

NUCLEAR MAGNETIC RESONANCE RESEARCH RESOURCE

2014 – 2015 Annual Report

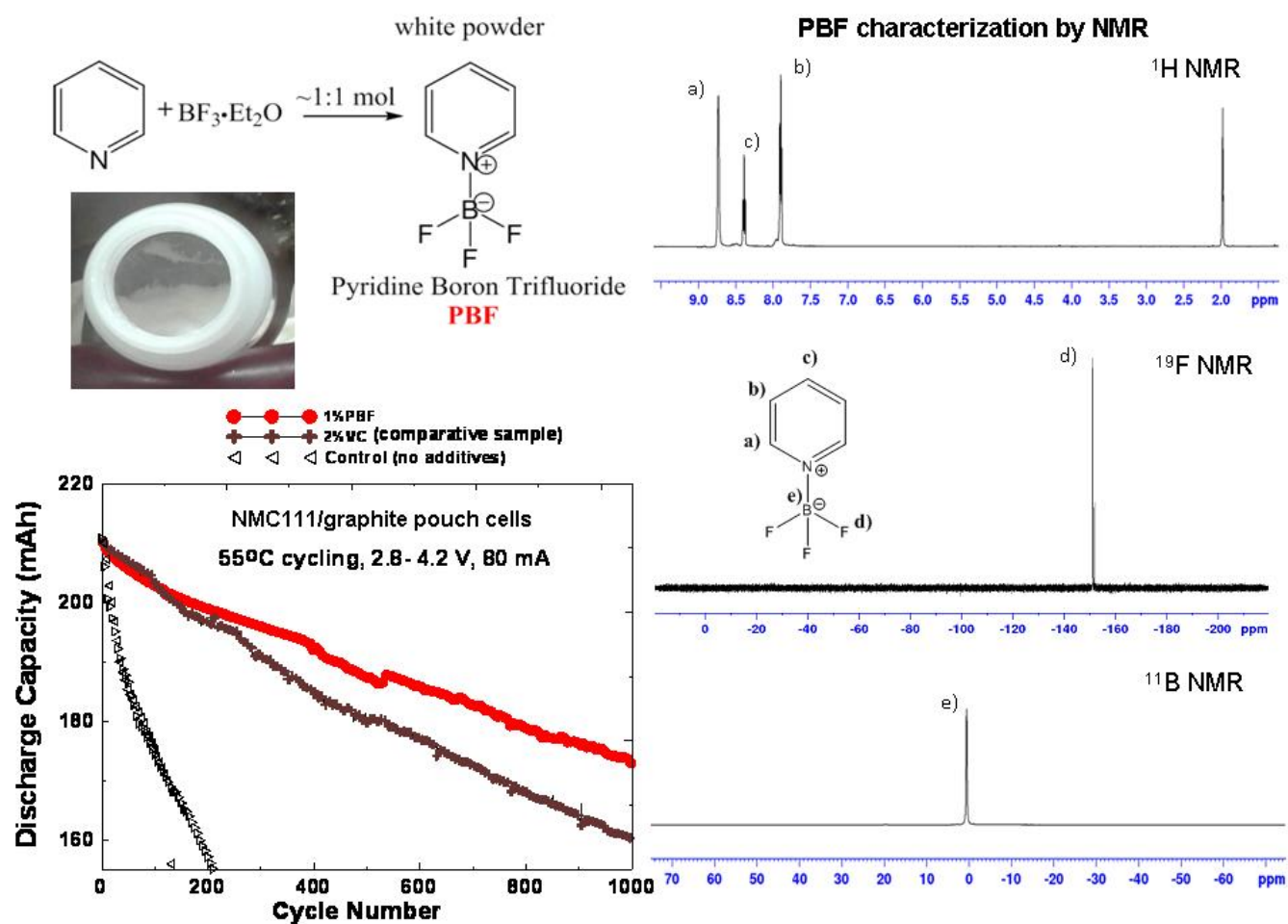


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About the cover: The new class of electrolyte additives -- Pyridine Boron Trifluoride (PBF) used in lithium ion batteries was synthesized in Dr. Jeff Dahn's group at Dalhousie University. The synthesized PBF was characterized by a Bruker AV300MHz spectrometer. The ¹H, ¹⁹F and ¹¹B NMR spectra indicated high purity of synthesized PBF additives. When 1 wt% PBF was added into carbonated-based electrolytes of Li[Ni_{1/3}Mn_{1/3}Co_{1/3}]O₂/graphite pouch cells, the cells demonstrated significantly promising cycling performance compared to those with 2 wt% Vinylene Carbonate (a common commercial additive) and control one after 1000 cycles at 55°C (2.8-4.2 V operating voltage).

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 2014-2015, the Centre assisted 40 research groups mostly drawn from the Atlantic Canada region but also including several international researchers, resulting in 58 publications, 125 conference presentations and 137 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 247 total students and a combined 269 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 ~9450 hours, with 7786 of these hours being devoted to solution-state NMR spectroscopy. 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 over *\$2.4-million in new external grant funds awarded* in the 2014-2015 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 \$11.4-million in external grant funding to Dalhousie researchers in the 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; recently elected for a second 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.

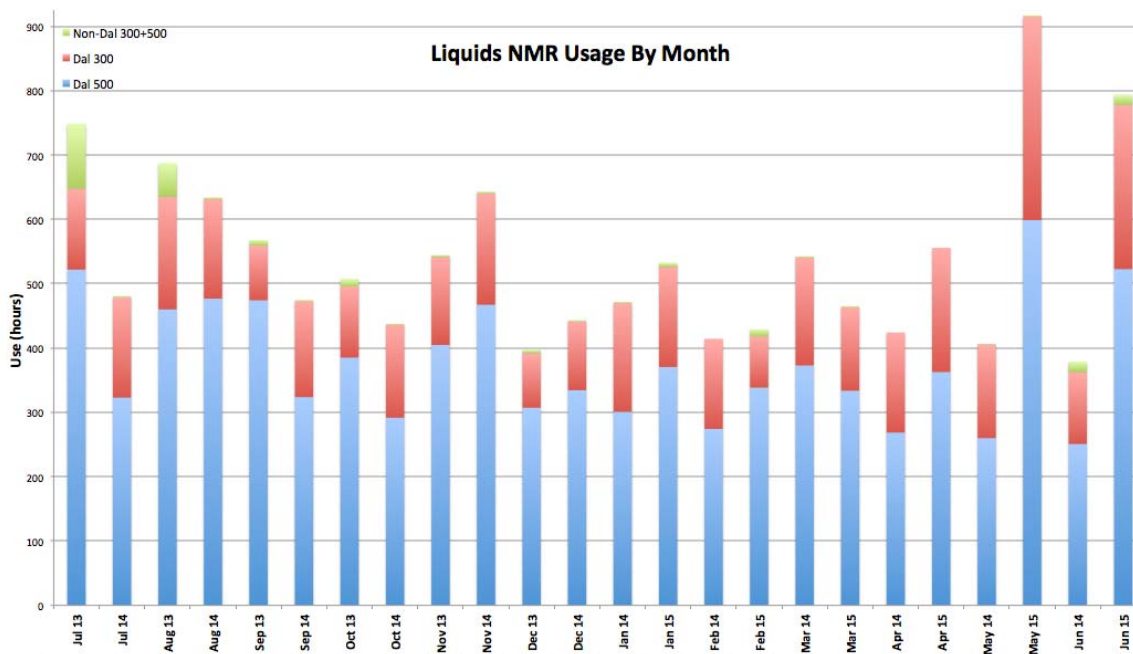
1.1 Mission Statement

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.

