

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

---

---

## Canadian NMR Research News Bulletin #5.1 Winter 2011

---

---

### Canadian NMR News



International Year of  
**CHEMISTRY**  
2011

#### 2011 International Year of Chemistry

January 2011 marks the beginning of the International Year of Chemistry. The Chemical Institute of Canada (CIC) is leading the Canadian

activities which will be devoted to the celebration of chemical sciences and will aim to reach over 500,000 Canadians.

We encourage all CIC members to get involved throughout the year. CIC has been active in planning events for 2011, some of which include:

- **Global Water Experiment**, connecting countries around the world to solve current water issues;
- **YouTube Video Contest**, giving high school students a chance to use their creativity in chemistry to win a \$2,500 scholarship;
- **Science Rendezvous**, a one day national event aiming to bring science to the public;
- **Public Lecture Series**, bringing Joe Schwarcz and Pierre Beaumier to speak on interesting topics in chemistry across Canada;
- **Canadian Chemistry Milestones**, celebrating significant contributions by Canadians. See the latest press release.

Local sections across the nation are organizing events in their communities. You can see what's happening in an area near you by following the Chemical Institute of Canada - International Year of Chemistry website for more information and to see how you can get involved

<http://www.iyc2011.ca>

CIC IYC Organizing Committee

---

#### In This Issue

- 1** Canadian NMR News
- 5** John A. Weil (1929–2010)
- 6** Recognition
- 7** NMR Theses Recently Defended
- 7** On the move
- 8** the 900 NMR Facility News
- 8** Upcoming NMR Events
- 9** New NMR Books
- 10** NMR Jobs and Vacancies
- 10** Canadian NMR Research Highlights
- 11** Recent NMR Publications
- 17** Contact us

---

#### 850 MHz NMR System at UBC

Bruker Corporation announced a major order from the University of British Columbia for its ultra-high field AVANCE™ III 850 spectrometer. The 850 MHz Nuclear Magnetic Resonance (NMR) magnet and spectrometer will enable researchers at the University of British Columbia and nearby Simon Fraser University to study the mechanisms of microbial diseases. Funds to purchase Canada's first 850 MHz actively-shielded compact NMR magnet were provided to the ASTRID (Advanced Structural Biology of Re-emerging Infectious Diseases) project by the Canada Foundation for Innovation, the British Columbia Knowledge Development Fund, and the University of British Columbia (UBC).

The AVANCE III 850 spectrometer is based on Bruker's new 850 MHz Ascend™ magnet that combines the key advantages of Bruker's well-established UltraShield™ Plus magnets with the

superior performance and greater convenience delivered by advanced superconductor technology. This further innovation has enabled the design of smaller magnet coils, resulting in a significant reduction in the size of the cryostat. The new Ascend magnets are therefore easier to site, even safer to run and offer reduced operating costs. With over 160 ultra-high field installations worldwide, Bruker has an unmatched track record in NMR magnet technology.

The AVANCE III 850 system includes Bruker's high-sensitivity CryoProbe™ technology, enabling researchers to perform measurements on very small quantities of sample. In addition it is equipped with Bruker's latest Efree™ probe technologies offering state-of-the-art research tools for the investigation of membrane proteins in biological solid-state NMR.

**Suzana K. Straus**, Associate Professor of Chemistry at UBC, commented: "In recent years developments in the field of solid state NMR have led to an emergence of biomolecular methods to investigate membrane proteins. With this new magnet and probe technology, we are now able to determine the full three-dimensional structures and to characterize the membrane interactions of a range of peptides and proteins of interest. This will have great impact on our knowledge of infectious diseases."

"The incredible sensitivity and dispersion of the CryoProbe equipped solution and solid-state 850 MHz spectrometer will enable ASTRID researchers to carry out challenging structural and dynamic studies of the complex biomolecular machines used by notorious pathogens, including methicillin resistant *Staphylococcus aureus*, *Pseudomonas aeruginosa*, and *Mycobacterium tuberculosis*," said **Lawrence McIntosh**, Professor of Biochemistry & Molecular Biology and Chemistry at the University of British Columbia.

*"University of British Columbia Orders Canada's First Compact 850 MHz NMR System from Bruker to Enable Research on Microbial Diseases"*

Vancouver, British Columbia, December 15, 2010 (press release)

<http://www.bruker-biospin.com/index.php?id=4291>

---

Submitted by Scott Kroeker (Manitoba)

## Solid-state NMR in the Sun

Pacifichem 2010, held December 15-20 in Honolulu, featured several NMR-themed symposia. In the Physical Chemistry division, "Solid-State NMR Methods and Applications in Inorganic Materials" consisted of four half-day oral sessions and a poster session. Topics included energy conversion and storage materials, catalysts, surfaces, glasses and semiconductors. We had 13 invited speakers, 19 contributed talks and 16 posters across a wide demographic and topical range. We had talks from graduate students and postdocs, as well as more established professors and researchers, with speakers coming from Canada, USA, Japan, South Korea, Germany, France and Taiwan. The sessions were well attended, averaging about 50 and maxing out at 100 (possibly because of one afternoon's deluge?). The talks and posters were of uniformly high quality and the question period was vigorous and engaging. Overall, the sessions were stimulating and brought together a good mix of enthusiastic NMR researchers in solid-state NMR of materials.

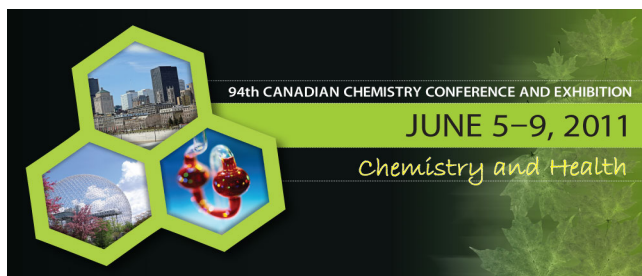


Pacifichem 2010: Rod Wasylshen, Helmut Eckert, John Ripmeester

-----  
**Jérémie Leclerc**, a Ph.D. student in the Michèle Auger's research group (Laval), has won one of the coveted student poster competition awards at Pacifichem 2010. His poster "Solid-state NMR spectroscopy reveals distinctive protein dynamics in closely related spider silks" was among of only 43 winners selected from more than 2000 student posters entered the competition and the only poster from Canada to win. *Congratulations, Jérémie!*

Read the news story at *C&EN*

<http://pubs.acs.org/subscribe/journals/cen/88/i51/html/8851news12.html>



## NMR events at CSC 2011

Dear Colleagues,

The 94<sup>th</sup> Canadian Chemistry Conference and Exhibition (**CSC 2011**) "Chemistry and Health" will be held in Montréal, Québec from June 5-9, 2011, as a joint effort of the Canadian Society for Chemistry and the four Montréal Universities, with the Université de Montréal Chemistry Department as the host. The CSC is the largest annual national event for chemical professionals attracting close to 2500 participants each year.

Canada is very dynamic in Nuclear Magnetic Resonance spectroscopy and to pursue the tradition, a **solid-state NMR workshop** organized by the National Ultrahigh Field NMR Facility for Solids

[http://nmr900.ca/events\\_e.html](http://nmr900.ca/events_e.html)

as well as two 1.5-day NMR symposia are scheduled to cover a wide range of applications and developments in the fields of solution and solid-state NMR.

Profs **Anthony Mittermaier** (McGill) and **Pierre Lavigne** (Université de Sherbrooke) are organizing the "**Solution NMR: Biomolecular structure, dynamics, and function**" symposium which includes, amongst a list of over 15 speakers, Charalampos Kalodimos (Rutgers), Brian Sykes (Alberta), Gary Shaw (Western Ontario) and Lawrence McIntosh (UBC).

Profs **Michel Lafleur** (Université de Montréal) and **Isabelle Marcotte** (Université du Québec à Montréal) are co-organizers of the symposium entitled "**Solid-state NMR: From materials to biomolecules**". So far, Marc Baldus (Utrecht), Vladimir Ladizhansky (Guelph), Bruce Balcom (New Brunswick), Valerie Booth (Memorial) and Ansgar Siemer (Columbia U.) have confirmed their presence as guest speakers.

