

NUCLEAR MAGNETIC RESONANCE RESEARCH RESOURCE

2012 – 2013 Annual Report

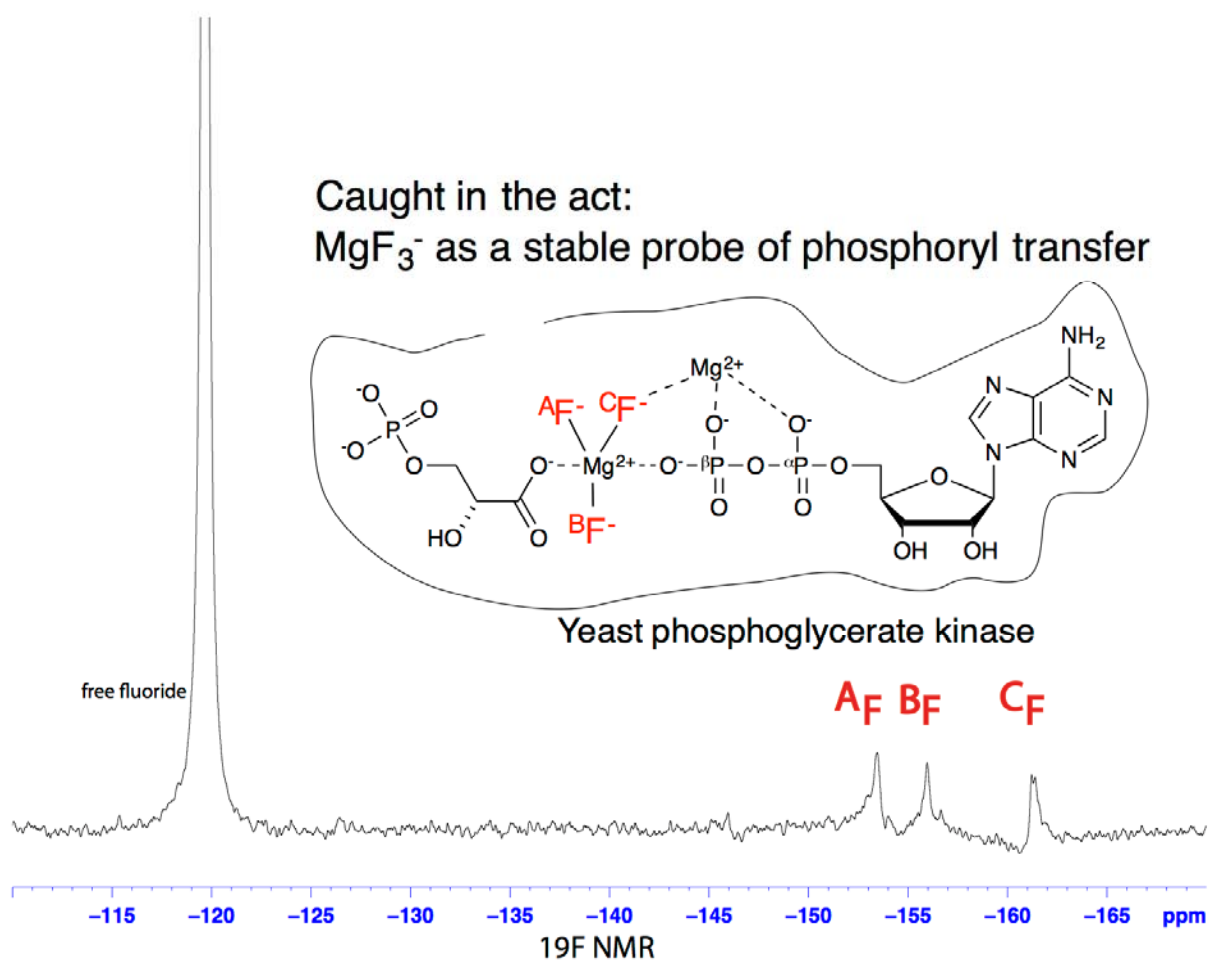


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About the cover: Caught in the Act: phosphoryl transfer is a ubiquitous process within biological systems for cell survival and communication. Using ¹⁹F NMR spectroscopy we demonstrate that the yeast glycolytic enzyme phosphoglycerate kinase invokes a trigonal bipyramidal transition state of phosphoryl transfer through the observation of a stable magnesium trifluoride complex. Authors: Nicole E. McCormick, Michael D. Lumsden, David L. Jakeman.

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 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, and facility maintenance. 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 2012-2013, the Centre assisted 42 research groups mostly drawn from the Atlantic Canada region but also including several international researchers, resulting in 58 publications, 150 conference presentations and 155 highly qualified personnel trained. Furthermore, teaching in the Department of Chemistry was supported in 4 undergraduate laboratories with 172 students, providing exposure to both the practical aspects of NMR spectroscopy and the nuances of data analysis. In total, use of the Centre's 4 NMR instruments was just over 9000 hours, with ~7483 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 *\$6.7-million in new external grant funds awarded* in the 2012-2013 fiscal year.

Using input from the NMR³ Centre staff (Dr. Jan Rainey, Director and Associate Professor in Biochemistry & Molecular and Chemistry; Dr. Mike Lumsden, Facility Coordinator; and, Dr. Ulli 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. Upgrade of 500 MHz high-resolution spectrometer: In the 2011 competition, an NSERC application for \$149,999 was awarded to a group of 6 NMR³ Users in the Research Tools and Instruments grant competition. This grant provided funds to upgrade our main solution-state NMR workhorse, the 500 MHz spectrometer, with a Bruker 5mm BBFO 500 MHz SmartProbe. This probe is a recent and innovative addition to the Bruker family of probes and offers marked increases in sensitivity, water suppression, and flexibility compared to the older BBO probe technology. Of particular interest is the ease of obtaining double resonance NMR data involving ¹⁹F and ¹H nuclei. For example, both ¹⁹F{¹H} experiments as well as ¹H{¹⁹F} experiments can be performed trivially (no recabling required) with this probehead. As part of this grant, an upgrade of the spectrometer (its "shim coils") was required to support installation of the SmartProbe. Delivery, instrument upgrade and installation occurred in December, 2012. The SmartProbe provides improved capabilities not only for routine instrument use (i.e. the default instrument configuration) but also provides new capabilities. In particular, observation of the ¹⁹F nucleus is made possible and this has already led to a rise in instrument use for non-routine bookings.

2. Decommissioning of AC 250 MHz - With the acquisition of our AV 300 MHz, which enjoyed its first full year of use in 2011-2012, usage of the older and less capable AC 250 MHz dwindled to almost zero. Our analysis of usage vs. upkeep costs (primarily keeping it filled with liquid nitrogen and helium cryogenics) indicated that this instrument was no longer sustainable. We therefore negotiated with Bruker Canada, Ltd. to decommission this and use it as a trade-in credit towards purchase of an autosampler for the 300 MHz spectrometer (item 1.2.3, below). In this decommissioning, we were careful to ensure that no capabilities were lost by carefully migrating capabilities such as low-temperature experiments over to the 300 MHz spectrometer and working with the primary users of these features to ensure that their research productivity was maintained.

