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

Canadian NMR Research News Bulletin #7.2
Spring 2013

Canadian NMR News

Submitted by Vlad Ladizhansky, Photo by Valerie Robertson

DNP-NMR at Guelph

Dear Colleagues,

I am pleased to announce that a new **395 GHz/600 MHz** Dynamic Nuclear Polarization (DNP) NMR spectrometer from Bruker has been installed in the University of Guelph NMR Centre. The instrument was purchased through funding from the Ontario Ministry of Economic Development and Innovation and the University of Guelph, with generous contribution by Bruker Canada.

Our DNP instrument is equipped with a triple resonance (^{1}H-^{13}C-^{15}N) low temperature 3.2 mm Magic Angle Spinning (MAS) solid-state NMR probe. The instrument will be available for all research groups in Canada and worldwide. The University of Guelph provides partial support for the NMR Centre Staff, but any additional costs (e.g., cryogens for magic angle spinning at 100K, etc) will have to be covered through user fees. Fee schedule will be finalized in the near future.

395 GHz/600 MHz DNP-NMR spectrometer, the University of Guelph NMR Centre

In This Issue

Applications of DNP to biosolids NMR and to NMR of materials are becoming widespread now. We would be very willing to assist you in using the DNP Facility, and encourage you to take advantage of this unique research opportunity.

Vlad Ladizhansky

Associate Professor
and Canada Research Chair II,
Department of Physics
University of Guelph,
50 Stone Road E, Guelph,
Ontario, Canada N1G 2W1
phone: 519-824-4120 Ext 53989
departmental fax: 519-836-9967
e-mail: vladizha@uoguelph.ca

Natalie Osborne "Getting a clearer image with advanced spectroscopy" *The Guelph Physics Department Chronicles*, Vol. 2, Issue 2, June 2012. download PDF:

http://www.physics.uoguelph.ca/docs/chronicles-2012-06.pdf

Submitted by Bob Berno, Steve Kornic

850 MHz NMR at the McMaster Biointerfaces Institute

The trucks and heavy machinery started arriving early one morning in mid-November 2012. With surgical precision, the new 850 MHz Bruker magnet and all the associated hardware and accessories were unpacked and moved to their final destination in the basement of the Arthur N. Bourns Building at McMaster University in Hamilton, ON. The magnet is now at field, and the spectrometer is being put through its paces.

The new 850 MHz NMR spectrometer was purchased using funds from the Canadian Foundation for Innovation (CFI) and the Province of Ontario. This NMR instrument is just one important and integral part of the newly created Biointerfaces Institute (BI) led by **Dr. John Brennan**, Professor and Canada Research Chair in Bioanalytical Chemistry and Biointerfaces, at McMaster University. http://tinyurl.com/cotqaag

Officially opened in April, 2013, the Biointerfaces Institute boasts a 10,000-square-foot facility equipped with cutting-edge instrumentation that will enable the rapid development of new biomaterials with many important applications. The BI focuses on the study and development of surfaces and interfaces of novel materials that have important and relevant biological activity.

The NMR spectrometer comes equipped with one solution state probe, a 5mm H/C/N TXI probe. For solids there are several MAS probes including a 4mm H/C/N HR-MAS probe, and E-Free probes with H/C/N and H/C/Si configurations. There is also a flat coil probe for oriented samples.

For more information, contact **Steve Kornic** at the Biointerfaces Institute at (905-525-9140 x20589)

http://biointerfaces.mcmaster.ca/

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

On behalf of the organizing committee, we would like to announce the 26th edition of the MOOT NMR Symposium in Kingston, Ontario. The meeting will be held in the new Abramsky House Medical School building at Queen's University on October 26th and October 27th, 2013. We will upload more information about the conference as it becomes available on the official symposium website. Visit often! http://www.mootnmr.org

Please direct any questions, comments or feedback about upcoming MOOT to chitayat@queensu.ca

We look forward to seeing you in October!

Your MOOT XXVI Organizing Committee,

Seth Chitayat and Gang Wu

Solid-State NMR Workshop at CSC 2013

The National Ultrahigh-Field NMR Facility for Solids and Bruker Canada are pleased to present the 8th Annual Solid-State NMR Workshop at the 96th Canadian Chemistry Conference and Exhibition in Quebec City (CSC 2013). The workshop will take place **Sunday, May 26, 2013, 13:00 - 19:00,** in the Québec City Convention Centre.

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.

Preliminary workshop program

Session 1

13:00-13:30 Younès Messaddeq (Université Laval)

13:30-14:00 Jun Xu (University of Western Ontario) "Determining the Number of Crystallographically Non-equivalent Sites for Each Element in MOF alfa-$Mg_3(HCOO)_6$ by Multinuclear Solid-State NMR at 21.1 T"

14:00-14:30 Kris Harris (McMaster University) "Solid-State NMR Studies of Lithium-Ion Battery Materials"

14:30-15:00 Kevin Burgess (University of Ottawa) "Alkaline-Earth Metal Solid-State NMR Study of Mg, Ca, and Sr Complexes in Organic Molecular Environments"

15:00-15:15 Coffee Break

Session 2

15:15-15:45 Michèle Auger (Université Laval) "^{2}H NMR study of the insertion of the myristoyl group of neuroral calcium sensor proteins in lipid bilayers"

15:45-16:15 Qasim Saleem (University of Toronto) "Lipids in motion: Lateral diffusion of lipids in bilayers measured via ^{31}P CODEX"

16:15-16:45 Martine Monette (Bruker Biospin)

16:45 Reception sponsored by **Bruker Canada**

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 2013 conference registration

WeNMR: Structural Biology on the Grid

(*Journal of Grid Computing*): The WeNMR (http://www.wenmr.eu) project is a European Union funded international effort to streamline and automate analysis of Nuclear Magnetic Resonance (NMR) and Small Angle X-Ray scattering (SAXS) imaging data for atomic and near-atomic resolution molecular structures. Conventional calculation of structure requires the use of various software packages, considerable user expertise and ample computational resources. To facilitate the use of NMR spectroscopy and SAXS in life sciences the WeNMR consortium has established standard computational workflows and services through easy-to-use web interfaces, while still retaining sufficient flexibility to handle more specific requests. Thus far, a number of programs often used in structural biology have been made available through application portals. The implementation of these services, in particular the distribution of calculations to a Grid computing infrastructure, involves a novel mechanism for submission and handling of jobs that is independent of the type of job being run. With over 450 registered users (September 2012), WeNMR is currently the largest Virtual Organization (VO) in life sciences. With its large and worldwide user community, WeNMR has become the first Virtual Research Community officially recognized by the European Grid Infrastructure (EGI).

