



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

Canadian NMR Research News Bulletin #5.2 Spring 2011

Guest Editorial

James Davis, Vladimir Ladizhansky
University of Guelph

Dear Colleagues,

Some of you may already know that the University of Guelph has been awarded a grant for a DNP-enhanced solid-state NMR spectrometer. The original application submitted to CFI in October of 2008 was a combined request for a Mass Spectrometry suite and a DNP instrument. The team of principal applicants with interests in various areas of life sciences was composed of ten researchers: Joseph Lam, Frances Sharom, Rod Merrill, Rickey Yada, Ryan Norris, Brenda Coomber, Kathrin Preuss, David Ma, James Davis, and Vladimir Ladizhansky, with an additional list of 20 researchers who supported the application.

Multidisciplinary Assessment Committee (MAC) was very excited about the DNP part of the proposal and ranked it very highly, but, despite this, our CFI application was not successful. However, the Ontario Ministry of Research and Innovation (MRI) supported the DNP initiative.



263 GHz Bruker Avance Solid-State DNP-NMR spectrometer (Credit: Bruker)

In This Issue

- 1** Guest Editorial
- 2** Canadian NMR News
- 5** Recognition
- 6** NMR Theses Recently Defended
- 6** On the move
- 7** the 900 NMR Facility News
- 7** Upcoming NMR Events
- 10** New Books
- 11** NMR Jobs and Vacancies
- 13** Canadian NMR Research Highlights
- 16** Recent NMR Publications
- 22** Contact us

Thanks to the Government of Ontario (MRI Ontario Research Fund - Research Infrastructure Program), Bruker Ltd., and the University of Guelph (College of Physical and Engineering Sciences, the Office of Research, and the University of Guelph NMR Centre), we were able to secure the funds in May 2010, received final approvals in December 2010, and submitted the order to Bruker in February 2011 for a 395 GHz/600 MHz (electron/proton frequency) solid-state DNP-NMR spectrometer. This will be the first commercial DNP-NMR instrument operating at 600 MHz. There is no final delivery date yet, but we anticipate the instrument to be operational before summer of 2012. All necessary renovations and installations have already been started, and are overseen by our NMR manager Valerie Robertson.

At Guelph, we are interested in solid-state NMR of membrane proteins. For those who don't follow the field of biological solid-state NMR

closely, recent developments in this area are truly impressive. About ten years ago, when one of the authors started his postdoc, solving a high-resolution structure of a simple tripeptide N-formyl-L-Met-L-Leu-L-Phe-OH by solid-state NMR methods was a major achievement (C.M. Rienstra et al, PNAS USA, **2002**, 99, 10260). In the last decade, the field has progressed enormously. Structure elucidation of insoluble proteins with molecular weights in the range of tens of kilodaltons, supramolecular aggregates, and membrane proteins has become quite common nowadays. Despite these developments, the applications to large proteins and protein complexes are severely limited by poor spectral sensitivity. The development of instrumentation and methodology for high-field DNP by Robert Griffin and co-workers at MIT, and the development of a commercial DNP spectrometer by Bruker is a break-through achievement that will help overcome the sensitivity problem.

Although applications of DNP in biosolids NMR seem to be much more widespread, and the DNP sensitivity enhancements in biomaterials are well documented in the literature (see, for example, V. Bajaj et al., PNAS USA **2009**, 106, 9244; P.C.A. van der Wel, JACS **2006**, 128, 10840), there is no doubt that other areas of NMR spectroscopy can benefit from it. One fine example was given by Lyndon Emsley and co-workers, who have recently demonstrated DNP-enhanced surface NMR (e.g., A. Lesage, JACS **2010**, 132, 15459).

The DNP-enhanced SSNMR instrument at Guelph will initially be equipped with a 3.2 mm H-C-N low temperature MAS probe, and will be available for use for all research groups in Canada and worldwide. Because of the limitations with probe tunability, applications will be initially limited to carbon- and nitrogen-detected spectroscopy (or nuclei with similar Larmor frequencies). We hope to be able to expand these capabilities to a wider range of nuclei, and encourage you to contact us to discuss additional opportunities.

We would like to invite you to use our new system at Guelph to take full advantage of DNP-NMR in your research.

Canadian NMR News

NSERC 2011 Competition Results

Natural Sciences and Engineering Research Council of Canada (**NSERC**) has announced results of the 2011 NSERC competition in the Discovery Grants Program (**DG**), Research Tools and Instruments Grants (**RTI**) and Scholarship programs. Some of the early results reported

Scott Kroeker (University of Manitoba) has his NSERC Discovery Grant "NMR Spectroscopy of Disordered Solids" renewed for five years.

Gang Wu (Queen's) has his NSERC Discovery Grant on "Oxygen-17 NMR of biological systems" renewed for five years.

David Bryce and colleagues from the University of Ottawa have received NSERC RTI funding for a console upgrade for 300 MHz solution NMR instrument at the Department of Chemistry.

Gang Wu and his colleagues at Queen's received NSERC RTI funding to replace two NMR probes at the Queen's NMR Facility.

Kevin Burgess and **Fred Perras** (University of Ottawa, Bryce lab) both have their NSERC Graduate Scholarships successfully renewed.

Submitted by Tim Burrow (Toronto)

NMR upgrades at the University of Toronto

The Department of Chemistry at the University of Toronto has ordered \$5.5M of new NMR spectrometers from Agilent Technologies to equip its new 4,000-square-foot NMR laboratory. The new spectrometers will be a **500 MHz** spectrometer, with 7600AS sample changer and XSens 13C sensitive cryogenically cooled probe, a **600 MHz** dual liquids and solids spectrometer and a **700 MHz** spectrometer with a H/F,CN Cold Probe, 7600AS sample changer and solids, biosolids and semi-solids probes.

"These new NMR systems will provide a vital boost to our new Centre for Spectroscopic Investigation of Complex Organic Molecules and Polymers (CSICOMP), increasing the range and scope of research in key areas," said Professor **Robert H. Morris**, Chair of the Chemistry Department.

More than 45 scientists as well as 300 graduate students and postdoctoral fellows will be able to use the facility for inorganic, organic, materials and bio-organic research, including broader investigations into the fate of fluorinated compounds in the environment. The new facility is supported by the Canada Foundation for Innovation and the Ontario Ministry of Research and Innovation.

"We are excited that the University of Toronto's new facility has chosen Agilent as its primary NMR equipment provider," said **Kevin Meldrum**, director, research products marketing for Agilent. "Agilent is dedicated to helping scientists meet all of their spectroscopy research needs and this agreement further illustrates that commitment."

