



— 2016-2017 Annual Report —

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About the cover: Biomolecular NMR spectroscopy relies on multiple experiments to complete the resonance assignment necessary to determine the atomic-resolution structure of a protein. The cover attempts to capture the iterative approach of using multiple NMR experiments to refine restraints and determine the structure of a protein. A hydrophobin protein is shown, the structure of which is initially poorly refined (bottom left) but after refinement using NMR data (indicated by the pulse program of a modified HNCACO experiment (Hiller et. al, (2015) PNAS 102:10876-81)) becomes well converged (centre). *Contributed by Calem Kenward and Dr. David Langelaan.*

Section 1 - Overview of NMR³ Centre and its Mission

The Nuclear Magnetic Resonance Research Resource (NMR³) supports users from the Atlantic region, primarily the Maritime Provinces, but also from across Canada and internationally. The Centre provides nuclear magnetic resonance spectroscopy (NMR) services to academic, industrial, and government users, in forms ranging from training users to perform hands-on experiments to data acquisition and interpretation to research collaboration. Housed in the Chemistry Building at Dalhousie University, the NMR³ currently hosts 4 NMR spectrometers with a variety of capabilities, ranging from 300 MHz for liquids to 700 MHz for solids. It has a staff of two Ph.D. level chemists, who work with the users on data acquisition and interpretation, alongside maintaining the instrumentation. In addition, the NMR³ partners with the proximal NRC-IMB lab in the operation of a 700 MHz spectrometer optimized for biological samples, and NMR³ users are allocated up to 30% of the time on this instrument. Because of the high concentration of small- to medium-sized universities in the Atlantic Region, the NMR³ plays a special role as a catalyst in enhancing research in the area, by providing both equipment and expertise in NMR that these universities cannot afford individually, and which would be highly redundant to provide at each. Dalhousie additionally benefits from this role in terms of the positive perception of our research intensiveness that is developed among the hands-on users from the other local universities, who are typically potential recruits for graduate or postgraduate studies.

NMR spectroscopy is the most important characterization technique available to chemists, biochemists and materials scientists, and is very important for many others including clinicians. Technological advances in the last decade have tremendously enhanced the value of NMR spectroscopic data and the variety of experiments now available. The Atlantic Region has a world-class reputation for research involving NMR spectroscopy and research that depends on NMR spectroscopy. In 2016-2017, the Centre assisted 32 research groups mostly drawn from the Atlantic Canada region but also including several international researchers, resulting in 50 publications, 2 patents, 83 conference presentations and 116 highly qualified personnel trained. Furthermore, teaching in the Departments of Chemistry and Biochemistry & Molecular Biology was supported in 7 undergraduate labs and 2 graduate labs with 182 total students and a combined 314 hours, providing exposure to both the practical aspects of NMR spectroscopy and the nuances of data analysis. In total, use of the Centre's 5 NMR instruments was ~8132 hours. The vast majority of instrument use was logged in experiments configured by trainees in support of externally funded research grants for Dalhousie University researchers. Perhaps the most concrete illustration of the critical and valuable nature of the services provided by our Centre is the fact that Dalhousie-based researchers identified NMR³ access as being essential in just over \$1.5-million in new external grant funds awarded in the 2016-2017 fiscal year. On a rolling basis, it should be further noted that NMR³ has been identified by users as being instrumental in the awarding of an additional \$21.7million in external grant funding to Dalhousie researchers in the 2015-2016 (>\$7.9-million), 2014-2015 (>\$2.4-million), 2013-2014 (>\$1.5-million), 2012-2013 (>\$6.7-million) and 2011-2012 (>\$3.2-million) fiscal years.

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

1.1 Mission Statement

The Nuclear Magnetic Resonance Research Resource (NMR³) is a research resource for nuclear magnetic resonance, with a client base distributed throughout the Atlantic region, primarily in the Maritime Provinces. The Centre was established as the Atlantic Region Magnetic Resonance Centre in 1982 through financial support from the Natural Sciences and Engineering Research Council of Canada (NSERC) and Dalhousie University and has enjoyed support from these and other sources throughout its history. The mission of the facility is to provide high-field nuclear magnetic resonance (NMR) spectral data and expertise to scientists in the Atlantic Region of Canada. The facility has enhanced numerous research programs and resulted in the training of numerous young scientists attending Universities in the Atlantic Region.

Deviation from original mission statement: with the demise of NSERC funding for facilities such as NMR³, we have been 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. It should be noted that a recent successful NSERC Research Tools & Instruments Operations and Maintenance support grant led by Dr. Josef Zwanziger will be providing an additional source of funding for our solid-state NMR operating costs, starting in the 2017-2018 fiscal year.

1.2 Current Year's Activity

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



Although our fee structure, predominantly based on hourly rates for instrument usage, was not modified (Section 4), income from User fees increased significantly in FY '16-'17 relative to the prior three fiscal years. Highly informative is the profile of our User fee income (shown graphically below including only Dal-based instrument user fees and not NRC 700 MHz user fees; fully profiled in Section 4), where it is clear that Industrial User fees, which were almost equally split between the liquids and solids usage in FY '16-'17, are an extremely important component of our total User Fee income at 20.7%. This represents a significant increase (namely, >\$12,000) over FY '15-'16, where industrial

use represented only 8% of User fee income, and was a record year for industrial usage relative to the past 4 fiscal years.



User Fee Income Breakdown

2. Full salary support: Our Strategic Initiatives Fund (SIF) support, thanks to spearheading by Dr. Mark Filiaggi, Associate Vice-President Research, means that we are currently receiving full salary support for Dr. Mike Lumsden (1 FTE) and Dr. Ulli Werner-Zwanziger (0.75 FTE). Over the reporting fiscal year, these funds were coupled with a Department of Chemistry position allocation (~2/3 of Dr. Mike Lumsden's salary) and funds obtained from the Faculty of Science because of Dr. Josef Zwanziger's Canada Research Chair (\$30,000 toward Dr. Ulrike Werner-Zwanziger's salary). The NMR³ top-up request from the SIF has been approved for the 2016-2017 Fiscal Year, with conditional budget approval for the 2017-2018 Fiscal Year, meaning that our user fees only need to cover non-salary expenses for these years. This conditional approval relies both upon the results of the annual Budget Advisory Committee report and upon NMR³ continuing to satisfy and maintain performance criteria. We have been told that our comprehensive annual report is an excellent means by which we can document this latter point, so are grateful to the users for their cooperation.

