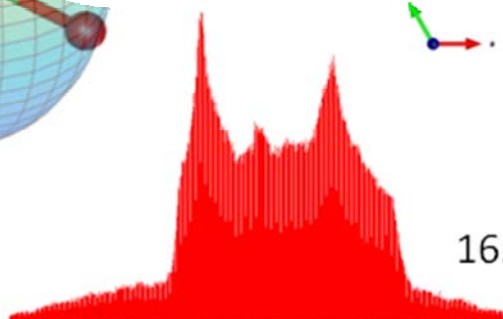
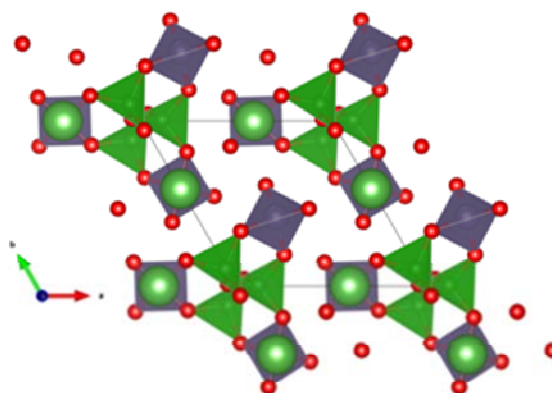
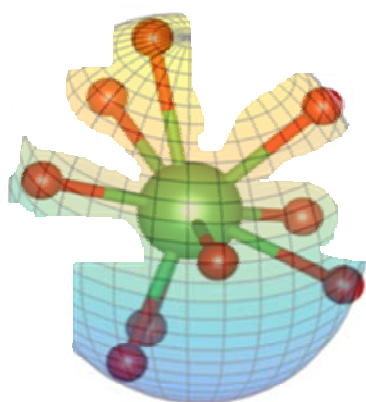


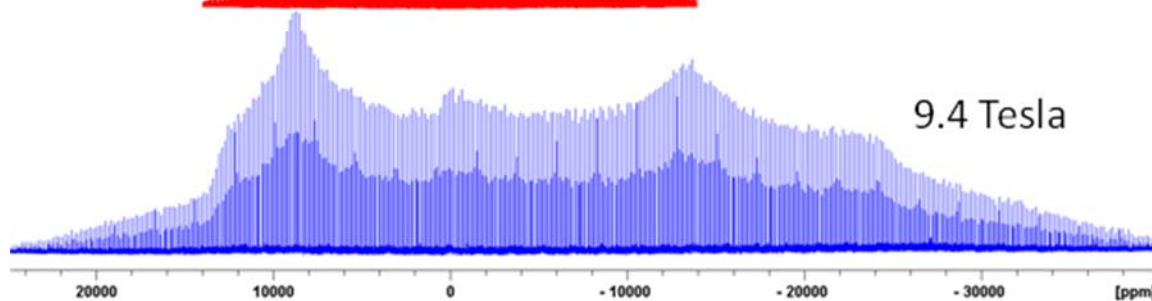
NUCLEAR MAGNETIC RESONANCE RESEARCH RESOURCE

2015 – 2016 Annual Report

^{39}La Solid State NMR Results of LaBGeO_5 Crystals



16.5 Tesla



9.4 Tesla

20000

10000

0

-10000

-20000

-30000

[ppm]

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About the cover: ¹³⁹La solid state NMR spectra of LaBGeO₅ crystals acquired at 16.5 T (top spectrum) and 9.4 T (bottom spectrum) by Alex Paterson in Professor Josef Zwanziger's group. Using static WURST-QCPMG experiments for wideline excitation, the experiment at two magnetic fields are used to separate chemical shift and quadrupole interactions. The ellipsoid fit to the LaO₉ coordination polyhedron is used to correlate distortions of the local structure to quadrupole and chemical shift parameters. In the crystal structure, the BO₄ tetrahedra (green) form a helix along the threefold screw axis which is (broadly) responsible for the ferroelectric properties of the crystal.

Section 1 - Overview of NMR³ Centre and its Mission

The Nuclear Magnetic Resonance Research Resource (NMR³) supports users from the Atlantic region, primarily the Maritime Provinces, but also from across Canada and internationally. The Centre provides nuclear magnetic resonance spectroscopy (NMR) services to academic, industrial, and government users, in forms ranging from training users to perform hands-on experiments to data acquisition and interpretation to research collaboration. Housed in the Chemistry Building at Dalhousie University, the NMR³ 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. level chemists, who work with the users on data acquisition and interpretation, alongside maintaining the instrumentation. In addition, the NMR³ partners with the proximal NRC-IMB lab in the operation of a 700 MHz spectrometer optimized for biological samples, and NMR³ 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 NMR³ 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, and which would be highly redundant to provide at each. 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.

NMR spectroscopy is the most important characterization technique available to chemists, biochemists and materials scientists, and is very important for many others including clinicians. Technological advances in the last decade have tremendously enhanced the value of NMR spectroscopic data and the variety of experiments now available. The Atlantic Region has a world-class reputation for research involving NMR spectroscopy and research that depends on NMR spectroscopy. In 2015-2016, the Centre assisted 36 research groups mostly drawn from the Atlantic Canada region but also including several international researchers, resulting in 60 publications, 8 patents, 163 conference presentations and 120 highly qualified personnel trained. Furthermore, teaching in the Departments of Chemistry and Biochemistry & Molecular Biology was supported in 5 undergraduate labs and 1 graduate lab with 207 total students and a combined 234 hours, providing exposure to both the practical aspects of NMR spectroscopy and the nuances of data analysis. In total, use of the Centre's 5 NMR instruments was ~8348 hours. The vast majority of instrument use 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 NMR³ access as being essential in just under *\$8-million in new external grant funds awarded* in the 2015-2016 fiscal year. On a rolling basis, it should be further noted that NMR³ has been identified by users as being instrumental in the awarding of an additional \$13.8-million in external grant funding to Dalhousie researchers in the 2014-2015 (>\$2.4-million), 2013-2014 (>\$1.5-million), 2012-2013 (>\$6.7-million) and 2011-2012 (>\$3.2-million) fiscal years.

Based upon input from the NMR³ Centre staff (Dr. Jan Rainey, Director (July 2011-Present; in the midst of a second elected 3-year term) and Professor in Biochemistry & Molecular Biology and Chemistry; Dr. Mike Lumsden, Facility Coordinator; and, Dr. Ulrike Werner-Zwanziger, Solid-state NMR Coordinator), policies regarding Centre usage protocols, user fees and decisions on instrument upgrades are made by the NMR³ User Group comprising an elected Chair (Dr. Mark Stradiotto, Alexander McLeod Professor of Chemistry, Dalhousie) and all Faculty who have paid user fees in the past Fiscal Year (Table provided in Section 3.1.1) are voting members of the User Group.

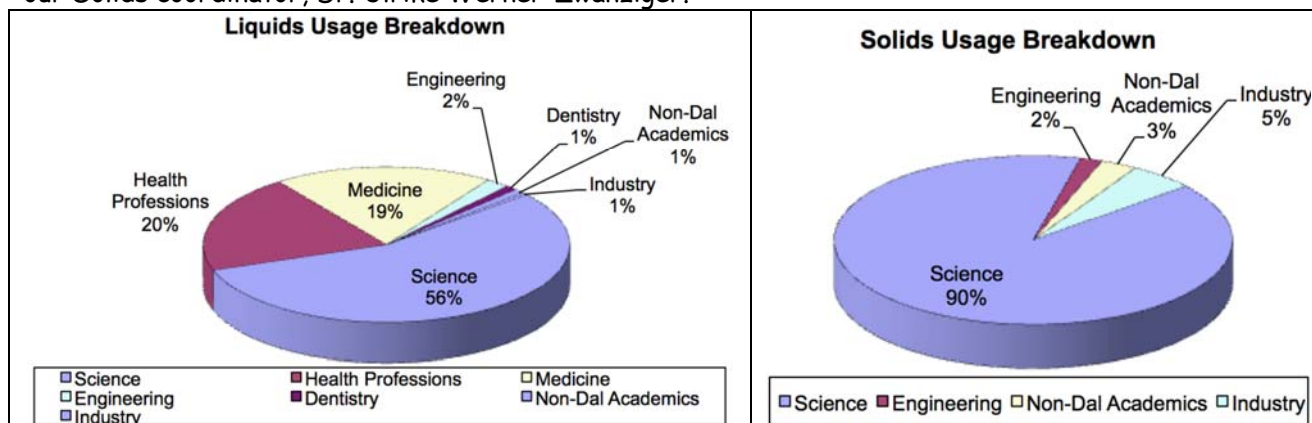
1.1 Mission Statement

The Nuclear Magnetic Resonance Research Resource (NMR³) is a research resource for nuclear magnetic resonance, 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 nuclear magnetic resonance (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.