3. Upgrading of Avance 300 MHz - The NMR³ Centre partnered with the Department of Chemistry (through allocation of teaching funds) to purchase an autosampler for the 300 MHz spectrometer, subsidized in small part by the trade in of our 250 MHz spectrometer (item 1.2.2, above). The 300

MHz was heavily used in daytime hours, but practically unused on evenings, overnight or weekends. Our intention is to facilitate rectifying of this disparate usage profile with the autosampler, allowing experiments to be queued up and configured to run all night. Currently, it is configured to run 1-2 overnight slots per week and is enjoying increased usage. Its function is quite similar to the autosampler on our 500 MHz instrument, meaning that users can be trained to use both instruments without implementation of entirely separate training programs. For teaching purposes, this will also allow very efficient use of the 300 MHz instrument.

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.

2. Explore ongoing support for facility staff salaries: We currently benefit from a strong level of support for the NMR³ facility from Dalhousie University in the form of partial salary support for our two PhD-level staff. Without these staff, the facility would cease to be functional and the major infrastructure housed within the facility would not be readily useable by the numerous research groups and trainees that depend upon them. The salary support we receive was cut at the beginning of the last Fiscal Year and is due to be cut again at the end of the present fiscal year, a situation which will lead to revenue recovery from other means - most notably, through increased user-fees from operating grants which are already stretched thin in many instances. While historically NMR³ was funded by NSERC, the cuts and changes to the Major Resources Support program make this impossible - even much larger national-level NMR facilities are now unable to obtain funding through these programs. CIHR has also stopped funding facilities such as NMR³. While we certainly keep on top of current funding opportunities, the only grant-oriented opportunity we are aware of that may provide some operating funding for NMR³ would be Infrastructure Operating Funds associated with a major CFI grant. Such a grant would require Dalhousie to prioritize upgrading and expansion of our NMR facilities, thus allowing this to proceed to the national competition. Even were this the case, however, the time frame of application and subsequent finalization is such that sustainability of the NMR³ usage profile is still in jeopardy the short term due to the impending funding cut to the facility by Dalhousie. In order to continue supporting our user-base optimally, including ensuring the *national competitiveness* for NSERC Discovery Grant or CIHR Operating Grant funding in terms of budgeting at a reasonable level for NMR spectroscopy aspects of researchers' programs, we will be seeking to both clarify the rationale for the cut to support that is upcoming and to look for means to rectify this. A major note is that while we appear to have a healthy surplus of funds, the major proportion of these funds have been earmarked by the NMR³ User Group as an emergency buffer in case of NMR magnet quenching. (Should a magnet quench, we would incur costs on the order \$10's of thousands to restore it to service - loss of any of our magnets from service would be catastrophic and majorly disruptive to the 42 research groups that rely on our facility.)

3. Dr. Ulrike Werner-Zwanziger will hold an NMR-class in the winter term. This class will emphasise the fundamental spin interactions, and will focus on solid-state NMR and its applications to Material Science. This class is targeted at the graduate and advanced undergraduate level of various faculties.

Section 2 - Centre Resources and Capabilities

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

Bruker/Tecmag AC - 250 MHz: Liquids Only**		
Magnet	Oxford 250/54 mm	
Console	Bruker AC with a Tecmag upgrade to a DSpect-F12 Data Acquisition System	
Channel 1	Broadband Transmitter	
Channel 2	¹ H and ¹⁹ F	
Probe 1	5mm QNP probe	Observe: ¹³ C, ³¹ P, ¹⁹ F/ decouple: ¹ H, switchable under software control
Temperature Control	B-VT1000	Includes a 25L liquid N ₂ dewar and an evaporator for generation of cold N ₂ gas.
Workstation	Dell Optiplex GX260 (Pentium 4) operating with Windows XP Pro SP2	
Spectrometer Software	NTNMR (Tecmag, Version 2.3.4 Build 30919)	

**Instrument decommissioned April 3, 2013.

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: ^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	

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

	positions. Equipped with a cooling option to cool samples down to 4°C.
Workstation	HP xw4600 operating with Red Hat Enterprise Linux (Release 4)
Spectrometer Software	TopSpin 2.1 pl4

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

Bruker DSX 400 MHz: Solids Only		
Magnet	Buker 400/89 UltraShield	
Console	Bruker Avance DSX	
Channels 1-3	Broadband Transmitter	
Probe 1	2.5mm MAS	^{69}Ga - ^{31}P / ^{19}F - ^1H
Probe 2	4mm HXY MAS	in dual mode: 45MHz - ^{31}P / ^1H Insert Pairs for X/Y (triple) mode: $^{31}\text{P}/^{11}\text{B}$, $^{31}\text{P}/^{27}\text{Al}$, $^{11}\text{B}/^{13}\text{C}$, $^{13}\text{C}/^{195}\text{Pt}$, $^{23}\text{Na}/^{29}\text{Si}$, $^6\text{Li}/^{29}\text{Si}$
Probe 3	4mm MAS	^{13}C - ^{31}P / ^{19}F - ^1H
Probe 4	7mm	^{15}N - ^{31}P / ^{19}F - ^1H
Probe 5	HP wideline probe	^{109}Ag - ^{31}P , high temperature design
Workstation	Silicon Graphics O ² operating with IRIX 6.3	
Spectrometer Software	XWIN-NMR 3.6 pl6	

AVANCE 700 MHz: Solids Only		
Magnet	Buker 700/54 UltraShield	
Console	Bruker Avance	
Channels 1-3	Broadband Transmitter	
Probe 1	2.5mm MAS	^{13}C - ^{31}P / ^{19}F - ^1H
Probe 2	4mm MAS	^{15}N - ^{13}C / ^{19}F - ^1H , ^{43}Ca
TriGamma™ Probe	3.2mm MAS	^{15}N - $^{29}\text{Si}/^{11}\text{B}$ - $^{31}\text{P}/^1\text{H}$
Triple Resonance Probe	4mm MAS	$^{29}\text{Si}/^{11}\text{B}/^1\text{H}$
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 , $^{47,49}\text{Ti}$, ^{89}Y , ^{87}Sr / ^{19}F - ^1H ,
EFREE Probe (contact Jan Rainey, if you are interested in using this probe).	5mm static solenoid	HCN/P
Workstation	Dell (Pentium) operating with RedHat Linux	
Spectrometer Software	XWIN-NMR 3.6 pl6	

