

NUCLEAR MAGNETIC RESONANCE RESEARCH RESOURCE

2011 – 2012 Annual Report

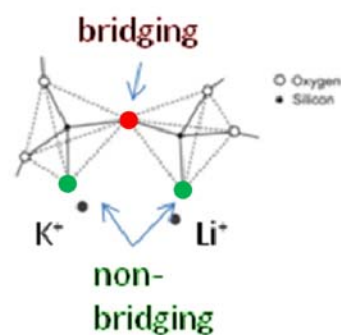
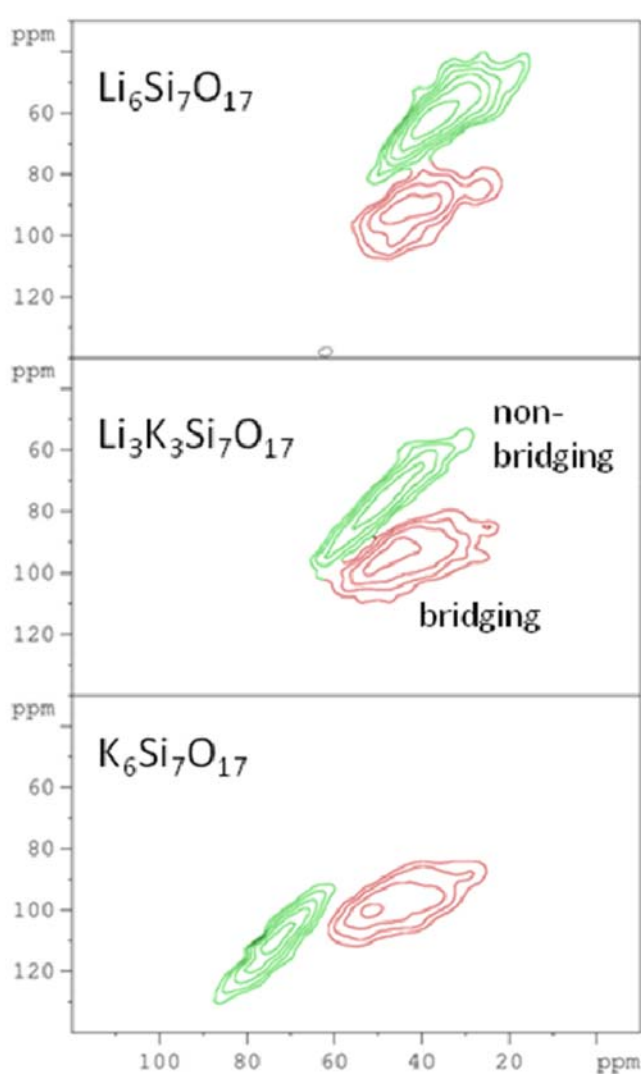


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About the cover: The spectra show ¹⁷O solid state NMR results on modified silicate glasses by Courtney Calahoo, Dr. Ulrike Werner-Zwanziger and Professor Josef Zwanziger. The glass composition has a pronounced influence on the position of the non-bridging oxygen nuclei in the vicinity of the lithium or potassium.

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 5 NMR spectrometers with a variety of capabilities, ranging from 250 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 2011-2012, the Centre assisted 39 research groups from a variety of locations throughout the Atlantic region, Canada, and North America, resulting in over 55 publications and nearly 150 highly qualified personnel trained. Furthermore, teaching in the Department of Chemistry was supported in 4 undergraduate laboratories with 175 students, 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 exceeded 8500 hours. The vast majority of instrument use was logged in experiments configured by trainees in support of externally funded research grants for Dalhousie University researchers. Perhaps the most concrete illustration of the critical and valuable nature of the services provided by our Centre is the fact that Dalhousie-based researchers identified NMR³ access as being essential in over *\$3.2-million in new external grant funds awarded* in the 2011-2012 fiscal year.

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. *NSERC RTI Award for 500 MHz Bruker SmartProbe:* An NSERC application for \$149,999 was awarded to a group of 6 NMR³ Users in the 2011 Research Tools and Instruments grant competition. This grant provides 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. This will arrive in the coming year, with more detail of our plans described in Section 1.3.1.

2. *User fee restructuring:* The shift in funding for NMR³ away from NSERC funding and towards an increased proportion of non-user fee income from Dalhousie University spurred us to reconsider the user fee model. Previously, all academic users paid one rate, regardless of home institution. We have modified the fee structure (detailed in Section 4.1) to better reflect the level of our income which comes from Dalhousie University in the form of salary support for our Facility Managers vs. for user fees. Essentially, users from other academic institutions may request that their institution pay an annual fee to become a "Supporting Institution" of the NMR³ Facility. This fee is reflective of both the historical level of usage by that institution and of the percentage of our revenue which comes from Dalhousie. Users at Supporting Institutions then pay identical hourly rates to Dalhousie users; those at other institutions pay full cost-recovery rates. Beyond academic users, NMR³ did not previously have a separate rate for users based at government laboratories, with these users paying academic rates. Other Canadian NMR facilities typically charge a rate more reflective of cost-recovery for government users, and we therefore similarly modified our fee structure. These changes in fee structure mean that Dalhousie University funds to NMR³ are not being used to subsidize use of the Centre by non-Dalhousie users.

1.3 Upcoming Year's Activity

1. *Upgrade of 500 MHz spectrometer and SmartProbe installation:* As described in Section 1.2.1, a major infrastructure award through the NSERC Research Tools & Instruments grant program has provided funds for an outstanding improvement for our 500 MHz spectrometer. As part of this grant, an upgrade of the spectrometer (its "shim coils") is required to support installation of the SmartProbe. Delivery, instrument upgrade and installation are expected in late-fall of 2012 or early-winter of 2013. Upon installation and thorough testing by the NMR³ Staff, outreach to the NMR³ user community will take place. We will fully publicize the new capabilities of our 500 MHz instrument and make users aware of the exciting new experimental possibilities. For the majority of users, there will be no visible change to the way in which they set up experiments, making a fully seamless transition. For users who want to take advantage of the new capabilities of the SmartProbe over and above our existing infrastructure, training will be performed on an individual basis by Staff member Dr. Mike Lumsden, with the level of intensity in training dependent upon the specific needs of the research group.

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 has dwindled to almost zero. Our analysis of usage vs. upkeep costs (primarily keeping it filled with liquid nitrogen and helium cryogenics) indicates that this instrument is no longer sustainable. We have therefore negotiated with Bruker Canada, Ltd. to decommission this and use it as a trade in for credit towards purchase of an autosampler for the 300 MHz spectrometer (item 1.3.3, below).

3. *Upgrading of Avance 300 MHz* - The NMR³ Centre has 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 1.3.2, above). The 300 MHz is currently heavily used in daytime hours, but practically unused on evenings, overnight or weekends. The autosampler will rectify this disparate usage profile, allowing experiments to be queued up and configured to run all night. This, in turn, will provide additional user fee revenue from the 300 MHz, allowing recovery of our expenditure (~\$21,755, taken from our currently healthy operating account, see Section 4.1) for the autosampler. Modest additional usage of the 300 MHz for 4.5 hours per day at the current rate of \$4.50 per hour would, for example, repay the expense of the autosampler in less than 3 years. Its function will be quite similar to the existing autosampler on our 500 MHz instrument, meaning that most users will already be trained to use the new infrastructure without implementation of a new training program.

