the deliverable in M18 = March 2017. At ESS we are also looking for other possible candidates for deuteration, such as amino acid surfactants, which have many applications as preservatives in cosmetics. The ESS is also collaborating with the observer partner ANSTO on the synthesis of per-deuterated phospholipids – a per-deuterated d_{82} -POPC was synthesized at the NDF in 2015, and on-going work focuses on polyunsaturated lipids.

Update ILL – Rachel Morrison

Rachel started work at ILL in July – she will work on task 5.2 – lipid extraction and characterization. She will continue the work of current ESS-ILL PhD student Robin Delhom who has already investigate



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the effect of growth conditions on the production of lipids in yeast. Rachel will work on *Gluconacetobacter* as an organism capable of producing both deuterated cellulose and PC lipids.

Update STFC

STFC has recruited Dr. Kun Ma from Oxford University, who will start as soon as the administrative processes allow. Work at ISIS has included upgrades to equipment including a GC-MS, microwave synthesis, deuterium NMR probe and method development such as medium-condition H/D exchange at reduced/T for e.g. *rac*-glycerol. ISIS has supported a number of non-UK user groups by synthesis of deuterated materials, e.g.

- A perdeuterated ligand for the nanomagnetism materials synthesis (Italy).
- Deuterated CTAB, SDS and nonionic surfactants (C12E6) to some non-UK Users (Sweden)
- The non-routine compounds we supplied to the non-UK users: e.g. Deuterated Oleic Triglyceride, Tween 80, 20, etc. (Sweden)
- Deuterated resorcinol -, Deuterated urea, Deuterated choline chloride (the Institute of Materials Sciences of Madrid (ICMM-CSIC, Spain).

More details can be found in the report on deliverable D5.2 (M12).

Update FZJ – Andreas Raba

Andreas has been working on the synthesis of isoprene, which needs to be very pure for the synthesis into polyisoprenes (D5.3), which form the basis of most synthetic rubbers but whose structure and properties depend on tight control of the reaction conditions, which determine what isomers are formed. In addition, the conducting polymer P3HT (D5.4) has been synthesized for use in studies of photovoltaic materials, to be continued with synthesis of novel P3HT based block copolymers.

Discussion – collaborations

Several possible collaborations were discussed:

- FZJ-ESS collaboration on polylactic acids – to arrange a meeting to discuss project goals and requirements for the monomers in terms of purity, characterization etc. Anna (&Hanna) to visit FZJ, hopefully also to meet Aachen University partner.
- ILL-ESS collaboration in lipid purification and analysis: Rachel to visit ESS to learn about methods and protocols set up here by Robin and to see facilities.
- FZJ-ISIS collaboration: to explore obtaining deuterated hexyl-compounds from ISIS for deuterating P3HT block copolymers.

Discussion – deliverables and reporting

The reporting was discussed and it was agreed to hold a WP meeting in January-February 2017 to prepare for the M18 reporting. Rachel at ILL to organize this.

In the meantime, each deliverable should be reported on the template available on the SINE2020 homepage log in section by the end of the month if it is due and sent to the WP leader/Miriam Förster. 6-monthly internal monitoring reports will be sent to ILL (Oct/Apr) including expenditure and progress.

User workshop 2017



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A user survey of the deuteration needs in Europe is one of the deliverables of the project, and for this it was agreed that the best way to activate the community is to hold a workshop. This will be in Lund around May-June 2017 and should encompass both chemical and biological deuteration to also explore the synergies. One member from each partner should participate in the organizing committee (Rachel ILL, Hanna/Anna ESS, Andreas FZJ, John Webster STFC), and should start working immediately on the program and speakers.

Decisions taken:

- 1) WP meeting to be held in January 2017 at ILL – Rachel to organise.
- 2) Survey prepared for workshop to activate community to give input
- 3) User workshop to be held in Lund May – June 2017
- 4) To set up a catalogue of deuterated products on SINE2020 website as resource for community.



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Tasks / responsables

Task # / Sub task #	Responsible person / entity
Example:	
Task1.1	John Wayne (ILL) with input on ABC from Jane Fonda (ESS) to study the selection of material XYZ. Expected achievement till next meeting in Silver City in 6mths time: Selection of material and first tests done
Task 1.2	X to exchange with Y bilaterally in order to set process and inform WP leader asap.

Deliverables (due in this period)

Deliverable #	Status
Example	
D1.1 Report on material study (Month 6)	Will be circulated to all just after meeting for comments