



National Ultrahigh-Field NMR  
Facility for Solids  
Centre national de RMN à  
ultrahaut champ pour les solides

## Canadian NMR Research News Bulletin #7.3 Summer 2013

### Guest Editorial

**David Bryce (Ottawa)**  
**Yining Huang (Western)**

Magnetic Resonance in Canada and *the Canadian Journal of Chemistry*

Earlier this year **Yining Huang** (Western) was named as the new Senior Editor of the *Canadian Journal of Chemistry* and **David Bryce** (Ottawa) was named the CJC Associate Editor for Magnetic Resonance and Molecular Spectroscopy.

Canada's magnetic resonance community is very strong and is recognized as such around the world. The *Canadian Journal of Chemistry* has published many important and highly-cited papers particularly in the field of NMR spectroscopy over the last several decades. In fact, a 2011 Thomson-Reuters Web of Knowledge analysis of the "relatedness" (a metric based on the strength of cited and citing relationships between journals) of other journals to *CJC* shows two NMR journals in the top ten. Two of the most cited *Can. J. Chem.* papers are NMR papers (by non-Canadians(!)): A.D. Buckingham's "Chemical Shifts in the Nuclear Magnetic Resonance Spectra of Molecules Containing Polar Groups" (**1960**, 38, 300) has been cited nearly 1000 times and R. K. Harris' "Comments on NMR Spectra of the  $X_nAA'X_n'$  Type" (**1964**, 42, 2275) nearly 700 times. Many of Ray Lemieux's important contributions to the NMR characterization of carbohydrates were published in the pages of

### In This Issue

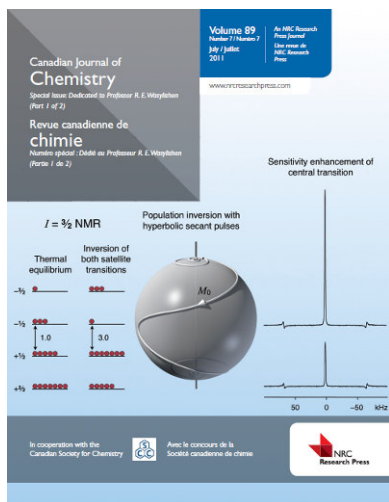
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*CJC*. Other Canadians including J.B. Stothers, T. Schaefer, W.G. Schneider (with co-author and Nobel Laureate John Pople), R.E. Wasylishen, J.A. Ripmeester, C.A. McDowell, and C.A. Fyfe have published some of their best work in Canada's own chemistry journal. Yet, in recent years, the popularity of *CJC* among Canadian authors has diminished. There are many reasons for this, including the desire to publish in what appear to be the 'highest impact' journals. While it is true that the infamous 'impact factor' is not a current strength *CJC*, the journal is very healthy and has several strengths. The cited half-life is greater than 10 years, indicating that contributions to *CJC* are of high quality and continue to garner citations long after their initial publication. *CJC*'s rejection rate approaches 70% and publication times have become highly competitive in the past two



years. Subscriptions to the journal are held in 175 countries, ensuring that articles are accessible.

With our recent appointments we hope to increase the rate of submissions to *CJC* particularly from Canadian researchers. One may ask why we should bother supporting *CJC*. Why shouldn't Canada have its own chemistry journal? Canada funds most of our research and we train Canadian students. Many other countries have their own chemistry journals, to name the few, *the Journal of the American Chemical Society* (USA), *Angewandte Chemie* (Germany), the *Australian Journal of Chemistry* (Australia). *CJC* is a not-for-profit journal. Canada has a strong reputation in chemistry, and a strong reputation in NMR. Yet Canadians publish twice as much in *Chem. Eur. J.* as they do in *CJC*. Canadians have also been quick to embrace start-up foreign journals like *Chemical Science*. The quality of *CJC*, and its associated metrics such as the impact factor, will only increase if Canadians like ourselves support the journal by submitting high-quality work.



This two-part special "NMR" issue of *CJC* published in 2011 and dedicated to Professor R.E. Wasylshen had attracted 35 NMR papers from Canadian and foreign researchers.

<http://www.nrcresearchpress.com/toc/cjc/89/7>  
<http://www.nrcresearchpress.com/toc/cjc/89/7>

## Canadian NMR News

### NSERC 2013 Competition Results

#### Discovery Grants

**Richard Epand** (McMaster) Membrane Interactions and Diacylglycerol Kinases

**Michael Gerken** (Lethbridge) Sulfur in Inorganic Fluorine Chemistry and the Development of a New Class of Weakly Coordinating Anions

**Michel Lafleur** (Montréal) Characterizing, Understanding and Exploiting lipid-lipid interactions

**Isabelle Marcotte** (Québec à Montréal) Nuclear magnetic resonance study of membrane interactions: from intact microorganisms to model membranes

**Igor Mastikhin** (New Brunswick) Magnetic Resonance Imaging of two-phase systems

**Lawrence McIntosh** (UBC) Glycosidases and Glycosyl Transferases

**Scott Prosser** (Toronto) Protein Functional Dynamics and Energy Landscapes

**Giles Santyr** (Western) Novel Approaches for Hyperpolarized Xenon-129 Magnetic Resonance Imaging

**Abdelhamid Sayari** (Ottawa) Nanostructured Materials for Separation and Catalysis

**Simon Sharpe** (Toronto) Structure, assembly, and biological activity of amyloid peptides and proteins

**George Shimizu** (Calgary) Synthesis and properties of metal organic frameworks

**Roderick Wasylshen** (Alberta) Magnetic Resonance Studies of Molecular Structure and Dynamics

**Anand Yethiraj** (Memorial) Tunable hydrodynamics and restricted motions: probing dynamics and the mechanisms of self-organization in soft matter

**Tom Ziegler** (Calgary) The development of new density functional based methods and their application to catalysis

**Josef Zwanziger** (Dalhousie) Structure/Property Relationships in Inorganic Glasses

*continued...*

## Discovery Accelerator Supplement

\$120,000 over three years

**Scott Prosser** (Toronto) Protein Functional Dynamics and Energy Landscapes

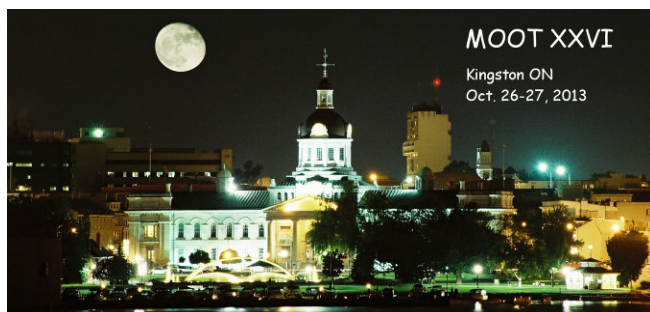
### Research Tools and Instruments (RTI)

**Kim Baines** (Western) Replacement Probe for Inova 600 MHz NMR Spectrometer

**Steve Bourgault, Isabelle Marcotte and Borhane Annabi** (Québec à Montréal) A protein purification platform for biochemistry and structural biology research

**Richard Epand** (McMaster) Isothermal titration calorimeter

**Scott Prosser** (Toronto) Essential Equipment for Membrane Protein Preparation and Purification



### MOOT XXVI NMR Symposium, Kingston, Ontario, October 26-27, 2013

On behalf of the organizing committee, we would like to announce the 26<sup>th</sup> edition of the MOOT NMR Symposium in Kingston, Ontario. The meeting will be held in the new Abramsky House Medical School building at Queen's University on October 26<sup>th</sup> and October 27<sup>th</sup>, 2013. The registration deadline is **September 15<sup>th</sup>**. For more information about the conference and registration details visit

<http://www.mootnmr.org>

Please direct any questions, comments or feedback about upcoming MOOT to [chitayat@queensu.ca](mailto:chitayat@queensu.ca)

We look forward to seeing you in October!