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/ dec.: 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)	

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 / dec.: ¹ H, z gradient coil and auto-tune / match accessory (ATMA)
Temperature Control	B-VT 3200	Includes a 25L liquid N ₂ dewar.
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	Observe: ¹⁴ N - ³¹ P / dec.: ¹ H z gradient coil and auto-tune / match accessory (ATMA)

Probe 2	5 mm TXI	Observe: ^1H / dec.: ^{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 pl4	

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 Biodegradation 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

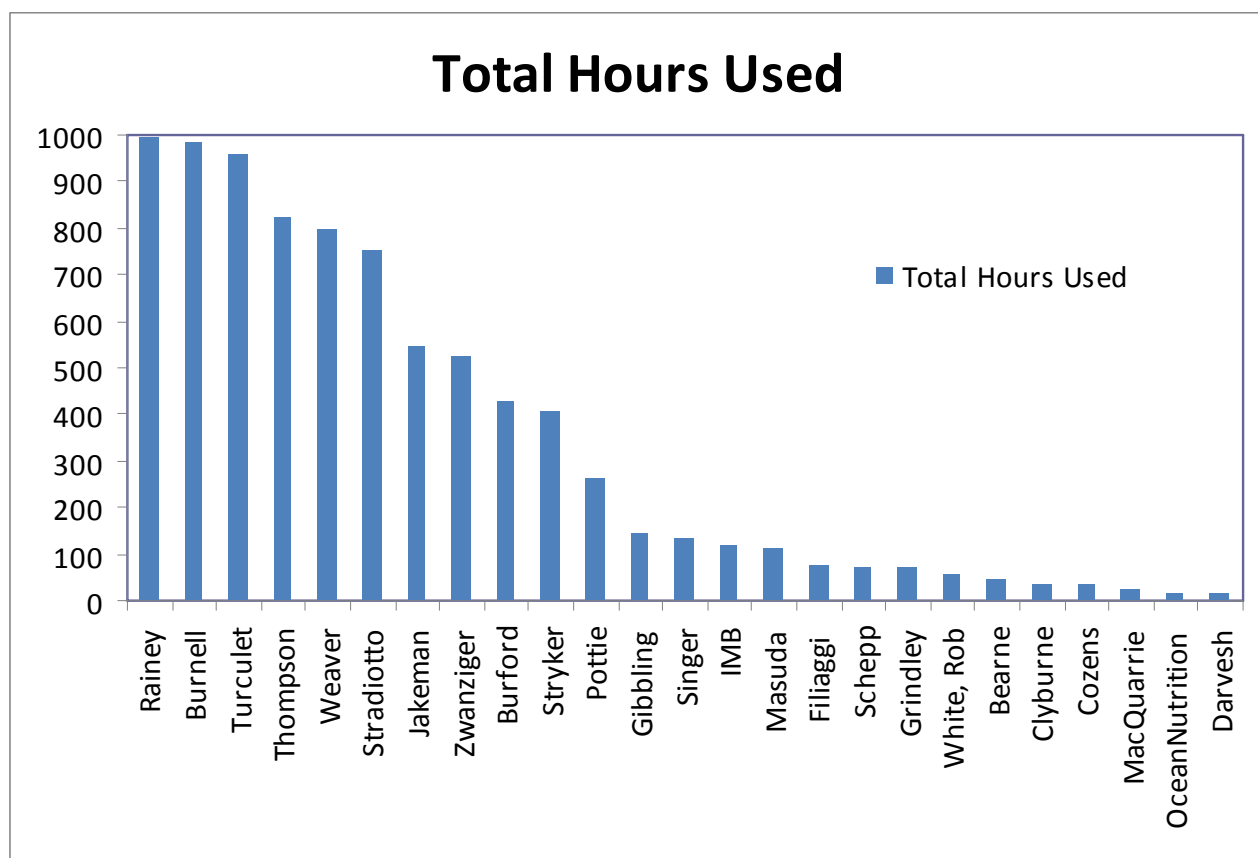
Position	Dalhousie	Supporting Maritime Institutions	Non-Supporting Maritime Institutions	Other	Government & Industry
Faculty Members	23	5	7	4	
NMR ³ Staff	2				
Instructors	3				
Research Associates	7				
Post-Docs	10	1			
PhD Students	30		1	3	
Masters Students	14	1	1		
Undergraduate Students	41	13	9		
Others	4				7

3.1.1 Faculty

Number	Name	Affiliation	Rank
1	Bearne, Stephen	Dalhousie University	Professor
2	Boyd, Daniel	Dalhousie University	Assistant Professor
3	Briand, Glen	Mount Allison University	Associate Professor
4	Bronstein, Lyuda	Indiana University, Bloomington, IN (USA)	Senior Scientist
5	Burford, Neil	Dalhousie University / UVIC	Professor
6	Burnell, Jean	Dalhousie University	Professor
7	Chatt, Ameres	Dalhousie University	Adjunct 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	Duffy, Stephen	Mount Allison University	Associate Professor
13	Duncan, Roy	Dalhousie University	Professor
14	Filiaggi, Mark	Dalhousie University	Associate Professor
15	Gibling, Martin	Dalhousie University	Professor
16	Grant, Andrew	Mount Allison University	Associate Professor
17	Grindley, Bruce	Dalhousie University	Adjunct Professor

18	Hanley, Jacob	Saint Mary's University	Associate Professor
19	Jakeman, David	Dalhousie University	Professor
20	Jha, Mukund	Nipissing University, North Bay, Ontario	Associate Professor
21	Lin, Tong-Jun	Dalhousie University	Professor
22	MacQuarrie, Stephanie	Cape Breton University	Assistant Professor
23	Masuda, Jason	Saint Mary's University	Associate Professor
24	McFarland, Sherri	Acadia University	Associate Professor
25	Messadeque, Younes	Université Laval, Quebec City, Quebec	Professor
26	Pottie, Ian	Mount Saint Vincent University	Associate Professor
27	Rainey, Jan	Dalhousie University	Associate 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	Weaver, Don	Dalhousie University	Professor
35	White, Mary Anne	Dalhousie University	Professor
36	White, Rob	Dalhousie University	Associate Professor
37	Wiesner, Ulrich	Cornell University, Ithaca, NY (USA)	Professor
38	Xia, Aibing	Mount Saint Vincent University	Associate Professor
39	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	Moya-Barrios, Reinaldo	Instructor
3	Whalen, Marc	Instructor

3.1.4 Research Associates, Post-Docs and Others

Number	Name	Affiliation	Position
1	Banfield, Scott	Dalhousie University	Research Associate
2	Bhattasali, Debabrata	Dalhousie University	Post-Doc