3. Conversion of Room 426B into a Resource for NMR Instruction and Centralized Data Processing: Since the decommissioning and removal of the Bruker AC-250 NMR spectrometer in 2012, Room 426B in the NMR³ facility has been used for storage. Although long been viewed as a potential resource for NMR-related training and tutorials, financial constraints and uncertainty over the past 4 years have prevented this from happening. With full salary support now achieved, the planned conversion of this space into such a resource has moved forward. Rooms 426-431 of the NMR³ facility now have integrated areas for NMR data acquisition (Room 431), NMR data processing (Room 430), sample preparation (Room 429) and instruction (Room 426B). Work on the conversion of this instruction space began late in the current reporting year and will continue into the next.

4. Solid-State NMR Instrument Upgrades: Thanks to a donation from Dr. Josef Zwanziger, the workstations and software of the two solid-state NMR spectrometers were upgraded from XWIN-NMR 3.6 to TopSpin 1 and 2, for the 400 MHz and 700 MHz spectrometers, respectively. These TopSpin software versions are the highest levels that the consoles can individually support.

1.3 Upcoming Year's Activity

1. Increase in Solids Coordinator FTE-level: Dr. Ulrike Werner-Zwanziger's position will be converted to 100% FTE, funded in part by the Faculty of Science, and in part by NMR³. The NMR³ portion is made up of a combination of SIF support from Dalhousie University and solid-state NMR user fees.

2. Replacement of aging air compressor: Thanks to a successful NSERC RTI application for major infrastructure improvements on our solids instruments led by Dr. Josef Zwanziger, together with Dr. Daniel Boyd, Dr. Jan Rainey, and Dr. Ulrike Werner-Zwanziger, the replacement of the aging air compressor essential for solid-state NMR instrumental operation is in the progress.

3. Operations and Maintenance Support for Research ssNMR instruments: Thanks to the successful application to the Operations and Maintenance Support for Research Equipment by Dr. Josef Zwanziger, in combination with the Institute of Research in Materials (IRM)/Clean Technologies Research Institute (CTRI), funding for a portion of the operational costs of the solid-state NMR spectrometers of the NMR³ has been possible. Starting April 1st, 2017 this support covers some consumables, especially cryogens.

4. Pursuit of instrument upgrade opportunities: All instruments in the NMR³ facility are operating with legacy Bruker consoles no longer supported by the vendor. To date, we have been fortunate to be able to work around this, but this remains a significant concern in the longer term should a more catastrophic hardware failure occur. In the case of the NMR³ solution-state NMR instruments, user fees have been set such that all normal operating expenses are more than met. Additional user fees are being collected to provide the capability to match funds in an infrastructure grant such as an NSERC RTI, ACOA AIF, etc. allowing for proactive replacement of console equipment. Solid-state instruments have been proactively upgraded in recent years through NSERC RTI and other opportunities, with an eye toward larger grant opportunities to upgrade the costlier consoles required for solids.

5. Conversion of Room 426B into a Resource for NMR Instruction and Centralized Data Processing: As mentioned in the previous section, work on the conversion of this space began late in the current reporting period. Several delays were encountered, including a significant delay in new carpet installation. The latter was due to the poor condition of the underlying floor, which was only discovered upon removal of the old flooring. With the new flooring now in place, the space conversion is expected to be completed during the Fall 2017 semester.

Section 2 - Centre Resources and Capabilities

Bruker AVANCE – 300 MHz: Liquids Only			
Magnet	Bruker 300/54mm on a TMC Anti-Vib	Bruker 300/54mm on a TMC Anti-Vibration Platform	
Console	Bruker Avance		
Channel 1	Broadband BLA2BB Amplifier (50 W ¹	H & 135 W ¹³ C)	
Channel 2	Broadband BLA2BB Amplifier (50 W ¹ H & 135 W ¹³ C)		
Probe 1	5 mm BBFO Observe: ¹⁴ N- ³¹ P & ¹⁹ F/decouple: ¹ H, z- gradient coil and auto-tune & match accessory (ATMA)		
Temperature Control	B-VT 3200	Includes a 25L liquid N_2 dewar.	
Automation	16 sample SampleXpress Lite		
Workstation	HP xw4600 operating with Windows XP Pro		
Spectrometer Software	TopSpin 2.1 pl8		

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

Bruker AVANCE – 500 MHz: Liquids Only			
Magnet	Spectrospin 500/54mm UltraShield w	ith 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 gradient coil and auto-tune & m accessory (ATMA)		
Probe 2	5 mm BBO Observe: ¹⁴ N - ³¹ P / decouple: ¹ gradient coil and auto-tune & n accessory (ATMA)		
Probe 3	5 mm TXI	Observe: ¹ H / decouple: ¹³ C and ¹⁵ N, Z-gradient coil.	
Temperature Control	B-VT 3200 Air pre-cooled with a BCU-05 chiller, includes a 25L liquid N ₂ dewar and ar exchange coil for generating cold N ₂		
Automation	60 sample B-ACS (Bruker Automation Control System)		
Workstation	HP xw4600 operating with Windows XP Pro		
Spectrometer Software	TopSpin 2.1 pl8		

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

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

Bruker DSX 400 MHz: Solids Only			
Magnet	Buker 400/89 UltraShield		
Console	Bruker Avance DSX		
Channels 1-3	Broadband Transmitter		
Probe 1	2.5mm MAS ⁶⁹ Ga- ³¹ P / ¹⁹ F- ¹ H		
Probe 2	4mm HXY MAS	in dual mode: 45MHz - ³¹ P / ¹ H Insert Pairs for X/Y (triple) mode: ³¹ P/ ¹¹ B, ³¹ P/ ²⁷ Al, ¹¹ B/ ¹³ C, ¹³ C/ ¹⁹⁵ Pt, ²³ Na/ ²⁹ Si, ⁶ Li/ ²⁹ Si	
Probe 3	4mm MAS	¹³ C- ³¹ P/ ¹⁹ F- ¹ H	
Probe 4	7mm	¹⁵ N- ³¹ P/ ¹⁹ F- ¹ H	
Probe 5	HP wideline probe	$^{109}\mathrm{Ag}-^{31}\mathrm{P}$, high temperature design	
Workstation	HP Z420 workstation		
Spectrometer Software	TopSpin 1.3 pl10		

