STAP Report
Samples and User Laboratory Services STAP
Virtual Sweden
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Panel members: Tamim Darwish, *ANSTO*, Karen Edler, *University of Bath,* Michelle Everett (outgoing chair), *SNS*, Jeremy Lakey, *Newcastle University*, Kim Lefmann, *University of Copenhagen* (absent), Ina Lommatzsch (incoming chair), *MLZ/FRMII*, Ron Smith, *ISIS*

The in person, Lund STAP was affected by the COVID-19 pandemic and therefore was held remotely with more interaction than the typical remote STAPs, but obviously less than usual in-person STAPs. We commend ESS for switching to this format quickly in order to continue the success of the project and for all the hard work and preparation that went into making this format work.

Charge:
Common Topics

- Overall progress towards completion of construction project "science support systems", including remaining in-kind deliveries and commissioning activities.
- Overall progress of on- and off-site labs and workshops, equipment, staffing, and capabilities.
- Updated guidelines on required instrument provisions including infrastructure, mechanical interfaces, utility supplies, control infrastructure, and sample workflow.
- Delivering collaborative research and development activities, including external grants, and proposed LENS priority action(s).
- Prioritising construction deliverables and operational activities following the COVID-19 crisis in view of ensuring Hot Commissioning in 2022 and First Science in 2023.

Sample and User Services

- Revision of policies related to user access, affiliation, and scientific publications to enable First Science.
- Participation in development of user office & proposal software tools.
- Suitability of minimal set of requirements for the user office & proposal software tools and the suggested implementation needs vs available resources adequate for hot commissioning in 2022 and first science in 2023.
- Operating deuteration support services and preparation for next pilot call in view of Hot Commissioning and First Science including prioritised access for COVID-19 research.
- Evaluation of laboratory spaces, equipment priorities and competences for (future) staff for lab services and method development.
- Progress on installing and using the on-site (user) laboratories including sample management during Hot Commissioning and towards First Science

DEMAX

First Call

The STAP would like to congratulate the DEMAX staff and management on the success of last year's proposal call, which showed an excellent demand of 19 proposals, given that it was their first call. This initial high demand from the scientific community clearly demonstrates that the DEMAX Team has marketed their capabilities really well. They have already positioned themselves in a healthy user base, which includes a good fraction of users from outside Sweden. This is a good resource to further help DEMAX in their own outreach activities through the research outputs and publications of these users. It has been proven by other deuteration facilities (e.g., NDF) that publication is an important multiplying factor in the networking and demand equation.

The deuterated molecules that were requested and approved are some of the most difficult molecules that can be requested from a deuteration facility and the STAP would like to commend the Team on being able to deliver such difficult molecules with the limited resources available. These types of deuterated molecules require a large amount of time and effort and therefore the justification for approving such molecules should be under strict scrutiny of their science impact to make sure that the effort of making them is well justified. It is strategically important to make sure there is a balance of easy and difficult deliverables to ensure fast research outputs that are essential for a newly established capability at ESS.

Second Call

When reviewing proposals for the second call, given the shortage of staff to execute chemical deuteration (which requires multiple skills and efforts), it is recommended that DEMAX narrow the variety of difficult deuterated molecules that they will provide and balance their supply with some "easier" products.

Due the current pandemic and the cancellation or postponement of beam-times, the facility should reprioritise their backlog from the first cycle and ensure they are working only on experiments that are scheduled (or"have already awarded beamtime" since scheduling may be a bit vague). Due to the shortage of resources (labour power), it is advised that the team focuses on some high value products (including speciality products from the facility), upscale their synthesis and provide the users with the minimum required amounts. If time is available, effort should be put into building up a stock of products which are often or likely to be requested (particularly those which are specialty products from this facility. Another approach that can be followed is to try and recover used samples (difficult to prepare ones) from users and re-purify them.