3	Chenu, Sebastien	Dalhousie University	Post-Doc
4	Craft, Cheryl	Institute Marine Biosciences	Gov/Industrial Scientist
5	Crain, Sheila	Institute Marine Biosciences	Gov/Industrial Scientist
6	Dodd, Angela	Saint Mary's University	
7	Fisher, Laural	Dalhousie University	Post-Doc
8	Hankinson, Rachael	Institute Marine Biosciences	Gov/Industrial Scientist
9	Harjani, Jitendra	Saint Mary's University	
10	Imam, Uddin	Dalhousie University	
11	Kehoe, Sharon	Dalhousie University	Post-Doc
12	Jahan, Nusrat	Institute Marine Biosciences	Gov/Industrial Scientist
13	Lu, Erhu	Dalhousie University	Research Associate
14	Marchal, Estelle	Dalhousie University	Post-Doc
15	McCormick, Nicole	Dalhousie University	Research Assistant
16	McGrath, Alaina	Dalhousie University	
17	Ngweniform, Pascaline	Dalhousie University	Post-Doc
18	Paul, Nawal	Dalhousie University	
19	Reed, Mark	Dalhousie University	Research Associate
20	Rinco, Olga	Dalhousie University	Visiting Professor
21	Robertson, Kathy	Saint Mary's University	
22	Sadaphal, Sandip	Saint Mary's University	
23	Sadeghi-khomani, Ali	Dalhousie University	Gov/Industrial Scientist
24	Sarker, Muzaddid	Dalhousie University	Post-Doc
25	Seto, Leslie	Dalhousie University	Technician
26	Smithen, Deborah	Dalhousie University	Post-Doc
27	Sonar, Swapnil	Saint Mary's University	Post-Doc
28	Stefanova, Roumiana	Institute Marine Biosciences	Gov/Industrial Scientist
29	Suarez, Erick	OceanNutrition	Gov/Industrial Scientist
30	Sun, Shengguo	Dalhousie University	Research Associate
31	Wheaton, Craig	Dalhousie University	Post-Doc
32	Wood, Thomas	Dalhousie University	Research Associate
33	Wu, Fan	Dalhousie University	Research Associate
34	Xu, Lingling	Dalhousie University	Visiting Researcher
35	Yadav, Arum	Dalhousie University	Research Associate
36	Zhang, Xiaofang	Dalhousie University	Post-Doc

3.2 Publications Associated with Centre (July 1, 2011 to June 30, 2012)

Summary of Publications

Publication Type	Number
Peer-reviewed Journal Articles	57
Non-refereed Publication	1

Peer-reviewed Journal Articles:

1. Alsabeh, PG; Lundgren, RJ; Longobardi, LE; Stradiotto, M, **Palladium-catalyzed synthesis of indoles via ammonia cross-coupling-alkyne cyclization**, Chemical Communications, 47(24), 6936-6938 (2011).
2. Alsabeh, PG; McDonald, R; Stradiotto, M, **Stoichiometric Reactivity Relevant to the Mor-DalPhos/Pd-Catalyzed Cross-Coupling of Ammonia and 1-Bromo-2-(phenylethynyl)benzene**, Organometallics, 31(3), 1049-1054 (2012).
3. Bendeif, EE; Matta, CF; Stradiotto, M; Fertey, P; Lecomte, C, **Can a Formally Zwitterionic Rhodium(I) Complex Emulate the Charge Density of a Cationic Rhodium(I) Complex? A Combined Synchrotron X-ray and Theoretical Charge-Density Study**, Inorganic Chemistry, 51(6), 3754-3769 (2012).
4. Bertolasi, V; Hunter, NJ; Vaughan, K, **An X-Ray Crystallographic Study of Five Compounds from a Series of 1,x-bis-(4-Oxo-3,4-dihydro-1,2,3-benzotriazin-3-yl)alkanes**, Journal of Chemical Crystallography, 41(8), 1105-1113 (2011).
5. Blair, AD; Hendsbee, AD; Masuda, JD, **1-(2,4,6-Triisopropylphenyl)ethanone**, Acta Crystallographica Section E - Structure Reports Online, 67(10), O2731 (2011).
6. Chenu, S; Werner-Zwanziger, U; Calahoo, C; Zwanziger, JW, **Structure and properties of NaPO₃-ZnO-Nb₂O₅-Al₂O₃ glasses**, Journal of Non-Crystalline Solids, 358(15), 1795-1805 (2012).
7. Chitnis, SS; MacDonald, E; Burford, N; Werner-Zwanziger, U; McDonald, R, **P-P Menshutkin preparation of prototypical phosphinophosphonium salts**, Chem. Com. 48(59), 7359-7361 (2012).
8. Chitnis, SS; Peters, B; Conrad, E; Burford, N; McDonald, R; Ferguson, MJ, **Structural diversity for phosphine complexes of stibenium and stibinidenium cations**, Chemical Communications, 47(45), 12331-12333 (2011).
9. Crawford, SM; Ali, AAS; Cameron, TS; Thompson, A, **Synthesis and Characterization of Fluorescent Pyrrolyldipyrinato Sn(IV) Complexes**, Inorganic Chemistry, 50(17), 8207-8213 (2011).
10. Donath, M; Conrad, E; Jerabek, P; Frenking, G; Frohlich, R; Burford, N; Weigand, JJ, **Ligand-Stabilized [P4]²⁺Cations**, Angewandte Chemie-International Edition, 51(12), 2964-2967 (2012).
11. Dupuis, SN; Robertson, AW; Veinot, T; Monro, SMA; Douglas, SE; Syvitski, RT; Goralski, KB; McFarland, SA; Jakeman, DL, **Synthetic diversification of natural products: semi-synthesis and evaluation of triazole jadomycins**, Chemical Science, 3(5), 1640-1644 (2012).
12. Dupuis, SN; Veinot, T; Monro, SMA; Douglas, SE; Syvitski, RT; Goralski, KB; McFarland, SA; Jakeman, DL, **Jadomycins Derived from the Assimilation and Incorporation of Norvaline and Norleucine**, Journal of Natural Products, 74(11), 2420-2424 (2011).
13. Ford, L; Atefi, F; Singer, RD; Scammells, PJ, **Grignard Reactions in Pyridinium and Phosphonium Ionic Liquids**, European Journal of Organic Chemistry, 5, 942-950 (2011).