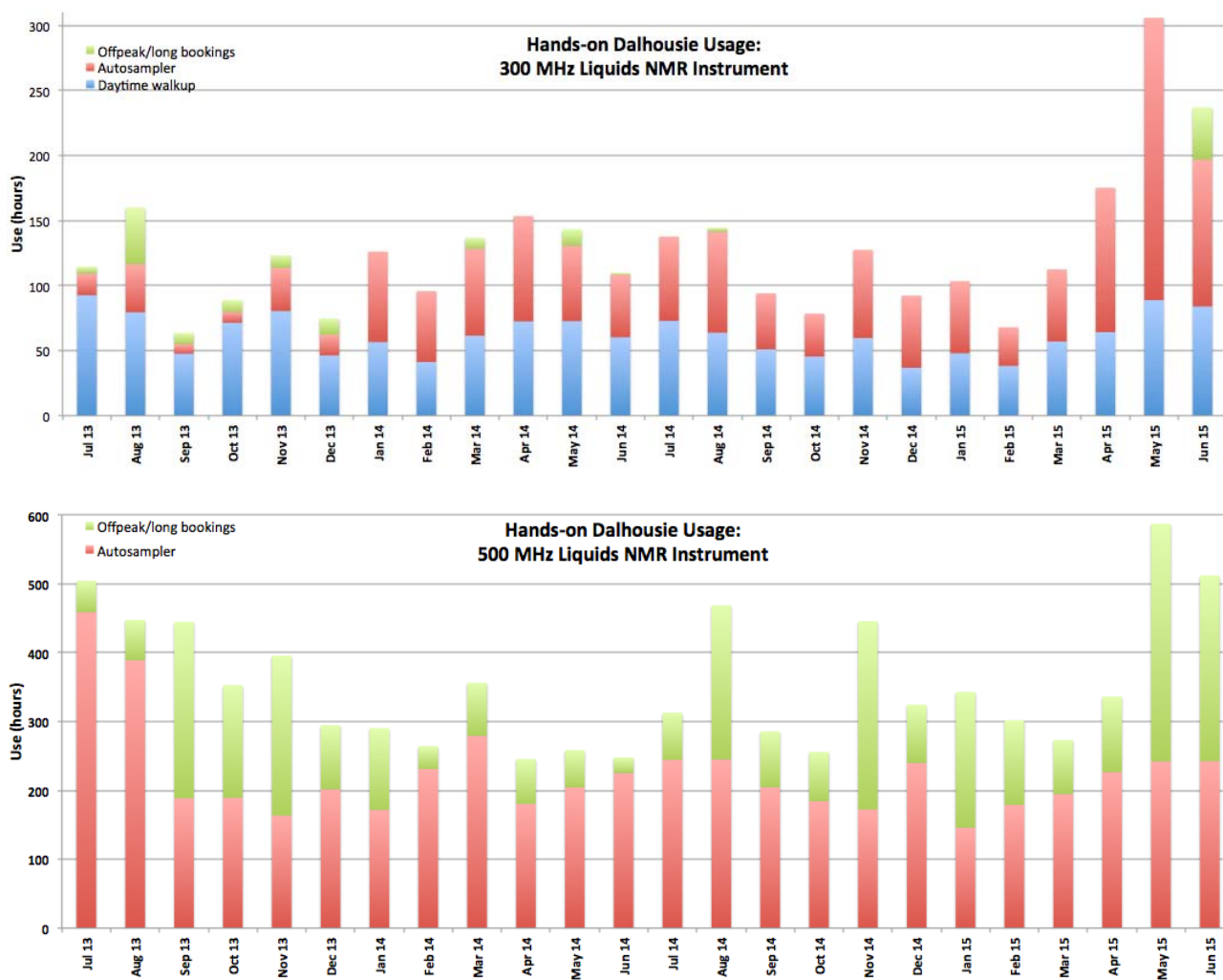
1.2 Current Year's Activity

1. Ongoing optimization of liquids NMR instrument usage: Our two solution-state NMR instruments both experienced increased usage in the 2014-2015 reporting year relative to 2013-2014. This is charted below on a monthly basis, with each month's usage from 2013-2014 shown beside the corresponding month in 2014-2015 - clearly there has been an increase in usage of our liquids instruments over the latter half of the 2014-2015 reporting period. This is definitely a positive trend to observe, since we have recently lost some of our major users through recruitment to other institutions and since Saint Mary's University installed an NMR instrument in 2013 (resulting in a



decrease in non-Dal usage from Fall 2013 onwards). Usage of both instruments also tends to be fairly consistent from month to month, indicating that we do not have significant periods of depressed usage. In the usage chart above, a trend of increased 300 MHz usage when 500 MHz usage is increased is

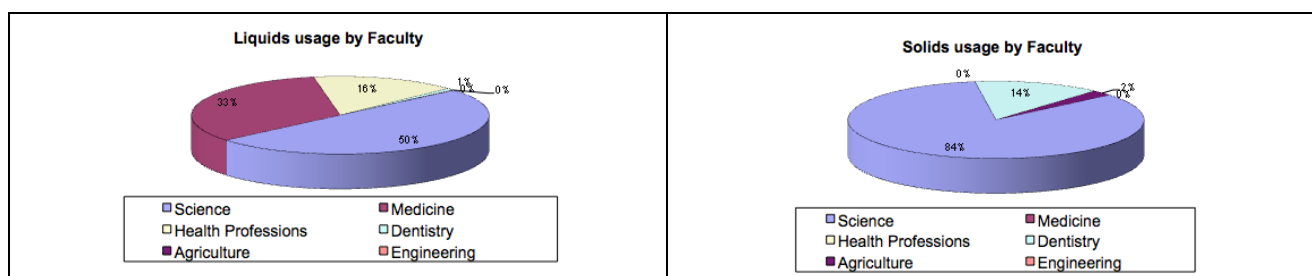
also apparent. Demand on the 500 MHz instrument definitely drives increased 300 MHz usage. In the 2013-2014 year, we began to target additional autosampler usage on our 300 MHz liquids instrument in order to better make use of the investment we had made in purchasing this autosampler. This, in turn, would lead to greater flexibility for usage of the 500 MHz in non-autosampler modality. This shift towards greater autosampler use on the 300 MHz began in January 2014. We are happy to note that this has continued in our current reporting year - usage profiles for each of the liquids instruments spanning both reporting years are provided below - and that usage in general has climbed.