AVANCE 700 MHz: Solids Only			
Magnet	Buker 700/54 UltraShield		
Console	Bruker Avance		
Channels 1-3	Broadband Transmitter		
Probe 1	2.5mm MAS	¹³ C- ³¹ P / ¹⁹ F- ¹ H	
Probe 2	4mm MAS	¹⁵ N- ¹³ C/ ¹⁹ F- ¹ H, ⁴³ Ca	
TriGamma™ Probe	3.2mm MAS	¹⁵ N- ²⁹ Si/ ¹¹ B- ³¹ P/ ¹ H	
Triple Resonance Probe	4mm MAS	²⁹ Si/ ¹¹ B/ ¹ H	
Low Gamma Probe	5mm MAS	Special inserts for ⁴³ Ca, ³⁹ K, ⁹¹ Zr, ¹⁰⁷ Ag, ⁶⁷ Zn, ²⁵ Mg, ¹³⁵ Ba, ³³ S, ¹⁴ N, ^{47,49} Ti, ⁸⁹ Y, ⁸⁷ Sr / ¹⁹ F- ¹ H,	
EFREE Probe (contact Jan Rainey, if you are interested in using this probe).	5mm static solenoid	HCN/P	
Workstation	HP Z420 workstation		
Spectrometer Software	TopSpin 2.1 pl8		

Section 3 - Detailed Description of Centre Activities

Position	Dalhousie	Supporting Maritime Institutions	Non-Supporting Maritime Institutions	Other	Government & Industry
Faculty Members	22	1	4	5	
NMR ³ Staff	2				
Instructors & TA's	12				
Post-Docs	11				
PhD Students	22	3		2	
Masters Students	27				
Undergraduate Students	24		1		
Others	13	1	3	4	14

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

3.1.1 Faculty

Number	Name	Affiliation	Rank
1	Anini, Younes	Dalhousie University	Associate Professor
2	Bearne, Stephen	Dalhousie University	Professor
3	Bronstein, Lyudmila	Indiana University	Adjunct Professor
4	Budge, Suzanne	Dalhousie University	Professor
5	Chick Jarrold, Caroline	Indiana University	Professor
6	Clyburne, Jason	St. Mary's University	Professor
7	Cozens, Frances	Dalhousie University	Associate Professor
8	Dahn, Jeff	Dalhousie University	Professor
9	Filiaggi, Mark	Dalhousie University	Associate Professor
10	Grant, Andrew	Mount Allison University	Associate Professor
11	Grindley, Bruce	Dalhousie University	Adjunct Professor
12	Jakeman, David	Dalhousie University	Professor
13	Langelaan, David	Dalhousie University	Assistant Professor
14	Kerr, Russell	University Prince Edward Island	Professor
15	Liu, Paul Xiang-Qin	Dalhousie University	Professor
16	McFarland, Sherri	Acadia University / University North Carolina	Professor
17	McMaster, Christopher	Dalhousie University	Professor
18	Miar, Younes	Dalhousie University	Assistant Professor
19	Obrovac, Mark	Dalhousie University	Professor

20	Rainey, Jan	Dalhousie University	Professor; NMR ³ Director
21	Schepp, Norm	Dalhousie University	Associate Professor
22	Siedle, Allen	Indiana University	Adjunct Professor
23	Speed, Alex	Dalhousie University	Assistant Professor
24	Stradiotto, Mark	Dalhousie University	Professor; NMR ³ User Group Chair
25	Thibault, Marie-Helene	Universite de Moncton	Professor
26	Thompson, Alison	Dalhousie University	Professor
27	Turculet, Laura	Dalhousie University	Associate Professor
28	White, Mary Anne	Dalhousie University	Professor
29	White, Rob	Dalhousie University	Associate Professor
30	Wiesner, Ulrich	Cornell University	Professor
31	Xia, Aibing	Mount Saint Vincent University	Associate Professor
32	Zwanziger, Josef	Dalhousie University	Professor

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



3.1.2 NMR³ staff

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

3.1.3 Industrial Users

Number	Name	Company Name	Notes
1	Areephong, Jetsuda	Appili Therapeutics	Trained Hands-On User
2	Banfield, Scott	Appili Therapeutics	Trained Hands-On User
3	Batchu, Pavan	Solid-State Pharma Inc	Trained Hands-On User
4	Fisher, Laural	Appili Therapeutics	Trained Hands-On User

5	Kaur, Jaspreet	Solid-State Pharma Inc	Trained Hands-On User
6	MacDonald, Elizabeth	Solid-State Pharma Inc	Trained Hands-On User
7	MacEachern, Lauren	Solid State Pharma Inc	Trained Hands-On User
8	Mayo, Robert Alex	Solid State Pharma Inc	Trained Hands-On User
9	Mohamed, Tarek	Appili Therapeutics	Trained Hands-On User
10	Petibon, Remi	Tesla Motors	Trained Hands-On User
11	Pourkhanjani, Ameneh	Solid-State Pharma Inc.	Trained Hands-On User
12	Russell, Stephanie	Appili Therapeutics	Trained Hands-On User
13	Su, Yeqing	Solid-State Pharma Inc	Trained Hands-On User
14	Sun, Shengguo	Appili Therapeutics	Trained Hands-On User
15		Apotex	Solid-state NMR
16		CARBONCURE	Solid-state NMR
17		Research & Productivity Council	Solid-state NMR
18		Tesla Motors	Solid-state NMR

3.1.4 Lab Instructors and TA's

Number	Name	Position
1	Adams, Matt	Teaching Assistant
2	Aish, Gaia	Lab Instructor
3	Aleman-Milan, Gianna	Lab Instructor
4	Huchenski, Blake	Teaching Assistant
5	Licht, Felicia	Teaching Assistant
6	Liu, Aaron	Teaching Assistant
7	Moya-Barrios, Reinaldo	Lab Instructor
8	Murray, Michael	Teaching Assistant
9	Noel, John	Teaching Assistant
10	Thompson, Lauren	Teaching Assistant
11	Tien, Chieh Hung	Teaching Assistant
12	Whalen, Marc	Lab Instructor

3.1.5 Research Associates, Post-Docs and Others

Number	Name	Affiliation	Position
1	Allen, Jennifer	Dalhousie University	Summer Researcher
2	Branch, Mackenzie	Dalhousie University	Visiting Researcher