Tsjerk A. Wassenaar (University of Calgary) **et al.** "WeNMR: Structural Biology on the Grid," *Journal of Grid Computing* **10** (2012) 743-767. **(Open access)** http://dx.doi.org/10.1007/s10723-012-9246-z

Life-saving NMR: Septic shock

NMR metabolomics research on pediatric septic shock by **Hans Vogel** and colleagues from the University of Calgary has been highlighted by *SpectroscopyNow.com*

David Bradley "Life-saving NMR: Septic shock" *SpectroscopyNow*, March 15, 2013 http://tinyurl.com/bl65mjb

Third U.S.-Canada Winter School on Biomolecular Solid-State NMR
Stowe, Vermont, January 5-11, 2013

The school materials and lectures are now available online for download

http://www.scs.illinois.edu/nmrwinterschool/course_materials.html

Suggested by Guy Bernard (Alberta)

***Nature* News Feature**
Volume 495 Number 7442, 28 March 2013
http://www.nature.com/nature/journal/v495/n7442/index.html

The future of publishing: A new page. A special issue of *Nature* looks at the transformation taking place in scientific publishing. *Nature* **495**, 425 (28 March 2013) http://dx.doi.org/10.1038/495425a

Richard Van Noorden "Open access: The true cost of science publishing" *Nature* **495**, 426–429 (28 March 2013) http://dx.doi.org/10.1038/495426a

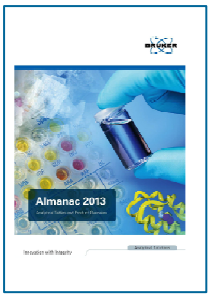
Richard Monastersky "Publishing frontiers: The library reboot" *Nature* **495**, 430–432 (28 March 2013) http://dx.doi.org/10.1038/495430a

Declan Butler "Investigating journals: The dark side of publishing" *Nature* **495**, 433–435 (28 March 2013) http://dx.doi.org/10.1038/495433a

to learn more visit

http://scholarlyoa.com/
http://scholarlyoa.com/publishers/
http://scholarlyoa.com/individual-journals/

Bruker Almanac goes digital



The Almanac has long been a Bruker tradition, having been published annually for three decades, and has over that time evolved into a modern reference aid, a handy guide to Bruker's vast range of technologies and solutions, and even become a digital aid for use on the iOS platform.

This year the **Bruker Almanac** has gone one step further, being relaunched as a free online ebook.

http://www.theresonance.com/2013/categories/academics/bruker-almanac-goes-digital

The Almanac App is also available for iPad, iPod and iPhone
https://itunes.apple.com/us/app/almanac/id367770786

Recognition

Professor **Lewis Kay** (University of Toronto) is the recipient of the **2013 Canadian Society for Chemistry E.W.R. Steacie Award.** The award is presented to a scientist who has made a distinguished contribution to chemistry while working in Canada.

Professor **Roderick Wasylishen** (University of Alberta) has been awarded the **2013 Kaplan Award for Excellence in Research**, the most prestigious University of Alberta research award.

Michael Brown "Kaplan Award: Chemistry pioneer shows researchers 'The Wasylishen Way'" *folio* Volume 50, issue 14, March 22, 2013
http://www.folio.ualberta.ca/article.cfm?v=104208&i=104377&a=4

Dr. **Glenn Facey** (NMR Facility Manager, University of Ottawa) has been awarded the **2013 President's Award for Service Excellence**.

Professor **Albert Berghuis** (McGill, Canada Research Chair in Structural Biology) has been appointed Chair of the Department of Biochemistry.

54th ENC Student Travel Awards

Following the long tradition, ENC has awarded 2013 Student Travel Stipends to support students attending the 54th ENC Conference April 14-19, 2013 in Asilomar, California. The

stipends were provided by the ENC, the Suraj P. Manrao Science Foundation, and by the generous contributions of sponsors. Among awardees there were several Canadian recipients including

Jasmine Viger-Gravel (University of Ottawa)
Daryl Good (University of Guelph)
Leayen Lam (University of Toronto)
Alan Manning (University of British Columbia)
Danielle Smiley (McMaster University)
Stanislav Veinberg (University of Windsor)

http://www.enc-conference.org

NMR Theses Recently Defended

Craig Markin (University of Alberta) March 2013

Supervisor: Prof. Leo Spyracopoulos

Ph.D. Biochemistry: "Molecular basis of ubiquitin chain synthesis and recognition"
http://hdl.handle.net/10402/era.30895

Brett Feland (University of Alberta) March 2013

Supervisor: Prof. Rod Wasylishen

M.Sc. Chemistry: "^{69}Ga and ^{71}Ga Solid-State NMR Studies of Six-Coordinate Gallium-Oxygen Complexes"

Bryan Lucier (University of Windsor) May 2013

Supervisor: Prof. Robert Schurko

Ph.D. Chemistry: "New Directions for Solid-State NMR of Insensitive Nuclei: Applications to Metal Nuclei in Inorganic Materials"

Canadian NMR Research Highlights

NMR paper in *Science*

R. Rosenzweig, S. Moradi, A. Zarrine-Afsar, J.R. Glover, L.E. Kay, "Unraveling the Mechanism of Protein Disaggregation Through a ClpB-DnaK Interaction," *Science* **339** (2013) 1080-1083.
http://dx.doi.org/10.1126/science.1233066

Abstract: HSP-100 protein machines, such as ClpB, play an essential role in reactivating protein aggregates that can otherwise be lethal to cells. Although the players involved are known, including the DnaK/DnaJ/GrpE chaperone system in bacteria, details of the molecular interactions are not well understood. Using methyl–transverse relaxation–optimized nuclear magnetic resonance spectroscopy, we present an atomic-resolution model for the ClpB-DnaK complex, which we verified by mutagenesis and functional assays. ClpB and GrpE compete for binding to the DnaK nucleotide binding domain, with GrpE binding inhibiting disaggregation. DnaK, in turn, plays a dual role in both disaggregation and subsequent refolding of polypeptide chains as they emerge from the aggregate. On the basis of a combined structural-biochemical analysis, we propose a model for the mechanism of protein aggregate reactivation by ClpB.

Science Perspective: **Helen R. Saibil,** "Machinery to Reverse Irreversible Aggregates," *Science* **339** (2013) 1040-1041.
http://dx.doi.org/10.1126/science.1236012

NMR papers in *Angewandte Chemie*

K. Yu, X. Liu, Q. Zeng, D.M. Leek, J. Ouyang, K.M. Whitmore, J.A. Ripmeester, Y. Tao, M. Yang, "Effect of Tertiary and Secondary Phosphines on Low-Temperature Formation of Quantum Dots," *Angewandte Chemie Int. Ed.* **52** (2013) 4823–4828.
http://dx.doi.org/10.1002/anie.201300568

P. Vallurupalli, L.E. Kay, "Probing Slow Chemical Exchange at Carbonyl Sites in Proteins by Chemical Exchange Saturation Transfer NMR Spectroscopy," *Angewandte Chemie Int. Ed.* **52** (2013) 4156–4159.
http://dx.doi.org/10.1002/anie.201209118

Cover article in *ChemMedChem*

N. Goudreau, R. Coulombe, A.-M. Faucher, C. Grand-Maitre, J.-E. Lacoste, C.T. Lemke, E. Malenfant, Y. Bousquet, L. Fader, B. Simoneau, J.-F. Mercier, S. Titolo, and S.W. Mason, "Monitoring Binding of HIV-1 Capsid Assembly Inhibitors Using ^{19}F Ligand-and ^{15}N Protein-Based NMR and X-ray Crystallography: Early Hit Validation of a Benzodiazepine Series," *ChemMedChem* **8** (2013) 405-414. **(Cover Article)**
http://dx.doi.org/10.1002/cmdc.201200580

Cover article in *Chemistry - A European Journal*

J. Xu, V.V. Terskikh, and Y. Huang, "Resolving Multiple Non-Equivalent Metal Sites in Magnesium-Containing Metal-organic Frameworks by Natural Abundance ^{25}Mg Solid-State NMR," *Chemistry - A European Journal* **19** (2013) 4432–4436. **(Cover Article)**

http://dx.doi.org/10.1002/chem.201300113

Four nonequivalent magnesium sites with very similar local Mg environments in a Mg-containing metal–organic framework, microporous α-$Mg_3(HCOO)_6$, have been resolved by ^{25}Mg natural-abundance triple-quantum magic-angle spinning (3QMAS) NMR spectroscopy at an ultrahigh magnetic field of 21.1 T.

