STAP Report
Users and Samples STAP
ESS HQ
2-3 April 2019

All panel members were in attendance: Karen Edler, *University of Bath,* Michelle Everett (chair), *SNS*, David Hess, *ILL*, Peter Holden, *ANSTO*, Kim Lefmann, *University of Copenhagen*, Ron Smith, *ISIS*. We welcome the addition of Ina Lommatzsch, *MLZ/FRMII*.

The STAP would like to thank ESS and SAD for the materials prepared and the progress made. SAD is on track to meet the needs of the facility. It has been noted the considerable progress we have seen since the STAP formation 3 years ago.

DEMAX

DEMAX has once again had a very successful year across all of its capabilities, in terms of productivity (16 crystallisation projects completed), capability development, establishment and maintenance of collaborations, and realisation of grant deliverables. There are clear signs of good progress, in terms of both service delivery and capability development, and grant activities have been executed well. Grant deliverables showed good alignment with user service-focused capability development, e.g., development of methods for enzymatic synthesis of labelled molecules (lactic acid and PLA) funded under SINE2020 and enzymatic modification of phospholipids (POPC) funded under Brightn**ess** WP2. These activities also showed good integration in the focus of the DEMAX pillars as they required both biodeuteration (biomass production, enzyme immobilisation and activity) and chemical deuteration (synthesis and/or separations) expertise. As the SINE2020 grant for DEUNET activities at the ESS passes into the final six months, it should be recorded that the grant has been a real success – leading to establishment of chemical deuteration at the ESS at reduced cost to the organisation and development of methods for lipid deuteration, cell component extraction and enzymatic methods for synthesis and molecular modification. DEUNET continues to expand its network beyond Europe with Australia and Japan already engaged and dialogue occurring with the US (Oak Ridge). The formation of the LENS Working Group 3 should help maintain momentum with DEUNET growth and efficacy.

Current lab and infrastructure arrangements are generally working well but there are issues on the horizon. In the current calendar year there is a clear path forward with a focus on servicing user proposals received in the first call and maturation of capability development.

Facilities, Infrastructure and Staff

Regarding the Chemical Deuteration lab set-up, SULF moves out of Medicon Village in 2020 and DEMAX will take over the payment of the lease which has been renegotiated at a rental of 600,000 SEK without DEMAX's involvement or knowledge. This appears an extraordinary sum and is approximately double the previous rental. The lease covers the Chemical Deuteration

lab, the Hydrogen Lab, and an office. One factor appears to be Medicon's desire to lease the office to a commercial client. Yielding the office may be possible but would require identification of an office in reasonable proximity to the Chemical Deuteration Lab so as to not waste time travelling to and from the office and lab. Relocating the Chemical Deuteration activities elsewhere is not attractive in the short term. Equipment for chemical synthesis and enzymatic modification of molecules is in place in the current lab and the landlord (STENA) provides waste handling services. Regarding characterisation of labelled molecules, the proximity to Lund University is advantageous. Chem D can access the NMR there on a fee-for-service basis and also the Mass Spectrometer. The former is working well but the latter involves a sub-optimal arrangement where ESS staff bring and install their own columns for each set of analyses. It is desirable that Chem D is funded to purchase a Gas Chromatograph- Mass Spectrometer (GC-MS) which would solve the issue with access to the Lund University Mass spectrometer and would enable relinquishment of the H- lab – currently required as the current GC (that does not have an MS detector) uses H for Flame Ionisation. **The option of relinquishing the Hydrogen lab and renegotiating the terms of the lease should be seriously considered (assuming that ESS shares the view that the rental is exorbitant and capacity to pay is an issue).**

Likewise, the current arrangement where the Biocrystallisation labs and office are located in LP3 at Lund University is very advantageous because of shared staff equipment and services. This arrangement is very cost effective and offers synergies with Lund University in terms of capabilities and expertise. It is still likely to be attractive beyond the life of the current lease (December 2020) which should be considered for renewal at the appropriate time (subject to evaluation of the future of LP3and its relationship with the Biodeuteration and Crystallisation effort).