Your MOOT XXVI Organizing Committee,  
Seth Chitayat and Gang Wu

## 20<sup>th</sup> ISMAR in Québec City in 2017

The 20<sup>th</sup> ISMAR (International Society of Magnetic Resonance) Conference will be held at the Québec City Convention Centre from July 23-28, 2017. **Michèle Auger**, Professor of Chemistry at Université Laval and **Jocelyn Guertin**, Sales Manager at the Québec City Convention Centre, presented Québec City's candidacy in Rio de Janeiro during the 18<sup>th</sup> ISMAR Conference last May.

**The International Society of Magnetic Resonance (ISMAR)** is the only international scientific organization that represents the whole range of the important research field of magnetic resonance (MR), in particular nuclear magnetic resonance (NMR), electron paramagnetic resonance (EPR), and magnetic resonance imaging (MRI). These and other MR-methods are used as main research tools in a very wide range of fields including physics, chemistry, life sciences, materials research and medicine. **ISMAR conferences** with typically more than 500 participants were held every three years beginning in 1971.

Today, ISMAR has a large number of active members from many countries throughout the world and has just increased the frequency of its meetings from triennial to **biennial**. Moreover, ISMAR offers **sponsorship** of conferences, workshops, and schools in all fields of magnetic resonance with emphasis on assisting rapidly growing MR communities and fostering young scientists.



ISMAR also administers Prizes and Honors for outstanding contributions to Magnetic Resonance, such as the **ISMAR Fellowship**

and the prestigious **ISMAR Prize** for senior scientists and the newly created **Anatole Abragam Prize** for outstanding young people who are within 5 years of completing their Ph.D. thesis.

We cordially invite you to become a Member and become active in keeping ISMAR alive and responsive to the ever young field of Magnetic Resonance.

<http://www.ismar.org/>

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### **Advances in Magnetic Resonance: From Stem Cells to Catalytic Surfaces**

In his editorial **Lyndon Emsley** (Associate Editor, *J. Am. Chem. Soc.*) reflects on the current state of magnetic resonance spectroscopy.

**Lyndon Emsley** "Advances in Magnetic Resonance: From Stem Cells to Catalytic Surfaces" *J. Am. Chem. Soc.* **135** (2013) 8089–8091. **(Editorial)**

<http://dx.doi.org/10.1021/ja404269a>

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### **Big Science vs. Little Science**

In their recent paper in *PLOS ONE* **Jean-Michel Fortin** and **David J. Currie** (University of Ottawa) analyzed the scientific output of Canadian researchers funded by NSERC. Perhaps to no surprise they have found that the amount of NSERC funding has little impact on scientific productivity (measured by publications), and the impact per dollar was actually lower for larger grants. Authors suggest funding university research as broadly as possible to maximize the outcome and research diversity.

**Jean-Michel Fortin, David J. Currie** "Big Science vs. Little Science: How Scientific Impact Scales with Funding," *PLOS ONE* **8** (2013) e65263. **(open access)**

<http://dx.doi.org/10.1371/journal.pone.0065263>

**Abstract** Agencies that fund scientific research must choose: is it more effective to give large grants to a few elite researchers, or small grants to many researchers? Large grants would be more effective only if scientific impact increases as an accelerating function of grant

size. Here, we examine the scientific impact of individual university-based researchers in three disciplines funded by the Natural Sciences and Engineering Research Council of Canada (NSERC). We considered four indices of scientific impact: numbers of articles published, numbers of citations to those articles, the most cited article, and the number of highly cited articles, each measured over a four-year period. We related these to the amount of NSERC funding received. Impact is positively, but only weakly, related to funding. Researchers who received additional funds from a second federal granting council, the Canadian Institutes for Health Research, were not more productive than those who received only NSERC funding. Impact was generally a decelerating function of funding. Impact per dollar was therefore lower for large grant-holders. This is inconsistent with the hypothesis that larger grants lead to larger discoveries. Further, the impact of researchers who received increases in funding did not predictably increase. We conclude that scientific impact (as reflected by publications) is only weakly limited by funding. We suggest that funding strategies that target diversity, rather than "excellence", are likely to prove to be more productive.

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### **Free online NMR databases**



the **Spectral Database for Organic Compounds** (SDBS) supported by the Japan's National Institute of Advanced Industrial Science and Technology (AIST) is a popular and free online tool containing reliable spectroscopic data for over 34000 organic compounds. The database contains six types of spectra, electron impact mass spectra (EI-MS), FT-IR, liquid-state  $^1\text{H}$  and  $^{13}\text{C}$  NMR, Raman and ESR.

[http://sdbs.riodb.aist.go.jp/sdbs/cgi-bin/cre\\_index.cgi](http://sdbs.riodb.aist.go.jp/sdbs/cgi-bin/cre_index.cgi)

Less known, SDBS database has recently branched into the **Solid-Sate NMR Spectral Database** (SSNMR\_SD) to the delight of all NMR folks working in the field. Even though much work lies ahead, SSNMR\_SD database has potential to become a rival of its sister database in many areas of materials research.

[http://riodb.ibase.aist.go.jp/ssnmr/index\\_eng.html](http://riodb.ibase.aist.go.jp/ssnmr/index_eng.html)



## Recognition

Professor **Richard Epand** (McMaster) is among nine recipients of the **2012 Barth Syndrome Foundation Research Grants**.

<http://www.barthsyndrome.org/english/view.asp?x=1705&mp=1648>

In early March 2013 **the Barth Syndrome Foundation, Inc.** announced the award of nine research grants to investigators in the US, Canada, and Europe. Since the 2002 season the Barth Syndrome Foundation, in consultation with its Scientific and Medical Advisory Board and with the support of the international affiliate chapters (Barth Syndrome Foundation of Canada, Barth Syndrome Trust {UK and Europe} and Association Barth France), has awarded over US \$2.7 million to more than 43 investigators worldwide in order to better understand this rare X-linked genetic disease characterized by cardiomyopathy, growth delay, muscle hypoplasia, neutropenia and extreme fatigue. This competitive grant program has resulted in many publications which are unraveling the details of this multi-faceted disease and are leading towards new ideas for treatment. Many of the past and present grant awardees will be attending the 7<sup>th</sup> International Barth Syndrome Foundation Scientific, Medical and Family Conference on June 23-28, 2014 in Clearwater, Florida.

<http://www.barthsyndrome.org/english/view.asp?x=1323&id=279>

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### 96<sup>th</sup> CSC Student Awards

**Fred Perras** (Bryce/Ottawa) won the 1<sup>st</sup> place prize (Physical/Theoretical Division) for his oral presentation at the 96<sup>th</sup> Canadian Chemistry Conference.

**Jasmine Viger-Gravel** (Bryce/Ottawa) won the second place poster prize (Physical Theoretical Division) at the 96<sup>th</sup> Canadian Chemistry Conference.

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### Scholarships and Fellowships

**Souryvanh Nirasay** (Marcotte/UQAM) has received a Ph.D. Scholarship from the *Fonds de recherche du Québec - Nature et technologies* (FQRNT).