We invite you to participate in the CSC2011 conference. More detail on the symposia, abstract submission and registration can be found on the conference website at <http://www.csc2011.ca>

**The deadline for abstract submission is February 15, 2011.**

NMR Symposia Organizers

---

## International Conference on Structural Genomics 2011

Dear Colleagues,

We are pleased to announce that registration is now open for the International Conference on Structural Genomics 2011, which will be held in Toronto, Canada on May 10-14, 2011. This meeting is the 6th in this series of biennial meetings of the International Structural Genomics Organization. The meeting is designed to serve as a forum to discuss the most recent developments in structural genomics, structural/chemical biology, and their impact on research in biology, medicine and disease. A substantial number of short talks will be selected from submitted poster abstracts. Also, a limited number of student travel fellowships will be available for travel to this meeting. Please see the website for further details <http://www.icsg2011.org>

**Abstract submission deadline is February 28, 2011.**

We hope to see you there!

Cheryl Arrowsmith - ICSG 2011 Organizer

Ted Baker, Stephen Burley, Dino Moras, Joel Sussman, Shigeyuki Yokoyama, Tom Terwilliger - ISGO Executive Committee

---

## ICSG 2011: Workshop on NMR Methods for Structural Biology

We are pleased to announce the Workshop on NMR Methods for Structural Biology at the International Conference on Structural Genomics 2011 in Toronto.

<http://www.icsg2011.org/workshop.php>

This workshop is organized by **Gaetano Montelione** (Rutgers), **Thomas Szyperski** (State University of New York) and **John Markley** (University of Wisconsin) and will

take place on Tuesday May 10, 2011 at the University of Toronto.

This workshop will survey technologies for structure/function investigations of proteins, developed in (or in collaboration with) structural genomics projects, that are ready for widespread use by the wider biological community. Topics will include: protein production and labeling by cell-based and cell-free approaches; automated assignment and secondary structure determination; reduced dimensionality approaches to NMR data collection; NMR structure validation; and, tools for data deposition, visualization, and querying from the BMRB and PDB.

Registration for the workshop is free to registered ICSG 2011 participants. Please visit <http://www.icsg2011.org> for ICSG 2011 meeting and workshop registration details

---

### MR microscopy conference in Beijing - ICMRM11

The 11<sup>th</sup> International Conference on Magnetic Resonance Microscopy will be held in Beijing, Aug 14-18, 2011.

<http://www.cup.edu.cn/icrm11/>

### Deadline for abstract submission is March 30, 2011.

The objectives of the ICMRM are to communicate recent developments in high-resolution, spatially resolved magnetic resonance methods and applications. Meeting strength stems from the eclectic background of participants and a diverse venue that has traditionally focused on non-clinical applications in science and engineering areas.

The 1<sup>st</sup> ICMRM was held in 1991 in Heidelberg and was originally known as the "Heidelberg Conference". It is the biannual conference of the Division of Spatially Resolved Magnetic Resonance of the Ampere Society.

Bruce J. Balcom, Professor  
the University of New Brunswick

---

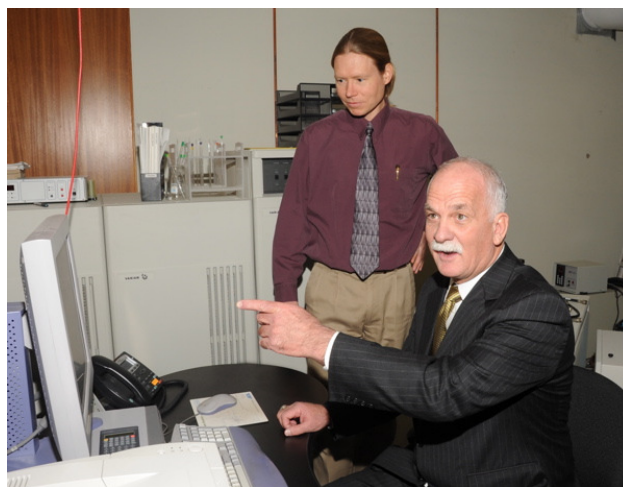
### A quantum spin on life

Read a feature story in the *Waterloo Region Record* about **Gina Passante**, a physics doctoral student working on NMR quantum computing at the University of Waterloo under the supervision of Raymond Laflamme.

<http://www.therecord.com/news/business/article/476771--a-quantum-spin-on-life>

---

**Scott Kroeker** hosted a distinguished party of politicians for an NMR lab tour associated with January's CFI LOF awards announcement. **The Honourable Vic Toews** (Minister of Public Safety), **Rod Bruinooge** (MP, Winnipeg South) and University of Manitoba dignitaries were treated to a demonstration of solid-state NMR. Mr. Toews opened his NMR account by running a Cs-133 MAS NMR spectrum of a model nuclear waste glass.



---

### H.L. Holmes Award 2011

Applications are being accepted for post-doctoral studies in chemistry, physics, biology or mathematics as they relate to medical and biological processes. Awards cover a one or two-year period, depending on available funding and the research proposal. An Award can have a monetary value of up to \$100,000 CDN per year. Please consult the following link for more information:

<http://www.nrc-cnrc.gc.ca/eng/about/holmes-awards.html>

**Application Deadline: February 28, 2011**

---

### NMR on Twitter

List of new solid-state NMR papers updated by Luke O'Dell (NRC-SIMS)

<http://twitter.com/solidstateNMR>

uOttawa NMR by Glenn Facey

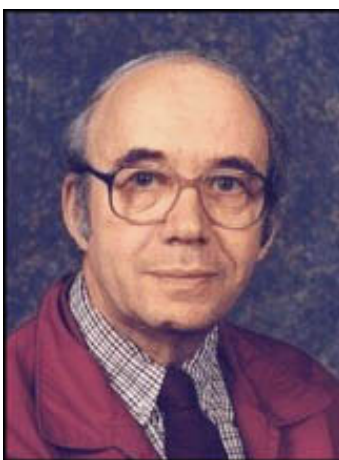
<http://twitter.com/uOttawaNMR>

NMR Wiki <http://twitter.com/nmrwiki>

nmr900 <http://twitter.com/nmr900>

Bruker <http://twitter.com/bruker>

Agilent <http://twitter.com/agilent>



### **Professor John A. Weil (1929-2010)**

Dr. John Ashley Weil, Professor Emeritus at the Department of Chemistry, the University of Saskatchewan, left us on 17 November 2010, after a period of hospitalization.

He was born 15 March 1929 near Hamburg, Germany. He, his mother, and his brother Claude Weil, fled Europe during the Nazi regime and arrived in the United States in 1940. John did his early education in a one room schoolhouse in the Catskill region of New York State, and then moved to Chicago, Illinois, where he completed high school in 1945.

John completed his doctorate in Chemical Physics at the University of Chicago in 1955, and then did a post-doctoral fellowship and taught at Princeton University. John was lured away to Argonne National Laboratory, near Chicago, where he worked on research for a dozen years, achieving the level of Senior Scientist. In 1971, he moved to the University of Saskatchewan to take up a tenured Professorship in Chemistry. In 1996, John formally retired from the University of Saskatchewan; but as Professor Emeritus, continued active research throughout the remainder of his life.

John was known internationally for his work on electron paramagnetic resonance (EPR) spectroscopy. Several generations of students were trained in his laboratories and he loved teaching and being surrounded by young people. John collaborated heavily with various research groups around the world; and published hundreds of papers, numerous book chapters, an EPR-NMR computer program, and several editions of an EPR textbook. He lectured all over the world. Sabbatical years were spent in New Zealand, Oxford, Bethlehem (PA), Chicago, and Urbana (IL).