3	Chevrier, Daniel	Dalhousie University	Post-Doc
4	Cranstone, Connor	Dalhousie University	Summer Researcher
5	Diaz, Carlos	University British Columbia	Summer Researcher
6	Douglas, Colin	Dalhousie University	Post-Doc
7	Eldesoky, Ahmed	University New Brunswick	Summer Researcher
8	Figliola, Carlotta	Dalhousie University	Post-Doc
9	Garaga, Mounesha	Dalhousie University	Post-Doc
10	Garcia, Anthony	Ecole Nationale Superieure de Chimie de Rennes, France	Visiting Researcher
11	Gaube, Sophie	Dalhousie University	Summer Researcher
12	Gu, Minglu	Dalhousie University	Summer Researcher
13	Hale, Dylan	Dalhousie University	Summer Researcher
14	Hall, David	Dalhousie University	Post-Doc
15	Jahan, Nusrat	Dalhousie University	Volunteer Researcher
16	Kelly, Josh	University Prince Edward Island	Technician
17	Lamont, Connor	Dalhousie University	Summer Researcher
18	Lynch, Kyle	Dalhousie University	Summer Researcher
19	McGuire, Ryan	Dalhousie University	Summer Researcher
20	Momeni, Arash	Dalhousie University	Post-Doc
21	O'Connell, Kathleen	Dalhousie University	Post-Doc
22	Ogawa, Takahiko	Dalhousie University	Post-Doc
23	Osmond, Travis	Mount Allison University	Research Assistant
24	Protheroe, Liam	Dalhousie University	Summer Researcher
25	Roberston, Kathy	St. Mary's University	Research Assistant
26	Said, Hammam	Dalhousie University	Summer Researcher
27	Simms, Gordon	Dalhousie University	Post-Doc
28	Subedi, Pankaj	Dalhousie University	Research Assistant
29	Versini, Antoine	ESPCI Paris, France	Visiting Researcher
30	Voth, Chris	University British Columbia	Visiting Researcher
31	Xia, Jian	Dalhousie University	Post-Doc
32	Zhu, Jian-She	Dalhousie University	Post-Doc

3.2 Publications Associated with Centre (July 1, 2016 to June 30, 2017)

Peer-Reviewed Journal Articles – total 50

1. Adams MR, Tien CH, Huchenski BSN, Ferguson MJ, & Speed AWH (**2017**) Diazaphospholene Precatalysts for Imine and Conjugate Reductions. *Angewandte Chemie-International Edition* <u>56</u>(22):6268-6271.

- Ahmed MY, Al-Khayat A, Al-Murshedi F, Al-Futaisi A, Chioza BA, Fernandez-Murray JP, Self JE, Salter CG, Harlalka GV, Rawlins LE, Al-Zuhaibi S, Al-Azri F, Al-Rashdi F, Cazenave-Gassiot A, Wenk MR, Al-Salmi F, Patton MA, Silver DL, Baple EL, McMaster CR, & Crosby AH (**2017**) A mutation of EPT1 (SELENOI) underlies a new disorder of Kennedy pathway phospholipid biosynthesis. *Brain* <u>140</u>:547-554.
- 3. Al-Mughaid H, Al-Zoubi RM, Khazaaleh M, & Grindley TB (**2017**) Assembly and inhibitory activity of monovalent mannosides terminated with aromatic methyl esters: The effect of naphthyl groups. *Carbohydrate Research* <u>446</u>:76-84.
- 4. Beh MHR, Douglas KIB, House KTE, Murphy AC, Sinclair JST, & Thompson A (**2016**) Robust synthesis of F-BODIPYs. *Organic & Biomolecular Chemistry* <u>14</u>(48):11473-11479.
- 5. Bhar P & Bearne SL (**2017**) Unexpected Side Product Formed during LDA-induced Phosphonylation of Uridine. *Chemistry Letters* <u>46(</u>4):609-611.
- Blensdorf T, Joenathan A, Hunt M, Werner-Zwanziger U, Stein BD, Mahmoud WE, Al-Ghamdi AA, Carini J, & Bronstein LM (2017) Hybrid composite polymer electrolytes: ionic liquids as a magic bullet for the poly(ethylene glycol)-silica network. *Journal of Materials Chemistry A* <u>5</u>(7):3493-3502.
- 7. Clark JSK, Lavoie CM, MacQueen PM, Ferguson MJ, & Stradiotto M (**2016**) A Comparative Reactivity Survey of Some Prominent Bisphosphine Nickel(II) Precatalysts in C-N Cross-Coupling. *Organometallics* <u>35(</u>18):3248-3254.
- 8. Clark JSK, Voth CN, Ferguson MJ, & Stradiotto M (**2017**) Evaluating 1,1'-Bis(phosphino)ferrocene Ancillary Ligand Variants in the Nickel-Catalyzed C-N Cross-Coupling of (Hetero)aryl Chlorides. *Organometallics* <u>36</u>(3):679-686.
- 9. Conroy BS, Weiss ER, Smith SP, & Langelaan DN (**2017**) Backbone H-1, C-13, and N-15 NMR resonance assignments of the Kruppel-like factor 4 activation domain. *Biomolecular Nmr Assignments* <u>11(1)</u>:95-98.
- 10. Ducatti DRB, Carroll MA, & Jakeman DL (**2016**) On the phosphorylase activity of GH3 enzymes: A beta-Nacetylglucosaminidase from Herbaspirillum seropedicae SmR1 and a glucosidase from Saccharopolyspora erythraea. *Carbohydrate Research* <u>435</u>:106-112.
- 11. Dufay JN, Fernandez-Murray JP, & McMaster CR (**2017**) SLC25 Family Member Genetic Interactions Identify a Role for HEM25 in Yeast Electron Transport Chain Stability. *G3-Genes Genomes Genetics* <u>7(</u>6):1861-1873.
- 12. Fernandez-Murray JP & McMaster CR (**2016**) Lipid synthesis and membrane contact sites: a crossroads for cellular physiology. *Journal of Lipid Research* <u>57</u>(10):1789-1805.
- 13. Filiaggi MJ & Momeni A (2017) Design and Optimization of Polyphosphate Coacervates for Use in Biomedical Devices. American Chemical Society Symposium (Coacervation: Physics, Chemistry and Biology).
- 14. Forget SM, Bushnell EAC, Boyd RJ, & Jakeman DL (**2016**) The acidity of beta-phosphoglucomutase monofluoromethylenephosphonate ligands probed by NMR spectroscopy and quantum mechanical methods. *Canadian Journal of Chemistry* <u>94</u>(11):902-908.
- 15. Forget SM, McVey J, Vining LC, & Jakeman DL (**2017**) Streptomyces venezuelae ISP5230 Maintains Excretion of Jadomycin upon Disruption of the MFS Transporter JadL Located within the Natural Product Biosynthetic Gene Cluster. *Frontiers in Microbiology* <u>8</u>.
- 16. Forget SM, Na J, McCormick NE, & Jakeman DL (**2017**) Biosynthetic 4,6-dehydratase gene deletion: isolation of a glucosylated jadomycin natural product provides insight into the substrate specificity of glycosyltransferase JadS. *Organic & Biomolecular Chemistry* <u>15</u>(13):2725-2729.
- 17. Forget SM, Robertson AW, Overy DP, Kerr RG, & Jakeman DL (**2017**) Furan and Lactam Jadomycin Biosynthetic

Congeners Isolated from Streptomyces venezuelae ISP5230 Cultured with N-epsilon-Trifluoroacetyl-L-lysine. *Journal of Natural Products* <u>80(</u>6):1860-1866.