**Michela Artizzu** (Marcotte/UQAM) was awarded an Undergraduate Student Scholarship from *the Create Training Program in Bionanomachines*.

**Jasmine Viger-Gravel** (Bryce/Ottawa) was awarded a *FQRNT Doctoral Scholarship*.

**Dr. Cory Widdifield** (Bryce/Ottawa) has received a prestigious *NSERC Postdoctoral Fellowship*. Cory is currently carrying out studies with Lyndon Emsley at ENS in Lyon.

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### NMR Theses Recently Defended

**Rebecca Jamieson** (University of Guelph)  
June 2013

Supervisor: Prof. Glenn Penner

**Ph.D. thesis:** "A Solid-state NMR Study of Tin and Phosphorus Containing Compounds"

External Examiner: Prof. Gillian Goward (McMaster)

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**Yeong Ju Noh** (University of Western Ontario)  
June 2013

Supervisor: Prof. Gary Shaw

**M.Sc. thesis:** "Structure of C-terminal Domain of Parkin, IBR-RING2"

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**Denis-Alexandre Trottier** (University of Waterloo) July 2013

Supervisor: Prof. Raymond Laflamme

**M.Sc. thesis:** "Liquid Crystal State NMR Quantum Computing – Characterization, Control and Certification"

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**Laure Soucémarianadin** (University of Alberta) July 2013

Supervisors: Prof. Sylvie Quideau (Renewable Resources) and Prof. Roderick Wasylshen (Chemistry)

**Ph.D. thesis:** "Black Carbon in Quebec Boreal Black Spruce Forests"

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## NMR Events

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### **ICMRM-12** 12<sup>th</sup> International Conference on Magnetic Resonance Microimaging

August 25-29, 2013, Fitzwilliam College,  
University of Cambridge, UK

<http://www.ceb.cam.ac.uk/ICMRM12>

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### **8<sup>th</sup> Alpine Conference on Solid-State NMR**

September 8-12, 2013, Chamonix Mont-Blanc,  
France

<http://www.alpine-conference.org>

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### **SMASH 2013** Small Molecule NMR Conference

Sept 22-25, 2013, Santiago de Compostela,  
Spain

<http://www.smashnmr.org/>

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### **MOOT XXVI NMR Symposium**

October 26-27, 2013, Queen's University,  
Kingston, ON

<http://www.mootnmr.org>

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5<sup>th</sup> Asia-Pacific NMR Symposium (**APNMR5**)  
and 9<sup>th</sup> Australian & New Zealand Society for  
Magnetic Resonance (**ANZMAG**) Meeting

October 27-30, 2013, Brisbane, Australia

<http://apnmr2013.org/>

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### **57<sup>th</sup> Conference on Magnetism and Magnetic Materials**

November 4-8, 2013, Denver, Colorado

<http://www.magnetism.org/>

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### **6<sup>th</sup> Annual GRASP Symposium**

November 25, 2013, McGill University,  
Montréal, QC, Canada

<http://grasp.mcgill.ca/english/conferences/conferences.html>

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### **PANIC 2014** Practical Applications of NMR in Industry Conference

February 3-5, 2014, Charlotte, NC

<http://www.panicnmr.com/>

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### **55<sup>th</sup> ENC**

March 23-28, 2014, Boston, MA

<http://www.enc-conference.org/>

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**CSC 2014**, the 97<sup>th</sup> Canadian Chemistry  
Conference and Exhibition  
"Chemistry from Sea to Sky"

June 1-5, 2014, Vancouver, B.C., Canada

<http://www.csc2014.ca/>

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### **56<sup>th</sup> Rocky Mountain Conference on Magnetic Resonance: Solid-State NMR Symposium & EPR Symposium**

July 13-17, 2014, Copper Mountain, Colorado

<http://www.rockychem.com/symposia/solid-state-nmr-symposium.html>

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**ICMRBS 2014**, the XXVI<sup>th</sup> International  
Conference on Magnetic Resonance in  
Biological Systems

August 24-29, 2014, Dallas, Texas

<http://www.icmrbs.org/>

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**Pacificchem 2015** The International  
Chemical Congress of Pacific Basin  
Societies

December 15-20, 2015, Honolulu, Hawaii, USA

<http://www.pacificchem.org/>

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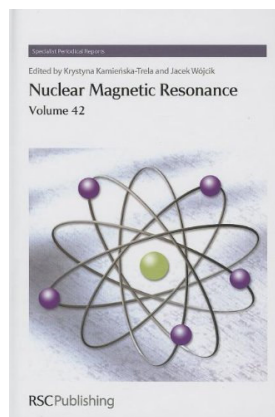
**ISMAR 2017** 20<sup>th</sup> ISMAR (International  
Society of Magnetic Resonance)  
Conference

July 23-28, 2017, Québec City, Québec,  
Canada

<http://www.ismar.org/>

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## New NMR Books from RSC



### Nuclear Magnetic Resonance: Volume 42 (Specialist Periodical Reports)

**Editors:** Krystyna Kamienska-Trela, Jacek Wojcik

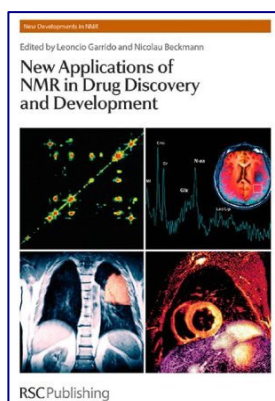
**Hardcover:** 415 pages  
**Language:** English  
**Publisher:** RSC (April, 2013)  
**ISBN:** 978-1849735773

<http://www.amazon.com/dp/1849735778>  
<http://www.amazon.ca/dp/1849735778>

**RSC:** With over 17,000 articles concerning NMR published per year, keeping up to date with the latest developments and applications of this technique can prove time-consuming. Now in its 42<sup>nd</sup> volume, the Specialist Periodical Report on NMR provides a digest of the current literature, compiled by experts in the field. The current volume devotes several chapters to the aspects and applications of spin-spin couplings, and biochemists will find separate chapters dedicated to proteins, lipids and carbohydrates. Further chapters discuss the latest developments in nuclear shielding, imaging and NMR in living systems. For a comprehensive account of the latest developments and research using NMR, look no further than Specialist Periodical Reports - Nuclear Magnetic Resonance. An essential book for NMR lab bench and university library shelf.

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<http://pubs.rsc.org/en/content/ebook/978-1-84973-577-3>



### New Applications of NMR in Drug Discovery and Development

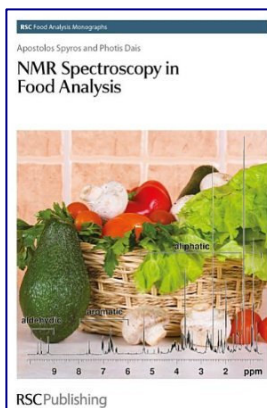
**Editors:** Leoncio Garrido, Nicolau Beckmann

**Hardcover:** 304 pages  
**Language:** English  
**Publisher:** RSC (July, 2013)  
**ISBN:** 978-1849734448

<http://www.amazon.com/dp/1849734445>  
<http://www.amazon.ca/dp/1849734445>

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<http://pubs.rsc.org/en/content/ebook/978-1-84973-444-8>



