Evaluation of the research infrastructure: Swedish NMR Centre (SNC), University of Gothenburg (GU)

Introduction

The evaluation aimed to review operations in accordance with University of Gothenburg GU's rules for systematic quality monitoring of research infrastructure. The assessment focused on the following criteria:

How are the rules and criteria for Research Infrastructure (RI) at GU 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 SwedNMR.

Evaluation of the leadership transition for the SNC.

Recommendations regarding continuation of operations (or, if applicable, discontinuation of

operations).

The evaluation has been performed on initiative from Marica Ericson, Head of Department of Chemistry and Molecular Biology, GU, i.e. the host unit, and is based on:

1. A thorough introduction to the GU, the SNC, and policy and rules for research infrastructures at the GOT provided by Marica Ericson in an online introductory meeting.

2. A self-evaluation report written by Göran Karlsson including appendixes with overview on users, research output 2021-2024, financial result 2021-Aug 2024 and a brief funding scheme from 2014-2026.

3. Interviews in person Göran Karlsson (Director), Cecilia Persson (lab manager), Björn Burmann (internal user, KMB), Björn Halleröd, (Advisor on research infrastructure for Chancellor at GOT), Göran Hilmersson (Dean at the faculty of Science), Erik Thomson (Deputy Head of Education), Per Sunnerhagen (Deputy Head of Research), Martina Nyström (Economist), on Zoom Thomas Vosegaard (chair of steering committee), Morten Grötli, (internal user, KMB), Lars Evenäs (user, Chalmers), Gustav Nestor (user, SLU), Axel Abelein (user Karolinska Institutet) and Anders Malmendal, (user, Roskilde univeristet, Dk).

Summary

The Swedish NMR Centre (SNC) is a research infrastructure that supports high-quality research, provides advanced PhD courses and workshops, and offers access to a wide range of spectrometers and services for studies on small molecules, biomolecules, metabolomes, and materials science.

Access to the infrastructure is available to all users via the SNC web portal. Rules, regulations, and access fees are clearly communicated to local, national, and international users from both academia and industry. Service pricing is considered from cheap to fair. User feedback consistently highlights satisfaction with the support provided. The equipment is regarded as

highly relevant to the user research needs, and the staff is unanimously described as highly competent and service-oriented.

The Swedish NMR Centre (SNC) is clearly to be classified as a university-wide research infrastructure and serves as a national node for SwedNMR, offering access to one of the most advanced NMR laboratories in Europe. It is unique within Sweden and benefits from support by both national and international funding bodies. However, its integration into the local academic environment at the GU warrants further discussion.

The leadership of the Swedish NMR Centre (SNC) has, over time, skillfully fostered strong collaborations and networks with other institutions. This has been crucial in securing external funding for upgrades and new equipment, as well as in retaining a highly skilled staff that provides exceptional user support. The total production of NMR hours amounts to 32,000, representing approximately 46% of the available hours per year, which marks a 10 percentage point increase since last external evaluation. The growth is foreseen to further increase in 2024, driven by walk-up usage and higher demand for DNP-NMR.

SNC is a partner in several national and international research infrastructure consortia focused on NMR, including SwedNMR (as coordinator), SciLifeLab, PANACEA-NMR, and R-NMR. Additionally, the in-house helium liquefaction system has been completed, achieving a helium recovery rate of 85-90%. Altogether ensuring a robust operational and funding plan for the coming years. Notably, the collaboration with AstraZeneca to acquire and operate a DNP-NMR setup, the only system of its kind in Scandinavia, serves as an exemplary partnership that meets the needs of both industry and academia.

Since 2021, over 120 scientific papers have been published, with NMR infrastructure playing a key role. One third of these papers were co-authored, and two thirds acknowledged SNC for its use or support.

An evaluation of the SNC leadership transition confirmed continuity, effectiveness, and alignment with objectives. Starting in 2025, the director role will be split into two: one for outreach and strategy, and one for daily operations. Both candidates are well-suited for their roles, with strong communication already in place, forming an optimal and dynamic team for steering SNC.

Thus, the facility is excellently managed, with well-established operations and fairly well financially secured the next couple of years. The SNC provides unique and adequate access with support that is top-level tailored to user needs. As a result, SNC is highly successful and serves as a role model for a well-run RI that should be continued and further supported. I believe that the SNC fully complies with the rules and criteria set for RI at the University of Gothenburg.

Observations and specific comments

Organization

The SNC is the coordinator of SwedNMR, which shares the same steering group. This structure should ideally create an efficient and transparent organization. However, it may be perceived as centralizing power at SNC, reducing national representation. This creates also some uncertainties regarding SwedNMR when Göran Karlsson steps down as director of SNC, even

though the process is internal to SNC. Clear communication with SwedNMR node members about the leadership transition at SNC is recommended.

The planned split of the director role into two positions—one for outreach and strategy, and one for daily operations—seems to ensure continuity, effectiveness, and motivated leadership for the facility. Björn Burmann will lead outreach and strategy, spending one day per week at SNC, with the remainder of his time at the host unit (CMB - Department of Chemistry and Molecular Biology). Cecilia Persson will lead daily operations, manage finances, and oversee human resources. Interviews reveal that both are motivated for their respective roles, already maintaining good communication, and showing strong commitment. Björn's continued involvement with CMB while stepping into the split director role is seen as a strength, fostering more relevance between SNC and CMB.

Operation

The SNC offers expert support, advanced and broad range of state-of-the-art spectrometers equipment, and technical assistance across a wide range of research fields, including structural biology, drug screening, metabolomics, materials science, and small molecule research.