Read the full press release by Agilent Technologies

<http://www.agilent.com/about/newsroom/presrel/2011/22mar-ca11021.html>

The opening of the CSICOMP facility is being scheduled to coincide with the **MOOT XXIV Symposium**, which will be held in Toronto, October 22-23. Agilent is working with **Simon Sharpe** and **Tim Burrow** to put together a daylong Agilent NMR Symposium and mixer on October 21st. More information will be posted on <http://www.spinsights.net/>

New NMR hardware at the University of Manitoba

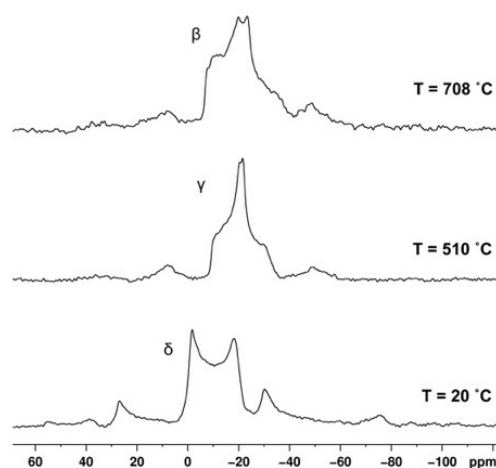
Scott Kroeker (Manitoba, Chemistry) has received a Bruker Avance III 400 widebore NMR spectrometer to accommodate a unique and the first in Canada laser-heated MAS probe built by Bruker capable of MAS experiments at temperatures exceeding 700°C (pictured)



This exciting new acquisition will be a big boost to NMR glass and minerals research projects underway in the Kroeker group.

The high-temperature MAS NMR probe is accompanied by a newly upgraded Avance III console for the 500 MHz standard bore magnet and a collection of new solid-state NMR probes designed to access low-gamma nuclei, very fast spinning MAS rates and broadband multi-resonance experiments. This infrastructure is supported by CFI.

²³Na MAS NMR of Na₂MoO₄ Phases



Web: Kroeker research group (pictures credit) <http://home.cc.umanitoba.ca/~kroekers/index.html>

Submitted by Henry Stronks (Bruker)

News from Bruker Canada

Alan Hume has been promoted to Bruker's North American Sales Manager. He will remain in Canada, and be responsible for BioSpin product lines in Canada, but he will also co-ordinate all the sales activities for NMR in the United States as well. Alan will have a team of sales people reporting to him and we wish him much success in his new role!



As a result, we are looking for a **new sales person** for Canada that will report to Alan Hume and assist him in sales activities in Canada. The job description is posted below (see *NMR Jobs* section).

Our continued growth in NMR in Canada is giving us the opportunity to hire an additional **service engineer** for installation and maintenance of our NMR product lines. This job announcement is also posted below.

Special Issue of *Solid State Nuclear Magnetic Resonance*

Solid-State NMR of Materials for Energy Storage and Conversion

Dear Friends and Colleagues,

Profs. **Eckert** and **Klinowski** have asked us to edit a special issue of *Solid State NMR*, with a focus in the area of NMR as applied to Materials for Energy Storage and Conversion. To this end, we would like to invite you to submit a manuscript for this special issue. Topics should include recent results on the development and use of solid-state NMR strategies for the characterization of energy materials, for example materials for use in lithium ion and rechargeable batteries in general, supercapacitors, polymer-electrolyte-membrane fuel cells, and solid-oxide fuel cells. We would like to include the wide variety of NMR methods that have been used in this field, their strengths, and avenues for further development. In an NMR-focused journal, it would also be appropriate to include some of the "how to" details or "tips and tricks" relevant to the successful implementation of the various NMR methods.

Please take these guidelines as suggestions only, and feel free to submit any original manuscript on a topic you feel would be appropriate to this community. The deadline for receipt of manuscripts will be **June 1, 2011**, and we anticipate publication around October/November 2011. Of course, all the manuscripts will be subject to strict peer-review procedures. Please feel free to contact us if you have any questions regarding potential topics, or any other concerns. We would appreciate hearing from you if you plan to submit a manuscript. Submission will be handled through the Elsevier web site. Author instructions and submission details can be found at <http://www.elsevier.com/>

With thanks and best regards

Clare P. Grey & Gillian R. Goward

7 Tesla clinical MRI at Western

Canada's first 7 Tesla clinical MRI scanner is now online at the University of Western Ontario. This instrument is located in the Robarts Research Institute's Centre for

Functional and Metabolic Mapping (CFMM) and is currently the highest magnetic field strength human MRI in Canada. The system is a head-only Siemens/Varian instrument for studies of brain structure and function, including the assessment of brain metabolism and physiology, cognitive function, and vascular dynamics. In 2005 the CFMM took delivery of a 9.4 Tesla Varian high-field small animal imaging system, the first of its kind in the world.

To learn more:

<http://cfmm.robarts.ca/>

<http://cfmm.robarts.ca/newsmodule/view/id/29/>

Science: Special Issue on Superconductivity

Science magazine celebrates the 100th anniversary of the discovery of superconductivity by **Heike Kammerlingh Onnes** in April 1911.

Science, 8 April 2011, volume 332, issue 6026
<http://www.sciencemag.org/content/332/6026.toc#SpecialIssue>

Even after one hundred years since discovery the research on the nature of superconductivity is ongoing, and in some systems is still a matter of heated debate. Recent NMR paper by researchers from McMaster on iron-based superconductors is attracting attention.

D.A. Torchetti, M. Fu, D.C. Christensen, K.J. Nelson, T. Imai, H.C. Lei, and C. Petrovic, "⁷⁷Se NMR investigation of the $K_xFe_{2-y}Se_2$ high-Tc superconductor (Tc=33 K)," *Phys. Rev. B* **83** (2011) 104508.

<http://dx.doi.org/10.1103/PhysRevB.83.104508>

The accompanying synopsis by the American Physical Society "*NMR uncovers missing magnetic fluctuations*"

<http://physics.aps.org/synopsis-for/10.1103/PhysRevB.83.104508>

The GE & Science Prize for Young Life Scientists

Attention Molecular Biology Ph.D. Graduates of 2010

Did you receive your Ph.D. in molecular biology in 2010? If so, apply for The GE & Science Prize for Young Life Scientists where you could win \$25,000 and be published in *Science*

magazine. You will win a trip to Sweden to accept your award at the Grand Hotel in Stockholm and participate in a seminar with Nobel Laureates. All it takes is a 1,000-word essay by **August 1, 2011**. Find out more at <http://www.gescienceprize.org>

Grand prize winner 2010

Mark Bates, born in Toronto Canada, received a B.Sc. degree in engineering physics from Queen's University, and an M.Sc. degree in physics from McGill University. Mark conducted his doctoral research at Harvard University, working under the guidance of Xiaowei Zhuang.



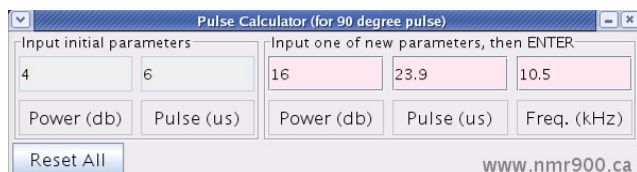
Bruker Spin Report #161

is available for download

http://www.bruker-biospin.com/spin_report.html

myPulse

Dr. **Eric Ye** (900 NMR Facility/University of Ottawa) has written an applet **myPulse** (*beta version*) to calculate the new 90 pulse length, power level and r.f. frequency based on known initial pulse parameters (us, dB) assuming the linear amplifier response. The applet is written in Phyton and works in the Bruker's TopSpin environment.



