

# Swedish NMR Centre at the University of Gothenburg

## Activity report 2023

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Göran Karlsson  
Director

## **Sammanfattning**

Under 2023 har Svenskt NMR-centrum gett stöd till 112 projekt och 58 forskare (PIs) från Göteborgs universitet samt andra nationella och internationella universitet, från regioner, industri eller annan icke-akademisk organisation. Användning av NMR-utrustningen har varit ca 34 000 timmar. Knappt 40% av tiden har använts för strukturbologi. Metabolomik och småmolekyler står för 17% vardera. Övrig tid fördelas huvudsakligen på materialvetenskap, DNP-NMR och industri.

Svenskt NMR-centrum har koordinerat forskningsinfrastrukturen SwedNMR-med stöd från vetenskapsrådet (VR) samt plattformen för integrerad strukturbologi inom SciLifeLab. Svenskt NMR-centrum har också deltagit i de VR-stödda forskningsinfrastrukturprojekten NBIS, CBCS och PPS samt, på EU-nivå, PANACEA och R-NMR.

Svenskt NMR-centrum har varit aktivt i utbildning på avancerad nivå, arrangerat kurser/workshops för doktorander och postdocs samt deltagit i olika outreach-aktiviteter.

De vetenskapliga resultaten presenteras i 38 artiklar i internationella tidskrifter. Omsättningen var 20,3 Mkr och resultatet blev 2177 kkr.

## **Summary**

During 2023, the Swedish NMR Center has provided support to 112 projects and 58 researchers (PIs) from the University of Gothenburg as well as other national and international universities, from regions, industry or other non-academic organizations. Use of the NMR equipment has been approximately 34,000 hours. Just under 40% of the time has been used for structural biology. Metabolomics and small molecules NMR account for 17% each. Remaining time is mainly divided between materials science, DNP-NMR and industry.

The Swedish NMR Center has coordinated the research infrastructure SwedNMR, funded by the research council (VR) and the platform for Integrated Structural Biology within SciLifeLab. The Swedish NMR Center has also participated in the VR-supported research infrastructure projects NBIS, CBCS and PPS as well as, at EU level, PANACEA and R-NMR.

The Swedish NMR center has been active in education at advanced level, arranged courses/workshops for doctoral students and postdocs and participated in several outreach activities

The scientific results are presented in 38 articles in international journals. The turnover was SEK 20.3 million and the result was SEK 2,177 thousand.

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## Instrumentation

The use of the NMR systems is higher compared to previous year. In total 33 800 hrs were booked (Fig 1). The increase is mainly due to the installation of the walk-up NMR system. This magnet was previously only marginally used. To a minor extent, the increase is due to the use of the DNP-NMR system.

The 900 MHz system 'Blue' (Bruker Avance III HD console, 3 mm TCI cryo-probe) has been used mostly for structure biology applications, as is the case both for the 800.1 system 'Indigo' (Bruker Avance III HD, SampleJet, 3 mm TCI cryo-probe) and the 700 MHz-system 'Green' (Bruker Avance III, SampleJet, 5 mm QCIF cryo-probe).

The 800.2 system 'Red' (Bruker Avance III HD console, SampleJet, 5 mm TXO cryo-probe) has to a larger extent been used for small molecules and materials science applications.

On the 600 MHz system 'White' (Bruker Avance III HD console, sample changer, room temp probe) the Bruker IVDr version was updated to 2.5, including implementation of diffusion-edited DIRE and JEDI experiments to be able to deliver GlycA, GlycB and SPC composite inflammation markers as well as lipoprotein profile and metabolite absolute concentrations.

The second 600 MHz system, 'Violet', upgraded in 2022 (Bruker NEO console, SampleJet, 5 mm QCIP cryoprobe, joint funding with the CMB department) was taken in full use early 2023. This was earlier than planned and was due to malfunction of the existing 400 MHz system at Campus Johanneberg.

The 400 MHz DNP-NMR system 'Pink' has been in extensive use during the year. Minor problems, *e.g.* a rotor crash, was successfully handled in-house. The 3.2 mm HCN DNP-NMR probe has been modified to allow  $^{19}\text{F}$  DNP-NMR. Planned service of the DNP gyrotron was carried out in February 2023. The current reporting model does not properly reflect the DNP-NMR usage. DNP-NMR is very much a handicraft. During 2023 effectively the DNP-NMR system should be considered as fully used.

Planned service of the five cryo-probes was carried out in June 2023. A negotiated price, SEK 147 000 (€ 13 000) per system was obtained from Bruker. For 2024, the possibility to service in-house or obtain service from a third party will be investigated.