14. Forget, SM; Bhattasali, D; Hart, VC; Cameron, TS; Syvitski, RT; Jakeman, DL, **Synthesis and enzymatic evaluation of ketose phosphonates: the interplay between mutarotation, monofluorination and acidity**, *Chemical Science*, 3(6), 1866-1878 (2012).
15. Gao, F; Stamp, CTM; Thornton, PD; Cameron, TS; Doyle, LE; Miller, DO; Burnell, DJ, **Selective formation of angular tricyclic compounds by ruthenium-mediated ring-rearrangement metathesis**, *Chemical Communications*, 48(2), 233-235 (2012).
16. Giffin, NA; Hendsbee, AD; Masuda, JD, **Rhodium carbonyl complexes of bulky, anionic nitrogen-based ligands: A comparison of donating ability**, *Journal of Organometallic Chemistry*, 696(13), 2533-2536 (2011).
17. Hendsbee, AD; Masuda, JD; Piorko, A, **(η^5)-Cyclopentadienyl)(η^6)-phenoxathiin 10,10-dioxide)iron(II) hexafluoridophosphate and phenoxathiin 10,10-dioxide**, *Acta Crystallographica Section C- Crystal Structure Communications*, 67(11), M351-M354 (2011).
18. Hendsbee, AD; Masuda, JD; Piorko, A, **[η^6]-1-Chloro-2-(pyrrolidin-1-yl)benzene](η^5)-cyclopentadienyl)iron(II) hexafluoridophosphate and (η^5)-cyclopentadienyl){2-[η^6]-2-(pyrrolidin-1-yl)phenyl]phenol}iron(II) hexafluoridophosphate**, *Acta Crystallographica Section C- Crystal Structure Communications*, 67(12), M391-M394 (2011).
19. Jakeman, DL, **Mechanisms of Glycosyltransferases: The In and the Out**, *Chembiochem*, 12(17), 2540-2542 (2011).
20. Jakeman, DL; Sadeghi-Khomami, A, **A beta-(1,2)-Glycosynthase and an Attempted Selection Method for the Directed Evolution of Glycosynthases**, *Biochemistry*, 50(47), 10359-10366 (2011).
21. Kassam, A; Burnell, DJ; Dahn, JR, **Lithiated 1,4,5,8-Naphthalenetetraol Formaldehyde Polymer, An Organic Cathode Material**, *Electrochemical and Solid State Letters*, 14(2), A22-A23 (2011).
22. Kehoe, S; Langman, M.; Abraham, B.; Zwanziger, U.; Boyd, D, **Composition-Structure-Property (Density and Cytocompatibility) for Experimental Embolic Particulates**, *Journal of Biomaterials Applications* (accepted June 2012).
23. Lavery, CB; McDonald, R; Stradiotto, M, **Efficient palladium-catalyzed synthesis of substituted indoles employing a new (silanyloxyphenyl)phosphine ligand**, *Chemical Communications*, 48(58), 7277-7279 (2012).
24. Liu, PY; Wu, YJ; Pye, CC; Thornton, PD; Poirier, RA; Burnell, DJ, **Facial Selectivity in the Diels-Alder Reactions of 2,2-Disubstituted Cyclopent-4-ene-1,3-dione Derivatives and a Computational Examination of the Facial Selectivity of the Diels-Alder Reactions of Structurally Related Dienes and Dienophiles**, *European Journal of Organic Chemistry*, 6, 1186-1194 (2012).
25. Lundgren, RJ; Hesp, KD; Stradiotto, M, **Design of New 'DalPhos' P,N-Ligands: Applications in Transition-Metal Catalysis**, *Synlett*, 17, 2443-2458 (2011).
26. Lundrigan, T; Baker, AEG; Longobardi, LE; Wood, TE; Smithen, DA; Crawford, SM; Cameron, TS; Thompson, A, **An Improved Method for the Synthesis of F-BODIPYs from Dipyrins and Bis(dipyrin)s**, *Organic Letters*, 14(8), 2158-2161 (2012).
27. Lundrigan, T; Crawford, SM; Cameron, TS; Thompson, A, **Cl-BODIPYs: a BODIPY class enabling facile B-substitution**, *Chemical Communications*, 48(7), 1003-1005 (2012).
28. Macdonald IR; Jollymore CT; Reid GA; Pottie IR; Martin E; Darvesh S, **Thioesters for the in vitro evaluation of agents to image brain cholinesterases**, *Journal of Enzyme Inhibition and Medicinal Chemistry*, (2012) in press.
29. MacDonald, E; Doyle, L; Burford, N; Werner-Zwanziger, U; Decken, A, **Stannylphosphonium Cations**, *Angewandte Chemie, International Edition*, 50, 11474-11477, S11474/1-S11474/16 (2011).

30. MacDonald, E; Doyle, L; Chitnis, SS; Werner-Zwanziger, U; Burford, B; Decken, A, **Me₃P complexes of p-block Lewis acids SnCl₄, SnCl₃⁺ and SnCl₂²⁺**, Chem. Com., 48(64), 7922-7924 (2012).
31. Macdonald, IR; Reid, GA; Joy, EE; Pottie, IR; Matte, G; Burrell, S; Mawko, G; Martin, E; Darvesh, S, **Synthesis and Preliminary Evaluation of PiperidinyI and PyrrolidinyI Iodobenzoates as Imaging Agents for Butyrylcholinesterase**, Molecular Imaging and Biology, 13(6), 1250-1261 (2111).
32. MacDonald, JL; Werner-Zwanziger, U; Chen, B; Zwanziger, JW; Forgeron, D, **A ⁴³Ca and ¹³C NMR study of the chemical interaction between poly(ethylene-vinyl acetate) and white cement during hydration**, Solid State NMR 40, 78-83, (2011).
33. MacInnis, MC; McDonald, R; Ferguson, MJ; Tobisch, S; Turculet, L, **Four-Coordinate, 14-Electron Ru-II Complexes: Unusual Trigonal Pyramidal Geometry Enforced by Bis(phosphino)silyl Ligation**, Journal of the American Chemical Society, 133(34), 13622-13633 (2011).
34. MacInnis, MC; McDonald, R; Turculet, L, **Synthesis and Characterization of Palladium Complexes Supported by an NPN-Phosphido Ancillary Ligand**, Organometallics, 30(23), 6408-6415 (2011).
35. Martin, V; Werner-Zwanziger, U; Zwanziger, JW; Dunlap, RA, **Correlation of structure and photoelastic response in tin phosphate glass**, International Journal of Applied Glass Science, 2, 282-289 (2011).
36. Marx, VM; Stoddard, RL; Heverly-Coulson, GS; Burnell, DJ, **Substituent-Controlled Reactivity in the Nazarov Cyclisation of Allenyl Vinyl Ketones**, Chemistry-A European Journal, 17(29), 8098-8104 (2011).
37. Moulins, JR; Burnell, DJ, **E/Z product distribution in the metathesis of allyl alcohol derivatives with a first generation ruthenium-based catalyst**, Tetrahedron Letters, 52(31), 3992-3994 (2011).
38. Nagar, M; Narmandakh, A; Khalak, Y; Bearne, SL, **Redefining the Minimal Substrate Tolerance of Mande late Racemase. Racemization of Trifluorolactate**, Biochemistry, 50(41), 8846-8852 (2011).
39. Ramezani, M; Resmer, KL; White, RL, **Glutamate racemization and catabolism in Fusobacterium varium**, Febs Journal, 278(14), 2540-2551 (2011).
40. Ramezani, M; White, RL, **Enantioselective catabolism of racemic serine: preparation of D-serine using whole cells of Fusobacterium nucleatum**, Tetrahedron: Asymmetry, 22(13), 1473-1478 (2011).
41. Resmer, KL; White, RL, **Metabolic footprinting of the anaerobic bacterium Fusobacterium varium using H-1 NMR spectroscopy**, Molecular Biosystems, 7(7), 2220-2227 (2011).
42. Ruddy, AJ; Mitton, SJ; McDonald, R; Turculet, L, **'Hemilabile' silyl pincer ligation: platinum group PSiN complexes and triple C-H activation to form a (PSiC)Ru carbene complex**, Chemical Communications, 48(8), 1159-1161 (2012).
43. Shin, K; Pandey, A; Anini, Y; Rainey, JK, **Differential apelin isoform production and involvement in obesity**, Regulatory Peptides, 177(S1), S32-S33 (2012).
44. Smithen, DA; Baker, AEG; Offman, M; Crawford, SM; Cameron, TS; Thompson, A, **Use of F-BODIPYs as a Protection Strategy for Dipyrins: Optimization of BF₂ Removal**, Journal of Organic Chemistry, 77(7), 3439-3453 (2012).
45. Smithen, DA; Cameron, TS; Thompson, A, **One-Pot Synthesis of Asymmetric Annulated Bis(pyrrole)s**, Organic Letters, 13(21), 5846-5849 (2011).
46. Sonar, S; Ambrose, K; Hendsbee, AD; Masuda, JD; Singer, RD, **Synthesis and application of Co(salen) complexes containing proximal imidazolium ionic liquid cores**, Canadian Journal of Chemistry, 90(1), 60-70 (2012).
47. Tardiff, BJ; Hesp, KD; Ferguson, MJ; Stradiotto, M, **Generation of [(IPr)Pd(PR₂Cl)] complexes via P-Cl reductive elimination**, Dalton Transactions, 41(26), 7883-7885 (2012).