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	27	6	4	5	
NMR ³ Staff	2				
Instructors	5				
Research Associates	4		1		
Post-Docs	16	2	2		
PhD Students	25				
Masters Students	21	3	1	1	
Undergraduate Students	31	16	4	1	
Others	14	9	2		2

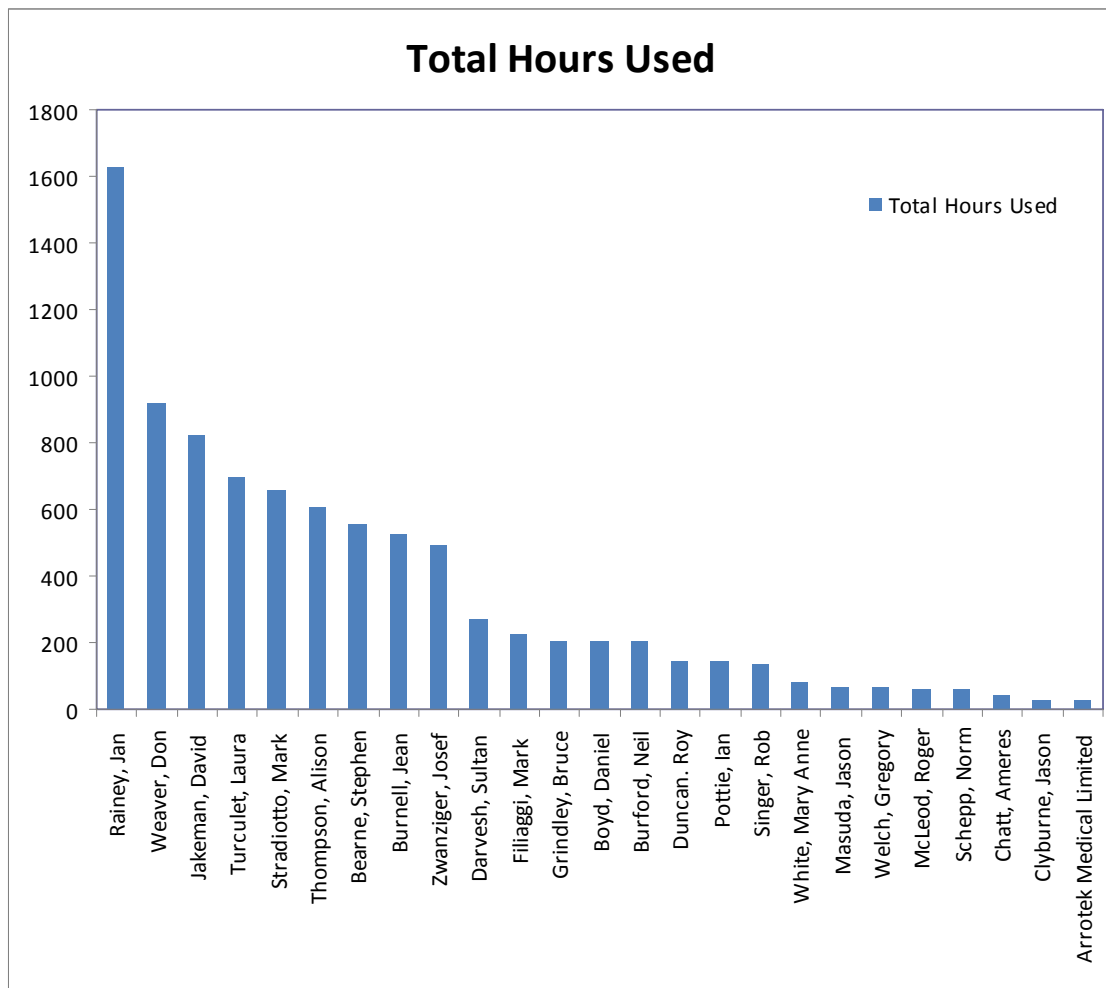
3.1.1 Faculty

Number	Name	Affiliation	Rank
1	Bearne, Stephen	Dalhousie University	Professor
2	Boyd, Daniel	Dalhousie University	Assistant Professor
3	Budge, Suzanne	Dalhousie University	Assistant Professor
4	Burford, Neil	Dalhousie University / UVIC	Professor
5	Burnell, Jean	Dalhousie University	Professor
6	Chatt, Ameres	Dalhousie University	Adjunct Professor
7	Clyburne, Jason	Saint Mary's University	Professor
8	Cozens, Frances	Dalhousie University	Associate Professor
9	Dahn, Jeff	Dalhousie University	Professor
10	Darvesh, Sultan	Dalhousie University	Professor
11	Duncan, Roy	Dalhousie University	Professor
12	Etkin, Nola	University of Prince Edward Island	Professor
13	Filiaggi, Mark	Dalhousie University	Associate Professor
14	Ghanem, Amyl	Dalhousie University	Associate Professor
15	Grindley, Bruce	Dalhousie University	Adjunct Professor
16	Hamam, Fayez	Taif University, Kingdom of Saudia Arabia	Assistant Professor
17	Jakeman, David	Dalhousie University	Professor; NMR ³ User Group Chair

18	Jha, Amitabh	Acadia University	Professor
19	Lin, Tong-Jun	Dalhousie University	Professor
20	MacQuarrie, Stephanie	Cape Breton University	Assistant Professor
21	Masuda, Jason	Saint Mary's University	Associate Professor
22	McLeod, Roger	Dalhousie University	Professor
23	Pottie, Ian	Mount Saint Vincent University	Associate Professor
24	Rainey, Jan	Dalhousie University	Associate Professor; NMR ³ Director
25	Rocherulle, Jean	Institut Universitaire de Technologie de Rennes, Rennes, France	Professor
26	Rupasinghe, Vasantha	Dalhousie University	Associate Professor
27	Sah, Ajay K.	Birla Institute of Technology & Science, Pilani, India	Assistant Professor
28	Schepp, Norm	Dalhousie University	Associate Professor
29	Singer, Rob	Saint Mary's University	Professor
30	Stradiotto, Mark	Dalhousie University	Professor
31	Thompson, Alison	Dalhousie University	Professor
32	Turculet, Laura	Dalhousie University	Associate Professor
33	Vaughan, Keith	Saint Mary's University	Professor
34	Vidovic, Drasko	Nanyang Technological University, Singapore	Professor
35	Weaver, Don	Dalhousie University	Professor
36	Welch, Gregory	Dalhousie University	Assistant Professor
37	Westcott, Steve	Mount Allison University	Professor
38	White, Mary Anne	Dalhousie University	Professor
39	White, Rob	Dalhousie University	Associate Professor
40	Wiesner, Ulrich	Cornell University, NY, USA	Professor
41	Xia, Aibing	Mount Saint Vincent University	Associate Professor
42	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	Aleman-Milan, Gianna	Instructor
2	McCahill, Jenny	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	Alharbi, Fayrooz	Dalhousie University	Volunteer Researcher

