Evaluation of the research infrastructure:

Swedish NMR Centre (SNC), University of Gothenburg

Introduction

The purpose of the evaluation was to review the operations as part of this research infrastructure's systematic quality monitoring. The assessment of the operations focused on the following criteria:

- How are the rules and criteria for Research Infrastructure at University of Gothenburg met?
- How are the activities developing?
- What are the benefits/opportunities for the Swedish NMR centre being part of larger infrastructure consortia, e.g., SciLifeLab and Swedstruct.
- Recommendations regarding continuation of operations (or, if applicable, discontinuation of operations).

The evaluation is based on:

1. A thorough introduction to the University of Gothenburg, the Swedish NMR Centre, and policy and rules for research infrastructures at the University of Gothenburg provided by Marica Ericson in an introductory meeting.
2. A self-evaluation report written by Gøran Karlsson including appendixes with overview on users, research output 2018-2020, financial result 2018-202 and a brief funding scheme from 2017-2025.
3. Interviews (Zoom) with Gøran Karlsson (Director), Cecilia Persson (lab manager), Anna Winkwist (internal user), Mikael Akke (external user and chair of steering committee), Gerhard Gröbner (representative from Umeå, and member of the steering committee), Staffan Schantz (representative from Astra Zeneca), Per Sunnerhagen (Acting deputy HoD), and Marica Ericson (assistant HoD).

Summary

The Swedish NMR centre (SNC) is an infrastructure supporting high quality research, also used in teaching, offering access to a wide range of spectrometers and services within biomolecular and material science research.

Access to the infrastructure is open to all users through the SNC web-portal. Rules, regulations and access fees are transparently communicated to the local, national and international users from academia and industry. The service prices are fair. Users report that they are satisfied with the support they receive, the equipment is relevant for their research, and the staff is repeatedly categorized as service minded.

The SNC RI is of strategic importance to all establishment levels (University/Faculty/Department-wide). It is unique in Sweden, with support from both national and international funding bodies. The integration into the local academic environment at UGOT should be discussed.

The SNC leadership has been very successful, and clever in establishing good collaborations and networks with other institutions. This has been key to secure external funding for upgrades and new equipment, and to maintain staff with a high level of expertise who provide excellent user support. Through these networks (e.g. KAW (2013-2020), and on-going SciLife and SWEDNMR) and in consultations within the SNC steering committee, the infrastructure has a convincing operational and funding plan for the next years. The SNC collaboration with Astra Zeneca for acquiring and running a DNP NMR setup that is unique in Scandinavia is a very interesting approach, where the partnership benefits needs of both industry and academia.

Thus, the facility is excellently run, its operation is well established and financially secured the next four years. The SNC provides unique and adequate access with support that is adapted to user needs. With this, the SNC is very successful and in many aspects a role model for a well-run RI that should be continued and further supported. We consider SNC to accurately meet the rules and criteria for Research Infrastructures at University of Gothenburg.

Observations and specific comments

Organization

The SNC has its core site at UGOT, with a satellite in Umeå. Both sites are supported with core funding from UGOT and UU, respectively, with separate budgets and complementary strategic and scientific focus. SNC strongly depends on additional external funding, SciLifeLab, KAW (until 2020) and SRC (SwedNMR, starting 2022). This has worked successfully in the past and at present, thanks to impressive and successful activities by the Director of SNC, Gøran Karlsson.

The coordination of SNC activities between UGOT and UU is done in monthly meetings.

A *Steering Committee (SC)*, appointed by the faculty of UGOT is chaired by Mikael Akke (U Lund) with representatives from other universities that access the SNC. The SC consults on scientific directions and monitors the budget. A SAB has been called in *ad hoc* in the past for specific strategic planning.

This governance of the SNC is not very clear and transparent and little information regarding this is documented on the web site of the SNC.

Operation

The SNC hosts a broad range of state-of-the-art spectrometers for various applications of NMR ranging from structural biology, drug screening to metabolomics and material science.
There is excellent, highly skilled and service-oriented staff to support users and their research projects. The SNC staff is fully dedicated to supporting users, with some of their time being also devoted for developing and improving methods that will improve the quality of user research projects.
Access for users is available by a transparent and efficient process. SNC staff evaluates the project proposals, performs risk assessment and gives advice on new projects to ensure quality and best practice. This is well appreciated by the users, who appreciate the streamlined application for projects, documentation of the experiments and implementation of SOPs. Users highly value the excellent professional support and willingness to implement new and advanced methods, in collaboration with the users to advance their projects. However, this usually involves a significant time investment by the staff and reduces overall capacities and/or slows response times for user projects.