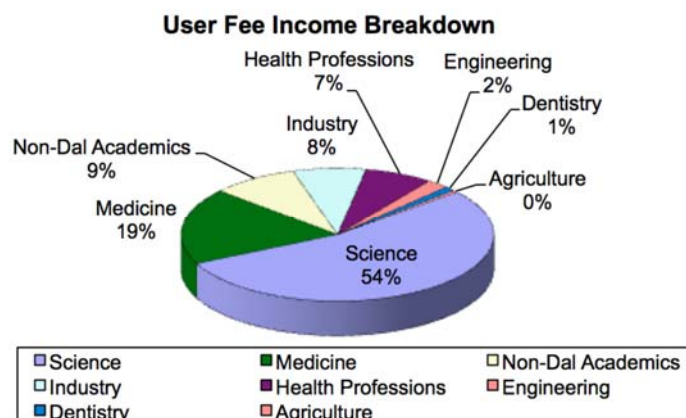
Deviation from original mission statement: with the demise of NSERC funding for facilities such as NMR³, we are now fully reliant upon funding from 3 sources: Dalhousie University, user fees and from "Supporting Institution" fees collected from other universities. Section 4.1 of the report fully describes the breakdown of these fees and the definition of Supporting Institution.

1.2 Current Year's Activity

1. Continued widespread usage: As in previous reporting years, NMR³ continues to experience broad usage from across Dalhousie and beyond. Although quite heavily tilted towards the Faculty of Science, particularly for the Solids facility, usage is clearly diverse. Particularly notable is the degree to which the Solids instruments are sought after by external users. This is an excellent indicator of the uniqueness of our Solids capabilities both in terms of instrumentation and in terms of the expertise of our Solids coordinator, Dr. Ulrike Werner-Zwanziger.



Also informative is the profile of our User fee income (detailed in Section 4), where it is clear that Industrial User fees, 77% of which came from Solids instrument usage, are an extremely important component of our total User Fee income at 8%. Dr. Ulrike Werner-Zwanziger's increase in position from 0.5-FTE to 0.75-FTE (point 1.2.3, later in this section) came only in the final quarter of the previous fiscal year. The additional 0.25-FTE of expert staff time now available in the Solids facility is therefore likely to lead to further industrial income for NMR³.



2. Full salary support currently achieved: Through an application for support from Dalhousie's Strategic Initiatives Fund (SIF) spearheaded by Dr. Mark Filiaggi, Associate Vice-President Research, NMR³ is currently receiving full salary support. These funds are coupled with a Department of Chemistry position allocation (~2/3 of Dr. Mike Lumsden's salary) and funds obtained from the Faculty of Science as a result of Dr. Josef Zwanziger's Canada Research Chair (a fixed \$30,000 toward Dr. Ulrike Werner-Zwanziger's salary). The NMR³ top-up request from the SIF has been approved for the 2015-2016 Fiscal Year, with conditional budget approval for the 2016-2017 and 2017-2018 Fiscal Years, meaning that our user fees only need to cover non-salary expenses for these years. This conditional approval relies both upon the results of the annual Budget Advisory Committee report and upon NMR³ continuing to satisfy and maintain performance criteria. We have been told that our comprehensive annual report is an excellent means by which we can document this latter point, so are grateful to the users for their cooperation.

3. Increase in Solids Coordinator FTE-level: As part of our proposal for SIF support, an increase from 0.5-FTE to 0.75-FTE for Dr. Ulrike Werner-Zwanziger's position was requested. The level of demand on Dr. Werner-Zwanziger's expertise and time was well beyond what was reasonable at a half-time level, with three-quarters time being a more accurate assessment of the time she commits. This request was fully approved, meaning that we are very fortunate to now officially have Dr. Werner-Zwanziger employed at a 0.75-FTE level. Without the SIF support, or a similar salary support program, this unfortunately would not have been financially viable.

1.3 Upcoming Year's Activity

1. Solids instruments upgrades: Thanks to a donation from Dr. Josef Zwanziger, the workstations and software of the two solid-state NMR spectrometers will be upgraded from XWIN-NMR 3.6 to TopSpin 1 and TopSpin 2, for the 400 MHz and 700 MHz spectrometers, respectively. These TopSpin software versions are the highest levels that the consoles can support. As of the time of writing, these upgrades are in progress.

2. NSERC RTI application: Dr. Josef Zwanziger together with Dr. Daniel Boyd, Dr. Jan Rainey and Dr. Ulrike Werner-Zwanziger, have submitted an NSERC-RTI application to the internal Dalhousie review committee for major infrastructure improvements on our Solids instruments. The funding proposes the replacement of the aging air compressor. The group is currently awaiting internal review results from Dalhousie University to proceed with the RTI submission to NSERC.

3. CFI Innovation Fund application: Dr. Jan Rainey (as project lead), along with other NMR³ users Drs. Stephen Bearne, Roy Duncan, David Langelaan, Paul Liu, and David Jakeman, are currently finalizing a CFI Innovation Fund application that would bring a third operational node to NMR³: a biomolecular NMR node, to be housed in the Life Sciences Research Institute on Summer Street. This would free up autosampler time on the 500 MHz, in particular, and provide many new NMR instrumental capabilities with a third, dedicated PhD-level NMR³ staff member.

4. CFI Innovation Fund application: CFI Innovation fund application with Dr. Daniel Boyd as Co-PI, being led by McGill (PI: Showan Nazhat), is associated with developing new glass materials for the release of inorganic therapeutics with applications in hard tissue repair / regeneration, hemostatic agents, and for interventional oncology. The request for funding includes the purchase of a fast spinning MAS probe head for the solid-state NMR³ spectrometers.

5. Operations and Maintenance Support for Research Equipment application: Dr. Josef Zwanziger, in combination with the Institute of Research in Materials, will submit a proposal to the new "Operations and Maintenance Support for Research Equipment" funding that will include some of the operational costs of the NMR³.

6. Conversion of Room 426B into a Resource for NMR Instruction and Centralized Data Processing: Since the decommissioning and removal of the Bruker AC-250 NMR spectrometer in 2012, Room 426B in the NMR³ facility has been used for storage. Although long been viewed as a potential resource for NMR-related training and tutorials, financial constraints and uncertainty over the past 4 years have prevented this from happening. As outlined in Section 1.2.2, with full salary support now achieved, the planned conversion of this space into such a resource will move forward. Consequently, rooms 426-431 of the NMR³ facility will have integrated areas for NMR data acquisition (Room 431), NMR data processing (Room 430), sample preparation (Room 429) and instruction (Room 426B).

Section 2 - Centre Resources and Capabilities

The following tables outline the current suite of NMR spectrometers managed by the NMR³:

Bruker AVANCE - 300 MHz: Liquids Only		
Magnet	Bruker 300/54mm on a TMC Anti-Vibration Platform	
Console	Bruker Avance	
Channel 1	Broadband BLA2BB Amplifier (50 W ¹ H & 135 W ¹³ C)	
Channel 2	Broadband BLA2BB Amplifier (50 W ¹ H & 135 W ¹³ C)	
Probe 1	5 mm BBFO	Observe: ¹⁴ N- ³¹ P & ¹⁹ F/decouple: ¹ H, z-gradient coil and auto-tune & match accessory (ATMA)
Temperature Control	B-VT 3200	Includes a 25L liquid N ₂ dewar.
Automation	16 sample SampleXpress Lite	
Workstation	HP xw4600 operating with Windows XP Pro	
Spectrometer Software	TopSpin 2.1 pl8	