This is a true service facility with excellent, highly skilled, and service-oriented staff dedicated to support users and their research projects. The SNC staff is fully committed to assisting users, with some of their time also focused on developing and improving methods, which will undoubtedly enhance the quality of user research projects.

Apart from metabolomics and structural biology applications, SNC staff have configured an instrument over the past year to be walk-up instrument for small molecule research, facilitating easier access for scientists at the host unit, CMB. The recent co-location of CMB next to SNC has expanded and deepened NMR usage for some scientists at CMB.

Users highly value the excellent professional support and the willingness to implement new and advanced methods, collaborating with them to advance their projects. Additionally, user have requested the possibility to purchase additional help for performing advanced analyses in their projects.

Clear rules are established for acknowledging staff in publications, based on their contributions to scientific collaborations (co-authorship) or service provision, such as providing data to the user (acknowledgement).

Funding

The financial support for the SNC is derived from a combination of institutional (basic fund) funds, user fees, and external grants. Basic funding comes from the Faculties of Science, the Sahlgrenska Academy, and the vice chancellor. In 2024, the total basic funding amounts to approximately 6 MSEK. However, starting in 2025, the Sahlgrenska Academy's funding (~1.5 MSEK) will cease. Despite this, the overall funding scheme seems well-balanced, and the situation for 2025 and 2026 is expected to be at a similar level to 2024. While this does not appear to affect the staffing situation, it may impact the console upgrade, which could threaten the capacity of SNC.

The implementation of overhead costs to the host unit is currently unclear, which could become a critical issue for SNC's operations and staff, potentially causing harm to a nationally important facility that has otherwise been economically well-managed for many years.

Another aspect is that SNC, with its relatively large budget, being connected to the host unit CMB, which has a more limited budget, could face significant economic challenges. This situation not only affects the financial stability of the host unit but also limits its strategic flexibility. Therefore, it does not seem logical for a university-wide infrastructure to be organized at the departmental level.

Strategic long-term planning

The host unit is currently developing new strategic plans, and SNC should be integrated into these plans to address the potential of unrealized users as well as widen the use of NMR within the host unit. This consideration will remain relevant regardless of the organizational level at which SNC is structured within GU.

The SNC focuses on three levels of hardware investments: low-level upgrades, such as new probes; medium-level investments, such as new console upgrades; and high-level advancements, such as ultra-high field NMR systems (>1 GHz). The first two levels of investments are realistic to achieve through local and national funding in coordination with SwedNMR. A new application to sustain and expand SwedNMR is currently under preparation.

However, the increasing sophistication of RIs demands highly skilled personnel and significant financial resources, with ultra-high field NMR systems (>1 GHz) exceeding costs of €15 million. Such an investment may require a Scandinavian or Nordic-wide consortium. Establishing SNC as a leading node within this consortium would create a realistic pathway to advancing ultra-high field NMR capabilities. This would enhance the attractiveness of SNC and the Nordic consortium for European collaborations and recruitment of top scientific research groups.

Given SNC's reputation and experience as a research infrastructure, it is a natural choice to take a leadership role in such a Nordic initiative.

As previously highlighted, SNC has successfully secured funding support through industrial partnerships, exemplified by its collaboration with AstraZeneca for the DNP setup. Additionally, regional partnerships, such as those with Chalmers or the new GoCo Health Innovation City, hold significant potential for future collaboration and funding opportunities.

SWOT Analysis

The SWOT analysis diagram from the self-evaluation report is presented below, with the detailed reflection available in the self-evaluation report itself. As the evaluator, I find it aligns well with the observations made during the on-site visit and recommend that readers review the reflections provided in the self-evaluation report.

	Helpful	Harmful
al origin	STRENGTHS	WEAKNESS
	Unique instrumentation	Ageing consoles
	Excellent staff expertise	Not fully booked
ern	Development in DNP,	Complex funding
<u>1</u>	relaxation/dynamics and Al	Many areas of activity
5	OPPORTUNITIES	THREATS
al origi	Next generation magnet	Lack of infrastructure strategy
	Dissolution DNP	OH-handling
ern	Interaction SwedNMR/SciLifeLab	No plan för PI recruitment
EXT		CMB economy – 8 year perspective

Figure: SWOT diagram from SNC self-evaluation report.

Recommendations

□ The first recommendation is a recurring theme in evaluation reports. Rather than reformulating it, I have chosen to cite it directly:

"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 forwardlooking 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."

- □ Currently, NMR is not included in the teaching portfolio at the host unit, CMB. To expand the local user base and enhance the relevance of NMR, it is recommended to evaluate the possibility of integrating NMR into the existing teaching portfolio at CMB. Here staff personal from SNC can be used. This integration could increase local usage of the SNC and provide broader benefits for GU.
- □ Artificial intelligence and machine learning are already integral part of daily operations at SNC. These technologies are crucial for future students to master, and SNC can play a key role by providing relevant case studies for education at the host unit, as well as across GU in general.
- □ Currently, staff scientists at SNC provide services to users, develop methods, and implement the latest NMR advancements. Their skills and expertise are also relevant for securing funding. Allowing them to take on smaller roles in applications they have

helped develop can further motivate them, ensuring continued competence and personal development, which benefits SNC, the host unit, and GU.

□ Currently, the number of PIs with a strong academic NMR background at GU is low. While SNC's broad range of NMR capabilities makes it an attractive facility, strategic recruitment is limited due to the current situation at the host unit. Earmarked funding from the faculty or vice chancellor level for the strategic recruitment of PIs with strong academic research in NMR would secure the development of SNC as a RI. Additionally, SNC could support emerging scientists in achieving tenure-track positions at SNC.

Date 7th of December, 2024

Finn auch

Finn L. Aachmann Professor NTNU