John received many honors, including: NSERC Longevity Award (2004 and 1994), Gerhard Herzberg Award from the Spectroscopy Society of Canada (2000), Fellow of the International EPR Society (1998), Distinguished Researcher Award at the University of Saskatchewan (1996), Erskine Lecturer at the University of Canterbury, NZ (1987), Doctor of Science degree awarded by the University of Saskatchewan (1985), Thorvaldson Professor (1983-1988), and Fulbright Scholar (1967-1968).

John passionately pursued outside interests in art, music, cultural aspects of quartz, stamp-collecting, skiing, collecting and writing about Inuit art, and travel. He enjoyed many of the spectacular places that the Earth has to offer. Dr. Weil was a dynamic, fascinating man, who will be much missed by family and friends throughout the world.

## Recognition

Submitted by Genevieve Seabrook (UHN)

On January 17<sup>th</sup> 2011, **Dr. Mitsu Ikura** received the 2010 Canadian Cancer Society "**Robert L. Noble Prize**" for his outstanding contributions to cancer research in Canada.



Dr. Ikura (right) receives the prize from Dr. Michael Wosnick; VP Research for Canadian Cancer Society and Scientific Director of the CCSRI

From the citation <http://www.cancer.ca>

"Dr. Ikura is an internationally recognized authority in the field of structural biology and has laid the groundwork for our understanding of signalling proteins such as cadherins and catenins and molecular signalling processes involved in human diseases such as cancer. His studies also provide excellent platforms for developing new drugs designed to interfere with the functioning of cancer cells.

Dr. Ikura is a senior scientist at the Ontario Cancer Institute and a professor at the University of Toronto. He received his PhD in macromolecular biophysics from Hokkaido University, Japan and pursued postdoctoral studies on multi-dimensional NMR spectroscopy of a calmodulin-kinase peptide complex at the National Institutes of Health.

Dr. Ikura has a Tier-1 Canada Research Chair in cancer structural biology and has been recognized by many awards and prizes including the William E. Rawls Prize, the International Research Scholar Award Howard Hughes Medical Institute, and the Premier's Research Excellence Award. He has published over 190 peer-reviewed papers and has been invited to speak at more than 200 international scientific conferences."

**Web:** the Ikura Laboratory  
<http://nmr.uhnres.utoronto.ca/ikura/index.html>

*About "Robert L. Noble" Prize:* The Robert L. Noble Prize is given for outstanding achievements in cancer research. It honours Dr Noble, an esteemed Canadian investigator whose research in the 1950s led to the discovery of vincristine, a widely-used anti-cancer drug. At the time, vincristine was one of the most effective treatments available for Hodgkin's disease.

---

### Canada Research Chairs in magnetic resonance renewed

In November 2010 the Government of Canada has announced an investment of \$275.6 million to fund 310 new or renewed Canada Research Chairs at 53 Canadian universities. This included renewal of four Chairs involved in magnetic resonance research.

**Cheryl Arrowsmith** (University of Toronto)  
Canada Research Chair Tier 1 in Structural Proteomics

**Mitsuhiko Ikura** (University of Toronto)  
Canada Research Chair Tier 1 in Cancer Structural Biology

**Pascale Legault** (Université de Montréal)  
Canada Research Chair Tier 2 in Structural Biology and Engineering of RNA

**Josef Zwanziger** (Dalhousie University)  
Canada Research Chair Tier 1 in the Nuclear Magnetic Resonance Studies of Materials

---

### Canada Research Chairs in MR

<http://www.chairs.gc.ca/>

Cheryl Arrowsmith (Toronto) Biochemistry  
Bruce Balcom (UNB) Multidisciplinary  
Valerie Booth (Memorial) Biochemistry  
Blaine Chronik (Western) Medical Physics  
Yining Huang (Western) Materials Science  
Mitsuhiko Ikura (Toronto) Molecular Biology  
Lewis Kay (Toronto) Biochemistry  
Vladimir Ladizhansky (Guelph) Biophysics  
Raymond Laflamme (Waterloo) Physics  
Pascale Legault (Montréal) Biochemistry  
Simon Sharpe (Toronto) Biochemistry  
Gary Shaw (Western) Structural Neurobiology  
Roderick Wasylishen (Alberta) Phys Chemistry  
Josef Zwanziger (Dalhousie) Phys Chemistry

---

## Recognition (cont'd)

**André Simpson**, Professor of chemistry at the University of Toronto Scarborough, has been elected a **Fellow of the Royal Society of Chemistry** (RSC)

<http://webapps.utoronto.ca/ose/story.php?id=2381>

**David L. Bryce**, an Associate Professor at the University of Ottawa, has been awarded **the 2011 CNC-IUPAC Travel Award**. Dr. Bryce will be an invited speaker at an IUPAC-sponsored meeting in August 2011 in Sigüenza, Spain: "IUCr Workshop - Categorizing Halogen Bonding and Other Noncovalent Interactions Involving Halogen Atoms".

[http://www.cnc-iupac.ca/awards11\\_e.html](http://www.cnc-iupac.ca/awards11_e.html)

## NMR Theses Recently Defended

*Congratulate your students here!*

**Vladimir Michaelis** (University of Manitoba), November 2010

Supervisor: Prof. Scott Kroeker  
Ph.D. thesis "Nuclear Magnetic Resonance Studies of Disorder and Local Structure in Borate and Germanate Materials"

**Jerrod Dwan** (University of Alberta), November 2010

Supervisor: Prof. Rod Wasylshen  
M.Sc. thesis "Investigating the  $^{197}\text{Au}$ - $^{31}\text{P}$  Spin-Spin Coupling Interactions in Gold-Phosphine Halides Using Solid-State Nuclear Magnetic Resonance, Spectral Simulations, and Quantum Chemistry Computations"

**Ming Wang** (University of Alberta), November 2010

Supervisor: Prof. Rod Wasylshen  
Ph.D. thesis "Applications of Magnetic Resonance Imaging for the Investigation of Water Refilling of Embolized Xylem Vessels in Plant Stem Segments and of Water Management in Operating Polymer Electrolyte Membrane Fuel Cells"

**Jasmine Viger-Gravel** (University of Ottawa), December 2010

Supervisor: Prof. David Bryce  
B.Sc. honours thesis: "Solid-state NMR Analysis of Halogen Bonding Involving Thiocyanates and Selenocyanates"

**Joseph Weiss** (University of Ottawa), December 2010

Supervisor: Prof. David Bryce  
M.Sc. thesis: "A Solid-State  $^{11}\text{B}$  NMR and Computational Study of Boron Electric Field Gradient and Chemical Shift Tensors in Boronic Acids and Boronic Esters"

## On the move

**Aaron Rossini**, after finishing his Ph.D. with Rob Schurko at the University of Windsor, Aaron has started a post-doctoral fellowship in the laboratory of Lyndon Emsley at the Ecole Normale Supérieure de Lyon in Lyon, France. Aaron's postdoctoral work is supported by a prestigious Marie Curie Fellowship he was awarded in 2010. Read a feature story about Aaron in the University of Windsor's *Daily News* <http://tinyurl.com/4rdc4ln>

**Vlad Michaelis** successfully defended his Ph.D. thesis in December 2010 in the Scott Kroeker's group (Manitoba) and has now joined the research group of Bob Griffin (MIT) with an NSERC PDF fellowship.

**Jasmine Viger-Gravel** completed her B.Sc. honours project in the group of David Bryce at the University of Ottawa in December 2010. She started her M.Sc. degree in the same group in January 2011.

**Ronald Soong** has recently accepted the position of NMR Scientist & NMR Manager at the University of Toronto Scarborough (UTSC) Environmental NMR Center. Dr. Soong completed his Ph.D in 2008 at the University of Toronto Mississauga under the guidance of Prof. Peter Macdonald. He then went on to do 2 years of postdoctoral studies at the University of Michigan with Prof. Ayyalusamy Ramamoorthy where Dr. Soong developed various cutting-edge multidimensional solid-state NMR techniques for membrane protein studies. At the UTSC Environment NMR Center, Dr. Soong will focus his research on the application of NMR in environmental science and metabolomics.