Recruitment of an additional staff member for Chemical Deuteration would offer the opportunity to expand both capacity and skill set. Having Anna Leung as the sole staff member dedicated to chemical synthesis represents a potential critical single-point- failure. A new recruit who has organic synthesis skills but also brings additional characterisation skills (say in NMR and/or MS) would add synthesis capacity but augment the expertise available in the group. We are uncertain of plans to recruit further for Biodeuteration but note that production so far has been at shake flask scale and any further recruitment might be an opportunity to acquire someone with bioreactor expertise to increase protein yields (and therefore staff time efficiency).

User Program

It is a considerable achievement for DEMAX to have moved into Operational Phase and to have successfully issued its first call for proposals since the last STAP. This is despite the time taken to secure approval of text for the on-line call. The materials and services offered represented a good balance between attractiveness and technical risk and at the time of writing the demand response was excellent. 19 proposals were received by the close of the call and this probably represents significant oversubscription.

Regarding the KPIs proposed, most are appropriate for deuteration activities. The KPI "How many neutron experiments are done with materials we supplied" could be problematic for several reasons: (a) DEMAX may successfully produce molecules as requested but has no control over whether they are put into the beam (b) how do you define an experiment – is it the total block of beam-time on one instrument? What if two instruments are used concurrently (SANS and USANS, SANS and reflectometry, SANS and dynamic measurements) – is that 1 or 2 experiments (c) how would you objectively verify number of experiments done (is the data collectible and verifiable?) (d) if the molecule(s) were used at various facilities over several years – how would you know (with the exception of the beam-time used to justify the proposal)? Other useful KPIs could include (1) Percentage success rate (how many proposals were technically unsuccessful (production wise) (2) Percentage of satisfied customers (to be defined based on feedback survey) (3) Number of user institutions – the range of institutions that are availing themselves of DEMAX services (count affiliations of all users on proposals done).

The question of characterisation of molecules (and in particular biomass extracts) produced for users and what documentation should be supplied was discussed with staff at the STAP and suggestions made (a matter of dialogue rather than being prescriptive here). Further questions could be discussed at the DEUNET meeting.
A request was made to provide input into content of the feedback survey (yet to be devised). Questions could include ones that address satisfaction with:

- quality of the molecule(s)
- quantity of the molecule(s)
- timing of delivery
- communication effectiveness
- proposal submission system
- ease of access to the service (DEMAX made it easy to obtain the product or service)
- How likely are you to recommend DEMAX to a friend or colleague?

We suggest a 5 point scale (so the middle is apparent and there are not too many choices which would spread/smear the data) and the use of descriptors for each point on the scale.

Commercial Access?
Regarding the question of commercial access to deuterated products, positive engagement with industrial users of neutrons would be of strategic and financial value. Demonstrating commercial demand is a good indicator of delivering value towards the application end of the value chain and is valued by most Governments (and funding bodies). A costing and pricing policy would need to be developed. Non-proprietary (or fundamental research) that is likely to be published, with co-authorship by DEMAX staff, could be charged at full cost recovery (staff time and other costs) or discounted initially if of strategic value or as a loss-leader to encourage engagement. Commercial (proprietary or confidential) proposals could be charged at

commercial rates (100% cost plus a mark-up). Ideally, consideration of this issue should be a driver for the ESS to develop an all-of-organisation policy on costing and pricing of industrial/commercial work. The sale of products to commercial vendors who will then on-sell, or further process and on-sell) is a more complex issue and should be approached cautiously. The sale of excess biomass or biomass extracts may be attractive and have little impact on availability of capacity for the user program. Aside from the need for development of a costing/pricing policy, care would need to be taken that it did not reduce capacity available for the user program beyond an acceptable point (which should be identified in advance). The sale of purified molecules to vendors would require further analysis of how neutron users are affected – whether by reduced availability of other labelled molecules through the user program or through having to pay more for them (through the vendors). Less tangible but important considerations include whether this type of sale would lead to a gradual degradation of DEMAX's reputation and the publication output of the facility if users became diverted to commercial vendors to a substantial degree.

