



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

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Canadian NMR Research  
News Bulletin #4.3  
Summer 2010

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### *Guest Editorial*

**Josef W. Zwanziger, Dalhousie University**

A recent and exciting development at Dalhousie University is the award of a new multi-investigator materials research program entitled **DREAMS (Dalhousie Research in Energy, Advanced Materials and Sustainability)**. This program is funded by an NSERC-sponsored Collaborative Research and Training Experience grant.

The purpose of DREAMS is to train a cohort of researchers (Masters and PhD students, undergraduate summer research students and postdoctoral fellows) at Dalhousie University who will address important aspects of energy production/storage and sustainability. DREAMS student researchers play a pivotal role in renewable energy production and storage as well as the sustainable production of

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environmentally acceptable or re-usable materials. The DREAMS cohort tackles some of the world's most important energy and sustainability problems through advanced materials research.

Both Canadian and international students in Chemistry, Physics or Mechanical Engineering are eligible for the DREAMS program. Students will be supervised by Dalhousie DREAMS team members **Heather Andreas** (Chemistry), **Jeff Dahn** (Physics/Chemistry), **Rich Dunlap** (Physics), **Dominic Groulx** (Mechanical Engineering), **Ian Hill** (Physics), **Harm Rotermund** (Physics), **Mary Anne White** (Chemistry/Physics) and **Joe Zwanziger** (Chemistry/Physics).

DREAMS trainees will carry out collaborative interdisciplinary research in Dalhousie's world-leading laboratories with innovative new courses and direct experience working with industrial partners. The DREAMS program is

designed to facilitate the transition of new researchers from trainees to productive participants in the worldwide economic community.

What differentiates DREAMS from other programs is its mix of traditional and non-traditional training. Students will complete new and novel graduate courses, such as

- Advances in Solar, Thermoelectric and Energy Harvesting Materials
- Advances in Battery, Fuel Cell and Supercapacitor Materials
- Sustainable Materials Issues

One of the most exciting aspects of the DREAMS program is the opportunity to work in industry. For example, each of our PhD students will spend two internships (work terms) of two to four months, in an external industrial or government lab. Working alongside industry researchers will provide valuable research experience and connections for future employment. External work term partners include labs both in Halifax, and around the world (for example Axion Power International and 3M in the USA, and Toshiba in Japan). Students' travel and accommodation expenses are covered by the DREAMS program.

DREAMS facilitates interdisciplinary and collaborative research. For example, PhD students will carry out research in two Dalhousie labs, and they will be jointly supervised by two or more members of the DREAMS team. This approach will greatly enhance their research skill set and their interdisciplinary experience.

Other novel approaches of the DREAMS program include training in non-traditional subjects such as IP issues, marketing aspects of materials, and how to be interviewed by the media, plus workshops on the transition to employment, such as résumé writing and interview skills.

The DREAMS program offers Dalhousie students an innovative mix of traditional and experiential learning that will help them to become some of the world's top young materials researchers.

Much more information about DREAMS, including application material, can be found at

<http://irm.dal.ca/DREAMS>

Finally, I would like to mention that the **MOOT** meeting, traditionally held in Ontario or Quebec, will for the first time be in Atlantic Canada, at Dalhousie University October 16 and 17. The MOOT NMR Symposium provides an informal environment for students, post-docs and faculty to present lectures and posters, discuss existing collaborations, and to establish new ones. Details can be found at

<http://structbio.biochem.dal.ca/jrainey/NMRMOOT/index.html>

## Canadian NMR News

Submitted by Kris Ooms (The King's University College)

### NMR spectroscopy at WCUCC

One great place for undergraduate research students to present their research in western Canada is the Western Canadian Undergraduate Chemistry Conference (WCUCC). This year the conference was held in Lethbridge, Alberta, May 7-8, 2010, and many high quality posters and talks were presented. The physical chemistry section of the conference was dominated by NMR spectroscopy. Among the posters and presentations were:

**Roxanne Shank** from Paul Hazendonk's group at the University of Lethbridge  
"Solution & Solid State NMR Spectroscopy: Applications in Radiopharmaceutical Chemistry"  
and "A Tale of Two Toxins: An NMR Study of the Trichothecenes T-2 and Deoxynivalenol"

**Alexandra Palech** from Rod Wasylishen's group at the University of Alberta  
"A Solid-State NMR study of Compounds Exhibiting Anomalous Thermal Expansion"

**Brandon Greer** from Scott Kroeker's group at the University of Manitoba  
"Ultrahigh Field NMR: A New Frontier for  $^{73}\text{Ge}$  NMR Spectroscopy"

**Jesse Vanderveen** from Kristopher Ooms' group at The King's University College

## "Multiple Quantum Filter NMR Spectroscopy of Hydrated Nafion Membranes"

All the talks and posters were well received by students and judges. Brandon and Jesse received the physical chemistry division prizes for best talk and poster, respectively. Congratulations to all who presented their work and demonstrated, yet again, the important place NMR research has in undergraduate education. Congratulations also go to Roxanne who was a co-organizer of the conference and won the most coveted of the door prizes, a copy of "NMR Crystallography".



WCUC 2010: Brandon, Jesse, Roxanne, Alexandra

Submitted by Gang Wu (Queen's)

### Special Issue of the *Canadian Journal of Chemistry* honouring Rod Wasylshen

The *Canadian Journal of Chemistry*, the Canadian Society for Chemistry's principal medium for publication of research, is preparing a special issue to honour the career contributions of Professor Roderick E. Wasylshen, Canada Research Chair in Physical Chemistry at the University of Alberta. The issue is scheduled to be published in July 2011.

Rod continues to have enormous impact on the field of NMR spectroscopy in Canada and worldwide. He has won numerous awards including the Gerhard Herzberg Award from the Spectroscopy Society of Canada, the John C. Polanyi Lecture Award, and the Alumni of Honour Award from the University of Waterloo. He has been elected as a Fellow of the Royal Society of Canada, a Killam Senior Fellow, a CIC Fellow, a Fellow of the American Association for the Advancement of Science,

and a Fellow of the International Society of Magnetic Resonance.

Rod's high-quality and prolific research output is evidenced by more than 300 peer-reviewed publications in top-notch scientific journals, as well as book chapters and reviews. Rod has consistently chosen to publish in the *Journal* and to promote the *Journal* among his colleagues. Beginning in 1969, Rod has published over 75 manuscripts in *Can. J. Chem.* Rod has also had a major impact on the training of the future generation of NMR spectroscopists in Canada.

The *Canadian Journal of Chemistry* is a monthly journal reporting current research findings in all branches of chemistry, including the traditional areas of analytical, inorganic, organic, and physical-theoretical chemistry and newer interdisciplinary areas such as materials science, spectroscopy, chemical physics, and biological, medicinal and environmental chemistry.

It is our pleasure to invite you to contribute an article, communication, or review article dedicated to Rod Wasylshen. All submitted manuscripts will be subject to normal peer review procedures. We anticipate and hope that this will be a very popular issue, and as such reach a large international audience.