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- 44. Tremblay ML, Xu LL, Sarker M, Liu XQ, & Rainey JK (**2016**) Characterizing Aciniform Silk Repetitive Domain Backbone Dynamics and Hydrodynamic Modularity. *International Journal of Molecular Sciences* <u>17</u>(8).
- 45. Wang L, Yin HM, Jabed MA, Hetu M, Wang CZ, Munro S, Zhu XL, Kilina S, McFarland SA, & Sun WF (**2017**) pi-Expansive Heteroleptic Ruthenium(II) Complexes as Reverse Saturable Absorbers and Photosensitizers for Photodynamic Therapy. *Inorganic Chemistry* <u>56</u>(6):3245-3259.
- 46. Wiethan C, Franceschini SZ, Bonacorso HG, & Stradiotto M (**2016**) Synthesis of pyrazolo 1,5-a quinoxalin-4(5H)-ones via one-pot amidation/N-arylation reactions under transition metal-free conditions. *Organic & Biomolecular Chemistry* <u>14(</u>37):8721-8727.
- 47. Wiethan C, Lavoie CM, Borzenko A, Clark JSK, Bonacorso HG, & Stradiotto M (**2017**) Ni and Cu-catalyzed one pot synthesis of unsymmetrical 1,3-di(hetero) aryl-1H-indazoles from hydrazine, o-chloro (hetero) benzophenones, and (hetero) aryl bromides. *Organic & Biomolecular Chemistry* <u>15</u>(23):5062-5069.
- 48. Wiethan C, Rosa WC, Bonacorso HG, & Stradiotto M (**2016**) Synthesis of tetra-substituted 5-trifluoromethylpyrazoles via sequential halogenation/palladium-catalyzed C-C and C-N cross-coupling. *Organic & Biomolecular Chemistry* <u>14</u>(7):2352-2359.

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3.3 Participation in Relevant Events for Research Dissemination

A total of **27 international** and **56 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
	14 international	13 student presentations at
	conference/symposium	the international level
	presentations by 10 professors	
What is the number of Centre personnel who participated in domestic events?	Professors/Associates & Number of Events	Students & Number of Events
	12 domestic	44 student presentations
	conference/symposium	
	presentations by 9 professors	

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

• 2nd Year Undergraduate

(1) CHEM 2401: "Organic Chemistry I" Instructor: Alison Thompson Course enrollment: 313

(2) CHEM 2402: "Organic Chemistry II" Instructor: Frances Cozens Course enrollment: 231

(3) CHEM 2304: "Introductory Physical Chemistry II" Instructor: Peng Zhang Course enrollment: 33

• 3rd Year Undergraduate

(1) BIOC 3700: "Biomolecular Chemistry" Instructors: Jan Rainey and Stephen Bearne Course enrollment: 40

(2) CHEM 3401: "Intermediate Organic Chemistry" Instructor: Alex Speed Course enrollment: 32 (3) CHEM 3404: "Physical Organic Chemistry and Spectroscopy" Instructor: Frances Cozens Course enrollment: 46

(4) CHEM 3103: "Intermediate Inorganic Chemistry" Instructor: Laura Turculet Course enrollment: 37

(5) CHEM 3801: "Experiential Learning in Chemistry" Instructor: Peter Wentzell Course enrollment: 5

• 4th Year Undergraduate

(1) CHEM 4402 (cross-listed with CHEM 5402): "Organic Structure Determination" Instructor: Norm Schepp Course enrollment: 25 (20 in 4402 and 5 in 5402)

(2) CHEM 4801: "Research Project Chemistry I" Instructor: Norm Schepp Course enrollment: 3

(3) CHEM 4901: "Honours Research Project" Instructor: Norm Schepp Course enrollment: 18

(4) CHEM 4602 (cross-listed with CHEM 5602): "Macromolecular Biophysics" Instructor: Jan Rainey Course enrollment: 7 (7 in 4602 and 0 in 5602)

(5) BIOC 4702 (cross-listed with BIOC 5702): "Macromolecular Biophysics" Instructor: Jan Rainey Course enrollment: 4 (1 in 4702 and 3 in 5702)

5th Year Graduate (1) CHEM 5120: "Advanced Organometallic Chemistry" Instructor: Mark Stradiotto Course enrollment: 8

3.5 Student Research Activities Related to the Centre Mission Statement

The following table summarizes the **79** student researchers who relied upon the NMR³ facility for progress in their research programs during the 2016-2017 reporting period. The table is made up of **27** Doctoral, **27** Masters, and **25** Undergraduate students.

	Student Name	Institution	Degree	Supervisor	Status	Thesis Title
1	Aboushawareb, Sarah	Dalhousie University	MSc	Stephen Bearne	Completed	Recognition of 'Minimal' Ligands by Enolase Superfamily Enzymes
2	Adams, Matt	Dalhousie University	MSc	Alex Speed	In-Progress	