2	Barry, Brian	Saint Mary's University	Post-Doc
3	Bhar, Palash	Dalhousie University	Post-Doc
4	Bhattasali, Debabrata	Dalhousie University	Post-Doc
5	Clement, Helen	Dalhousie University	Research Assistant
6	Crain, Sheila	Institute for Marine Biosciences	Gov/Industrial Scientist
7	Crawford, Sarah	Dalhousie University	Post-Doc
8	Dodd, Angela	Saint Mary's University	Visiting Researcher
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	Gomez, Alwyn	Saint Mary's University	Research Assistant
14	Harjani, Jitendra	Saint Mary's University	Research Assistant
15	Hassan, Sami	Dalhousie University	Post-Doc
16	Hawco, Cassandra	Dalhousie University	Research Assistant
17	Houlihan, Pat	Saint Mary's University	Research Assistant
18	Hurisso, Bitu	Saint Mary's University	Post-Doc
19	Jahan, Nusrat	Dalhousie University	Volunteer Researcher
20	Kajetanowicz, Aleksandra	Dalhousie University	Volunteer Researcher
21	Krebs, Maria	Saint Mary's University	Visiting Researcher
22	Lefsay, Abir	Dalhousie University	Post-Doc
23	Lu, Erhu	Dalhousie University	Research Associate
24	MacLeod, Erin	Saint Mary's University	Research Assistant
25	Marchal, Estelle	Dalhousie University	Post-Doc
26	Maughan, Ellen	Saint Mary's University	Research Assistant
27	McCormick, Nicole	Dalhousie University	Research Assistant
28	McGrath, Alaina	Dalhousie University	Research Assistant
29	Miller, Kimberly	Dalhousie University	Research Assistant
30	Mohammed, Ameruddin	Dalhousie University	Post-Doc
31	Naidu, Ajaya	Acadia University	Post-Doc
32	Pal, Mohan	Dalhousie University	Post-Doc
33	Paul, Nawal	Dalhousie University	Research Associate
34	Pericherla, Kasi	Acadia University	Visiting Researcher
35	Qi, Yuxin	Dalhousie University	Volunteer Researcher
36	Ramsaywack, Sharwatie	Mount Allison University	Post-Doc

37	Rana, Neha	Acadia University	Visiting Researcher
38	Russell, Stephanie	Dalhousie University	Visiting Researcher
39	Sarker, Muzaddid	Dalhousie University	Post-Doc
40	Schranck, Johannes	Dalhousie University	Exchange Student
41	Seto, Leslie	Dalhousie University	Technician
42	Smithen, Deborah	Dalhousie University	Post-Doc
43	Srinivasan, Priya	University de Moncton	Research Associate
44	Suarez, Erick	OceanNutrition	Gov/Industrial Scientist
45	Sun, Shengguo	Dalhousie University	Research Associate
46	Todd, Angela	Saint Mary's University	Research Assistant
47	Ullah, Zia	Dalhousie University	Post-Doc
48	Valliant, Esther	Dalhousie University	Post-Doc
49	Wheaton, Craig	Dalhousie University	Post-Doc
50	Wu, Fan	Dalhousie University	Research Assistant
51	Xin, Jun	Dalhousie University	Research Associate
52	Zhang, Xiaofang	Dalhousie University	Post-Doc

3.2 Publications Associated with Centre (July 1, 2012 to June 30, 2013)

Peer-reviewed Journal Articles – total 58:

1. Alsabeh, PG; Lundgren, RJ; McDonald, R; Seechurn, CCCJ; Colacot, TJ; Stradiotto, M, **An Examination of the Palladium/Mor-DalPhos Catalyst System in the Context of Selective Ammonia Monoarylation at Room Temperature**, Chemistry-A European Journal, 19, 2131-2141 (2013).
2. Alsabeh, PG; Stradiotto, M; Neumann, H; Beller, M, **Aminocarbonylation of (Hetero)aryl Bromides with Ammonia and Amines using a Palladium/DalPhos Catalyst System**, Advanced Synthesis & Catalysis, 354, 3065-3070 (2012).
3. Beaton, SA; Jiang, PM; Melong, JC; Loranger, MW; Mohamady, S; Veinot, TI; Jakeman, DL, **The Effect of Bisphosphonate Acidity on the Activity of A Thymidyltransferase**, Organic and Biomolecular Chemistry, 11, 5473-5480 (2013).
4. Boudreau, J; Courtemanche, MA; Marx, VM; Burnell, DJ; Fontaine, FG, **Ambiphilic molecules for trapping reactive intermediates: interrupted Nazarov reaction of allenyl vinyl ketones with Me₂PCH₂AlMe₂**, Chemical Communications, 48, 11250-11252 (2012).
5. Chenu, S; Werner-Zwanziger, U; Calahoo, C; Zwanziger, JW, **Structure and properties of NaPO₃-ZnO-Nb₂O₅-Al₂O₃ glasses**, Journal of Non-Crystalline Solids, 358, 1795-1805 (2012).
6. Chitnis, SS; Burford, N; Ferguson, MJ, **2,2-Bipyridine Complexes of Antimony: Sequential Fluoride Ion Abstraction from SbF₃ by Exploiting the Fluoride Ion Affinity of Me₃Si⁺**, Angewandte Chemie-International Edition, 52, 2042-2045 (2013).

7. Chitnis, SS; Carpenter, YY; Burford, N; McDonald, R; Ferguson, MJ, **Assembly of a cyclo-Tetrastibinotetraphosphonium Tetracation by Reductive Elimination**, *Angewandte Chemie-International Edition*, 52, 4863-4866 (2013).
8. Chitnis, SS; MacDonald, E; Burford, N; Werner-Zwanziger, U; McDonald, R, **P-P Menschutkin preparation of prototypical phosphinophosphonium salts**, *Chemical Communications*, 48, 7359-7361 (2012).
9. Crawford, SM; Alsabeh, PG; Stradiotto, M, **Palladium-Catalyzed Mono-alpha-arylation of Carbonyl-Containing Compounds with Aryl Halides using DalPhos Ligands**, *European Journal of Organic Chemistry*, 6042-6050 (2012).
10. Darvesh, S, **Butyrylcholinesterase radioligands to image Alzheimer's disease brain**, *Chemico-Biological Interactions*, 203, 354-357 (2013).
11. Donath, M; Conrad, E; Jerabek, P; Frenking, G; Frohlich, R; Burford, N; Weigand, JJ, **Ligand-Stabilized [P4]2+ Cations**, *Angewandte Chemie-International Edition*, 51, 2964-2967 (2012).
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3.3 Participation in relevant events for research dissemination