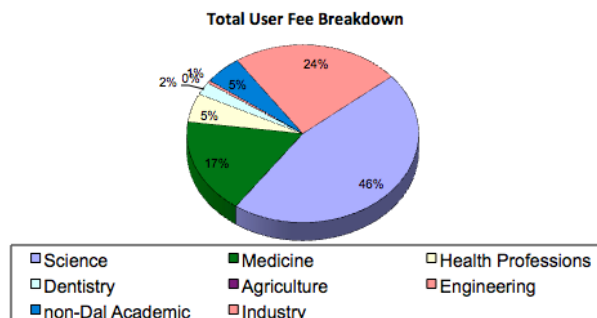
2. User fee adjustment: During the 2014-2015 fiscal year, we expended the surplus in our day-to-day operating account. This triggered a reconsideration of our User Fees to ensure that they were sufficient to cover our expenses. As we are in the process of actively lobbying for salary support for Drs. Lumsden and Werner-Zwanziger through sources other than User Fees, we initially calculated our new User Fee structure to *meet all costs except salary*. During this process, at the explicit request of the User Group, we moved to an accounting system where costs and revenue are considered separately for our Liquids Facility and our Solids Facility. Some costs are shared between the two facilities; however, by far the largest portion of our non-salary costs is instrument-specific - each instrument has unique upkeep and maintenance costs, where unfortunately the Solids instruments have greater fixed costs.

Following this analysis, our Liquids User Fee structure remains unchanged – all non-salary costs were being met (and modestly exceeded) with our current fees and under current profiles of usage. Our Solids User Fee structure, on the other hand, required a major overhaul in order to meet non-salary expenses. These new User Fees came into effect Apr. 1, 2015. If academic and industrial usage continues at historical levels, we are confident that the current User Fees will be sufficient to meet our non-salary costs.

3. Expansion of "support fee" system to tier hourly rates: Over 50% of our revenue comes in the form of salary support through a Department of Chemistry position (covering ~69% of Dr. Lumsden's salary) and from the Faculty of Science (~62% of Dr. Werner-Zwanziger's salary through support of Professor Joe Zwanziger's Canada Research Chair.) For context, the usage profiles of our Liquids and Solids facilities in the 2014-2015 reporting period are shown below.



Although quite heavily tilted towards the Faculty of Science, particularly for the Solids facility, usage is clearly diverse. Also informative is the profile of our User Fee income (detailed in Section 4), where it is clear that Industrial User fees, 92% of which came from Solids instrument usage, are an extremely important component of our total User Fee income at ~24%.



Given this picture of diverse usage drawn from across Dalhousie, and beyond, to begin to better reflect the salary support that is received directly through Chemistry and Science vs. the lack of support from other areas of Dalhousie, we introduced an annual "support fee" system based upon the Faculty/College in which a researcher is housed. Effectively, any Dalhousie researcher from outside of the Faculty of Science is asked to pay a higher annual fee (\$250) than those within Science (\$100). This is effectively an extension of the model used for our "supporting institution" fee for non-Dalhousie users, where an annual fee (\$500) is levied. All academic users from Dalhousie or beyond then pay one of two classes of hourly user fee: a lower "supporting user" hourly rate; or, a higher rate if they choose not to pay the annual support fee. This has, correspondingly, allowed us to recover some additional cost from users housed outside of the Faculty of Science; in future, we will assess the appropriateness of this model of facility access (and the magnitude of fees) based upon the level(s) of

salary support received from various sources moving forward. *Note: these fees were levied in the 2015-2016 Fiscal Year, so do not appear in the current financial report.*

4. Solids coordinator leave: Dr. Werner-Zwanziger was on leave without pay from the facility during the reporting year (July 2014-June 2015). Dr. Margaret Hanson-Clarke, a postdoctoral fellow with Dr. Josef Zwanziger, was acting solid-state NMR coordinator during Dr. Werner-Zwanziger's absence. Dr. Werner-Zwanziger spent the year at the University of California, Santa Barbara conducting research with the group of Dr. Brad Chmelka. She has now returned and is again coordinating all aspects of the Solids facility and is looking forward to applying her new knowledge about materials and pulse sequences to projects involving NMR³.

5. Uninterruptable power supplies: After lengthy waits, our Liquids facility has a new uninterruptable power supply (UPS) serving both instruments and our Solids facility has a new set of UPS batteries. Both facilities are therefore well protected again for short losses of power. Beyond ensuring smoothness in instrument operation, this is key for our instrument longevity since the electronics in NMR instruments (particularly in aged consoles such as ours) can be quite sensitive to power loss and spikes upon return.

6. Data Processing & Analysis Room: During the fall of 2014, the facility purchased a new Windows 7 work-station, an HP LaserJet P1606dn printer, and a processing license for Bruker's TopSpin 3.2.6 NMR software. Subsequently, former NMR³ office space (Room 430) was converted into an NMR data processing and analysis room. The space currently contains two processing stations and multiple versions of TopSpin all networked to the new printer. Other software products are available for spectral analysis in this space, including Bruker's "Dynamics Center" and gNMR for spin-system analysis. In addition, the NMR³ web (for remote automation updates) and ftp (for remote data retrieval) services were migrated to the newer and more robust Windows 7 system.

1.3 Upcoming Year's Activity

1. Address salary support shortfall: Our budget, assuming historical usage profiles of the various instruments, is now balanced in all aspects except salary. We are awaiting the results of an application by Dr. Mark Filiaggi for support funding for NMR³ and other key university core facilities from the Dalhousie upper administration. Should the upper administration not move forward with core facility funding, we will be revisiting a variety of other strategies to ensure that our salary expenses are covered without further increasing user fees. Our user fees are already either comparable to or well above many other universities of similar research intensity - ideally we can maintain our competitiveness in this regard, given the general dwindling of grant funds from NSERC and CIHR.

