Users and Samples STAP closeout report
ESS HQ Lund, Sweden
6-7 March 2018

Panel members present: Karen Edler, *University of Bath*, Michelle Everett (chair), *SNS*, David Hess, *ILL*, Peter Holden, *ANSTO*, Kim Lefmann, *University of Copenhagen*, Ron Smith, *ISIS*
Attending SE STAP: Marek Bartkowiak, *PSI*; Absent: Giovanna Cicognani, *ILL*

Introduction

The Scientific and Technical Advisory Panel (STAP) would like to thank the Scientific Activities Division (SAD) for all the hard work put into presenting their progress. Strides have clearly been made toward the ultimate goal of a fully functioning user facility. The Scientific Advisory Committee (SAC) suggestion of Fall 2017 was to have STAP meetings twice a year prior to the SAC meetings. This was discussed and received favorably. In order to save time for the STAP members and money for ESS, one of these meetings will take place electronically.

User Labs – Radioactive Materials Lab (RML)

With the news of the in-kind contact moving on from the University of Tartu, some assurance should be given from the University to ensure a smooth handover for the provision of in-kind glove boxes. A new contact should be identified and discussions had to be sure they are on the same page as was the previous contact.

The building design presented for D08 looks to give better options for the RML and is accepted. The STAP gives its support for moving the door for the changeover room. This will be a favorable change for the safety aspect of this lab.

There was a lot of discussion about budget. Consider leveraging other groups as much as possible. For the RML, could the gamma spec be supplied by the radiological group? Ultimately radiation safety should lie in their hands and therefore this equipment would be most beneficial to their operations.

Instrument specific labs

The interaction between the protein crystallography instrument NMX and the deuteration platform DEMAX is a good model to follow for coordination efforts. SAD should find people whose research interests/backgrounds are aligned with the research of the instrument and have that person be the link. Instrument teams should provide work flows. Ask them to write work aides for how exactly the instrument specific lab will be used. SAD can then better understand the needs and be the source of information for implementation and safety. This discussion brought up an interesting point about communication. It was stated by multiple instrument scientists that there was a policy not communicated about sample handling at the instrument. Please be aware that policies should be communicated in many different ways and many different times.

Access Policy, Strategy

DEMAX offers a small scale opportunity to flesh out policies on access and to get SAD in the mindset of doing the same for instrument access. Prioritization of DEMAX proposals should be

on the basis of highest probability of demonstrating the values of ESS investment in DEMAX that is enabling high quality science and on clear differentiation from capability offered elsewhere.

Scientific Coordination and User Office (SCUO) software

Consideration for SCUO software has increased considerably since the last STAP meeting. Having said that, it still has a very long way to go, all the way in fact, as work on it has not yet begun. The STAP is encouraged by the data management division, DMSC's, commitment to have a functional software option for the start of DEMAX operations in 2019. DEMAX should get together with DMSC now and discuss basic requirements. With such a short amount of time and no employee in place yet, the idea of using a software that already exists is encouraged. DMSC has the right attitude; this will be the first public call for ESS and ESS needs this to look professional. ESS has long since said that their goal is to improve on the snags of other facilities. Here is a prime opportunity for that. Paper and pencil is not ideal, for managing personal information, nor for metrics which will clearly be needed for sponsor reporting.

The STAP commends the MAX IV collaboration on a common portal.

We like the idea of a DOI associated with proposals in order to data-mine the facility history. It facilitates data management for users and allows tracking for safety, both externally and internally.

SULF -General User labs

The extra costs for utilities expected by Conventional Facilities (CF) tax an already tight budget. More money must be provided to pay for these installations such as electrical outlets and ethernet ports. It has never been in the project plan for other divisions to pay for utilities that are clearly within the remit of conventional facilities. As well, provision for a budget needs to be determined to accommodate unforeseen expenses due to construction such as changes to the labs for safety, e.g., non-opening windows and how to deal with that. Other costs that have come to light include site training for contractors and VAT on labor.

Tempering expectations for equipment is one way to cope with a strapped budget. Plan to provide money for basic day 1 equipment for preparation and characterization of samples. For the next meeting it would be useful to have gone through one typical experiment per area of instrument and list each item needed throughout the workflow.