This cover article features results obtained using the 21.1 T solid-state NMR spectrometer at the National Ultrahigh-Field NMR Facility for Solids (Ottawa, ON). If you are interested in using this spectrometer in your research please contact us at terskikhv@nrc-cnrc.gc.ca

NMR papers in *PNAS*

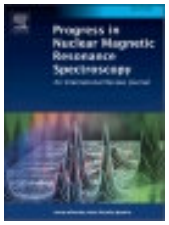
K. Shin, K.A. Udachin, I.L. Moudrakovski, D.M. Leek, S. Alavi, C.I. Ratcliffe, and J.A. Ripmeester, "Methanol incorporation in clathrate hydrates and the implications for oil and gas pipeline flow assurance and icy planetary bodies" *Proc. Natl. Acad. Sci. USA* **110** (2013) online.
http://dx.doi.org/10.1073/pnas.1302812110

M.J. Smith, B.G. Neel, and M. Ikura, "NMR-based functional profiling of RASopathies and oncogenic RAS mutations," *Proc. Natl. Acad. Sci. USA* **110** (2013) 4574-4579.
http://dx.doi.org/10.1073/pnas.1218173110

Reviews in *Soft Matter*

J. Dobnikar, A. Snezhko and A. Yethiraj, "Emergent colloidal dynamics in electromagnetic fields," *Soft Matter* **9** (2013) 3693-3704. **(Review Article)**
http://dx.doi.org/10.1039/C3SM27363F

Progress in NMR Spectroscopy



U.H.N. Dürr, R. Soong, A. Ramamoorthy, "When detergent meets bilayer: birth and coming of age of lipid bicelles," *Progress in Nuclear Magnetic Resonance Spectroscopy* **69** (2013) 1-22. **(Invited Review)**
http://dx.doi.org/10.1016/j.pnmrs.2013.01.001

Review in *FEBS Journal*

F.J. Amador, P.B. Stathopulos, M. Enomoto, M. Ikura, "Ryanodine Receptor Calcium Release Channels: Lessons from structure-function studies," *FEBS Journal* (2013) online. **(Review)**
http://dx.doi.org/10.1111/febs.12194

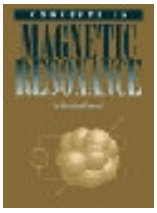
Review in *Solid State Nuclear Magnetic Resonance*

F.A. Perras, J. Viger-Gravel, K.M.N. Burgess, D.L. Bryce, "Signal Enhancement in Solid-State NMR of Quadrupolar Nuclei," *Solid State Nuclear Magnetic Resonance* **51-52** (2013) 1–15. **(Review)**
http://dx.doi.org/10.1016/j.ssnmr.2012.11.002

Review in *Molecular and Cellular Endocrinology*

D. Létourneau, A. Lefebvre, P. Lavigne, J.-G. LeHoux, "STARD5 specific ligand binding: Comparison with STARD1 and STARD4 subfamilies," *Molecular and Cellular Endocrinology* **371** (2013) 20-25. **(Review)**
http://dx.doi.org/10.1016/j.mce.2013.01.004

Review in *Concepts in Magnetic Resonance*



A.D. Bain, "NMR quadrupole liouvillians for arbitrary spin: Exact symbolic expressions and perturbation solutions," *Concepts in Magnetic Resonance Part A* **42A** (2013) 45–58.

http://dx.doi.org/10.1002/cmr.a.21259

Dr. William (Bill) George Schneider

(1915 - 2013)

Former President wrote the book on nuclear magnetic resonance & led NRC through period of growth

Bill Schneider's life was the fabric that makes up the colours of Canadian history. Wooed to Saskatchewan by the Dominion Lands Act and its promise of free land for newcomers, his Austrian grandparents spent their first years struggling to survive. Schneider's father, who had never completed grade school, eventually married and secured a good-sized farm near Wolseley, Sask. where young William George *"Bill"* was born.

Hardship was the young family's constant companion. At the age of 4, during the Spanish flu epidemic of 1918-20, the man who would someday lead the country's national research facility found himself motherless, helping his siblings care for crops and animals. His father's eventual decision to remarry would reshape the family's fortunes. Reminiscing on his childhood, Bill Schneider credited his new stepmother – who valued education above all else – with encouraging all six children to aspire to the highest education possible, even if meant considerable sacrifice for the family. Bill Schneider pursued his education against the sombre backdrop of the Great Depression.

The young farmer eventually left a one-room schoolhouse to attend Luther College in Regina, where he spent the last of his five years obtaining university credits.

From there, Schneider was headed to the University of Saskatchewan, where he would room with two other students (including yet-to-be named Nobel Laureate Henry Taube) and take summer campus jobs to make ends meet. During his senior years, a bursary from the National Research Council (NRC) would help pay the costs associated with obtaining a B. Sc. (Honours) in 1937 and an M. Sc. in 1939.

That Fall, the young researcher began his PH.D studies at McGill University under the supervision of Chemistry Department Chair Otto Maass who, at the time, also served as an advisor to the Department of National Defense (DND) and the NRC. The looming threat of war would direct their research.

When Canada declared war on Germany in 1939, Maass immediately sent his student a telegram advising him not to enlist. His skills were needed for critical defense-related research in a classified program underway with DND. Schneider immediately got to work synthesizing a number of compounds in order to develop strategies against the enemy's suspected imminent use of poisonous gases with highly toxic fluorine compounds.

Though his focus would eventually be directed towards non-military projects to fulfill his Doctoral degree, Schneider's early research in poisonous gasses (including radio-active mustard gas and Lewisite) continued through his post-doctoral work at NRC and at Harvard, ending only when the American military identified another defense priority – that of urgently defending the Allied Forces who were enduring submarine attacks along the Atlantic coast.

Bill Schneider now found himself working with the Woods Hole Oceanographic Institute (WHOI) - the U.S. army's primary naval research arm - in weaponry testing and the development of improved measures for underwater explosives. It was during this time (from 1943 to 1946), and during a complex exercise to recover a capsized boat, that Schneider's innate leadership abilities became evident. The impact of Schneider's overall work during the war earned him a Certificate of Appreciation for outstanding contribution from the U.S. War Department and the U.S. Navy Department.

In 1946, Bill Schneider joined NRC to set up a Physical Chemistry Section in the Chemistry Division, under the direction of Dr. E.W.R. Steacie. After seven years of conducting top secret research, Schneider is said to have taken pleasure in the challenge of developing a peace-

time research program built around intermolecular forces and interactions and methods of investigation, including high resolution nuclear magnetic resonance. His book, *"High Resolution Nuclear Magnetic Resonance,"* the first comprehensive volume on the emerging discipline of High-resolution NMR Spectroscopy was co-authored with Nobel Laureate, John Pople, and Harold Bernstein in 1959.