3	Alharbi, Mona	Dalhousie University	PhD	Jan Rainey	Left	
4	Alsharif, Salman	Dalhousie University	BSc	David Jakeman	Left	
5	Ampaw, Anna	Dalhousie University	MSc	David Jakeman	Completed	The Expression of 19F- Labeled Beta- Phospholucomutase and the Evaluation of its Inhibitors
6	Aronitz, Elise	Dalhousie University	BSc	Alison Thompson	In-Progress	
7	Beaucage, Peter	Cornell University	PhD	Ulrich Wiesner	In-Progress	
8	Beh, Michael	Dalhousie University	MSc	Alison Thompson	In-Progress	
9	Bennett, Raymond	Dalhousie University	BSc	Frances Cozens	Completed	Production & Characterization of BODIPY-based Carbocations Using Laser Flash Photolysis
10	Burke, Luke	Dalhousie University	BSc	Alison Thompson	Completed	Synthesis of aza- dipyrrins and their C- and O-aza-BODIPY Analogues
11	Carroll, Madison	Dalhousie University	MSc	David Jakeman	In-Progress	
12	Charlton, Michael	Dalhousie University	BSc	Alex Speed	Completed	Exploring the Reactivity Potential of Cationic and Fluorinated Diazaphospholenes
13	Christopherson, Cheyenne	Dalhousie University	BSc	Alex Speed	Completed	Synthesis of Boron Bis(amino)cyclopropylid ene Carbene Adducts for use in Asymmetric Hydrogenation Catalysis
14	Clark, Farren	Dalhousie University	BSc	David Jakeman	In-Progress	
15	Clark, Jillian	Dalhousie University	MSc	Mark Stradiotto	In-Progress	
16	Cole, Laura	Dalhousie University	MSc	Alison Thompson	Left	
17	Diaz-Rodriguez, Roberto	Dalhousie University	BSc	Alison Thompson	In-Progress	
18	Easton, Nicole	Dalhousie University	BSc	Stephen Bearne	In-Progress	
19	Ellis, Leah	Dalhousie University	PhD	Jeff Dahn	In-Progress	
20	Firth, Ben	Dalhousie University	BSc	Robert White	Completed	Fragmentation Mechanisms of Gas Phase α-oxocarboxylate Hydrazones via Collision- Induced Dissociation Mass Spectrometry
21	Forget, Stephanie	Dalhousie University	PhD	David Jakeman	In-Progress	

22	Gatien, Alex	Dalhousie University	MSc	Mark Stradiotto	In-Progress	
23	Gauthier, Roby	Dalhousie University	PhD	Jeff Dahn	In-Progress	
24	Giffen, Kristen	Dalhousie University	BSc	Alex Speed	Completed	Exploring the Ability of N-Heterocyclic Phosphones to Activate and Deliver bis(pinacolato)diboron and Allyl Pinacolborate to Unsaturated Compounds
25	Gracious, Shayne	Dalhousie University	BSc	Bruce Grindley	Left	
26	Greening, Sarah	Dalhousie University	MSc	Alison Thompson	In-Progress	
27	Groves, Brandon	Dalhousie University	PhD	Alison Thompson	Completed	The Synthesis of Prodigiosene-Based Anticancer Reagents and Development of Reactions for Dipyrrin- Based Molecules
28	Hagar, Mostafa	Dalhousie University	BSc	Bruce Grindley	Completed	Mechanistic Aspects of N-bromosuccinimide- Mediated Dibutylstannylene Acetal Oxidation Towards N-H Bond Oxidative Addition of Amines
29	Harris, Emily	Dalhousie University	MSc	Suzanne Budge	In-Progress	
30	Hollenhorst, Helia	Dalhousie University	MSc	Laura Turculet	In-Progress	
31	Huchenski, Blake	Dalhousie University	MSc	Alex Speed	In-Progress	
32	Hung Tien, Chieh	Dalhousie University	MSc	Alex Speed	In-Progress	
33	Hynes, Toren	Dalhousie University	BSc	Jeff Dahn	In-Progress	
34	Igboeli, Hope	University Prince Edward Island	PhD	Russell Kerr	In-Progress	
35	Jee, Alison	Dalhousie University	BSc	David Jakeman	Completed	
36	Johnsen, Ann	Dalhousie University	BSc	Alison Thompson	In-Progress	
37	Kelly, Colin	Dalhousie University	MSc	Laura Turculet	In-Progress	
38	Kenward, Calem	Dalhousie University	BSc	Jan Rainey	Completed	Optimizing ¹⁹ F-labelled Indole Incorporation into Apelin Receptor to Probe Local Conformation, Dynamics, and Ligand Binding in a GPCR by NMR Spectroscopy

39	Kim, Min Joon	Dalhousie University	BSc	Alison Thompson	Completed	Development of New Methodology for the Reduction of 2- Thionoester Pyrroles Pre-Catalyst Systems
40	Kirshenbaum, Maxine	Dalhousie University	BSc	Bruce Grindley	In-Progress	
41	Knopf, Philipp	Dalhousie University	BSc	Stephen Bearne	Completed	Entropic Effects on the Binding to the Active Site of <i>Clostridium sticklandii</i> proline racemase
42	Kohle, Ferdinand	Cornell University	PhD	Ulrich Wiesner	In-Progress	
43	Lavoie, Chris	Dalhousie University	MSc	Mark Stradiotto	In-Progress	
44	Lee, Diane	Dalhousie University	BSc	Alex Speed	Completed	The use of Bis(amino)cyclopropenyl idene Carbene-Borane Adducts for Catalyst of Diels-Alder Reaction
45	Lefsay, Abir	Dalhousie University	PhD	Ameres Chatt	Completed	Development of Liquid Chromotographic and Mass Spectrometric Methods for the Identification of Chlorinated Triacylglycerols in Natural Oils
46	Liang, Leon	University Prince Edward Island	PhD	Russell Kerr	In-Progress	
47	Lindeperg, Fabien	Dalhousie University	PhD	Laura Turculet	In-Progress	
48	Liu, Aaron	Dalhousie University	MSc	Jeff Dahn	In-Progress	
49	Lundrigan, Travis	Dalhousie University	PhD	Alison Thompson	In-Progress	
50	Ma, Lin	Dalhousie University	MSc	Jeff Dahn	In-Progress	
51	Macaulay, Casper	Dalhousie University	PhD	Laura Turculet	In-Progress	
52	MacLeod, Jeanna	Dalhousie University	MSc	David Jakeman	In-Progress	
53	MacNeil, Grant	Dalhousie University	MSc	Jan Rainey	In-Progress	
54	MacQueen, Preston	Dalhousie University	PhD	Mark Stradiotto	In-Progress	
55	McCluskey, Greg	Dalhousie University	PhD	Stephen Bearne	In-Progress	
56	McCoy, Ryan	Saint Mary's University	BSc	Jason Clyburne	In-Progress	
57	McDonald, Nicholas	Dalhousie University	MSc	Rob White	In-Progress	