The STAP was asked to supply suggestions for mandatory equipment. Here is a list in no particular order.

- Glove boxes – Apart the glove box(es) in the RML, one glove box for handling solid state samples and one glove box that allows the handling of solvents should be available. Glove boxes can be quite labour-intensive, it is suggested to keep their number as low as possible. It should be verified with SE if at least one of the boxes needs to be specifically designed to take up some SE equipment.
- Enclosure/fume hood for handling nano-powders
- Freeze-dryer

- Centrifuge – Up to ca. 15.000 rpm for 15 and 50 ml falcons must be available. An ultra-centrifuge might be useful.
- Rotary evaporator – at least one, better two
- (Vacuum) ovens – A good number of ovens with an operating temperature up to 200-250°C must be available, including vacuum ovens. In addition cleaning rooms should be equipped (with more specious) ovens for drying glassware.
- Furnaces – One standard laboratory chamber furnace (1300°C) and one tube furnace (1300-1500°C) should be sufficient. Independent heating zones for the latter as well as equipment for heating under gas or vacuum can be useful.
- UV-Vis spectrophotometer – One spectrophotometer with interchangeable sample compartments should be available, including a thermostated sample compartment. In addition, a NanoDrop or equivalent portable instrument for small sample volumes must be available.
- FTIR – An entry-level model equipped with a diamond ATR should be sufficient for most user related applications. It may be useful (not only for IR applications) to have the equipment for preparing pellets (press + die) available. One could consider investing in a more sophisticated model that can later be extended with a FTIR microscope or that can be used for protein FTIR, etc.
- Light scattering – An easy to use DLS instrument like a Malvern must be available, preferably one which combines DLS and Zeta potential. A more sophisticated instrument for dynamic and static light scattering will certainly be interesting, especially for internal research. However, training users on such an instrument is more time consuming. (could be acquired with the SANS instruments)
- Spin coater
- UV Ozone cleaner
- Plasma cleaner
- Tip sonicator
- Quartz crystal micro balance
- Langmuir troughs – may need to be custom-built to work with (Si) blocks used on the refractometers.
- Ellipsometer (could maybe be acquired with the reflectometry instruments)
- Rheometer (could maybe be acquired with SANS/reflectometry instruments for use with Neutrons)
- Density meter
- Versatile microscope
- HPLC system
- Ultra-pure water systems – should be available in every sample preparation lab
- Laboratory Fridges (8°C) and -20°C freezers, one -80°C freezer
- Chillers & vacuum pumps – It will be useful to have some backup recirculating coolers/heaters and vacuum pumps available.

Well done on ways you have tried thus far to engage with local universities for “nice to have.” This will be the smart track forward on these pieces of equipment. While considering the budget, do not underestimate the magnitude and expense of the consumables that will be needed, e.g., ultrapure water, D2O, gases for glove boxes. As mentioned previously for the

RML, leverage science interests to encourage equipment bought by instruments and PIs for their research.

Scientists managing SULF are currently on 0.5 (Monika) and 0.4 (Melissa) positions and they raised themselves the question whether to stay on 0.5 or whether to go on a full position in the future. With the start of the user programme, SULF scientists should go on a full position. The fear is that as a 0.5 SULF and 0.5 instrument scientist it will be difficult to manage both tasks and one or the other will suffer in the end.

A three compartment cold room (-25°C, -18°C, 1°C) was presented with costs of around 100k €. While there is certainly a need for a good number of freezers (around -20°C), one should consider if there is a real necessity for a sub-zero cold room, especially with a division in -18°C and -25°C sections. Here some money could be saved (in acquisition and operation) by choosing a simple cold room operated just above 4°C.

DEMAX

Equipment acquisition has progressed well and is appropriate and necessary. Further equipment is required, and the acquisitions proposed in 2018 are appropriate (i.e. Parr Reactors to help service Chemical Deuteration user needs arising from the first and subsequent proposal calls, a microscope for cold room viewing of protein crystals and an incubator to ensure constant access for proposals work – in the context of currently having to book incubator time with LP3 at Lund University).