Schneider was named Director of the Division of Pure Chemistry (1963-65), Vice-President, Scientific (1965-67) and finally, President of NRC (1967-80). He never lost his love of hands-on research. If he could not pursue it full time, he would tell close friends, he felt his effectiveness would be greatly diminished. Many suspected that Schneider's greatest (and perhaps only) regret about his eventual appointment as President of NRC was that his new duties would end his work in the laboratory.

NRC breaks new ground with Schneider at the helm

Bill Schneider's tenure as President of NRC was marked, in part, by the oil crisis and resulting energy crunch of the 1970s. To help Canada respond to these challenges, NRC took the lead in developing technologies focused on energy conservation and renewable resources. Work on solar energy, wind energy and biomass would soon follow, though these programs became less urgent when the oil crisis was over.

Recognizing the need to help foster the development of science and engineering in Quebec universities (the former McGill student had always been concerned by the fact that science in the province had only become secularized during Quebec's "Quiet Revolution" of the 60s), Schneider led the development of a number of NRC-created programmes de ratrappage ("catch up" programs) to accelerate the emergence of a scientific-based academic community. Soon, NRC would build a laboratory (the former Industrial Materials Institute) in Boucherville, Quebec.

It was also under Schneider's presidency that NRC became the lead agency for contracting the private-sector design and construction of Canadarm, the robotic arm commissioned by NASA for use on the U.S. Space Shuttle. "Up until that time, we had an embryonic space program and one of (NRC's) policies was that we needed to get industry involvement to take on contracts for space hardware. With this one major initiative, aerospace was established at NRC," Schneider explained. It remains one of the most important NRC portfolios today.

This period also witnessed the emergence of a large science infrastructure in Canada, with NRC now responsible for operating all of the country's astronomical observatories. The Canada-France telescope was created in Hawaii and the TRIUMF project began one of the world's leading subatomic physics laboratories. After Herzberg won the Nobel Prize in 1971, NRC decided to combine all its astronomy related research activities into an institute and the Herzberg Institute of Astrophysics was born. Other regionally- based institutes (such as the Institute of Cold Ocean Engineering) would soon follow.

The need to foster closer links to industry led to the creation of NRC's Industrial Research Assistance Program (IRAP) and the merging of the Technical Information Service with the National Science Library to become the new Canada Institute for Scientific and Technical Information (CISTI). When Bill Schneider finally retired in 1980, he continued to foster a close relationship to industry by becoming a chemical consultant himself and establishing a biotechnology company in Ottawa.

Over the years Bill Schneider received many honours and awards, including Fellowships in the Royal Society (London), the Royal Society of Canada (RSC) and the Chemical Institute of Canada. He received a Doctor of Laws degree with Pierre Elliot Trudeau and then UN Secretary, U Thant in 1968 from the University of Alberta. The RSC presented him with the Henry Marshall Tory Medal in 1969. He was president of the International Union of Pure and Applied Chemistry from 1983 to 1985, and was named an Officer in the Order of Canada in 1976.

Bill Schneider remained close to NRC and often attended functions at Sussex Drive. On June 1, 2006, the researcher proudly celebrated his 91st birthday during the grand opening ceremony of a facility commemorating his contributions. The W.G. Schneider Building (M-40), a state-of-the-art Nuclear Magnetic Resonance (NMR) facility, is located at NRC's Montreal Road campus and still bears his name.

Bill Schneider passed away peacefully in Ottawa on February 18, 2013 at the age of 97.

courtesy of NRC Canada, used with permission

NMR Events

Submitted by Bruce Balcom

ICMRM-12: 12th International Conference on Magnetic Resonance Microimaging

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

The chairs and organising committee are pleased to announce the first call for abstracts for ICMRM12, to be held at Fitzwilliam College, Cambridge, UK. Detailed information about the conference and abstract submission can be found at http://www.ceb.cam.ac.uk/ICMRM12

Location The conference will be held in the historic City of Cambridge at Fitzwilliam College, one of the 28 undergraduate colleges of the University of Cambridge. The conference dinner will be held in the Great Hall at Trinity College. Cambridge is within easy reach of London (<50 mins by train from King's Cross station) and its major airports and is even closer to Stansted Airport (~30 mins by train)

Provisional Programme ICMRM12 will open with an education session on Sunday 25th August 2013 at 11:00 am and will close on Thursday 29th August 2013 at 5:00pm. In addition to oral and poster sessions, there will be plenary speakers as well as keynote presentations by a number of invited speakers. There will also be a session dedicated to the Colloquium on Mobile NMR (CMMR).

Plenary speakers: Lucio Frydman, Klaas Prüssmann and Warren S. Warren

We are pleased to confirm the following **invited speakers:** Stephen Blackband, Sarah Codd, Simon Duckett, Axel Haase, Jürgen Hennig, Peter Jakob, Katsumi Kose, Malcolm Levitt, Ben Newling, John Pauly, Daniel Topgaard

Abstract Submissions Submissions for oral and poster presentations at ICMRM12 are now invited. Please access the ICMRM12 website for detailed information about abstract submissions.
http://www.ceb.cam.ac.uk/ICMRM12

Important Dates

14 May 2013: Deadline for abstract submission for oral presentations

15 July 2013: Deadline for abstract submission for poster presentations

25 June 2013: Early bird registration deadline

Sponsors and Exhibitors Please contact us to discuss opportunities for sponsorship and exhibitions during ICMRM12.

Contact ICMRM12 Administration:
tricia@paceprojects.co.uk

We look forward to welcoming you to ICMRM12 in 2013. Regards,

Professor Lynn Gladden,
Dr Andy Sederman,
ICMRM12 Chairs
http://www.ceb.cam.ac.uk/ICMRM12

18th Triennial ISMAR Conference

May 19-24, 2013, Rio de Janeiro, Brazil
http://www.ismar2013.net/

8th Solid-State NMR Workshop at CSC 2013

May 26, 2013, Québec, QC, Canada
http://nmr900.ca/events_e.html

CSC 2013, the 96th Canadian Chemistry Conference and Exhibition "Chemistry without Borders"

May 26-30, 2013, Québec, QC, Canada
http://www.csc2013.ca/

Computational Aspects of Metabolomic NMR Gordon Research Seminar

June 1-2, 2013, West Dover, VT
http://www.grc.org/programs.aspx?year=2013&program=grs_bionmr

Computational Aspects - Biomolecular NMR Gordon Research Conference

June 2-7, 2013 West Dover, VT
http://www.grc.org/programs.aspx?year=2013&program=bionmr

7th Annual VIVA NMR Symposium

June, 2013, University of Victoria, Victoria B.C.