Bruker AVANCE - 500 MHz: Liquids Only		
Magnet	Spectrospin 500/54mm UltraShield with anti-vibration posts	
Console	Bruker Avance	
Channel 1	Broadband (300 Watt BLAXH)	
Channel 2	¹ H and ¹⁹ F (100 Watt BLAXH)	
Channel 3	Broadband (300 Watt BLAX)	
Probe 1	5 mm BBO SmartProbe	Observe: ¹⁴ N- ³¹ P & ¹⁹ F/decouple: ¹ H, z-gradient coil and auto-tune & match accessory (ATMA)
Probe 2	5 mm BBO	Observe: ¹⁴ N - ³¹ P / decouple: ¹ H, z-gradient coil and auto-tune & match accessory (ATMA)
Probe 3	5 mm TXI	Observe: ¹ H / decouple: ¹³ C and ¹⁵ N, Z-gradient coil.
Temperature Control	B-VT 3200	Air pre-cooled with a BCU-05 chiller, also includes a 25L liquid N ₂ dewar and an exchange coil for generating cold N ₂ gas.
Automation	60 sample B-ACS (Bruker Automation Control System)	
Workstation	HP xw4600 operating with Windows XP Pro	
Spectrometer Software	TopSpin 2.1 pl8	

Bruker AVANCE III - 700 MHz: Liquids Only**		
Magnet	Spectrospin 700/54mm UltraShield Plus with anti-vibration posts	
Console	Bruker Avance-III	
Channel 1	Broadband (500 Watt)	
Channel 2	^1H and ^{19}F (100 Watt)	
Channel 3	Broadband (500 Watt)	
Channel 4	Broadband (300 Watt)	
Probe 1	5 mm TCI Cryoprobe	Observe: ^1H / decouple: ^{13}C and ^{15}N , with z gradient coil and auto-tune / match accessory (ATMA). ^1H , ^2H (lock), and ^{13}C preamps cryogenically cooled.
Probe 2	1.7 mm TCI Cryoprobe	Observe: ^1H / decouple: ^{13}C and ^{15}N , with z gradient coil and auto-tune / match accessory (ATMA). ^1H , ^2H (lock), and ^{13}C preamps cryogenically cooled.
Probe 3	5 mm BBO	Observe: ^{15}N - ^{31}P / decouple: ^1H , z gradient coil and auto-tune / match accessory (ATMA).
Temperature Control	B-VT 3000	Air pre-cooled with a BCU-05 chiller. Also includes a 25L liquid nitrogen dewar and a nitrogen exchange coil for generating cold N_2 gas. All probes equipped with BTO2000 accessory
Automation	SampleJET - accommodates up to 5 x 96 tubes + 47 individual positions. Equipped with a cooling option to cool samples down to 4°C.	
Workstation	HP xw4600 operating with Red Hat Enterprise Linux (Release 4)	
Spectrometer Software	TopSpin 2.1 pl4	

**Instrument sited at the NRC Institute for Marine Biondiagnostics NMR lab located adjacent to Dalhousie. The spectrometer is jointly owned and operated with this NMR lab.

Bruker DSX 400 MHz: Solids Only		
Magnet	Buker 400/89 UltraShield	
Console	Bruker Avance DSX	
Channels 1-3	Broadband Transmitter	
Probe 1	2.5mm MAS	^{69}Ga - ^{31}P / ^{19}F - ^1H
Probe 2	4mm HXY MAS	in dual mode: 45MHz - ^{31}P / ^1H Insert Pairs for X/Y (triple) mode: $^{31}\text{P}/^{11}\text{B}$, $^{31}\text{P}/^{27}\text{Al}$, $^{11}\text{B}/^{13}\text{C}$, $^{13}\text{C}/^{195}\text{Pt}$, $^{23}\text{Na}/^{29}\text{Si}$, $^6\text{Li}/^{29}\text{Si}$

Probe 3	4mm MAS	^{13}C - ^{31}P / ^{19}F - ^1H
Probe 4	7mm	^{15}N - ^{31}P / ^{19}F - ^1H
Probe 5	HP wideline probe	^{109}Ag - ^{31}P , high temperature design
Workstation	Silicon Graphics O ² operating with IRIX 6.3	
Spectrometer Software	XWIN-NMR 3.6 pl6 (upgrade to TopSpin 1 in progress)	

AVANCE 700 MHz: Solids Only		
Magnet	Buker 700/54 UltraShield	
Console	Bruker Avance	
Channels 1-3	Broadband Transmitter	
Probe 1	2.5mm MAS	^{13}C - ^{31}P / ^{19}F - ^1H
Probe 2	4mm MAS	^{15}N - ^{13}C / ^{19}F - ^1H , ^{43}Ca
TriGamma TM Probe	3.2mm MAS	^{15}N - ^{29}Si / ^{11}B - ^{31}P / ^1H
Triple Resonance Probe	4mm MAS	^{29}Si / ^{11}B / ^1H
Low Gamma Probe	5mm MAS	Special inserts for ^{43}Ca , ^{39}K , ^{91}Zr , ^{107}Ag , ^{67}Zn , ^{25}Mg , ^{135}Ba , ^{33}S , ^{14}N , $^{47,49}\text{Ti}$, ^{89}Y , ^{87}Sr / ^{19}F - ^1H ,
EFREE Probe (contact Jan Rainey, if you are interested in using this probe).	5mm static solenoid	HCN/P
Workstation	Dell (Pentium) operating with RedHat Linux	
Spectrometer Software	XWIN-NMR 3.6 pl6 (upgrade to Topspin 2 in progress)	

Section 3 - Detailed Description of Centre Activities

3.1 Core Group of Personnel Affiliated With or Residing Within the Centre

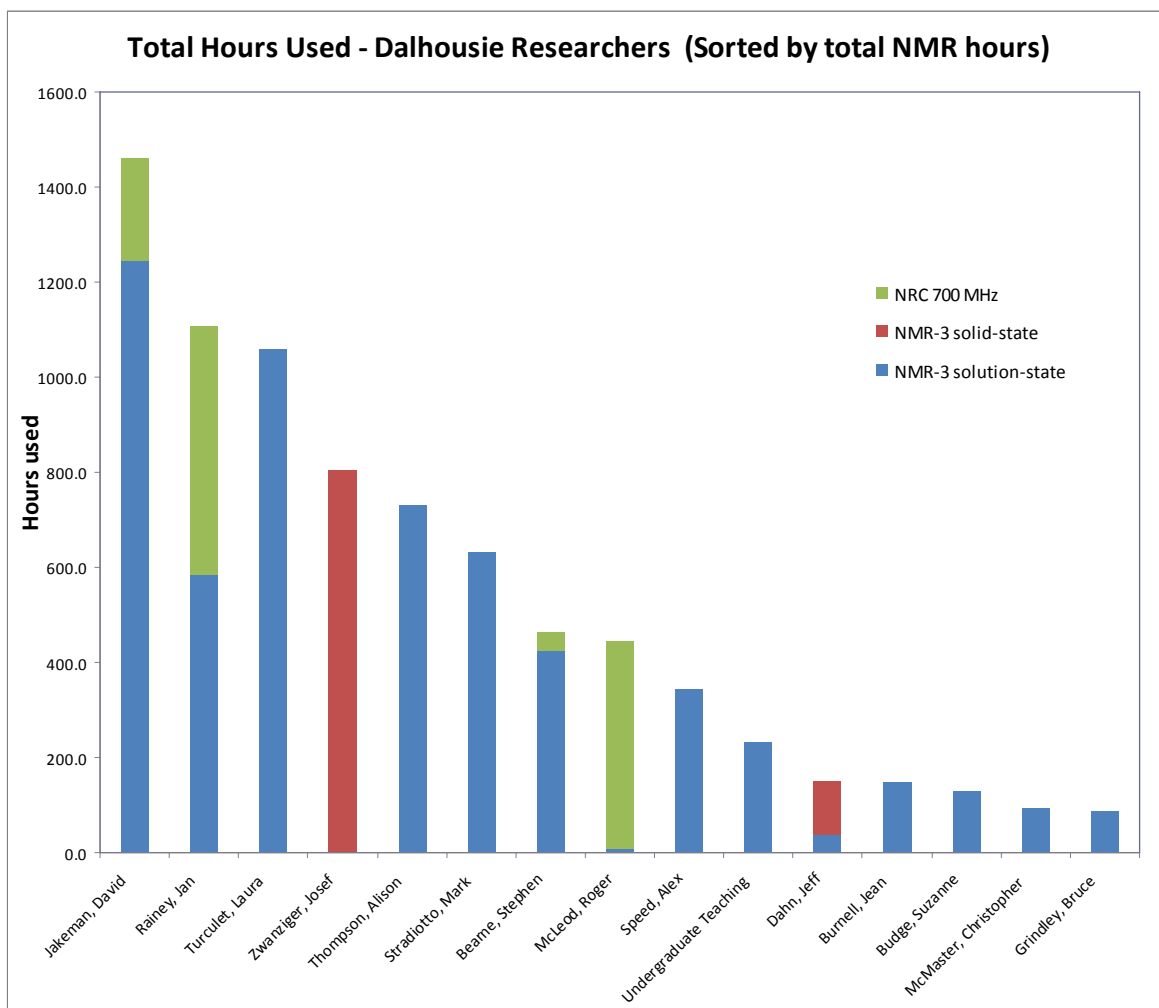
Position	Dalhousie	Supporting Maritime Institutions	Non-Supporting Maritime Institutions	Other	Government & Industry
Faculty Members	26	2	4	4	
NMR ³ Staff	2				
Instructors & TA's	14				
Post-Docs	17	1			
PhD Students	22			1	
Masters Students	24	3			
Undergraduate Students	31	2	3		
Others	5	2	1	7	12