There are clear rules established on acknowledging staff in publications, depending on the contributions of staff as part of a scientific collaboration (co-authorship) or service provision with handing over data to the user (acknowledgement).

The facility aims to follow and establish Open Science and FAIR principles, – this is also requested by SciLifeLab. There are professional systems and procedures established for storage and analysis. Similar systems to handle sensitive (e.g., patient) data are currently being established.

Funding
Financial support of the SNC relies on a combination of institutional (university) funds, income from user fees and external grants. This is a complex operation, that, however, functions well. Staff usually obtain permanent positions, for which funding is currently secured until 2025/26. This is nevertheless a problematic situation as potentially staff needs to be downsized if some external funding would be no longer available. It will be important that UGOT is aware of this situation and can potentially provide backup to ensure an efficient operation of the SNC.

Strategic long-term planning
The presented strategic plans are sensible and convincing. The ambition to install a high-end magnet >1 GHz) within SNC and offer this to the users is timely and relevant. This should be part of a national strategy as is, in fact, considered with the SWEDNMR project, which is just starting.

SNC has been successful in getting funding support with industrial partners (AZ for the DNP), which is an impressive success and may also lead ways for future upgrades of instrumentation.

SWOT analysis
Strength: SNC is well equipped, has highly skilled staff with world-leading expertise, who are well appreciated by users.

Weaknesses: Funding support for permanent staff is complex and could endanger the operation of SNC and its user support. The institutional integration of SNC at UGOT should be addressed. Procedures for handling of sensitive data should be finalized.

Opportunities: SNC is already well-established and networked in national and European consortia, additional interactions and collaborations with biobank and mass spec services could increase the impact and visibility.

Threats: Funding of staff and maintenance/acquisition of new instrumentation is secure for a midterm perspective. A more sustainable funding will be desirable. Stronger integration and support of clinical studies with metabolomics will be important.

Recommendations

- The organizational structure of the SNC is complex due to the involvement with several networks, e.g. SciLifeLab, SWEDNMR, and partners, such as the NMR node in Umeå. Although this is visualized on the web-pages, it would be beneficial for future evaluations if the report includes more specific information on this.
- The Steering Committee (SC) meets twice a year to discuss strategic planning and the budget of SNC, in addition to ad hoc discussions with the chair on specific questions. The SC can, when necessary, call-in advice from a Scientific Advisory Board (SAB). For transparency, we would advise

that these organizational structures are visible within the web-portal, and that their mandates are described. Names and affiliations of the committee/board members should also be listed.

- SNC should perform regular user evaluations to monitor the service provided, also enabling input on new technologies, equipment and services that the infrastructure should consider implementing into their strategic plans.
- SNC should look for solutions to current bottle necks. Lag-time for metabolomics projects is reported to be up to several months, although the use of the metabolomics dedicated spectrometer is reported to have a yearly average use of 35%. Post processing and analyses of such data are demanding. Could this be improved by training more staff/reallocating staff, increase staff, initiate collaborations with bioinformatics groups or obtain additional support for personnel funding from large user projects? Also, perhaps training courses and workshops could help users to become more self-sufficient.
- Access to the infrastructure is provided through applications submitted online from the web-portal. Up to now, the infrastructure has had capacity to take on all requests. User requests and spectrometer usage should be closely monitored to provide input for strategic decisions on new purchases/upgrades and phasing out of equipment, in discussions with the steering committee. Are the routines for distributing projects between Gothenburg and Umeå sufficient?
- Some users receive training to do hands-on NMR-experiments on their own. Collating this learning material or combining the training for several users could be more time efficient and should be considered.
- SNC has been organized at the Department level the last years. SNC is a high-end infrastructure, which the Department should recognize as an asset. As an advanced high-end research infrastructure requires continuous maintenance, upgrades and new investments and experienced associated staff. This is financially demanding, and requires careful and forward-looking strategic planning. Notably, SNC has been extremely clever in securing external funding through their active networking and the director is to be congratulated for these achievements.

  The university has an important role in the long-term predictability of the operations by their contributions to basic financing for the infrastructure. It is therefore important that the Department establishes good routines for their responsibility as a host unit (according to the rules for research infrastructures at the university of Gothenburg, Styrdokument Dnr 2014/631). This would also include expertise to support and maintain the infrastructure, and to facilitate efficient communication between the research infrastructure and the faculty/vice chancellor level where basic funding is provided. Given that SNC has support from two faculties (Natural Science and Medical) it might be appropriate that strategic planning and budget of SNC will be discussed in an annual meeting involving the director and faculties at the vice chancellor level.
- Systems for safe storage, processing and transfer of sensitive data to handle GDPR regulations needs to be finalized and articulated on the web-page.

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