

NUCLEAR MAGNETIC RESONANCE RESEARCH RESOURCE

2013 – 2014 Annual Report

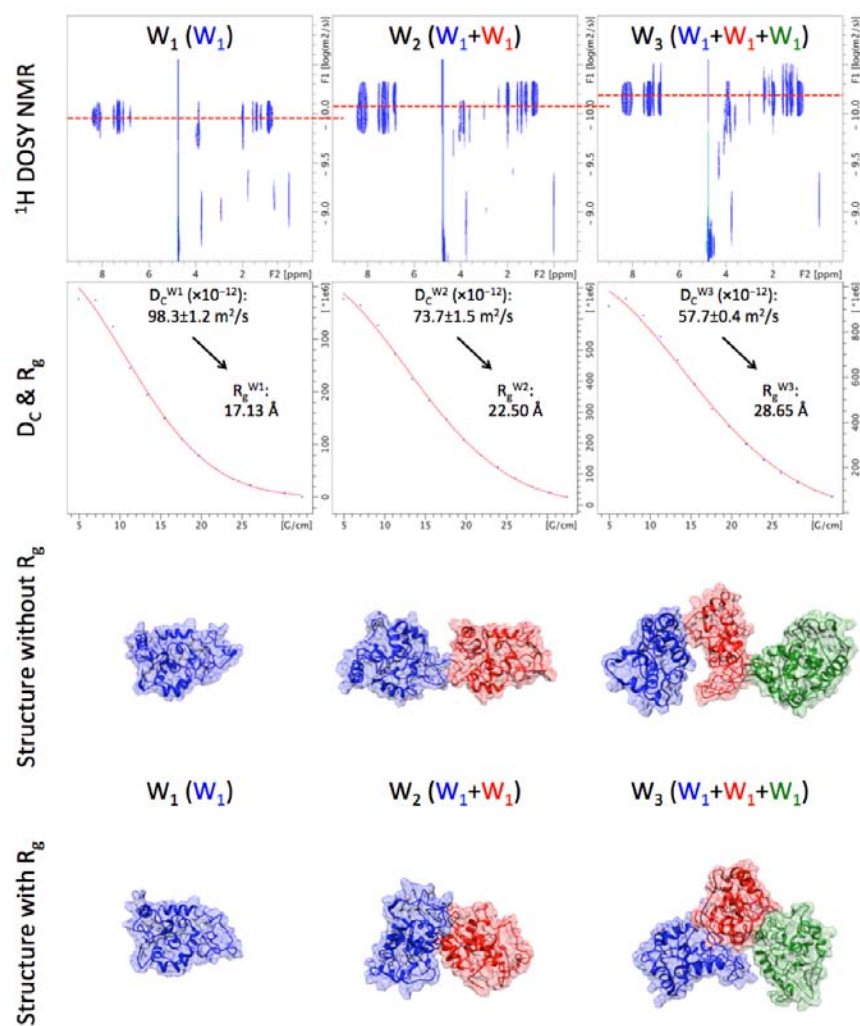


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About the cover: Compactly folded "beads-on-a-string" architecture of spider wrapping silk protein AcSp1. Constructs of differing numbers of concatenated 200-amino acid repetitive domains ($W_1 = 1$ repeat; $W_2 = 2$ repeats; $W_3 = 3$ repeats) were characterized by diffusion-ordered NMR spectroscopy (DOSY). Heteronuclear backbone walk NMR experiments show a strikingly modular structure. Translational diffusion coefficient (D_c) values determined using DOSY NMR indicate that W_n proteins are not ideal spheres, ellipsoids or cylinders. Use of a radius of gyration (R_g) restraint, based on DOSY-derived D_c values, improved the agreement between structure calculations and experimental data, revealing a compactly folded beads-on-a-string architecture for spider wrapping silk. (Figure prepared by Dr. Muzaddid Sarker in Jan Rainey's research group.)

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 2013-2014, the Centre assisted 46 research groups mostly drawn from the Atlantic Canada region but also including several international researchers, resulting in 69 publications, 141 conference presentations and 153 highly qualified personnel trained. Furthermore, teaching in the Department of Chemistry was supported in 4 undergraduate laboratories with 167 students and 186 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 ~9700 hours, with 8427 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 *\$1.5-million in new external grant funds awarded* in the 2013-2014 fiscal year. On a rolling basis, it should be further noted that NMR³ has been identified as being instrumental in awarding of an additional \$9.9-million in external grant funding to Dalhousie researchers in the 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 Associate 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. The current elected User Group Chair is Dr. David Jakeman (Professor, Dalhousie Pharmacy and Chemistry) 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.

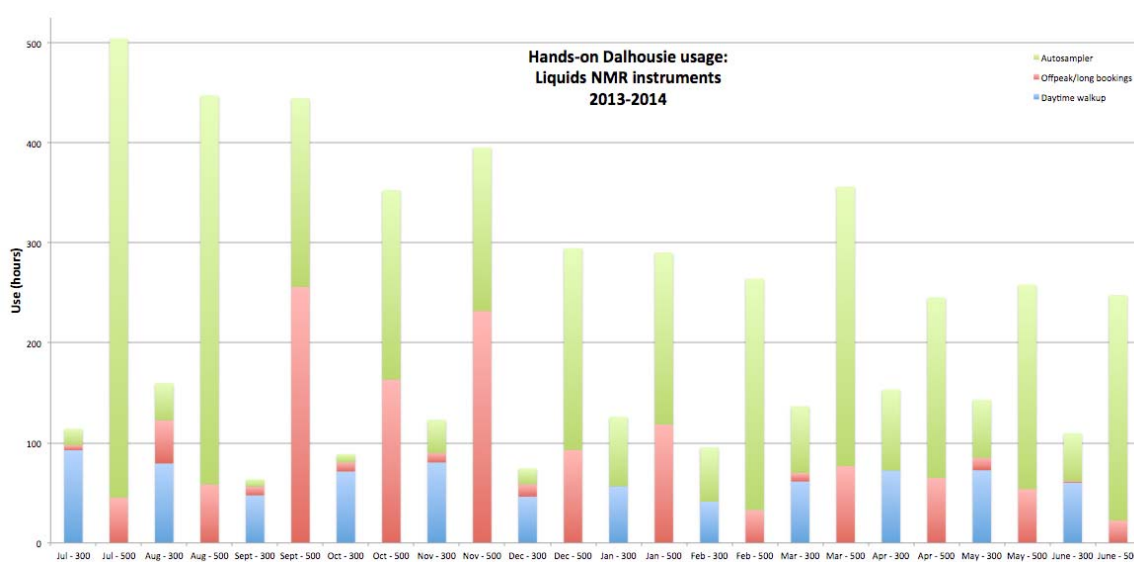
1.1 Mission Statement

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 continuous 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. Encourage more diverse instrument usage: The workhorse instrument of NMR³ is the AV500 MHz solution-state NMR instrument. This is reflected in usage dynamics, covering 4308 hours of the total 7176 hours of the four Dalhousie-based instruments. Three major classes of experiment are performed: (1) routine experiments configured by individual users in a semi-automated modality (via autosampler, first-come-first-served basis with classes 2 and 3 pre-empting these experiments); (2) hands-on experiments for samples with limited lifetime or requiring special handling (via bookable slots available at 4 pm 5 days per week); and, (3) hands-on experiments requiring either a non-standard instrument configuration or an 8 hour to several day period of acquisition (via bookable slots following a schedule set quarterly by Dr. Lumsden in consultation with Dr. Rainey and the User Group.) NMR³ faces an ongoing juggling act between, in particular, classes 1 and 3 of usage. Class 1 usage can, in some part, also be accommodated by the 300 MHz instrument. This was made more feasibly in the previous fiscal year when the NMR³ Centre partnered with the Department of Chemistry (through allocation of teaching funds) to purchase an autosampler for the 300 MHz spectrometer, providing functionality quite similar to the autosampler on our 500 MHz instrument. Unfortunately, despite this upgrade, in the early part of the report year, off-peak and autosampler usage on the 300 MHz instrument was negligible to minimal. (Daytime usage on the 300 MHz is hands-on and fully bookable to users, and tends to be heavily used throughout the year.) We therefore implemented a campaign to encourage off-peak 300 MHz usage through both increased autosampler availability and a decrease of hourly user fees in hopes that this would provide ongoing momentum for 300 usage, increasing the proportion of off-peak time used and providing additional availability of the 500 MHz for non-routine purposes. As illustrated in the following chart, this was highly successful:



Implementation of the new 300 MHz policies began in January, and the above plot of usage profile demonstrates clearly that this led to a major increase in autosampler usage on this instrument that remained consistent for the first 6 months of the year. Notably, this change in policy was accompanied by an increase in the number of "class 3" booking slots available on the 500 MHz. No major concerns have been raised by the User Group as a result of this potential decrease in 500 MHz time, with good uptake of the 300 MHz appearing to compensate.