A total of 38 international and 112 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
	21 international conference/symposium presentations by 14 professors & 1 NMR ³ staff member.	17 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
	32 domestic conference/symposium presentations by 14 professors	80 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: 256

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

Instructor: Peng Zhang

Course enrollment: 63

- **3rd Year Undergraduate**

(1) BIOC 3700.03: "Biomolecular Chemistry"

Instructors: Jan Rainey and Stephen Bearne

Course enrollment: 43

(2) CHEM 3401.03: "Intermediate Organic Chemistry"

Instructor: Norm Schepp
Course enrollment: 30

(3) CHEM 3404.03: "Intermediate Organic Chemistry: Physical Organic Chemistry and Spectroscopy"
Instructors: Fran Cozens and Norm Schepp
Course enrollment: 29

(4) CHEM 3103.03: "Intermediate Inorganic Chemistry"
Instructors: Marc Whalen
Course enrollment: 50

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

(1) BIOC 4702.03 / CHEM 4602.03: "Biophysical Characterization of Macromolecules"

Instructor: Jan Rainey

Course enrollment: 2 in BIOC 4702, 4 in CHEM 4602; also offered as BIOC 5702 and CHEM 5702 - no graduate enrollment in 2012-2013.

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

Instructor: Bruce Grindley

Course enrollment: 11

3.5 Student research activities related to the Centre mission statement

The following table summarizes the 103 student researchers who relied upon the NMR³ facility for progress in their research programs during the 2012-2013 reporting period. The table is made up of 25 Doctoral, 26 Masters, and 52 Undergraduate students.

	Student Name	Institution	Degree	Supervisor	Status	Thesis Title
1	Abdelkhalik, Ashraf	Acadia University	MSc	Amitabh Jha	In-Progress	
2	Aish, Gaia	Dalhousie University	MSc	David Jakeman	In-Progress	
3	Alfareed, Ahmed	Saint Mary's University	BSc	Jason Masuda	Left	
4	Alsabeh, Pamela	Dalhousie University	PhD	Mark Stradiotto	In-Progress	
5	Ambrose, Kenson	Saint Mary's University	BSc	Rob Singer	In-Progress	
6	Ardagh, Giselle	Dalhousie University	BSc	Jean Burnell	Left	
7	Bach, Ryan	Cape Breton University	BSc	Stephanie MacQuarrie	In-Progress	
8	Baker, Alex	Dalhousie University	BSc	Alison Thompson	Completed	Tin (IV) Chloride as a New Reagent for the Deprotection of Benzyl Esters

9	Bates, Jamie	Dalhousie University	BSc	Fran Cozens	Completed	The Solvent Effects on the Single-Photon Absorption of a Benzoxadiazole Derivative: A Preliminary Study for Two-photon Absorption Analysis
10	Blair, Amber	Saint Mary's University	BSc	Jason Masuda	Left	
11	Bourque, Alex	Dalhousie University	PhD	Mary Anne White	In-Progress	
12	Bouwhuis, Rachel	McMaster University	BSc	Rob White	Left	
13	Bow, Jean-Paul	Dalhousie University	BSc	Mark Stradiotto	Completed	Design of New N-Heterocyclic Carbene/Phosphine Ligands for use in Palladium-Catalyzed Cross-Coupling Reactions
14	Calahoo, Courtney	Dalhousie University	PhD	Joe Zwanziger	In-Progress	
15	Chowdhury, Barsha	Dalhousie University	BSc	Fran Cozens	In-Progress	
16	Comeau, Patricia	Dalhousie University	PhD	Mark Filiaggi	In-Progress	
17	Cook, Earl	Dalhousie University	MSc	Mark Stradiotto	In-Progress	
18	Corcoran, Shawna	Cape Breton University	BSc	Stephanie MacQuarrie	In-Progress	
19	D'Arcy, Duncan	Dalhousie University	BSc	Sultan Darvesh	Left	
20	Dickey, Brett	Dalhousie University	MSc	Daniel Boyd	In-Progress	
21	Doyle, Kirstin	Saint Mary's University	BSc	Jason Clyburne	Left	
22	Doyle, Lauren	Dalhousie University	BSc	Laura Turculet	Left	
23	Forget, Stephanie	Dalhousie University	MSc	David Jakeman	In-Progress	
24	Gallant, Chris	Dalhousie University	BSc	Laura Turculet	Left	
25	Groves, Brandon	Dalhousie University	MSc	Alison Thompson	In-Progress	Competitive Inhibition of <i>Schizosaccharomyces pombe</i> Serine Racemase by α -Hydroxymethylserine
26	Harty, Matthew	Dalhousie University	BSc	Stephen Bearne	Completed	

27	Hendsbee, Art	Dalhousie University	MSc	Greg Welch	In-Progress	
28	Hollenhorst, Helia	Dalhousie University	BSc	Alison Thompson	In-Progress	
29	Ingram, Leanne	Mount Saint Vincent University	BSc	Sultan Darvesh	Left	
30	Jaeschke, Alyssa	Mount Saint Vincent University	MSc	Ian Pottie	In-Progress	
31	Jollymore, Courtney	Mount Saint Vincent University	MSc	Ian Pottie	In-Progress	
32	Kelly, Colin	Dalhousie University	MSc	Laura Turculet	In-Progress	
33	Keyes, Lauren	Saint Mary's University	BSc	Jason Masuda	Completed	Zirconocene Derivatives for Dehydrocoupling of Acetylenes and Carbene-Phosphinidene Adducts and their Metal Complexes
34	Khalyapin, Ilya	Dalhousie University	BSc	Donald Weaver	Completed	
35	Khanal, Mandar	Dalhousie University	MSc	Stephen Bearne	Completed	Inhibition of the Prostate Cancer Biomarker Methylacetyl-coa Racemase (Amacr) by Novel Substrate-Product Analogues
36	Kilcup, Nancy	Dalhousie University	PhD	Daniel Boyd	In-Progress	
37	Kitching, Elizabeth	Dalhousie University	BSc	Greg Welch	In-Progress	
38	Lavery, Chris	Dalhousie University	PhD	Mark Stradiotto	In-Progress	
39	Lavoie, Chris	Saint Mary's University	BSc	Rob Singer	In-Progress	
40	LeFort, Francois	Dalhousie University	PhD	Jean Burnell	In-Progress	
41	Loranger, Matthew	Dalhousie University	PhD	David Jakeman	In-Progress	
42	Lundrigan, Travis	Dalhousie University	PhD	Alison Thompson	In-Progress	
43	Macaulay, Casper	Dalhousie University	BSc	Greg Welch	In-Progress	
44	MacDonald, Elizabeth	Dalhousie University	PhD	Neil Burford	In-Progress	
45	MacDonald, Ian	Dalhousie University	PhD	Sultan Darvesh	In-Progress	