59th ICASS International Conference on Analytical Sciences and Spectroscopy & **Spectr'Atom 2013** Conference (June 25-28, 2013)

June 26-28, 2013, Le Grand Lodge Mont Tremblant, Mont-Tremblant, Québec
http://csass.org/ICASS.html

AMPERE NMR School

June 23-29, 2013, Poznan, Poland
http://www.staff.amu.edu.pl/~school/

EUROMAR 2013

30 June - 5 July, 2013, Crete, Greece
http://www.euromar2013.org/

NMRCM 2013 International Symposium and Summer School "NMR in Condensed Matter" 10th meeting "NMR in Life Sciences"

July 8-12, 2013, St. Petersburg, Russia
http://nmr.phys.spbu.ru/nmrcm

55th Rocky Mountain Conference on Magnetic Resonance (EPR Symposium)

July 28-August 1, 2013, Denver, Colorado
http://www.rockychem.com/

ICMRM-12 12th International Conference on Magnetic Resonance Microimaging

August 25-29, 2013, Fitzwilliam College, University of Cambridge, UK
http://www.ceb.cam.ac.uk/ICMRM12

8th Alpine Conference on Solid-State NMR

September 8-12, 2013, Chamonix Mont-Blanc, France
http://www.alpine-conference.org

SMASH 2013 Small Molecule NMR Conference

Sept 22-25, 2013, Santiago de Compostela, Spain http://www.smashnmr.org/

MOOT XXVI NMR Symposium

October 26-27, 2013, Queen's University, Kingston, ON
http://www.mootnmr.org

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

October 27-30, 2013, Brisbane, Australia
http://apnmr2013.org/

57th Conference on Magnetism and Magnetic Materials

November 4-8, 2013, Denver, Colorado
http://www.magnetism.org/

6th Annual GRASP Symposium

November 25, 2013, McGill University, Montréal, QC, Canada
http://grasp.mcgill.ca/english/conferences/conferences.html

55th ENC

March 23-28, 2014, Boston, MA
http://www.enc-conference.org/

CSC 2014, the 97th Canadian Chemistry Conference and Exhibition
"Chemistry from Sea to Sky"

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

56th Rocky Mountain Conference on Magnetic Resonance: Solid-State NMR Symposium & EPR Symposium

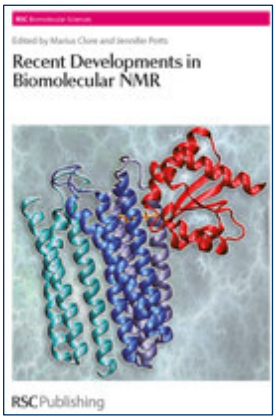
July 13-17, 2014, Copper Mountain, Colorado
http://www.rockychem.com/symposia/solid-state-nmr-symposium.html

ICMRBS 2014, the XXVIth International Conference on Magnetic Resonance in Biological Systems
August 24-29, 2014, Dallas, Texas
http://www.icmrbs.org/

Pacifichem 2015 The International Chemical Congress of Pacific Basin Societies

December 15-20, 2015, Honolulu, Hawaii, USA
http://www.pacifichem.org/

New NMR Books



Recent Developments in Biomolecular NMR

Marius Clore (Editor), Jennifer Potts (Editor)

Hardcover: 364 pages
Language: English
Publisher: RSC, August 2012
ISBN: 978-1849731201

http://www.amazon.com/dp/1849731209
http://www.amazon.ca/dp/1849731209

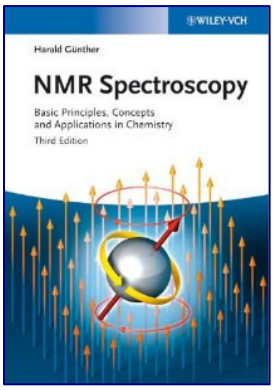
RSC: NMR spectroscopy is widely used in biomolecular science particularly for structure determination of proteins, nucleic acids and carbohydrates. Much of the innovation within NMR spectroscopy has been within the field of protein NMR spectroscopy, an important technique in structural biology. Filling a gap in the literature, this book will draw together experts in the field to discuss the real advances in NMR methods that have occurred or have an impact on the biomolecular field in the last few years. The coverage will include recent developments in using NMR for determination of protein structures, membrane proteins, the dynamics of RNA and advances in NMR in drug discovery. Edited by leading biological NMR spectroscopists, the book will be an essential reference for researchers in industry and academia interested in or joining this bioanalytical field.

Table of contents
http://pubs.rsc.org/en/Content/eBook/978-1-84973-120-1

This book is part of the RSC Series of books on *New Developments in NMR*.
Editor-in-Chief: William S. Price (Australia), Series Editors: **Bruce Balcom (Canada)**, István Furó (Sweden), Maili Liu (China), Masatsune Kainosho (Japan).

To learn more and to see other books from this series
http://www.rsc.org/shop/books/series/91.asp?seriesid=91

NMR Spectroscopy: Basic Principles, Concepts and Applications in Chemistry



Harald Günter (Author)

Paperback: 687 pages
Language: English
Publisher: Wiley-VCH; 3rd edition (May 13 2013)
ISBN: 978-3527330003

http://www.amazon.com/dp/3527330003
http://www.amazon.ca/dp/3527330003

Wiley: The third edition of the popular classic retains the clear style and excellent didactical, highly practical approach. It explains this complex topic without mathematical equations, making it ideal for those students who do not have a strong mathematical background, but want to understand the fundamentals of NMR and work with the method in an efficient and accurate way. The contents have been completely revised and updated with approximately 25% new material, including new chapters on biological NMR and on other nuclei, outdated methods are replaced by current ones, and new developments have been added.

Table of contents:

The Physical Basis of the Nuclear Magnetic Resonance Experiment Part I.

The Proton Magnetic Resonance Spectra of Organic Molecules.

Experimental Aspects of Nuclear Magnetic Resonance Spectroscopy.

Chemical Shift and Spin-Spin Coupling as Functions of Structure.

The Analysis of High-Resolution Nuclear Magnetic Resonance Spectra.

The Influence of Molecular Symmetry and Chirality on Proton Magnetic Resonance Spectra.

The Physical Basis of the Nuclear Magnetic Resonance Experiment Part II: Fourier Transform and Pulse Nuclear Magnetic Resonance.

Two-Dimensional Nuclear Magnetic Resonance Spectroscopy.

The Influence of Dynamic Effects on ^{1}H Nuclear Magnetic Resonance Spectra.

Selected Experimental Techniques of Nuclear Magnetic Resonance Spectroscopy.

^{13}C Nuclear Magnetic Resonance Spectroscopy.

Other Important Nuclei (Including ^{15}N, ^{31}P, ^{17}O and Metal Nuclei)

Techniques for Studying Biological Macromolecules

Appendix/Bibliography/Solutions to Exercises/Index

NMR Jobs and Vacancies

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

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

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

Interested students should contact Prof. Isabelle Marcotte at: marcotte.isabelle@uqam.ca

Prof. Isabelle Marcotte, Ph.D.
Department of Chemistry
Université du Québec à Montréal
PO Box 8888, Downtown Station
Montréal (QC)
H3C 3P8 Canada
T. 1-514-987-3000 #5015
F. 1-514-987-4054
marcotte.isabelle@uqam.ca

Postdoctoral Research Associate in In-Vivo NMR Spectroscopy

Environmental NMR Centre, Department of Chemistry, University of Toronto at Scarborough, Toronto, Ontario, Canada
http://www.scar.utoronto.ca/~asimpson/

Project Description: The project will, in collaboration with Bruker Biospin Corporation, Environment Canada and the National Water Research Institute to pioneer in-vivo NMR technologies and applications to elucidate environment stressors. Development of both low speed MAS approaches and static approaches will be developed for small organisms that are key to understanding aquatic toxicity at the molecular-level. In terms of MAS, the environmental NMR Center is equipped with a range of Comprehensive Multiphase NMR probes (CMP-NMR) (J. Magn. Reson. 2012; 217:61-76). CMP NMR is a new area of NMR spectroscopy that incorporates solid-state, semi-solids (HR-MAS) and solution-state NMR into a single approach. When applied to an organism in-vivo, all bonds in all phases can be detected providing a high resolution overview of everything in a living system. In terms of static system, specimen cells have already been developed that feed and oxygenate organisms inside NMR spectrometers permitting them to be studied indefinitely in a non-stressed state.