2. Research published in Science: Dr. Ulrike Werner-Zwanziger worked closely with a research team led by Dr. Jason Clyburne from Saint Mary's University, to understand how nature uses carbon-capture to tame cyanide poisons. Using solid-state NMR, Dr. Werner-Zwanziger provided key evidence in the discovery of the formation of cyanofornate. This simple ion - which is formed when cyanide bonds to carbon dioxide - is a by-product of the fruit-ripening process that has evaded detection for decades. Following the publication in *Science* (**344** (6179), 75-78 (2014)), this work was featured in the media from local to international levels, including reports in Chemistry Today, Chemistry and Engineering News, Canadian NMR Research, the Chronicle Herald, and Canadian Chemistry News.

3. New contract with NRC negotiated: During the previous fiscal year, a new contract was negotiated with the NRC for access to the 700 MHz high-resolution NMR spectrometer. This was negotiated ~12 months after the previous contract expired due to delays at the NRC in drawing up a new contract, meaning that access to this instrument by Dalhousie users was extremely limited over the reporting year and was all billed retroactively at the new rates (recall that Dalhousie purchased and owns the cryoprobes employed in this instrument, so is a major stakeholder). User fees in the new contract have been simplified to a single hourly rate, vs. the previous distinction between "long" and "short" experiments. This means that the hourly rate for short experiments has dropped dramatically (from \$29/hour + HST to \$10.63/hour + HST), while that for long experiments has increased by ~19%. Access issues for Dalhousie users have been worked out such that after-hours access is again made possible in the new contract.

4. Major revamp of the NMR³ website: After attending web training courses and in consultation with the Chemistry Department's computer support specialist, Ryan MacKinnon, a major restructuring of the NMR³ facility website was undertaken. In September of 2013, migration of the old site to Adobe Communique 5 (CQ5) was completed. Adobe CQ5 is a large-scale web content and digital asset

management system in use and supported by the Dalhousie Web team. The migration ensured online branding and content consistency with other Dalhousie-based websites and, in addition, provided many new and enhanced tools for communicating with the users of the facility. You can visit the facility's new and improved website at <http://www.dal.ca/diff/nmr3.html>.

1.3 Upcoming Year's Activity

1. Improve high-resolution NMR facility reliability through restoration of uninterruptible power supply (UPS): Included with the installation of the AVANCE 500 MHz spectrometer in 2003 was a 6 kVA UPS. UPS systems installed with NMR spectrometers serve a number of important power functions, including stabilizing the line voltage, correcting line voltage spikes, and maintaining power to the spectrometer via batteries during short power outages. All of these functions improve the reliability and stability of a spectrometer (and therefore improve data quality) and increase longevity. Unfortunately, the 6 kVA UPS failed last year and the repair cost proved to be exceedingly high. Therefore, we plan to purchase a new UPS system this year; sized such that it will be able to service both the AVANCE 300 and 500 high-resolution NMR spectrometers. **Note:** although the UPS system was purchased early in the reporting year, we have experienced major delays in scheduling of Facilities Management to complete the installation. We had hoped to make this upgrade in the current reporting year, but instead have been able to do so for the upcoming reporting year.

2. Revisit hourly user fees: On the basis of a loss in University support of funding for Dr. Lumsden's salary (from 85% to 69%), the facility is facing an impending budget crunch. As such, we will be revisiting the hourly fees charged on all instruments on the basis of both covering salaries and other expenses (consumables and maintenance.) We expect to propose a new set of user fees for discussion with and ratification by the User Group in the Fall of 2014. The goal will be to ensure that a balanced budget is achieved and that a healthy contingency fund remains to cover costs should an unlikely, but possible, catastrophic instrument quench occur. We will also continue to explore options for further funding from University sources, vs. individual research grants. A large-scale CFI application led by Alison Thompson is under review - this would alleviate many of these budgetary issues in the short term (~5 year period), but we need to work under the assumption that we must balance the budget based upon our current usage profile and income sources.

3. Solids coordinator leave arrangements: Dr. Werner-Zwanziger will be on leave without pay from the facility for a one year period (July 2014-June 2015). Dr. Margaret Hanson-Clarke, a postdoctoral fellow with Dr. Josef Zwanziger, will be employed as acting solid-state NMR coordinator on the same part-time basis during Dr. Werner-Zwanziger's absence. Dr. Hanson-Clarke and Dr. Werner-Zwanziger will be in frequent contact with regard to day-to-day operations, while Dr. Rainey will maintain oversight of Dr. Hanson-Clarke in terms of general NMR³ operations.

4. NRC NMR access issues: Unfortunately, access to the 700 MHz instrument co-purchased by Dalhousie remains sporadic and unpredictable. At present, there is a shutdown of the NRC Biological Magnetic Resonance Facility. Even data previously acquired by Dalhousie users (at significant cost) is not accessible. Ramifications of the current shutdown are significant for several Dalhousie-based NMR users and underline the need for more reliably available instrumentation with better oversight and reporting to the Dalhousie (and greater NMR³) community than is provided through intermittent access at the NRC.

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 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	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 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	^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 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 - ^1H

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

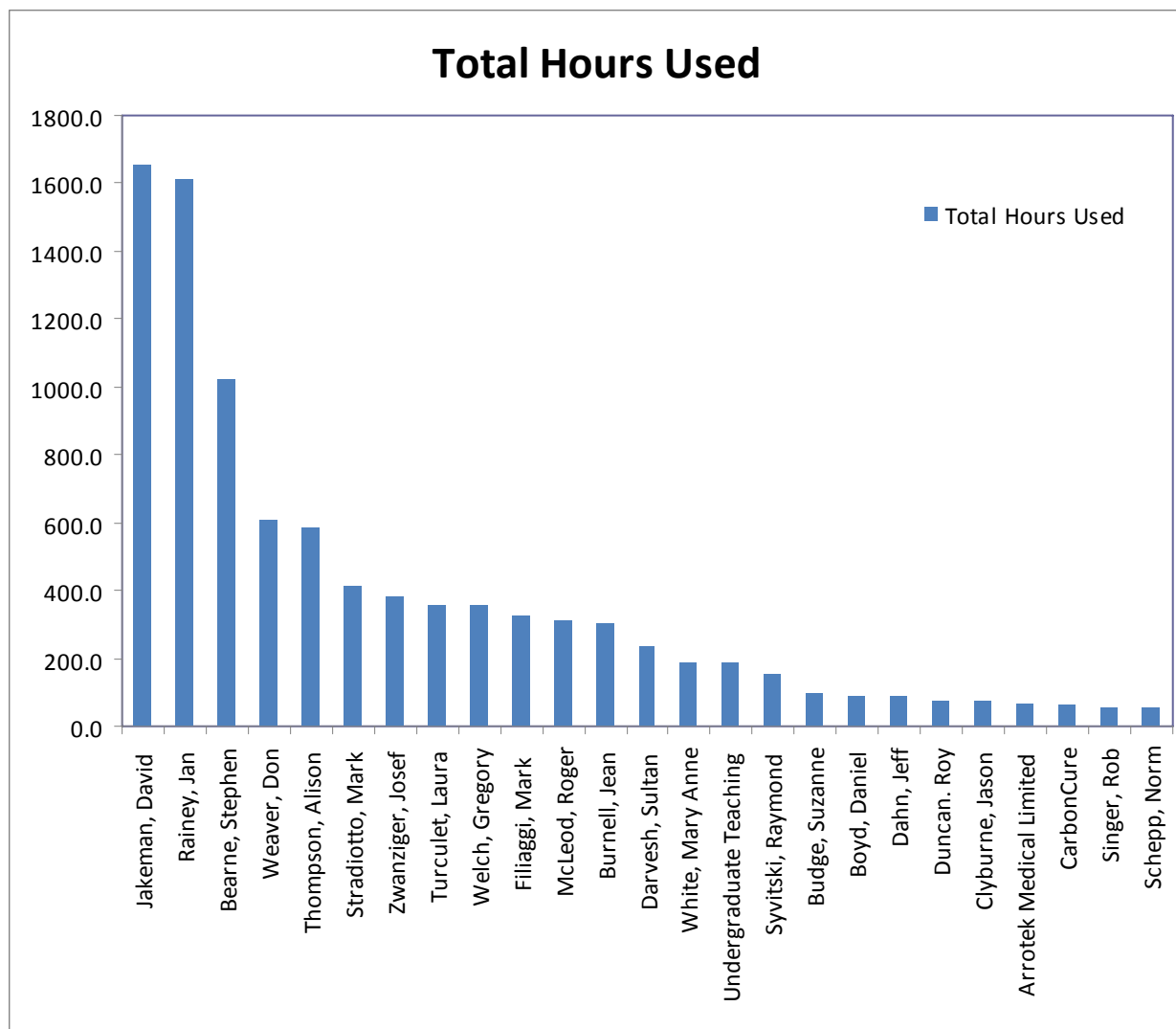
Position	Dalhousie	Supporting Maritime Institutions	Non-Supporting Maritime Institutions	Other	Government & Industry
Faculty Members	29	5	5	7	
NMR ³ Staff	2				
Instructors	5				
Research Associates	7				
Post-Docs	20	2	1		
PhD Students	32		1		
Masters Students	29	2	1		
Undergraduate Students	21	12			
Others	16	4	2		3