Instructions to Authors can be viewed at the journal web site:

[http://pubs.nrc-cnrc.gc.ca/eng/journals/forauthors\\_cjc.html](http://pubs.nrc-cnrc.gc.ca/eng/journals/forauthors_cjc.html)

**Please confirm by e-mail to Judy Murdoch** if you intend to submit a manuscript  
[jmurdoch@uwo.ca](mailto:jmurdoch@uwo.ca)

and submit your contribution via the online submission program as soon as possible and not later than **November 1, 2010** at <http://pubs.nrc-cnrc.gc.ca/cjc/osprey>

Please suggest at least three suitable reviewers two of which must be from a North American research institution in your cover letter or in the space provided in Osprey.

Sincerely,

Yining Huang, University of Western Ontario  
[yhuang@uwo.ca](mailto:yhuang@uwo.ca)

David Bryce, University of Ottawa  
[dbryce@uottawa.ca](mailto:dbryce@uottawa.ca)

Gang Wu, Queen's University  
[gang.wu@chem.queensu.ca](mailto:gang.wu@chem.queensu.ca)

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Submitted by Bob Berno (McMaster)

## Don Hughes' Memorial Photos

Hello everyone.

Thanks to all of you who could attend the memorial service for Don in early June. I know I enjoyed seeing all of you and sharing stories.

We posted a slide show of photos that were taken during the service. In case you haven't had a chance to look through these, please take a couple of minutes to have a look.

<http://tinyurl.com/3a9w7tx>

*One of the last papers by Don Hughes submitted shortly before his death and dedicated to his memory*

**A.D. Bain, D.W. Hughes, C.K. Anand, Z. Nie, V.J. Robertson**, "Problems, artifacts and solutions in the INADEQUATE NMR experiment," *Magnetic Resonance in Chemistry* **48** (2010) 630-641.

<http://dx.doi.org/10.1002/mrc.2639>

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## PROCESS web-server

**PROCESS** (**P**rotein **S**tructure **E**valuation **S**uite & **S**erver) web server has been created by **David Wishart** and colleagues from the University of Alberta. The server is designed to evaluate and validate protein structures solved by either X-ray crystallography or NMR spectroscopy. PROCESS is intended to serve as a tool that can be used by structure biologists as well as database curators to assess and validate newly determined protein structures.

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

**M. Berjanskii, Y. Liang, J. Zhou, P. Tang, P. Stothard, Y. Zhou, J. Cruz, C. Macdonell, G. Lin, P. Lu, D.S. Wishart**, "PROCESS: a protein structure evaluation suite and server," *Nucleic Acids Res* **38** (2010) 633-640.

<http://dx.doi.org/10.1093/nar/gkq375>

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## NMR: Nobel work if you can get it

*Chemistry World* has published a candid interview with **Richard Ernst**, a winner of the 1991 Nobel Prize in chemistry for his contribution to the development of NMR.

<http://www.rsc.org/chemistryworld/News/2010/July/13071002.asp>

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## An NMR Spectrometer for \$187

**Carl Michal** from the Department of Physics & Astronomy at the University of British Columbia has published a do-it-yourself recipe for a low-cost NMR spectrometer operating in the Earth's magnetic field. Using widely available parts and supplies you can now build your personal fully-functioning NMR instrument for less than \$200!

**C.A. Michal** "A low-cost spectrometer for NMR measurements in the Earth's magnetic field," *Meas. Sci. Technol.* **21** (2010) 105902.

<http://dx.doi.org/10.1088/0957-0233/21/10/105902>

Web: <http://www.physics.ubc.ca/~michal/>

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## Radio-Canada: interview with David Bryce

**Les Chercheurs:** Dans le cadre de notre série sur les Chercheurs, nous recevons cette semaine **David Bryce**, professeur agrégé au Département de chimie et chercheur au Centre de recherche et d'innovation en catalyse de l'Université d'Ottawa.

<http://tinyurl.com/27wt299>

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## Magnetic Personalities!

"The spotlight on science" project by the Faculty of Science at McMaster is "spotlighting" areas of interest in the various departments.

<http://www.science.mcmaster.ca/spotlight/>

Most recently the program featured the McMaster's Nuclear Magnetic Resonance Facility. Watch the interview with **Bob Berno** and several graduate students from the Department of Chemistry & Chemical Biology.

<http://tinyurl.com/372lzjk>

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## Canadian NMR blogs and news sites

Solid-State NMR Literature Blog  
(Rob Schurko's group, Windsor)  
<http://ssnmr.blogspot.com/>

Glenn Facey's NMR Blog  
<http://u-of-o-nmr-facility.blogspot.com/>

Canadian NMR News  
<http://nmr900.blogspot.com/>

## NMR Theses Recently Defended

*Congratulate your students here!*

**Adrian Weber** (Chemistry, UBC), July 2010  
Supervisor: Elliott Burnell  
External examiner: Rod Wasylshen attended  
Ph.D. thesis: "Chemical Physics and the Condensed Phase: NMR Studies in a Liquid-Crystal Testing Ground"

**Hiyam Hamaed** (University of Windsor), May 2010  
Supervisor: Robert Schurko  
Ph.D. thesis: "Solid-State NMR Spectroscopy of Unreceptive Nuclei in Inorganic and Organic Systems"

**Alan MacGregor** (University of Windsor), May 2010  
Supervisor: Robert Schurko  
M.Sc. thesis: "Development and Application of Techniques for the Acquisition of Ultra-Wideline Solid-State NMR Spectra"

## Recognition

**Lewis Kay**, Professor of Biochemistry, Molecular Genetics and Chemistry at the Departments of Biochemistry, Molecular Genetics and Chemistry, University of Toronto, has been named a **2010 Fellow of the Royal Society** (U.K.).

<http://www.news.utoronto.ca/health-and-medicine/u-of-t-research-elected-to-royal-society-uk.html>

*From the citation:* "NMR has made a major impact in the study of the structures and properties of biomolecules. Lewis Kay and his group at the University of Toronto have developed many of the recent technical advances that have pushed the size limit of protein complexes that can be examined by NMR spectroscopy beyond 500 kDa. For example, methyl-TROSY has been used by the Kay group to elucidate the structure and aspects of the dynamics of the 670 kDa 20S proteasome core particle. In addition, Kay and his group have delineated the detailed consequences of the binding of ligands to proteins; in the case of aspartate transcarbamoylase, for example, they have defined the nature of the allostery associated with the binding of nucleotide effector molecules. Professor Kay's laboratory has also developed the theoretical framework for the

important step of relating protein dynamics to thermodynamics. The methods developed in his laboratory have been used by his group and others to study molecular recognition, protein stability and the energetics of ligand binding. His group has also developed methods for studying the invisible excited states of proteins by NMR and is applying them to furthering our understanding of protein folding and conformational dynamics. Lewis Kay's contributions will continue to provide insights into protein structures and their fluctuations that will carry on elucidating further their biological functions for many years to come."

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**David Cory**, formerly a professor of nuclear engineering at the Massachusetts Institute of Technology, has been appointed **Canada Excellence Research Chair** in Quantum Information Processing at the Institute for Quantum Computing of the University of Waterloo. Cory's research at IQC is expected to contribute toward the world's first generation of practical quantum devices. At the MIT's Francis Bitter Magnet Laboratory David Cory was leading development of innovative nuclear magnetic resonance methods for quantum information processing and advanced engineering.

[http://www.iqc.ca/institute/news\\_fulltext.php?id=159](http://www.iqc.ca/institute/news_fulltext.php?id=159)

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**Josef Zwanziger**, Professor of Chemistry at Dalhousie University in Halifax and a Canada Research Chair in NMR studies of materials, has joined the board of Editors of the *Journal of Non-Crystalline Solids*.