58	McIntyre, Logan	University Prince Edward Island	PhD	Russell Kerr	In-Progress	
59	Murphy, Luke	Dalhousie University	PhD	Laura Turculet	In-Progress	
60	Murray,Vivian	Dalhousie University	MSc	Jeff Dahn	In-Progress	
61	Nix, Hayden	Dalhousie University	MSc	Mark Filiaggi	Left	
62	Noel, John	Dalhousie University	PhD	Mary Anne White	In-Progress	
63	Paterson, Alex	Dalhousie University	PhD	Josef Zwanziger	In-Progress	
64	Power, Emma	Dalhousie University	BSc	Josef Zwanziger	In-Progress	
65	Qin, Teng Fei	Dalhousie University	MSc	Norman Schepp	In-Progress	
66	Rotta-Loria, Nicolas	Dalhousie University	PhD	Mark Stradiotto	In-Progress	
67	Sawarzky, Ryan	Dalhousie University	MSc	Mark Stradiotto	In-Progress	
68	Shin, Kyungsoo	Dalhousie University	PhD	Jan Rainey	In-Progress	
69	Song, Qinyan	Dalhousie University	PhD	Paul Liu	In-Progress	
70	Spencer, Shannon	Dalhousie University	BSc	Younes Miar	Completed	Metabolomics for reproduction traits in mink
71	Srinivasan, Pooja	Dalhousie University	MSc	Stephen Bearne	In-Progress	
72	Sulekha, Anamika	Dalhousie University	PhD	Jan Rainey	In-Progress	
73	Tassone, Joseph	Dalhousie University	PhD	Mark Stradiotto	In-Progress	
74	Thompson, Lauren	Dalhousie University	MSc	Jeff Dahn	In-Progress	
75	Wang, Yukun	Dalhousie University	PhD	Mark Obrovac	In-Progress	
76	Weber, Rochelle	Dalhousie University	MSc	Jeff Dahn	In-Progress	
77	Welsh, Erin	Dalhousie University	BSc	Alex Speed	In-Progress	
78	Xia, Wei	Dalhousie University	PhD	Suzanne Budge	In-Progress	

79	Xiong, Deijun	Dalhousie University	PhD	Jeff Dahn	In-Progress		
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3.6 Outreach Strategy

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

Anyone wishing to become a hands-on user of a high-resolution NMR spectrometer at the NMR³ is first required to read the NMR³ facility safety guide and pass an online test consisting of 10 questions. Subsequently, users can take a 1 h training course on the AVANCE 300 and/or the AVANCE 500 using the sample changer. Both 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 most researchers via Dr. Mike Lumsden. The exceptions are the Dalhousie groups of Professors Jan Rainey, Paul Xiang-Qin Liu, Roy Duncan and David Jakeman from the Departments of Biochemistry & Molecular Biology and the College of Pharmacy. Many individuals from these groups have been trained to use the spectrometer themselves. Additionally, training courses are provided by NRC staff for researchers requesting walk-up access to the 700 MHz spectrometer using ICON-NMR and the SampleJET. A number of researchers from the groups of Professors Alison Thompson, David Jakeman, Jan Rainey, and Stephen Bearne are trained and have walk-up access to the spectrometer.

Access to the Bruker Avance 400 and 700 MHz NMR spectrometers for solids is handled differently than for the solution-state NMR spectrometers, because solid-state NMR is more technically challenging than solution-state NMR and experiments carried out in our facility tend to be non-routine in nature. Because of the different usage 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 and Saint Mary's University.
- (3) Those, whose research centers around solid-state NMR.

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

2. During the Fall 2016 semester, the NMR³ facility mentored a 3rd year Undergraduate Student as part of the requirements for the course: CHEM 3801 "Experiential Learning in Chemistry". During the semester, **Roberto Diaz-Rodriquez** spent ~8 hours per week with Drs. Mike Lumsden and Ulrike Werner-Zwanziger, learning about many fundamental aspects of both high-resolution and solid-state NMR spectroscopy in a hands-on fashion. The curriculum included a background theory and hardware section, a survey of common NMR experiments in both solids and liquids as well as an overview of data processing techniques. At the end of the term, Roberto was provided with an unknown

molecule and tasked with determining its structure using the techniques and training he was exposed to throughout the term.

3. Outreach also takes the form of detailing NMR³ capabilities during regional, national and international seminars. During the past reporting period, NMR³ Director Jan Rainey did so in NMR-intensive invited talks at the University of Saskatchewan, Saint Mary's University, the Annual Meeting of the Biophysical Society of Canada, and at the Canadian Society for Chemistry (CSC) Conference. NMR³ Solid-State Coordinator Ulli Werner-Zwanziger also highlighted the solid-state NMR capabilities of the NMR³ at the 13th International Conference on the Structure of Non-Crystalline Materials (NCM-13) and at the MOOT 29 NMR Conference in Charlottetown, Prince Edward Island.

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

- On October 4, 2016, Dr. Mike Lumsden hosted a group of 11 students from the Dalhousie class BIOC 4702/5702 and CHEM 4602/5602 and provided hands-on demonstrations of high-resolution NMR techniques such as water suppression, RF pulse length calibration, and T1/T2 measurements.
- On October 12, 2016, NMR³ facility staff hosted a group of 17 undergraduate students from Saint Mary's University and explained/demonstrated the basic principles of high-resolution and solid-state NMR spectroscopy.

5. On November 22nd, 2016, Dr. Mike Lumsden gave an invited lecture to the Dalhousie BIOC 4702/5702 and CHEM 4602/5602 class entitled "Diffusion NMR Spectroscopy".

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

3.7 Technology Development, Patent, Industry Collaborations or Commercialization Activities

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

- Artificial Spider Aciniform Silk Proteins, Methods of Making and Uses Thereof. Liu, X-Q., <u>Rainey, J.K.</u>, Weatherbee-Martin, N. and Xu, L. *United States Provisional Patent 62/287,564*. Filed Jan. 27, 2016; Patent Cooperation Treaty application *PCT/CA2017/050099* Filed Jan. 27, 2017.
- 2. Polyphosphate Glass Microspheres, Methods of Making and Uses Thereof. Mark Filiaggi and Arash Momeni Boroujeni, U.S. Patent Application No. 62/233,646 filed September 28, 2015; International application published as WO 2017/054076 (April 6, 2017).

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

- The pure shift NMR technique PSYCHE (Pure Shift Yielded by CHirp Excitation) was setup on the AVANCE 500 liquids spectrometer during the reporting period. The PSYCHE experiment, like other experiments in this class, yields ¹H spectra containing resonances due to chemical shifts only (singlets with no multiplicity information). This results in considerable simplification of congested and otherwise difficult to decipher spectra.
- A double-presat experiment was setup on the AVANCE 500 liquids spectrometer. This experiment allows researchers to attenuate two dominant signals (normally solvent) instead of the usual limitation of one.
- Routine 1D ²⁷Al observe experiments were setup and made available to all researchers on the AVANCE 300 liquids spectrometer.