3.1.1 Faculty

Number	Name	Affiliation	Rank
1	Bearne, Stephen	Dalhousie University	Professor
2	Boyd, Daniel	Dalhousie University	Assistant Professor
3	Bronstein, Lyudmila	Indiana University	Professor
4	Brooks, Su-Ling	Dalhousie University	Associate Professor
5	Budge, Suzanne	Dalhousie University	Assistant Professor
6	Burford, Neil	Dalhousie University / Uvic	Professor
7	Burnell, Jean	Dalhousie University	Professor
8	Clyburne, Jason	Saint Mary's University	Professor
9	Cozens, Frances	Dalhousie University	Associate Professor
10	Dahn, Jeff	Dalhousie University	Professor
11	Darvesh, Sultan	Dalhousie University	Professor
12	Duncan, Roy	Dalhousie University	Professor
13	Filiaggi, Mark	Dalhousie University	Associate Professor
14	Ghanem, Amyl	Dalhousie University	Associate Professor
15	Grindley, Bruce	Dalhousie University	Adjunct Professor
16	Jakeman, David	Dalhousie University	Professor; NMR ³ User Group Chair
17	Jha, Amitabh	Acadia University	Professor

18	Jha, Mukund	Nipissing University	Associate Professor
19	Li, Kecheng	University of New Brunswick	Professor
20	Lin, Tong-Jun	Dalhousie University	Professor
21	MacQuarrie, Stephanie	Cape Breton University	Assistant Professor
22	Masuda, Jason	Saint Mary's University	Associate Professor
23	McFarland, Sherri	Acadia University	Professor
24	McLeod, Roger	Dalhousie University	Professor
25	Obrovac, Mark	Dalhousie University	Associate Professor
26	Pincock, James	Dalhousie University	Adjunct Professor
27	Price, Gordon	Dalhousie University	Assistant Professor
28	Pottie, Ian	Mount Saint Vincent University	Associate Professor
29	Rainey, Jan	Dalhousie University	Associate Professor; NMR ³ Director
30	Ramanathan, Vaidhya	Indian Institute of Science Educ. & Res., India	Professor
31	Rocherullé, Jean	Institut Universitaire de Technologie de Rennes, Rennes, France	Professor
32	Schepp, Norm	Dalhousie University	Associate Professor
33	Singer, Rob	Saint Mary's University	Professor
34	Stradiotto, Mark	Dalhousie University	Professor
35	Syvitski, Raymond	Dalhousie University	Adjunct Professor
36	Thompson, Alison	Dalhousie University	Professor
37	Turculet, Laura	Dalhousie University	Associate Professor
38	Udenigwe, Chibuike	Dalhousie University	Assistant Professor
39	Vaughan, Keith	Saint Mary's University	Professor
40	Weaver, Don	Dalhousie University / Toronto	Professor
41	Welch, Gregory	Dalhousie University	Assistant Professor
42	White, Mary Anne	Dalhousie University	Professor
43	White, Rob	Dalhousie University	Associate Professor
44	Wiesner, Ulrich	Cornell University, NY, USA	Professor
45	Zodrow, Erwin	Cape Breton University	Professor
46	Zwanziger, Josef	Dalhousie University	Professor

The usage profile for the heaviest user groups (top 25) 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 Instructors

Number	Name	Position
1	Aish, Gaia	Instructor
2	Aleman-Milan, Gianna	Instructor
3	Moya-Barrios, Reinaldo	Instructor
4	Padmos, Dan	Instructor
5	Whalen, Marc	Instructor

3.1.4 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	Barry, Brian	Saint Mary's University	Post-Doc
5	Bhar, Palash	Dalhousie University	Post-Doc
6	Borzenko, Andrey	Dalhousie University	Post-Doc
7	Brown, David	Mycodex Group Incorporated	Government/Industrial
8	Crawford, Sarah	Dalhousie University	Post-Doc
9	Fisher, Laural	Dalhousie University	Post-Doc
10	Garrison, David	Mount Saint Vincent University	Research Assistant
11	Ghosh, Ramprasad	Dalhousie University	Post-Doc
12	Giroux, Alexander	Dalhousie University	Volunteer Researcher
13	Hanson-Clarke, Margaret	Dalhousie University	Post-Doc
14	Hassan, Muhammad Sami	Dalhousie University	Post-Doc
15	Hawco, Cassandra	Dalhousie University	Research Assistant
16	Hilborn, Jim	Dalhousie University	Volunteer Researcher
17	Hollenhorst, Helia	Dalhousie University	Volunteer Researcher
18	Hurisso, Bitu	Saint Mary's University	Post-Doc
19	Kajetanowicz, Aleksandra	Dalhousie University	Volunteer Researcher
20	Kim, Chris	Dalhousie University	Post-Doc
21	Lobb, Kevin	Dalhousie University	Visiting Researcher
22	Lu, Erhu	Dalhousie University	Research Associate
23	MacLeod, Erin	Saint Mary's University	Research Assistant
24	MacQueen, Preston	Dalhousie University	Research Assistant
25	Marchal, Estelle	Dalhousie University	Post-Doc
26	Maughan, Ellen	Saint Mary's University	Research Assistant
27	McCahill, Jenny	Dalhousie University	Research Associate
28	McCormick, Nicole	Dalhousie University	Research Assistant
29	Miller, Kimberly	Dalhousie University	Research Assistant
30	Mohammed, Ameruddin	Dalhousie University	Post-Doc
31	Mugica, Odei	Dalhousie University	Exchange Student

32	Naidu, Ajaya	Acadia University	Post-Doc
33	Ness, Matthew	Research & Productivity Council	Government/Industrial
34	Nie, Mengyun	Dalhousie University	Post-Doc
35	Ogawa, Takahiko	Dalhousie University	Post-Doc
36	Pal, Mohan	Dalhousie University	Post-Doc
37	Paul, Nawal	Dalhousie University	Research Associate
38	Pericherla, Kasi	Acadia University	Visiting Researcher
39	Rana, Neha	Acadia University	Visiting Researcher
40	Russell, Stephanie	Dalhousie University	Visiting Researcher
41	San Juan, Ronan	Dalhousie University	Post-Doc
42	Sarker, Muzaddid	Dalhousie University	Post-Doc
43	Sawatzky, Ryan	Dalhousie University	Research Assistant
44	Schranck, Johannes	Dalhousie University	Exchange Student
45	Smithen, Deborah	Dalhousie University	Post-Doc
46	Sparavalo, Sara	Dalhousie University	Technician
47	Sun, Shengguo	Dalhousie University	Research Associate
48	Todd, Angela	Saint Mary's University	Research Assistant
49	Ullah, Zia	Dalhousie University	Post-Doc
50	Valliant, Esther	Dalhousie University	Post-Doc
51	Walton, Scott	Enovex Corporation	Government/Industrial
52	Wang, Yaohui	Dalhousie University	Post-Doc
53	Wheaton, Craig	Dalhousie University	Post-Doc
54	Wu, Fan	Dalhousie University	Research Assistant
55	Xin, Jun	Dalhousie University	Research Associate

3.2 Publications Associated with Centre (July 1, 2013 to June 30, 2014)

Peer-Reviewed Journal Articles – total 69

1. Alsabeh, P. G.; Lundgren, R. J.; McDonald, R.; Seechurn, C. C. C. J.; Colacot, T. J.; Stradiotto, M., **An Examination of the Palladium/Mor-DalPhos Catalyst System in the Context of Selective Ammonia Monoarylation at Room Temperature**. *Chem-Eur J* 2013, *19*(6), 2131-2141.
2. Alsabeh, P. G.; Stradiotto, M., **Addressing Challenges in Palladium-Catalyzed Cross-Couplings of Aryl Mesylates: Monoarylation of Ketones and Primary Alkyl Amines**. *Angew Chem Int Edit* 2013, *52*(28), 7242-7246.
3. Ambrose, K.; Hurisso, B. B.; Singer, R. D., **Recyclable ionic liquid tagged Co(salen) catalysts for the oxidation of lignin model compounds**. *Can J Chem* 2013, *91*(12), 1258-1261.
4. Beaton, S. A.; Jiang, P. M.; Melong, J. C.; Loranger, M. W.; Mohamady, S.; Veinot, T. I.; Jakeman, D. L. **The**