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**David Bryce** (University of Ottawa) has been invited to serve as a member of the NSERC Chemistry Evaluation Group for a three year term beginning this fall. This coincides with the end of a successful three-year term for **Gang Wu** (Queen's University).

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**Fred Perras** (Bryce Group, University of Ottawa) has been awarded **the CSC prize** for his poster entitled "Exploring the Validity of Common Assumptions Made in the Characterization of *J* Coupling Tensor Anisotropies" which was presented at the Ottawa-Carleton Chemistry Institute Day on May 28, 2010.

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**Rob Attrell** (Bryce Group, University of Ottawa) has been awarded **the 2010 Hypercube Scholar prize** for his honours

thesis entitled "A Solid-State Halogen NMR and Computational Study of Quadrupolar and Chemical Shift Tensors in Anilinium Halide Salts Exhibiting Halogen Bonding".

## On the move

**Albin Otter**, an NMR Laboratory Supervisor at the Chemistry Department of the University of Alberta, has retired after 26 years with the Department. *Happy retirement, Albin!*

**Lawson Miller** (Memorial University) has joined the **Kroeker** group (U of Manitoba) for the summer as part of the Inorganic Chemistry Exchange (ICE) program. His research involves using NMR to probe devitrification products in model nuclear waste glasses. The 2010 ICE Workshop will be held at the University of Manitoba, August 19-20.

## the 900 NMR Facility News

### Facility Steering Committee membership

The National Ultrahigh-Field NMR Facility for Solids wishes to extend its sincere thanks to **Yining Huang** (University of Western Ontario), the outgoing member of the Facility Steering Committee who served in 2006-2010. Yining has done a great job as the representative for Ontario Universities. His valuable insights and suggestions have certainly helped to improve the Facility and broaden its user base.

The Facility is pleased to announce that **Gang Wu** (Queen's) has been appointed to serve on the Facility Steering Committee as the representative for Ontario Universities for the next three years. Gang Wu is a long-time facility user and his first-hand experience will be very useful in managing the Facility. *Welcome aboard, Gang!*

### NMR Facility Annual Report 2009-2010

Dear NMR Facility Users, we are preparing our 2009-2010 Annual Report and we would like to receive the following information from you:

1) a brief progress report for each of your research projects. Please prepare a separate

report for each project, regardless of whether the project has ended or not. Each report should illustrate for non-NMR specialists major project findings and should normally not exceed one-two pages (text and figures) (preferably MS Word format, or an ASCII text + figures separately). Selected progress reports will be included in the printed version of the Annual Report.

2) all 2009-2010 research publications featuring results from the 900 instrument (published, accepted, submitted)

3) invited lectures and oral presentations in 2009-2010

4) poster presentations in 2009-2010

5) 2009-2010: Honor thesis, Ph.D. thesis and similar works by your students using the 900 results (please indicate name of the student, department, title of thesis, date of the defense)

6) any other relevant information you may consider useful including in our report

Let me know if any questions, and thank you for your contribution!

On behalf of the Facility Steering Committee,  
Victor Terskikh

Email: [terskikhv@nrc-cnrc.gc.ca](mailto:terskikhv@nrc-cnrc.gc.ca)

### Travel support program for students and young scientists

Students and young scientists from Canadian Universities are welcome to apply for a travel stipend towards full or partial reimbursement of their travel expenses incurred while visiting the 900 Facility. All requests should be submitted by a supervisor in advance of the trip and include a cost estimate. Requests should be forwarded to the Facility manager for review and approval by the Steering Committee.

[http://nmr900.ca/policies\\_e.html](http://nmr900.ca/policies_e.html)

#### Recent Travel Grant Recipients

**Patrick Walsh** (University of Toronto)

**Kathryn Hotke** (Redeemer University College)

**Margaret Hanson** (University of Western Ontario)

**Alexandra Palech** (University of Alberta)

## Upcoming NMR Events

Let everyone know about upcoming NMR-related events at your University or Lab. NMR conference announcements are also welcome.

# MOOT XXIII

## MINI NMR SYMPOSIUM

### MOOT XXIII Second Announcement

The 23<sup>rd</sup> Annual MOOT NMR Symposium will take place at Dalhousie University in Halifax, Nova Scotia on **October 16 and 17<sup>th</sup>, 2010**.

The MOOT NMR Symposium provides an informal environment for students, post-docs and faculty to present lectures and posters, discuss existing collaborations, and to establish new ones. It has traditionally been a regional gathering of NMR spectroscopists from Ontario and Quebec but has been expanding to include NMR Spectroscopists from the Maritimes. As a result, MOOT XXIII will be hosted for the first time outside of its traditional region; on the East coast in beautiful Halifax, Nova Scotia! We welcome you to check out and bookmark our website for the most up-to-date information:

<http://structbio.biochem.dal.ca/jrainey/NMRMOOT/index.html>

### Notices:

(1) Registration and submission of titles for oral/poster presentations are open as of June 30, 2010. The deadline for both is **September 15, 2010**. Visit the registration menu item on our website where registration information can be provided via Word document or fillable PDF.

(2) Be sure and register for the banquet, to be held Saturday evening at the Halifax Citadel National Historic Site on Citadel Hill - overlooking the downtown core of Halifax and the harbour.  
<http://www.pc.gc.ca/eng/lhn-nhs/ns/halifax/index.aspx>

(3) A big thank you to all of our confirmed sponsors, including Bruker BioSpin Canada, Agilent Technologies (formally Varian), Sigma-Aldrich Canada, New Era Enterprises, National Ultrafigh-Field NMR Facility for Solids (Canada), and Suraj Manrao. If you wish to

sponsor this meeting, please contact Joe Zwanziger at [jzwanzig@dal.ca](mailto:jzwanzig@dal.ca)

### Reminders:

(1) Accommodations - a block of rooms has been reserved at **Atlantica** at a rate of \$129 per night, including parking, and is based on 1-4 person occupancy. See the website for additional details and reservation deadlines.  
<http://www.atlantichotelhalifax.com>

(2) Travel - a 10% discount has been arranged with **WestJet** for your flight to MOOT XXIII. Again, additional details are on the website.

If you have any questions, comments or feedback about this year's MOOT and/or website, please let us know by email at [mootnmr@gmail.com](mailto:mootnmr@gmail.com)

We look forward to seeing you in October!

Your MOOT XXIII Organizing Committee:

Mike Lumsden  
Joe Zwanziger  
Jan Rainey  
Ulli Werner-Zwanziger

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Submitted by Scott Kroeker (Manitoba)

### Pacifichem 2010: Registration is open

The 2010 International Chemical Congress of Pacific Basin Societies **Pacifichem 2010** will take place in Honolulu, Hawaii, December 15-20, 2010 and will be hosted by the Canadian Society for Chemistry (CSC).

Registration and housing reservation for Pacifichem 2010 is now open. The deadline for early bird registration is **November 1, 2010**.