46	MacLean, Mark	Dalhousie University	MSc	Mark Stradiotto	Completed	Rational Structural Diversification and Application of DalPhos Ligands for use in Challenging C-N Cross-Coupling Reactions
47	MacQueen, Preston	Cape Breton University	BSc	Stephanie MacQuarrie	In-Progress	
48	Makramalla, Miller	Saint Mary's University	BSc	Jason Clyburne	Left	
49	Martinez-Farina, Camilo	Dalhousie University	MSc	David Jakeman	In-Progress	
50	McAfee, Seth	Dalhousie University	MSc	Greg Welch	In-Progress	Synthesis of a Linker-Arm Version of <i>Borrelia burgdorferi</i> Glycolipid 1, an Antigenic Glycolipid in Lyme Disease
51	McClennan, Billy	Saint Mary's University	BSc	Jason Masuda	In-Progress	
52	McDonald, Rory	Dalhousie University	BSc	Bruce Grindley	Completed	
53	McGrath, Trevor	Saint Mary's University	BSc	Rob Singer	In-Progress	
54	Meier-Stephenson, Felix	Dalhousie University	PhD	Donald Weaver	In-Progress	Synthetic Methodology for the Preparation of Prodigiosenes Modified at the B-ring
55	Melanson, Jennifer	Dalhousie University	PhD	Alison Thompson	In-Progress	
56	Milosevich, Natalia	Dalhousie University	BSc	Alison Thompson	Completed	
57	Mishra, Vinyak	Dalhousie University	BSc	Jean Burnell	Left	
58	Mitton, Samuel	Dalhousie University	PhD	Laura Turculet	In-Progress	Rhodium and Iridium Pincer Complexes Supported by Bis(phosphino)silyl Ligation: Applications in Bond Cleavage Chemistry
59	Momeni, Arash	Dalhousie University	PhD	Mark Filiaggi	In-Progress	
60	Morgan, Erin	Dalhousie University	PhD	Laura Turculet	Completed	
61	Morgan, Tim	Dalhousie University	PhD	Jean Burnell	In-Progress	
62	Moulins, Jonathan	Dalhousie University	PhD	Jean Burnell	In-Progress	
63	Murphy, Luke	Saint Mary's University	MSc	Jason Clyburne	In-Progress	

64	Murrell, Emily	Dalhousie University	BSc	Jean Burnell	Completed	Trapping of the Cationic Intermediate of the Nazarov Reaction by Pyrrole and by Thiophenes
65	Naserifard, Nikrooz	Saint Mary's University	BSc	Jason Masuda	In-Progress	
66	Orrell, Kathleen	Dalhousie University	BSc	Jan Rainey	In-Progress	
67	Patterson, Robin	Dalhousie University	BSc	Bruce Grindley	Completed	Synthesis of a Glycolipid as a Possible Vaccine for Lyme Disease
68	Paul, Michelle	Saint Mary's University	BSc	Rob Singer	In-Progress	
69	Payne, Abby	Dalhousie University	BSc	Greg Welch	Left	
70	Pettipas, Shauna	Dalhousie University	BSc	Mark Stradiotto	Left	
71	Prudhoe, Christine	Saint Mary's University	BSc	Rob Singer	Completed	Phosphonium Ionic Liquid Based Salen Ligands for use in Catalysis
72	Qin, Teng Fei	Dalhousie University	BSc	Norman Schepp	Completed	Synthesis and Photochemistry of 7-Methyl-4-Nitrobenzofurazan
73	Rashid, Ahmed	Dalhousie University	BSc	Stephen Bearne	Completed	Synthesis of Thioesters using Methyl Acetyl Phosphate in Aqueous Conditions
74	Reda, Alexandra	Dalhousie University	MSc	Roger McLeod	In-Progress	
75	Reid, Marla	Dalhousie University	MSc	Amyl Ghanem	In-Progress	
76	Robertson, Andrew	Dalhousie University	PhD	David Jakeman	In-Progress	
77	Robinson-Enebeli, Stephen	Saint Mary's University	BSc	Jason Masuda	In-Progress	
78	Rock, Chris	University of Prince Edward Island	BSc	Nola Etkin	Completed	
79	Romao, Carl	Dalhousie University	PhD	Mary Anne White	In-Progress	
80	Rotta-Loria, Nicolas	Dalhousie University	BSc	Mark Stradiotto	Completed	Synthesis and Application of a New Series of P,O-DalPhos Ligands For Use in Transition Metal-Catalyzed Bond Forming Reactions

81	Roy, Alexander	Dalhousie University	MSc	Stephen Bearne	Completed	Catalysis by Extremozymes: Comparing Orotidine-Monophosphate Decarboxylases from Psychrophiles, Mesophiles, and Thermophiles
82	Ruddy, Adam	Dalhousie University	PhD	Laura Turculet	In-Progress	
83	Ruzic-Gauthier, Michael	Dalhousie University	MSc	Norman Schepp	In-Progress	
84	Ryan, Meaghan	Dalhousie University	BSc	Norman Schepp	Completed	Synthesis and Characterization of Two-Photon Absorbing Push-Pull Organic Chromophores.
85	Sehgal, Chandni	Dalhousie University	BSc	Sultan Darvesh	Left	
86	Simms, Gordon	Dalhousie University	PhD	Donald Weaver	In-Progress	
87	Soley, Jacob	Dalhousie University	BSc	Sultan Darvesh	Completed	
88	Soni, Kiran	Bilra Institute Tech & Science	MSc	Ajay Sah	In-Progress	
89	Sparavalo, Sara	Dalhousie University	BSc	Jan Rainey	Completed	Synthesis of a Recombinant Collagen-Mimetic Peptide (Gly-Pro-Pro) by <i>Escherichia coli</i> Expression Systems
90	Stone, Jeremy	Saint Mary's University	BSc	Jason Clyburne	In-Progress	
91	Subedi, Pankaj	Dalhousie University	MSc	Fran Cozens	In-Progress	
92	Sudan, Sudansu	Dalhousie University	MSc	Vasanth Rupasinghe	Completed	Antiproliferative Properties of Acylated Derivatives of Quercetin-3-O-Glucoside
93	Timm, Matthew	Mount Saint Vincent University	BSc	Ian Pottie	Completed	
94	Toulany, Amir	Dalhousie University	BSc	Fran Cozens	Left	
95	Tovstiga, Tara	Dalhousie University	MSc	Rob White	In-Progress	
96	Tremblay, Marie	Dalhousie University	PhD	Jan Rainey	In-Progress	