- effect of bisphosphonate acidity on the activity of a thymidyltransferase.** *Org Biomol Chem* 2013, *11* (33), 5473-5480.
5. Chitnis, S. S.; Burford, N.; Decken, A.; Ferguson, M. J., **Coordination Complexes of Bismuth Inflatates with Tetrahydrofuran and Diphosphine Ligands.** *Inorg Chem* 2013, *52* (12), 7242-7248.
 6. Chitnis, S. S.; Burford, N.; McDonald, R.; Ferguson, M. J., **Prototypical Phosphine Complexes of Antimony(III).** *Inorg Chem* 2014, *53* (10), 5359-5372.
 7. Chitnis, S. S.; Carpenter, Y. Y.; Burford, N.; McDonald, R.; Ferguson, M. J., **Assembly of a cyclo-Tetrastibinotetraphosphonium Tetracation by Reductive Elimination.** *Angew Chem Int Edit* 2013, *52* (18), 4863-4866.
 8. Comeau, P.; Filiaggi, M. J., **Incorporating strontium improves therapeutic potential of calcium polyphosphate delivery matrices for osteomyelitis treatment.** Proceedings of the 31st Annual Meeting of the Canadian Biomaterials Society, Halifax, June 2014. 2014.
 9. Comeau, P.; Filiaggi, M. J., **Incorporation of strontium into amorphous calcium polyphosphate matrices improves the local tuneability of vancomycin delivery.** Proceedings of the 60th Annual Meeting of the Orthopaedic Research Society, New Orleans, LA, March 2014. 2014.
 10. Crawford, S. M.; Lavery, C. B.; Stradiotto, M., **BippyPhos: A Single Ligand With Unprecedented Scope in the Buchwald-Hartwig Amination of (Hetero) aryl Chlorides.** *Chem-Eur J* 2013, *19* (49), 16760-16771.
 11. Gillis, E. A. L.; Grossert, J. S.; White, R. L., **Rearrangements Leading to Fragmentations of Hydrocinnamate and Analogous Nitrogen-Containing Anions Upon Collision-Induced Dissociation.** *J Am Soc Mass Spectr* 2014, *25* (3), 388-397.
 12. Groves, B. R.; Crawford, S. M.; Lundrigan, T.; Matta, C. F.; Sowlati-Hashjin, S.; Thompson, A., **Synthesis and characterisation of the unsubstituted dipyrin and 4,4-dichloro-4-bora-3a,4a-diaza-s-indacene: improved synthesis and functionalisation of the simplest BODIPY framework.** *Chem Commun* 2013, *49* (8), 816-818.
 13. Harroun, S. G.; Abraham, T. J.; Prudhoe, C.; Zhang, Y. T.; Scammells, P. J.; Brosseau, C. L.; Pye, C. C.; Singer, R. D., **Electrochemical surface-enhanced Raman spectroscopy (E-SERS) of novel biodegradable ionic liquids.** *Phys Chem Chem Phys* 2013, *15* (44), 19205-19212.
 14. Harty, M.; Nagar, M.; Atkinson, L.; LeGay, C. M.; Derksen, D. J.; Bearne, S. L., **Inhibition of serine and proline racemases by substrate-product analogues.** *Bioorg Med Chem Lett* 2014, *24* (1), 390-393.
 15. Hawco, C. L. A.; Marchal, E.; Uddin, M. I.; Baker, A. E. G.; Corkery, D. P.; Dellaire, G.; Thompson, A., **Synthesis and biological evaluation of prodigiosene conjugates of porphyrin, estrone and 4-hydroxytamoxifen.** *Bioorgan Med Chem* 2013, *21* (19), 5995-6002.
 16. Hemeon, I.; Durand, A.; Singer, R. D., **Houben-Weyl Methods of Molecular Transformations.** In *Science of Synthesis Silyl Zinc Reagents*, 2013; Vol. Volume 4, pp 141-149.
 17. Hendsbee, A.; Vaughan, K., **1,8,10,17-Tetraazapentacyclo[8.8.1.1(8,17).0(2,7).0(11,16)]icosane X-ray crystal structure revisited.** *J Mol Struct* 2013, *1050*, 1-4.
 18. Hendsbee, A. D.; Macaulay, C. M.; Welch, G. C., **Synthesis of an H-ggregated thiophene-phthalimide based small molecule via microwave assisted direct arylation coupling reactions.** *Dyes Pigments* 2014, *102*, 204-209.
 19. Hendsbee, A. D.; Sun, J. P.; Rutledge, L. R.; Hill, I. G.; Welch, G. C., **Electron deficient diketopyrrolopyrrole dyes for organic electronics: synthesis by direct arylation, optoelectronic characterization, and charge carrier mobility.** *J Mater Chem A* 2014, *2* (12), 4198-4207.
 20. Holthausen, M. H.; Knackstedt, D.; Burford, N.; Weigand, J. J., **Phosphenium-Insertion and Chloronium-Addition Reactions Involving the cyclo-Phosphanes (t-BuP)(n) (n=3, 4).** *Aust J Chem* 2013, *66* (10), 1155-1162.
 21. Issa, M. E.; Hall, S. R.; Dupuis, S. N.; Graham, C. L.; Jakeman, D. L.; Goralski, K. B., **Jadomycins are cytotoxic to ABCB1-, ABCC1-, and ABCG2-overexpressing MCF7 breast cancer cells.** *Anti-Cancer*

- Drug 2014, 25(3), 255-269.
22. Joenathan, A. T.; Mathews, K. L.; Wirey, M.; Beeram, S.; Werner-Zwanziger, U.; Baker, L. A.; Carini, J. P.; Bronstein, L. M., **Composite polymer electrolytes for lithium ion batteries which contain tricoordinate boron for enhanced conductivity and transference numbers**. Abstr Pap Am Chem S 2013, 246.
 23. Jollymore, C. T.; Macdonald, I. R.; Pottie, I. R.; Martin, E.; Darvesh, S., **Evaluation of a Butyrylcholinesterase Ligand, Nmethyl-4-piperidinyl-4-fluorobenzoate, for use in Human Tissues**. Alzheimer's and Dementia 2013, 9(4S), P42, P385.
 24. Kennedy, K. L.; Gibling, M. R.; Eble, C. F.; Gastaldo, R. A.; Gensel, P. G. ; Werner-Zwanziger, U.; Wilson, R. A., **Lower Devonian Coaly Shales of Northern New Brunswick, Canada: Plant Accumulations in the Early Stages of Terrestrial Colonization**. *Journal of Sedimentary Research*, 2013, 83[11-12], 1202-1215.
 25. Macdonald, I. R.; Reid, G. A.; Pottie, I. R.; Martin, E.; Darvesh, S., **Visualizing Alzheimer's Pathology with Cholinesterase Imaging Agents**. Alzheimer's and Dementia 2013, 9(4S), P32, P197.
 26. Karpichev, Y.; Jahan, N.; Paul, N.; Petropolis, C. P.; Mercer, T.; Grindley, T. B.; Marangoni, D. G., **The micellar and surface properties of a unique type of two-headed surfactant - Pentaerythritol based di-cationic surfactants**. *J Colloid Interf Sci* 2014, 423, 94-100.
 27. Kelly, C. M.; Ruddy, A. J.; Wheaton, C. A.; Sydora, O. L.; Small, B. L.; Stradiotto, M.; Turculet, L., **Synthesis, structural characterization, and reactivity of Cp*Ru(N-phosphinoamidinate) complexes**. *Can J Chem* 2014, 92(3), 194-200.
 28. Lavery, C. B.; Rotta-Loria, N. L.; McDonald, R.; Stradiotto, M., **Pd2dba3/Bippyphos: A Robust Catalyst System for the Hydroxylation of Aryl Halides with Broad Substrate Scope**. *Adv Synth Catal* 2013, 355(5), 981-987.
 29. Lefsay, A. M.; Guy, R. D.; Chatt, A.; White, R. L., **Synthesis and tandem mass spectrometry of chlorinated triacylglycerols**. *Chem Phys Lipids* 2013, 174, 55-63.
 30. Little, V. R.; Tingley, R.; Vaughan, K., **Triazene Derivatives of (1,x)-Diazacycloalkanes. Part X. Synthesis and Characterization of a series of 1,4-Di[2-aryl-1-diazenyl]-2,5-dimethylpiperazines**. *Can J Chem* 2014, 92, 665-669.
 31. Loranger, M. W.; Beaton, S. A.; Lines, K. L.; Jakeman, D. L., **Thiophosphate and thiophosphonate analogues of glucose-1-phosphate: synthesis and enzymatic activity with a thymidyltransferase**. *Carbohydr Res* 2013, 379, 43-50.
 32. Loranger, M. W.; Forget, S. M.; McCormick, N. E.; Syvitski, R. T.; Jakeman, D. L., **Synthesis and Evaluation of L-Rhamnose 1C-Phosphonates as Nucleotidyltransferase Inhibitors**. *J Org Chem* 2013, 78(19), 9822-9833.
 33. Lu, E.; Yadav, A.; Weaver, D. F.; Reed, M. A., **An Efficient Method for the Protection of Aromatic Amines with Benzostabase and Its Utility in Anionic Aromatic Transformations**. *Synlett* 2013, 24(17), 2259-2262.
 34. Lund, K. L. A. R.; Thompson, A., **Synthesis of Symmetric meso- H- Dipyrin Hydrobromides from 2-Formylpyrroles**. *Synlett* 2014, 25(8), 1142-1144.
 35. Lundrigan, T.; Cameron, T. S.; Thompson, A., **Activation and deprotection of F-BODIPYs using boron trihalides**. *Chem Commun* 2014, 50(53), 7028-7031.
 36. Ma, K; Werner-Zwanziger, U; Zwanziger, J; Wiesner, U, **Controlling Growth of Ultrasmall Sub-10 nm Fluorescent Mesoporous Silica Nanoparticles**, *Chemistry of Materials*, 25, 677-691 (2013).
 37. MacQueen, P. M.; Bach, R. A.; MacLean, C. T. P.; MacQuarrie, S. L., **Effective One-Step Synthesis of Silica Supported 1,3-Dibutylimidazolium Acetate for Carbon Dioxide Capture**. *J Phys Chem C* 2014, 118(10), 5239-5242.
 38. Marchal, E.; Smithen, D. A.; Uddin, M. I.; Robertson, A. W.; Jakeman, D. L.; Mollard, V.; Goodman, C. D.; MacDougall, K. S.; McFarland, S. A.; McFadden, G. I.; Thompson, A., **Synthesis and antimalarial activity of prodigiosenes**. *Org Biomol Chem* 2014, 12(24), 4132-4142.