48. Tardiff, BJ; McDonald, R; Ferguson, MJ; Stradiotto, M, **Rational and Predictable Chemoselective Synthesis of Oligoamines via Buchwald-Hartwig Amination of (Hetero)Aryl Chlorides Employing Mor-DalPhos**, *Journal of Organic Chemistry*, 77(2), 1056-1071 (2012).
49. Tardiff, BJ; Stradiotto, M, **Buchwald-Hartwig Amination of (Hetero)aryl Chlorides by Employing Mor-DalPhos under Aqueous and Solvent-Free Conditions**, *European Journal of Organic Chemistry*, 21, 3972-3977 (2012).
50. Thornton, PD; Burnell, DJ, **Isomerization of the (E)-Alkene of a Conjugated Enyne During Intramolecular Pauson-Khand Cyclization**, *European Journal of Organic Chemistry*, 26, 4989-4992 (2011).
51. Thornton, PD; Cameron, TS; Burnell, DJ, **Vinyllogous anionic processes in the formation and interconversion of tetracyclic ring systems**, *Organic & Biomolecular Chemistry*, 9(9), 3447-3456 (2011).
52. Top, D; Read, JA; Dawe, SJ; Syvitski, RT; Duncan, R, **Cell-Cell Membrane Fusion Induced by p15 Fusion-associated Small Transmembrane (FAST) Protein Requires a Novel Fusion Peptide Motif Containing a Myristoylated Polyproline Type II Helix**, *Journal of Biological Chemistry*, 287, 3403-3414 (2012).
53. Twibanire, JK; Grindley, TB, **Efficient and controllably selective synthesis of esters using peptide coupling agents**, *Organic Letters*, 13(12), 2988-2991 (2011).
54. Twibanire, JK; Grindley, TB, **Polyester dendrimers**, *Polymers*, 4(1), 794-879 (2012).
55. Warren, SC; Perkins, MR; Adams, AM; Kamperman, M; Burns, AA; Arora, H; Herz, E; Suteewong, T; Sai, H; Li, Z; Werner, J; Song, J; Werner-Zwanziger, U; Zwanziger, JW; Graetzel, M; Di Salvo, FJ; Wiesner, U, **A silica sol-gel design strategy for nanostructured metallic materials**, *Nature Materials*, 11, 460-467 (2012).
56. Werner-Zwanziger, U; Chapman, K; Zwanziger, JW, **Multinuclear NMR Study of Zinc Dicyanide**, *Zeitschrift für Physikalische Chemie*, (2012) in print.
57. Xu, L; Tremblay, M-L; Meng, Q; Liu, X-Q; Rainey, JK, **^1H , ^{13}C and ^{15}N NMR assignments of the aciniform spidroin (AcSp1) repetitive domain of *Argiope trifasciata* wrapping silk**, *Biomolecular NMR Assignments*, 6(2), 147-151 (2012).

Non-refereed publication:

Boutilier, J. and Duncan, R. (2011). The Reovirus Fusion-Associated Small Transmembrane (FAST) Proteins: Virus-Encoded Cellular Fusogens. In "Current Topics in Membranes: Membrane Fusion" vol. 68, p. 107-140. L. V. Chernomordik and M. Koslov (eds.). Elsevier.

3.3 Participation in relevant events for research dissemination

A total of 34 international and 68 domestic conference or symposium presentations were reported by professors and students, using and relying upon data collected at the Centre.

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

Professors/Associates & Number of Events	Students & Number of Events
18 international conference/symposium presentations by 10 professors	16 student presentations at the international level
Professors/Associates & Number of Events	Students & Number of Events
18 domestic conference/symposium presentations by 9 professors	50 student presentations

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

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"

Instructor: Robert White

Course enrollment: 204

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

Instructors: Josef Zwanziger, Mary Anne White, and Gianna Aleman-Milan

Course enrollment: 61

- **3rd Year Undergraduate**

(1) BIOC 3700.03: "Biomolecular Chemistry"

Instructors: Jan Rainey and Stephen Bearne

Course enrollment: 54

(2) CHEM 3401.03: "Intermediate Organic Chemistry"

Instructor: Norm Schepp

Course enrollment: 36

(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: 49

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

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

Instructor: Jean Burnell

Course enrollment: 14 undergraduates in 4402 and 6 graduate students in 5402, respectively

- **Graduate**

(1) PHYS 6250.03: "Experimental Techniques in Materials Science"

Instructor: Josef Zwanziger (for NMR component)

Course enrollment: 12

(2) CHEM 6457.015 / BIOC 6703.015: "Magnetic Resonance Techniques for Drug Design and Development" Instructor: Ray Syvitski

Course enrollment: 4

(3) CHEM 6362.015 / BIOC 6702.015: "Topics in High Resolution NMR"

Instructor: Jan Rainey with some guest lectures by NMR³ staff member Mike Lumsden

Course enrollment: 3 students + 2 audits

3.5 Student research activities related to the Centre mission statement

The following table summarizes the 113 student researchers who relied upon the NMR³ facility for progress in their research programs during the 2011-2012 reporting period. The table is made up of 34 Doctoral, 15 Masters, and 64 Undergraduate students.