Reposted from <http://www.chem.ualberta.ca/>

The Department of Chemistry, University of Alberta is delighted to announce that **Mr. Mark Miskolzie** has been appointed as our NMR

Laboratory Supervisor, effective November 1, 2010. Mark has a long association with the department, having first earned his BSc (Specialization) in 1999 and then his MSc in Physical Chemistry (supervisor: Dr. George Kotovych) in December 2002. From January to June 2003, he worked as a Research Assistant in Dr. Kotovych's lab and in July 2003, he took up the position as the NMR Service Lab Coordinator under the tutelage of Dr. Albin Otter. During that period, Mark earned a reputation as a dedicated and proactive employee with extremely strong technical skills coupled with a courteous and professional attitude. These characteristics made Mark an obvious successor to the position. Given his long association with the NMR Facility, the department is very fortunate to have hired Mark and is confident he is the right person to take on the challenge.

## the 900 NMR Facility News



### 2009-2010 Annual Report

The 2009/10 Annual Report of the National Ultrahigh-Field NMR Facility for Solids is available in print and for download at [http://nmr900.ca/annual\\_e.html](http://nmr900.ca/annual_e.html)

To request a printed copy please forward your mailing address to the Facility manager.

### NMR Facility Celebrates 100 Publications

On January 28, 2011 another milestone was reached with the acceptance of the 100<sup>th</sup> peer-reviewed publication enabled by the 900 NMR Facility. The record did not stay long, however, as the very next day two more papers have been accepted, and the current tally now stands at 103, 13 papers already this year alone.

[http://nmr900.ca/publications\\_e.html](http://nmr900.ca/publications_e.html)

The scientific output of the NMR Facility over the last five years has been undeniably impressive, and would not be possible without many enthusiastic Facility users, but also without hard work and dedication of the Facility staff and continuing support from our shareholders.

## Upcoming NMR Events

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



**ISMRR** Workshop "Ultra-high field systems and applications: 7T and beyond"

21-23 February 2011, Lake Louise, Alberta, Canada. Registration is open <http://www.ismrm.org/workshops/UltraHighField10/>

### Biophysical Society 55<sup>th</sup> Annual Meeting

March 5-9, 2011, Baltimore, Maryland  
**Special event:** Biophysical Society of Canada Mixer, Sunday, March 6, 2011, 6:00-7:00 PM  
<http://www.biophysics.org/2011meeting>

### Agilent Users' Meeting before the 52<sup>nd</sup> ENC

April 8-9, 2011, Santa Clara, California  
<http://www.chem.agilent.com/en-US/Events/en-US/Pages/enc11usermeeting.aspx>

### Bruker Pre-ENC NMR Workshops and Breakfast Symposium

April 9-10, 2011, Monterey, California  
<http://www.bruker-biospin.com/enc11.html>

### 52<sup>nd</sup> ENC

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



**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>



**ICSC 2011: Workshop on NMR Methods for Structural Biology**  
May 10, 2011, University of Toronto, Ontario, Canada <http://www.icsg2011.org>



**International Conference on Structural Genomics 2011**, ISGO  
Conference May 10-14, 2011, Toronto, Ontario, Canada <http://www.icsg2011.org>

**Abstract submission deadline is February 28, 2011**

**Registration is open until April 15, 2011**

---

## **Biomolecular NMR - Computational Aspects Gordon Research Conference**

May 22-27, 2011, Lucca (Barga), Italy  
**Registration deadline April 24, 2011**  
<http://www.grc.org/programs.aspx?year=2011&program=bionmr>

---

## **SMARTER 2 Workshop**

May 23-27, 2011, University of Aveiro, Portugal  
<http://smarter.web.ua.pt/>

---

## **6<sup>th</sup> Solid-State NMR Workshop at CSC 2011**

June 5, 2011, Montréal, Quebec, Canada  
[http://nmr900.ca/events\\_e.html](http://nmr900.ca/events_e.html)

---

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

June 5-9, 2011, Montréal, Quebec, Canada  
**Abstract deadline February 15, 2011**  
<http://www.csc2011.ca/>

---

## **Magnetic Resonance - Methods and Applications Gordon Research Seminar**

June 11-12, 2011, Biddeford, Maine, USA  
**Registration deadline May 14, 2011**  
[http://www.grc.org/programs.aspx?year=2011&program=grs\\_magr](http://www.grc.org/programs.aspx?year=2011&program=grs_magr)

---

## **Magnetic Resonance Gordon Research Conference**

June 12-17, 2011, Biddeford, Maine, USA  
**Registration deadline May 15, 2011**  
<http://www.grc.org/programs.aspx?year=2011&program=magres>

---

## **53<sup>rd</sup> Rocky Mountain Conference on Analytical Chemistry** (EPR Symposium only)

July 24-28, 2011, Snowmass, Colorado  
<http://www.rockychem.com/>

---

## **ICMRM11 - MR microscopy conference**

August 14-18, 2011, Beijing, China  
<http://www.cup.edu.cn/icrm11/>

---

## **EUROMAR 2011**

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

---

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

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

---

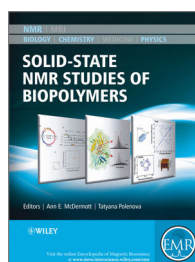
## **SMASH 2011** Small Molecule NMR Conference

September 11-15, 2011, Chamonix, France  
<http://www.smashnmr.org/>

---

## **New NMR Books**

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



---

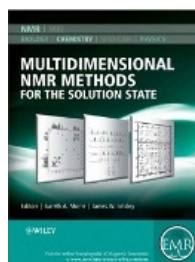
### **Solid State NMR Studies of Biopolymers**

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/>



---

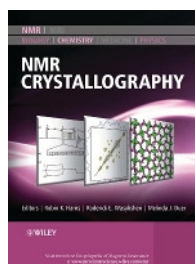
### **Multidimensional NMR Methods for the Solution State**

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>



---

### **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/>

## NMR Jobs and Vacancies

### 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

### C&EN News of the Week: Elevating Oxygen

Two recent NMR papers by **Gang Wu** (Queen's) and coworkers are highlighted by *Chemical & Engineering News* in their first issue of 2011.

<http://pubs.acs.org/cen/news/89/i01/8901notw4.html>

Both papers deal with  $^{17}\text{O}$  NMR in large protein complexes, in solution and in solid state. New research approaches proposed by Gang Wu and his team have potential to significantly advance the field of protein NMR spectroscopy.

**Jianfeng Zhu and Gang Wu**, "Quadrupole Central Transition  $^{17}\text{O}$  NMR Spectroscopy of Biological Macromolecules in Aqueous Solution," *Journal of the American Chemical Society* **133** (2011) 920-932.

<http://dx.doi.org/10.1021/ja1079207>

**Jianfeng Zhu, Eric Ye, Victor Terskikh, and Gang Wu**, "Solid-State  $^{17}\text{O}$  NMR Spectroscopy of Large Protein-Ligand Complexes," *Angewandte Chemie International Edition* **49** (2010) 8399-8402. **(Cover Article)**

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

Part of this research was made possible using resources of the National Ultrahigh-Field NMR Facility for Solids. For the complete list of research publications enabled by the Facility

[http://nmr900.ca/publications\\_e.html](http://nmr900.ca/publications_e.html)

### Cover article in *Structure*

DAXX protein, also known as a "death-associated factor", is an important player in many cell cycle processes. However the detailed molecular structure of this important protein has not been reported. In this cover article in *Structure*



#### **Lawrence McIntosh**

(UBC) and his team has discovered using NMR spectroscopy that the C-terminal half of DAXX is intrinsically disordered, whereas the N-terminal portion contains a well-folded helical bundle domain. This important work provides a structural foundation for understanding the diverse functions of DAXX.