2. NSERC RTI application: Dr. Josef Zwanziger together with Dr. D. Boyd, Dr. J. Dahn, Dr. J. Rainey and Dr. Ulrike Werner-Zwanziger, have prepared an NSERC-RTI application to the internal Dalhousie review committee for major infrastructure improvements on our Solids instruments. The major component is a fast spinning Magic Angle Spinning probe head tunable to a wide range of nuclei (¹⁵N - ³¹P/ ¹⁹F - ¹H) serving important projects such as glassy, bio-, and battery materials. In addition, funding is included to replace the aging air compressor and to upgrade the spectrometer software to modern standards. The group is currently awaiting internal review results from Dalhousie University to proceed with the RTI submission to NSERC

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 ^1H & 135 W ^{13}C)	
Channel 2	Broadband BLA2BB Amplifier (50 W ^1H & 135 W ^{13}C)	
Probe 1	5 mm BBFO	Observe: ^{14}N - ^{31}P & ^{19}F /decouple: ^1H , 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 pl6	

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	^1H 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: ^1H , z-gradient coil and auto-tune & match accessory (ATMA)
Probe 2	5 mm BBO	Observe: ^{14}N - ^{31}P / decouple: ^1H , z-gradient coil and auto-tune & match accessory (ATMA)
Probe 3	5 mm TXI	Observe: ^1H / 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 pl6
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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	¹ H and ¹⁹ F (100 Watt)	
Channel 3	Broadband (500 Watt)	
Channel 4	Broadband (300 Watt)	
Probe 1	5 mm TCI Cryoprobe	Observe: ¹ H / decouple: ¹³ C and ¹⁵ N, with z gradient coil and auto-tune / match accessory (ATMA). ¹ H, ² H (lock), and ¹³ C preamps cryogenically cooled.
Probe 2	1.7 mm TCI Cryoprobe	Observe: ¹ H / decouple: ¹³ C and ¹⁵ N, with z gradient coil and auto-tune / match accessory (ATMA). ¹ H, ² H (lock), and ¹³ C preamps cryogenically cooled.
Probe 3	5 mm BBO	Observe: ¹⁵ N - ³¹ P / decouple: ¹ H, 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 Biodiagnostics 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- ¹ H

Probe 2	4mm HXY MAS	in dual mode: 45MHz - ³¹ P / ¹ H Insert Pairs for X/Y (triple) mode: ³¹ P/ ¹¹ B, ³¹ P/ ²⁷ Al, ¹¹ B/ ¹³ C, ¹³ C/ ¹⁹⁵ Pt, ²³ Na/ ²⁹ Si, ⁶ Li/ ²⁹ Si
Probe 3	4mm MAS	¹³ C- ³¹ P/ ¹⁹ F- ¹ H
Probe 4	7mm	¹⁵ N- ³¹ P/ ¹⁹ F- ¹ H
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	

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- ¹ H
Probe 2	4mm MAS	¹⁵ N- ¹³ C/ ¹⁹ F- ¹ H, ⁴³ Ca
TriGamma™ Probe	3.2mm MAS	¹⁵ N- ²⁹ Si/ ¹¹ B- ³¹ P/ ¹ H
Triple Resonance Probe	4mm MAS	²⁹ Si/ ¹¹ B/ ¹ H
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} Ti, ⁸⁹ Y, ⁸⁷ Sr / ¹⁹ F- ¹ H,
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	

Section 3 - Detailed Description of Centre Activities

3.1 Core Group of Personnel affiliated with or residing within the Centre

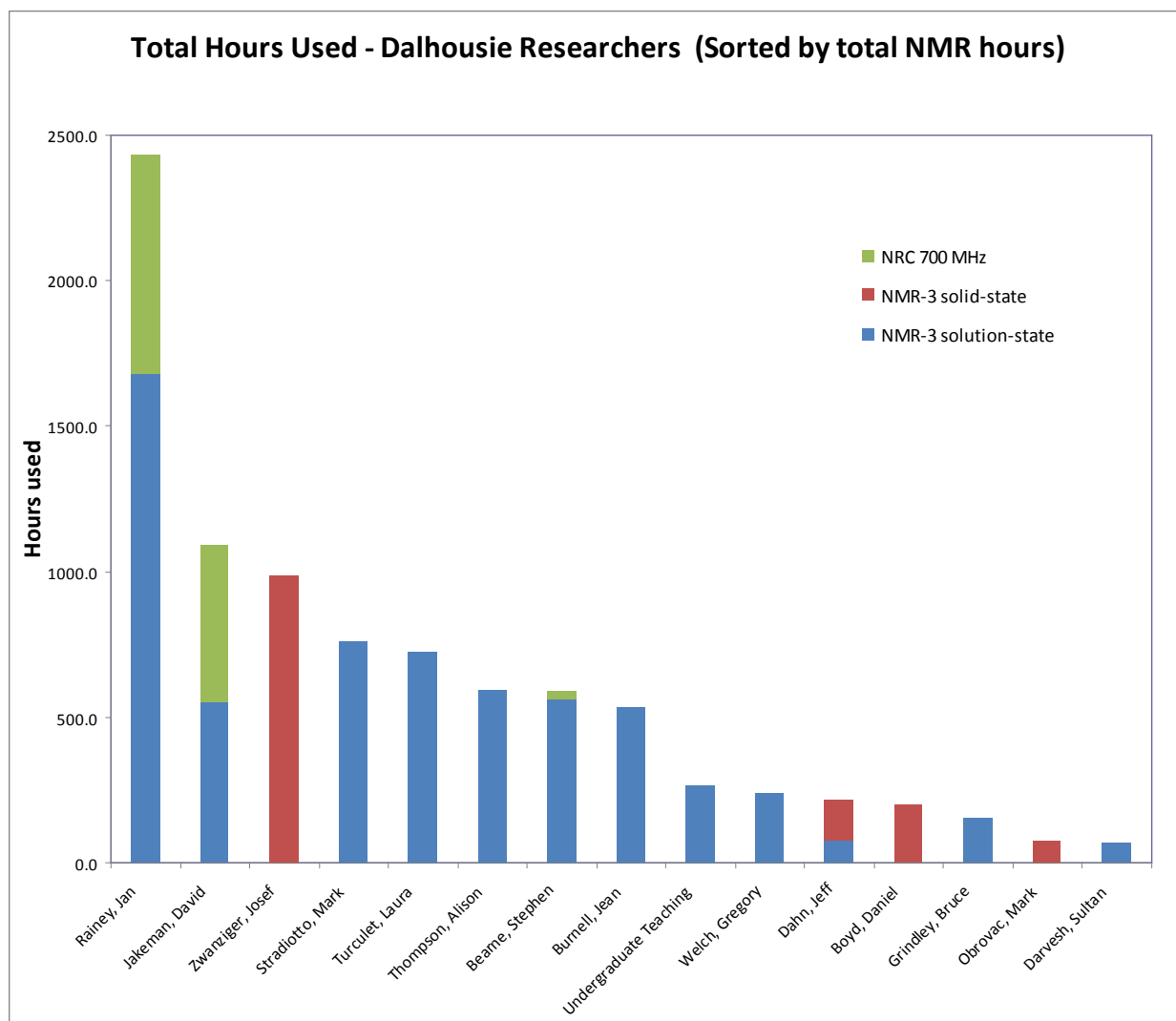
Position	Dalhousie	Supporting Maritime Institutions	Non-Supporting Maritime Institutions	Other	Government & Industry
Faculty Members	30	1	5	4	
NMR ³ Staff	2				
Instructors & TA's	11				
Research Associates	4		1		
Post-Docs	20		1		
PhD Students	30			1	
Masters Students	31	1	1		
Undergraduate Students	22	2	4		
Others	11		1	2	5