39. Marchal, E.; Uddin, M. I.; Smithen, D. A.; Hawco, C. L. A.; Lanteigne, M.; Overy, D. P.; Kerr, R. G.; Thompson, A., **Antimicrobial activity of non-natural prodigiosenes**. *Rsc Adv* 2013, *3*(45), 22967-22971.
40. Mathews, K. L.; Budgin, A. M.; Beeram, S.; Joenathan, A. T.; Stein, B. D.; Werner-Zwanziger, U.; Pink, M.; Baker, L. A.; Mahmoud, W. E.; Carini, J. P.; Bronstein, L. M., **Solid polymer electrolytes which contain tricoordinate boron for enhanced conductivity and transference numbers**. *J Mater Chem A* 2013, *1*(4), 1108-1116.
41. Mitton, S. J.; McDonald, R.; Turculet, L., **Facile intramolecular silicon-carbon bond activation at Pt-O and Pt-II centers**. *Polyhedron* 2013, *52*, 750-754.
42. Momeni, A.; Filiaggi, M. J., **Synthesis and characterization of different chain length sodium polyphosphates**. *J Non-Cryst Solids* 2013, *382*, 11-17.
43. Momeni, A.; Filiaggi, M. J., **Comprehensive Study of the Chelation and Coacervation of Alkaline Earth Metals in the Presence of Sodium Polyphosphate Solution**. *Langmuir* 2014, *30*(18), 5256-5266.
44. Momeni, A.; Filiaggi, M. J., **In vitro degradation of polyphosphate gels**. *Proceedings of the 31st Annual Meeting of the Canadian Biomaterials Society, Halifax, June 2014*. 2014.
45. Momeni, A.; Filiaggi, M. J., **Rheological properties of polyphosphate gels**. *Proceedings of the 31st Annual Meeting of the Canadian Biomaterials Society, Halifax, June 2014*. 2014.
46. Murphy, L. J.; Robertson, K. N.; Harroun, S. G.; Brosseau, C. L.; Werner-Zwanziger, U.; Moilanen, J.; Tuononen, H. M.; Clyburne, J. A. C., **A Simple Complex on the Verge of Breakdown: Isolation of the Elusive Cyanofomate Ion**. *Science* 2014, *344*(6179), 75-78.
47. Nagar, M.; Lietzan, A. D.; St Maurice, M.; Bearne, S. L., **Potent Inhibition of Mandelate Racemase by a Fluorinated Substrate-Product Analogue with a Novel Binding Mode**. *Biochemistry-Us* 2014, *53*(7), 1169-1178.
48. Pal, M.; Bearne, S. L., **Inhibition of glutamate racemase by substrate-product analogues**. *Bioorg Med Chem Lett* 2014, *24*(5), 1432-1436.
49. Pandey, A.; Sarker, M.; Liu, X. Q.; Rainey, J. K., **Small expression tags enhance bacterial expression of the first three transmembrane segments of the apelin receptor**. *Biochemistry and cell biology = Biochimie et biologie cellulaire* 2014, *92*(4), 269-78.
50. Pericherla, K.; Jha, A.; Khungar, B.; Kumar, A., **Copper-Catalyzed Tandem Azide-Alkyne Cycloaddition, Ullmann Type C-N Coupling, and Intramolecular Direct Arylation**. *Org Lett* 2013, *15*(17), 4304-4307.
51. Pericherla, K.; Kumar, A.; Jha, A., **Povarov-Reductive Amination Cascade to Access 6-Aminoquinolines and Anthrazolines**. *Org Lett* 2013, *15*(16), 4078-4081.
52. Rastogi, S.; Marchal, E.; Uddin, I.; Groves, B.; Colpitts, J.; McFarland, S. A.; Davis, J. T.; Thompson, A., **Synthetic prodigiosenes and the influence of C-ring substitution on DNA cleavage, transmembrane chloride transport and basicity**. *Org Biomol Chem* 2013, *11*(23), 3834-3845.
53. Rastogi, S.; Thompson, A.; Davis, J., **Transmembrane ion transporters derived from various natural products**. *Abstr Pap Am Chem S* 2013, *246*.
54. Robertson, A. P. M.; Burford, N.; McDonald, R.; Ferguson, M. J., **Coordination Complexes of Ph₃Sb(2+) and Ph₃Bi(2+): Beyond Pnictonium Cations**. *Angew Chem Int Edit* 2014, *53*(13), 3480-3483.
55. Robertson, A. P. M.; Friedmann, J. N.; Jenkins, H. A.; Burford, N., **Exploring structural trends for complexes of Me₂E(OSO₂CF₃)(₂) (E = Si, Ge, Sn) with pyridine derivatives**. *Chem Commun* 2014, *50*(59), 7979-7981.
56. Robertson, A. P. M.; Gray, P. A.; Burford, N., **Interpnictogen Cations: Exploring New Vistas in Coordination Chemistry**. *Angew Chem Int Edit* 2014, *53*(24), 6050-6069.
57. Ruddy, A. J.; Kelly, C. M.; Crawford, S. M.; Wheaton, C. A.; Sydora, O. L.; Small, B. L.; Stradiotto, M.; Turculet, L., **(N-Phosphinoamidinate)Iron Pre-Catalysts for the Room Temperature Hydrosilylation of Carbonyl Compounds with Broad Substrate Scope at Low Loadings**. *Organometallics* 2013, *32*(19), 5581-5588.