The purpose of this applet is similar to the popular Bruker's **pulse** program, however the initial parameter input is manual, i.e. does not automatically use $p1$ (us) and $p1$ (dB) values from the currently open dataset.

Please enquire if you would like to test this applet and to provide your comments and suggestions

Email: terskikhv@nrc-cnrc.gc.ca

SpinWorks update

SpinWorks 3.1.8 (February 10, 2011)
Improved baseline correction routine (Whittiker Smoother). The FID display routine has been improved, and the window function is now displayed with the FID. Small bug fixes.

For most recent SpinWorks news and the download link

<http://nmrwiki.org/wiki/index.php?title=SpinWorks>

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>

Recognition

André Simpson, Associate Professor of chemistry at the University of Toronto Scarborough, has been awarded **the 2011 CSC W.A.E. McBryde Medal** for his research in the development of nuclear magnetic resonance (NMR) spectroscopy with the specific objective to address environmental problems at a molecular level.

From the citation: "Andre Simpson obtained his PhD from the University of Birmingham, U.K. then moved to the U.S. completing two postdoctoral fellowships, first at Mississippi State and then at Ohio State University. Simpson is an associate professor at the University of Toronto. He is best known for his research developing nuclear magnetic resonance-based methods to study the structure and interactions in complex environmental mixtures. His research has helped understand how and why different carbon pools respond to climate change and unravel the complexities of contaminant fate and toxicity in the environment. Simpson has published more than 60 refereed articles since

his first journal publication in 2000 and contributed to 12 book chapters. In 2004, he co-founded the Environmental NMR Centre at the University of Toronto, a first of its kind in Canada. In 2008 he was ranked in the "Ten to Watch for in 2008" by the Toronto Star. Later in the same year he was awarded the Royal Society of Chemistry/Society for Environmental and Toxicology and Chemistry – Environmental Science Award, a global award recognizing outstanding contributions to the field."

Read the announcement at http://www.chemistry.ca/index.php?ci_id=1953&la_id=1

David Bryce, Associate Professor at the University of Ottawa, has been awarded **the 2011 Young Researcher of the Year Award** presented by the University of Ottawa. The Young Researcher of the Year Awards are presented annually to two University of Ottawa faculty members who have made exceptional contributions to research and training students. Each award is accompanied by a \$10,000 research grant.

From the citation: "David Bryce is an associate professor in the Department of Chemistry. He received the award in the pure and applied science category for his contributions in the field of nuclear magnetic resonance. He has already established himself as a leader on the international scene within his field. His research focuses on nuclear magnetic resonance (NMR) spectroscopy, specifically, solid-state NMR and quantum mechanical calculations of NMR parameters."

Read the announcement at http://www.media.uottawa.ca/mediaroom/news-details_2239.html

Canadian recipients of the 52nd ENC student travel stipend awards

April 10-15, 2011, Asilomar, California

James Longstaffe, University of Toronto

Brent Pautler, University of Toronto

Roxanne Shank, University of Lethbridge

Leigh Spencer, McMaster University

Carl S. Tan, Carleton University

Meaghan Ward, University of Guelph

NMR Theses Recently Defended

Stan Giesbrecht (University of Manitoba)
Supervisor: Prof. Scott Kroeker
B.Sc. Honours thesis: "Nuclear Magnetic Resonance Studies of Natural Borate Minerals"

Mélanie Ouellette (University of Ottawa)
Supervisor: Prof. David Bryce
B.Sc. Honours thesis: "Solid-State Chlorine-35 NMR and Computational Study of Nucleobase Hydrochlorides, Acetylcholine Chloride, and N,N-Dimethylmethyleiminium Chloride"

On the move

Kamal Mroué, after finishing his Ph.D. with Bill Power at the University of Waterloo, Kamal has joined the Ramamoorthy Group at the University of Michigan, Ann Arbor. Kamal is working on development of novel solid-state NMR techniques to characterize membrane proteins, bone materials, and nanomaterials, and on quantum chemical calculations of anisotropic NMR interaction tensors to extract structural information on biomolecular systems.

Congratulations to Bryce lab alumnus **Joseph Weiss**, M.Sc., on his new job at ACD Labs in Toronto!

Aurore Lebrun and **Prisca Hendarsa**, visiting students from France, have joined David Bryce's lab for the summer.

Dr. Se-Woung Oh, a visiting professor from Mokpo National University, South Korea, has joined Bryce's lab for a period of one year.

Graham Cree (Carleton) is a summer student at NRC-SIMS in Ottawa working with Andreas Brinkmann.

After finishing her Ph.D. with flying colours in the Schurko group (Windsor) and receiving the Governor General's Gold Medal, **Hiyam Hamaed** is now in Europe, at the University of St. Andrew's in Scotland, where she is involved with NMR in lithium-ion batteries research.

Read a feature story about Hiyam in the University of Windsor's *Taking Action* <http://tinyurl.com/6jqseys>

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

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

Travel support program for students and young scientists

Students and young scientists from Canadian Universities are welcome to apply for a travel stipend towards 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

Recent Travel Grant Recipients

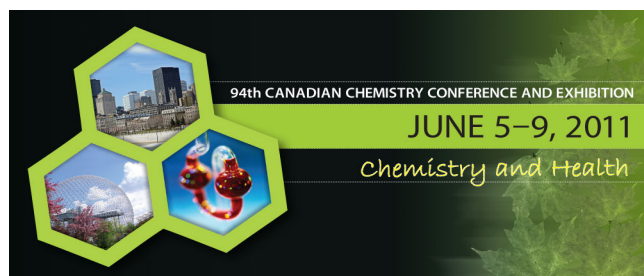
Leigh Spencer (McMaster University)

Bryan Lucier (University of Windsor)

Marcel Hildebrand (University of Windsor)

Stanislav Veinberg (University of Windsor)

Upcoming NMR Events



NMR events at CSC 2011

Dear Colleagues,

The 94th 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 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 (PT5), June 6-7.

<http://abstracts.csc2011.ca/vdv00011.htm>

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**" (PT7), June 7-8.

<http://abstracts.csc2011.ca/vdv00011.htm>

We invite you to participate in the CSC2011 conference. More detail on the symposia, registration and accommodation can be found on the conference website at

<http://www.csc2011.ca>

NMR Symposia Organizers



Solid-State NMR Workshop at CSC 2011

The National Ultrahigh-Field NMR Facility for Solids and Bruker Canada are pleased to present the 6th Annual Solid-State NMR Workshop at the 94th Canadian Chemistry Conference and Exhibition in Montreal. The workshop will take place on **Sunday afternoon, June 5, 2011** in the *Palais des congrès de Montréal*.

This annual Canadian solid-state NMR event focuses on the latest developments in solid-state NMR spectroscopy with emphasis on practical aspects and applications in materials

and life sciences. The workshop will be of interest not only to NMR spectroscopists, but also to students and other researchers interested in using modern NMR techniques in their research practice.

