Nuclear Magnetic Resonance Research Resource
2020 Annual Report

Introduction

The Nuclear Magnetic Resonance Research Resource (NMR^3) provides nuclear magnetic resonance (NMR) spectroscopy services to academic, industrial, and government users, in a multitude of forms ranging from training researchers to perform hands-on experiments to data processing and interpretation to research collaboration. Housed in the Chemistry Building at Dalhousie University, the NMR^3 currently hosts 4 NMR spectrometers with a variety of capabilities, ranging from 300 MHz for liquids to 700 MHz for solids. It has a staff of two Ph.D. chemists, who work with the users on data acquisition, interpretation, and publishing, alongside maintaining the instrumentation. In addition, the NMR^3 partners with the proximal NRC-IMB lab in the operation of a 700 MHz spectrometer optimized for biological samples, and NMR^3 users are allocated up to 30% of the time on this instrument. Because of the high concentration of small- to medium-sized universities in the Atlantic Region, the NMR^3 plays a special role as a catalyst in enhancing research in the area, by providing both equipment and expertise in NMR that these universities cannot afford individually. Dalhousie additionally benefits from this role in terms of the positive perception of our research intensiveness that is developed among the hands-on users from the other local universities, who are typically potential recruits for graduate or postgraduate studies. In addition, NMR^3 provides services to area government laboratories, industry, and start-ups. Most recently, and with special permission due to the shut-down, NMR^3 provides analytical support for the high priority Covid-19 research.

Mission

The Nuclear Magnetic Resonance Research Resource (NMR^3) is a research resource for NMR, with a client base distributed throughout the Atlantic region, primarily in the Maritime Provinces. The Centre was established as the Atlantic Region Magnetic Resonance Centre in 1982 through financial support from the Natural Sciences and Engineering Research Council of Canada (NSERC) and Dalhousie University and has enjoyed support from these and other sources throughout its history. The mission of the facility is to provide high-field NMR spectral data and expertise to scientists in the Atlantic Region of Canada. The facility has enhanced numerous research programs and resulted in the training of numerous young scientists attending Universities in the Atlantic Region.

Organizational Structure

The NMR^3 Centre staff consists of:

- Dr. Jan Rainey, Director (July 1, 2011 – June 30, 2020) and Professor in Biochemistry & Molecular Biology and Chemistry (on sabbatical spring 2020)
- Dr. Josef Zwanziger, interim Director (January 2020 – June 30, 2020) and Professor in Chemistry and Physics
- Dr. Mike Lumsden, Facility Coordinator
- Dr. Ulrike Werner-Zwanziger, Solid-state NMR Coordinator

The **Director** is elected by the Users Committee and is appointed for a three-year term. He/she is normally a faculty member of Dalhousie University, Department of Chemistry with duties that include the preparation of grant applications to support the operation of the Centre as well as the promotion of the Centre to outside users and the preparation of reports, including the Annual Report.

The **Facility Coordinator** is a staff member of the Department of Chemistry of Dalhousie University. He/she will be selected by the NMR^3 User Committee, in consultation with the Director and the Chair of the Chemistry Department. Her/his duties include overseeing the day-to-day operation of the Centre, including the supervision and support of hands-on users, implementing equipment training programs, scheduling the equipment and liaising with lab instructors and TA's in the delivery of teaching labs making use of the NMR spectrometers.

The **Solid-State NMR Coordinator** oversees the operation of the solid-state NMR instrumentation including all aspects of research, as well as instrument maintenance and repairs, administration, and other solid-state NMR lab organization.

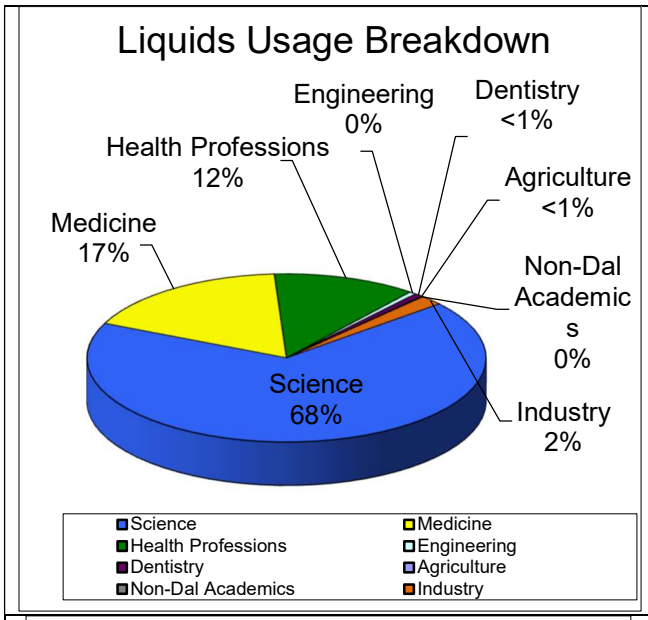
Policies regarding NMR^3 Centre usage protocols, user fees and decisions on instrument upgrades are made by the **NMR^3 User Committee** (UC). This group is led by an elected Chair (at present, Dr. Alex Speed, Professor of Chemistry, Dalhousie) who serves a term of no more than three years. The voting members of the UC are those academic researchers who have paid user fees to the Centre within the preceding 12 months. This committee sets the overall policy of the Centre, is the ultimate decision-making body and meets at least semi-annually to consider the annual report and other business arising during the year.