58. Schranck, J.; Tlili, A.; Alsabeh, P. G.; Neumann, H.; Stradiotto, M.; Beller, M., **Palladium-Catalysed Carbonylative α -Arylation of Acetone and Acetophenones to 1,3-Diketones**. *Chem-Eur J* 2013, *19* (38), 12624-12628.
59. Smithen, D. A.; Forrester, A. M.; Corkery, D. P.; Dellaire, G.; Colpitts, J.; McFarland, S. A.; Berman, J. N.; Thompson, A., **Investigations regarding the utility of prodigiosenes to treat leukemia**. *Org Biomol Chem* 2013, *11* (1), 62-68.
60. Sun, J. P.; Hendsbee, A. D.; Eftaiha, A. F.; Macaulay, C.; Rutledge, L. R.; Welch, G. C.; Hill, I. G., **Phthalimide-thiophene-based conjugated organic small molecules with high electron mobility**. *J Mater Chem C* 2014, *2* (14), 2612-2621.
61. Tovstiga, T. E.; Gillis, E. A.; Grossert, J. S.; White, R. L., **Characterization of Multiple Fragmentation Pathways Initiated by Collision-induced Dissociation of Multifunctional Anions Formed by Deprotonation of 2-Nitrobenzenesulfonylglycine**. *J Mass Spectrom* 2014, *49*, 168-177.
62. Tran, T.; Jahan, N.; Marangoni, D. G.; Grindley, T. B., **Synthesis of surfactants based on pentaerythritol. II. Anionic gemini surfactants**. *Can J Chem* 2013, *91* (11), 1085-1092.
63. Twibanire, J. D. K.; Grindley, T. B., **Polyester Dendrimers: Smart Carriers for Drug Delivery**. *Polymers-Basel* 2014, *6* (1), 179-213.
64. Twibanire, J. D. K.; Huestis, M. P.; Grindley, T. B., **AB(3) building blocks for the synthesis of polyester dendrimers**. *Tetrahedron Lett* 2014, *55* (23), 3436-3439.
65. Wheaton, C. A.; Bow, J. P. J.; Stradiotto, M., **New Phosphine-Functionalized NHC Ligands: Discovery of an Effective Catalyst for the Room-Temperature Amination of Aryl Chlorides with Primary and Secondary Amines**. *Organometallics* 2013, *32* (21), 6148-6161.
66. Wheaton, C. A.; Stradiotto, M., **Probing the utility of palladium complexes supported by morpholine-functionalized N-heterocyclic carbene ligands in Buchwald-Hartwig amination**. *Can J Chem* 2013, *91* (8), 755-762.
67. Whittleton, S. R.; Boyd, R. J.; Grindley, T. B., **How Do Nucleophiles Accelerate the Reactions of Dialkylstannylene Acetals? The Effects of Adding Fluoride to Dialkoxidi-n-butylstannanes**. *J Phys Chem A* 2013, *117* (47), 12648-12657.
68. Zhang, X. F.; Werner-Zwanziger, U.; Boyd, D., **Correlation between Structural and Mechanical Properties of Zn-loaded Multi-component Borogermanate Glasses**. *Proceedings of the 12th International Conference on the Structure of Non-Crystalline Materials, Trento, Italy, 2013* 2013.
69. Zodrow, E. L.; D'Angelo, J. A.; Werner-Zwanziger, U.; Chen, B., **Hair-trichomes-files and spectrochemistry of *Macroneuropteris scheuchzeri* (Basal Cantabrian, Sydney Coalfield, Canada)** *Paleontographica, Abt. B: Palaeobotany - Paleophytology* 2014, *290* [4-6], 141-153.

3.3 Participation in relevant events for research dissemination

A total of 35 international and 106 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
--	-----------------------------

What is the number of Centre personnel who participated in domestic events?

16 international conference/symposium presentations by 9 professors	19 student presentations at the international level
Professors/Associates & Number of Events	Students & Number of Events
34 domestic conference/symposium presentations by 12 professors	72 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 2402.03: "Introductory Organic Chemistry: Reactivity of Functional Groups"

Instructors: Jean Burnell and James Pincock

Course enrollment: 298

(2) CHEM 2304.03: "Introductory Physical Chemistry II"

Instructor: Peng Zhang

Course enrollment: 59

- **3rd Year Undergraduate**

(1) BIOC 3700.03: "Biomolecular Chemistry"

Instructors: Jan Rainey and Stephen Bearne

Course enrollment: 51

(2) CHEM 3401.03: "Intermediate Organic Chemistry"

Instructor: Bruce Grindley

Course enrollment: 27

(3) CHEM 3404.03: "Intermediate Organic Chemistry: Physical Organic Chemistry and Spectroscopy"

Instructors: Fran Cozens

Course enrollment: 34

(4) CHEM 3103.03: "Intermediate Inorganic Chemistry"

Instructors: Marc Whalen

Course enrollment: 47

- **4th Year Undergraduate (cross-listed with a graduate class)**

(1) CHEM 4402.03 (cross-listed with CHEM 5402.03): "Organic Structure Determination"

Instructor: Bruce Grindley

Course enrollment: 10

- **Graduate**

(1) CHEM 6354: "Topics in Nuclear Magnetic Resonance"

Instructor: Ulrike Werner-Zwanziger

Course enrollment: 4

3.5 Student research activities related to the Centre mission statement

The following table summarizes the 98 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 33 Doctoral, 32 Masters, and 33 Undergraduate students.

	Student Name	Institution	Degree	Supervisor	Status	Thesis Title
1	Aish, Gaia	Dalhousie University	MSc	David Jakeman	Completed	The Synthesis and Enzymatic Evaluation of Biologically Relevant Sugar 1-Phosphonates
2	Alsabeh, Pamela	Dalhousie University	PhD	Mark Stradiotto	Completed	The Development of Catalysts for the Monoarylation of Ammonia and Related Challenging Cross-Coupling Reactions
3	Ambrose, Kenson	Saint Mary's University	BSc	Rob Singer	Completed	Oxidation of Lignin Model Compounds Using Ionic Liquid-Based Salen Metal Complexes
4	Baker, Alex	Dalhousie University	BSc	Alison Thompson	Completed	
5	Bates, Jamie	Dalhousie University	MSc	Fran Cozens	In-Progress	
6	Bourque, Alex	Dalhousie University	PhD	Mary Anne White	Completed	Investigations of Reversible Thermochromism in Three-Component Systems
7	Calahoo, Courtney	Dalhousie University	PhD	Joe Zwanziger	In-Progress	
8	Chisholm, Alicia	Dalhousie University	BSc	Mark Stradiotto	In-Progress	
9	Chowdhury, Barsha	Dalhousie University	BSc	Fran Cozens	In-Progress	
10	Comeau, Patricia	Dalhousie University	PhD	Mark Filiaggi	In-Progress	
11	Cook, Earl	Dalhousie University	MSc	Mark Stradiotto	In-Progress	
12	Doyle, Kirstin	Saint Mary's University	BSc	Jason Clyburne	In-Progress	

13	Fielden, Ryan	Dalhousie University	MSc	Mark Obrovac	In-Progress	
14	Forget, Stephanie	Dalhousie University	MSc	David Jakeman	In-Progress	
15	Galbraith, Justine	Dalhousie University	PhD	Joe Zwanziger	In-Progress	
16	Gong, Min	Dalhousie University	MSc	Chibuike Udenigwe	In-Progress	
17	Groves, Brandon	Dalhousie University	MSc	Alison Thompson	In-Progress	
18	Hargreaves, Breanna	Dalhousie University	BSc	Mark Stradiotto	In-Progress	
19	Harty, Matthew	Dalhousie University	MSc	Stephen Bearne	In-Progress	
20	Hendsbee, Art	Dalhousie University	MSc	Greg Welch	In-Progress	
21	Hoey, Marshall	Dalhousie University	MSc	Laura Turculet	In-Progress	
22	Huchenski, Blake	Dalhousie University	BSc	Bruce Grindley	In-Progress	
23	Ingram, Leanne	Mount Saint Vincent University	BSc	Ian Pottie	In-Progress	
24	Jaeschke, Alyssa	Mount Saint Vincent University	MSc	Ian Pottie	In-Progress	
25	Jollymore, Courtney	Dalhousie University	PhD	Sultan Darvesh	In-Progress	
26	Kelly, Colin	Dalhousie University	MSc	Laura Turculet	In-Progress	
27	Keyes, Lauren	Saint Mary's University	BSc	Jason Masuda	Completed	
28	Kilcup, Nancy	Dalhousie University	PhD	Daniel Boyd	In-Progress	
29	Kitching, Elizabeth	Dalhousie University	BSc	Greg Welch	In-Progress	
30	Lavery, Chris	Dalhousie University	PhD	Mark Stradiotto	Completed	The Development and Application of New Palladium Catalysts in Challenging C-N and C-O Bond Forming Reactions Phosphonium Ion Salen Based Derivatives for use in Catalysis
31	Lavoie, Chris	Saint Mary's University	BSc	Rob Singer	Completed	
32	LeFort, Francois	Dalhousie University	PhD	Jean Burnell	In-Progress	