Workshop program

Session 1 (Palais, room 513D)

13:00-13:25 Steven Hartman (Brock University) "NMR Studies of Nitrogen- and Aluminum-doped Silicon Carbide Polytypes"

13:25-13:50 Luke O'Dell (Steacie Institute for Molecular Sciences, NRC Canada) "New Possibilities for ^{14}N Overtone NMR Spectroscopy"

13:50-14:15 Yining Huang (University of Western Ontario) " ^{67}Zn Solid-State NMR Characterization of Zn Environments in Metal-Organic Frameworks"

14:15-14:40 Frank Engleke (Bruker)

14:40-15:00 Coffee Break

Session 2 (Palais, room 513D)

15:00-15:25 Alexandre Arnold (Université du Québec à Montréal) "Structure Determination of Collagen and Silk-Type Environments in the Blue Mussel *Mytilus Edulis* Byssal Threads"

15:25-15:50 Patrick Walsh (The Hospital for Sick Children, University of Toronto) "Solid State NMR Characterization of a Soluble Prion Protein Octamer"

15:50-16:15 Karen Johnston (University of Windsor) "A ^{35}Cl Solid-State NMR Study of Transition-Metal Organometallic Complexes Using Ultra-High Field NMR"

16:15-16:40 Robert Attrell (University of Ottawa) "Chlorine-35 and Bromine-81 Solid-State NMR Spectroscopic Study of Haloanilinium Halide Salts"

16:45 Reception sponsored by **Bruker Canada** (Palais, room 512F)

Registration for the NMR Workshop is free but space is limited. To register please forward your name and affiliation to Victor Terskikh

Email: Victor.Terskikh@nrc-cnrc.gc.ca

Note that the NMR Workshop registration is separate and independent from the CSC 2011 conference registration

5th Annual VIVA NMR symposium

Dear Colleagues,

I am pleased to announce that the 5th **VIVA (VIctoria VAncouver)** NMR Symposium is to take place at St. John's College, UBC, Friday, July 29th, 2011.



The scope of this one day symposium is to bring together NMR users, researchers and managers from western Canada and the north-west of the USA to share information on topics of general NMR interest and to foster the development of an NMR community. Talks or poster presentations by graduate students working in any aspects of NMR are especially encouraged. **Deadline for registration is July 15th, 2011.**

Further details and registration info are available at

<http://www.chem.ubc.ca/viva/index.html>

We look forward to seeing you all again.
Sincerely

Zhicheng (Paul) Xia

Department of Chemistry,
University of British Columbia



The Seventh International Conference on Borate Glasses, Crystals and Melts will be held in Halifax from **August 21-25, 2011**. This is the first time this triennial meeting will be held in Canada, with previous locations including Japan, Italy, Bulgaria, UK and USA. The meeting will have a strong solid-state NMR component, as members of the organizing committee include Joe Zwanziger (conference chair), Randy Youngman, Sabyasachi Sen and Scott Kroeker. Invited speakers include Hellmut Eckert and Sung Keun Lee.

For more information and to register:
<http://www.regonline.com/borate7>



We are pleased to announce that the MOOT XXIV NMR Symposium will take place **October 22nd-23rd** (2011) in Toronto, Ontario, hosted at the Hospital for Sick Children and the University of Toronto. The MOOT NMR Symposium has traditionally been a meeting bringing together nuclear magnetic resonance spectroscopists from across Ontario, Quebec, and more recently the Maritimes and the nearby United States. This trainee-oriented meeting aims to give blossoming researchers the opportunity to present their research to the close-knit Canadian NMR community. Talks and posters will be held at the Hospital for Sick Children, located in the Discovery District of downtown Toronto, and the banquet will be held at historic Hart House on the University of Toronto campus.

In addition, **Agilent Technologies** will be holding a day long symposium and mixer the day before this year's MOOT (Oct. 21). More information regarding the agenda and location for this symposium will be posted soon and available on <http://www.spinsights.net>

We are working to update the conference website. Detailed information will be available shortly at <http://www.mootnmr.org> with registration and abstract submission for posters and talks opening in early June 2011.

A block of rooms has been reserved at the **Delta Chelsea**, conveniently located within a 5-minute walk of the conference venue, at a rate of \$129/night (double occupancy) - booking details will be posted to the conference website later in May. **Porter Airlines** offers a 20% discount on all fare classes for attendees travelling to Toronto for the MOOT NMR Symposium.

If you have comments, inquiries, or would like to be added to the MOOT email list, please send a message to mootnmr@gmail.com

We look forward to seeing you in October!

Sharpe lab

Molecular Structure and Function Programme,
Hospital for Sick Children / Department of
Biochemistry, University of Toronto

Biomolecular NMR - Computational Aspects Gordon Research Conference

May 22-27, 2011, Lucca (Barga), Italy
<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/>

6th Solid-State NMR Workshop at CSC 2011

June 5, 2011, Montréal, Quebec, Canada
http://nmr900.ca/events_e.html

CSC 2011, the 94th Canadian Chemistry Conference and Exhibition

June 5-9, 2011, Montréal, Quebec, Canada
<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

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>

AMPERE NMR School

June 19-25, 2011, Zakopane, Poland
Registration deadline May 15, 2011
<http://www.staff.amu.edu.pl/~school/index.html>

53rd Rocky Mountain Conference on Analytical Chemistry (EPR Symposium only)

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

5th Annual VIVA NMR Symposium

July 29, 2011, St. John's College, UBC, Vancouver, B.C.

Registration is open until July 15, 2011

<http://www.chem.ubc.ca/viva/index.html>

ICMRM11 - MR microscopy conference

August 14-18, 2011, Beijing, China
<http://www.cup.edu.cn/icmrm11/>

 **NANUC 2011 NMR BootCamp**
Biomolecular NMR Training Course

August 15-20, 2011, Edmonton, AB
http://www.nanuc.ca/nmrbootcamp/2011_NMR_BootCamp/Welcome.html

 **Borate 7**
7th International Conference on Borate
Glasses, Crystals and Melts

August 21-25, 2011, Halifax, Canada
<http://www.regonline.com/borate7>

EUROMAR 2011

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


7th Alpine Conference on Solid-State NMR


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

SMASH 2011 Small Molecule NMR Conference

September 18-21, 2011, Chamonix, France
<http://www.smashnmr.org/>

 **Agilent NMR Symposium**
October 21, 2011, Toronto, Canada
<http://www.spinsights.net>

 **MOOT XXIV NMR Symposium**
October 22-23, 2011, Toronto, Canada
<http://www.mootnmr.org>

 **CSChe 2011**, the 61st Canadian Chemical
Engineering Conference

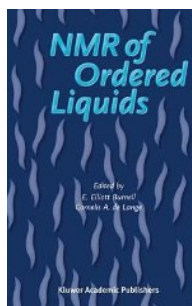
October 23-26, 2011, London, Ontario, Canada
Abstract deadline May 31, 2011
<http://www.csche2011.ca>