Canadian NMR will be well represented by four symposia focusing on biological systems, polymers and inorganic materials. The technical program of Pacifichem 2010 and the full list of speakers are now available online at <http://www.pacifichem2010.org>

For the complete NMR symposia schedules <http://pacifichem.abstractcentral.com/planner.jsp> no need to login, just hit "search" and enter "nmr" in "Session Title Search"

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## ***NMR Symposia at Pacifichem 2010***

**NMR Spectroscopy of Polymers - Innovative NMR Strategies for Complex Macromolecular Systems** (Symposium #12)  
Peter Macdonald, University of Toronto

**Biomolecular Structure and Dynamics - Recent Advances in NMR** (Symposium #43)  
Mitsuhiko Ikura, Ontario Cancer Institute

**Advances in Solid-State NMR of Biological Molecules** (Symposium #58) Michèle Auger,  
Université Laval

**Solid-State NMR Methods and Applications in Inorganic Materials** (Symposium #228)  
Scott Kroeker, University of Manitoba

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 **3<sup>rd</sup> IUPAC International Conference on Green Chemistry**

August 15-18, 2010, Ottawa, ON  
<http://www.icgc2010.ca/>

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**ICMRBS 2010** the XXIV<sup>th</sup> International Conference on Magnetic Resonance in Biological Systems

August 22-27, 2010, Cairns, Australia  
<http://www.icmrbs2010.org/>

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**SMASH 2010** Small Molecule NMR Conference

September 26-29, 2010, Portland, Oregon, USA  
<http://www.smashnmr.org/main.asp>

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 **MOOT XXIII NMR Symposium**

October 16-17, 2010, Dalhousie University, Halifax  
<http://structbio.biochem.dal.ca/jrainey/NMRMOOT/index.html>

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 **2010 UK NMR BootCamp**

November 1-4, 2010, University of Birmingham, U.K.  
[http://www.nanuc.ca/nmrbootcamp/2010\\_NMR\\_BootCamp/Welcome.html](http://www.nanuc.ca/nmrbootcamp/2010_NMR_BootCamp/Welcome.html)

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 **Pacifichem 2010** The International Chemical Congress of Pacific Basin Societies

December 15-20, 2010, Honolulu, Hawaii, USA  
<http://www.pacifichem.org/>

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**Frontiers of NMR Biology**

Keystone Symposium  
January 8-13, 2011, Big Sky, MT

Abstract Deadline: 15<sup>th</sup> September 2010  
Registration Deadline: 9<sup>th</sup> November 2010  
<http://www.keystonesymposia.org/>

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**52<sup>nd</sup> ENC**

April 10-15, 2011, Asilomar, California  
<http://www.enc-conference.org/>

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 **19<sup>th</sup> ISMRM** — Scientific Meeting and Exhibition of the International Society for Magnetic Resonance in Medicine

May 7-13, 2011, Montreal, Quebec, Canada  
<http://www.ismrm.org>

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 **CSC 2011**, the 94<sup>th</sup> Canadian Chemistry Conference and Exhibition

June 5-9, 2011, Montréal, Quebec, Canada  
<http://www.csc2011.ca/>

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**Magnetic Resonance Gordon Research Conference**

June 12-17, 2011, Biddeford, Maine, USA  
<http://www.grc.org/>

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**EUROMAR 2011**

August 21-25, 2011, Frankfurt, Germany  
<http://euromar2011.org/>

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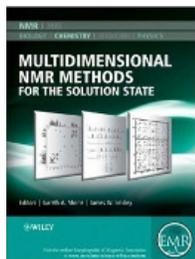
**7<sup>th</sup> Alpine Conference** on Solid-State NMR

September 11-15, 2011, Chamonix Mont-Blanc, France  
<http://www.alpine-conference.org>

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## New Books

*Disclaimer: For your information only. In this bulletin we are not endorsing any products or services.*



### Multidimensional NMR Methods for the Solution State

Gareth A. Morris (Editor)  
James W. Emsley (Editor)  
**Hardcover:** 580 pages  
**Publisher:** Wiley; June 2010  
**Language:** English  
**ISBN:** 978-0470770757

<http://www.amazon.com/dp/0470770759>  
<http://www.amazon.ca/dp/0470770759>

*Wiley:* "Multidimensional NMR methods have transformed the way in which solution state NMR is used to elucidate the structures of chemical and biochemical systems. The first book covering new developments in nearly a decade, this much-needed resource explains recent experimental methods for the rapid measurement of multidimensional solution-state NMR spectra. With articles written by key developers of the techniques, the coverage deals with both the theoretical tools and the latest practical applications, giving an unmatched guide to students, researchers, technicians, and anyone else working with NMR techniques today"

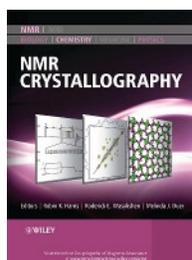
### Canadian contributions

**A.D. Bain** "COSY: Quantitative Analysis,"  
Chapter 13, pp. 167-176.  
<http://dx.doi.org/10.1002/9780470034590.emrstm0095>

**T.T. Nakashima and R.E.D. McClung**  
"Heteronuclear Shift Correlation Spectroscopy,"  
Chapter 22, pp. 289-304.  
<http://dx.doi.org/10.1002/9780470034590.emrstm0209>

**R. Muhandiram and L.E. Kay** "3D HMQC-NOESY, NOESY-HMQC, and NOESY-HSQC,"  
Chapter 25, pp. 335-350.  
<http://dx.doi.org/10.1002/9780470034590.emrstm0563>

The complete **Table of Contents** is available  
[http://media.wiley.com/product\\_data/excerpt/59/04707707/0470770759.pdf](http://media.wiley.com/product_data/excerpt/59/04707707/0470770759.pdf)

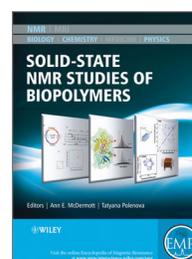


### NMR Crystallography

Robin K. Harris (Editor)  
Roderick E. Wasylshen (Editor)  
Melinda J. Duer (Editor)  
**Hardcover:** 520 pages  
**Publisher:** Wiley; January 2010  
**Language:** English  
**ISBN:** 978-0470699614

<http://www.amazon.com/dp/0470699612/>  
<http://www.amazon.ca/dp/0470699612/>

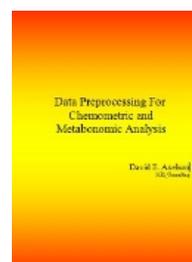
*Coming in October, 2010*



### Solid State NMR Studies of Biopolymers

Anne E. McDermott (Editor)  
Tatyana Polenova (Editor)  
**Hardcover:** 592 pages  
**Publisher:** Wiley; October 2010  
**Language:** English  
**ISBN:** 978-0470721223

<http://www.amazon.com/dp/0470721227/>  
<http://www.amazon.ca/dp/0470721227/>



### Data Preprocessing for Chemometric and Metabonomic Analysis

by **David E. Axelson**  
**Softcover:** 420 pages  
**Publisher:** MRi Consulting, Kingston, Ontario; July 30, 2010  
**Language:** English  
**ISBN:** 978-1926825618

<http://www.chemometrics-analysis.com/>

*D. Axelson:* "The best preprocessing methods will be the ones that ultimately produce a robust model with the most accurate predictive ability. Unfortunately, there are no particularly straightforward rules to guide investigators to the best selection of preprocessing options; the subsequent trial and error optimization process may be quite time consuming and confusing. However, spending little or no time investigating preprocessing options is likely to result in less than optimal results. The primary objective of this book is to present a relatively focused outline of the major options available for data analysis, with an emphasis on the advantages and disadvantages of the techniques discussed. "

The complete **Table of Contents** is available  
[http://www.chemometrics-analysis.com/Book\\_brochure1.pdf](http://www.chemometrics-analysis.com/Book_brochure1.pdf)

## NMR Jobs and Vacancies

### **NMR Scientist at the Environmental NMR Centre, University of Toronto Scarborough**

The Environmental NMR Centre and the Department of Physical and Environmental Sciences at the University of Toronto Scarborough are seeking a Senior NMR Research Associate to oversee the daily operation, training, and management of the Environmental NMR Centre. The position has a very large research and development component and the candidate is expected to work closely in and with the facilities Directors to maintain the centre at the cutting-edge of Environmental NMR globally and be central to pioneering new developments in NMR in general.