**E. Escobar-Cabrera, D.K.W. Lau, S. Giovinazzi, A.M. Ishov, L.P. McIntosh**, "Structural Characterization of the DAXX N-Terminal Helical Bundle Domain and Its Complex with Rassf1C," *Structure* **18** (2010) 1642-1653. **(Cover Article)**

<http://dx.doi.org/10.1016/j.str.2010.09.016>

### NMR paper in *Angewandte Chemie*

**L. Shi, I. Kawamura, K.-H. Jung, L.S. Brown, and V. Ladizhansky**, "Conformation of a Seven-Helical Transmembrane Photosensor in the Lipid Environment," *Angewandte Chemie International Edition* **50** (2011) 1302-1305.

<http://dx.doi.org/10.1002/anie.201004422>

### Two NMR papers in *PNAS*

**L. Zheng, P.B. Stathopoulos, R. Schindl, G.-Y. Li, C. Romanin, and M. Ikura**, "Auto-inhibitory role of the EF-SAM domain of STIM proteins in store-operated calcium entry," *Proc. Natl. Acad. Sci. USA* **108** (2011) 1337-1342.

<http://dx.doi.org/10.1073/pnas.1015125108>

**M.T.J. Smith, J. Meissner, S. Esmonde, H.J. Wong, and E.M. Meiering**, "Energetics and mechanisms of folding and flipping the myristoyl switch in the  $\beta$ -trefoil protein, hisactophilin," *Proc. Natl. Acad. Sci. USA* **107** (2010) 20952-20957.

<http://dx.doi.org/10.1073/pnas.1008026107>

---

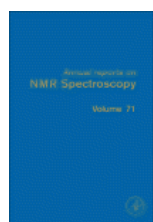
## Encyclopedia of Magnetic Resonance: new entries

**J.A. Ripmeester**, "Forty-Plus Years of Research in Solid-State NMR Spectroscopy", *Encyclopedia of Magnetic Resonance* (2010).  
<http://dx.doi.org/10.1002/9780470034590.emrhp1041>

**R.M. Henkelman**, "MRI: A Quantitative Measurement?" *Encyclopedia of Magnetic Resonance* (2010).  
<http://dx.doi.org/10.1002/9780470034590.emrhp1024>

---

## Annual Reports on NMR Spectroscopy

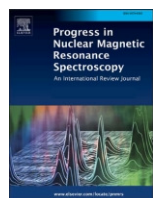


**William P. Power** "High-Resolution Magic Angle Spinning—Enabling Applications of NMR Spectroscopy to Semi-Solid Phases," *Annual Reports on NMR Spectroscopy* **72** (2011) 111-156. **(Invited Review)**

<http://dx.doi.org/10.1016/B978-0-12-385857-3.00003-7>

---

## Progress in NMR Spectroscopy



**A.D. Bain and B. Berno**, "Liouvillians in NMR: the Direct Method Revisited," *Progress in Nuclear Magnetic Resonance Spectroscopy* (2011) accepted. **(Invited Review)**

<http://dx.doi.org/10.1016/j.pnmrs.2010.12.002>

---

## Review

**R.Y. Dong** "Recent developments in biaxial liquid crystals: An NMR Perspective," *International Journal of Modern Physics B* **24** (2010) 4641-4682. **(Review)**  
<http://dx.doi.org/10.1142/S0217979210056487>



**H. Han, A.V. Ouriadov, E. Fordham, B.J. Balcom**, "Direct Measurement of Magnetic Field Gradient Waveforms," *Concepts in Magnetic Resonance Part A* **36A** (2010) 349-360.

<http://dx.doi.org/10.1002/cmr.a.20194>

---

## 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

**M. McDonald, V. Booth, and M.R. Morrow**, "Orientation and Dynamics of Synthetic Transbilayer Polypeptides Containing GpATM Dimerization Motifs," *Biophysical Journal* **100** (2011) 656-664.  
<http://dx.doi.org/10.1016/j.bpj.2010.12.3725>

**M. Sarker, J. Rose, M. McDonald, M.R. Morrow, and V. Booth**, "Modifications to Surfactant Protein B Structure and Lipid Interactions under Respiratory Distress Conditions: Consequences of Tryptophan Oxidation," *Biochemistry* **50** (2011) 25-36.  
<http://dx.doi.org/10.1021/bi101426s>

---

## NRC-IMB

**E.R. Suárez, P.F. Mugford, A.J. Rolle, I.W. Burton, J.A. Walter, J.A. Kralovec**, "<sup>13</sup>C-NMR regioisomeric analysis of EPA and DHA in fish oil derived triacylglycerol concentrates," *JAOCs, Journal of the American Oil Chemists' Society* **87** (2010) 1425-1433.  
<http://dx.doi.org/10.1007/s11746-010-1638-2>

**R.A. Perez, N. Rehmman, S. Crain, P. Leblanc, C. Craft, S. MacKinnon, K. Reeves, I.W. Burton, J.A. Walter, P. Hess, M. Quilliam, J.E. Melanson**, "The preparation of certified calibration solutions for azaspiracid-1, -2, and -3, potent marine biotoxins found in shellfish," *Analytical and Bioanalytical Chemistry* **398** (2010) 2243-2252.  
<http://dx.doi.org/10.1007/s00216-010-4161-2>

---

## Dalhousie University

**X. Zhang, J.W. Zwanziger**, "Design and Applications of an in situ Electrochemical NMR Cell," *Journal of Magnetic Resonance* **208** (2011) 136-147.  
<http://dx.doi.org/10.1016/j.jmr.2010.10.013>

**B. Chen, U. Werner-Zwanziger, J.W. Zwanziger, M.L.F. Nascimento, L. Ghussn, E.D. Zanotto**, "Correlation of network structure with devitrification mechanism in lithium and sodium diborate glasses," *Journal of Non-Crystalline Solids* **356** (2010) 2641-2644.  
<http://dx.doi.org/10.1016/j.jnoncrysol.2010.04.053>

---

### University of New Brunswick

**C.E. Muir, B.J. Lowry and B.J. Balcom**, "Measuring diffusion using the differential form of Fick's law and magnetic resonance imaging," *New J. Phys.* **13** (2011) 015005. (**Special Issue** "Focus on the Physics of Magnetic Resonance on Porous Media")  
<http://dx.doi.org/10.1088/1367-2630/13/1/015005>

**O.V. Petrov, G. Erslund, B.J. Balcom**, " $T_2$  distribution mapping profiles with phase encode MRI," *Journal of Magnetic Resonance* (2011) accepted.  
<http://dx.doi.org/10.1016/j.jmr.2010.12.006>



**H. Han, A.V. Ouriadov, E. Fordham, B.J. Balcom**, "Direct Measurement of Magnetic Field Gradient Waveforms," *Concepts in Magnetic Resonance Part A* **36A** (2010) 349-360.

<http://dx.doi.org/10.1002/cmr.a.20194>

---

### McGill University

**P.J. Farber, A. Mittermaier**, "Concerted dynamics link allosteric sites in the PBX homeodomain," *Journal of Molecular Biology* **405** (2011) 819-830.  
<http://dx.doi.org/10.1016/j.jmb.2010.11.016>

**Q. Liu and K. Gehring**, "Heterodimerization of BAK and MCL-1 Activated by Detergent Micelles," *Journal of Biological Chemistry* **285** (2010) 41202-41210.  
<http://dx.doi.org/10.1074/jbc.M110.144857>

**A. Matte, G. Kozlov, J.F. Trempe, M.A. Currie, D. Burk, Z. Jia, K. Gehring, I. Ekiel, A.M. Berghuis, M. Cygler**, "Preparation and characterization of bacterial protein complexes for structural analysis," *Advances in protein chemistry and structural biology* **76** (2009) 1-42. (**review**)  
[http://dx.doi.org/10.1016/S1876-1623\(08\)76001-2](http://dx.doi.org/10.1016/S1876-1623(08)76001-2)