It is a good idea to have an early and rapid internal feasibility review before it goes out to peer review. Reject the impossible or nearly impossible projects quickly so that time is not wasted, and users can move on by modifying their experiments or sourcing alternatives. The next stage is to provide a guidance to external reviewers at the peer review stage of the difficulty in providing the deuterated materials requested, e.g., some estimated measure in terms of FTE months. Include information on whether or not it's a risky synthesis or has been done many times before. For biodeuteration, users should include evidence of preliminary data (yield / difficulty) from non-deuterated purification. A preference should be given to providing high yield cell pastes for further purification in host lab.

Execution time of one year should be the general maximum, maybe regulated by possible existing beamtime awards, if users come with a well-planned, mature and low risk request these should be

prioritised. The main thing is to keep review times as short as possible to enable users to switch their plans if unsuccessful.

Staffing

DEMAX should mitigate the risk of single point failure and loss of key personnel in all three different capabilities of the team: chemical deuteration, biodeuteration and crystallisation. The maternity leave replacement should happen quickly. Also, is Oliver being replaced? This position should be back-filled as well. There is a risk of losing the user demand that has already been achieved from the first round if discontinuation occurs between the user base and the facility for more than a year. The EoI approach is a good mitigation of this risk. DEMAX's first proposal call and deliveries were well received in the community. This is a great first scientific success for ESS, so ESS needs to take care and support DEMAX's efforts considering they have been mostly funded by finding money outside of ESS.

For further mitigation, it is recommended that the facility continues to engage the users through negotiating partial production of deuterated molecules. This can be done by providing the necessary deuterated precursory compounds. If possible, users could continue synthesis and production of the final compound.

As stated in the previous STAP report a second chemist now and a biologist for the long term is recommended. The second chemist would definitely benefit from training at another D-Lab, especially if the Parr experts at DEMAX are not available to train the new recruits. The training can be practical if it's for a short period of time. A good synthetic chemist wouldn't require much training. Training on chemical deuteration is required on the Parr reactors, sample analysis and characterisation. The current coverage of protein / DNA production and crystallisation is 0.5 FTE from Lund Uni LP3 plus Zoe working on crystallisation. There is a strong demand for these services which supports the recruitment of a biologist FTE to ensure strength in this area. This was evident in the first call.

Strategy

It is important for the deuteration capability at DEMAX to develop and maintain its differentiation from other deuteration laboratories. The crystallisation and yeast lipids extraction capabilities are good examples and they should be reinforced and maintained. This will bring new demand and build the user trust in requesting other small deuterated organic molecules. This differentiation is important in giving recognition for the funders to keep funding the facility.

The capacity and demand should be carefully assessed at each round: sitting out 1 pillar every now and then to allow for staff recruitment & training or equipment commissioning is supported by the STAP. Deliverables should be measured by effort time and delivery time. The facility should encourage users to contact staff and discuss feasibility of their requests and more importantly the minimum amounts of products needed before submitting their proposals. This will minimize the feasibility assessment time and ensure ordering and stocking of reagents that may require long time to arrive.

Some basic remarks about supporting first science, any biomaterials should be well proven and well behaved. From experience on working up target station 2 at ISIS there will be enough to worry about without fearing that the sample won't remain in solution on the beam line. Since ESS should provide science that is unobtainable elsewhere the biological samples can be well tried and boring to start with. Furthermore with higher fluxes, each minute fixing a sample on the beamline is much more costly than on slower sources.

COVID-19

The COVID-19 is important work. We commend the effort. When the first project gets going, get a press release out. Relevance is always good for science. To mitigate down time caused by the pandemic, we recommended prioritizing the C19 proposals and anything left over from the first call. DEMAX could also take this time to consider specializing in a molecule that the other D-labs do not, as well as scaling up production of molecules you know you will need.