The Environmental NMR Centre currently houses two unique, Bruker BioSpin NMR systems. The first is a fully hyphenated 2D-HPLC-SPE-NMR-MS, and is novel both in Canada and Environmental Research in general. The second system has capabilities to perform in situ multiphase NMR analyses of heterogeneous samples that contain solid, gel and solution phase samples, the hardware is globally unique and being co-developed directly with Bruker BioSpin. The Centre focuses on the development and application of NMR techniques to study a range of environmental problems. The current topics of research include: environmental metabolomics, LC-SPE-NMR-MS applications to complex environmental mixtures, in vivo NMR spectroscopy imaging, hyperpolarization, DNP, development of multiphase NMR methods (solids, HR-MAS, solutions NMR as a single technique). In addition, the Centre focuses on the development and application of novel NMR approaches to complex systems (including soils, ocean sediments, atmospheric deposits (particles, rain, snow, glacial ice), cells, tissues, small organisms and other environmental matrices) to better understand structure and environmental reactivity.

After an initial probationary period, this will be a continuing full-time appointment.

The NMR scientist will report to the Chair of the Department and work closely with the Director and Associate Director of the Environmental NMR Centre. The research associate will be responsible for instrument maintenance, training of graduate students/postdoctoral fellows/visiting scientists assist in writing grant applications to upgrade the centre and co-publication of research with the facility's principal investigators and collaborators. The candidate will also be expected to lead research projects publishing both as a primary and secondary author. The successful candidate will take an active role in all aspects of the research of the NMR Centre

and will strive to ensure that he/she becomes recognized as a leader in the field of Environmental NMR spectroscopy.

The candidate will also be involved in undergraduate thesis supervision in the Department's chemistry program and will be encouraged to apply to instruct one course in the undergraduate chemistry program on a yearly basis. The candidate will also oversee the operation/maintenance of a teaching/research Departmental NMR system (Bruker BioSpin 500MHz Avance) and ensure that faculty and students can acquire high quality data required for the teaching and research programs. These duties will include the set up of new experiments, training of students and faculty, maintenance and calibration. Candidates should note that the departmental NMR system is fully automated (BACS) with a single automatic tuning and matching probe (ATM) and that the department has only a small number of users, once running smoothly should require minimal intervention on a daily basis.

Applicants must have a Ph.D. in Chemistry or related discipline with a very strong background in NMR spectroscopy and a drive/passion for the development of NMR spectroscopy. In exceptional circumstances, an established leader in the field with a MSc degree but more than 10 years of experience may be considered. In addition, experience with metabolomics, chromatography, mass spectrometry and working with complex biological and/or environmental systems are a strong assets. Experience with pulse programming, custom processing of NMR data (MATLAB, ACD, etc.) and programming/webpage design is also beneficial. Experience with Bruker instruments is very important and the ideal candidate will have experience in (or enthusiastic to learn) all areas of NMR including solutions, HR-MAS, solids and imaging.

Salary will be commensurate with the candidate's qualifications and experience.

Applicants should send a cover letter, curriculum vitae, a statement of research, a statement of teaching and three letters of reference to:

**Rose Jones** (Assistant to the Chair)  
NMR Scientist Search Committee  
Department of Physical & Environmental Sciences  
University of Toronto Scarborough  
1265 Military Trail  
Toronto, Ontario M1C 1A4

Email submissions should be sent to [rjones@utsc.utoronto.ca](mailto:rjones@utsc.utoronto.ca)

Unfortunately, applications that are not accompanied by at least three references cannot be considered. We will start reviewing applications

beginning **September 13, 2010**, although the search will remain open until the position is filled.

The University of Toronto is strongly committed to diversity within its community and especially welcomes applications from visible minority group members, women, Aboriginal persons, persons with disabilities, members of sexual minority groups, and others who may contribute to the further diversification of ideas.

All qualified candidates are encouraged to apply; however, Canadians and permanent residents will be given priority.

Physical and Environmental Sciences, UTSC  
<http://www.utsc.utoronto.ca/~physsci/>

Andre Simpson research group  
<http://www.utsc.utoronto.ca/~asimpson/>

Myrna Simpson research group  
<http://www.utsc.utoronto.ca/~msimpson/>

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### **Postdoctoral position, University of Toronto Mississauga**

A postdoctoral position is available for a Canadian Institutes of Health Research funded project in the laboratory of **Professor Voula Kanelis** at the University of Toronto Mississauga (UTM). The successful candidate will investigate the nucleotide binding domains (NBDs) of the sulfonyl urea receptors (SURs) using biophysical approaches, including NMR spectroscopy. SUR proteins are ABC transporters that form the regulatory subunits of ATP-sensitive potassium (KATP) channels. We are studying the effects of disease-causing mutations in the SUR NBDs on their stability, structure, and interactions with other regions in the SURs and in KATP channels. A Ph.D. in biochemistry or a related discipline is required. Candidates should have experience with protein expression and purification and protein NMR spectroscopy.

Located 30 km west of downtown Toronto, The University of Toronto Mississauga (<http://www.utm.utoronto.ca>) is a campus of the University of Toronto (<http://www.utoronto.ca>), the largest research University in Canada. UTM provides all of the advantages of research at the University of Toronto, while additionally providing a smaller, friendly campus environment in a beautiful natural setting by the Credit River.

Our newly renovated and well-equipped laboratory contains all the equipment necessary for protein biochemistry and fluorescence spectroscopy. Other equipment (CD spectrophotometer, isothermal titration calorimeter, differential scanning calorimeter) is available in the Center for Applied

Bioscience and Biotechnology at the University of Toronto Mississauga. NMR experiments will be performed primarily on a Varian 600 MHz spectrometer equipped with a cryoprobe at UTM. We also have access to high-field spectrometers located at the University of Toronto NMR facility.

Interested applicants should submit their CV, contact information for three references, and a description of previous research experience to **Voula Kanelis**

[voula.kanelis@utoronto.ca](mailto:voula.kanelis@utoronto.ca)

Assistant Professor  
Department of Chemical and Physical Sciences,  
University of Toronto Mississauga

3359 Mississauga Road North  
South Building, Room 4042  
Mississauga, ON, L5L 1C6

PHONE: 905-569-4542  
FAX: 905-828-5425  
<http://www.utm.utoronto.ca/7319.html>

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### **University of British Columbia**

The Michael Smith Laboratories (**MSL**) and the Centre for High-throughput Biology (**CHiBi**) at the University of British Columbia are jointly launching a major recruiting initiative and invite applications for **six new faculty positions**. These full-time tenure-track positions will be filled primarily at the Assistant Professor level but exceptional candidates at a higher rank may be considered. The six new faculty will be located in exceptional research space at the centre of campus within a highly interdisciplinary and collaborative environment that includes biological and physical scientists and engineers, as well as proteomics and bioinformatics experts. The closing date for all applications is **September 14, 2010**.