### NMR Spectroscopy in Food Analysis

**Editors:** Apostolos Spyros, Photis Dais

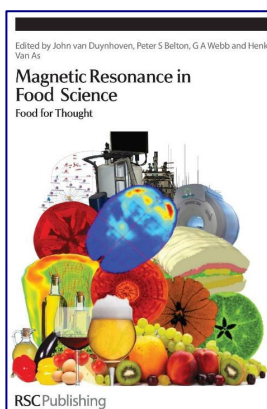
**Hardcover:** 220 pages  
**Language:** English  
**Publisher:** RSC (October, 2012)  
**ISBN:** 978-1849731751

<http://www.amazon.com/dp/1849731756>  
<http://www.amazon.ca/dp/1849731756>

**RSC:** During the last two decades, the use of NMR spectroscopy for the characterization and analysis of food materials has flourished, and this trend continues to increase today. Currently, there exists no book that fulfils specifically the needs of food scientists that are interested in adding or expanding the use of NMR spectroscopy in their arsenal of food analysis techniques. Current books and monographs are rather addressed to experienced researchers in food analysis providing new information in the field. This book, written by acknowledged experts in the field, fills the gap by offering a day to day NMR guide for the food scientist, affording not only the basic theoretical aspects of NMR spectroscopy, but also practical information on sample preparation, experimental conditions and data analysis. Current developments in the field covered in this book are the availability of solid state NMR experiments such as CP/MAS and HR-MAS NMR for the analysis of semisolid foods.

#### Table of contents

<http://pubs.rsc.org/en/content/ebook/978-1-84973-175-1>



### Magnetic Resonance in Food Science: From Food to Thought

**Editors:** John van Duynhoven, Peter S. Belton, G.A. Webb, Henk van As

**Hardcover:** 220 pages  
**Language:** English  
**Publisher:** RSC (April, 2013)  
**ISBN:** 978-1849736343

<http://www.amazon.com/dp/1849736340>  
<http://www.amazon.ca/dp/1849736340>

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<http://pubs.rsc.org/en/content/ebook/978-1-84973-634-3>

## NMR Software

Reposted with permission. Originally published on <http://www.theresonance.com/>

May 29, 2013 // Structural Biology

### Assisted NMR Data Interpretation in Synthetic Chemistry

"The research group of Prof. H el ene Lebel at the Universit e de Montr eal focuses on catalysis in synthetic organic chemistry. The major aim of her research is the development of novel synthetic methodologies using organometallic complexes as catalysts. As well as a strong background in organic and organometallic chemistry, this research also requires the use of sophisticated techniques such as NMR spectroscopy, mass spectrometry and X-ray crystallography, in order to identify reaction pathways and verify reaction products."

**Authors:** Johan Bartholom eus<sup>1</sup>, Martine Monette<sup>2</sup>, Rajeev Kumar<sup>2</sup>, Sandra Groscurth<sup>3</sup>, H el ene Lebel<sup>1</sup>

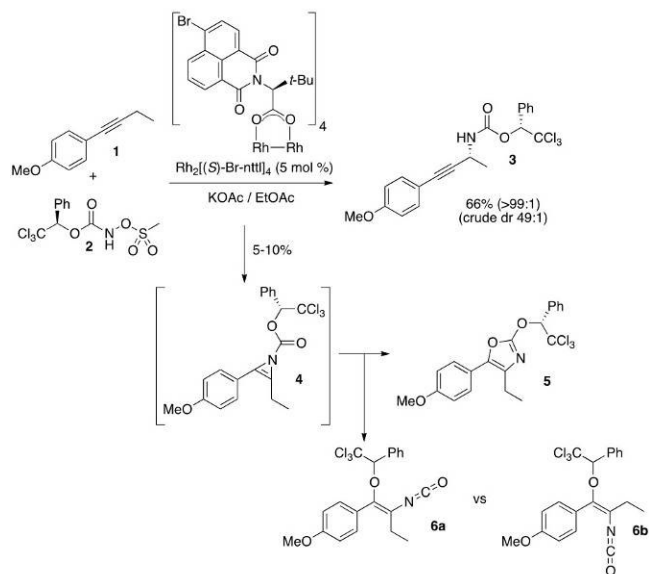
<sup>1</sup> Universit e de Montreal, <sup>2</sup> Bruker BioSpin Canada, <sup>3</sup> Bruker BioSpin Switzerland

One of Prof. Lebel's current research topics aims to synthesize chiral amines via a C-H insertion reaction, using a novel chiral N-methanesulfonyloxycarbamate **[1]**.

For instance, reaction of alkyne **1** with reagent **2** in the presence of a chiral rhodium dimer led to chiral amine **3** in good yields and high stereoselectivity (See **Figure 1**).

As these propargylic C-H amination reactions typical yield around 60-65% of the desired product, they looked at the by-products formed during this reaction. One of them was isolated in the 5-10% yield.

As <sup>1</sup>H NMR spectra reveals the presence of the ethyl group, as well as the proton alpha to the CCl<sub>3</sub> group, they hypothesized a reaction with the alkyne moiety to form <sup>1</sup>H-azirine **4**, which is known to rearrange and form the corresponding oxazole **5**. The full interpretation of the NMR spectra would have been quite complex, and giving the small amount of material obtained (few mg) the suitable crystals for X-ray crystal structure analysis would have been particularly challenging.



**Figure 1:** Stereoselective and regioselective rhodium-catalyzed propargylic C-H amination reaction

In order to support the chemist in this complex but essential routine task, Bruker developed powerful software tools for interactive and assisted NMR data analysis.

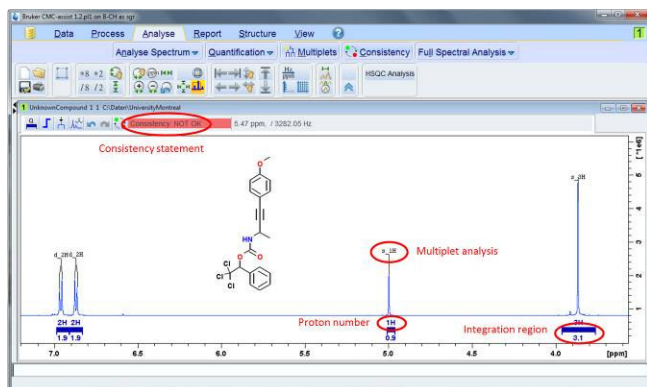
In most cases, verification of reaction products is based on molecular mass determination and the interpretation of NMR spectra, typically 1D proton spectra. With the aid of Bruker's CMC-assist software solution, these 1D proton spectra can be processed and analyzed at the push of a button. Instead of having to concentrate on the appropriate processing method and then having to analyze the spectrum manually step by step, the CMC-assist software performs these tasks and provides a consistency statement within a few seconds.

In the case of the stereospecific reaction (**Figure 1**), the automated spectra interpretation first confirms that structure **3** and experimental data are not in agreement.

In order to identify the actual synthesized compound a complete structure elucidation was performed. Based on the information from additional NMR data such as 1D <sup>13</sup>C, HSQC, HMBC and COSY spectra, the software CMC-se assists with the process of structure elucidation by analyzing the spectra automatically, translating the NMR correlations into atomic



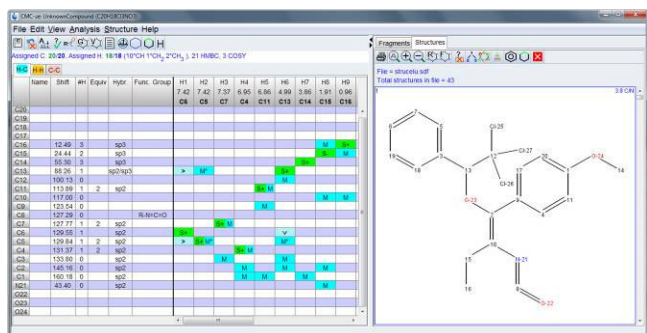
connectivities and proposing possible structures that fit all experimental data.