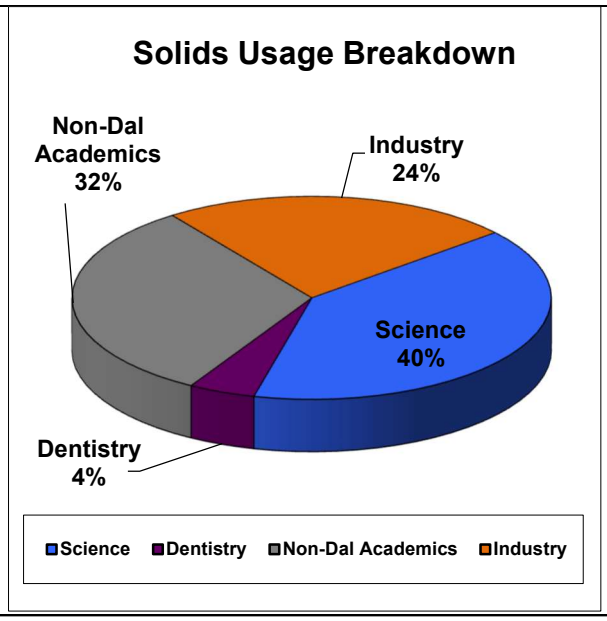
Key Research Outcomes and Activities

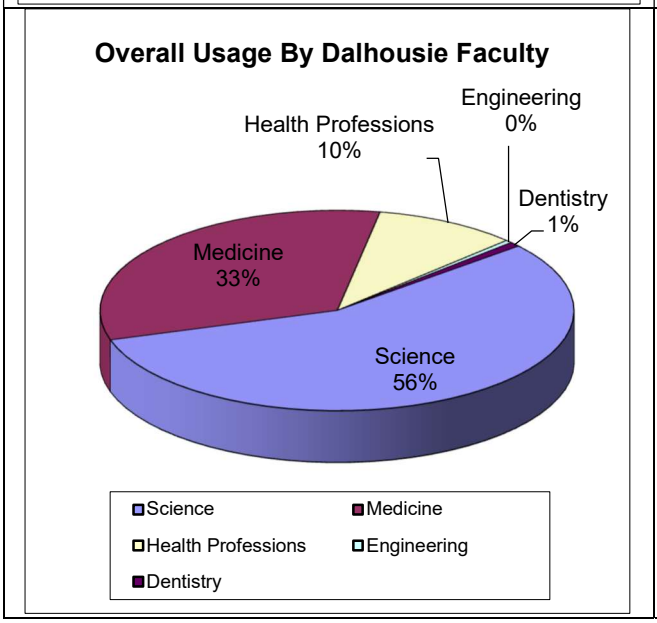
In the past year, the NMR^3 Facility served a total of 135 users from 29 research groups in addition to 20 customers from Government and Industry.

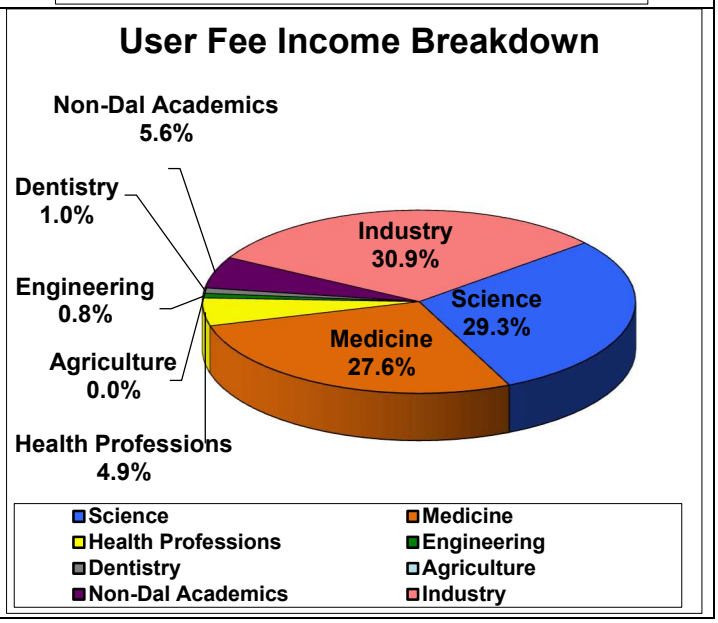
Position	Dalhousie	Other Maritime Institutions	Other Academic Institutions	Government & Industry
Faculty Members	22	6	1	
NMR^3 Staff	2			
Instructors & TA's	12			
Post-Docs	9		1	
PhD Students	23	3		
Masters Students	23	1		
Undergraduate Students	29	1		
Others	8		1	20