For more information see the PDF poster (76 kB)  
[http://www.msl.ubc.ca/pdfs/faculty\\_employment/six\\_faculty\\_poster.pdf](http://www.msl.ubc.ca/pdfs/faculty_employment/six_faculty_poster.pdf)

Web: <http://www.msl.ubc.ca/>  
Web: <http://www.chibi.ubc.ca/>

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### **Listings of NMR jobs and vacancies**

Canadian NMR Jobs  
[http://nmr900.ca/nmr\\_jobs.html](http://nmr900.ca/nmr_jobs.html)

NMR Wiki  
<http://nmrwiki.org/wiki/index.php?title=Category:Jobs>

NMR jobs on the NMR Information Server  
<http://www.spincore.com/nmrjobs/>

AMPERE mailing list

<https://listes.sc.univ-paris-diderot.fr/sympa/info/nmr>

NMR jobs on SpectroscopyNow.com

<http://www.spectroscopynow.com/coi/cda/list.cda?type=Job&chld=0>

FG-MR Jobs

<http://fgmrjobs.blogspot.com/>

## Canadian NMR Research Highlights

Research highlights and most recent NMR publications by Canadian research teams.

### Opportunities for studying polymorphs and cement-based materials via $^{43}\text{Ca}$ solid-state NMR



Calcium is an important component in diverse materials and biochemicals. However, NMR spectroscopy of the only spin-active calcium isotope,  $^{43}\text{Ca}$ , is notoriously challenging due to its low natural abundance (0.14 %), low resonance frequency, and quadrupolar nature.

Recently, researchers from the University of Ottawa, the NRC Steacie Institute for Molecular Sciences (SIMS-NRC), and Dalhousie University have independently reported advances in studies of inorganic polymorphs and cement-based materials using Ca-43 solid-state NMR spectroscopy.

"In spite of the great complexity of the calcium silicate chemistry involved in the hydration of Portland cement, we have shown that  $^{43}\text{Ca}$  solid-state NMR provides useful new insights into cement chemistry", says **Igor Moudrakovski** (SIMS-NRC) of his collaboration with the Institute for Research in Construction (SIMS-IRC). **Josef Zwanziger** (Dalhousie) and his academic and industrial partners have similarly applied  $^{43}\text{Ca}$  NMR in their project on the development, optimization and commercialization of high performance cement based composite materials.

Zwanziger explains, "we are trying to understand the nature of the composite-cement interface, and the mechanisms of toughening and strengthening in concrete composites. Calcium NMR is one of the many tools which is shedding light on the nature of

the interface." At the University of Ottawa, **David Bryce** and his research group have demonstrated the utility of calcium NMR in understanding polymorphism in solids. This work has implications for understanding biomaterials as well as inorganic materials.

Because  $^{43}\text{Ca}$  NMR in solid state requires a very strong magnetic field for sensitivity reasons, all these experiments were carried out at the National Ultrahigh-Field NMR Facility for Solids, a national user facility managed by the University of Ottawa and housed on NRC's Ottawa campus, which houses Canada's only 21.1 T (900 MHz) NMR spectrometer.

The latest calcium NMR research has been published in *PCCP* and *J. Am. Chem. Soc.*, and a perspective on the state of the field is now available in *Dalton Transactions* (Bryce, 2010).

**David L. Bryce** "Calcium Binding Environments Probed by  $^{43}\text{Ca}$  NMR Spectroscopy," *Dalton Transactions* (2010) online. (**cover article**)

<http://dx.doi.org/10.1039/c0dt00416b>

**Igor Moudrakovski, Rouhollah Alizadeh, James J. Beaudoin**, "Natural abundance high field  $^{43}\text{Ca}$  solid state NMR in cement science," *Physical Chemistry Chemical Physics* **12** (2010) 6961-6969.

<http://dx.doi.org/10.1039/c000353k>

**David L. Bryce, Elijah B. Bultz, and Dominic Aebi**, "Calcium-43 Chemical Shift Tensors as Probes of Calcium Binding Environments. Insight into the Structure of the Vaterite  $\text{CaCO}_3$  Polymorph by  $^{43}\text{Ca}$  Solid-State NMR Spectroscopy," *Journal of the American Chemical Society* **130** (2008) 9282-9292.

<http://dx.doi.org/10.1021/ja8017253>

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### Lymphoma NMR Research

**Cheryl Arrowsmith** and her group at the Ontario Cancer Institute took part in a multidisciplinary study of human lymphoma involving research teams from seven different departments from Universities in Canada and U.S. Using structure-based analysis of lymphoma proteins they were able to identify small molecules which may potentially serve as lymphoma inhibitors. This research is a practical step in finding new cancer

treatments. Not surprisingly, their paper in *Cancer Cell* has attracted considerable attention in science media.

<http://www.uhnresearch.ca/news/php/readarticle.php?id=26187>

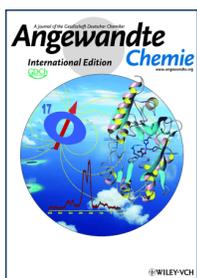
<http://www.sciencedaily.com/releases/2010/04/100412124955.htm>

**L.C. Cerchietti, A.F. Ghetu, X. Zhu, G.F. Da Silva, S. Zhong, M. Matthews, K.L. Bunting, J.M. Polo, C. Farès, C.H. Arrowsmith, S.N. Yang, M. Garcia, A. Coop, A.D. MacKerell, G.G. Privé, A. Melnick,** "A Small-Molecule Inhibitor of BCL6 Kills DLBCL Cells In Vitro and In Vivo," *Cancer Cell* **17** (2010) 400-411.

<http://dx.doi.org/10.1016/j.ccr.2009.12.050>

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### Cover article in *Angewandte Chemie*



Low concentration and poor sensitivity often hinder or make impossible solid-state  $^{17}\text{O}$  NMR in large biomolecular systems. In this cover article in *Angewandte Chemie* **Gang Wu** (Queen's) and co-workers from the University of Ottawa and NRC Canada show that at an

ultrahigh magnetic field of 21 T the high-quality solid-state  $^{17}\text{O}$  NMR spectra can be obtained for large protein–ligand complexes of up to 300 kDa in size. Complementary multinuclear  $^{17}\text{O}$ ,  $^{27}\text{Al}$ , and  $^{13}\text{C}$  NMR data obtained in this work have aided in the structural refinement for an ovotransferrin-bound Al-oxalate complex.

**J. Zhu, E. Ye, V. Tersikh, and G. Wu,** "Solid-State  $^{17}\text{O}$  NMR Spectroscopy of Large Protein-Ligand Complexes," *Angewandte Chemie International Edition* (2010) online.

**(Cover Article)**

<http://dx.doi.org/10.1002/anie.201002041>



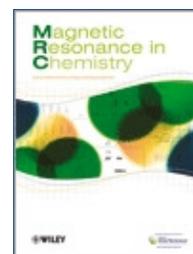
This is a **ninth cover article** featuring results obtained using resources of the National Ultrahigh-Field NMR Facility for Solids.

