

DEMAX: initial operations

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Joint SEE/samples/labs STAP meeting 2018

Outline



- Future (2019-2022) – labs, equipment, competences
- Initial operation, 1st call for DEMAX proposals
- Challenges during initial ops period

DEMAX Current 2018



	Biodeuteration	Crystallization	Chem Deuteration
Lab space	✓	✓	✓
Equipment	✓	✓ (minor needs)	✓ (minor needs)
Staff	0.4 SZF <i>0.3 FTE @ LP3</i>	0.4 SZF <i>0.2 FTE @ LP3</i>	1 AL 0.5 HWK Part-time MSc

* 0.5 FTE shared technician with LP3 (24 mo. research contract)

DEMAX Future 2019-2022



	Biodeuteration	Crystallisation	Chem Deuteration
Lab space	✓	✓	✓
Equipment	✓	✓	✓
Staff			
2019	1.0 ZF; 0.5 FTE (ESS/LP3)		1.0 AL; 1.0 HWK
2020	1.0 ZF; 1.0 FTE (ESS/LP3)		1.0 AL; 1.0 HWK
2021-2022	1.0 ZF; 2.0 FTE (ESS/LP3)		1.0 AL; 1.0 HWK
<i>2023 (steady state)</i>	<i>(4 FTE)</i>		<i>(3 FTE)</i>

Initial operations 2019-2020 period



- We are in good shape to start initial operations
- Call for proposals, review and execution according to scheme below.
- Focused call: deuterated bacterial cell paste, purified deuterated protein, crystallization support for proteins, chemical deuteration (lactic acid or analogues, pyruvate, lipids/surfactants-to be defined during 2018)

	03-19	04-19	05-19	06-19	07-19	08-19	09-19	10-19	11-19	12-19	01-20	02-20	03-20	04-20
1	OPEN	REVIEW	IN PROG	IN PROG	IN PROG	IN PROG	IN PROG	IN PROG						
2							OPEN	REVIEW	IN PROG	IN PROG	IN PROG	IN PROG	IN PROG	IN PROG

- Call will go out via ESS website and community mailing lists
- Proposal scoring & tracking to be done "pencil & paper" for 2019 & 2020 (i.e. Excel)
- Project & reagent delivery will be discussed at bi-weekly meetings, shipped out as soon as available

Initial operations 2019-2020 period



- Technical, safety, and feasibility reviews will be done by ESS staff (Involve: SULF, DEMAX)
- Scientific merit will be reviewed by small external review board, each proposal will have 3 reviewers
- For access, applicants should either show **a**warded beamtime, submitted proposal or indicate an intent to use the material at existing neutron facilities
- Authorship vs. acknowledgements will be handled in a rational, case-by-case basis

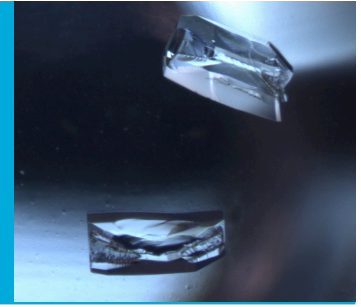
Initial operations 2019-2020 period



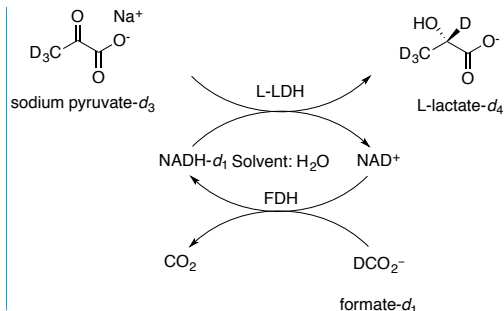
- We aim to accommodate ~12-18 proposals total
- 5-8 crystallization proposals, 5 biodeuteration (biomass and/or D-protein), 2-5 chemical deuteration (depending on complexity)
- Bio & chem deuteration runs as a service, crystallization a mixed (service & access)



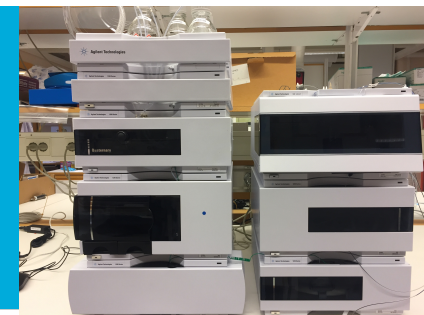
Biodeuteration & Crystallization Initial Ops



- ZF (1.0) Tech (0.5 - 1.0) able to cover required activities in initial ops period 2019-2020
- Significant overlap in competence, LP3 can cover gaps
- Competences covered: molecular biology, cell culturing, protein production, crystallization, biophysical characterization.
- Can continue to cover, but with limited capacity
- 2022-23: remaining 2 FTEs to be recruited



Chemical deuteration – Initial Ops



- Chemical deuteration: AL (1.0), HWK (0.5) - able to cover requirements for initial proposal rounds 2019-2020
- Competence exists to synthesise/purify/analyse perdeuterated lipids, surfactants, well-defined other small molecules
- Can continue to expand competence 2021-2022 focusing on the same types of molecules, but with limited capacity
- 2023: polymer/organic synthesis chemist to be recruited (unless chemical deuteration strategy changes)

Challenges



- Lab space – we need a continuous, stable home
- Coordination between bio & chem deuteration for using deuterated bio materials
- DEUNET – continued coordination and buy-in from partner facilities
- Scientific review committee members (volunteers?)
- Staffing – is it an appropriate plan (for now – 2021)?