53rd ENC

April 15-20, 2012, Miami, FL
<http://www.enc-conference.org/>

New NMR Books

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



NMR of Ordered Liquids
E.E. Burnell (Editor)
C.A. de Lange (Editor)
Paperback: 488 pages
Publisher: Springer; 1st ed.
Softcover of orig. ed. 2003
edition (July, 2011)
Language: English
ISBN: 978-9048163052

<http://www.amazon.com/dp/9048163056>
<http://www.amazon.ca/dp/9048163056>

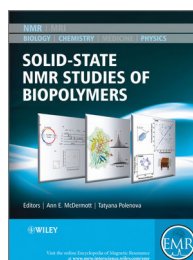
Springer: **NMR of Ordered Liquids** gives a unique overview of the scope and limitations of the NMR of oriented liquids, based on contributions from acknowledged experts in the field. The book consists of four sections:

-detailed general introduction which covers the basic principles and sophisticated experimental techniques;

-wide variety of applications ranging from NMR studies of small atoms and molecules in anisotropic liquids to the utilization of residual dipolar couplings for structure determination of biological molecules;

-summary of the sophisticated theoretical treatments, computer simulations, and phenomenological models for anisotropic intermolecular interactions that are widely used in the analysis of experimental results;

-overview of the dynamical aspects and relaxation processes relevant for orientationally ordered molecules.



Solid State NMR Studies of Biopolymers

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

NMR Jobs and Vacancies

Bruker Ltd. (Canada) - Technical Sales Representative

Bruker Ltd. manufactures, distributes and services the world's most comprehensive range of magnetic resonance research tools enabling life science, materials science, analytical chemistry, process control and clinical research advanced analytical magnetic resonance instruments including Nuclear Magnetic Resonance (NMR), preclinical MRI and EPR.

We are currently seeking a BioSpin Technical Sales Representative to join our team of professionals in a dynamic environment. If you are an innovative problem solver focused on customers and have the ability take initiative and work independently, this is a tremendous opportunity! As a member of the Bruker Sales Team you will put your scientific background combined with your outstanding selling skills to accelerate sales in Bruker BioSpin Products; specifically NMR, MRI, and EPR Spectrometers. Bruker Ltd. offers competitive salary and benefits packages.

Candidate Qualifications:

- BSc Degree or equivalent in chemistry, sciences or engineering. Advanced degree preferred.
- Technical/sales experience with Nuclear Magnetic Resonance (NMR) and/or experience in the scientific instrumentation business preferred
- Good organization and capability to keep detailed records
- Outstanding written and verbal communication skills. Preference may be given to bilingual (English/French) candidates
- Ability to interface with all levels within an organization for both internal and external customers
- Demonstrated capabilities to assure good customer relations through actions and communication skills
- Strong team work skills in a virtual environment with various departments including Service, Applications, Finance and other Sales representatives
- Valid Canadian driver's license and ability to travel extensively across Canada, US and occasionally Internationally

Essential Responsibilities:

- Managing the Canadian Magnetic Resonance marketplace by meeting sales and service targets
- Organizing and facilitating instrument demonstrations and managing customer events
- Issuing quotations, responding to public tenders and negotiating contracts
- Identifying and sourcing new business resulting in the growth of the territory at or above quota
- Ensuring excellent customer support

To apply online

<http://www.workopolis.com/EN/job/13101510?uc=E12>

or forward your resume to the attention of **Mr.**

Brian Stoddart

Email: brian.stoddart@hrbsolutions.ca

Bruker Ltd. (Canada) - Service Representative

Bruker Ltd. manufactures, distributes and services the world's most comprehensive range of magnetic resonance research tools enabling life science, materials science, analytical chemistry, process control and clinical research advanced analytical magnetic resonance instruments including Nuclear Magnetic Resonance (NMR), preclinical MRI and EPR. We are currently seeking a BioSpin Service Representative to join our team of professionals in a dynamic environment. If you are an innovative problem solver focused on customers and have the ability take initiative and work independently, this is a tremendous opportunity! Bruker Ltd. offers competitive salary and benefits packages.

Candidate Qualifications:

- Bachelor's degree (or higher) in Electronic/Electrical Engineering, Chemistry or Physics
- Working knowledge of Nuclear Magnetic Resonance (NMR), preclinical MRI and EPR would be a definite asset
- Demonstrated capabilities to assure good customer relations through actions and communication skills
- Ability to work independently and exhibit excellent time management skills
- Proven problem solving and trouble shooting skills
- Strong team work skills in a virtual environment with various departments including Sales, Finance and other Service representatives
- Ability to travel extensively across Canada and occasionally Internationally

Essential Responsibilities:

- Provide on-site installations, testing, training and customer support for the Bruker BioSpin product
- Conduct routine/ preventative maintenance
- Diagnosing problems by in-depth trouble shooting and provide service for repair of these complex systems
- Instruct and train customers in the operation and maintenance of the systems

Interested applicants should forward their resume to the attention of **Mr. Brian Stoddart**

Email: brian.stoddart@hrbsolutions.ca

University of Alberta, Faculty Position

Proteomics/Metabolomics and Structural Biology of Human Disease

Faculty of Medicine & Dentistry - Department of Biochemistry

Competition No. - A104413899

Closing Date - Will remain open until filled

The Department of Biochemistry in the Faculty of Medicine and Dentistry invites applications for tenure-track or tenured positions in Functional Proteomics, Metabolomics and the Structural Biology of Proteins involved in human diseases.

The successful candidates will be expected to conduct research, teach undergraduate and graduate students, supervise graduate students and post-doctoral fellows and seek external funding. Priority will be given to researchers using proteomics, metabolomics and/or structural biological approaches to address fundamental biological questions. Major areas of strength of the Department and Faculty are in cardiovascular research, diabetes, cancer, cellular and molecular biology, cell signaling, structural biology of proteins and enzymes, lipid biochemistry and membrane biology (see also <http://www.biochem.ualberta.ca>). New laboratory space will be available within the Katz Research Innovation Facility of the University of Alberta. Significant infrastructure for mass spectrometry, NMR (<http://www.nanuc.ca>) and X-ray crystallography is already available, and funds from the Canada Foundation for Innovation, the Faculty of Medicine and Dentistry and Province of Alberta have been secured to expand and update existing instrumentation.

Applicants must have a PhD and/or MD, with a track record in the application of proteomics, metabolomics and/or structural biology to molecular discoveries associated with human disease. Candidates are invited to submit a curriculum vitae, a detailed statement of research program, a sample of published work and the names of three references (who will only be approached with permission). Consideration of applications will commence after April 25, 2011; however, the competition will remain open until the positions are filled.

How to Apply

Mail Dr. Charles Holmes, Professor and Chair
Department of Biochemistry
4-74 Medical Sciences Building
University of Alberta
Edmonton, Alberta, Canada T6G 2H7

<http://www.careers.ualberta.ca/Competition/A104413899/>

All qualified candidates are encouraged to apply; however, Canadians and permanent residents will be given priority. The University of Alberta hires on the basis of merit. We are committed to the principle of equity in employment. We welcome diversity and encourage applications from all qualified women and men, including persons with disabilities, members of visible minorities, and Aboriginal persons.

