

WP5 Chemical Deuteration Meeting

Date: 5th May 2018

Attendees:

Anna Leung

Giovanna Fragneto

John Webster

Peixun Li

Marek Jura

Hanna Wacklin-Knecht (by Skype)

Jürgen Allgaier (by Skype)

Thomas Hellweg

Location: Parma, Italy

ISIS

- peptide synthesiser: C8-C12 chains deuterated; working on longer. H-amino acids; will move to d-amino acids. Plan to chemically deuterate them and separate them using chiral column on prep flash LC system (new). 2 racemic already and isoleucine.
- deuteration methodology: 1. H-cube. 2. Microwave synthesiser. 3. Supercritical parr.
- 44 requests this round. As discussed at last meeting they reached out to network partners (FZJ) for help with proposals they cannot fulfil themselves.
- Peixun visiting FZJ next week to discuss one potential collaboration that has come from a user proposal (this is beyond the scope of the SINE2020 deliverables).
- EU proposals (historical) completed for SE DK DE Italy Spain
- Next ISIS User meeting (UK focus) March-May 2019

ILL

- hydrogenous and deuterated yeasts grown with h- & d-palmitic acid and h-oleic acid (a desaturation is observed in all cases). Haven't tried with stearic to see if oleic is produced, will try as soon as new post-doc arrives
- GC set-up installed and started to use
- new post-doc Krishna Batchu to begin hopefully mid-June 2018 (experiencing visa issue problems)
- deliverable 5.9 due Sept 2018, moved to month 42, March 2019

ESS

- lipase/phospholipase work is progressing with the completion of Masters Thesis project in the DEULAB. This work will continue with a four-month contract after summer
- ongoing work to modify glycerides and phospholipids
- HPLC system installed for unsaturated FA separation
- More interaction with the bio deuteration part of DEMAX
- Some info missing from DEUNET – requested from responsible partners
- J-PARC would like to join next user meeting; ANSTO offered to host

-Newsletter prepared by Alison Mader of ILL from the info on Deuteration.net; to be distributed soon. Discussion of how to do this considering changes to privacy and facility newsletters.

FZJ

- polylactic acid synthesis going well in collaboration with Aachen
- lactide synthesis has been improved using anhydrous conditions
- D and L-lactide-d have been synthesised. Noted that analysis is more problematic because of the inherent sensitivity differences between 1H and 2H NMR
- Synthesised polylactic acid has a narrow MWD as desired

GENERAL

- Thomas Hellweg suggested we publish a review at the end of the sine2020 period
- ISIS to send the case studies they already have re industry engagement
- ILL would like to write one about antibiotics but wonder if it is too fundamental. They also have an industry engagement person so Giovanna will liaise with them
- Thomas Hellweg will continue on DEUNET advisory panel until the end of the SINE period
- Agreement that we should ask the same to the other members; ask Karen Edler to be an official member; and Jian Lu to be chairperson (Thomas will do this if Jian declines)
- ISIS user meeting: could also have a WP5 meeting. Not to be co-hosted by DEUNET this time (feedback from their users)
- Giovanna: can we combine with lipid bilayers which should happen next year some time?
- Decision is that DEUNET will need to have a user meeting which is separate to ISIS. Either at ILL or ESS. Need to apply for funding for institutes/see what funding is left in SINE/consider other funding opportunities
- ISIS, ILL and ESS agreed it would be possible to attend an ANSTO/AUS user meeting though not to be involved in the organisation. Later though it was discovered that we cannot use SINE funds for travel outside of Europe. Giovanna to confirm this and Anna to communicate to Peter Holden next week
- Anna to feedback to others about whether the next period report is cumulative or not
- HWK/AL to see about 3 – continuing membership of advisory panel (except Thomas who has already agreed)

FEEDBACK from advisory panel

(WP5 specific):

- Minor delays but have hired a competent workforce and progress has been smooth
- Specific molecules, access to EU users, meetings
- DEUNET platform: share materials and knowledge; provide user access. Database (?) and survey. Post-SINE2020 and Brexit sustainability?
- Deuterated PLA: possible tech transfer (pharma?)
- High impact on doing better neutron experiments for all (mainly soft matter and bio) users

(General):

-Include success indicators in reports for non-experts (ie almost complete, progress made, finished)

-Sustainability – comment on this. Is there a role for facilities? Critical mass for lobbying? For maintaining expertise this is important. For some WP there is an obvious argument for continuation eg DEUNET