**Figure 2:** 1D  $^1\text{H}$  spectrum analyzed by the automated structure verification software CMC-assist. Although the signals in the spectrum do not match the expected molecular structure, the spectrum gets analyzed with respect to peak integration, proton number determination and multiplet analysis.

Although structure elucidation still requires some manual interaction, the software CMC-se speeds up the process significantly and provides a convenient tool to both handle the data and to identify the unknown structure.

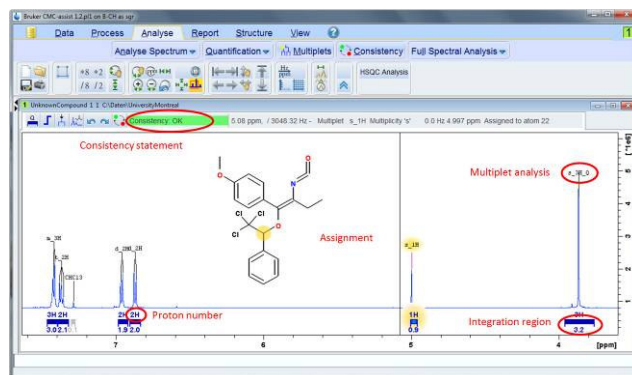
In the case of the by-product obtained from the amination reaction, initially assigned as 5, CMC-se readily identified the actual synthesized compound. By providing the CMC-assist software with the newly identified reaction product, the automated structure verification then confirms the consistency of spectrum and structure.



**Figure 3:** Complete structure elucidation assisted by the software CMC-se.

Isocyanate 6a was assigned as the by-product, instead of the expected oxazole 5. This information was relevant to Prof. Lebel's group,

as it showed that the  $^1\text{H}$ -azirine 4 rearrange in an unexpected fashion, and thus could help them in designing novel reaction pathways.



**Figure 4:** 1D  $^1\text{H}$  spectrum analyzed by the automated structure verification software CMC-assist. The assignment can be visualized by hovering the mouse over any peak and the corresponding atom of the molecule will be highlighted. In order to document the spectrum interpretation, different reports can be generated and attached to the records in the lab notebook. In addition, the spectrum description can be readily exported as publication string in various journal formats.

This stereospecific organic reaction, performed at Prof. Lebel's lab as part of her research on the development of novel synthetic strategies, represents a typical example of the daily work of a chemist.

Nowadays the chemistry underlying syntheses such as this is quite complex. Ideally the chemist should not be additionally occupied by the interpretation of the NMR data.

With the chemist in mind Bruker has further developed the software packages CMC-assist – for automated structure verification, and CMC-se – for computer aided structure elucidation. As shown by Prof. Lebel's example, these software packages reliably analyze NMR spectra, significantly speeding up the process of analytical data interpretation.

[1] **Hélène Lebel, Carl Trudel, Cédric Spitz**, "Stereoselective intermolecular C–H amination reactions," *Chem. Commun.* **48** (2012) 7799–7801.

<http://dx.doi.org/10.1039/c2cc33689h>

See original post and high-resolution figures:

<http://tinyurl.com/pmhq3hq>

## NMR Jobs and Vacancies

### PhD/MSc positions in solid-state NMR, Université du Québec à Montréal

We are looking for **two** motivated and dynamic PhD or MSc candidates to join our Laboratory of NMR of Biological Systems as early as May 2013. Candidates must be interested in membrane physico-chemistry and NMR spectroscopy with biological applications and have a background in chemistry or biochemistry or related field.

The research projects concern the in vivo NMR study of the interaction of drugs and environmental contaminants with microorganisms such as bacteria and microalgae, as well as the development of model cell membranes to study specific interactions with membrane components. Students will have full access to 400 and 600 MHz NMR spectrometers as well as infrastructure for bacterial and microalgal cell growth.

Interested students should contact Prof. Isabelle Marcotte at:

[marcotte.isabelle@uqam.ca](mailto:marcotte.isabelle@uqam.ca)

**Prof. Isabelle Marcotte**, Ph.D.  
Department of Chemistry  
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### University of Toronto, Predoctoral or Postdoctoral Position in Protein NMR and MRI (Autumn 2013)

Our biomolecular engineering laboratory is located within the Clinical Imaging Research department at the Sunnybrook Research Institute and is associated with the Departments of Medical Biophysics and Pharmaceutical Sciences at the University of Toronto. Our group plans to recruit a Ph.D. candidate or a Postdoctoral Fellow with experience in either protein NMR [familiar with protein expression, deuteration and protein isotope-labeling methods] or MRI approaches [small animal imaging with contrast agents] to develop new MRI contrast agents able to

detect metabolic events, immune and inflammatory responses and/or tumour foci in vivo. The applicant will interface with chemists and molecular biologists in our laboratory that are developing biomolecules as imaging probes and/or therapeutic agents. This individual will also be involved in collaborations between our laboratory and several MRI groups on site involved in pre-clinical and clinical MRI research. Instrumentation within our Imaging research group includes both pre-clinical and clinical MRI instruments as well as state-of-the-art ultrasound and SPECT/PET/CT instruments.

**Qualifications:** M.Sc. or Ph.D. in Protein NMR or with practical experience in MRI techniques involving contrast agents performed on small animals. The applicant must have one or more publications proving that he/she has a practical knowledge of such techniques and must be willing to work with animals. Interested individuals should forward their CV and a cover letter by email to **Dr. Jean Gariépy** and have two letters of recommendation sent separately to the same email address by referees.

**Prof. Jean Gariépy**, Ph.D.  
Departments of Medical Biophysics &  
Pharmaceutical Sciences  
University of Toronto  
SRI Research Chair in Biomolecular  
Engineering  
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Phone: (416) 480-5704 / Fax: (416) 480-5714

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### M.Sc. or Ph.D. position in solid-state NMR at the University of Ottawa

Highly motivated candidates interested in physical chemistry and/or NMR spectroscopy are invited to apply for a M.Sc. or Ph.D. in the group of **Prof. David Bryce** at the University of Ottawa  
<http://mysite.science.uottawa.ca/dbryce/>

Research in solid-state NMR in the Bryce group covers a variety of areas including the development of the spectroscopy of

traditionally difficult quadrupolar nuclei, applications of double-rotation NMR, applications to weak interactions including halogen bonding, and the study of polymorphism. Experimental work is complemented by quantum chemical studies. Interested students should contact Prof. Bryce directly at [dbryce@uottawa.ca](mailto:dbryce@uottawa.ca)

Please note that due to budgetary constraints, the position is open only to Canadian students.

Prof. **David L. Bryce**, Ph.D.  
Department of Chemistry  
10 Marie Curie Private  
University of Ottawa  
Ottawa, Ontario K1N6N5  
Canada  
Phone 613-562-5800 ext 2018  
Fax 613-562-5170  
Email [dbryce@uottawa.ca](mailto:dbryce@uottawa.ca)  
Web <http://mysite.science.uottawa.ca/dbryce/>

Two **postdoctoral positions** are available to work in the Biomembrane Structure Unit, in the Biochemistry Department at Oxford University, UK.