Regarding Covid, DEMAX could look at it as a chance to get processes and R&D in place, maybe produce some raw materials or standard reagents. Engaging with your users at this stage would be a good approach. It is encouraged to work with them on data analysis and paper publication. You have had a good amount of pull from your users in the first round, it would be appropriate to prepare plans for a push approach during the shutdown period. Working on your outreach and case studies and the impact of the work done so far is a good strategy in this particular time. Furthermore, it is unlikely that lots of beamtime will be awarded soon so there is likely to be an extended quiet period. ISIS is also heading for a long shutdown (TS1 will be off for 14 months from 4th January 2021 (this starting date is likely to slip...); TS2 will be off for only 8 months from the starting date) so that demand may not resume for awhile.

Lab Spaces

The lab spaces and services that DEMAX has at LU and MV are well-suited to their needs. The STAP encourages ESS to support this as a long-term home for DEMAX. They have access to much needed instrumentation that ESS will most likely never have and it doesn't make sense for this team to buy and support such instrumentation. The NMR and mass spectrometer access are very essential for the facility. Managing the access through other groups would definitely be beneficial for the facility and will free up significantly the repair and maintenance budget and even the operation budget for operating and maintaining such instruments. There are no suitable locations on the ESS site for DEMAX labs, a project de-scoping decision made by ESS with the guarantee that off-site lab space would be funded.

SCUO

Software

The Scientific Coordination and User office achieved a success with the 2nd DEMAX call and the software development effort. Carina from the user office and the STAP would like to recognize the extraordinary effort from DMSC who not only worked hard to implement what was requested, but also asked insightful questions to help ensure the solutions met the needs. As well, the DEMAX team was crucial to developing the processes that are implemented to date.

DMSC has done a fantastic job of getting the user office software off the ground. Unfortunately, when assessing the requirements from all groups (most of them not even provided yet) and the remaining work, it is most likely that the user office software will not be ready for first science. This is disappointing and concerning. As you have heard this STAP say so many times in the past years, the user office software does SO MUCH heavy lifting, from user's personally identifiable information, to travel planning for users, to sample tracking, to safety signatures, to proposal review, and on and on. Many different roles at ESS will use this software daily. The STAP urges ESS to support an additional 1.0 FTE to this effort. In the meantime, we suggest ranking software requirements in a way that they can be staged for development and implementation. If different software packages are used (e.g. a mix of in-house and commercial) ensure that file formats etc. allow information to be exchanged between them. Carina has begun the tedious process of who will need engagement. This is a very useful exercise. All the included

parties will need to dedicate time to supplying their requirements. It is not for SCUO to supply requirements for others. Every group needs to feel the urgency of this. And just a reminder, the policy documents will be the guidance for how the software is mapped out.

Outreach and Performance
The interaction within the user community is appropriate and encouraged, e.g., joint user meeting, conferences. It is a challenge to stay relevant when there isn't an operating facility, and the pandemic will certainly add complexity. Moving to virtual conferences and symposia is commended.

Deciding on Key Performance Indicators is supported by the STAP. The ESFRI report is sensible to follow. The STAP also recommended that SCUO get with funding agencies and see what KPIs they look for. These are needed for software requirements. Plan for them from the beginning.

Policies and Guidelines
SCUO presented policy documents to the STAP last year for discussion. The STAP has been recommending that these policies be developed and accepted for many reports now. These policies are the building blocks of the entire user program. As you know, building blocks go down first and lay a foundation that supports all other building efforts. Only one of the documents that we reviewed last year has made it all the way through to Council. The STAP strongly recommends the prioritization of the approval and implementation of these policies and guidelines. They are stuck at various stages of review, i.e., SMT, SAC, Council, please get them moving.

There was quite a discussion with SCUO following the user office software concerning the definition of a sample (as opposed to starting materials) as it relates to entering information into the proposal system. It was intended that we discuss this with SULF, but unfortunately the time didn't allow. It would be great if ESS could make the reporting for "samples" much easier than is currently the case elsewhere. Firstly, it is suggested that samples need not be explained in detail at the proposal stage which should instead concentrate on any obvious safety issues that may prevent the award of beam time. Later, during scheduling, the detailed safety assessment should deal separately with laboratory materials/ reagents/ etc and "samples". In many examples in soft matter and biology the facility will need to manage the delivery of a number of raw materials (buffers, detergents, biologicals, dry salts etc) which will need to be covered by chemical/biological safety rules. These will then give rise to a completely different set of things still called "samples" which have been in the beam and only these need to be subject to radiological safety rules. The word "sample" is best kept here to align itself with solid condensed matter samples.