The support the NMR^3 facility provides is reflected in the scientific output. In the last year, 54 publications have appeared using NMR^3-produced data, as well as 6 PhD theses, 3 M.Sc. theses, various honours theses, and 74 conference presentations. The Centre assisted 29 research groups, mostly drawn from the Atlantic Canada region but also including several international researchers, resulting in 111 highly qualified personnel trained. Furthermore, teaching in the Departments of Chemistry and Biochemistry & Molecular Biology was supported in 6 undergraduate labs and 2 graduate labs with 105 total students and a combined 192 hours, providing exposure to both the practical aspects of NMR spectroscopy and the nuances of data analysis. Access to NMR spectrometers has been critical for one patent application from faculty within Dalhousie University (Prof. Jeff Dahn) and at least one industrial patent application by a local start-up company (Coloursmith Labs Inc.). In total, use of the Centre's 5 NMR instruments was ~5943 hours. Most of the instrument usage was logged in experiments configured by trainees in support of externally funded research grants for Dalhousie University researchers. Perhaps the most concrete illustration of the critical and valuable nature of the services provided by our Centre is the fact that Dalhousie-based researchers identified NMR^3 access as being essential in just over ***$2.4-million in new external grant funds awarded*** in the reporting year. In addition to servicing the NMR needs of the academic community of the Atlantic Region and beyond, the highly specialized instrumentation has supported local and national industrial research. In particular, the specialized solid-state NMR instrumentation and excellent support staff has attracted collaborations worldwide, including users from the United States, Europe, and Asia.









Community Impact

Thanks to a broad range of instrumentation, expert staff, and a world-class reputation for excellence in NMR spectroscopy and research that relies on it, the NMR³ facility has had an impact on a **broad spectrum of scientific communities**. As supported by the data in the previous section, these range from guiding undergraduate students in teaching labs and research projects to collaborating and publishing with high-level scientists and faculty within Dalhousie and beyond.

Dalhousie Undergraduate students and those of regional Universities are positively impacted by NMR³ both from a teaching and a research perspective. In the previous academic year, five different undergraduate courses made direct use of the NMR spectrometers for teaching/data acquisition purposes, logging nearly 200 hours of spectrometer time. In addition, many Honours research projects and experiential learning students from a variety of Faculties are reliant upon NMR³ for progress and success.

Dalhousie Graduate students from a broad range of research disciplines rely upon NMR^3 for their research pursuits. Because NMR spectroscopy is such a diverse technique, graduate students in chemistry, physics, biochemistry, materials science, and engineering and beyond benefit from the facility's infrastructure and expertise. With training of HQP a key focus, most of these graduate students use the spectrometers in a hands-on fashion. In the reporting year, 46 Dalhousie graduate students have used the facility.

Post-Doctoral Fellows and other high-level Scientists from Dalhousie University, regional, and international institutions have taken advantage of our instrumentation and expertise, both in form of training of HQPs as well as obtaining research results through collaboration. These researchers originate from a variety of Dalhousie University departments, including Chemistry, Physics, and Biochemistry and Molecular Biology, and international institutions such as Indiana University (USA) and Friedrich-Schiller-University (Germany).

Research programs for many **Academics Beyond Dalhousie** are enhanced by NMR^3. Because of the high concentration of small- to medium-sized universities in the region, the NMR^3 plays a special role as a catalyst in enhancing research in the area by providing both advanced infrastructure and expertise that these universities do not possess individually. Dalhousie additionally benefits from this role in terms of the positive perception of our research intensiveness that is developed among the hands-on users from the other local universities, who are typically potential recruits for graduate or postgraduate studies. In the reporting year there have been active collaborations with laboratories at Saint Mary's University, University of New Brunswick, and Cape Breton University as well as international institutions.

Ongoing strong collaborations with a variety of **Industry & Startups** has had a mutually beneficial impact as well as on the local economy. These collaborations include ongoing projects of scientists trained for hands-on-use, mostly on the liquid state NMR instruments by companies such as Tesla and Solid State Pharma, as well as occasional service support on the solid state instrumentation to companies such as Solid State Pharma and Research Productivity Council (New Brunswick). Recent results obtained on the solid state NMR spectrometers were crucial for the patent application of Coloursmith Labs Inc.