The budget for consumables has been increased which is a positive action that helps deliver maximum value for the staff levels currently available in DEMAX

Advertising of the proposal call for 2019 is critical and many suggestions on how to reach the existing community and potential new users were discussed. The STAP would suggest consideration of increasing the length of the call from 1 month to 6 or 8 weeks. The timing (March and September) seems appropriate and we agree with the reasons given for the timing (immediately after many neutron calls). Care needs to be taken not to unintentionally exclude achievable proposals or opportunities by the way in which the capability on offer is described.

Expression of interest outside the agreed scope of the call is strongly recommended as this may offer unanticipated opportunities to label molecules within DEMAX capabilities that had not been anticipated. It may also identify opportunities to partner for capability development and could help inform decisions on future capability development (what molecules are wanted). Expressions of interest may also reveal new users and broaden DEMAX's network and influence. Demonstration of high demand is important and so care must be taken to not exclude proposals (even if it is decided that they cannot be done this round).

It is recommended that approving one Biodeuteration and one Chemical Deuteration proposal early in the call under discretion be considered in order to have a quick and efficient start-up of official operations in the first month/weeks of the 6 month operational period.

Thought needs to be given to how feedback on completion of deuteration proposals will be collected and assessed. In the initial calls (prior to availability of final User Office software) a simple survey (e.g. using Survey Monkey) would be an interim solution.

The collaboration between LP3 and DEMAX for biodeuteration and the access to space, equipment and expertise that it offers is critical for the short to medium term success of Biodeuteration and is very much a positive leveraging of investment. The original budget allocated to establish Biodeuteration lab facilities (elsewhere) is not sufficient and would not lead to a capability level equal to that available in the LP3 arrangement. It should be noted that although the arrangement is stable, it rests on LP3's future as a facility in Lund University. Should LP3 cease, a considerable part of the advantage would be lost, although LU Biology Department would still have much to offer equipment wise.

To ensure continuity of capability provision by the Chemical Deuteration Team the lease for Medicon Village needs to be concluded quickly. Moving elsewhere is not preferred in the short term but if necessary would need to be done in time for capability provision for the 2019 Proposal call. It should be noted that a move in the short term would also jeopardize successful completion of DEUNET deliverables.

Extras

The PO system does not seem to support an efficient and realistic method of buying things. Procurement processes are currently inefficient, unpredictable and untraceable. Issues include delegations, resource limitation in purchasing and the perception that large projects are more urgent. This increases the burden on staff time and reduces efficiency in experimental planning and execution. In addition, small purchases should not need upper management authorization. Team members throughout the organization who have had some basic procurement training should have authority to spend money up to a threshold such as €5,000. This approval is very much a waste of senior staff time.

A test beamline for crystal alignment is necessary for single crystal users. Access to it and scheduling for it in the proposal system will be a must.

Has the user office discussed with the instruments mail-in programs for routine experiments? How does beam time allocation look? As requirements will be needed by DMSC very soon, the user office policies need to be developed. Scheduling, proposals, access modes are all parts of the user program. Consider some high level outlines, flow charts or use cases to facilitate requirements lists. It would be unfortunate to push so hard for SCUO software and not be ready with the needs.

SULF presented an idea for multiple turnstiles around target building entrances to minimize queues from hand and foot monitoring. This change is supported and will ease the movement of people in and out of the building. If this is a radiation protection issue, what is the plan for loading bays and roll up doors? Large equipment must get into the instrument hall and clearly a turnstile is not an option.

As was mentioned in the revised report last year, consideration of how to deal with activated and contaminated sample environments should be given. Let's address this at the next STAP and discuss some options for a path forward, as well as share some facility procedures.

Conclusion

Thanks to the STAP members for their time and consideration. As it seems to be beneficial to staff time and budget, we discussed keeping the Users and Samples STAP joint with the Sample Environment (SE) STAP. This works well, but places Marek in a situation where he has to be in two places at once, and therefore has chosen to stay with SE. Thank you Marek for your contribution and we look forward to hearing from you as you keep us in the loop on the SE progress.