[http://nmr900.ca/nmr\\_jobs.html#oxford](http://nmr900.ca/nmr_jobs.html#oxford)

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Canadian NMR News  
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## Canadian NMR Research Highlights

### NMR paper in *Science*

**J.-F. Trempe, V. Sauvé, K. Grenier, M. Seirafi, M.Y. Tang, M. Ménade, S. Al-Abdul-Wahid, J. Krett, K. Wong, G. Kozlov, B. Nagar, E.A. Fon, K. Gehring**, "Structure of Parkin Reveals Mechanisms for Ubiquitin Ligase Activation," *Science* **340** (2013) 1451-1455.  
<http://dx.doi.org/10.1126/science.1237908>

*Science Editor's Summary: Parkin Enhanced?* Inactivation of parkin, an E3 ubiquitin ligase, is responsible for a familial form of Parkinson's disease and may be involved in sporadic forms as well. **Trempe et al.** (p. 1451, published online 9 May) present the crystal structure of full-length parkin in an autoinhibited configuration. Guided by the structure, mutations were designed that activated parkin both in vitro and in cells. Because parkin is neuroprotective, the structure provides a framework for enhancing parkin function as a therapeutic strategy in Parkinson's disease.

### NMR paper in *Angewandte Chemie*

**A. Mainz, T.L. Religa, R. Sprangers, R. Linser, L.E. Kay, and B. Reif**, "NMR Spectroscopy of Soluble Protein Complexes at One Mega-Dalton and Beyond," *Angew. Chem. Int. Ed.* **52** (2013) 8746-8751.  
<http://dx.doi.org/10.1002/anie.201301215>

### NMR paper in *Nature Structural & Molecular Biology*

**T. Moldoveanu, C.R. Grace, F. Llambi, A. Nourse, P. Fitzgerald, K. Gehring, R.W. Kriwacki and D.R. Green**, "BID-induced structural changes in BAK promote apoptosis," *Nature Structural & Molecular Biology* **20** (2013) 589-597.  
<http://dx.doi.org/10.1038/nsmb.2563>

### NMR papers in *PNAS*

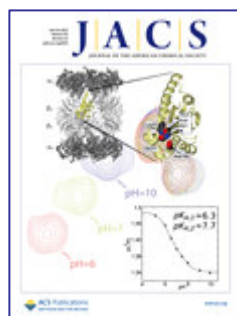
**A. Sekhar and L.E. Kay**, "NMR paves the way for atomic level descriptions of sparsely populated, transiently formed biomolecular conformers," *Proc. Natl. Acad. Sci. USA* **110** (2013) 12867-12874. (**Perspective**)  
<http://dx.doi.org/10.1073/pnas.1305688110>

**C. Li, M. Enomoto, A.M. Rossi, M.-D. Seo, T. Rahman, P.B. Stathopoulos, C.W. Taylor, M. Ikura, and J.B. Ames,** "CaBP1, a neuronal Ca<sup>2+</sup> sensor protein, inhibits inositol trisphosphate receptors by clamping intersubunit interactions," *Proc. Natl. Acad. Sci. USA* **110** (2013) 8507–8512.

<http://dx.doi.org/10.1073/pnas.1220847110>

**K. Shin, K.A. Udachin, I.L. Moudrakovski, D.M. Leek, S. Alavi, C.I. Ratcliffe, and J.A. Ripmeester,** "Methanol incorporation in clathrate hydrates and the implications for oil and gas pipeline flow assurance and icy planetary bodies," *Proc. Natl. Acad. Sci. USA* **110** (2013) 8437–8442.

<http://dx.doi.org/10.1073/pnas.1302812110>



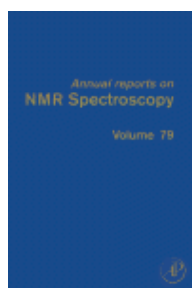
Cover article in the  
*Journal of the American  
Chemical Society*

**A. Velyvis and L.E. Kay,** "Measurement of Active Site Ionization Equilibria in the 670 kDa Proteasome Core Particle Using Methyl-TROSY NMR," *J. Am. Chem. Soc.* **135** (2013) 9259–9262.

<http://dx.doi.org/10.1021/ja403091c>

### Annual Reports on NMR Spectroscopy

**I.L. Moudrakovski** "Recent Advances in Solid-State NMR of Alkaline Earth Elements," *Annual Reports on NMR Spectroscopy* **79** (2013) 129–240. **(Invited Review)**



<http://dx.doi.org/10.1016/B978-0-12-408098-0.00004-5>

### Review in *Environmental Reviews*

**B.P. Lankadurai, E.G. Nagato, and M.J. Simpson,** "Environmental Metabolomics: An Emerging Approach to Study Organism Responses to Environmental Stressors," *Environmental Reviews* (2013) accepted. **(Review)**

<http://dx.doi.org/10.1139/er-2013-0011>

### Reviews in *FEBS Journal*

**Z. Bozoky, M. Krzeminski, P.A. Chong and J.D. Forman-Kay,** "Structural changes of CFTR R region upon phosphorylation: a plastic platform for intra- and inter-molecular interactions," *FEBS Journal* (2013) online. **(Review)**

<http://dx.doi.org/10.1111/febs.12422>

**D. Gagné, N. Doucet,** "Structural and functional importance of local and global conformational fluctuations in the RNase A superfamily," *FEBS Journal* (2013) online. **(Review)**

<http://dx.doi.org/10.1111/febs.12371>

**F.J. Amador, P.B. Stathopoulos, M. Enomoto, M. Ikura,** "Ryanodine Receptor Calcium Release Channels: Lessons from structure-function studies," *FEBS Journal* (2013) online. **(Review)**

<http://dx.doi.org/10.1111/febs.12194>

### Review in *Accounts of Chemical Research*

**R.W. Schurko,** "Ultra-Wideline Solid-State NMR Spectroscopy," *Acc. Chem. Res.* (2013) online. **(Review)**

<http://dx.doi.org/10.1021/ar400045t>

### Review in *Trends in Analytical Chemistry*

**D.S. Wishart,** "Characterization of biopharmaceuticals by NMR spectroscopy," *Trends in Analytical Chemistry* **48** (2013) 96–111. **(Review)**

<http://dx.doi.org/10.1016/j.trac.2013.03.009>

### NMR Research highlighted by *the Canadian Chemical News*

*New technique improves NMR spectroscopy*  
May/June 2013 Physical Chemistry

<http://www.cheminst.ca/magazine/news/new-technique-improves-nmr-spectroscopy>

**F.A. Perras and D.L. Bryce,** "Measuring Dipolar and J Coupling Between Quadrupolar Nuclei Using Double-Rotation NMR," *Journal of Chemical Physics* **138** (2013) 174202.

<http://dx.doi.org/10.1063/1.4802192>



## Recent NMR Publications

most recent NMR publications by Canadian research groups as they appear on <http://nmr900.ca> website. This list should not be considered complete. You are encouraged to let us know of your recent publications as they become available.