Background: Often, numerous environmental contaminants are found at low levels which in isolation are non-lethal but combined exhibit toxicities that are difficult to evaluate. In the long term they may be very hazardous to animal, plant and human populations, as their affects are often detected too late, and after physical symptoms become widespread. This project will develop in-vivo NMR that will permit "molecular fingerprinting" approaches that directly measure the changes in a living organism as a direct response to its surroundings. This research aims to develop tools that can answer the key question "Is a particular contaminated environment safe for life?" and understand how and why certain chemicals are toxic. Preliminary results demonstrate the approaches that can efficiently and quantitatively asses the stress in natural populations months/years before conventional reproduction tests as-well as explaining the source of the stress and its biochemical implications. Furthermore, such "early warning systems" could potentially being used to predict and permit treatment of disease at its very early stages before symptoms are apparent.

In addition, to monitoring the changes in the organism, specific NMR experiments will also be developed to identify binding sites of anthropogenic contaminants in-vivo. This is made possible due to globally unique hardware developed between the Environmental NMR Center and Bruker Biospin (leading manufacturer of NMR technology). It is worth mentioning that these approaches have wide spread applicability in general not just for contaminants but understand how any molecule (for example drugs, nutrition) bind in-vivo and thus represent an extremely powerful molecular tool for chemical/biochemical/medical research in general.

The candidate must have a strong background in NMR spectroscopy ideally with expertise in solid-state, HR-MAS and solution-state NMR. Expertise in one area is sufficient as long the candidate is willing and interested in learning all areas of NMR spectroscopy. The candidate must be open minded and willing to work with very complex in-vivo systems. The candidate should be willing to learn to design novel pulse programs that combine aspects from solution-state and solid-state NMR. Candidates will need to draw upon and integrate a range of concepts including saturation transfer, diffusion editing, cross-polarization dynamics, relaxation filters, isotope filtering with 1-3D NMR spectroscopy to access specific key molecular interactions from within complex matrices. The candidate will have

access to a range of state of-the-art equipment at the Environmental NMR center including prototype multiphase probes and hardware, as well as solid-state, HR-MAS, liquid-state, cryoprobes, micro-imaging, and hyphenated (2D-HPLC-SPE-NMR-MS(Q-q-Tof) NMR spectrometers.

The project will be carried out in close collaboration with Bruker BioSpin and candidate may be asked to spend time at Bruker headquarters in the U.S. assisting in building larger diameter MAS probes as required (typically 1 month per year). Previous probe building experience is not required. At present we have number of fully working prototypes but are working on further development of new probe designs with Bruker.

The candidate should have an interest in environmental chemistry and/or willingness to learn key issues in this field. Due to the very technical nature of the project the position is specifically suited to a gifted and open-minded NMR spectroscopist rather than an environmentalist with NMR experience. The candidate must be willing to travel and may be expected to lead visits with graduate students to the Bruker BioSpin Corporation headquarters and the National Water Research Institute as/if required. In addition, the candidate, along with the center manager and directors, will be expected to act as a general NMR resource for graduate students, and collaborators in the Environmental NMR Center, and assist with training, data acquisition, processing and interpretation on projects as required. The Environmental NMR Center is highly collaborative and such involvement will nearly always result in the post-doctoral fellow becoming a co-author in any research in which they assisted.

Application: Candidates should send a complete C.V. including a publication list, a statement outlining their suitability and their interest in the position. Candidates should arrange to have 3 references sent directly. Applications without the appropriate references have to be considered incomplete and cannot be considered. Applications and references should be sent to

Professor André Simpson, FRSC
Director of the Environmental NMR Center
Department of Chemistry
Division of Physical and Environmental Sciences
University of Toronto at Scarborough
1265 Military Trail, Toronto, MIC 1A4

or e-mailed as a PDF attachment to
andre.simpson@utoronto.ca

All applications and references will be reviewed once complete. We aim to fill the position by July 1st 2013.

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

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

Research in solid-state NMR in the Bryce group covers a variety of areas including the development of the spectroscopy of traditionally difficult quadrupolar nuclei, applications of double-rotation NMR, applications to weak interactions including halogen bonding, and the study of polymorphism. Experimental work is complemented by quantum chemical studies. Interested students should contact Prof. Bryce directly at dbryce@uottawa.ca

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

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

Ph.D. and Postdoctoral NMR positions

Two postdoc positions in oriented sample (OS) and MAS solid-state NMR of helical membrane proteins, National High Magnetic Field Laboratory, Tallahassee, FL
http://nmr900.ca/nmr_jobs.html#nhmfl

Postdoctoral Scientist in NMR of Materials and Processes, RWTH Aachen University, Aachen, Germany
http://nmr900.ca/nmr_jobs.html#aachen

Postdoctoral position in NMR spectroscopy of protein(s) involved in transcriptional regulation Institut de Recherche Interdisciplinaire, CNRS, Lille, France
http://nmr900.ca/nmr_jobs.html#iri

Postdoc in high-pressure solution-NMR, University of California, Davis
http://nmr900.ca/nmr_jobs.html#UCDavis

PhD positions in materials research and solid-state NMR at TUT and KIT (Tallinn, Estonia / Karlsruhe, Germany)
http://nmr900.ca/nmr_jobs.html#tutkit

Recent NMR Publications

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

Memorial University of Newfoundland

L. MacEachern, A. Sylvester, A. Flynn, A. Rahmani, and M.R. Morrow, "Dependence of Bicellar system phase behavior and dynamics on anionic lipid concentration," *Langmuir* **29** (2013) 3688–3699. http://dx.doi.org/10.1021/la305136q

J. Dobnikar, A. Snezhko and A. Yethiraj, "Emergent colloidal dynamics in electromagnetic fields," *Soft Matter* **9** (2013) 3693-3704. **(Review Article)** http://dx.doi.org/10.1039/C3SM27363F

S. Barhoum, V. Booth and A. Yethiraj, "Diffusion NMR Study of Complex Formation in Membrane-Associated Peptides," *European Biophysics Journal* **42** (2013) 405-414. http://dx.doi.org/10.1007/s00249-013-0890-4

Dalhousie University

D.N. Langelaan, T. Reddy, A.W. Banks, G. Dellaire, D.J. Dupré, J.K. Rainey, "Structural features of the apelin receptor N-terminal tail and first transmembrane segment implicated in ligand binding and receptor trafficking," *Biochimica et Biophysica Acta (BBA) - Biomembranes* **1828** (2013) 1471–1483. http://dx.doi.org/10.1016/j.bbamem.2013.02.005

K. Ma, U. Werner-Zwanziger, J. Zwanziger and U. Wiesner, "Controlling growth of ultra-small sub-10nm fluorescent mesoporous silica nanoparticles," *Chemistry of Materials* **25** (2013) 677–691. http://dx.doi.org/10.1021/cm303242h

E.L. Zodrow, R. Helleur, U. Werner-Zwanziger, B. Chen, J.A. D'Angelo, "Spectrochemical study of coalified *Trigonocarpus grandis* (Pennsylvanian tree-fern ovule, Canada): Implications for fossil-organ linkage," *International Journal of Coal Geology* **109-110** (2013) 24–35. http://dx.doi.org/10.1016/j.coal.2013.01.013