University of Alberta

PhD student or Postdoctoral fellow with NMR experience and interest in Microbial Glycobiology

A PhD or postdoctoral position is available immediately at the University of Alberta. The successful candidate will be jointly supervised by **Dr. Roderick Wasylshen** (Department of Chemistry and Canada Research Chair in Physical Chemistry) <http://ramsey.chem.ualberta.ca/>

and **Dr. Christine Szymanski** (Department of Biological Sciences and Alberta Ingenuity Centre for Carbohydrate Science) http://www.biology.ualberta.ca/faculty/christine_szymanski/

The student will be involved in a multidisciplinary project examining bacterial capsular polysaccharides and developing new techniques to examine bacterial-host interactions using high-resolution magic-angle spinning NMR.

The NMR Facilities in the Department of Chemistry are well equipped for the collaborative research project. Specifically we have access to a Varian 600 with a nanoprobe for magic-angle spinning experiments. Details of the other NMR spectrometers in the Department can be found at: <http://nmr.chem.ualberta.ca/> and <http://ramsey.chem.ualberta.ca/>

Applicants should have a strong background in NMR and biological chemistry. Knowledge of solid-state NMR, molecular modeling and NMR programming would be an asset.

Interested applicants should send a single PDF document containing a CV, one-page statement of research interests and contact information of three references to Email cszymans@ualberta.ca

University of Prince Edward Island

Chemistry Graduate Student Position in Flax Lignan Metabolomics

A M.Sc. graduate student position is available immediately in the Chemistry Department, University of Prince Edward Island, to investigate flax SDG (secoisolariciresinol diglucoside) lignan biosynthesis and glycosylation. This project is part of the Total Utilization Flax GENomics (**TUFGEN**) Project funded by Genome Canada, Genome Prairies and other sponsors. It will involve the use of state-of-the-art phytochemical and metabolomic technologies for the isolation and characterization of flax lignan species found in wild and mutant lines.

Applicants must have a B.Sc. in Chemistry, Phytochemistry, Biochemistry, or other relevant disciplines in biology or chemistry. Experience/knowledge required for this position, include, but are not limited to, the understanding of plant metabolite extractions, basic analytical chemistry skills, and a strong understanding of one or more of chromatography (LC/GC), MS and NMR. A strong understanding in statistics/metabolomics would be an asset.

Candidates should possess good written and verbal English skills, be self-motivated, and demonstrate an ability to work as part of an interactive group. Interested candidates should contact **Dr. Chris Kirby** (chris.kirby@agr.gc.ca) and/or **Dr. Jason McCallum** (jason.mccallum@agr.gc.ca) and the selected applicant will be invited to apply for admission to the Master's program at UPEI. He/She will be co-supervised by Agriculture and Agri-Food Canada scientists (Kirby and McCallum) as well as UPEI **Prof. Russ Kerr**. The research will be conducted in AAFC laboratories located within the Institute of Nutritional Sciences and Health (NRC-INH building on UPEI campus), which has a vibrant scientific community and offers cutting-edge facilities for plant molecular biology, phytochemistry, UPLC-MS, NMR, and bioactive compounds research. We are offering a stipend starting at \$18,000 per annum. Applicants should send a letter outlining their research interests, career goals, a copy of their student record (unofficial transcripts), curriculum vitae, and contact information for three references to Dr. Chris Kirby and/or Dr. Jason McCallum. For additional details, please send inquiries to the provided email addresses.

Listings of NMR jobs and vacancies

Canadian NMR Jobs

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

The Human Serum Metabolome

An ambitious project is underway by a large international group of scientists led by **David Wishart** (Alberta) to identify and characterize all metabolites in human body. NMR plays a prominent role in this research along with other analytical techniques. Their most recent report published in *PLoS ONE* concerns with metabolites found in human blood, more than 4000 identified so far.

N. Psychogios, D.D. Hau, J. Peng, A.C. Guo, R. Mandal, S. Bouatra, I. Sinelnikov, R. Krishnamurthy, R. Eisner, B. Gautam, N. Young, J. Xia, C. Knox, E. Dong, P. Huang, Z. Hollander, T.L. Pedersen, S.R. Smith, F. Bamforth, R. Greiner, B. McManus, J.W. Newman, T. Goodfriend, D.S. Wishart, "The Human Serum Metabolome," *PLoS ONE* **6** (2011) e16957. (**open access article**) <http://dx.doi.org/10.1371/journal.pone.0016957>

Abstract: "Continuing improvements in analytical technology along with an increased interest in performing comprehensive, quantitative metabolic profiling, is leading to increased interest pressures within the metabolomics community to develop centralized metabolite reference resources for certain clinically important biofluids, such as cerebrospinal fluid, urine and blood. As part of an ongoing effort to systematically characterize the human metabolome through **the Human Metabolome Project**, we have undertaken the task of characterizing the human serum metabolome. In doing so, we have combined targeted and non-targeted NMR, GC-MS and LC-MS methods with computer-aided literature mining to identify and quantify a comprehensive, if not absolutely complete, set of metabolites commonly detected and quantified (with today's technology) in the human serum metabolome. Our use of multiple metabolomics platforms and technologies allowed us to substantially enhance the level of metabolome coverage while critically assessing the relative strengths and weaknesses of these platforms or technologies. Tables containing the complete set of 4229 confirmed and highly probable human serum compounds, their concentrations, related literature references

and links to their known disease associations are freely available at <http://www.serummetabolome.ca>

This research has been recently highlighted by ACCN, the Canadian Chemical News http://www.accn.ca/index.php?ci_id=2582&la_id=1

To read the interview with David Wishart <http://tinyurl.com/6bqde7p>

Nature News: Breaking the protein rules

One of the textbook concepts in molecular biology is that proteins fold up spontaneously to form the most energetically stable three-dimensional structures. These folded proteins are presumed structurally rigid, which is important for their unique functionality, e.g. as enzymes. There are indications, however, mostly coming from NMR studies, that many important proteins exist in disordered form. A news feature in the recent issue of *Nature* discusses implications of this potentially far-reaching finding. Among cited examples of intrinsically disordered proteins is the NMR study on Sic1 protein by **Julie Forman-Kay** and her group at the University of Toronto/SickKids.

T. Chouard "Structural biology: Breaking the protein rules," *Nature* **471** (2011) 151-153. <http://dx.doi.org/10.1038/471151a>

Cover article in Chemistry - A European Journal



B.J. Greer, V.K. Michaelis, M.J. Katz, D.B. Leznoff, G. Schreckenbach, S. Kroeker, "Characterising Lone-Pair Activity of Lead(II) by ^{207}Pb Solid-State NMR: Coordination Polymers of $[\text{N}(\text{CN})_2]^-$ and $[\text{Au}(\text{CN})_2]^-$ with Terpyridine

Ancillary Ligands," *Chemistry - A European Journal* **17** (2011) 3609-3618. <http://dx.doi.org/10.1002/chem.201002913>

PCCP lists 25 most cited Canadian research articles

Physical Chemistry Chemical Physics has announced that the Canadian Society for Chemistry (CSC) is now one of its co-owner

societies. To celebrate this new partnership, PCCP has created a collection of 25 top cited articles from authors based in Canada to showcase some of the great Canadian research published in PCCP.