Commitment to Equity Diversity & Inclusion

The NMR^3 labs are open to all users with training, without exception. Last year, of the 102 hands-on users (that is, users working in-person in the labs and under guidance from the staff), some 47 were female and 20 were in racially visible minority groups. With a staff that is itself diverse, we believe that NMR^3 is successful in providing an inclusive, supportive laboratory environment that helps all users achieve scientific success.

Operations

Opportunities for our ongoing operations include the following:

1. Our interaction with local industry was very successful over the last year and we foresee increasing it. We plan to rejuvenate the practice of an annual NMR workshop day, with an emphasis on partnerships with industry, and featuring some of recent successes (Solid State Pharma, Coloursmith Labs, Tesla).

2. We are in the process of renewing one instrument, with more in the pipeline—having more up-to-date equipment will help expand the facility use, both by opening up access to new methods, and reducing the amount of time the staff must spend on maintenance.

Barriers include:

1. The current and ongoing helium supply uncertainty is of large concern to the NMR^3 facility. All spectrometers rely on liquid helium to keep the super-conducting magnets in operation, so lack of supply has existential consequences. In addition, the supply uncertainty has financial consequences as significant price increases have been predicted by the supply companies. Dalhousie's Core Funding has supported the NMR3 Facility by directing funding towards the purchase of a helium capture and liquefaction instrumentation. The process of planning and purchasing this instrumentation is ongoing.

2. During the preparation of this report, the University was closed due to the Covid-19 pandemic. The details and timeframe concerning resumption of research activities remains unclear but what is clear is that the day-to-day operations of NMR^3 will be impacted, particularly for the high-resolution NMR spectrometers where there is a large **hands-on** user base. The interim Director and Facility staff have been devising a re-opening plan which will convey details about new sanitation procedures, the use of PPE, and maintaining 2 m of social distancing while working in the NMR room. By virtue of some important covid-19 research taking place at Dalhousie that is making use of the NMR spectrometers, these guidelines are being tested prior to the broader re-opening.

3. The continuing uncertainty in salary support for the NMR3 staff leads to artificially high user rates, so much so that use is actually suppressed on the solids side. While both staff members are in T-10, NSGEU positions, neither position is fully funded by the university. Therefore, rates are kept artificially high as a hedge against loss of core funding, which has led a number of users especially on the solids side to send samples to other facilities. If the core funding situation could be stabilized, particularly by funding these full time staff positions, rates could be brought more in line with other institutions and usage would increase.

Goals/Plans for Upcoming Calendar Year

1. *Replacement of aging spectrometer console for solid state NMR spectrometer:* Thanks to a successful NSERC RTI application for major infrastructure improvements on our solids instruments led by Dr. Josef Zwanziger together with Dr. Daniel Boyd, Dr. Jan Rainey, Dr. Jason Clyburne (SMU) and Dr. Ulrike Werner-Zwanziger, the replacement of the aging Bruker 400 MHz DSX solid state NMR console is in the progress. The bid has been awarded to Tecmag Inc. and was close to shipment at the end of March. The Covid-19 shutdown has halted the delivery. We expect it now within a few months. Given the current difficult situation, the installation will likely be done by the solid state NMR coordinator with remote help from the company. Initial training will take place remotely and in person at a later date.

2. *Helium recovery system:* Thanks to funding from Dalhousie University, funding to purchase a helium recovery system for the ssNMR instruments has been granted. Planning has taken considerable time from the fall onwards. Unfortunately, also, this project has been delayed by the Covid-19 shutdown. We hope to resume the bidding process as soon as longer presence in the laboratories is allowed and outstanding issues can be addressed. Considerations are on the way on how to possibly tie in the liquid state NMR magnets.

3. *NMR Research Day:* Plans are being drafted to organize an NMR workshop. Originally, we had hoped to hold this workshop in June, but here also the Covid-19 shutdown enforced a modification of the plans. Given all the current uncertainties this plan will be revisited later.

4. A variety of *initiatives are underway to bring new infrastructure* to NMR^3. First, a CFI JELF/CRC application by Professor Alison Thompson to upgrade and expand our existing liquids facility, by adding a 400 MHz spectrometer for liquids, should be deciding upon soon. This instrument will be installed in the 4th floor lab area. Second, Professor Zwanziger is a co-PI on a CFI IF proposal led by Professor Michael Freund, that, if successful, will add a very low field spectrometer to the ground floor lab dedicated to the study of batteries and battery materials. Finally, Professor Jan Rainey is a co-PI on a multi-institution CFI IF application by Professor Jan Rainey which would bring new solution- and solid-state biomolecular capabilities, with primary installation site in the LSRI.