3.1.1 Faculty

Number	Name	Affiliation	Rank
1	Bearne, Stephen	Dalhousie University	Professor
2	Boyd, Daniel	Dalhousie University	Associate Professor
3	Bronstein, Lyudmila	Indiana University	Senior Scientist
4	Budge, Suzanne	Dalhousie University	Professor
5	Burnell, Jean	Dalhousie University	Professor Emeritus
6	Chatt, Amares	Dalhousie University	Adjunct Professor
7	Clyburne, Jason	Saint Mary's University	Professor
8	Cozens, Frances	Dalhousie University	Associate Professor
9	Dahn, Jeff	Dalhousie University	Professor
10	Darvesh, Sultan	Dalhousie University	Professor
11	Ducatti, Diogo	Federal University of Parana, Brazil	Professor
12	Duncan, Roy	Dalhousie University	Professor
13	Filiaggi, Mark	Dalhousie University	Associate Professor
14	Grindley, Bruce	Dalhousie University	Adjunct Professor
15	Jakeman, David	Dalhousie University	Professor
16	Liu, Paul Xiang-Qin	Dalhousie University	Professor
17	Jha, Amitabh	Acadia University	Professor
18	MacQuarrie, Stephanie	Cape Breton University	Associate Professor
19	McFarland, Sherri	Acadia University	Professor

20	McLeod, Roger	Dalhousie University	Professor
21	McMaster, Christopher	Dalhousie University	Professor
22	Plucknett, Kevin	Dalhousie University	Professor
23	Rainey, Jan	Dalhousie University	Professor; NMR ³ Director
24	Ramanathan, Vaidhya	Indian Institute of Science Educ. & Res., India	Professor
25	Rohde, John	Dalhousie University	Assistant Professor
26	Schepp, Norm	Dalhousie University	Associate Professor
27	Singer, Rob	Saint Mary's University	Professor
28	Speed, Alex	Dalhousie University	Assistant Professor
29	Stradiotto, Mark	Dalhousie University	Professor; NMR ³ User Group Chair
30	Thompson, Alison	Dalhousie University	Professor
31	Turculet, Laura	Dalhousie University	Associate Professor
32	White, Mary Anne	Dalhousie University	Professor
33	White, Rob	Dalhousie University	Associate Professor
34	Wiesner, Ulrich	Cornell University, NY, USA	Professor
35	Xia, Aibing	Mount Saint Vincent University	Associate Professor
36	Zwanziger, Josef	Dalhousie University	Professor

The usage profile for the heaviest Dalhousie user groups (top 15) is shown in the bar graph:



3.1.2 NMR³ staff

Number	Name	Position
1	Lumsden, Michael	Facility Coordinator
2	Werner-Zwanziger, Ulrike	Solid-State NMR Coordinator

3.1.3 Industrial Users

Number	Name	Company Name	Notes
1	Areephong, Jetsuda	Appili Therapeutics	Trained Hands-On User
2	Banfield, Scott	Appili Therapeutics	Trained Hands-On User
3	Batchu, Pavan	Solid-State Pharma Inc	Trained Hands-On User
4	Fisher, Laural	Appili Therapeutics	Trained Hands-On User
5	Hayes, Cameron	Solid-State Pharma Inc	Trained Hands-On User
6	Hilborn, Jim	Heritage Memorials Ltd.	

7	Kehoe, Sharon	ABK Biomedical	
8	MacEachern, Lauren	Solid State Pharma Inc	Trained Hands-On User
9	Ness, Matthew	Research & Productivity Council	
10	Russell, Stephanie	Appili Therapeutics	Trained Hands-On User
11	Sardella, Dan	Apotex	
12	Sun, Shengguo	Appili Therapeutics	Trained Hands-On User

3.1.4 Lab Instructors and TA's

Number	Name	Position
1	Aish, Gaia	Lab Instructor
2	Aleman-Milan, Gianna	Lab Instructor
3	Berryman, Victoria	Lab Instructor
4	Ellis, Sarah	Teaching Assistant
5	Huchenski, Blake	Teaching Assistant
6	Liu, Aaron	Teaching Assistant
7	McDonald, Nicholas	Teaching Assistant
8	Moya-Barrios, Reinaldo	Lab Instructor
9	Noel, John	Teaching Assistant
10	Sawarzky, Ryan	Teaching Assistant
11	Subedi, Pankaj	Teaching Assistant
12	Vanya Ewart, Kathryn	Lab Instructor
13	Whalen, Marc	Lab Instructor
14	Zaky, Mariam	Teaching Assistant

3.1.5 Research Associates, Post-Docs and Others

Number	Name	Affiliation	Position
1	Bhar, Palash	Dalhousie University	Post-Doc
2	Borzenko, Andrey	Dalhousie University	Post-Doc
3	Douglas, Colin	Dalhousie University	Post-Doc
4	Figliola, Carlotta	Dalhousie University	Post-Doc
5	Garaga, Mounesha	Dalhousie University	Post-Doc
6	Garcia, Anthony	Ecole Nationale Supérieure de Chimie de Rennes, France	Visiting Researcher
7	Ghosh, Goutam	Acadia University	Post-Doc

8	Hall, David	Dalhousie University	Post-Doc
9	Huchenski, Blake	Dalhousie University	Research Assistant
10	Kahwaji, Samer	Dalhousie University	Post-Doc
11	Marchal, Estelle	Dalhousie University	Post-Doc
12	McCormick, Nicole	Dalhousie University	Research Assistant
13	Mfoumou, Etienne	Nova Scotia Community College	Research Scientist
14	Momeni, Arash	Dalhousie University	Post-Doc
15	Monro, Susan	Acadia University	Research Assistant
16	Morash, Ben	Dalhousie University	Summer Researcher
17	Nie, Mengyun	Dalhousie University	Post-Doc
18	Ogawa, Takahiko	Dalhousie University	Post-Doc
19	Orrell, Kathleen	Dalhousie University	Summer Researcher
20	Pal, Mohan	Dalhousie University	Post-Doc
21	Robertson, Andrew	Dalhousie University	Research Assistant
22	Rusalovsky, Olexiy	Ottawa University	Summer Researcher
23	Sarker, Muzaddid	Dalhousie University	Post-Doc
24	Shi, Ge	Acadia University	University Staff
25	Simms, Gordon	Dalhousie University	Post-Doc
26	Tremblay, Marie	Dalhousie University	Research Assistant
27	Valliant, Esther	Dalhousie University	Post-Doc
28	Versini, Antoine	ESPCI Paris, France	Visiting Researcher
29	Voth, Chris	University British Columbia	Visiting Researcher
30	Wentzell, Jordan	Lakehead University	Summer Researcher
31	Wiethan, Carson	Universidade Federal de Santa Maria, Brazil	Exchange Student
32	Winter, Sherany	Universiteit Leiden, Netherlands	Exchange Student
33	Xia, Jian	Dalhousie University	Post-Doc
34	Zhu, Jian-She	Dalhousie University	Post-Doc

3.2 Publications Associated with Centre (July 1, 2015 to June 30, 2016)

Peer-Reviewed Journal Articles – total 60

1. Al-Mughaid H, Al-Zoubi RM, Paul NK, & Grindley TB (2015) Unique tetrameric and hexameric mannoside clusters prepared by click chemistry. *Carbohydrate Research* 417:27-33.