33	Lefsay, Abir	Dalhousie University	PhD	Ameres Chatt	In-Progress	
34	Lindeperg, Fabien	Dalhousie University	PhD	Laura Turculet	In-Progress	
35	Loranger, Matthew	Dalhousie University	PhD	David Jakeman	Completed	The Design and Synthesis of Phosphate-Based Inhibitors of Nucleotidyl-transferases
36	Lund, Katie	Dalhousie University	MSc	Alison Thompson	In-Progress	
37	Lundrigan, Travis	Dalhousie University	PhD	Alison Thompson	In-Progress	
38	Ma, Lin	Dalhousie University	MSc	Jeff Dahn	In-Progress	
39	Macaulay, Casper	Dalhousie University	BSc	Greg Welch	Completed	The Design, Synthesis, and Characterization of Asymmetric, Truncated & Electron Deficient Small Molecule Semiconductors
40	MacDonald, Elizabeth	Dalhousie University	PhD	Neil Burford	Completed	Cationic and Dicationic Phosphine Complexes of Tin and Germanium
41	MacDonald, Ian	Dalhousie University	PhD	Sultan Darvesh	Completed	Synthesis and Evaluation of Butyrylcholinesterase Ligands for Molecular Neuroimaging
42	MacIntyre, Logan	Dalhousie University	BSc	David Jakeman	In-Progress	
43	Martinez-Farina, Camilo	Dalhousie University	MSc	David Jakeman	In-Progress	
44	McAfee, Seth	Dalhousie University	MSc	Greg Welch	In-Progress	
45	McClennan, Billy	Saint Mary's University	BSc	Jason Masuda	In-Progress	
46	McCluskey, Greg	Dalhousie University	PhD	Stephen Bearne	In-Progress	
47	McConnell, Mandy	Dalhousie University	BSc	Sultan Darvesh	Completed	Synthesis and Evaluation of Diphenyl Carbamates for Imaging Alzheimer's Disease Pathology
48	McGrath, Trevor	Saint Mary's University	BSc	Rob Singer	Completed	Ionic Organocatalysis
49	Meier-Stephenson, Felix	Dalhousie University	PhD	Donald Weaver	Completed	A New Theory of Alzheimer's Disease

50	Melanson, Jennifer	Dalhousie University	PhD	Alison Thompson	In-Progress	
51	Milosevich, Natalia	Dalhousie University	BSc	Alison Thompson	Completed	
52	Mishra, Vinayak	Dalhousie University	BSc	Mark Stradiotto	Completed	
53	Mitton, Samuel	Dalhousie University	PhD	Laura Turculet	Completed	Synthesis and Reactivity of Group 10 Silyl Pincer Complexes
54	Momeni, Arash	Dalhousie University	PhD	Mark Filiaggi	In-Progress	
55	Morash, Ben	Dalhousie University	BSc	Jan Rainey	In-Progress	
56	Morgan, Tim	Dalhousie University	PhD	Jean Burnell	In-Progress	
57	Morrison, Zachary	Dalhousie University	BSc	Stephen Bearne	In-Progress	
58	Moulins, Jonathan	Dalhousie University	PhD	Jean Burnell	Completed	Synthesis of Heterocycles via Chemoselective Geminal Acylation of Methoxyoxazolidines, E/Z Isomerization in the Metathesis of Allyl Alcohol Derivatives with a First Generation Ruthenium Catalyst, and Interception of Nazarov Reaction Intermediates of Allenyl Vinyl Ketones with Arenes Isolation and Characterization of the Elusive Cyanofomate Ion and the Dependence of its Stability on Solvent Dielectric Constant
59	Murphy, Luke	Saint Mary's University	MSc	Jason Clyburne	In-Progress	
60	Namespetra, Andrew	Dalhousie University	MSc	Greg Welch	In-Progress	
61	Naserifard, Nikrooz	Saint Mary's University	BSc	Jason Masuda	In-Progress	
62	O'Connell, Kathleen	Dalhousie University	PhD	Daniel Boyd	In-Progress	
63	Orrell, Kathleen	Dalhousie University	BSc	Jan Rainey	In-Progress	
64	Pandey, Aditya	Dalhousie University	PhD	Jan Rainey	In-Progress	

65	Paterson, Alex	Dalhousie University	MSc	Joe Zwanziger	In-Progress	
66	Patterson, Robin	Dalhousie University	MSc	Jan Rainey	In-Progress	
67	Paul, Michelle	Saint Mary's University	BSc	Rob Singer	In-Progress	
68	Payne, Abby-Jo	Dalhousie University	MSc	Greg Welch	In-Progress	
69	Pelletier, Andre	University of New Brunswick	PhD	Kecheng Li	In-Progress	
70	Periyapperuma, Kalani	Dalhousie University	MSc	Mark Obrovac	In-Progress	
71	Petibon, Remi	Dalhousie University	PhD	Jeff Dahn	In-Progress	
72	Pitman, Logan	Dalhousie University	BSc	Greg Welch	Completed	Design and Synthesis of Narrow Band Gap Small Molecules Based Upon iso-Indigo Building Blocks Using Furan, 1-Methyl-Pyole and Thiophene as Bridging Structures for Organic Solar Cells
73	Prudhoe, Christine	Saint Mary's University	BSc	Rob Singer	Completed	
74	Qin, Teng Fei	Dalhousie University	MSc	Norman Schepp	In-Progress	
75	Romao, Carl	Dalhousie University	PhD	Mary Anne White	In-Progress	
76	Reda, Alexandra	Dalhousie University	MSc	Roger McLeod	In-Progress	
77	Regan, Gemma	Dalhousie University	BSc	Stephen Bearne	In-Progress	
78	Reid, Marla	Dalhousie University	MSc	Amyl Ghanem	In-Progress	
79	Robertson, Andrew	Dalhousie University	PhD	David Jakeman	In-Progress	
80	Robinson-Enebeli, Stephen	Saint Mary's University	BSc	Jason Masuda	In-Progress	
81	Rotta-Loria, Nicolas	Dalhousie University	MSc	Mark Stradiotto	In-Progress	
82	Ruddy, Adam	Dalhousie University	PhD	Laura Turculet	In-Progress	
83	Ruzic-Gauthier, Michael	Dalhousie University	MSc	Norman Schepp	Completed	Cleavage of Duplex DNA Using Two-Excitation of N-Alkylpyridine Thiones

84	Ryan, Meaghan	Dalhousie University	BSc	Norman Schepp	Completed	
85	Sainuddin, Tariq	Acadia University	MSc	Sherri Mcfarland	In-Progress	
86	Scott, Ellie	Dalhousie University	BSc	Jan Rainey	Completed	The Expression, Purification, and Biophysical Characterization of Transmembrane Segments 1-3 of the Apelin Receptor Synthesis and Evaluation of Butyrylcholinesterase Pyridone Ligands as Molecular Imaging Agents for Alzheimer's Disease
87	Sehgal, Chandni	Dalhousie University	BSc	Sultan Darvesh	Completed	
88	Shin, Kyungsoo	Dalhousie University	PhD	Jan Rainey	In-Progress	
89	Shu, Weixi	Dalhousie University	MSc	Gordon Price	In-Progress	
90	Simms, Gordon	Dalhousie University	PhD	Donald Weaver	In-Progress	
91	Soley, Jacob	Dalhousie University	BSc	Sultan Darvesh	In-Progress	
92	Stone, Jeremy	Saint Mary's University	BSc	Jason Clyburne	In-Progress	
93	Subedi, Pankaj	Dalhousie University	MSc	Fran Cozens	In-Progress	
94	Tovstiga, Tara	Dalhousie University	MSc	Rob White	Completed	Novel Fragmentation Processes of 2-Nitrobenzenesulfonyl Amino Acid Anions
95	Tremblay, Marie	Dalhousie University	PhD	Jan Rainey	In-Progress	
96	Xia, Wei	Dalhousie University	MSc	Suzanne Budge	In-Progress	
97	Xiong, Deijun	Dalhousie University	PhD	Jeff Dahn	In-Progress	
98	Zaky, Mariam	Dalhousie University	BSc	Jean Burnell	Completed	Nazarov Cyclization Reactions of Allenyl Aryl Ketones

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 required to first attend a 1.5 h lecture on a variety of basics, including safety in an NMR laboratory, proper sample preparation, locking, shimming, etc. Attendance at the lecture and passing the concluding multiple-choice quiz is a prerequisite for getting hands-on training. 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 exception to this statement is the NMR savvy research group of Professor Jan Rainey from the Department of Biochemistry & Molecular Biology at Dalhousie. Individuals from this group have been trained to use the spectrometer themselves. Additionally, training courses are provided for researchers requesting walk-up access to the 700 MHz spectrometer using ICON-NMR and the SampleJET. Students and postdoctoral fellows from the research groups of Professors David Jakeman, Alison Thompson, Don Weaver, Stephen Bearne, and Jan Rainey 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 stem from the research group of Professors Josef Zwanziger and Jan Rainey. Their 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 University of Toronto, the University of Toronto at Mississauga, and in the School of Biomedical Engineering at Dalhousie.