97	Twibanire, Jean D'Amour K.	Dalhousie University	PhD	Bruce Grindley	Completed	Synthesis of Novel Types of Polyester Glycodendrimers and the Development and Applications of an Efficient Alternative to Multistep Regioselective Esterification in Diols and Polyols
98	Vuailat, Guillaume	Dalhousie University	BSc	Greg Welch	Completed	Quinoxaline-Based Small Molecules and Polymers for Plastic Solar Cells
99	Warden, Hunter	Dalhousie University	BSc	Jean Burnell	Completed	Acid-Mediated 6- π Electrocyclization to Form a Seven- Membered Ring Antioxidant and Cytoprotective Properties of Long Chain Fatty Acid Acyated Flavonoids
100	Warnakulasuriya, Sumudu	Dalhousie University	MSc	Vasanth Rupasinghe	Completed	
101	Weale, Mike	Dalhousie University	MSc	Laura Turculet	Left	
102	Xia, Wei	Dalhousie University	MSc	Suzanne Budge	In- Progress	
103	Xiong, Deijun	Dalhousie University	PhD	Jeff Dahn	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 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 McMaster University (Hamilton, ON), the Hospital for Sick Children (Toronto, ON), the National High Magnetic Field Laboratory at Florida State University (Tallahassee, USA), Université Laval (Québec, QC) and the University of Oxford (Oxford, UK).

3. NMR³ facility staff occasionally conduct tours of the facility for visitors, typically high school groups and/or first year university science students. On March 27, 2013, Dr. Mike Lumsden hosted a group of ~ 20 1st year Dalhousie Chemistry students and explained/demonstrated the basic principles of high-resolution NMR spectroscopy.

3.7 Technology Development, patent or commercialization activities

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

1. **Radiopaque Embolic Agents.** Published 02.08.2012. Publication number: WO/2012/101524.
Principal Inventor: Daniel Boyd

2. **Carbamate Compounds and Methods of use in Diseases of the Nervous System.** US provisional patent application Serial No. 61/697,114 filed Sept 5, 2012. Principal Inventor: Sultan Darvesh
3. **Phenothiazine Compounds and Methods of use in Diseases of the Nervous System.** Provisional patent application Serial No. 61/736,146 filed December 12, 2012. Principal Inventor: Sultan Darvesh
4. **Long Chain Polyphosphate Embolic Composition.** U.S. Patent Application No. 61/722,422 filed November 5, 2012. Principal Inventor: Mark Filiaggi
5. **Silanyloxyaryl Phosphine Ligand and Uses Thereof in C-N Cross-Coupling.** PCT/CA2013/050315 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. **Anticancer Therapeutic Effect of Acylated Derivatives of Phloridzin.** Provisional US patent filing. Principal Inventor: Vasantha Rupasinghe
8. **Compositions and Methods of Treating Amyloid Disease.** Principal Inventor: Don Weaver
 - US patent 8,420,640 issued Apr 16, 2013
 - New Zealand patent 591896 issued Jul 2, 2013
 - National phase in Feb 2011 (application numbers in parentheses):
 Canada (2735158) - examination not yet requested
 European Patent Office (09810663) - grant intended; waiting for grant pub & validation
 Israel (211425) - OA response filed
 Australia (2009285591) - examination requested
 Japan (2011525235) - examination requested
 Hong Kong (1111728.3) - grant intended; will pay issue fee upon UK validation at EPO
 China (200980138688) - OA response filed
9. **Compounds and Methods of Treating Amyloid Disease.** Principal Inventor: Don Weaver
 - US provisional patent application 61/448,969 filed Mar 3, 2011
 - International patent application PCT/US12/27399 filed Mar 2, 2012
 - National phase in Sep 2013 (application numbers in parentheses): US (14/002,031), Canada (TBD)
10. **Benzofurazan Compounds and Methods.** Principal Inventor: Don Weaver
 - US provisional patent application 61/693,011 filed Aug 24, 2012
 - International patent application PCT/US13/56220, filed Aug 22, 2013
11. **Antioxidant Inhibitors of Amyloid Aggregation.** Principal Inventor: Don Weaver
 - US provisional patent application 61/811,136 filed Apr 12, 2013
12. **Antimicrobial/adjvant compounds and methods.** Principal Inventor: Don Weaver
 - US provisional patent application 61/448,682 filed Mar 3, 2011
 - International patent application PCT/CA2012/050130 filed Mar 2, 2012
 - National phase Sep 2013: pending in US, Canada (31 month deadline Oct 2013 will include pending in EPO, Japan, Korea, China, India, South Africa, Australia, New Zealand, and Hong Kong)

The NMR³ facilities were central to the Don Weaver lab's focus on the design and development of new chemical entities for the treatment of Alzheimer's disease (AD). In the past two years, this group has synthesized and characterized 320 new chemical entities as putative therapeutics for AD. The NMR

facilities were central to the characterization of these compounds. The activities of these compounds resulted in the Weaver lab receiving a \$4.7M grant from the Wellcome-Trust. Once these agents were produced in Weaver's academic lab, they were ultimately transferred to Treventis Corp, a start-up biotech company. Thus, the NMR³ has been important in the development of new agents that led to knowledge translation and commercialization.

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

1. The Research and Productivity Council (Fredicton, NB) is using our 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 our 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 soild-state NMR

3 Dr. Ulrike Werner-Zwanziger presented solid-state NMR capabilities at the "Nova Scotia CLEANTECH & MATERIALS Industry Research Connector" on April 30, 2013. This workshop was organized by Kevin Buchan - Dalhousie, Richard Isnor - NSERC, Lauren MacDonald - ACOA, and Jeff Stockhausen - NRC-IRAP. It offered industries and academic researcher the possibility to highlight industrial research interests and to outline academic research capabilities. Representatives of several research funding and economic development agencies, including ACOA, NRC-IRAP, MITACS, and NSERDT were also present. This workshop lead to one industrial collaboration between NMR³ and CARBONCURE (3 of 3.7).

Dr. Ulrike Werner-Zwanziger also attended the Ocean Industry Show Case, but no contacts involving NMR were formed during this event.

4. Dr. Jan Rainey continued a collaboration initiated by an NSERC Engage Grant with Toronto-based Vive Crop Protection to investigate their primary nanoparticle product by NMR spectroscopy. Experiments were performed by a postdoctoral fellow (Dr. Muzaddid Sarker) and had academically-oriented goals, so this did not result in industrial user fees. Instead, this resulted in a grant-in-aid to Dr. Rainey's group and cost-recovery for the University in the form of the associated overhead.

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. 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, 2012 – March 31, 2013)

4.1 2012-2013 Financial Report

Financial support in '12-'13 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 during the 2012/2013 FY were unchanged from the previous year and are provided below.