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### **Magnetic Resonance in Chemistry: a computational issue**

*Magnetic Resonance in Chemistry* is putting together a special issue on "the Quantum-Chemical Calculations and their applications".

Many papers from this issue, including several invited contributions from Canadian groups, are already available online.



**D.H. Brouwer, I.L.**

**Moudrakovski, R.J.**

**Darton, R.E. Morris,** "Comparing quantum chemical calculation methods for structural investigation of zeolite crystal structures by solid-state NMR spectroscopy", *Magnetic Resonance in Chemistry* (2010) online.

**(Invited Article, Special Issue)**

<http://dx.doi.org/10.1002/mrc.2642>

**D.L. Bryce,** "A computational investigation of J couplings involving  $^{27}\text{Al}$ ,  $^{17}\text{O}$ , and  $^{31}\text{P}$ ,"

*Magnetic Resonance in Chemistry* (2010) online. **(Invited Article, Special Issue)**

<http://dx.doi.org/10.1002/mrc.2630>



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### **Renaissance of DNP**

Dynamic Nuclear Polarization (DNP) effect is based on the transfer of the large electron spin polarization to nuclear spins, thus DNP has a potential of significantly boosting NMR sensitivity, both in solids and

in the liquid state. There has been recently a surge of interest in DNP mostly driven by advances in instrumentation. It was very timely, that *Physical Chemistry Chemical Physics* had decided to put together a special DNP-themed issue, which is now available online. This issue, guest-edited by leading experts in DNP, **Robert Griffin** and **Thomas Prisner**, represents a comprehensive overview of the modern state-of-the-art DNP instrumentation and research.

<http://tinyurl.com/3xzqpf>

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### **Progress in NMR Spectroscopy**



**D.S. Wishart** "Interpreting Protein Chemical Shift Data," *Progress in Nuclear Magnetic Resonance Spectroscopy* (2010) in press. **(Invited Review)**

<http://dx.doi.org/10.1016/j.pnmrs.2010.07.004>

## Recent NMR Publications

We are listing here most recent NMR publications by Canadian research groups as they appear on the [www.nmr900.ca](http://www.nmr900.ca) website. Although we are doing our best keeping track of your publications, this list should not be considered complete. You are encouraged to let us know of your recent publications as they become available.

### Memorial University of Newfoundland

**Md.N. Uddin and M.R. Morrow**, "Bicellar Mixture Phase Behavior Examined by Variable-Pressure Deuterium NMR and Ambient Pressure DSC," *Langmuir* **26** (2010) 12104-12111. <http://dx.doi.org/10.1021/la1014362>

### Dalhousie University

**M.L. Tremblay, A.W. Banks, J.K. Rainey**, "The predictive accuracy of secondary chemical shifts is more affected by protein secondary structure than solvent environment," *Journal of Biomolecular NMR* **46** (2010) 257-270. <http://dx.doi.org/10.1007/s10858-010-9400-5>

**T. Reddy, X.J. Li, L. Fliegel, B.D. Sykes, J.K. Rainey**, "Correlating structure, dynamics, and function in transmembrane segment VII of the Na<sup>+</sup>/H<sup>+</sup> exchanger isoform 1," *Biochimica Et Biophysica Acta-Biomembranes* **1798** (2010) 94-104. <http://dx.doi.org/10.1016/j.bbamem.2009.06.025>

### University of New Brunswick

**J. Zhang, B.J. Balcom**, "Parallel-plate RF resonator imaging of chemical shift resolved capillary flow," *Magnetic Resonance Imaging* **28** (2010) 826-833. <http://dx.doi.org/10.1016/j.mri.2010.03.033>

**A.B. Tayler, A.J. Sederman, B. Newling, M.D. Mantle, L.F. Gladden**, "'Snap-shot' velocity vector mapping using echo-planar imaging," *Journal of Magnetic Resonance* **204** (2010) 266-272. <http://dx.doi.org/10.1016/j.jmr.2010.03.006>

### McGill University

**Q. Liu, T. Moldoveanu, T. Sprules, E. Matta-Camacho, N. Mansur-Azzam, K. Gehring**, "Apoptotic Regulation by MCL-1 through Heterodimerization," *Journal of Biological Chemistry* **285** (2010) 19615-19624. <http://dx.doi.org/10.1074/jbc.M110.105452>

**A.Y. Denisov, E. Kloser, D.G. Gray, A.K. Mittermaier**, "Protein alignment using cellulose nanocrystals: practical considerations and range of application," *J Biomol NMR* **47** (2010) 195-204. <http://dx.doi.org/10.1007/s10858-010-9423-y>

**S. Barelier, J. Pons, K. Gehring, J.-M. Lancelin and I. Krimm**, "Ligand Specificity in Fragment-Based Drug Design," *J. Med. Chem.* **53** (2010) 5256-5266. <http://dx.doi.org/10.1021/jm100496j>

### Université de Montréal

**Y.J. Wang, H. Therien-Aubin, W.E. Baille, J.T. Luo, X.X. Zhu**, "Effect of molecular architecture on the self-diffusion of polymers in aqueous systems: A comparison of linear, star, and dendritic poly(ethylene glycol)s," *Polymer* **51** (2010) 2345-2350. <http://dx.doi.org/10.1016/j.polymer.2010.03.047>

**V. Delfosse, P. Bouchard, E. Bonneau, P. Dagenais, J.F. Lemay, D.A. Lafontaine, P. Legault**, "Riboswitch structure: an internal residue mimicking the purine ligand," *Nucleic Acids Research* **38** (2010) 2057-2068. <http://dx.doi.org/10.1093/nar/gkp1080>

### NRC-SIMS

**A. Guerrero-Martinez, D. Avila, F.J. Martinez-Casado, J.A. Ripmeester, G.D. Enright, L. De Cola, and G. Tardajos**, "Solid Crystal Network of Self-Assembled Cyclodextrin and Nonionic Surfactant Pseudorotaxanes," *J. Phys. Chem. B* (2010) ASAP. <http://dx.doi.org/10.1021/jp105808j>

**S. Pawsey, K.K. Kalebaila, I. Moudrakovski, J.A. Ripmeester and S.L. Brock**, "Pore Structure and Interconnectivity of CdS Aerogels and Xerogels by

Hyperpolarized Xenon NMR", *J. Phys. Chem. C* **114** (2010) 13187–13195.  
<http://dx.doi.org/10.1021/jp103157t>

 **J. Zhu, E. Ye, V. Terskikh, and G. Wu**, "Solid-State  $^{17}\text{O}$  NMR Spectroscopy of Large Protein-Ligand Complexes", *Angewandte Chemie International Edition* (2010) online. **(Cover Article)**  
<http://dx.doi.org/10.1002/anie.201002041>

**M.A. Arshad, Y.K. Soon, J.A. Ripmeester**, "Quality of soil organic matter and C storage as influenced by cropping systems in northwestern Alberta, Canada," *Nutrient Cycling in Agroecosystems* (2010) in press.  
<http://dx.doi.org/10.1007/s10705-010-9377-1>