<http://tinyurl.com/3cdr4uy>

Five articles on this list are from Canadian NMR research groups, including four papers enabled in part by the National Ultrahigh-Field NMR Facility for Solids.



C.M. Widdifield and D.L. Bryce, "Crystallographic Structure Refinement with Quadrupolar Nuclei: a Combined Solid-State NMR and GIPAW DFT Example Using MgBr_2 ," *Physical Chemistry Chemical Physics* **11** (2009) 7120-7122.

<http://dx.doi.org/10.1039/b911448n>



D.H. Brouwer, S. Alavi and J.A. Ripmeester, "NMR Crystallography of p-tert-Butylcalix[4]arene Host-Guest Complexes Using ^1H Complexation-Induced Chemical Shifts," *Physical Chemistry Chemical Physics* **10** (2008) 3857-3860. **(Cover Article)**

<http://dx.doi.org/10.1039/b805326j>



L.A. O'Dell and R.W. Schurko, "Static solid-state ^{14}N NMR and computational studies of nitrogen EFG tensors in some crystalline amino acids," *Physical Chemistry Chemical Physics* **11** (2009) 7069-7077.

<http://dx.doi.org/10.1039/b906114b>

S. Cadars, D.H. Brouwer and B.F. Chmelka, "Probing local structures of siliceous zeolite frameworks by solid-state NMR and first-principles calculations of ^{29}Si - ^{29}Si scalar couplings," *Physical Chemistry Chemical Physics* **11** (2009) 1825-1837.

<http://dx.doi.org/10.1039/b815361b>



M.A.M. Forgeron and R.E. Wasylishen, "Molybdenum magnetic shielding and quadrupolar tensors for a series of molybdate salts: a solid-state ^{95}Mo NMR study," *Physical Chemistry Chemical Physics* **10** (2008) 574-581.

<http://dx.doi.org/10.1039/b713276j>

NMR papers in Nature journals

A.M. Souza, J.F. Zhang, C.A. Ryan, R. Laflamme, "Experimental magic state distillation for fault-tolerant quantum computing," *Nature Communications* **2** (2011) 169. <http://dx.doi.org/10.1038/ncomms1166>

L.A. Freiburger, O.M. Baettig, T. Sprules, A.M. Berghuis, K. Auclair, A.K. Mittermaier, "Competing allosteric mechanisms modulate substrate binding in a dimeric enzyme," *Nature Structural & Molecular Biology* **18** (2011) 288-294. <http://dx.doi.org/10.1038/nsmb.1978>

Progress in NMR Spectroscopy



L.A. O'Dell "Direct Detection of Nitrogen-14 in Solid-State NMR Spectroscopy," *Progress in Nuclear Magnetic Resonance Spectroscopy* (2011) accepted. **(Invited Review)**

<http://dx.doi.org/10.1016/j.pnmrs.2011.04.001>

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

A.J. Simpson, D.J. McNally, M.J. Simpson "NMR Spectroscopy in Environmental Research: From Molecular Interactions to Global Processes," *Progress in Nuclear Magnetic Resonance Spectroscopy* **58** (2011) 97-175. **(Invited Review)** <http://dx.doi.org/10.1016/j.pnmrs.2010.09.001>

Perspectives in Magnetic Resonance

L.E. Kay, "Solution NMR Spectroscopy of Supra-Molecular Systems, Why Bother? A Methyl TROSY View," *Journal of Magnetic Resonance* **210** (2011) 159-170. <http://dx.doi.org/10.1016/j.jmr.2011.03.008>

NMR papers in PNAS

R. Selvaratnam, S. Chowdhury, B. VanSchouwen, and G. Melacini, "Mapping allostery through the covariance analysis of NMR chemical shifts," *Proc. Natl. Acad. Sci. USA* **108** (2011) 6133-6138. <http://dx.doi.org/10.1073/pnas.1017311108>

M. Dey, A. Velyvis, J.J. Li, E. Chiu, D. Chiovitti, L.E. Kay, F. Sicheri, and T.E. Dever, "Requirement for kinase-induced conformational change in eukaryotic initiation factor 2a (eIF2a) restricts phosphorylation of Ser51," *Proc. Natl. Acad. Sci. USA* **108** (2011) 4316-4321. <http://dx.doi.org/10.1073/pnas.1014872108>

Review

R.M. Epand and R.F. Epand, "Bacterial membrane lipids in the action of antimicrobial agents," *J. Pept. Sci.* **17** (2011) 298-305. **(Review)** <http://dx.doi.org/10.1002/psc.1319>

Faculty 1000 evaluations

Launched in 2002, **the Faculty of 1000** (F1000) project identifies and evaluates the most important articles in biology and medical research. The selection process comprises the world's leading scientists and clinicians who post-publication peer review the best of the articles they read and explain their importance. <http://f1000.com/>

Some of the most recent Canadian NMR publications evaluated by the Faculty 1000

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* **49** (2011) 151-161. <http://dx.doi.org/10.1007/s10858-011-9473-9>
F1000 evaluation <http://f1000.com/9856956>

D.M. Korzhnev, T.L. Religa, W. Banachewicz, A.R. Fersht, L.E. Kay, "A Transient and Low-Populated Protein-Folding Intermediate at Atomic Resolution", *Science* **329** (2010) 1312-1316. <http://dx.doi.org/10.1126/science.1191723>
F1000 evaluation <http://f1000.com/5349956>

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>
F1000 evaluation <http://f1000.com/7874956>

Recent NMR Publications

We are listing here most recent NMR publications by Canadian research groups as they appear on the 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. Sarker, D. Jackman, and V. Booth, "Lung Surfactant Protein A (SP-A) Interactions with Model Lung Surfactant Lipids and an SP-B Fragment," *Biochemistry* (2011) accepted. <http://dx.doi.org/10.1021/bi200167d>

Dalhousie University

C.D.L. Saunders, L.E. Longobardi, N. Burford, M.D. Lumsden, U. Werner-Zwanziger, B. Chen, and R. McDonald, "Comprehensive Chemical Characterization of Complexes Involving Lead-Amino Acid Interactions," *Inorg. Chem.* **50** (2011) 2799-2810. <http://dx.doi.org/10.1021/ic101892x>

D.N. Langelaan, P. Ngweniform, J.K. Rainey, "Biophysical characterization of G-protein coupled receptor-peptide ligand binding," *Biochem Cell Biol.* **89** (2011) 98-105. <http://dx.doi.org/10.1139/O10-142>

Y. Carpenter, N. Burford, M.D. Lumsden, and R. McDonald, ³¹P NMR Studies Demonstrating the Assembly of catena-Phosphorus Frameworks from Chlorophosphinochlorophosphonium Cations," *Inorg. Chem.* **50** (2011) 3342-3353. <http://dx.doi.org/10.1021/ic102150s>