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	Brooks, Su-Ling	Dalhousie University	Associate Professor
5	Budge, Suzanne	Dalhousie University	Professor
6	Burnell, Jean	Dalhousie University	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	Duncan, Roy	Dalhousie University	Professor
12	Filiaggi, Mark	Dalhousie University	Associate Professor
13	Grindley, Bruce	Dalhousie University	Adjunct Professor
14	He, Quan	Dalhousie University	Assistant Professor
15	Jakeman, David	Dalhousie University	Professor
16	Liu, Paul Xiang-Qin	Dalhousie University	Professor
17	MacQuarrie, Stephanie	Cape Breton University	Associate Professor

18	McFarland, Sherri	Acadia University	Professor
19	Moore, Robert	Dalhousie University	Professor Emeritus
20	Obrovac, Mark	Dalhousie University	Professor
21	Price, Gordon	Dalhousie University	Associate Professor
22	Rainey, Jan	Dalhousie University	Professor; NMR ³ Director
23	Ramanathan, Vaidhya	Indian Institute of Science Educ. & Res., India	Professor
24	Roger, Andrew	Dalhousie University	Professor
25	Rohde, John	Dalhousie University	Assistant Professor
26	Savidge, Rodney	University New Brunswick	Professor
27	Schepp, Norm	Dalhousie University	Associate Professor
28	Simpson, Alastair	Dalhousie University	Professor
29	Singer, Rob	Saint Mary's University	Professor
30	Stradiotto, Mark	Dalhousie University	Professor; NMR ³ User Group Chair
31	Thompson, Alison	Dalhousie University	Professor
32	Turculet, Laura	Dalhousie University	Associate Professor
33	Vidovic, Drasko	Singapore	Professor
34	Weaver, Don	Dalhousie University / Toronto	Professor
35	Welch, Gregory	Dalhousie University	Assistant Professor
36	White, Mary Anne	Dalhousie University	Professor
37	White, Rob	Dalhousie University	Associate Professor
38	Wiesner, Ulrich	Cornell University, NY, USA	Professor
39	Xia, Aibing	Mount Saint Vincent University	Associate Professor
40	Zwanziger, Josef	Dalhousie University	Professor

The usage profile for the heaviest Dalhousie user groups (top 15) is shown below 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	Brown, David	Mycodev Group Inc	
2	Hilborn, Jim	Heritage Memorials Ltd.	
3	MacEachern, Lauren	Solid State Pharma Inc	Trained Hands-On User

4	Ness, Matthew	Research & Productivity Council	
5	Ullah, Zia	NeuroQuest	Trained Hands-On User

3.1.4 Lab Instructors and TA's

Number	Name	Position
1	Aish, Gaia	Instructor
2	Aleman-Milan, Gianna	Instructor
3	Berryman, Victoria	Instructor
4	Chisholm, Rory	Instructor
5	Iaboni, Douglas	Teaching Assistant
6	Liu, Aaron	Teaching Assistant
7	Moya-Barrios, Reinaldo	Instructor
8	Padmos, Dan	Instructor
9	Whalen, Marc	Instructor
10	Yang, Rui	Teaching Assistant
11	Zheng, Lituo	Teaching Assistant

3.1.5 Research Associates, Post-Docs and Others

Number	Name	Affiliation	Position
1	Areephong, Jetsuda	Dalhousie University	Research Associate
2	Banfield, Scott	Dalhousie University	Research Associate
3	Barrionuevo, Manoel	Dalhousie University	Exchange Student
4	Bhar, Palash	Dalhousie University	Post-Doc
5	Borzenko, Andrey	Dalhousie University	Post-Doc
7	Davis, Mallory	Dalhousie University	Volunteer Researcher
8	Douglas, Colin	Dalhousie University	Post-Doc
9	Figliola, Carlotta	Dalhousie University	Post-Doc
10	Fisher, Laural	Dalhousie University	Post-Doc
11	Hagar, Mostafa	Dalhousie University	Volunteer Researcher
12	Hall, David	Dalhousie University	Post-Doc
13	Hanson-Clarke, Margaret	Dalhousie University	Post-Doc
14	Harris, Emily	Dalhousie University	Summer Researcher
15	Hasan, Sami	Dalhousie University	Post-Doc

17	Hurisso, Bitu	Saint Mary's University	Post-Doc
18	Kim, Chris	Dalhousie University	Post-Doc
19	Kirshenbaum, Maxine	Dalhousie University	Volunteer Researcher
21	Marchal, Estelle	Dalhousie University	Post-Doc
22	McCormick, Nicole	Dalhousie University	Research Assistant
23	Monro, Susan	Acadia University	Research Associate
24	Morrison, Zachary	Dalhousie University	Summer Researcher
25	Mugica, Odei	Dalhousie University	Exchange Student
26	Na, Jungwook	Dalhousie University	Summer Researcher
28	Nie, Mengyun	Dalhousie University	Post-Doc
29	Ogawa, Takahiko	Dalhousie University	Post-Doc
30	Pal, Mohan	Dalhousie University	Post-Doc
31	Paul, Nawal	Dalhousie University	Research Associate
32	Rusalovsky, Olexiy	Ottawa University	Summer Researcher
33	San Juan, Ronan	Dalhousie University	Post-Doc
34	Sarker, Muzaddid	Dalhousie University	Post-Doc
35	Shi, Ge	Acadia University	University Staff
36	Smithen, Deborah	Dalhousie University	Post-Doc
37	Sparavalo, Sara	Dalhousie University	Technician
38	Sun, Shengguo	Dalhousie University	Research Associate
40	Valliant, Esther	Dalhousie University	Post-Doc
41	Wang, Yaohui	Dalhousie University	Post-Doc
42	Wentzell, Jordan	Lakehead University	Summer Researcher
43	Wiethan, Carson	Dalhousie University	Visiting Researcher
44	Xia, Jian	Dalhousie University	Post-Doc
45	Zhu, Jian-She	Dalhousie University	Post-Doc

3.2 Publications Associated with Centre (July 1, 2014 to June 30, 2015)

Peer-Reviewed Journal Articles – total 58

1. Baker AEG, Marchal E, Lund KLAR, & Thompson A (2014) The use of tin(IV) chloride to selectively cleave benzyl esters over benzyl ethers and benzyl amines. *Canadian Journal of Chemistry* 92(12):1175-1185.
2. Borzenko A, Rotta-Loria NL, MacQueen PM, Lavoie CM, McDonald R, & Stradiotto M (2015) Nickel-Catalyzed Monoarylation of Ammonia. *Angewandte Chemie-International Edition* 54(12):3773-3777.
3. Bourque AN & White MA (2015) Control of thermochromic behaviour in crystal violet lactone (CVL)/alkyl gallate/alcohol ternary mixtures. *Canadian Journal of Chemistry* 93(1):22-31.