**C. Riedinger, J. Boehringer, J.-F. Trempe, E.D. Lowe, N.R. Brown, K. Gehring, M.E.M. Noble, C. Gordon, and J.A. Endicott**, "Structure of Rpn10 and Its Interactions with Polyubiquitin Chains and the Proteasome Subunit Rpn12," *Journal of Biological Chemistry* **285** (2010) 33992-34003.  
<http://dx.doi.org/10.1074/jbc.M110.134510>

---

### Health Canada

**N. Panjwani, D.J. Hodgson, S. Sauve, Y. Aubin**, "Assessment of the Effects of pH, Formulation and Deformulation on the Conformation of Interferon Alpha-2 by NMR," *Journal of Pharmaceutical Sciences* **99** (2010) 3334-3342.  
<http://dx.doi.org/10.1002/jps.22105>

---

### University of Ottawa

**H. Mohammadi-Manesh, S. Alavi, T.K. Woo and B. Najafi**, "Molecular Dynamics Simulation of NMR Powder Lineshapes of Linear Guests in Structure I Clathrate Hydrates" *Phys.Chem.Chem.Phys.* **13** (2011) 2367-2377.  
<http://dx.doi.org/10.1039/C0CP01920H>

---

### NRC-SIMS



**O.B. Lapina, D.F. Khabibulin, and V.V. Terskikh**, "Multinuclear NMR Study of Silica Fiberglass Modified with Zirconia," *Solid State Nuclear Magnetic Resonance* (2011) online.  
<http://dx.doi.org/10.1016/j.ssnmr.2010.12.002>



**L.A. O'Dell, R.W. Schurko, K.J. Harris, J. Autschbach, and C.I. Ratcliffe**, "Interaction Tensors and Local Dynamics in Common Structural Motifs of Nitrogen: A Solid-state  $^{14}\text{N}$  NMR and DFT Study," *J. Am. Chem. Soc.* **133** (2011) 527-546.  
<http://dx.doi.org/10.1021/ja108181y>



**L.A. O'Dell and C.I. Ratcliffe**, "Crystal Structure Based Design of Signal Enhancement Schemes for Solid-State NMR of Insensitive Half-Integer Quadrupolar Nuclei," *Journal of Physical Chemistry A* **115** (2011) 747-752.  
<http://dx.doi.org/10.1021/jp111531e>

**R. Alizadeh, J.J. Beaudoin, L. Raki, V. Terskikh,** "C-S-H/polyaniline nanocomposites prepared by in situ polymerization", *Journal of Materials Science* **46** (2011) 460-467.  
<http://dx.doi.org/10.1007/s10853-010-4918-1>

**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* **89** (2011) 71-79.  
<http://dx.doi.org/10.1007/s10705-010-9377-1>


**H. Lu, T. Kawasaki, T. Ukita, I. Moudrakovski, T. Fujii, S. Noguchi, T. Shimada, M. Nakamizu, J. Ripmeester, C. Ratcliffe,** "Particle-size effect on the saturation of methane hydrate in sediments – Constrained from experimental results," *Marine and Petroleum Geology* (2011) accepted.  
<http://dx.doi.org/10.1016/j.marpetgeo.2010.11.007>

**H. Lu, T.D. Lorenson, I.L. Moudrakovski, J.A. Ripmeester, T.S. Collett, R.B. Hunter, C.I. Ratcliffe,** "The characteristics of gas hydrates recovered from BPXA-DOE-USGS Mount Elbert Gas Hydrate Stratigraphic Test Well, Alaska North Slope," *Marine and Petroleum Geology* **28** (2011) 411-418.  
<http://dx.doi.org/10.1016/j.marpetgeo.2010.01.002>

**J.A. Ripmeester,** "Forty-Plus Years of Research in Solid-State NMR Spectroscopy", *Encyclopedia of Magnetic Resonance* (2010).  
<http://dx.doi.org/10.1002/9780470034590.emrhp1041>

---

## Queen's University

 **J. Zhu and G.Wu,** "Quadrupole Central Transition  $^{17}\text{O}$  NMR Spectroscopy of Biological Macromolecules in Aqueous Solution," *Journal of the American Chemical Society* **133** (2011) 920-932.  
**(C&EN News of the Week)**  
<http://dx.doi.org/10.1021/ja1079207>

**J.Y.C. Lau, T. Olding, G. Wu and L.J. Schreiner,** "Fricke dosimetry of irradiated sugar by  $^1\text{H}$  NMR relaxation," *Journal of Physics: Conference Series* **250** (2010) 012096.  
<http://dx.doi.org/10.1088/1742-6596/250/1/012096>

---

## University of Toronto

**J. Shloush, J.E. Vlassov, I. Engson, S. Duan, V. Saridakis, S. Dhe-paganon, B. Raught, Y. Sheng, and C.H. Arrowsmith,** "Structural and Functional Comparison of the RING Domains of Two p53 E3 Ligases, Mdm2 and Pirh2," *Journal of Biological Chemistry* **286** (2011) 4796-4808.  
<http://dx.doi.org/10.1074/jbc.M110.157669>

**S. Ko, H. Kim, J. Yun, A. Yee, C.H. Arrowsmith, C. Cheong, W. Lee,** "Solution structure of MTH1821, a putative structure homologue to RNA polymerase  $\alpha$  subunit from *Methanobacterium thermoautotrophicum*," *Proteins: Structure, Function and Bioinformatics* (2011) in press.  
<http://dx.doi.org/10.1002/prot.22956>

**J.R. Brender, R.P.R. Nanga, N. Popovych, R. Soong, P.M. Macdonald, A. Ramamoorthy,** "The amyloidogenic SEVI precursor, PAP248-286, is highly unfolded in solution despite an underlying helical tendency," *Biochimica et Biophysica Acta (BBA) - Biomembranes* (2011) accepted.  
<http://dx.doi.org/10.1016/j.bbamem.2011.01.010>

**G. Bouvignies, D.F. Hansen, P. Vallurupalli, and L.E. Kay,** "Divided-Evolution-Based Pulse Scheme for Quantifying Exchange Processes in Proteins: Powerful Complement to Relaxation Dispersion Experiments," *J. Am. Chem. Soc.* **133** (2011) ASAP.  
<http://dx.doi.org/10.1021/ja109589y>

**X. Feng, K. Hills, A.J. Simpson, J.K. Whalen, M.J. Simpson,** "The role of biodegradation and photo-oxidation in the transformation of terrigenous organic matter," *Organic Geochemistry* (2011) accepted.  
<http://dx.doi.org/10.1016/j.orggeochem.2011.01.002>

**L. Zheng, P.B. Stathopoulos, R. Schindl, G.-Y. Li, C. Romanin, and M. Ikura,** "Auto-inhibitory role of the EF-SAM domain of STIM proteins in store-operated calcium entry," *Proc. Natl. Acad. Sci. USA* **108** (2011) 1337-1342.  
<http://dx.doi.org/10.1073/pnas.1015125108>

**A. Lemak, A. Gutmanas, S. Chitayat, M. Karra, C. Farès, M. Sunnerhagen, C.H. Arrowsmith,** "A novel strategy for NMR resonance assignment and protein structure

determination," *Journal of Biomolecular NMR* **49** (2011) 27-38.  
<http://dx.doi.org/10.1007/s10858-010-9458-0>

**L. Kaustov, H. Ouyang, M. Amaya, A. Lemak, N. Nady, S. Duan, G.A. Wasney, Z. Li, M. Vedadi, M. Schapira, J. Min and C.H. Arrowsmith,** "Recognition and Specificity Determinants of the Human Cbx Chromodomains," *Journal of Biological Chemistry* **286** (2011) 521-529.  
<http://dx.doi.org/10.1074/jbc.M110.191411>

**A.S. Pinheiro, J.A. Marsh, J.D. Forman-Kay, and W. Peti,** "Structural Signature of the MYPT1-PP1 Interaction," *J. Am. Chem. Soc.* **133** (2011) 73-80.  
<http://dx.doi.org/10.1021/ja107810r>