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### Agriculture and Agri-Food Canada, Charlottetown

**C.W. Kirby, T. Wu, R. Tsao, J.L. McCallum,** "Isolation and structural characterization of unusual pyranoanthocyanins and related anthocyanins from Staghorn sumac (*Rhus typhina* L.) via UPLC-ESI-MS,  $^1\text{H}$ ,  $^{13}\text{C}$ , and 2D NMR spectroscopy," *Phytochemistry* (2013) online.  
<http://dx.doi.org/10.1016/j.phytochem.2013.06.017>

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### Boehringer Ingelheim (Canada) Ltd, Laval

**S.R. LaPlante, N. Aubry, G. Bolger, P. Bonneau, R. Carson, R. Coulombe, C. Sturino, P.L. Beaulieu,** "Monitoring Drug Self-Aggregation and Potential for Promiscuity in Off-target *In vitro* Pharmacology Screens by a Practical NMR Strategy," *Journal of Medicinal Chemistry* (2013) accepted.  
<http://dx.doi.org/10.1021/jm4008714>

**S.R. Laplante, F. Bilodeau, N. Aubry, J.R. Gillard, J. O'Meara, R. Coulombe,** "N- versus O-alkylation: Utilizing NMR methods to establish reliable primary structure determinations for drug discovery," *Bioorganic and Medicinal Chemistry Letters* **23** (2013) 4663-4668.  
<http://dx.doi.org/10.1016/j.bmcl.2013.06.007>

**S.R. LaPlante, R.J. Carson, J.R. Gillard, N. Aubry, R. Coulombe, S. Bordeleau, P.R. Bonneau, M. Little, J.A. OMeara, and P.L. Beaulieu,** "Compound Aggregation in Drug Discovery: Implementing a Practical NMR Assay for Medicinal Chemists," *Journal of Medicinal Chemistry* **56** (2013) 5142-5150.  
<http://dx.doi.org/10.1021/jm400535b>

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### Université de Sherbrooke

**D. Létourneau, A. Lorin, A. Lefebvre, J. Cabana, P. Lavigne, J.-G. LeHoux,** "Thermodynamic and solution state NMR characterization of the binding of secondary

and conjugated bile acids to STARD5," *Biochimica et Biophysica Acta (BBA) - Molecular and Cell Biology of Lipids* (2013) online.  
<http://dx.doi.org/10.1016/j.bbalip.2013.07.005>

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### INRS-Institut Armand-Frappier

**D. Gagné, N. Doucet,** "Structural and functional importance of local and global conformational fluctuations in the RNase A superfamily," *FEBS Journal* (2013) online. **(Review)**  
<http://dx.doi.org/10.1111/febs.12371>

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**I.E. Gulerez, K. Gehring,** "X-ray crystallography and NMR as tools for the study of protein tyrosine phosphatases," *Methods* (2013) accepted.  
<http://dx.doi.org/10.1016/j.ymeth.2013.07.032>

**J.-F. Trempe, V. Sauvé, K. Grenier, M. Seirafi, M.Y. Tang, M. Ménade, S. Al-Abdul-Wahid, J. Krett, K. Wong, G. Kozlov, B. Nagar, E.A. Fon, K. Gehring,** "Structure of Parkin Reveals Mechanisms for Ubiquitin Ligase Activation," *Science* **340** (2013) 1451-1455.  
<http://dx.doi.org/10.1126/science.1237908>

**A. Kumar, D.C. Burns, M.S. Al-Abdul-Wahid, and G.A. Woolley,** "A Circularly Permuted Photoactive Yellow Protein as a Scaffold for Photoswitch Design," *Biochemistry* **52** (2013) 3320-3331.  
<http://dx.doi.org/10.1021/bi400018h>

**T. Moldoveanu, C.R. Grace, F. Llambi, A. Nourse, P. Fitzgerald, K. Gehring, R.W. Kriwacki and D.R. Green,** "BID-induced structural changes in BAK promote apoptosis," *Nature Structural & Molecular Biology* **20** (2013) 589-597.  
<http://dx.doi.org/10.1038/nsmb.2563>

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### University of Ottawa

**F.A. Perras and D.L. Bryce,** "Symmetry-Amplified *J* Splittings for Quadrupolar Spin Pairs: A Solid-State NMR Probe of Homoatomic Covalent Bonds," *Journal of the American Chemical Society* **135** (2013) accepted.  
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<http://dx.doi.org/10.1039/c3ce40875b>



**C.M. Widdifield, G. Cavallo, G.A. Facey, T. Pilati, J. Lin, P. Metrangolo, G. Resnati and D.L. Bryce,** "Multinuclear Solid-State Magnetic Resonance as a Sensitive Probe of Structural Changes upon the Occurrence of Halogen Bonding in Co-Crystals," *Chemistry - A European Journal* **19** (2013) online.  
<http://dx.doi.org/10.1002/chem.201300809>



**K.M.N. Burgess, Y. Xu, M.C. Leclerc, and D.L. Bryce,** "Insight into Magnesium Coordination Environments in Benzoate and Salicylate Complexes through  $^{25}\text{Mg}$  Solid-State NMR Spectroscopy," *Journal of Physical Chemistry A* **117** (2013) 6561–6570.  
<http://dx.doi.org/10.1021/jp405145b>

**A. Ahmadalinezhad, R. Tailor, and A. Sayari,** "Molecular-Level Insights into the Oxidative Degradation of Grafted Amines," *Chemistry - A European Journal* **19** (2013) 10543–10550.  
<http://dx.doi.org/10.1002/chem.201300864>

**H. Mohammadi-Manesh, S. Alavi, T.K. Woo, B. Najafi,** "Computational prediction of temperature dependence of  $^{13}\text{C}$  NMR lineshapes of planar molecules in structure I clathrate hydrates," *Journal of the Iranian Chemical Society* **10** (2013) 659–667.  
<http://dx.doi.org/10.1007/s13738-012-0198-9>

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## NRC Canada



**K.E. Johnston, C.A. O'Keefe, R.M. Gauvin, J. Trébosc, L. Delevoye, J.-P. Amoureux, N. Popoff, M. Taoufik, K. Oudatchin, and R.W. Schurko,** "A Study of Transition-Metal Organometallic Complexes Combining  $^{35}\text{Cl}$  Solid-State NMR Spectroscopy and  $^{35}\text{Cl}$  NQR Spectroscopy and First-Principles DFT Calculations," *Chemistry - A European Journal* **19** (2013) online.  
<http://dx.doi.org/10.1002/chem.201301268>

**F.L. Lin, E. Vinogradov, C. Deng, S. Zeller, B.A. Green, K.U. Jansen, V. Pavliak,** "Identification of the Common Antigenic Determinant Shared by Streptococcus pneumoniae Serotypes 33A, 35A and 20 Capsular Polysaccharides," *Carbohydrate Research* (2013) accepted.  
<http://dx.doi.org/10.1016/j.carres.2013.08.001>



**X. Kong, M. Shan, V.V. Terskikh, I. Hung, Z. Gan, and G.Wu,** "Solid-State  $^{17}\text{O}$  NMR of Pharmaceutical Compounds: Salicylic Acid and Aspirin," *Journal of Physical Chemistry B* **117** (2013) online.  
<http://dx.doi.org/10.1021/jp405233f>

**R.G. Lees-Miller, J.A. Iwashkiw, N.E. Scott, A. Seper, E. Vinogradov, S. Schild, M.F. Feldman,** "A common pathway for O-linked protein-glycosylation and synthesis of capsule in *Acinetobacter baumannii*," *Molecular Microbiology* (2013) accepted.  
<http://dx.doi.org/10.1111/mmi.12300>

**I.L. Moudrakovski** "Recent Advances in Solid-State NMR of Alkaline Earth Elements," *Annual Reports on NMR Spectroscopy* **79** (2013) 129–240. (Invited Review)  
<http://dx.doi.org/10.1016/B978-0-12-408098-0.00004-5>



**P. He, J. Xu, V.V. Terskikh, A. Sutrisno, H.-Y. Nie, and Y. Huang,** "Identification of Non-equivalent Framework Oxygen Species in Metal-organic Frameworks by  $^{17}\text{O}$  Solid-state NMR," *Journal of Physical Chemistry C* **117** (2013) online. (Cover Article) <http://dx.doi.org/10.1021/jp403512m>