Liquids Hourly Rates: Hands-On Usage			
	Academics @ Dal & Supporting Institutions¹	Academics @ Non-Supporting Institutions¹	Government/Industry
Tecmag/AC 250	\$4.50	\$20.00	\$65.00
AV 300	\$4.50	\$20.00	\$65.00
AV 500	\$5.50	\$24.00	\$130.00
AV III 700	\$9.00/\$29.00 ²	See Footnote 3	See Footnote 3

Liquids Hourly Rates: Service			
	Dal Academics	Non-Dal Academics	Government/Industry
Tecmag/AC 250	\$6.75	\$30.00	\$100.00
AV 300	\$6.75	\$30.00	\$100.00
AV 500	\$8.25	\$36.00	\$200.00
AV III 700	\$13.50/\$33.50 ²	See Footnote 3	See Footnote 3

Solids Hourly Rates: All Instruments			
	Academics @ Dal & Supporting Institutions¹	Academics @ Non-Supporting Institutions¹	Government/Industry
Hands-On / Collaborative⁴	\$6.50	\$11.50	\$65.00
Service	\$10.00	\$17.25	\$100.00

Additional Charges	
Service	Charge
Packing Rotors for Solid-State NMR	\$10 per Rotor
Packing Air-Sensitive Samples for Solid-State NMR	\$50 per Rotor
Preparing High Resolution NMR Samples ⁵	\$10 per Sample
Processing NMR Spectra ⁶	\$10/\$20 per Experiment
Nonroutine Processing Requests (i.e. lineshape fits, simulations, predictions)	\$10 per Experiment
Structural Assignments / Spectral Interpretation / Literature Searches	\$50 per Hour

1 Details concerning the classification of Supporting vs Non-Supporting Institutions is available from NMR³. 2 Short runs (< 4 hours ; up to 30% of Dal's time) are charged at \$29 per hour and long runs at \$9 per hour (up to 70% of Dal's time). 3 All non-Dalhousie users must approach BMRF staff directly to determine fees and access to the AV III 700 instrument. 4 These rates assume either independent hands-on usage or collaborative usage with Dr. Werner-Zwanziger being co-author if level of contribution merits. 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

For liquids NMR service work (data acquired by a NMR³ staff member), note that a clear distinction in fees is made between Dalhousie and non-Dalhousie academics, with the latter paying a significantly higher amount. However, for both hands-on liquids usage (the researcher uses the equipment and obtains the data him/herself) and solid-state NMR 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 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 by St. Mary's University in the previous FY but extending to the end of the current FY.

4.2 Grants directly related to the mission statement of NMR³ and awarded within the 2012-2013 Fiscal Year

In total, **\$6,736,580 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. Users from other Nova Scotia universities also identified \$443,994 in grant funds awarded in the 2012-2013 Fiscal Year with the same type of reliance upon and/or budgeting for use of the NMR³ Centre. 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.

Grants Awarded to Dalhousie-Based Users

Principal Applicant: **Sultan Darvesh**

- Dalhousie Medical Research Foundation - Equipment Grant. "Radio-TLC or radio-HPLC system for detection and purification of radiotracers for diagnosis and treatment of Alzheimer disease and multiple sclerosis." (\$24,504; 1 year)
- CIHR - Operating Grant. "Butyrylcholinesterase Ligands as Potential Radiopharmaceuticals for Brain Imaging in Dementia." (\$129,297/year; 3 years)
- CDHA - Research Fund Grant. "A pilot study to evaluate butyrylcholinesterase radioligands as molecular imaging agents for multiple sclerosis." (\$14,999; 1 year)
- Multiple Sclerosis Society of Canada - endMS Summer Research Assistantship Grant. "Synthesis and evaluation of butyrylcholinesterase pyridone ligands as molecular imaging agent for Multiple sclerosis." (\$5,000; 1 year)

Principal Applicant: **David Jakeman**

- CIHR - Operating Grant. "Rhamnose biosynthesis: alternative antibacterial targets" (\$146,284/year, 3 years)

Principal Applicant: **Jan Rainey**

- Dalhousie Medical Research Foundation - Equipment Grant. "Time-resolved fluorescence spectroscopy instrumentation to characterize intermolecular interactions, catalysis, protein folding and metabolic processes." (\$29,817/year; 1 year)
- National High Magnetic Field Laboratory (Tallahassee, USA) - Magnet Time & Travel Support. "Solid-state NMR characterization of recombinant spider wrapping silk." (5 days of 600 MHz instrument time = \$780 at NMR3 hourly rate; \$1200 in travel support)
- Vive Crop Protection - Grant in Aid. "Follow-up on NSERC Engage Grant." (\$1,260 including overhead; 1 year)

Principal Applicant: **Mark Stradiotto**

- Springboard Atlantic - Innovation Mobilization Program Award. "Phosphino silyl ether ligands for metal-catalyzed cross-coupling catalysis" (\$20,000; 1 year)
- GreenCentre - Proof-of-Principle Grant. "Phosphino silyl ether ligands for metal-catalyzed cross-coupling catalysis." (\$20,000; 1 year)

Principal Applicant: **Alison Thompson**

- NSERC - Research Tools & Instruments. "Inert Atmosphere Thin-Film Deposition Systems for the Fabrication of Organic Films and Devices via Solution and Thermal Evaporation Techniques." (\$149,583; 1 year)
- NSHRF - Development Grant. "Development of Innovative Models and Inhibitors of Enzymes Along the Heme Synthetic Pathway." (\$15,000; 1 year)

Principal Applicant: **Laura Turculet**

- Chevron Philips Chemical Company. "Application of Proprietary Phosphinoamidates in Iron-catalyzed Hydrosilylation (Turculet L. & Stradiotto M.; \$45,000 USD)
- NSERC - Discovery Grant. "Harnessing the Unusual Reactivity of Transition Metal Complexes Supported by Multidentate Silyl and Phosphido Ligands." (\$45,000/year; 5 years)

Principal Applicant: **Don Weaver**

- Wellcome-Trust-UK. "Design and Optimisation of New Chemical Entities that Prevent the Neurotoxic Oligomerization and Misfolding of both β -amyloid and tau Proteins: A Disease Modifying Therapeutics Approach for Alzheimer's Dementia." (\$4,687,824 over three years)

Principal Applicant: **Greg Welch**

- NSERC - Discovery Grant. "Development of Soluble Small Molecules for use in Plastic Solar Cells" (\$35,000/year; 5 years)

Principal Applicant: **Josef Zwanziger**

- NSERC - Discovery Grant. "Structure/Property Correlations in Inorganic Glasses." (\$99,000/year; 5 years)

Grants Awarded to NMR³ Users at Supporting Institutions

Principal Applicant: **Rob Singer**

- CFI - LOF. "New 300 MHZ NMR" (with Jason Masuda and Jason Clyburne; \$429,468; 1 year)
- St. Mary's University Faculty of Graduate Studies and Research. "Task Specific Ionic Liquids." (\$2000/year, 2 years)
- Springboard Atlantic. "Green Formulation for Antifouling Marine Paint" (\$10,526; 1 year)