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

- On August 8, 2013, Dr. Mike Lumsden was filmed in a video shoot where he demonstrated the operation of the AV-300 MHz spectrometer as well as outlining important topics associated with NMR spectrometer usage such as safety in a NMR lab, proper sample preparation techniques, etc. This video was made available to a number of undergraduate labs making use of the facility for teaching.
- On October 22, 2013, 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. **Butyrylcholinesterase ligands as diagnostic tools and treatment for diseases of the nervous system.** European Patent #2320891 (Great Britain, France and Germany), Issued November 18, 2013. Principal Inventor: Sultan Darvesh
2. **Butyrylcholinesterase ligands as diagnostic tools and treatment for diseases of the nervous system.** Hong Kong Patent # HK1157227 issued February 7, 2014. Principal Inventor: Sultan Darvesh
3. **Carbamate compounds and methods of use in diseases of the nervous system.** International Publication Number WO/2014/039526 (World Intellectual Property Organization), Issued March 13, 2014. Principal Inventor: Sultan Darvesh
4. **Silanyloxyaryl Phosphine Ligand and Uses Thereof in C-N Cross-Coupling.** PCT/CA2013/050315. Principal Inventor: Mark Stradiotto
5. **Novel Catalyst** PCT/US2011/061130 (*covers the DalPhos ligand family*). Published 26 September 2013: US 2013/0253185 A1. Principal Inventor: Mark Stradiotto
6. **Diversification of the Edaravone Structure via Palladium-Catalyzed Hydrazine Cross-Coupling with Application in Inhibiting Beta Amyloid Aggregation.** US Patent and Trademark Office Provisional Application Number 61/811,136 (filed 12 April 2013). Principal Inventor: Mark Stradiotto
7. D. Boyd used solid-state NMR to examine the effects of γ -irradiation and accelerated aging on the composition-structure-property relationships for radiopaque embolic microspheres. The microspheres in question are the basis for a new medical device company in Halifax called **ABK Biomedical** (a spin out from Dalhousie). NMR³ was crucial to advance the technology to regulatory approval and preclinical validation.
8. **Antifouling Marine Paints.** Provisional Patent filed in US Patent and Trademark Office (USPTO), March 20, 2014 application #: 61/968,305. Principal Inventor: Rob Singer (Saint Mary's University)

2. The solid-state NMR instruments have been used with five different companies in collaboration with NMR³ expert staff member Dr. Ulrike Werner-Zwanziger:

1. The Research and Productivity Council (Fredericton, NB) is using NMR³ solid-state ¹³C NMR capabilities to test processing and design of polymers.
2. ABK Biomedical Ltd. (Halifax, NS), under the leadership of Professor D. Boyd, has employed NMR³ solid-state ²⁹Si NMR for the characterization of treatments of medical glasses.
3. Together with Dr. Mark MacDonald from CARBONCURE (Halifax, NS), Dr. Ulrike Werner-Zwanziger investigated the possibility to characterize the form of carbon captured by solid-state NMR.
4. Together with Enovex (Saint John, New Brunswick), Dr. Werner-Zwanziger applied ¹³C solid state NMR to proprietary materials.
5. For the Mycodev Group Inc. (Fredericton, New Brunswick) Dr. Ulrike Werner-Zwanziger applied ¹³C solid state NMR to proprietary materials.

3. Dr. Jan Rainey has continued collaborating with Toronto-based Vive Crop Protection (initially via an NESRC Engage Grant, in follow up by grant-in-aid funding from Vive) to investigate their primary nanoparticle product (AllosperserTM nanoparticles) by NMR spectroscopy. In the past reporting year, new experiments and data analysis were carried out providing exciting insight into the actual chemistry involved in Allosperser formation, fundamental knowledge not previously available to Vive. Based on these new findings, there is strong potential for a follow up collaborative research grant.

3.8 Other Activities related to Knowledge Exchange or Mobilization

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, 2013 – March 31, 2014)

4.1 2013-2014 Financial Report

Financial support in '13-'14 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 15% and the University 85% of the Coordinator's full salary and benefits. Also, the facility paid 35% of the Solid-State NMR Coordinator's salary with the remainder being paid through CRC funding. Other direct costs of the facility this past FY included magnet cryogenics, 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)			
	Academics @ Dal & Supporting Institutions¹	Academics @ Non-Supporting Institutions¹	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 2	See Footnote 2

Liquids Service Fees (per Sample)		
	All Academics	Government/Industry
AV-300 & AV-500	\$10.00	\$50.00
AV III 700	\$15.00	See Footnote 2

Solids Hourly Rates: All Instruments			
	Academics @ Dal & Supporting Institutions¹	Academics @ Non-Supporting Institutions¹	Government/Industry
Hands-On / Collaborative³	\$6.50	\$11.50	\$65.00
Service	\$10.00	\$17.25	\$100.00

Additional Charges			
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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 ⁴	\$10 per Sample
Preparing High Resolution NMR Samples ⁵	\$10 per Sample
Processing NMR Spectra ⁶	\$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 Details concerning the classification of Supporting vs Non-Supporting Institutions is available from NMR³. 2 All non-Dalhousie users must approach BMRB staff directly to determine fees and access to the AV III 700 instrument. 3 These rates assume either independent hands-on usage or collaborative usage with Dr. Werner-Zwanziger being co-author if level of contribution merits. 4 This fee applies to both hands-on/collaborative as well as service samples. 5 Deuterated solvent costs are not included in this service. 6 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 previous reporting period, a number of fee changes were implemented:

- For the AV-300 autosampler, the standard usage rate was reduced for a limited time in order to encourage increased usage of this relatively new piece of equipment.
- Also for the AV-300 autosampler, a priority rate (double the standard usage rate) was introduced to allow a given researcher to "jump to the front of the line" of the automation queue.
- The model for billing high-resolution NMR service work was modified during the current reporting period. The old model of a higher hourly rate for magnet time was abandoned in favor of implementing a per sample fee for all high-resolution NMR service work. Consequently, high-resolution NMR magnet time is billed at the same hourly rate regardless of whether the experimentation is performed hands-on (the researcher uses the equipment and obtains the data him/herself) or as a service (data is acquired by a NMR³ staff member).
- The rate for AV-III 700 MHz usage was changed to \$10.63 per hour, regardless of experiment length. The previous two-tier rate structure for short vs. long experiments was discontinued.
- In the solid-state NMR lab, a \$10 per sample fee was incorporated to help offset the rising costs of solid-state NMR consumables.

Note that for both liquid and solid-state NMR hands-on usage, non-Dal academics have the possibility of paying the lower Dal academic rate providing their institution supports NMR³. Any academic institution outside of Dalhousie can become classified as an NMR³ Supporting Institution by paying a flat-rate annual fee of \$500 to support NMR³ costs. Payment entitles any academic user from that institution to perform hands-on use of NMR³ facilities at the Dalhousie rate for the remainder of the

current fiscal year. Note that during the current FY, the \$500 support fee was paid by Mount Saint Vincent University and St. Mary's University.

4.2 Grants directly related to the mission statement of NMR³ and awarded within the 2013-2014 Fiscal Year

In total, **\$1,528,776 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 two reporting periods (since beginning to report aggregate grant funding, an additional **>\$9.9-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

Principal Applicant: **Roy Duncan**

- CIHR - Operating Grant: "Membrane curvature sensors, inducers and microdomains in reovirus-mediated syncytium formation." (\$145,851/year; 5 years)

Principal Applicant: **Greg Welch**

- NSERC - Engage Grant: "Synthesis of organic polymers and oligomers relevant to the electronics industry using silica supported palladium heterogeneous catalysts." (\$25,000 for 1 year)
- Next Energy Technologies-Industrial Grant: "Design and synthesis of new organic materials to improve the thermal and chemical stability of organic solar cells." (\$100,000 for 18 months)

Principal Applicant: **Mark Stradiotto**

- NSERC - Discovery Grant: "Advancing Late Metal Catalysis: DalPhos Ligand Design, Mechanism, and New Reactivity" (\$84,000/year; 5 years)
- Chevron Phillips Chemical Company: "Application of Proprietary Phosphinoamidates in Catalysis" (\$70,000 USD for 1 year, 50% in collaboration with Laura Turculet)

Principal Applicant: **Jan Rainey**

- Nova Scotia Health Research Foundation: "Scotia Support Grant". (\$25,000/year; 2 years; 50% in collaboration with R. Duncan)
- NSERC - Research Tools and Instruments Grant: "A Total Internal Reflection Fluorescence (TIRF) Microscope for the Maritimes."(\$53,522)

Principal Applicant: **Raymond Syvitski**

- MITACS - Accelerate Grant: "NMR characterization of amyloid beta peptide interactions with lead compound. (\$45,000 for 1 year, with V. Ewart)

Principal Applicant: **Sultan Darvesh**

- Brain Repair Centre - Knowledge Translation Grant: "Butyrylcholinesterase Neuroimaging Ligands for Early and Definitive Diagnosis of Alzheimer's Disease." (\$29,999 for 1 year, with S. Beyea, C. Bowen.)

Principal Applicant: **Bruce Grindley**

- Green Centre Canada - Proof of Principle Grant: "Gemini Synthesis New Process Improvements" (\$6000 for 1 year)

Grants Awarded to NMR³ External Users

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

- CBU Research Project (RP) Grant: "New Ionic Liquid-Modified Mesoporous Silicas as Recyclable Materials for L-Proline Catalyzed Aldol Reaction." (\$8000 for 1 year)