4. Ciechonska M & Duncan R (2014) Reovirus FAST proteins: virus-encoded cellular fusogens. *Trends in Microbiology* 22(12):715-724.
5. Comeau PA & Filiaggi MJ (2015) Calcium polyphosphate precipitation - A strategy to tune the chain length of the glass and control the subsequent release of vancomycin. *Materials Chemistry and Physics* 159:56-63.
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3.3 Participation in relevant events for research dissemination

A total of 37 international and 88 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
	23 international conference/symposium presentations by 13 professors	14 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
	19 domestic conference/symposium presentations by 13 professors	69 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: 318

(2) CHEM 2402: "Organic Chemistry II"

Instructor: Frances Cozens

Course enrollment: 247

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

Instructor: Peng Zhang

Course enrollment: 88

- **3rd Year Undergraduate**

(1) BIOC 3700: "Biomolecular Chemistry"

Instructors: Jan Rainey and Stephen Bearne

Course enrollment: 35

(2) CHEM 3401: "Intermediate Organic Chemistry"

Instructor: Bruce Grindley

Course enrollment: 48

(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: 55

- **4th Year Undergraduate**

(1) CHEM 4901: "Honours Research Project"

Instructor: Norm Schepp

Course enrollment: 5

(2) BIOC 4702 (cross-listed with BIOC 5702/CHEM 5602): "Macromolecular Biophysics"

Instructor: Jan Rainey

Course enrollment: 9

3.5 Student research activities related to the Centre mission statement

The following table summarizes the 92 student researchers who relied upon the NMR³ facility for progress in their research programs during the 2013-2014 reporting period. The table is made up of 31 Doctoral, 33 Masters, and 28 Undergraduate students.

	Student Name	Institution	Degree	Supervisor	Status	Thesis Title
1	Adams, Matt	Dalhousie University	BSc	Jean Burnell	In-Progress	
2	Ampaw, Anna	Dalhousie University	MSc	David Jakeman	In-Progress	

3	Bates, Jamie	Dalhousie University	MSc	Fran Cozens	Left	
4	Beh, Michael	Dalhousie University	MSc	Alison Thompson	In-Progress	
5	Bennett, Leah	Acadia University	BSc	Sherri McFarland	In-Progress	
6	Chisholm, Alicia	Dalhousie University	BSc	Mark Stradiotto	In-Progress	
7	Chowdhury, Barsha	Dalhousie University	BSc	Fran Cozens	In-Progress	
8	Comeau, Patricia	Dalhousie University	PhD	Mark Filiaggi	Completed	Novel Fabrication of a Calcium Polyphosphate Delivery Matrix for Treatment of Osteomyelitis and Bone Regeneration
9	Cook, Earl	Dalhousie University	MSc	Mark Stradiotto	Left	
10	Dickey, Brett	Dalhousie University	PhD	Daniel Boyd	In-Progress	
11	Ellis, Leah	Dalhousie University	PhD	Jeff Dahn	In-Progress	
12	Fielden, Ryan	Dalhousie University	MSc	Mark Obrovac	Completed	Layered Oxide Phases for Sodium-Ion Battery Electrodes
13	Forget, Stephanie	Dalhousie University	MSc	David Jakeman	In-Progress	
14	Garrison, David	Mount Saint Vincent	BSc	Ian Pottie	Completed	Investigation of Triisopropyl Propanenitronate with Acetals
15	Gong, Min	Dalhousie University	MSc	Chibuike Udenigwe	In-Progress	
16	Groves, Brandon	Dalhousie University	MSc	Alison Thompson	In-Progress	
17	Harding, Tommy	Dalhousie University	PhD	Alastair Simpson	In-Progress	
18	Hargreaves, Breanna	Dalhousie University	BSc	Mark Stradiotto	In-Progress	
19	Harty, Matthew	Dalhousie University	MSc	Stephen Bearne	In-Progress	
20	Hendsbee, Arthur	Dalhousie University	MSc	Greg Welch	Left	
21	Hoey, Marshall	Dalhousie University	MSc	Laura Turculet	In-Progress	
22	Hollenhorst, Helia	Dalhousie University	BSc	Laura Turculet	In-Progress	

23	Huchenski, Blake	Dalhousie University	BSc	Bruce Grindley	Completed	Synthesis of a Vaccine Against Lyme Disease Derived from BbGL1
24	Hurshman, Colby	Dalhousie University	BSc	David Jakeman	In-Progress	
25	Jaeschke, Alyssa	Mount Saint Vincent University	MSc	Ian Pottie	Completed	Development of the Nitronate Nazarov Reaction from Phenyl Nitromethane
26	Jee, Alison	Dalhousie University	BSc	David Jakeman	In-Progress	
27	Jollymore, Courtney	Dalhousie University	PhD	Sultan Darvesh	Left	
28	Kahwaji, Samer	Dalhousie University	PhD	Mary Anne White	In-Progress	
29	Kajetanowicz, Aleksandra	Dalhousie University	BSc	Alison Thompson	In-Progress	
30	Kelly, Colin	Dalhousie University	MSc	Laura Turculet	In-Progress	
31	Kenward, Calem	Dalhousie University	BSc	Jan Rainey	In-Progress	
32	Kilcup, Nancy	Dalhousie University	PhD	Daniel Boyd	In-Progress	
33	Kitching, Elizabeth	Dalhousie University	BSc	Greg Welch	In-Progress	
34	Kim, Min Joon	Dalhousie University	BSc	Alison Thompson	In-Progress	
35	Knopf, Philipp	Dalhousie University	BSc	Stephen Bearne	In-Progress	
36	Kottwitz, Haila	Dalhousie University	MSc	John Rohde	In-Progress	
37	Land, Michael	Saint Mary's University	BSc	Jason Clyburne	In-Progress	
38	Lavoie, Chris	Dalhousie University	MSc	Mark Stradiotto	In-Progress	
39	LeBlanc, Danielle	Dalhousie University	BSc	Jan Rainey	Completed	Biophysical Characterization of the C-Terminal Tail of the Apelin Receptor
40	LeFort, Francois	Dalhousie University	PhD	Jean Burnell	In-Progress	
41	Lefsay, Abir	Dalhousie University	PhD	Ameres Chatt	In-Progress	
42	Lindeperg, Fabien	Dalhousie University	PhD	Laura Turculet	In-Progress	