V. Martin, B. Wood, U. Werner-Zwanziger, J.W. Zwanziger, "Structural aspects of the photoelastic response in lead borate glasses," *Journal of Non-Crystalline Solids* **357** (2011) 2120-2125. <http://dx.doi.org/10.1016/j.jnoncrysol.2011.01.042>

H. Al-Mughaid, K.N. Robertson, U. Werner-Zwanziger, M.D. Lumsden, T.S. Cameron and T.B. Grindley, "2-Propynyl 2,3,4,6-tetra-O-acetyla-D-mannopyranoside," *Acta Crystallographica Section C* **C67** (2011) o60-o63. <http://dx.doi.org/10.1107/S010827011005225X>

University of New Brunswick

F. Marica, S.A.B. Jofré, K.U. Mayer, B.J. Balcom, T.A. Al, "Determination of Spatially-Resolved Porosity, Tracer Distributions and Diffusion Coefficients in Porous Media Using MRI Measurements and Numerical Simulations," *Journal of Contaminant Hydrology* (2011) accepted. <http://dx.doi.org/10.1016/j.jconhyd.2011.04.008>

Z. Zhang, A.E. Marble, R.P. MacGregor, J. Martin, H. Wang, B.J. Balcom, "Zero-mode TEM parallel-plate resonator for high-resolution thin film magnetic resonance imaging," *Canadian Journal of Chemistry* **89** (2011) online. **(Special Issue)** <http://dx.doi.org/10.1139/V11-018>

G. LaPlante, J.C. Garcia-Naranjo, B.J. Balcom, "Real-time cure monitoring of an epoxy/polyamidoamine system with unilateral magnetic resonance," *NDT&E International* **44** (2011) 329-334. <http://dx.doi.org/10.1016/j.ndteint.2010.11.002>

K.V. Romanenko, B.J. Balcom, "Permeability mapping in porous media by magnetization prepared centric-scan SPRITE," *Exp Fluids* **50** (2011) 301-312. <http://dx.doi.org/10.1007/s00348-010-0923-z>

McGill University

B. Fortier-McGill, V. Toader, and L. Reven, "Chain Dynamics of Water-Saturated Hydrogen-Bonded Polymer Complexes and Multilayers," *Macromolecules* **44** (2011) 2755-2765. <http://dx.doi.org/10.1021/ma102907w>

R. Yang, S.A. Gaidamakov, J.W. Xie, J. Lee, L. Martino, G. Kozlov, A.K. Crawford, A.N. Russo, M.R. Conte, K. Gehring, R.J. Maraia, "La-Related Protein 4 Binds Poly(A), Interacts with the Poly(A)-Binding Protein MLE Domain via a Variant PAM2w Motif, and Can Promote mRNA Stability," *Molecular and Cellular Biology* **31** (2011) 542-556. <http://dx.doi.org/10.1128/MCB.01162-10>

L.A. Freiburger, O.M. Baettig, T. Sprules, A.M. Berghuis, K. Auclair, A.K. Mittermaier, "Competing allosteric

mechanisms modulate substrate binding in a dimeric enzyme," *Nature Structural & Molecular Biology* **18** (2011) 288-294.
<http://dx.doi.org/10.1038/nsmb.1978>

Université de Montréal

M.-A. Gagnon, M. Lafleur, "Comparison of the structure and the transport properties of low-set and high-set curdlan hydrogels," *Journal of Colloid and Interface Science* **357** (2011) 419-427.
<http://dx.doi.org/10.1016/j.jcis.2011.02.033>

G.D. Tomasso, P. Lampron, P. Dagenais, J.G. Omichinski, P. Legault, "The ARiBo tag: a reliable tool for affinity purification of RNAs under native conditions," *Nucleic Acids Research* **39** (2011) e18.
<http://dx.doi.org/10.1093/nar/gkq1084>


Université du Québec à Montréal

D.E. Warschawski, A.A. Arnold, M. Beaugrand, A. Gravel, É. Chartrand, I. Marcotte, "Choosing membrane mimetics for NMR structural studies of transmembrane proteins," *Biochimica et Biophysica Acta (BBA) - Biomembranes* (2011) online.
<http://dx.doi.org/10.1016/j.bbamem.2011.03.016>

Boehringer Ingelheim (Canada)

C.T. Lemke, N. Goudreau, S. Zhao, O. Hucke, D. Thibeault, M. Llinas-Brunet, and P.W. White, "Combined X-ray, NMR, and Kinetic Analyses Reveal Uncommon Binding Characteristics of the Hepatitis C Virus NS3-NS4A Protease Inhibitor BI 201335," *Journal of Biological Chemistry* **286** (2011) 11434-11443.
<http://dx.doi.org/10.1074/jbc.M110.211417>


University of Ottawa

 **C.M. Widdifield and D.L. Bryce,** "A Multinuclear Solid-State Magnetic Resonance and GIPAW DFT Study of Anhydrous Calcium Chloride and its Hydrates," *Canadian Journal of Chemistry* (2011) online. (Special Issue)
<http://dx.doi.org/10.1139/V11-009>

P.A. Kerneghan, S.D. Halperin, D.L. Bryce, and K.E. Maly, "Postsynthetic modification of an imine-based microporous organic network,"

Canadian Journal of Chemistry **89** (2011) 577-582.
<http://dx.doi.org/10.1139/V11-014>


R.G.B. Bouwé, I.K. Tonlé, S.Letaief, E. Ngameni, C. Detellier, "Structural characterization of 1,10-phenanthroline-montmorillonite intercalation compounds and their application as low-cost electrochemical sensors for Pb(II) detection at the sub-nanomolar level," *Applied Clay Science* **52** (2011) 258-265.
<http://dx.doi.org/10.1016/j.clay.2011.02.028>

 **J. Zhu, E. Ye, V. Terskikh, and G. Wu,** "Experimental Verification of the Theory of Nuclear Quadrupole Relaxation in Liquids over the Entire Range of Molecular Tumbling Motion," *Journal of Physical Chemistry Letters* **2** (2011) 1020-1023.
<http://dx.doi.org/10.1021/jz200296g>

NRC-SIMS

D.L.A.G. Grimminck, S.K. Vasa, W.L. Meerts, A.P.M. Kentgens, A. Brinkmann, "EASY-GOING DUMBO on-spectrometer optimisation of phase modulated homonuclear decoupling sequences in solid-state NMR," *Chemical Physics Letters* (2011) accepted.
<http://dx.doi.org/10.1016/j.cplett.2011.04.079>

L.A. O'Dell "Direct Detection of Nitrogen-14 in Solid-State NMR Spectroscopy," *Progress in Nuclear Magnetic Resonance Spectroscopy* (2011) accepted. (Invited Review)
<http://dx.doi.org/10.1016/j.pnmrs.2011.04.001>

 **J. Zhu, E. Ye, V. Terskikh, and G. Wu,** "Experimental Verification of the Theory of Nuclear Quadrupole Relaxation in Liquids over the Entire Range of Molecular Tumbling Motion," *Journal of Physical Chemistry Letters* **2** (2011) 1020-1023.
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