**G. Song, M.H.B. Hayes, E.H. Novotny, A.J. Simpson,** "Isolation and fractionation of soil humin using alkaline urea and dimethylsulphoxide plus sulphuric acid," *Naturwissenschaften* **98** (2011) 7-13.  
<http://dx.doi.org/10.1007/s00114-010-0733-4>

**L.L. Mao, P.B. Stathopoulos, M. Ikura, M. Inouye,** "Secretion of human superoxide dismutase in Escherichia coli using the condensed single-protein-production system," *Protein Science* **19** (2010) 2330-2335.  
<http://dx.doi.org/10.1002/pro.512>

**J. Yuk, J.R. McKelvie, M.J. Simpson, M. Spraul, A.J. Simpson,** "Comparison of 1-D and 2-D NMR techniques for screening earthworm responses to sub-lethal endosulfan exposure," *Environmental Chemistry* **7** (2010) 524-536.  
<http://dx.doi.org/10.1071/EN10084>

**E. Kupce, L.E. Kay, and R. Freeman,** "Detecting the "Afterglow" of  $^{13}\text{C}$  NMR in Proteins Using Multiple Receivers," *J. Am. Chem. Soc.* **132** (2010) 18008-18011.  
<http://dx.doi.org/10.1021/ja1080025>

**J.L. Kitevski-LeBlanc, F. Evanics and R.S. Prosser,** "Optimizing  $^{19}\text{F}$  NMR protein spectroscopy by fractional biosynthetic labeling," *Journal of Biomolecular NMR* **48** (2010) 113-121.  
<http://dx.doi.org/10.1007/s10858-010-9443-7>

**H. Mizuno, T.K. Mal, M. Wälchli, T. Fukano, M. Ikura, A. Miyawaki,** "Molecular basis of

photochromism of a fluorescent protein revealed by direct  $^{13}\text{C}$  detection under laser illumination," *Journal of Biomolecular NMR* **48** (2010) 237-246.  
<http://dx.doi.org/10.1007/s10858-010-9453-5>

---

## McMaster University

**L.J.M. Davis, I. Heinmaa, B.L. Ellis, L.F. Nazar and G.R. Goward,** "Influence of particle size on solid solution formation and phase interfaces in  $\text{Li}_{0.5}\text{FePO}_4$  revealed by  $^{31}\text{P}$  and  $^7\text{Li}$  solid state NMR spectroscopy," *Phys. Chem. Chem. Phys.* (2011) online.  
<http://dx.doi.org/10.1039/c0cp01922d>

**A.D. Bain, C.K. Anand, Z. Nie,** "Exact Solution of the CPMG Pulse Sequence with Phase Variation Down the Echo Train: Application to  $R_2$  Measurements," *Journal of Magnetic Resonance* (2011) accepted.  
<http://dx.doi.org/10.1016/j.jmr.2011.01.009>



**A.D. Bain and B. Berno,** "Liouvillians in NMR: the Direct Method Revisited," *Progress in Nuclear Magnetic Resonance Spectroscopy* (2011) accepted. **(Invited Review)**  
<http://dx.doi.org/10.1016/j.pnmrs.2010.12.002>

**J. Milojevic, G. Melacini,** "Stoichiometry and Affinity of the Human Serum Albumin-Alzheimer's A-beta Peptide Interactions," *Biophys J.* **100** (2011) 183-192.  
<http://dx.doi.org/10.1016/j.bpj.2009.08.028>

**R.J. Kalbasi, A.R. Massah, F. Zamani, A.D. Bain, B. Berno,** "Metal (Co, Mn)-amine-functionalized mesoporous silica SBA-15: synthesis, characterization and catalytic properties in hydroxylation of benzene", *J Porous Mater* (2011) online.  
<http://dx.doi.org/10.1007/s10934-010-9400-6>

---

## University of Guelph

**Y. Fan, L. Shi, V. Ladizhansky and L.S. Brown,** "Uniform isotope labeling of a eukaryotic seven-transmembrane helical protein in yeast enables high-resolution solid-state NMR studies in the lipid environment," *Journal of Biomolecular NMR* (2011) online.  
<http://dx.doi.org/10.1007/s10858-011-9473-9>

**L. Shi, I. Kawamura, K.-H. Jung, L.S. Brown, and V. Ladizhansky**, "Conformation of a Seven-Helical Transmembrane Photosensor in the Lipid Environment," *Angewandte Chemie International Edition* **50** (2011) 1302-1305.  
<http://dx.doi.org/10.1002/anie.201004422>

---

### University of Waterloo



**W.P. Power** "High-Resolution Magic Angle Spinning—Enabling Applications of NMR Spectroscopy to Semi-Solid Phases," *Annual Reports on NMR Spectroscopy* **72** (2011) 111-156. **(Invited Review)**

<http://dx.doi.org/10.1016/B978-0-12-385857-3.00003-7>

**M.T.J. Smith, J. Meissner, S. Esmonde, H.J. Wong, and E.M. Meiering**, "Energetics and mechanisms of folding and flipping the myristoyl switch in the  $\beta$ -trefoil protein, hisactophilin," *Proc. Natl. Acad. Sci. USA* **107** (2010) 20952-20957.  
<http://dx.doi.org/10.1073/pnas.1008026107>

**O. Moussa, C.A. Ryan, D.G. Cory, R. Laflamme**, "Testing Contextuality on Quantum Ensembles with One Clean Qubit," *Physical Review Letters* **104** (2010) 160501(4).  
<http://dx.doi.org/10.1103/PhysRevLett.104.160501>

---

### University of Western Ontario

**B. Chen and Y. Huang**, "Formation of Microporous Material  $\text{AlPO}_4\text{-18}$  under Dry-Gel Conversion Conditions," *Microporous and Mesoporous Materials* (2011) accepted.  
<http://dx.doi.org/10.1016/j.micromeso.2011.02.002>

**D.E. Spratt and G.S. Shaw**, "Association of the Disordered C-terminus of CDC34 with a Catalytically-bound Ubiquitin," *Journal of Molecular Biology* (2011) accepted.  
<http://dx.doi.org/10.1016/j.jmb.2011.01.047>

**L. Santamaria-Kisiel and G.S. Shaw**, "Identification of regions responsible for the open conformation of S100A10 using chimaeric S100A11–S100A10 proteins," *Biochemical Journal* **434** (2011) 37–48.  
<http://dx.doi.org/10.1042/BJ20100887>

---

### University of Windsor



**L.A. O'Dell, R.W. Schurko, K.J. Harris, J. Autschbach, and C.I.**

**Ratcliffe**, "Interaction Tensors and Local Dynamics in Common Structural Motifs of Nitrogen: A Solid-state  $^{14}\text{N}$  NMR and DFT Study," *J. Am. Chem. Soc.* **133** (2011) 527–546. <http://dx.doi.org/10.1021/ja108181y>

**A.W. MacGregor, L.A. O'Dell, R.W. Schurko**, "New Methods for the Acquisition of Ultra-Wideline Solid-State NMR Spectra of Spin-1/2 Nuclides," *Journal of Magnetic Resonance* **208** (2011) 103-113.  
<http://dx.doi.org/10.1016/j.jmr.2010.10.011>



**A.J. Rossini, I. Hung, S.A. Johnson, C. Sleboznick, M. Mensch, P.A.**

**Deck, and R.W. Schurko**, "Solid-State  $^{91}\text{Zr}$  NMR Spectroscopy Studies of Zirconocene Olefin Polymerization Catalyst Precursors," *J. Am. Chem. Soc.* **132** (2010) 18301–18317.  
<http://dx.doi.org/10.1021/ja107749b>

---

### University of Manitoba

**A.R. Geisheimer, J.E.C. Wren, V.K. Michaelis, M. Kobayashi, K. Sakai, S. Kroeker, and D.B. Leznoff**, "Aggregation of  $[\text{Au}(\text{CN})_4]^-$  Anions: Examination by Crystallography and  $^{15}\text{N}$  CP-MAS NMR and the Structural Factors Influencing Intermolecular  $\text{Au}\cdots\text{N}$  Interactions," *Inorg. Chem.* (2011) ASAP.  
<http://dx.doi.org/10.1021/ic101782v>