3. Industry Collaborations: Solid-State NMR collaborates on proprietary research with:

- CarbonCure Technologies
- Research and Productivity Council
- Tesla-Canada and
- Apotex

3.8 Other Activities Related to Knowledge Exchange or Mobilization

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

- A new document describing how to perform 1D 1 H- 19 F HOESY experiments on the AV-500.
- Significant updates to the following documents were made during the reporting period:
 - Acquiring ²H NMR Spectra on the AV300 Spectrometer (version 1.5, July 2016)
 - High-Temperature NMR on the AV-300 (version 1.5.1, December 2016)
 - Low-Temperature NMR on the AV-300 (version 1.8, July 2016)

2. Given the popularity of online social networking programs and the communication tools these programs provide, in 2012 the NMR³ facility joined Twitter @nmr3_mike. Although email communication with facility personnel is still widely used, followers of NMR³ receive important facility updates, education, and NMR-related information via "tweets". The number of followers of the NMR³ facility has now reached **202**.

3. A successful collaboration between the Halifax-based startup company, CarbonCure Technologies, and Dr. Ulrike Werner-Zwanziger, which used solid-state NMR spectroscopy in the NMR3 to characterize the molecular level cement structure following carbon capture and storage was featured by the Clean Technologies Research Institute (CTRI) website (https://www.dal.ca/dept/ctri/for-industry.html).

4. An NSERC Engage Grant spurred collaboration between NMR³ Director Dr. Jan Rainey and Sackville, NB-based Soricimed Biopharma Inc. began in the prior reporting period, employing high-resolution NMR spectroscopy experiments for structural biology characterization of bioactive peptides of key importance to Soricimed.

Section 4 – Financial Information (April 1, 2016 – March 31, 2017)

4.1 2016-2017 Financial Report

Financial support in '16-'17 came from a total of 2 broad sources: (1) Dalhousie University and (2) User Fees. Again, this FY, Dalhousie funded the total salary costs of the facility and we remain extremely grateful for this expanded salary support during the past two FY's. The Faculty of Science paid 69% of the Coordinator's salary and benefits with the remaining 31% covered by a new Dalhousie Strategic Initiative Fund (SIF). As well, 42% of the Solid-State NMR Coordinator's salary and benefits was paid by the Faculty of Science in support of Professor Joe Zwanziger's Canada Research Chair. The remaining 58% came from our SIF allocation. Direct costs of the facility this past FY included magnet cryogens, lab supplies, computing costs, and all expenses associated with service, maintenance and upgrades.

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

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

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

Solids Hourly Rates: All Instruments			
	Tier 1 Academic Rates ¹	Tier 2 Academic Rates ²	Government/Industry
Hands-On / Collaborative ⁵	\$18.50	\$33.00	\$100.00
Service	\$28.50	\$50.00	\$125.00

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

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

4.2 Grants Directly Related to the Mission Statement of NMR³ Awarded Within the 2016-2017 Fiscal Year

In total, **\$1,535,552** in new grant funds were awarded to Dalhousie University researchers in grants identified by the Centre users as relying upon preliminary data acquired at NMR³ and/or including use of the NMR³ Centre as part of the grant budget. It should be noted that this includes a multi-institution CFI (~\$6.2-million of \$21-million total to Dalhousie); the drug discovery aspects of this CFI project certainly has a clear tie to NMR spectroscopy. It should also be noted that the grants listed below are only newly awarded grants, not ongoing research grants – this is therefore a one year "snapshot" of the critical nature of NMR³ for Dalhousie's competitiveness to capture grant funds. Over the previous four reporting periods (since beginning to report aggregate grant funding), an additional >**\$21.7-million in grant funds has been attributed by Dalhousie users as relying upon the ability to access NMR³ facilities.**

Grants Awarded to Dalhousie–Based NMR³ Users in FY 2016-2017

Principal Applicant: Stephen Bearne

- NSERC Discovery Grant: "Role of Binding Determinants in Enzyme Catalysis", S,L. Bearne (\$180,000 over 5 years)
- NSERC Research Tools & Instruments Grant: "Differential Scanning Calorimeter for Protein Studies", with 5 others including NMR³ users X-Q. Liu and J.K. Rainey (\$143,590)

Principal Applicant: David Jakeman

 Canadian Institutes of Health Research – Project Grant: "Rhamnose Biosynthesis: Alternative Antibacterial Targets" (\$703,000 over 5 years)

Principal Applicant: David Langelaan

• Dalhousie Medical Research Foundation – Capital Equipment Grant: "Equipment for an X-ray crystallography pipeline" (\$23,704)

Principal Applicant: Jan Rainey

- Beatrice Hunter Cancer Research Institute Bridge Funds: "Structure Determination of an Intrinsically Disordered Viral Oncogene", with J. Corcoran (Principal Applicant) (\$15,000; 20%)
- NSERC Idea to Innovation: "Scale-Up and Optimization of Recombinant Spider Wrapping Silk Fibre and Yarn Production", with X-Q. Liu (\$125,000; 50%)
- Springboard Atlantic Innovation Mobilization Program: "Automated Spinning of Yarn from Recombinant Spider Wrapping Silk Fibres for Application in Textiles", with X-Q. Liu (\$20,000 Proof-of-Concept Funding; 50%)
- NSERC Engage Grant: "Biophysical Characterization of Soricidin" (\$25,000)

Principal Applicant: Mark Filiaggi

- Innovacorp Early Stage Commercialization Fund: "Polyphosphate Glass Microsphere for Clinical Use" (\$50,000 -March 13, 2017: March 13, 2018)
- NSERC Discovery Grant: "Comprehensive study of Inorganic Polyphosphates for Biomedical Engineering Applications" (\$135,000 total: April 1, 2016 March 31, 2021)
- NSERC Engage Grant: "Developing Resorbable and Drug-Eluting Embolization Microspheres" (\$25,000: April 1, 2016 October 1, 2016)

Principal Applicant: Mark Stradiotto

• Chevron Phillips Chemical: "Application of a Proprietary Ligand Class", 50% with Laura Turculet (\$65,000 USD for 2016-2017)

Principal Applicant: Younes Anini

• Canadian Fertility and Andrology Society (CFAS): "Validation of Nuclear Magnetic Resonance Spectroscopy to Identify Novel Biomarkers for Infertility" (\$5,000: 10/2016 – 10/2017)

Grants Awarded to NMR³ External Users

Principal Applicant: Andrew Grant (Mount Allison University)

- NSERC Connect Grant: travel to a working gold mine in Newfoundland (\$5,000: January 2017 for 2 months)
- NSEC-IRAP Project: "Alternative Methods of Gold Adsorption" (\$5,000 March 2017)