Publications and DOIs

This is an important but regrettably necessary topic: a lot of users fail to acknowledge facility use or staff contribution (whether through co-authorship which generally is appropriate in the case of deuterated molecule production, or by text in the acknowledgements). This is frequently the reality and each facility is searching for the best way to deal with this. Try to track each user via the User Office/Proposal System and send reminder emails. A failure by a user to provide co-authorship or acknowledgement should lead to a request for that practice to change. Repeat offenders could receive a second warning which includes the possibility of access restrictions. The use of DOIs for individual batches of deuterated molecules may not work well. A certificate of analysis with a unique identifier might work better in terms of communication with the user. As DEMAX is a unique name, tracking use not acknowledged in publications should still be possible as offenders still usually give the source of the molecule in the methods section. DOIs for molecules may not be worth the effort and would be complicated but this is ultimately DEMAX's decision and developments in DOI use in Europe are a relevant consideration.

SULF

SULF is progressing well, is on track and well managed. The STAP was asked to address chemical safety in the charge. Those comments can be found in the general topics section below. SULF is working toward being the lab subject matter experts, SMEs, for ESS. There has been a lot of movement toward collaborations within ESS. These efforts are supported at this stage. They are a good opportunity to supplement funding and to work out processes of lab work that establish communities and harmonization of practices. Obviously the main task will change with the user program and this is just a note to be mindful. One ESS – One Lab will be promoted by collaborations within - such as the accelerator collaboration.

The construction coordinator is a good appointment for ESS. We suggest weekly, onsite standup meetings to cover what has been done during the last week, and what is proposed for the following week. This should be a quick catchup of what transpired over the previous week and future plans. This should be a way to catch any build issue that will hinder the overall function/plan of the lab spaces. These walk throughs will serve as a way to keep you current. These meetings would also be useful to the SE platforms.

SCUO

Guesthouse vs. Hotel
Once ESS is running and enough instruments are commissioned to have reliable user numbers, a guesthouse will be a good choice. It offers more flexibility regarding cancellation and rebooking, where in hotels you often have to pay fees. Users can benefit from networking in a guesthouse arrangement. They are all together, whereas staying in hotels they can be spread around the city not making possible the opportunity to talk to each other. The User Office saves time on booking by not having to call ten hotels because they are fully booked. Rates can be better and expected. In general, users are content with a quite simple guesthouse – at hotels they expect more and complain often afterwards. The reimbursement process will be less burdensome when the costs of the rooms are directly paid. Another advantage of an on-site guesthouse vs hotels in town is the shorter time it takes users to get between their accommodation and experiment, giving the opportunity to grab a few hours of sleep (in a bed, rather than falling asleep in a chair on the beamline) during intensive experiments.

A guesthouse would not be needed right away. As long as only a few users are visiting ESS, no guesthouse is needed. Utilise hotels during the early period. Consider starting from about 50 rooms and going up to 75/100. Consider the measurement time of a typical experiment and the size of a typical experiment team in total number determination. It is strongly advised that you establish one central check-in and that it includes a security/safety personnel be present 24/7. If the User Office provides all necessary documents to this check in (for example in a folder, where you can find the access badge etc.), the safety personnel can hand this over to the user. Perhaps users can find some kind of a door code and/or safe code in order to fetch the room key by himself there.

GENERAL TOPICS

We encourage you to finalize the user policy as well as the publication policy as soon as possible. It is on this that you will base all further steps. We look forward to seeing the draft access policy as discussed.

The STAP was asked to comment on the eminent value engineering exercise. It is hard to imagine that much more could be cut from the SULF budget. They have already started to tap

into outside funding for acquiring scientific equipment. What is seen as the operations allotment? Would it be possible to have monies in the first 3 years to buy more expensive equipment from the ops budget? As is, there is just enough for the most basic equipment such as glovebox, hoods, tables, balances.