**E. Vinogradov, F. Valence, E. Maes, I. Jebava, V. Chuat, S. Lortal, T. Grard, Y. Guerardel, I. Sadovskaya,** "Structural studies of the cell wall polysaccharides from three strains of *Lactobacillus helveticus* with different autolytic properties: DPC4571, BROI and LH1," *Carbohydrate Research* (2013) accepted.  
<http://dx.doi.org/10.1016/j.carres.2013.05.020>

**K. Shin, K.A. Udachin, I.L. Moudrakovski, D.M. Leek, S. Alavi, C.I. Ratcliffe, and J.A. Ripmeester,** "Methanol incorporation in clathrate hydrates and the implications for oil and gas pipeline flow assurance and icy planetary bodies," *Proc. Natl. Acad. Sci. USA* **110** (2013) 8437–8442.  
<http://dx.doi.org/10.1073/pnas.1302812110>

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## Queen's University



**X. Kong, M. Shan, V.V. Terskikh, I. Hung, Z. Gan, and G.Wu,** "Solid-State  $^{17}\text{O}$  NMR of Pharmaceutical Compounds:

Salicylic Acid and Aspirin," *Journal of Physical Chemistry B* **117** (2013) online.

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**Y. Li, Z.Y. Ni, R. Guo, Y. Wu, M. Dong, F. Sauriol, Q.W. Shi, Y.C. Gu, B. Cong,** "A new taxane from the needles of *Taxus cuspidata*," *Chemistry of Natural Compounds* **49** (2013) 277-280.

<http://dx.doi.org/10.1007/s10600-013-0581-5>

**Y.-F. Li, Y. Kang, S.-B. Ko, Y. Rao, F. Sauriol, and S. Wang,** "Highly Congested Donor-Acceptor P-B Compound: Synthesis and Properties of a BMe<sub>2</sub>- and a PPh<sub>2</sub>-Functionalized 1,8-Naphthalene," *Organometallics* **32** (2013) 3063-3068.

<http://dx.doi.org/10.1021/om4002846>

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## University of Toronto

**M. Whitfield Åslund, G.L. Stephenson, A.J. Simpson, M.J. Simpson,** "Comparison of earthworm responses to petroleum hydrocarbon exposure in aged field contaminated soil using traditional ecotoxicity endpoints and  $^1\text{H}$  NMR-based metabolomics," *Environmental Pollution* **182** (2013) 263-268.

<http://dx.doi.org/10.1016/j.envpol.2013.07.026>

**J.L. Kitevski-LeBlanc, J. Hoang, W. Thach, S.T. Larda, and R.S. Prosser,** " $^{19}\text{F}$  NMR Studies of a Desolvated Near-Native Protein Folding Intermediate," *Biochemistry* (2013) accepted.

<http://dx.doi.org/10.1021/bi4010057>

**O. Pisani, K.M. Hills, D. Courtier-Murias, A.J. Simpson, N.J. Mellor, E.A. Paul, S.J. Morris, M.J. Simpson,** "Molecular level analysis of long term vegetative shifts and relationships to soil organic matter composition," *Organic Geochemistry* **62** (2013) 7-16.

<http://dx.doi.org/10.1016/j.orggeochem.2013.06.010>

**A. Mainz, T.L. Religa, R. Sprangers, R. Linser, L.E. Kay, and B. Reif,** "NMR Spectroscopy of Soluble Protein Complexes at One Mega-Dalton and Beyond," *Angew. Chem. Int. Ed.* **52** (2013) 8746-8751.

<http://dx.doi.org/10.1002/anie.201301215>

**A. Sekhar and L.E. Kay,** "NMR paves the way for atomic level descriptions of sparsely populated, transiently formed biomolecular conformers," *Proc. Natl. Acad. Sci. USA* **110** (2013) 12867-12874. **(Perspective)**

<http://dx.doi.org/10.1073/pnas.1305688110>

**B.P. Lankadurai, E.G. Nagato, and M.J. Simpson,** "Environmental Metabolomics: An Emerging Approach to Study Organism Responses to Environmental Stressors," *Environmental Reviews* (2013) accepted. **(Review)**

<http://dx.doi.org/10.1139/er-2013-0011>

**Z. Bozoky, M. Krzeminski, P.A. Chong and J.D. Forman-Kay,** "Structural changes of CFTR R region upon phosphorylation: a plastic platform for intra- and inter-molecular interactions," *FEBS Journal* (2013) accepted. **(Review)**

<http://dx.doi.org/10.1111/febs.12422>

**S.T. Larda, K. Simonetti, M.S. Al-Abdul-Wahid, S. Sharpe, and R.S. Prosser,** "Dynamic equilibria between monomeric and oligomeric misfolded states of the mammalian prion protein measured by  $^{19}\text{F}$  NMR," *J. Am. Chem. Soc.* **135** (2013) 10533-10541.

<http://dx.doi.org/10.1021/ja404584s>

**P. Vallurupalli, G. Bouvignies, L.E. Kay,** "A Computational Study of the Effects of  $^{13}\text{C}$ - $^{13}\text{C}$  Scalar Couplings on  $^{13}\text{C}$  CEST NMR Spectra: Towards Studies on a Uniformly  $^{13}\text{C}$ -Labeled Protein," *ChemBioChem* (2013) online.

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**C. Li, M. Enomoto, A.M. Rossi, M.-D. Seo, T. Rahman, P.B. Stathopoulos, C.W. Taylor, M. Ikura, and J.B. Ames,** "CaBP1, a neuronal  $\text{Ca}^{2+}$  sensor protein, inhibits inositol trisphosphate receptors by clamping intersubunit interactions," *Proc. Natl. Acad. Sci. USA* **110** (2013) 8507-8512.

<http://dx.doi.org/10.1073/pnas.1220847110>

**E.G. Nagato, J.C. D'eon, B.P. Lankadurai, D.G. Poirier, E.J. Reiner, A.J. Simpson, M.J. Simpson,** <sup>1</sup>H NMR-based metabolomics investigation of *Daphnia magna* responses to sub-lethal exposure to arsenic, copper and lithium," *Chemosphere* (2013) online.  
<http://dx.doi.org/10.1016/j.chemosphere.2013.04.085>

**T.H. Kim, K.Y. Chung, A. Manglik, A.L. Hansen, R.O. Dror, T.J. Mildorf, D.E. Shaw, B.K. Kobilka, and R.S. Prosser,** "The Role of Ligands on the Equilibria Between Functional States of a G Protein-Coupled Receptor," *J. Am. Chem. Soc.* **135** (2013) 9465–9474.  
<http://dx.doi.org/10.1021/ja404305k>

**A. Kumar, D.C. Burns, M.S. Al-Abdul-Wahid, and G.A. Woolley,** "A Circularly Permuted Photoactive Yellow Protein as a Scaffold for Photoswitch Design," *Biochemistry* **52** (2013) 3320–3331.  
<http://dx.doi.org/10.1021/bi400018h>

**B.A. Cottrell, M.Gonsior, L.M. Isabelle, W. Luo, V. Perraud, T.M. McIntire, J.F. Pankow, P. Schmitt-Kopplin, W.J. Cooper, A.J. Simpson,** "A Regional Study of the Seasonal Variation in the Molecular Composition of Rainwater," *Atmospheric Environment* **77** (2013) 588–597.  
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