Number	Student Name	Institution	Degree	Supervisor	Status	Thesis Title
1	Aish, Gaia	Dalhousie University	MSc	David Jakeman	In-Progress	
2	Ali, Malik	Dalhousie University	BSc	Rob White	In-Progress	
3	Alsabeh, Pamela	Dalhousie University	PhD	Mark Stradiotto	In-Progress	
4	Ambrose, Kenson	Saint Mary's University	BSc	Rob Singer	Completed	Oxidation of a Lignin Model Compound Using Salen-Cobalt Derivatives
5	Anderson, Katharine	Dalhousie University	PhD	Donald Weaver	In-Progress	
6	Ardagh, Giselle	Dalhousie University	BSc	Jean Burnell	Completed	Nazarov Reactivity of Allenyl Vinyl Ketones with Terminal Substitution of the Allene Moiety
7	Baker, Alex	Dalhousie University	BSc	Alison Thompson	In-Progress	

8	Bateman, Mary	Dalhousie University	BSc	Fran Cozens	In-Progress	
9	Bennett, Matthew	Cape Breton Univeristy	BSc	Stephanie MacQuarrie	In Progress	
10	Bennett, Sarah	Dalhousie University	PhD	Alison Thompson	Completed	Dipyrins, Pyrrolyldipyrins, Prodigiosenes and Their Complexes
11	Blair, Amber	Saint Mary's University	BSc	Jason Masuda	In-Progress	
12	Calahoo, Courtney	Dalhousie University	PhD	Josef Zwanziger	In-Progress	
13	Chauhan, Owen	Dalhousie University	BSc	Jean Burnell	Completed	Intramolecular Interception of the Nazarov Reaction of Allenyl Vinyl Ketones with Arenes
14	Chitnis, Saurabh	Dalhousie University/UVIC	PhD	Neil Burford	In-Progress	
15	Chowdhury, Saptarshi	Dalhousie University	BSc	Alison Thompson	In-Progress	
16	Comeau, Patricia	Dalhousie University	PhD	Mark Filiaggi	In-Progress	
17	Cook, Earl	Mount Saint Vincent University	BSc	Aibing Xia	Completed	
18	Coolen, Stacy	Mount Saint Vincent University	BSc	Ian Pottie	In-Progress	
19	Cuthbert, Tyler	Saint Mary's University	BSc	Rob Singer	In-Progress	
20	Daley, Erika	Saint Mary's University	BSc	Rob Singer	In-Progress	
21	D'Arcy, Duncan	Mount Saint Vincent University	BSc	Ian Pottie	In-Progress	
22	Dexter, Graham	Dalhousie University	BSc	Jean Burnell	Completed	Nazarov Reactions Intercepted by Oxygen-substituted Dienes
23	Doyle, Chris	Dalhousie University	BSc	Jan Rainey	In-Progress	
24	Doyle, Lauren	Dalhousie University	BSc	Neil Burford	Completed	Synthesis and Reactivity of Late Metal Complexes Featuring Novel PSiN Mixed Donor Tridentate Ligands
25	Dupuis, Stephanie	Dalhousie University	MSc	David Jakeman	In-Progress	
26	Durand, Alanna	Saint Mary's University	BSc	Rob Singer	In-Progress	

27	Feldman, Erin	Dalhousie University	BSc	David Jakeman	In-Progress	
28	Flemming, Kelli	Dalhousie University	BSc	Stephen Bearne	In-Progress	
29	Forget, Stephanie	Dalhousie University	MSc	David Jakeman	In-Progress	
30	Giffin, Nick	Saint Mary's University	MSc	Jason Masuda	Completed	Synthesis and Reactivity of Low-Valent Group 14-15 Compounds
31	Groves, Brandon	Dalhousie University	MSc	Alison Thompson	In-Progress	
32	Hart, Catherine	Dalhousie University	BSc	David Jakeman	In-Progress	
33	Hawco, Cassandra	Dalhousie University	MSc	Alison Thompson	In-Progress	
34	Hendsbee, Art	Saint Mary's University	BSc	Jason Masuda	Completed	Reactions of Low Valent Main Group Compounds With Chalcogen Containing Species
35	Hirtle, Jordan	Dalhousie University	BSc	Jan Rainey	In-Progress	
36	Jaeschke, Alyssa	Mount Saint Vincent University	BSc	Ian Pottie	Completed	Investigation of the Nitronate-Nazarov Cyclization
37	Jollymore, Courtney	Mount Saint Vincent University	MSc	Ian Pottie	In-Progress	
38	K. Twibanire, Jean D'Amour	Dalhousie University	PhD	Bruce Grindley	In-Progress	
39	Kelly, Sean	Mount Saint Vincent University	BSc	Ian Pottie	In-Progress	
40	Kennedy, Kirsten	Dalhousie University	MSc	Martin Gibling	In-Progress	
41	Keyes, Lauren	Saint Mary's University	BSc	Jason Masuda	In-Progress	
42	Khanal, Mandar	Dalhousie University	MSc	Stephen Bearne	In-Progress	
43	Knackstedt, Dane	Dalhousie University	BSc	Neil Burford	In-Progress	
44	Langelaan, David	Dalhousie University	PhD	Jan Rainey	Completed	Structural Studies Of Apelin And Its Receptor As Well As The Characteristics And Causes Of Membrane Protein Helix Kinks
45	Lavery, Chris	Dalhousie University	PhD	Mark Stradiotto	In-Progress	

46	Ledemi, Yannick	Universite Laval, QC	PhD	Younes Messadeque	In-Progress	
47	LeFort, Francois	Dalhousie University	MSc	Jean Burnell	In-Progress	
48	Lefsay, Abir	Dalhousie University	PhD	Ameres Chatt	In-Progress	
49	Lines, Katie	Dalhousie University	BSc	David Jakeman	In-Progress	
50	Longobardi, Lauren	Dalhousie University	BSc	Mark Stradiotto	In-Progress	
51	Loranger, Matthew	Dalhousie University	PhD	David Jakeman	In-Progress	
52	Lucas, Stewart	Dalhousie University	BSc	Neil Burford	In-Progress	
53	Lundrigan, Travis	Dalhousie University	PhD	Alison Thompson	In-Progress	
54	Ma, Kai	Cornell University, USA	PhD	Ulrich Wiesner	In-Progress	
55	MacDonald, Elizabeth	Dalhousie University	PhD	Neil Burford	In-Progress	
56	MacDonald, Ian	Mount Saint Vincent University	PhD	Ian Pottie	In-Progress	
57	MacDonald, Sarah	Saint Mary's University	BSc	Jason Masuda	In-Progress	
58	MacInnis, Morgan	Dalhousie University	PhD	Laura Turculet	Completed	Synthesis, Reactivity, and Catalytic Applications of Ruthenium and Palladium Complexes Supported by New Pincer Ligands
59	MacIntosh, Ian	Saint Mary's University	BSc	Jason Clyburne	In-Progress	
60	MacLean, Mark	Dalhousie University	MSc	Mark Stradiotto	In-Progress	
61	Makramalla, Miller	Saint Mary's University	BSc	Jason Clyburne	In-Progress	
62	Martinez-Farina, Camilo	Dalhousie University	BSc	David Jakeman	Completed	Investigations into the Biosynthesis of Novel Jadomycins
63	Marx, Vanessa	Dalhousie University	PhD	Jean Burnell	Completed	Development of the Interrupted Nazarov Cyclization of Allenyl Vinyl Ketones, with Application to the Total Synthesis of the Cyclooctane Natural Product Roseadione