43	Lund, Katie	Dalhousie University	MSc	Alison Thompson	In-Progress	
44	Lundrigan, Travis	Dalhousie University	PhD	Alison Thompson	In-Progress	
45	Ma, Kai	Cornell University, USA	PhD	Ulrich Wiesner	In-Progress	
46	Ma, Lin	Dalhousie University	MSc	Jeff Dahn	Completed	Studies of the Effects of Electrolyte Additives on the Reactivity between Charged Electrodes and Electrolytes in Li-Ion Batteries Using Accelerating Rate Colarimetry
47	Macaulay, Casper	Dalhousie University	MSc	Laura Turculet	In-Progress	
48	MacDonald, Kathleen	Dalhousie University	PhD	Daniel Boyd	In-Progress	
49	MacIntyre, Logan	Dalhousie University	BSc	David Jakeman	Completed	Modified Culture Conditions to Produce Novel Jadomycins
50	MacQueen, Preston	Dalhousie University	PhD	Mark Stradiotto	In-Progress	
51	Martinez-Farina, Camilo	Dalhousie University	MSc	David Jakeman	Completed	Investigations into the Biosynthesis, Derivatization, and Purification of Jadomycins
52	McAfee, Seth	Dalhousie University	MSc	Greg Welch	Left	
53	McCain, Julia	Acadia University	BSc	Sherri McFarland	In-Progress	
54	McClennan, Billy	Saint Mary's University	BSc	Jason Clyburne	In-Progress	
55	McCluskey, Greg	Dalhousie University	PhD	Stephen Bearne	In-Progress	
56	McDonald, Nicholas	Dalhousie University	MSc	Rob White	In-Progress	
57	Melanson, Jennifer	Dalhousie University	PhD	Alison Thompson	In-Progress	
58	Momeni, Arash	Dalhousie University	PhD	Mark Filiaggi	Completed	Developing an Injectable in-situ-forming Calcium Polyphosphate System as a Hemostatic Agent

59	Morash, Ben	Dalhousie University	BSc	Jan Rainey	Completed	The NMR Chemical Shift Standard DSS Exhibits Concentration-Dependent Behavior in both Aqueous and Micellar Solution
60	Morgan, Tim	Dalhousie University	PhD	Jean Burnell	In-Progress	
61	Murphy, Luke	Dalhousie University	PhD	Laura Turculet	In-Progress	
62	Nagar, Mitesh	Dalhousie University	PhD	Stephen Bearne	Completed	Mandelate Racemase: Insights into Substrate Tolerance, Novel Inhibitor Binding Modes, and the Role of Binding Determinants
63	Namespetra, Andrew	Dalhousie University	MSc	Greg Welch	Completed	A Study of Photoactive Materials for Solution-Processed Thin-Film Solar Cells
64	O'Connell, Kathleen	Dalhousie University	PhD	Daniel Boyd	In-Progress	
65	Orrell, Kathleen	Dalhousie University	BSc	Jan Rainey	Completed	Probing the Local Conformational Environment within Recombinant <i>Argiope Trifasciata</i> Aciniform Silk Protein by ¹⁹ F NMR
66	Pandey, Aditya	Dalhousie University	PhD	Jan Rainey	In-Progress	
67	Panther, Scott	Dalhousie University	BSc	Jean Burnell	In-Progress	
68	Paterson, Alex	Dalhousie University	PhD	Joe Zwanziger	In-Progress	
69	Patterson, Robin	Dalhousie University	MSc	Jan Rainey	In-Progress	
70	Payne, Abby-Jo	Dalhousie University	MSc	Greg Welch	Left	
71	Periyapperuma, Kalani	Dalhousie University	MSc	Mark Obrovac	Completed	Development of a New Cell Design for Metal Battery Research and Investigating Electrode Materials and Electrolyte Systems for Mg Batteries
72	Petibon, Remi	Dalhousie University	PhD	Jeff Dahn	In-Progress	
73	Qin, Teng Fei	Dalhousie University	MSc	Norman Schepp	In-Progress	

74	Romao, Carl	Dalhousie University	PhD	Mary Anne White	Completed	Thermoelastic Properties of Materials with Negative Coefficients of Thermal Expansion
75	Reda, Alexandra	Dalhousie University	MSc	Roger McLeod	Completed	Structural Characterization of 20 kDa Lipid-Binding Fragments of Apolipoprotein B100
76	Regan, Gemma	Dalhousie University	BSc	Stephen Bearne	Completed	Development of a Probe for Active Site-Directed Activity Profiling
77	Robertson, Andrew	Dalhousie University	PhD	David Jakeman	Completed	Exploring Jadomycin Biosynthesis in <i>Streptomyces Venezuelae</i>
78	Rotta-Loria, Nicolas	Dalhousie University	MSc	Mark Stradiotto	In-Progress	
79	Ruddy, Adam	Dalhousie University	PhD	Laura Turculet	Completed	Synthesis, Characterization, and Reactivity of Transition Metal Complexes Supported by Heteropolydentate Ligation
80	Sainuddin, Tariq	Acadia University	MSc	Sherri Mcfarland	In-Progress	
81	Sawarzky, Ryan	Dalhousie University	MSc	Mark Stradiotto	In-Progress	
82	Shin, Kyungsoo	Dalhousie University	PhD	Jan Rainey	In-Progress	
83	Simms, Gordon	Dalhousie University	PhD	Donald Weaver	Completed	The Discovery of a Novel Series of Amyloid- β Antiaggregants Based on the Structure of 3-Hydroxyanthranilic Acid: A Detailed Analysis of the Mechanism of Action Underpinning Antiaggregant Activity
84	Soley, Jacob	Dalhousie University	BSc	Sultan Darvesh	Completed	Development of Radiolabeled Cholinesterase Ligands for Imaging of Alzheimer's Disease Pathology
85	Subedi, Pankaj	Dalhousie University	MSc	Fran Cozens	In-Progress	
86	Timm, Matthew	Mount Saint Vincent	BSc	Aibing Xia	In-Progress	

87	Tremblay, Marie	Dalhousie University	PhD	Jan Rainey	Completed	The Structural Characterization of <i>Argiope trifasciata</i> Spider Wrapping Silk by Solution-State NMR
88	Wilkes, Britney	Dalhousie University	BSc	Mark Obrovac	In-Progress	
89	Xia, Wei	Dalhousie University	MSc	Suzanne Budge	In-Progress	
90	Xiong, Deijun	Dalhousie University	PhD	Jeff Dahn	In-Progress	
91	Yaphe, Hannah	Dalhousie University	BSc	Stephen Bearne	In-Progress	
92	Zaky, Mariam	Dalhousie University	MSc	Jean Burnell	In-Progress	

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 groups of Professors Jan Rainey, Paul Xiang-Qin Liu, Roy Duncan and Andrew Roger from the Department of Biochemistry & Molecular Biology at Dalhousie. 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 research seminars at the western University and the University of Prince Edward Island; NMR³ Solid-State Coordinator Ulli Werner-Zwanziger did so at the University of California, Santa Barbara.