2. Blackburn GM, Hagele G, Hottgenroth A, Ivory AJ, Jakeman DL, & Spiske R (2016) Automated lineshape analysis of complex NMR spectra for a novel synthetic tetrafluorobisphosphonate, a

potential ligand for phosphoglycerate kinase. *Phosphorus Sulfur and Silicon and the Related Elements* **191**(3):367-372.

3. Comeau PA & Filiaggi MJ (2016) Structural analysis of $x\text{SrO}-(50-x)\text{CaO}-50\text{P}(2)\text{O}(5)$ glasses with $x=0, 5$, or 10 mol% for potential use in a local delivery system for osteomyelitis treatment. *Materials Science & Engineering C-Materials for Biological Applications* **58**:639-647.

4. Culf AS, Yin HM, Monroe S, Ghosh A, Barnett DA, Ouellette RJ, Cuperlovic-Culf M, & McFarland SA (2016) A spectroscopic study of substituted anthranilic acids as sensitive environmental probes for detecting cancer cells. *Bioorganic & Medicinal Chemistry* **24**(5):929-937.

5. Dai XD, Liu XQ, & Meng Q (2015) Segmental expression and C-terminal labeling of protein ERp44 through protein trans-splicing. *Protein Expression and Purification* **112**:29-36.

6. Dai XD, Xun QJ, Liu XQ, & Meng Q (2015) Cysteine-free non-canonical C-intein for versatile protein C-terminal labeling through trans-splicing. *Applied Microbiology and Biotechnology* **99**(19):8151-8161.

7. Darvesh S (2016) Butyrylcholinesterase as a Diagnostic and Therapeutic Target for Alzheimer's Disease. *Curr Alzheimer Res*.

8. Fernandez CV, O'Connell C, Ferguson M, Orr AC, Robitaille JM, Knoppers BM, & McMaster CR (2015) Stability of Attitudes to the Ethical Issues Raised by the Return of Incidental Genomic Research Findings in Children: A Follow-Up Study. *Public Health Genomics* **18**(5):299-308.

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10. Ford L, Ylijoki KEO, Garcia MT, Singer RD, & Scammells PJ (2015) Nitrogen-Containing Ionic Liquids: Biodegradation Studies and Utility in Base-Mediated Reactions. *Australian Journal of Chemistry* **68**(6):849-857.

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3.3 Participation in Relevant Events for Research Dissemination

A total of **38** international and **125** domestic conference or symposium presentations were reported by professors and students, using and relying upon data collected at the Centre.

What is the number of Centre personnel who participated in international events?	Professors/Associates & Number of Events	Students & Number of Events
	18 international conference/symposium presentations by 11 professors	20 student presentations at the international level
What is the number of Centre personnel who participated in domestic events?	Professors/Associates & Number of Events	Students & Number of Events
	31 domestic conference/symposium presentations by 14 professors	94 student presentations

3.4 Courses Taught by Members of the Centre with Significant Content Related to the NMR³ Mission Statement

- **2nd Year Undergraduate**

(1) CHEM 2401: "Organic Chemistry I"

Instructor: Alison Thompson

Course enrollment: 366

(2) CHEM 2402: "Organic Chemistry II"

Instructor: Frances Cozens

Course enrollment: 277

(3) CHEM 2304: "Introductory Physical Chemistry II"

Instructor: Peng Zhang

Course enrollment: 35

- **3rd Year Undergraduate**

(1) BIOC 3700: "Biomolecular Chemistry"

Instructors: Jan Rainey and Stephen Bearne

Course enrollment: 35

(2) CHEM 3401: "Intermediate Organic Chemistry"

Instructor: Alex Speed

Course enrollment: 43

(3) CHEM 3404: "Physical Organic Chemistry and Spectroscopy"

Instructor: Norm Schepp

Course enrollment: 47

(4) CHEM 3103: "Intermediate Inorganic Chemistry"

Instructor: Marc Whalen

Course enrollment: 51

(5) CHEM 3801: "Experiential Learning in Chemistry"

Instructor: Peter Wentzell

Course enrollment: 11

• **4th Year Undergraduate**

(1) CHEM 4402 (cross-listed with CHEM 5402): "Organic Structure Determination"

Instructor: Jean Burnell

Course enrollment: 31 (20 in 4402 and 11 in 5402)

(2) CHEM 4801: "Research Project Chemistry I"

Instructor: Norm Schepp

Course enrollment: 1

(3) CHEM 4901: "Honours Research Project"

Instructor: Norm Schepp

Course enrollment: 20

3.5 Student Research Activities Related to the Centre Mission Statement

The following table summarizes the **86** student researchers who relied upon the NMR³ facility for progress in their research programs during the 2015-2016 reporting period. The table is made up of 23 Doctoral, 27 Masters, and 36 Undergraduate students.

	Student Name	Institution	Degree	Supervisor	Status	Thesis Title
1	Aboushawareb, Sarah	Dalhousie University	MSc	Stephen Bearne	In-Progress	
2	Adams, Matt	Dalhousie University	BSc	Alex Speed	Completed	Synthesis and Catalytic Ability of N-Heterocyclic Phosphines
3	AlHarbi, Salma	Acadia University	MSc	Amitabh Jha	Completed	Synthetic Studies on 1,3-Diketones Leading to Novel Curcumin Analogs
4	AlJaroudi, Zainab	Acadia University	MSc	Amitabh Jha	Completed	Synthesis of Substituted 6,6a-Dihydroisoindolo[2,1-a]quinolin11(5H)-ones
5	Alsharif, Salman	Dalhousie University	BSc	David Jakeman	In-Progress	
6	Ampaw, Anna	Dalhousie University	MSc	David Jakeman	In-Progress	

7	Aronitz, Elise	Dalhousie University	BSc	Alison Thompson	In-Progress	
8	Beh, Michael	Dalhousie University	MSc	Alison Thompson	In-Progress	
9	Bennett, Leah	Acadia University	BSc	Sherri McFarland	Completed	
10	Bennett, Raymond	Dalhousie University	BSc	Frances Cozens	In-Progress	
11	Burke, Luke	Dalhousie University	BSc	Alison Thompson	In-Progress	
12	Calahoo, Courtney	Dalhousie University	PhD	Josef Zwanziger	Completed	Structure-Property Relations of Mixed-Alkali and Ion-Exchange Silicate Glasses
13	Carroll, Madison	Dalhousie University	MSc	David Jakeman	In-Progress	
14	Charlton, Michael	Dalhousie University	BSc	Alex Speed	In-Progress	
15	Chisholm, Alicia	Dalhousie University	BSc	Mark Stradiotto	Completed	Investigations of Multi-Component, One-Pot, C-N Bond-Forming Reactions with Gold, Palladium, and Nickel Catalysts
16	Clark, Farren	Dalhousie University	BSc	David Jakeman	In-Progress	
17	Clark, Jillian	Dalhousie University	BSc	Mark Stradiotto	Completed	Nickel Catalyzed Mono-arylation of Amines: A Comparison of Two Effective Pre-catalyst Systems
18	Easton, Nicole	Dalhousie University	BSc	Stephen Bearne	In-Progress	
19	Ellis, Leah	Dalhousie University	PhD	Jeff Dahn	In-Progress	
20	Firth, Ben	Dalhousie University	BSc	Robert White	In-Progress	
21	Forget, Stephanie	Dalhousie University	MSc	David Jakeman	In-Progress	
22	Gracious, Shayne	Dalhousie University	BSc	Bruce Grindley	In-Progress	
23	Greening, Sarah	Dalhousie University	MSc	Alison Thompson	In-Progress	
24	Groves, Brandon	Dalhousie University	MSc	Alison Thompson	In-Progress	
25	Hagar, Mostafa	Dalhousie University	BSc	Bruce Grindley	In-Progress	