University of New Brunswick

I.V. Mastikhin, A. Arbabi, "Transiently porous medium: Magnetic Resonance Imaging studies of acoustic cavitation," *Microporous and Mesoporous Materials* (2013) online. http://dx.doi.org/10.1016/j.micromeso.2013.02.042

C.E. Muir, B.J. Balcom, "A comparison of magnetic resonance imaging methods for fluid content imaging in porous media," *Magnetic Resonance in Chemistry* (2013) online. http://dx.doi.org/10.1002/mrc.3947

T.D. Humphries, K.T. Munroe, T.M. DeWinter, C.M. Jensen, G.S. McGrady, "NMR spectroscopic and thermodynamic studies of the etherate and the α, α', and γ phases of AlH_3," *International Journal of Hydrogen Energy* **38** (2013) 4577–4586. http://dx.doi.org/10.1016/j.ijhydene.2013.01.096

Université Laval

F. Otis, M. Auger, and N. Voyer, "Exploiting Peptide Nanostructures to Construct Functional Artificial Ion Channels," *Acc. Chem. Res.* (2013) online. http://dx.doi.org/10.1021/ar400044k

J.-F. Labbé, T. Lefèvre, A.-A. Guay-Bégin and M. Auger, "Structure and membrane interactions of the β-amyloid fragment 25–35 as viewed using spectroscopic approaches," *Phys. Chem. Chem. Phys.* **15** (2013) 7228-7239. http://dx.doi.org/10.1039/c3cp44623a

Y. Ledemi, B. Bureau, G.Le Caër, L. Calvez, C. Roiland, G. Tricot, P. Florian, V. Nazabal, D. Massiot, "^{71}Ga NMR in chalcogenide and chalco-halide glasses," *Journal of Non-Crystalline Solids* (2013) online. http://dx.doi.org/10.1016/j.jnoncrysol.2013.03.038

J. Leclerc, T. Lefèvre, M. Gauthier, S.M. Gagné and M. Auger, "Hydrodynamical properties of recombinant spider silk proteins: Effects of pH, salts and shear, and implications for the spinning process," *Biopolymers* (2013) accepted. http://dx.doi.org/10.1002/bip.22218

Boehringer Ingelheim (Canada) Ltd, Laval

N. Goudreau, C.T. Lemke, A.-M. Faucher, C. Grand-Maître, S. Goulet, J.-E. Lacoste, J. Rancourt, E. Malenfant, J.-F. Mercier, S. Titolo, and S.W. Mason, "Novel Inhibitor Binding Site Discovery on HIV-1 Capsid N-Terminal Domain by NMR and X-ray Crystallography," *ACS Chem. Biol.* (2013) online. http://dx.doi.org/10.1021/cb400075f

N. Goudreau, O. Hucke, A.-M. Faucher, C. Grand-Maître, O. Lepage, P.R. Bonneau, S.W. Mason, S. Titolo, "Discovery and Structural Characterization of a New Inhibitor Series of HIV-1 Nucleocapsid Function: NMR Solution Structure Determination of a Ternary Complex Involving a 2:1 Inhibitor/NC Stoichiometry," *Journal of Molecular Biology* (2013) online. http://dx.doi.org/10.1016/j.jmb.2013.02.022

N. Goudreau, R. Coulombe, A.-M. Faucher, C. Grand-Maitre, J.-E. Lacoste, C.T. Lemke, E. Malenfant, Y. Bousquet, L. Fader, B. Simoneau, J.-F. Mercier, S. Titolo, and S.W. Mason, "Monitoring Binding of HIV-1 Capsid Assembly Inhibitors Using ^{19}F Ligand- and ^{15}N Protein-Based NMR and X-ray Crystallography: Early Hit Validation of a Benzodiazepine Series," *ChemMedChem* **8** (2013) 405-414. **(Cover Article)** http://dx.doi.org/10.1002/cmdc.201200580

Université du Québec à Trois-Rivières

M. Veillette, K. Bichel, P. Pawlica, S.M.V. Freund, M.B. Plourde, Q.T. Pham, C. Reyes-Moreno, L.C. James, L. Berthoux, "The V86M mutation in HIV-1 capsid confers resistance to TRIM5alpha by abrogation of cyclophilin a-dependent restriction and enhancement of viral nuclear import," *Retrovirology* **10** (2013) 25. http://dx.doi.org/10.1186/1742-4690-10-25

Université de Sherbrooke

D. Létourneau, A. Lefebvre, P. Lavigne, J.-G. LeHoux, "STARD5 specific ligand binding: Comparison with STARD1 and STARD4 subfamilies," *Molecular and Cellular Endocrinology* **371** (2013) 20-25. **(Review)** http://dx.doi.org/10.1016/j.mce.2013.01.004

Université du Québec à Montréal

A.E. Gravel, A.A. Arnold, E.J. Dufourc, I. Marcotte, "An NMR investigation of the structure, function and role of the hERG channel selectivity filter in the long QT syndrome," *BBA - Biomembranes* **1828** (2013) 1494–1502. http://dx.doi.org/10.1016/j.bbamem.2013.02.012

McGill University

R. Vinaik, G. Kozlov, K. Gehring, "Structure of the Non-Catalytic Domain of the Protein Disulfide Isomerase-Related Protein (PDIR) Reveals Function in Protein Binding," *PLoS ONE* **8** (2013) e62021. http://dx.doi.org/10.1371/journal.pone.0062021

J. Milette, V. Toader, E. Soulé, R.B. Lennox, A.D. Rey, and L. Reven, "A Molecular and Thermodynamic View of the Assembly of Gold Nanoparticles in Nematic Liquid Crystal," *Langmuir* **29** (2013) 1258–1263. http://dx.doi.org/10.1021/la304189n

A. Caballero, S. Bennett, C.J. Serpell and P.D. Beer, "Iodo-imidazolium salts: halogen bonding in crystals and aniontemplated pseudorotaxanes," *Cryst Eng Comm* **15** (2013) 3076-3081. http://dx.doi.org/10.1039/c2ce26020d

Université de Montréal

L. Volpon, M.J. Osborne, H. Zahreddine, A.A. Romeo, K.L.B. Borden, "Conformational changes induced in the eukaryotic translation initiation factor eIF4E by a clinically relevant inhibitor, ribavirin triphosphate," *Biochem. Biophys. Res. Commun.* (2013) online. http://dx.doi.org/10.1016/j.bbrc.2013.03.125

N. Goudreau, R. Coulombe, A.-M. Faucher, C. Grand-Maitre, J.-E. Lacoste, C.T. Lemke, E. Malenfant, Y. Bousquet, L. Fader, B. Simoneau, J.-F. Mercier, S. Titolo, and S.W. Mason, "Monitoring Binding of HIV-1 Capsid Assembly Inhibitors Using ^{19}F Ligand- and ^{15}N Protein-Based NMR and X-ray Crystallography: Early Hit Validation of a Benzodiazepine Series," *ChemMedChem* **8** (2013) 405–414. **(Cover Article)** http://dx.doi.org/10.1002/cmdc.201200580

University of Ottawa

F.A. Perras and D.L. Bryce, "Measuring Dipolar and J Coupling Between Quadrupolar Nuclei Using Double-Rotation NMR," *Journal of Chemical Physics* **138** (2013) 174202. http://dx.doi.org/10.1063/1.4802192