64	McPherson, Alex	Saint Mary's University	BSc	Jason Clyburne	In-Progress	
65	Melanson, Jennifer	Dalhousie University	PhD	Alison Thompson	In-Progress	
66	Mills, Harriet	Dalhousie University	BSc	Alison Thompson	Completed	Creating Chirality at the α -Carbon Atom of a Pyrrole Using a Tripeptide Chiral Catalyst
67	Mishra, Vinayak	Dalhousie University	BSc	Fran Cozens	In-Progress	
68	Mitton, Samuel	Dalhousie University	PhD	Laura Turculet	In-Progress	
69	Momeni, Arash	Dalhousie University	PhD	Mark Filiaggi	In-Progress	
70	Morgan, Erin	Dalhousie University	PhD	Laura Turculet	In-Progress	
71	Morgan, Tim	Dalhousie University	PhD	Jean Burnell	In-Progress	
72	Moulins, Jonathan	Dalhousie University	PhD	Jean Burnell	In-Progress	
73	Moussa, Nabil	Dalhousie University	BSc	Rob White	In-Progress	
74	Muchechedi, Hillary	Dalhousie University	MSc	Alison Thompson	In-Progress	
75	Murphy, Luke	Saint Mary's University	BSc	Jason Clyburne	Completed	Carbon Dioxide Capture with Amines in Non-Volatile Solvents and the Effect of Sulfur Dioxide on the Absorbent
76	Nijssen, Kathryn	Dalhousie University	BSc	Donald Weaver	In-Progress	
77	Offman, Matthew	Dalhousie University	BSc	Alison Thompson	In-Progress	
78	Pandey, Aditya	Dalhousie University	PhD	Jan Rainey	In-Progress	
79	Parvizi Omran, Raha	Dalhousie University	BSc	Bruce Grindley	Completed	The Synthesis of an Antigen Against Lyme Disease
80	Penwell, Will	Dalhousie University	BSc	Norman Schepp	In-Progress	
81	Peters, Brendan	Dalhousie University	MSc	Neil Burford	In-Progress	
82	Pettipas, Shauna	Dalhousie University	BSc	Norman Schepp	In-Progress	
83	Prudhoe, Christine	Saint Mary's University	BSc	Rob Singer	In-Progress	

84	Rajora, Maneesha	Dalhousie University	BSc	Jean Burnell	In-Progress	
85	Rashid, Ahmed	Dalhousie University	BSc	Neil Burford	In-Progress	
86	Resmer, Kelly	Dalhousie University	PhD	Rob White	Completed	Metabolic Studies of <i>Fusobacterium varium</i> Using NMR Spectroscopy
87	Robertson, Andrew	Dalhousie University	PhD	David Jakeman	In-Progress	
88	Romao, Carl	Dalhousie University	PhD	Mary Anne White	In-Progress	
89	Roy, Alexander	Dalhousie University	BSc	Stephen Bearne	In-Progress	
90	Ruddy, Adam	Dalhousie University	PhD	Laura Turculet	In-Progress	
91	Ruzic-Gauthier, Michael	Dalhousie University	BSc	Norman Schepp	In-Progress	
92	Sanford, Jessica	Mount Saint Vincent University	BSc	Aibing Xia	Completed	
93	Sharpe, James	Dalhousie University	BSc	Neil Burford	In-Progress	
94	Simms, Gordon	Dalhousie University	PhD	Donald Weaver	In-Progress	
95	Smith-Halverson, Duncan	Dalhousie University	BSc	Norman Schepp	In-Progress	
96	Speckert, Matthew	Dalhousie University	BSc	Jan Rainey	Completed	A positive influence: Investigating the importance of key residues within the apelin peptides in the context of the membrane catalysis model
97	Stamp, Craig	Dalhousie University	PhD	Jean Burnell	In-Progress	
98	Subedi, Pankaj	Dalhousie University	BSc	Fran Cozens	Completed	The Development of a Probe Molecule to Monitor the Behavior and Reactivity of Photochemically Generated Hydroxyl Radical
99	Sun, Yao	Cornell University, USA	PhD	Ulrich Wiesner	In-Progress	
100	Tait, Mary	Cape Breton University	BSc	Stephanie MacQuarrie	In-Progress	
101	Tang, Timothy	Dalhousie University	BSc	Norman Schepp	In-Progress	

102	Tardiff, Ben	Dalhousie University	PhD	Mark Stradiotto	Completed	Palladium-Catalyzed Amine Synthesis: Chemoselectivity and Reactivity Under Aqueous Conditions
103	Thomas, Allison	Mount Saint Vincent University	BSc	Ian Pottie	In-Progress	
104	Tilley, Ryan	Dalhousie University	BSc	Fran Cozens	Completed	Synthesis of β -Sulfur Substituted Radical Precursors
105	Toulany, Amir	Dalhousie University	BSc	Fran Cozens	Completed	Reactivity of Alkoxy Radicals in Solution and in Zeolites: Synthesis of N-(alkoxy)pyridine-2-Thione and the Study of their Photogenerated Alkoxy Radicals
106	Tovstiga, Tara	Dalhousie University	MSc	Rob White	In-Progress	
107	Tremblay, Marie-Laurence	Dalhousie University	PhD	Jan Rainey	In-Progress	
108	Tucker, Lloyd	Dalhousie University	BSc	Alison Thompson	In-Progress	
109	Ward, Sarah	Dalhousie University	MSc	Donald Weaver	Completed	The Development of Exogenous Anticonvulsants and Endogenous Uracil-Based Antiepileptic Agents
110	Weale, Mike	Dalhousie University	MSc	Laura Turculet	In-Progress	
111	Weingartshofer, Tony	Dalhousie University	BSc	David Jakeman	In-Progress	
112	Wilson, David	Dalhousie University	BSc	Donald Weaver	Completed	Synthesis of β -aryl- β -alanine Analogues for Development of Therapeutics for Substance Dependence
113	Zenko, Ben	Dalhousie University	BSc	Donald Weaver	Completed	Amino Acid Derived β -amyloid Antiaggregants: An Examination of the Structure-Activity Relationship of L-phenylalanine and L-tryptophan Analogues

3.6 Outreach Strategy

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. Next, researchers are introduced to the AC/Tecmag-250 spectrometer in 2 x 1 h sessions in small groups. After demonstrating proficiency and competency on the AC/Tecmag-250, 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 occasionally 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 and 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, Bruce Grindley, 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 liquid state NMR spectrometers, because solid state NMR is barely routine in our facility and 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.

3.7 Technology Development, patent or commercialization activities

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

1. U.S. provisional patent submitted 61/637,387. (Title redacted for IP reasons). Principal investigator: Mark Stradiotto.
2. U.S. Provisional Application 61/437,566 filed January 28, 2012 : Title: RADIOPAQUE EMBOLIC PARTICLES. Principal investigator: Daniel Boyd.