SULF
Labs – onsite and off
SULF has had many successes since we last met. The onsite lab fit out is continuing quite well. Congratulations on the excellent project management. The 3 month buffer before COVID is evidence of this. The onsite schedule for Sanber, walk throughs and handoffs, is a lot of work for the whole team, but absolutely worth it. It is commended. The interactions with CF and Sanber are well managed. SULF plans to move to onsite labs in the fall, given that installations are allowed to continue. They have a well thought out, staged plan to move based on what utilities will be available when and have clear plans for handing off the MV lab to DEMAX.

One lab for ESS is a strategy to offer scientific expertise in characterization to the whole of ESS. This is great for securing favor throughout the organization. Two examples of projects so far include the

examination of rad hard lubricants to be used in the target and concrete analysis for shielding materials. These activities reinforce the point that SULF is building functional chemistry labs for the whole of ESS, not just workbenches for users to 'fill their sample cans' and are well supported by the STAP. The plan to grow equipment and expertise in tandem will serve the users well.

Budget

The STAP always encourages getting money from other places, as the budget for SULF is too lean, so well done on receiving the Human Frontiers Science Grant, which is external validation of the work being planned. Well done on fostering such a great relationship with the UK that they will permanently loan SULF much needed characterization equipment. This is a boon for ESS. As well the FLUCO projects with Alice (shared tech) are going well and are supported by both STAPs. This facilitates the opportunity to further synergies between working labs and working experiments.

The 10% operations budget cut is a minus to an already too small budget. Just one example is sample cans, i.e. whether sample can inventories sit with SULF or with SE, for sure these costs are massive. Please look into a ramp up in the SULF budget commensurate with the ramp up of instruments and users.

Staffing

This team is taking up the slack in a lot of areas that are not related to their mission. Some of these efforts need to be examined and absorbed by ESS facilities. A dedicated waste management handler is necessary for the whole facility. There will be a lot of complicated waste for all the divisions. This needs to be handled at the facility level. This is the same for deliveries. The burden of receiving deliveries is high on these teams. It is understood that ESS is still a construction site and the facilities do not have ownership of the whole site but look forward to the future and support shipping and receiving from a facility level. Consider the staff plan for SULF in general here. It won't be long before SULF will need after hours on call to support operations.

As previously mentioned, the STAP has started to discuss and give input into what the sample handling, flow and management could look like in the software. Care must be taken for SULF to retain control of these. A system where the samples (and materials needed to prepare samples) remain the property of the experimenters is a good model. Involvement of radiation safety in this sample intake process is one example where things could go horribly wrong, e.g., radioactive samples turn up at ESS without anyone having accepted the responsibility of them. Users should have clear procedures /flow charts to fill out the right forms and enter the required information. Users often visit several different facilities each year and understandably get confused as to who needs what information, so make it simple and clear. Panel members are willing to act as guinea pigs to test the usability of these systems. This will make life of the SULF team easier too. This is certainly needed for the SCUO software effort. We are asking SULF to start looking into this. The handling documentation is in place, so there is something to build on.

GENERAL

We have expressed concern over the ESH and OSH support in the past and we are happy to report that some key hires has made the safety effort superb and appropriate for the type of work we done. Well done health and safety team.

The STAP appreciates the clear information given in the presentations and the reports, as well the reports with highlighted questions for advice are helpful guidance.

In conclusion, DEMAX operations has delivered excellent science and are on track to continue. SULF is handling a lot of extras with grace and is well on track for project delivery. SCUO is making great progress, don't let the delay of the software come home to roost on them. The effort to making ESS a success is clearly evident in the accomplishments the STAP sees from each meeting to the next.