 **D.H. Brouwer, I.L. Moudrakovski, R.J. Darton, R.E. Morris**, "Comparing quantum chemical calculation methods for structural investigation of zeolite crystal structures by solid-state NMR spectroscopy", *Magnetic Resonance in Chemistry* (2010) online. **(Invited Article, Special Issue)**  
<http://dx.doi.org/10.1002/mrc.2642>

 **I. Moudrakovski, R. Alizadeh, J.J. Beaudoin**, "Natural abundance high field  $^{43}\text{Ca}$  solid state NMR in cement science," *Physical Chemistry Chemical Physics* **12** (2010) 6961–6969.  
<http://dx.doi.org/10.1039/c000353k>

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#### NRC-IBS

**J. Kubler-Kielb, E. Vinogradov, C. Mocca, V. Pozsgay, B. Coxon, J.B. Robbins and R. Schneerson**, "Immunochemical studies of *Shigella flexneri* 2a and 6, and *Shigella dysenteriae* type 1 O-specific polysaccharide-core fragments and their protein conjugates as vaccine candidates," *Carbohydrate Research* **345** (2010) 1600–1608.  
<http://dx.doi.org/10.1016/j.carres.2010.05.006>

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#### University of Ottawa

 **J. Zhu, E. Ye, V. Terskikh, and G. Wu**, "Solid-State  $^{17}\text{O}$  NMR Spectroscopy of Large Protein-Ligand Complexes", *Angewandte Chemie International Edition* (2010) online. **(Cover Article)**  
<http://dx.doi.org/10.1002/anie.201002041>

**T. Ducat and N.K. Goto**, " $^1\text{H}$ ,  $^{13}\text{C}$ ,  $^{15}\text{N}$  chemical shift assignments for the *Neisseria gonorrhoeae* MinE regulator of cell division septum placement", *Biomolecular NMR Assignments* (2010) online.  
<http://dx.doi.org/10.1007/s12104-010-9247-4>

**D.L. Bryce**, "A computational investigation of J couplings involving  $^{27}\text{Al}$ ,  $^{17}\text{O}$ , and  $^{31}\text{P}$ ", *Magnetic Resonance in Chemistry* (2010) online. **(Invited Article, Special Issue)**  
<http://dx.doi.org/10.1002/mrc.2630>

 **D.L. Bryce** "Calcium Binding Environments Probed by  $^{43}\text{Ca}$  NMR Spectroscopy", *Dalton Transactions* (2010) in press. **(Cover Article)**  
<http://dx.doi.org/10.1039/c0dt00416b>

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#### Queen's University

 **J. Zhu, E. Ye, V. Terskikh, and G. Wu**, "Solid-State  $^{17}\text{O}$  NMR Spectroscopy of Large Protein-Ligand Complexes", *Angewandte Chemie International Edition* (2010) online. **(Cover Article)**  
<http://dx.doi.org/10.1002/anie.201002041>

**B.M. Cossairt, C.C. Cummins, A.R. Head, D.L. Lichtenberger, R.J. F. Berger, S.A. Hayes, N.W. Mitzel and G. Wu**, "On the Molecular and Electronic Structures of  $\text{AsP}_3$  and  $\text{P}_4$ ", *J. Am. Chem. Soc.* **132** (2010) 8459–8465.  
<http://dx.doi.org/10.1021/ja102580d>

**S. Martic, G. Wu, and S. Wang**, "Interactions of cytidine with  $\text{N}_2$ -functionalized guanosines and cytidine – cytidine exchange involving a GC pair - NMR and fluorescence spectroscopic study", *Can. J. Chem.* **88** (2010) 524–532.  
<http://dx.doi.org/10.1139/V10-040>

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#### University of Toronto

**B. Wu, T. Skarina, A. Yee, M.C. Jobin, R. Dileo, A. Semesi, C. Fares, A. Lemak, B.K. Coombes, C.H. Arrowsmith, A.U. Singer, A. Savchenko**, "NleG Type 3 Effectors from Enterohaemorrhagic *Escherichia coli* Are U-Box E3 Ubiquitin Ligases", *PLoS Pathogens* **6** (2010) e1000960 (1–17).  
<http://dx.doi.org/10.1371/journal.ppat.1000960>

**T.L. Religa, L.E. Kay**, "Optimal methyl labeling for studies of supra-molecular systems", *J Biomol NMR* **47** (2010) 163–169.  
<http://dx.doi.org/10.1007/s10858-010-9419-7>

**A.J. Baldwin, T.L. Religa, D.F. Hansen, G. Bouvignies and L.E. Kay**, "<sup>13</sup>C-HD<sub>2</sub> Methyl Group Probes of Millisecond Time Scale Exchange in Proteins by <sup>1</sup>H Relaxation Dispersion: An Application to Proteasome Gating Residue Dynamics", *J. Am. Chem. Soc.* **132** (2010) 10992–10995.  
<http://dx.doi.org/10.1021/ja104578n>

**G. Bouvignies, D.M. Korzhnev, P. Neudecker, D.F. Hansen, D. Flemming, M.H.J. Cordes, L.E. Kay**, "A simple method for measuring signs of H-1(N) chemical shift differences between ground and excited protein states", *Journal of Biomolecular NMR* **47** (2010) 135–141.  
<http://dx.doi.org/10.1007/s10858-010-9418-8>

**X. Xu, H. Sun, M.J. Simpson**, "Concentration- and time-dependent sorption and desorption behavior of phenanthrene to geosorbents with varying organic matter composition", *Chemosphere* **79** (2010) 772–778.  
<http://dx.doi.org/10.1016/j.chemosphere.2010.03.027>

**J.G. Longstaffe, M.J. Simpson, W. Maas and A.J. Simpson**, "Identifying Components in Dissolved Humic Acid That Bind Organofluorine Contaminants using <sup>1</sup>H{<sup>19</sup>F} Reverse Heteronuclear Saturation Transfer Difference NMR Spectroscopy", *Environ. Sci. Technol.* **44** (2010) 5476–5482.  
<http://dx.doi.org/10.1021/es101100s>

**C.M. Byrne, M.H.B. Hayes, R. Kumar, E.H. Novotny, G. Lanigan, K.G. Richards, D. Fay, A.J. Simpson**, "Compositional Changes in the Hydrophobic acids fraction of Drainage Water from Different Land Management Practices", *Water Research* **44** (2010) 4379–4390.  
<http://dx.doi.org/10.1016/j.watres.2010.05.055>

**P. Walsh, P. Neudecker and S. Sharpe**, "Structural Properties and Dynamic Behavior of Nonfibrillar Oligomers Formed by PrP(106–126)", *J. Am. Chem. Soc.* **132** (2010) 7684–7695.  
<http://dx.doi.org/10.1021/ja100431q>

**D.F. Hansen, P. Neudecker and L.E. Kay**, "Determination of Isoleucine Side-Chain Conformations in Ground and Excited States of Proteins from Chemical Shifts", *J. Am. Chem. Soc.* **132** (2010) 7589–7591.  
<http://dx.doi.org/10.1021/ja102090z>

**B.G. Pautler, A.J. Simpson, D.J. McNally, S.F. Lamoureux and M.J. Simpson**, "Arctic Permafrost Active Layer Detachments Stimulate Microbial Activity and Degradation of Soil Organic Matter", *Environmental Science & Technology* **44** (2010) 4076–4082.  
<http://dx.doi.org/10.1021/es903685j>

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