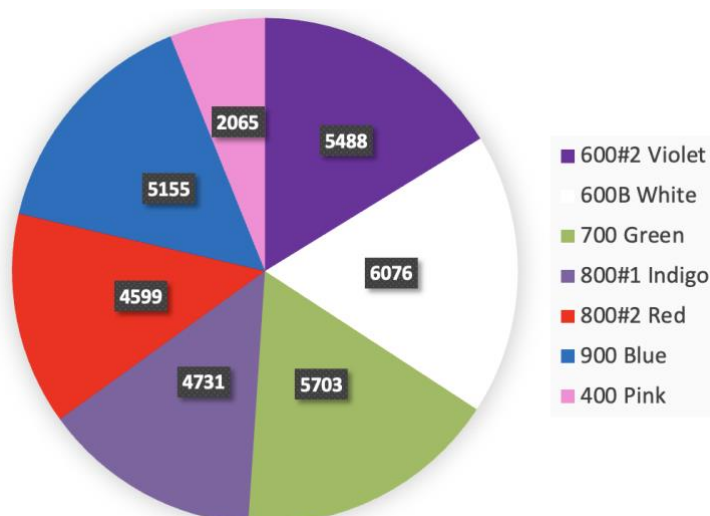


Figure 1. Spectrometer use (hrs) per spectrometer during 2023.

### **Additional instrumentation and installations**

In accordance with earlier recommendations, two old systems (500 MHz & 600 MHz non-shielded Oxford magnet with Agilent/Varian consoles, respectively) were discharged and decommissioned in May. Peripheral equipment and consoles have been removed, currently only the magnets remain in the spectrometer hall.

The helium liquefier was upgraded in January 2023 with a capacity of liquefying 35 L per day. An attempt to operate an intermediate 500 L transfer dewar was tried during the summer, but the helium losses during transfer were too severe. In 2023, 7600 L helium were liquefied. The losses are estimated to ca 10%.

The installation of the Insight system for in-cell NMR applications has been delayed due to delivery problems from the vendor.

### **Personnel**

The staff comprised eight senior staff scientists (sv. 1:e forskningsingenjör) at the start of 2023. Cecilia Person is the Facility manager (0.5 FTE). Two FTE (full time equivalents) were allocated for operations in the Protein Production Sweden (PPS) and the Chemical Biology Consortium Sweden (CBCS) research infrastructures, respectively and 0.2 FTE were supported from the NBIS research infrastructure. One staff scientist resigned in May and one staff scientist was on sick leave between June and October. A new recruitment with start in 2024 was made and a temporary replacement was recruited for six months.

The service area metabolomics has been supported by 1.5 FTE senior staff scientists, DNP-NMR was effectively supported by 0.75 FTEs. Service for small molecules has been relatively high, 1 FTE, mostly due to installation of the walk-up system. The support for structural biology has been 1 FTE. Spectrometer maintenance and helium handling are included in this numbers.

In April 2023 a postdoc was employed in the EU research infrastructure project PANACEA for two years, and M.Sc. A research assistant was employed during 7 months (June-December) in the SciLifeLab “BeyondFold” project. B.Sc. An internship from University of Marseille, was organized at the Swedish NMR Center during the period June-August, 2023.

### **Usage per application area**

The total usage includes walk-up, SNC methods development, service, maintenance and losses due to e.g. late cancellations. Applications in structural biology account for 38% of total spectrometer time. Metabolomics accounts for 17 %, Small Molecules including use of the walk-up system accounts for 17 %. Materials Science required 5%, DNP-NMR 3,4 % and Fragment based screen 2 %. The remaining time was spent on internal use at the Swedish NMR Centre (Methods development, 5%), spectrometer maintenance and implementation (7%) and losses due to e.g. cancellations (7%).

The Science Faculty used 38% of spectrometer time, the Sahlgrenska Academy 12%, other academic users used 20% and industry 9%. The 20% of academic use outside the university of Gothenburg includes ALL major Swedish universities.

During 2023, 58 researchers (PIs) received access or support from the Swedish NMR Centre. Of these, 24 (41%) were women. The use is distributed among 112 projects of varying scope. Structural biology dominates (35) projects, followed by small molecules

(21), metabolomics (20), materials science (13), DNP-NMR (10) Fragment based screen (3), Methods development (7) and teaching (3).

### **Publications**

The Swedish NMR Centre was acknowledged or had co-authors in 38 peer reviewed articles. Highlights where the Swedish NMR Centre was acknowledged are *e.g.*

-*Structure of Glycans by NMR Spectroscopy*, published in *Chemical Review*

-*Disulfide-Bond-Induced Structural Frustration and Dynamic Disorder in a Peroxiredoxin from MAS NMR* published in *JACS*,

Two examples with co-authors from the Swedish NMR Centre are *e.g.*

-*Insulin thermostability in a real world setting*, published in *The Lancet Diabetes & Endocrinology*

-*Atomic-level structure determination of amorphous molecular solids by NMR*, published in *Nature Communications*.

Out-reach and competence development is described in other sections below.

### **Activity, outreach and competence development**

During 2023, the Swedish NMR Centre coordinated or participated in several national and international research infrastructures. Activities and period of activity for research infrastructures funded by the Swedish Research Council are:

-SwedNMR (general NMR, 2022-2026, coordinator)

-CBCS (chemical biology, 2022-2026),

-PPS (protein production, 2022-2026) and

-NBIS (bioinformatics, 2023-2028)

The Swedish NMR Centre is a unit within SciLifeLab (2021-2024) and also coordinates the Integrated Structural Biology platform within SciLifeLab.