2. The solid-state NMR instruments have been used with two different companies, where three different researchers have collaborated with NMR³ expert staff member Dr. Ulrike Werner-Zwanziger:

1. The specialized low gamma probe head at relatively high field strengths, as well as our unique combination of nuclei that can be studied together has lead to a (proprietary) service work for Styker Orthobiologics with two different researchers within the company.
2. For Silver's Agencies Dr. Ulrike Werner-Zwanziger has helped identify the origin of materials involved in spillage on a ship. This work might be part of a law suit in the future, since large damages were incurred in the incidents.

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 June of 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, 2011 – March 31, 2012)

4.1 Financial Report

Financial support in '11-'12 came from a total of 3 sources: (1) Dalhousie University (2) User Fees and (3) a newly instated "Supporting Institution Fee" (described below). This past year, the University paid the Coordinator's full salary and benefits. The facility paid 42% of the Solid-State NMR Coordinator's salary with the remainder paid by the Faculty of Science in support of Dr. Josef Zwanziger's Canada Research Chair in NMR Studies of Materials. Other direct costs of the facility this past FY included magnet cryogenics, lab supplies, computing costs, and all expenses associated with service and maintenance.

In January of 2012, the facility revised its fee structure. An outline of the posted user fees applicable at the end of the current reporting period is provided below.

Liquids Hourly Rates: Hands-On Usage			
	Academics @ Dal & Supporting Institutions ¹	Academics @ Non-Supporting Institutions ¹	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 Institutions ¹	Academics @ Non-Supporting Institutions ¹	Government/Industry
Hands-On / Collaborative ⁴	\$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 initial, 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. In each subsequent fiscal year, the requested annual fee for that institution is calculated using a formula that is based upon the percent usage of NMR time in the previous fiscal year by all users from that institution. This payment entitles academic users to continued hands-on access to the NMR³ instruments at the Dalhousie rates over that year. Further details are provided on the facilities website. Note that during the current FY, the \$500 support fee was paid by Saint Mary's University.

4.2 Grants directly related to the mission statement of NMR³ and awarded within the 2011-2012 Fiscal Year:

In total, **\$3,201,973 in new grant funds** were awarded to Dalhousie University researchers in grants identified by the Centre user 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 \$35,526 in grant funds awarded in the 2011-2012 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:

Chevron Phillips Chemical. "Application of a Proprietary Ligand Class in Cross-Coupling Catalysis." **Co-applicants: M. Stradiotto and L. Turculet.** (\$40,000; 1 year)

CIHR - Operating Grant. "Developing Inhibitors of Bacterial and Trypanosomal CTP Synthases"
Principal Applicant: S.L. Bearne. (\$138,474/year; 5 years).

CIHR/Nova Scotia Health Research Foundation/Dalhousie UIMRF - Regional Partnership Program Operating Grant. "Synthesis and Evaluation of Butyrylcholinesterase Ligands for Brain Imaging in Dementia." **S. Darvesh (Principal Applicant), I. Pottie, S. Burrell:** (\$107,246; 1 year)

Dalhousie Medical Research Foundation - Adopt a Researcher Program. "Synthesis and Brain evaluation of butyrylcholinesterase ligands as diagnostic and therapeutic agents for Alzheimer disease, Equipment grant for drug discovery in Alzheimer's disease." **Principal Applicant - S. Darvesh.** (\$50,000/year; 2 years)

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." **Principal Applicant - S. Darvesh.** (\$24,504; 1 year)

CIHR - Operating Grant. "Butyrylcholinesterase Ligands as Potential Radiopharmaceuticals for Brain Imaging in Dementia." **S. Darvesh (Principal Applicant), I. Pottie, S. Burrell** (\$129,297/year; 3 years)

France-Canada Research Fund. "Low-Melting High Strength Glass for Solar Cell Applications."
Principal Applicant - J.W. Zwanziger. (\$10,000/year; 2 years)

Innovacorp Early Stage Commercialization Fun. "Commercialization of CaP Liquid Embolic System." **MJ Filiaggi [Principal Applicant], A Momeni, R Abraham.** (\$49,500; 1 year).

Nova Scotia Health Research Foundation - Establishment Grant. "Stimuli responsive glass ionomer cements for ART." **Principal Applicant: D. Boyd.** (\$49,333/year; 3 years).

NSERC - Collaborative Health Research Program. "An Interdisciplinary Approach Towards the Development of a Disease-stabilizing Treatment for Alzheimer's Disease" **Co-applicants: M. Stradiotto and D.F. Weaver.** (\$225,500/year; 2 years).

NSERC - Discovery Grant. "Cyclization reactions in synthetic organic chemistry." **Principal Applicant: D.J. Burnell.** (\$70,000/year; 5 years).

NSERC - Discovery Grant. "Synthesis and Applications of Biologically Active Carbohydrate Derivatives and Related Compounds." **Principal Applicant - T.B. Grindley.** (\$35,000/year; 5 years)

NSERC - Discovery Grant. "Understanding, engineering and exploiting protein self-assembly." **Principal Applicant - J.K. Rainey.** (\$28,000/year; 5 years)

NSERC - Discovery Grant. "Synthesis and Applications of Pyrroles, Dipyrins and their Complexes." **Principal Applicant - A. Thompson.** (\$55,000/year; 5 years)

NSERC - Engage Grant. "Developing NMR spectroscopic methods to characterize polymer nanoparticles and their cargo." **Principal Applicant - J.K. Rainey.** (\$25,000; 1 year)

NSERC - Engage Grant. "Direct Preparation of Key Intermediates in Heterocycle Synthesis Employing Novel Pd-Catalyzed Alpha-Arylation." **Principal Applicant - M. Stradiotto.** (\$24,500; 1 year)

NSERC - Interaction Grant. "Exploration of potential collaboration with Vive Nano Inc." **Principal Applicant - J.K. Rainey.** (\$1,964; 1 year).

NSERC - Research Tools & Instruments. "A SmartPROBE for NMR studies." **D.L. Jakeman (Principal Applicant), S.L. Bearne, T.B. Grindley, J.K. Rainey, M.J. Stradiotto & A. Thompson.** (\$149,999; 1 year)

Springboard Innovation Mobilization Program Award (Proof of Concept). "Glycerol-based Surfactants: An Entirely New Suite of High-performance Green Surfactant Compounds with Multiple Industrial and Commercial Applications." **G. D. Marangoni and T.B. Grindley** (\$20,000; 1 year)

Springboard Innovation - Mobilization Program Award. "Phosphino silyl ether ligands for metal-catalyzed cross-coupling catalysis" **Principal Applicant - M. Stradiotto.** (\$20,000; 1 year)

Grants awarded to NMR³ users located at other Nova Scotia Universities (user fee rate category specified in each case):

NSERC - Engage Grant. "Metal and Organic Sensing with Biomass from BioEnergy Inc." **Principal Applicant - S. MacQuarrie (Cape Breton University - not currently a supporting institution).** (\$25,000; 1 year)

Springboard Atlantic. "Green Marine Antifouling Agents" **Principal Applicant - R. Singer (St. Mary's University - a supporting institution).** (\$10,526; 1 year)