DMSC

Software development saw definite progress and is headed in a good direction. Having something ready for the DEMAX call is commended. There is still a fair bit of functionality needed to serve purpose, but it was a good effort on a short amount of time. Please be reminded that some of the basics of operations and access policies will need to be incorporated in the software from the onset. Those decisions should be made in the near future. Other thoughts for the software development include:

- Integrating other aspects into the user software is advised, Sample Tracker, Radiation Protection, Safety Training, Access badges. Within the scope of the access badge system, at the User Office one can have a look at all aspects of a user while the other departments can use their "part" of the system. Don't forget to discuss the needs of those other groups before programming.
- Think early on about help-pages: will HELP be provided within the system or on separate web pages? The User Office will be saved from a lot of time-consuming calls from users struggling with the system.
- Avoid "free fields" that can be completed as the user wishes. It is difficult dealing with them and it takes a lot of time to correct them into useful text. Try to use drop down lists or checkboxes as much as possible.
- Guide the users plainly on what has to be done when – users do not always understand what you mean, make it elementary.
- Give the user status information within the system or via email.

Perhaps, start with a UML (unified modeling language) of what you will need in general and get deeper into the modules in discussion with those who are involved in each module. At first launch, it can be simple. Create something that you can put more flesh on easily and customize once the demands increase, e.g., new instruments, new workflows. It is very important to have a system that can be adapted as needs change.

ESH

It has become a recurring theme to comment on how ESH does not appear to be meeting the expected needs of scientific and technical activities (across the SAD platforms). There is a typical understanding in most scientific facilities of the expectations of ESH and those somehow are not quite aligning at ESS. It is great news that there is recruitment underway for a chemical safety officer. We encourage fast onboarding. Unfortunately, it has been a long time coming (one year since we reported on it) and meanwhile there are a number of scientific and technical activities occurring across the lab. The ESH staff at LU was called out as meeting expectations.

We suggest SAD work with ESH management on understanding the misalignment. This will pave a way forward for the new hire. The new hire should spend quality time with LU ESH staff to get an understanding of what is needed to provide safety advice and sign off. It is understood that SAD management is ultimately responsible that work is handled safely. However, it is the responsibility of ESH to assess processes and deem them safe from a legal and best-known practices standpoint. Therefore, it would be appropriate to recognize members of the SULF team and other SAD staff as SMEs on aspects of chemical laboratory practice, technician related practice and hazard identification that would work with the legal side. SAD should offer up documentation for ESH to "ok" and ESH should sign off on them. Look for solutions that are fit for purpose and achieve compliance. It would also be appropriate to recognize and access SMEs elsewhere such as at LU. This should establish what is appropriate practice and lead to harmonization across ESS. This is particularly important for when the user program starts when many SMEs will visit (optics). The system needs to be in place for SOUP to minimize sample approval time.

Procurement/Logistics

Logistics seems to be where it needs to be with regard to shipping needs. The addition of shipping same day is fantastic. As for procurement, we will reiterate some of our comments from last year regarding the procurement process. Ordering should be easy, fast and trackable. From an end user perspective, the envelope orders (understood to be emergency only) should be the normal order mode for amounts up to 5KEuro or so. A software system that allows for same day catalogue ordering is a must. Just as anyone can get online and order products from home, there must be a way to do this at ESS. We all work at very different facilities in many different countries and we all have the ability to order things with quick turnaround times. This is a pretty standard capability. There should be many end users who have the ability to place orders such as admins, group leads, team leads, various delegated staff. For those who do not have a buying role, they should be able to forward shopping carts to those who do. It is advised to look for a way to allow employees to get on, order something, and the order go out same day or next day at the latest. Please review and reevaluate the approval process. Obviously budget holders are ultimately responsible, but delegation of buying and approving should be much less clunky. As well, budget holders do not have an easy way to see the current state of their money. A system whereby staff can login and look at real time data of financial accounts makes for more responsible spending. If this system needs time for development, it is advised that the financial division train the end users on a way to pull needed reports for spending and budget planning.

In a restatement from previous STAP reports: There must be a way to make this process better. Other facilities have found a way. They must reach out for solutions and revamp their policies and tools in order to accommodate a large staff with obvious needs to ensure facility success.

CONCLUSION

Overall the work done on the SAD project is notable. We look forward to watching the user program develop and seeing the labs come to life as SAD ramps up toward operations.