**V.K. Michaelis and S. Kroeker**, " $^{73}\text{Ge}$  Solid-State NMR of Germanium Oxide

Materials: Experimental and Theoretical Studies," *Journal of Physical Chemistry C* **114** (2010) 21736–21744.  
<http://dx.doi.org/10.1021/jp1071082>

---

### University of Alberta

**O. Julien, J.R. Beadle, W.C. Magee, S. Chatterjee, K.Y. Hostetler, D.H. Evans, and B.D. Sykes**, "Solution Structure of a DNA Duplex Containing the Potent Anti-Poxvirus Agent Cidofovir," *J. Am. Chem. Soc.* **133** (2011) ASAP.  
<http://dx.doi.org/10.1021/ja109823e>

**T.C. Bjorndahl, G.-P. Zhou, X.i Liu, R. Perez-Pineiro, V. Semenchko, F. Saleem, S. Acharya, A. Bujold, C.A. Sobsey, and D.S. Wishart,** "Detailed Biophysical Characterization of the Acid-induced PrPc to PrP<sup>B</sup> Conversion Process," *Biochemistry* (2011) accepted.  
<http://dx.doi.org/10.1021/bi101435c>

**O. Julien, P. Mercier, C.N. Allen, O. Fiset, C.H.I. Ramos, P. Lagüe, T.M.A. Blumenschein, B.D. Sykes,** "Is there nascent structure in the intrinsically disordered region of troponin I?," *Proteins: Structure, Function, and Bioinformatics* (2011) accepted.  
<http://dx.doi.org/10.1002/prot.22959>

**C.E. Norris, S.A. Quideau, J.S. Bhatti and R.E. Wasylshen,** "Soil carbon stabilization in jack pine stands along the Boreal Forest Transect Case Study," *Global Change Biology* **17** (2011) 480-494.  
<http://dx.doi.org/10.1111/j.1365-2486.2010.02236.x>



**D.S. Wishart** "Interpreting Protein Chemical Shift Data," *Progress in Nuclear Magnetic Resonance Spectroscopy* **58** (2011) 62-87.  
**(Invited Review)**

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

**I.M. Robertson, Y.B. Sun, M.X. Li, B.D. Sykes,** "A structural and functional perspective into the mechanism of Ca<sup>2+</sup>-sensitizers that target the cardiac troponin complex," *J. Molecular and Cellular Cardiology* **49** (2010) 1031-1041.  
<http://dx.doi.org/10.1016/j.yjmcc.2010.08.019>

**C.J. Markin, L.F. Saltibus, M.J. Kean, R.T. McKay, W. Xiao, and L. Spyropoulos,** "Catalytic Proficiency of Ubiquitin Conjugation Enzymes: Balancing pKa Suppression, Entropy, and Electrostatics," *J. Am. Chem. Soc.* **132** (2010) 17775-17786.  
<http://dx.doi.org/10.1021/ja105267w>

**B.N. Ametaj, Q. Zebeli, F. Saleem, N. Psychogios, M.J. Lewis, S.M. Dunn, J.G. Xia, D.S. Wishart,** "Metabolomics reveals unhealthy alterations in rumen metabolism with increased proportion of cereal grain in the diet of dairy cows," *Metabolomics* **6** (2010) 583-594.  
<http://dx.doi.org/10.1007/s11306-010-0227-6>

**J. Tzeng, B.L. Lee, B.D. Sykes and L. Fliegel,** "Structural and Functional Analysis of Transmembrane Segment VI of the NHE1 Isoform of the Na<sup>+</sup>/H<sup>+</sup> Exchanger," *Journal of Biological Chemistry* **285** (2010) 36656-36665.  
<http://dx.doi.org/10.1074/jbc.M110.161471>

---

### University of Calgary

**O.F. Bathe, R. Shaykhtudinov, K. Kopciuk, A.M. Weljie, A. McKay, F.R. Sutherland, E. Dixon, N. Dunse, D. Sotiropoulos and H.J. Vogel,** "Feasibility of Identifying Pancreatic Cancer Based on Serum Metabolomics," *Cancer Epidemiol Biomarkers Prev* **20** (2011) 140-147.  
<http://dx.doi.org/10.1158/1055-9965.EPI-10-0712>

**M.G. Hobbs, C.J. Knapp, P.T. Welsh, J. Borau-Garcia, T. Ziegler, R. Roesler,** "Anionic N-heterocyclic carbenes with N,N'-Bis(fluoroaryl) and N,N'-bis(perfluoroaryl) substituents," *Chemistry - A European Journal* **16** (2010) 14520-14533.  
<http://dx.doi.org/10.1002/chem.201001698>

**H. Ishida, and H.J. Vogel,** "The Solution Structure of a Plant Calmodulin and the CaM-binding Domain of the Vacuolar Calcium-ATPase BCA1 Reveals a New Binding and Activation Mechanism," *Journal of Biological Chemistry* **285** (2010) 38502-38510.  
<http://dx.doi.org/10.1074/jbc.M110.131201>

---

### University of British Columbia

**K.H. Kim, H.-S. Kang, M. Okon, E. Escobar-Cabrera, L.P. McIntosh, M. Paetzl,** "Structural characterization of *Escherichia coli* BamE, a lipoprotein component of the beta-barrel assembly machinery complex," *Biochemistry* **50** (2011) 1081-1090.  
<http://dx.doi.org/10.1021/bi101659u>

**S.K. Straus, W.R.P. Scott, C.D. Schwieters, D.A. Marvin,** "Consensus structure of Pf1 filamentous bacteriophage from X-ray fibre diffraction and solid-state NMR," *European Biophysics Journal* (2011) in press.  
<http://dx.doi.org/10.1007/s00249-010-0640-9>

**J.T.J. Cheng, J.D. Hale, M. Elliott, R.E.W. Hancock, S.K. Straus,** "The Importance of Bacterial Membrane Composition in the Structure and Function of Aurein 2.2 and

selected Variants," *BBA - Biomembranes* **1808** (2011) 622-633.  
<http://dx.doi.org/10.1016/j.bbamem.2010.11.025>

**A.C.J. Weber, X. Yang, R.Y. Dong, E.E. Burnell**, "The smectic effect on solute order parameters rationalized by double Maier-Saupe Kobayashi-McMillan theory," *Journal of Chemical Physics* **132** (2010) 034503.  
<http://dx.doi.org/10.1063/1.3291486>

**R.Y. Dong** "Recent developments in biaxial liquid crystals: An NMR Perspective," *International Journal of Modern Physics B* **24** (2010) 4641-4682. **(Review)**  
<http://dx.doi.org/10.1142/S0217979210056487>

**E. Escobar-Cabrera, D.K.W. Lau, S. Giovinazzi, A.M. Ishov, L.P. McIntosh**, "Structural Characterization of the DAXX N-Terminal Helical Bundle Domain and Its Complex with Rassf1C," *Structure* **18** (2010) 1642-1653. **(Cover Article)**  
<http://dx.doi.org/10.1016/j.str.2010.09.016>

**J.L. Figueirinhas, G. Feio, C. Cruz, M. Lehmann, C. Kohn, R.Y. Dong**, "Nuclear magnetic resonance spectroscopic investigations of phase biaxiality in the nematic glass of a shape-persistent V-shaped mesogen," *Journal of Chemical Physics* **133** (2010) 174509.  
<http://dx.doi.org/10.1063/1.3496491>

## Contact us

You are invited to forward your thoughts and suggestions about this News Bulletin to

Victor Terskikh, Manager  
National Ultrahigh-field NMR Facility for Solids

1200 Montreal Road M-40  
Ottawa ON, K1A 0R6

Tel. (613) 998-5552

Fax: (613) 990-1555

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