26	Hargreaves, Breanna	Dalhousie University	BSc	Mark Stradiotto	In-Progress	
27	Harris, Emily	Dalhousie University	MSc	Suzanne Budge	In-Progress	
28	Harty, Matthew	Dalhousie University	MSc	Stephen Bearne	Completed	Studying the Role of the Divalent Metal Cation Activator of the Cambialistic Enzyme Mandelate Racemase
29	Hoey, Marshall	Dalhousie University	MSc	Laura Turculet	Completed	Synthesis of Transition Metal Complexes Supported by Mixed Donor PSiP' Bis-Phosphino Silyl Pincer Ligands
30	Hollenhorst, Helia	Dalhousie University	BSc	Laura Turculet	Completed	Indole Pincer Rhodium and Iridium PSiP Complexes: Progress Towards N-H Bond Oxidative Additions of Amines
31	Huang, Shuya	Dalhousie University	BSc	Jan Rainey	Completed	Characterizing peptide-membrane interactions of the recently discovered peptide hormone Apela
32	Hung Tien, Chieh	Dalhousie University	BSc	Alex Speed	Completed	Dealkylation and Halogenation of Tertiary Amines by s-Triazine Derivatives
33	Hurshman, Colby	Dalhousie University	BSc	David Jakeman	Completed	Synthesis of Novel Phosphono Glucose 1-phosphate analogues to Inhibit Bacterial Cell Wall Biosynthesis
34	Hynes, Toren	Dalhousie University	BSc	Jeff Dahn	In-Progress	
35	Jee, Alison	Dalhousie University	BSc	David Jakeman	Completed	
36	Johnsen, Ann	Dalhousie University	BSc	Alison Thompson	In-Progress	
37	Jones, Christina	Mount Saint Vincent	BSc	Aibing Xia	In-Progress	
38	Kajetanowicz, Aleksandra	Dalhousie University	BSc	Alison Thompson	Completed	Synthesis of F-aza BODIPYs and Conversion of F-aza-BODIPYs to X-aza-BODIPYs
39	Kelly, Colin	Dalhousie University	MSc	Laura Turculet	In-Progress	
40	Kenward, Calem	Dalhousie University	BSc	Jan Rainey	In-Progress	
41	Kirshenbaum, Maxine	Dalhousie University	BSc	Bruce Grindley	In-Progress	

42	Kim, Min Joon	Dalhousie University	BSc	Alison Thompson	In-Progress	
43	Knopf, Philipp	Dalhousie University	BSc	Stephen Bearne	In-Progress	
44	Kottwitz, Haila	Dalhousie University	MSc	John Rohde	Completed	Mechanisms of Colonization Resistance to <i>Shigella flexneri</i>
45	Land, Michael	Saint Mary's University	BSc	Jason Clyburne	Completed	New Electron-Rich Diketiminic Ligands: An Experimental & Computational Investigation on the Isolation of Reactive Species
46	Lavoie, Chris	Dalhousie University	MSc	Mark Stradiotto	In-Progress	
47	LeFort, Francois	Dalhousie University	PhD	Jean Burnell	Completed	Studies of Ring Forming Reactions: Geminal Acylation, Nazarov Cyclization and Cyclohexyne Reactions
48	Lefsay, Abir	Dalhousie University	PhD	Ameres Chatt	In-Progress	
49	Lindeperg, Fabien	Dalhousie University	PhD	Laura Turculet	In-Progress	
50	Lund, Katie	Dalhousie University	MSc	Alison Thompson	Completed	Towards the Synthesis of Di- and Tri-Pyrrolic Compounds
51	Lundrigan, Travis	Dalhousie University	PhD	Alison Thompson	In-Progress	
52	Ma, Kai	Cornell University, USA	PhD	Ulrich Wiesner	In-Progress	
53	Macaulay, Casper	Dalhousie University	MSc	Laura Turculet	In-Progress	
54	MacLeod, Jeanna	Dalhousie University	MSc	David Jakeman	In-Progress	
55	MacQueen, Preston	Dalhousie University	PhD	Mark Stradiotto	In-Progress	
56	McCain, Julia	Acadia University	BSc	Sherri McFarland	Completed	Synthesis & Characterization of Cyclometalated Ru(II) Complexes for Applications in Photoactivated Cancer Therapy
57	McClennan, Billy	Saint Mary's University	BSc	Jason Clyburne	In-Progress	
58	McCluskey, Greg	Dalhousie University	PhD	Stephen Bearne	In-Progress	

59	McDonald, Nicholas	Dalhousie University	MSc	Rob White	In-Progress	
60	Melanson, Jennifer	Dalhousie University	PhD	Alison Thompson	Completed	Functionalization of Mono- and Dipyrrolic Compounds
61	Morgan, Tim	Dalhousie University	PhD	Jean Burnell	Completed	Selectivity in the Interrupted Nazarov Reaction
62	Murphy, Luke	Dalhousie University	PhD	Laura Turculet	In-Progress	
63	Na, Jungwook	Dalhousie University	BSc	David Jakeman	Completed	Construction of Deletion Mutants of <i>Streptomyces venezuelae</i> ISP5230 to Investigate the Biosynthesis of Novel Glycosylated Jadomycins
64	Noel, John	Dalhousie University	PhD	Mary Anne White	In-Progress	
65	O'Connell, Kathleen	Dalhousie University	PhD	Daniel Boyd	Completed	High Borate Glasses for the Controlled Release of Therapeutic Metal Ions
66	Pandey, Aditya	Dalhousie University	PhD	Jan Rainey	Completed	Expression, Purification and Biophysical Characterization of Large Fragments of the Apelin Receptor Enabling Delineation of a Juxtamembrane Helix with Amphipathicity Necessary for Plasma Membrane Localization
67	Paterson, Alex	Dalhousie University	PhD	Josef Zwanziger	In-Progress	
68	Patterson, Robin	Dalhousie University	MSc	Jan Rainey	Completed	Probing Membrane Catalyzed Apelin-Receptor Interactions by Fluorescence Spectroscopy
69	Petibon, Remi	Dalhousie University	PhD	Jeff Dahn	Completed	Study of the Reactivity of Electrolyte Solvents & Additives in Li-Ion Cells and Design of New Electrolyte Blends
70	Poehls, Jan	Dalhousie University	PhD	Mary Anne White	In-Progress	
71	Qin, Teng Fei	Dalhousie University	MSc	Norman Schepp	In-Progress	
72	Rotta-Loria, Nicolas	Dalhousie University	MSc	Mark Stradiotto	In-Progress	

73	Said, Hammam	Dalhousie University	BSc	Bruce Grindley	Completed	Attachment of BbGL1 Derivatives Using a Linker Arm Attached to O-3 of Galactose as a Route to a Potential Lyme Disease Vaccine
74	Sainuddin, Tariq	Acadia University	MSc	Sherri Mcfarland	Completed	Development of Ru(II) Polypyridyl Complexes Containing TI-Expansive Functional Ligands as Photosensitizers for Photodynamic Therapy
75	Sawarzk, Ryan	Dalhousie University	MSc	Mark Stradiotto	In-Progress	
76	Shin, Kyungsoo	Dalhousie University	PhD	Jan Rainey	In-Progress	
77	Sinclair, Jocelyn	Dalhousie University	BSc	Josef Zwanziger	In-Progress	
78	Song, Qinyan	Dalhousie University	PhD	Paul Liu	In-Progress	
79	Subedi, Pankaj	Dalhousie University	MSc	Fran Cozens	Completed	The Two-Photon Excitation Fluorescence (TPEF) Enhancement of Dipolar Organic Chromophores in Y Zeolites
80	Tassone, Joseph	Dalhousie University	PhD	Mark Stradiotto	In-Progress	
81	Toutsenko, Serge	Dalhousie University	BSc	Bruce Grindley	Completed	Synthesis of O-2 Attached Linker-arm Derivatives of BbGL1 for Protein Attachment in the Development of a Vaccine for Lyme Disease
82	Xia, Wei	Dalhousie University	PhD	Suzanne Budge	In-Progress	
83	Xiong, Deijun	Dalhousie University	PhD	Jeff Dahn	In-Progress	
84	Yaphe, Hannah	Dalhousie University	BSc	Stephen Bearne	Completed	Developing a sensitive, continuous, and direct assay for α -methylacyl-CoA racemase
85	Zaky, Mariam	Dalhousie University	MSc	Jean Burnell	Completed	Exploration of the Nazarov Cyclization Reaction
86	Zheng, Lituo	Dalhousie University	MSc	Jeff Dahn	Completed	Phosphorus-Based Negative Electrodes for Sodium-Ion Batteries

3.6 Outreach Strategy

1. Training of HQP is the key component of NMR³ outreach activities. As the following sections describe in more detail, training on the instruments is provided for on-site use, and in addition our staff assist with NMR training and support at our regional partner universities.