At EU level, the Swedish NMR Centre participates in the research infrastructures PANACEA (2021-2025) and R-NMR (2022-2025).

Within the University of Gothenburg, apart from setting up the walk-up system, all users at the department of Chemistry and Molecular Biology and users at Chalmers received hands-on training in small groups.

The advanced course on NMR, KEM840, was co-organized at the Swedish NMR Centre.

The internal methods development was to a large extent focused on benchmarking, and implementation of relaxation experiments and methods for  $t_1$  noise suppression. New methods for quantification of inflammation biomarkers were implemented as part of the upgrade to IVDr 2.5.

Within SwedNMR, two topical meetings focusing on  $^{13}\text{C}$  and  $^{15}\text{N}$  relaxations were organized in Gothenburg (March 13-14) and Lund (April 18-19) respectively. The meetings were followed up by a mini-symposium on protein relaxation organized as a

satellite to the European Biophysics Society meeting in Stockholm (July 30, ca 40 participants). These events are part of the competence development for staff scientists.

An international workshop on artificial intelligence in NMR (AI in NMR, September 24-29) was organized at the Swedish NMR Centre: The workshop was attended by ca 20 postdocs and PhD students.

The SwedNMR annual meeting with ca 100 participants was organized in Uppsala (May 3-5).

The Umeå node will conduct a national users survey for the SwedNMR annual report.

Within the ISB platform of SciLifeLab, a strategy meeting was organized in Hällsnäs outside Gothenburg (January 26-27), focusing on platform operations during 2023- and 2024.

The ISB annual users meeting (Stockholm, December 6) attracted more than 60 participants and was followed up by a second strategy meeting (December 7) where the SciLifeLab operations during 2025-2028 were discussed.

The BeyondFold project focused on the use of AlphaFold together with NMR based protein dynamics.

Clinical metabolomics was addressed in two projects focusing on QC of biobanked sampled, and inflammation markers in long covid, respectively.

The collaborative project FragCor, where fragment based screen was applied to identify potential hits against Covid 19 Nsp5/Mpro was finished.

Within PANACEA, two trans-national (TA) projects were received. In the joint research activity (JRA), the first DNP-NMR spectra showing <sup>19</sup>F DNP were recorded.

In the R-NMR project, the Swedish NMR Centre assisted in the evaluation of a survey and a report on GDPR, participated in the discussions and gave a presentation on aspects of remote access to NMR spectrometers.

### **Funding and economic result 2023**

Locally, the Swedish NMR Centre received basic funding from the Sciences faculty, the Sahlgrenska Academy and the vice chancellor. In addition, strategic co-financing (30-50%) of external funding is provided from the vice chancellor (25% and the Science faculty (5-25%), connected to external grants from other funding bodies, e.g. the research council (50%), SciLifeLab (30%) and EU (the difference in real overhead and the 20% approved by EU).

The Swedish NMR Centre also receives funding from SciLifeLab, the research council (SwedNMR, PPS, CBCS; NBIS) and from EU (PANACEA, R-NMR).

The profit and loss account for the Swedish NMR Centre in 2023 is reported in table 1. The results follow the budget reasonably well. On the revenue side, *sales* increase by SEK

1.3 million SEK, largely due to metabolomics. Principles for accounting of co-financing are being discussed. On the *expenditure* side, salaries and other personnel costs are slightly below budget (SEK 1.3 million), due to delayed recruitments and sick leave. Operating costs are SEK 1.1 million over budget (especially costs for helium and consumption mtrl), but also premises costs deviate significantly (+0.7 million SEK). Internal co-financing is under discussion. The result (2 163 thousand SEK) is considerably higher than budget. The main reasons are better sales and changes in accounting of co-funding. Sales now contributes 17% of expenditures.

<b>Profit and loss account</b>	<b>Budget</b>	<b>Result</b>	<b>%</b>
Faculty funding	4 952	4 993	100
Sales	2 200	3 471	158
Internal grants	1 500	1 514	101
Grants	5 680	7 086	125
Co-financing	2 464	3 650	148
Financial revenues		143	
Accrual of project	1569	1 497	95
Hasselblad Found*	500		(incl in grants)
<b>Revenues</b>	<b>20 169</b>	<b>22 355</b>	<b>111%</b>
Salaries	9 057	7 871	87
Change holiday debt	0	24	
Other personnel costs	325	180	55
Running costs	4 083	5 194	127
Co-financing	1 304	888	68
Overhead costs		223	
Premises	2 600	3 262	125
Financial costs	0	16	
Depreciations	2 852	2 533	89
<b>Expenditures</b>	<b>20 171</b>	<b>20 193</b>	<b>100</b>
<b>Total</b>	<b>0</b>	<b>2 163</b>	



## Publikations 2023

Scientific reports where the Swedish NMR Centre was acknowledged (1-26) or co-authored by staff from the Swedish NMR Centre (27-38).

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