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

- On September 30, 2014, Drs. Mike Lumsden and Muzaddid Sarker (a PDF with Professor Jan Rainey) provided high-resolution NMR experiment demonstrations to 10 Dalhousie students from the BIOC 4702 course (cross-listed with BIOC 5702/CHEM 5602).
- On October 22, 2014, NMR³ facility staff hosted a group of ~ 14 undergraduate students from Saint Mary's University and explained/demonstrated the basic principles of high-resolution and solid-state NMR spectroscopy.

3.7 Technology Development, patent or commercialization activities

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

1. **Olefin Hydroboration.** US 2014/293,833. Principal Inventor: Mark Stradiotto
2. **Antifouling Marine Paints** US 2014/968,305. Principal Inventors: Robert Singer and John Steele
3. **Butyrylcholinesterase Ligands as Diagnostic Tools and Treatment for Diseases of the Nervous System** US Patent #8,795,630, Issued August 5, 2014. Principal Inventor: Sultan Darvesh

4. **Butyrylcholinesterase Ligands as Diagnostic Tools and Treatment for Diseases of the Nervous System** Japanese Patent #5734853 Issued April 24, 2015. Principal Inventor: Sultan Darvesh

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:

- A 1D ¹H-¹⁹F HOESY experiment (Heteronuclear NOESY) was setup on the AVANCE 500, an experiment that capitalizes on the capabilities of the BBFO SmartProbe installed in this spectrometer.
- Implementation of the WURST-QCPMG pulse sequence on the Avance 700, yielding ultra-wide quadrupolar spectra and permitting the study of ¹³⁵Ba, ¹³⁹La and ²⁰⁹Bi nuclei in the solid-state.
- A NMR technique designed to detect the binding of small molecules to large receptors called WaterLOGSY was set up and made routinely available.

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 for ²H NMR observe on the AV500 and AV300 instruments.
- Creation of the "AVANCE 500 Experiment List"; a tabulation of all available NMR experiments on the AV500, along with brief descriptions of the purpose of each experiment and a listing of the default parameters.
- Significant updates to the documents for data retrieval from the facility ftp server (version 2.0, March 2015) as well as the NMR3 facility user guide (version 5.0, April 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 on twitter now also receive important updates and information via "tweets".

Section 4 – Financial Information (April 1, 2014 – March 31, 2015)

4.1 2014-2015 Financial Report

Financial support in '14-'15 came from a total of 3 sources: (1) Dalhousie University (2) User Fees and (3) a "Supporting Institution Fee" (described below). This past year, the facility paid 31% and the University 69% of the Coordinator's full salary and benefits. Also, the facility paid 20% of the Solid-State NMR Coordinator salary with the remaining 80% paid by the Faculty of Science in support of Professor Joe Zwanziger's Canada Research Chair. Other direct costs of the facility this past FY included magnet cryogens, lab supplies, computing costs, and all expenses associated with service and maintenance.

User fees at the conclusion of the reporting period are provided 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	\$10 per Rotor
Packing Air-Sensitive Samples for Solid-State NMR	\$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
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

Compared to the 2013-2014 reporting period, changes to the user fee structure are as follows:

- 1) **Hourly Rate Increases for Solid-State NMR Usage:** These changes were implemented on April 1, 2015 and were calculated on the basis of a historical analysis of solid-state NMR billable hours vs. solid-state NMR non-salary expenses (cryogenics, maintenance, repairs, etc). The rates were increased to a level calculated to cover non-salary operational costs of the two solid-state NMR spectrometers. A similar analysis was performed for the high-resolution NMR spectrometers with the conclusion that high-resolution NMR rates did not require adjustment.
- 2) **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 this year, 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 and awarded within the 2014-2015 Fiscal Year

In total, **\$2,453,340 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 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 **>\$11.4-million in grant funds has been attributed by Dalhousie users as relying upon the ability to access NMR³ facilities.**

Grants Awarded to Dalhousie-Based Users

Applicant: **Bruce Grindley**

- Green Centre Canada Grant: "Large Scale Synthesis of Gemini Surfactants and Surfactant Building Blocks Based on Pentaerythritol" (\$11,000 for 1 year)

Applicant: **Jan Rainey**

- NSERC - Research Tools and Instruments: "A Light Scattering Instrument for Characterizing of (Bio)molecule and Supramolecular Assembly Size, Shape, and Oligomerization State" (\$131,720)
- NSERC - Engage: "Optimized NMR Spectroscopy-Based Screening for Bioactives from Natural Product Libraries" (\$25,000)
- NSERC - Interaction Grant: "Exploration of Potential Collaboration with Nautilus Biosciences Inc" (\$735)

Applicant: **Mark Filiaggi**

- Dalhousie Faculty of Dentistry Research Fund Grant: "New Strategies for Improving the Cohesiveness of Calcium Polyphosphate as a Liquid Embolic Agent" (\$9,830)

Applicant: **Mark Stradiotto**

- Chevron Phillips Chemical Company: "Application of a Proprietary Ligand Class" (\$60,000 USD for 1 year, 50% in collaboration with Laura Turculet)

Applicant: **Mary Anne White**

- NSERC - Discovery Grant: "Fundamental Science for Future Materials Applications" (\$59,000/year; 5 years)

Applicant: **Paul Xiang-Qin Liu**

- NSERC - Discovery Grant: "Intein-Catalyzed Protein Splicing: Functional Versatility and Utility" (\$52,000/year; 5 years)

Applicant: **Rob White**

- NSERC - Discovery Grant: "Elucidation of Bacterial and Mass Spectral Pathways" (\$30,000/year; 5 years)

- NSERC - Engage: "Elaboration of Differential Mobility Spectrometry using Isomeric Ions and Computational Chemistry" (\$25,000)

Applicant: **Roy Duncan**

- CIHR - "Membrane Curvature Sensors, Inducers, and Microdomains in Reovirus-mediated Syncytium Formation" (\$145,851/year; 5 years)

Applicant: **Sultan Darvesh**

- Dalhousie Faculty of Medicine: "Dalhousie Medical Research Foundation Irene MacDonald Sobey Chair in Curative Approaches to Alzheimer's Disease" (\$70,000/year; 5 years)
- Canadian Consortium for Neurodegeneration in Aging, Canadian Institutes of Health Research: "Early Synaptic Changes and Metabolomics" (\$78,400/year; 5 years)

Grants Awarded to NMR³ External Users

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

- NSERC - Discovery Grant: "Catalysis, Separations, and New Methodologies Using Ionic Liquids" (\$20,000/year; 5 years)
- Faculty of Graduate Studies and Research, Saint Mary's University: "Organocatalysis in Ionic Liquids" (\$3,000)

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

- Cape Breton University - Research Project (RP) Grant: "A Brief Investigation of the Organocatalytic Abilities of Allenes" (\$8,000)