Anyone wishing to become a hands-on user of a high-resolution NMR spectrometer at the NMR³ is first required to read the NMR³ facility safety guide and pass an online test consisting of 10 questions. Subsequently, users can take a 1 h training course on the AVANCE 300 and/or the AVANCE 500 using the sample changer. Both of these training courses also finish with a short quiz or a practical exam. Further advanced training is provided for students requiring more specialized NMR experiments. In particular, advanced training is available for the hands-on use of the 500 spectrometer without the sample changer, and for performing variable temperature NMR experiments on the AVANCE 300. In addition to spectrometer training, classroom tutorial sessions are held when demand warrants on the basics of processing 1D and 2D NMR data with Bruker's software package called TopSpin.

Hands-on access to the 700 MHz spectrometer located at NRC is currently provided to the majority of researchers via Dr. Mike Lumsden. The exceptions are the Dalhousie groups of Professors Jan Rainey, Paul Xiang-Qin Liu, Roy Duncan and Roger McLeod from the Departments of Microbiology & Immunology and Biochemistry & Molecular Biology. A number of individuals from these groups have been trained to use the spectrometer themselves. Additionally, training courses are provided by NRC staff for researchers requesting walk-up access to the 700 MHz spectrometer using ICON-NMR and the SampleJET. A number of researchers from the groups of Professors Alison Thompson, David Jakeman, Jan Rainey, and Stephen Bearne are trained and have walk-up access to the spectrometer.

Access to the Bruker Avance 400 and 700 MHz NMR spectrometers for solids is handled differently than for the solution-state NMR spectrometers, because solid-state NMR is more technically challenging than solution-state NMR and experiments carried out in our facility tend to be non-routine in nature. Because of the different user profiles, users basically fall into one of three groups:

- (1) Those who require solid-state NMR spectroscopy only once, or rarely during their graduate careers and are not from Dalhousie University. This category also includes remote industry and government users.
- (2) Those who require solid-state NMR occasionally, but do not use it as a main tool of their research. These users are typically from Dalhousie University.
- (3) Those, whose research centers around solid-state NMR.

For the first group, solid-state NMR spectra are provided by Dr. Ulrike Werner-Zwanziger, often without the presence of the researcher. The results are typically given in report form whose detail concerning the interpretation depends on the solid-state NMR expertise of the user. For the second group, solid-state NMR spectroscopy is typically performed by Dr. Ulrike Werner-Zwanziger in collaboration with and in the presence of the user. Training, more in the form of teaching is done during the acquisition of the experiments. This form of collaboration allows for more tailored research and interpretation. The final group of users typically stems from the research group of Professor Josef Zwanziger. His students and Postdoctoral Fellows become proficient enough to conduct their experiments independently. Due to the non-routine form of their research, training here is done more in the form of collaboratively developing the experiments and determining their experimental

parameters, which the users can then apply to their research materials. Some users become so independent, that they can develop experiments on their own.

2. Outreach also takes the form of detailing NMR³ capabilities during regional, national and international seminars. During the past reporting period, NMR³ Director Jan Rainey did so in NMR-intensive invited talks at Soricimed Biopharma Inc. and at the Canadian Society for Chemistry Conference (CSC). NMR³ Solid-State Coordinator Ulli Werner-Zwanziger also highlighted the solid-state NMR capabilities of the NMR³ at the CSC and at the 13th International Conference on the Structure of Non-Crystalline Materials (NCM-13).

3. NMR³ facility staff occasionally provides tours of the facility for visitors, typically high school groups and/or undergraduate science students.

- On October 14, 2015, NMR³ facility staff hosted a group of ~ 18 undergraduate students from Saint Mary's University and explained/demonstrated the basic principles of high-resolution and solid-state NMR spectroscopy.

4. Dr. Ulrike Werner-Zwanziger engages in general science outreach at Clayton Park Junior High School, by presenting lectures "Rocks Talk" with practical demonstrations.

3.7 Technology Development, Patent or Commercialization Activities

1. Patents involving researchers identified as being supported by NMR³:

1. **Artificial Spider Aciniform Silk Proteins, Methods of Making and Uses Thereof.** United States Provisional Patent 62/287,564. Principal Inventors: Jan Rainey, Paul Liu, Lingling Xu and Nathan Weatherbee-Martin.
2. **Butyrylcholinesterase Ligands as Diagnostic Tools and Treatment for Diseases of the Nervous System.** Australian Patent #2009285584, Canadian Patent #2,735118 and Israeli Patent Application 211347. Principal Inventor: Sultan Darvesh
3. **Metal-based Thiophene Photodynamic Compounds and Their Use.** US Patent No. 9,345,769. Principal Inventor: Sherri McFarland
4. **Nickel Cross-Coupling.** CA 2016/050622. Principal Inventor: Mark Stradiotto
5. **Polyphosphate Glass Microspheres, Methods of Making and Uses Thereof.** US Patent Application No 62/233,646. Principal Inventor: Mark Filiaggi
6. **Treatment of Familial Exudative Vireoretinopathy through Inhibition of S1PR2 by Small Molecules.** Principal Inventor: Christopher McMaster

2. NMR³ staff are often called upon to setup (and sometimes make routinely available) novel and/or highly specialized NMR experimentation to solve a variety of research problems. During the current reporting period, the following experiments were implemented on NMR³ spectrometers for the first time:

- The 2D ¹H-¹³C HECAD-¹H¹³C HSQC experiment (**HE**teronuclear **C**ouplings from **A**scii-**D**omain experiments with **E**-cosy type cross peaks) was setup on the AVANCE 500 liquids spectrometer, an experiment designed to measure both the magnitude of ¹H-¹³C long range J-couplings and their relative signs.

- Cross spectrometer acquisition on the solid-state NMR spectrometers was set up and used to obtain NMR data on quadrupolar nuclei in two different field strength with the same pulse sequences to separate quadrupole and chemical shift contributions.
- A constant-time semi-selective HMBC was implemented on both the AV500 and 300 liquids spectrometers, an experiment designed to improve the resolution achieved in the indirect dimension of the standard HMBC in order to facilitate structure elucidation.
- A number of Shigemi tubes were purchased during the reporting period and made available to NMR³ researchers. These tubes increase the sensitivity of NMR experiments obtained for liquid samples when the amount of sample available is limited by reducing the minimum solvent volume necessary.
- ¹⁹F T₁/T₂ experiments were setup and optimized on the AV500 spectrometer, experiments that take full advantage of the BBFO SmartProbe on this spectrometer.

3.8 Other Activities Related to Knowledge Exchange or Mobilization

1. The NMR³ facility maintains a significant library of instruction documents as a means to support its trained hand-on users to perform NMR experimentation independently. The majority of these documents can be accessed via the NMR³ website (<http://www.dal.ca/diff/nmr3/documents.html>). In addition, hard copies are available within the facility itself. During the current reporting period, a number of updates and additions were made to this library, including:

- A new instruction document describing how to obtain ³¹P Saturation Transfer Experiments on the AV-300, an experiment designed to detect slow chemical exchange.
- A document describing how researchers can restart the AV-500 autosampler after a critical error.
- Significant updates to the following documents were made during the reporting period:
 - Multiplet analysis using TopSpin
 - Power-cycling the AV-300 spectrometer (version 1.3, August 2015)
 - Power-Cycling the AV-500 spectrometer (version 1.3.1, August 2015)

2. Given the popularity of online social networking programs and the communication tools these programs provide, in 2012 the NMR³ facility joined Twitter @nmr3_mike. Although email communication with facility personnel is still widely used, followers of NMR³ receive important facility updates, education, and NMR-related information via "tweets". The number of followers of the NMR³ facility has now reached **141**.

3. The breadths of solid-state NMR research conducted in the NMR3 was featured in a series of tweets by the Institute of Research in Materials and re-tweeted by the NMR3 and, among others, the National Ultrahigh-field NMR Facility for Solids.

Section 4 – Financial Information (April 1, 2015 – March 31, 2016)

4.1 2015-2016 Financial Report

Financial support in '15-'16 came from a total of 3 broad sources: (1) Dalhousie University (2) User Fees and (3) and Support Fees (described below). This past FY, Dalhousie funded the total salary costs of the facility and we are extremely grateful for this expanded salary support. The Faculty of Science paid 69% of the Coordinator's salary and benefits with the remaining 31% covered by a new Dalhousie Strategic Initiative Fund (SIF). As well, 62% of the Solid-State NMR Coordinator's salary and benefits was paid by the Faculty of Science in support of Professor Joe Zwanziger's Canada Research Chair. The remaining 38% was also paid from the SIF. Direct costs of the facility this past FY included magnet cryogenes, lab supplies, computing costs, and all expenses associated with service, maintenance and upgrades.

User fees at the conclusion of the reporting period were unchanged from a year earlier and are summarized in the following tables:

Liquids Magnet Time (per Hour)			
	Tier 1 Academic Rates¹	Tier 2 Academic Rates²	Government/Industry
AV 300 Autosampler	\$3.50	\$20.00	\$100.00
AV-300 Priority	\$7.00	\$40.00	\$200.00
AV-300 Hands-On	\$4.50	\$20.00	\$100.00
AV 500	\$5.50	\$24.00	\$130.00
AV III 700	\$10.63	See Footnote 3	See Footnote 3

Liquids Service Fees (per Sample)⁴		
	All Academics	Government/Industry
AV-300 & AV-500	\$10.00	\$50.00
AV III 700	\$15.00	See Footnote 3

Solids Hourly Rates: All Instruments			
	Tier 1 Academic Rates¹	Tier 2 Academic Rates²	Government/Industry
Hands-On / Collaborative⁵	\$18.50	\$33.00	\$100.00
Service	\$28.50	\$50.00	\$125.00

Additional Charges	
Service	Charge
Packing Rotors for Solid-State NMR - Standard	\$10 per Rotor
Packing Rotors for Solid-State NMR - Special Handling	\$50 per Rotor
Fee to Cover Solid-State NMR Consumables ⁶	\$10 per Sample
Preparing High Resolution NMR Samples ⁷	\$10 per Sample
Processing NMR Spectra ⁸	\$10/\$20 per Experiment
Deuterated Solvents	Cost
Nonroutine Processing Requests (i.e. lineshape fits, simulations, predictions)	\$10 per Experiment
Staff Work (i.e. Structural Assignments / Spectral Interpretation / Literature Searches / Report Writing)	\$50 per Hour

1 Tier 1 rates are charged to all academic researchers who pay the appropriate annual support fee (\$100 for Dalhousie FoS researchers, \$250 for Dalhousie non-FoS researchers, and \$500 per Institution for all non-Dalhousie researchers). 2 Tier 2 rates are charged to all academic researchers who elect NOT to pay the annual support fee described in 1. 3 All non-Dalhousie users must approach BMRF staff directly to determine fees and access to the AV III 700 instrument. 4 Per sample fees for high-resolution NMR service requests are in addition to the base hourly rate for magnet time outlined above. 5 These rates assume either independent hands-on usage or collaborative usage with Dr. Werner-Zwanziger being co-author if level of contribution merits. 6 This fee applies to both hands-on/collaborative as well as service samples. 7 Deuterated solvent costs are not included in this service. 8 Within a given fiscal year, the first 20 experiments processed within a research group are billed at \$10 per experiment. All experiments over and above the first 20 are billed at \$20 per experiment

Tier 1 vs. Tier 2 Academic Rates

Prior to April 1, 2015, only academics at Universities other than Dalhousie had a two tier rate structure for usage of the NMR³ facility resources. Lower rates were charged whenever their Institution paid an annual \$500 support fee. In April of 2015, this idea of a two tier rate structure tied to financial support of NMR³ was expanded to also include Dalhousie researchers. Dalhousie researchers within the Faculty of Science are now charged the lower (Tier 1) rates upon payment of a \$100 annual support fee; the fee is \$250 for researchers in all other Faculties. The support fee is not mandatory; researchers may elect to not pay the fee and instead pay the higher (Tier 2) hourly rates.

4.2 Grants Directly Related to the Mission Statement of NMR³ Awarded Within the 2015-2016 Fiscal Year

In total, **\$7,926,802 in new grant funds** were awarded to Dalhousie University researchers in grants identified by the Centre users as relying upon preliminary data acquired at NMR³ and/or including use of the NMR³ Centre as part of the grant budget. It should be noted that this includes a multi-

institution CFI (~\$6.2-million of \$21-million total to Dalhousie); the drug discovery aspects of this CFI project certainly has a clear tie to NMR spectroscopy. It should also be noted that the grants listed below are only newly awarded grants, not ongoing research grants - this is therefore a one year "snapshot" of the critical nature of NMR³ for Dalhousie's competitiveness to capture grant funds. Over the previous three reporting periods (since beginning to report aggregate grant funding, an additional **>\$13.8-million in grant funds has been attributed by Dalhousie users as relying upon the ability to access NMR³ facilities.**

Grants Awarded to Dalhousie-Based NMR³ Users

Applicant: Alison Thompson

- NSERC - Research Tools and Instruments: "High-Resolution Tandem Mass Spectrometer for Small Molecule and Bioanalysis Research", with 10 others (\$150,000)
- Nova Scotia Health Research Foundation (NSHRF) - Scotia Support Grant: "Medicinal Chemistry (Graduate Training Program)", with D. Jakeman and M. Stradiotto (\$49,600 for 2 years)
- Beatrice Hunter Cancer Research Institute: Seed Grant: "Characterizing 18F-BODIPYs in vivo and in vitro", with K. Brewer (\$10,000 for 1 year)

Applicant: Christopher McMaster

- Canadian Foundation for Innovation: "Research Program for Rare Pediatrics Diseases", with K. Boycott (PI) and J. Michaud (\$21,012,964 for 5 years; Dalhousie portion ~\$6.2-million)
- CIHR Operating Grant: "A Novel Antibiotic Class to treat Diabetic Ulcer Infections", with D. Weaver (\$715,250 for 5 years)

Applicant: David Jakeman

- Glyconet: "Novel Inhibitors that Block Rhamnose Biosynthesis and Rhamnosyltransferase Activities" (\$55,000 for 1 Year)
- NSERC Engage: "Chemoenzymatic Methods to Prepare N-glucuronides for use in Drug Discovery" (\$25,000 for 6 months)

Applicant: Jan Rainey

- Nova Scotia Health Research Foundation (NSHRF) - Scotia Support Grant: "Support of a Research Team Providing Training in Membrane Protein Structure-Function Correlation", with R. Duncan (\$50,000; 50%; renewal)
- Dalhousie Medical Research Foundation (DMRF) - Equipment Grant: "A Microviscometer for Accurate Characterization of Protein-Lipid, Protein-Ligand, and Protein-Protein Interactions", with 2 others (\$20,933; 55%)
- Springboard Atlantic - Innovation Mobilization Program: "Recombinant Spider Aciniform Silk Production and its use as Surgical Sutures", with X-Q. Liu (\$20,000 proof-of-concept funding with \$13,067 in cash and remainder in kind + \$12,542 patent and legal funding; 50%)
- NSERC - Connect Grant: "Exploration of Potential Collaboration with Soricimed Biopharma Inc." (\$477)

Applicant: Mark Stradiotto

- NSERC - Idea to Innovation Grant: "Pad-DalPhos: A New Ligand Class for Nickel-Catalyzed Cross-Coupling", (\$125,000 for 2015-2017; 100%)

- Chevron Phillips Chemical - Renewal: "Application of a Proprietary Ligand Class", with L. Turculet (\$48,000 CDN Current Year - \$273,000 USD 2012-2016; 50%)

Applicant: **Stephen Bearne**

- Nova Scotia Health Research Foundation (NSHRF) - Scotia Support Grant, with C. Blouin (\$50,000 over 2 years)

Applicant: **Sultan Darvesh**

- Dalhousie Medical Research Foundation Irene MacDonald Sobey Chair in Curative Approaches to Alzheimer's Disease - Faculty of Medicine, Dalhousie University (\$350,000 for 2014-2019)

Grants Awarded to NMR³ External Users

Principal Applicant: **Robert Singer (Saint Mary's University)**

- NSERC - Engage Grant: "Sustainable Additive Manufacturing Materials from Waste Biomass" (\$25,000 for 1 year)

Principal Applicant: **Stephanie MacQuarrie (Cape Breton University)**

- NSERC - DDG: "Non-Covalently Bound Heterogeneous Catalysts" (\$20,000 for 1 year)
- Cape Breton University Spring RP: "Proline Functionalized Biocarbon" (\$8,000)