J. Viger-Gravel, S. Leclerc, I. Korobkov and D.L. Bryce, "Correlation Between ^{13}C Chemical Shifts and the Halogen Bonding Environment in a Series of Solid para-Diiodotetrafluorobenzene Complexes," *CrystEngComm* **15** (2013) 3168-3177. http://dx.doi.org/10.1039/C3CE26750D

J. Yuk, K.L. McIntyre, C. Fische, J. Hicks, K.L. Colson, E. Lui, D. Brown, J.T. Arnason, "Distinguishing Ontario ginseng landraces and ginseng species using NMR-based metabolomics," *Analytical and Bioanalytical Chemistry* **405** (2013) 4499-4509. http://dx.doi.org/10.1007/s00216-012-6582-6

F.A. Perras, J. Viger-Gravel, K.M.N. Burgess, D.L. Bryce, "Signal Enhancement in Solid-State NMR of Quadrupolar Nuclei," *Solid State Nuclear Magnetic Resonance* **51-52** (2013) 1–15. **(Review)** http://dx.doi.org/10.1016/j.ssnmr.2012.11.002

NRC Canada

M.B. Perry, L.L. MacLean, M. Gottschalk, V. Aragon, E. Vinogradov, "Structure of the capsular polysaccharides and lipopolysaccharides from *Haemophilus parasuis* strains ER-6P (serovar 15) and Nagasaki (serovar 5)," *Carbohydrate Research* (2013) accepted. http://dx.doi.org/10.1016/j.carres.2013.04.023

P.Jr. Morin, D. Ferguson, L.M. LeBlanc, M.J.G. Hébert, A.F. Paré, J. Jean-François, M.E. Surette, M. Touaibia, and M. Cuperlovic-Culf, "NMR Metabolomics Analysis of the Effects of 5-Lipoxygenase Inhibitors on Metabolism in Glioblastomas," *J. Proteome Res.* (2013) online. http://dx.doi.org/10.1021/pr400026q

L. Wang, E.V. Vinogradov and A.J. Bogdanove, "Requirement of the Lipopolysaccharide O-Chain Biosynthesis Gene *wxocB* for Type III Secretion and Virulence of *Xanthomonas oryzae* pv. Oryzicola," *Journal of Bacteriology* **195** (2013) 1959-1969. http://dx.doi.org/10.1128/JB.02299-12

T.L. Spencer, L.A. O'Dell, I.L. Moudrakovski, and G.R. Goward, "Dynamics of Ag^+ Ions in $RbAg_4I_5$ Probed Indirectly Via ^{87}Rb Solid-State NMR," *Journal of Physical Chemistry C* **117** (2013) online. http://dx.doi.org/10.1021/jp3125928

E. Vinogradov, M. Frimmelova, R. Toman, "Chemical structure of the carbohydrate backbone of the lipopolysaccharide from *Piscirickettsia salmonis*," *Carbohydrate Research* (2013) accepted. http://dx.doi.org/10.1016/j.carres.2013.04.010

J. Kubler-Kielb, E. Vinogradov, "Reinvestigation of the structure of *Brucella* O-antigens," *Carbohydrate Research* (2013) accepted. http://dx.doi.org/10.1016/j.carres.2013.03.021

K. Yu, X. Liu, Q. Zeng, D.M. Leek, J. Ouyang, K.M. Whitmore, J.A. Ripmeester, Y. Tao, M. Yang, "Effect of Tertiary and Secondary Phosphines on Low-Temperature Formation of Quantum Dots," *Angewandte Chemie International Edition* **52** (2013) 4823–4828. http://dx.doi.org/10.1002/anie.201300568

E. Altman, V. Chandan, J. Li, E. Vinogradov, "Lipopolysaccharide structure of *Helicobacter pylori* serogroup O:3," *Carbohydrate Research* **366** (2013) 33–37. http://dx.doi.org/10.1016/j.carres.2012.11.004

C.V. Bowen, D. DeBay, H.S. Ewart, P. Gallant, S. Gormley, T.T. Ilenchuk, U. Iqbal, T. Lutes, M. Martina, G. Mealing, N. Merkley, S. Sperker, M.J. Moreno, C. Rice, R.T. Syvitski, J.M. Stewart, "In Vivo Detection of Human TRPV6-Rich Tumors with Anti-Cancer Peptides Derived from Soricidin," *PLoS ONE* **8** (2013) e58866. http://dx.doi.org/10.1371/journal.pone.0058866

K. Yu, P. Ng, J. Ouyang, Md.B. Zaman, A. Abulrob, T.N. Baral, D. Fatehi, Z.J. Jakubek, D. Kingston, X. Wu, X. Liu, C. Hebert, D.M. Leek, and D.M. Whitfield, "Low-Temperature Approach to Highly

Emissive Copper Indium Sulfide Colloidal Nanocrystals and Their Bioimaging Applications," *ACS Appl. Mater. Interfaces* **5** (2013) 2870–2880.
http://dx.doi.org/10.1021/am302951k

E. Papulovskiy, A.A. Shubin, V.V. Terskikh, C. Pickard and O.B. Lapina, "Theoretical and experimental insights into applicability of solid-state ^{93}Nb NMR in catalysis," *Physical Chemistry Chemical Physics* **15** (2013) 5115-5131.
http://dx.doi.org/10.1039/c3cp44016h

J. Xu, V.V. Terskikh, and Y. Huang, "Resolving Multiple Non-Equivalent Metal Sites in Magnesium-Containing Metal-organic Frameworks by Natural Abundance ^{25}Mg Solid-State NMR," *Chemistry - A European Journal* **19** (2013) 4432–4436. **(Cover Article)**
http://dx.doi.org/10.1002/chem.201300113

L.A. O'Dell, I.L. Moudrakovski, "A Combined Ultra-wideline Solid-state NMR and DFT Study of ^{137}Ba Electric Field Gradient Tensors in Barium Compounds," *Chemical Physics Letters* **565** (2013) 56–60.
http://dx.doi.org/10.1016/j.cplett.2013.02.040

L.A. O'Dell and A. Brinkmann, "^{14}N overtone NMR spectra under magic angle spinning: Experiments and numerically exact simulations," *Journal of Chemical Physics* **138** (2013) 064201.
http://dx.doi.org/10.1063/1.4775592

Queen's University

Q. Luo, J. Cao, D. Tang, D. Wu, Y. Huang, J. Xiang, F. Wang, X. Liu, G. Wu, "Lipophilic thioguanosine: an anion receptor for cesium fluoride," *Journal of Fluorine Chemistry* **150** (2013) 67–71.
http://dx.doi.org/10.1016/j.jfluchem.2013.02.020

B. Pluvinage, S. Chitayat, E. Ficko-Blean, D.W. Abbott, J.M. Kunjachen, J. Grondin, H.L. Spencer, S.P. Smith, A.B. Boraston, "Conformational analysis of StrH, the surface-attached exo-β-D-N-acetylglucosaminidase from *Streptococcus pneumonia*," *Journal of Molecular Biology* **425** (2013) 334–349.
http://dx.doi.org/10.1016/j.jmb.2012.11.005

University of Toronto

K.M. Hart, A.L. Kulakova, C. Allen, A.J. Simpson, S.F. Oppenheimer, H. Masoom, D. Courtier-Murias, R. Soong, L.A. Kulakov, B.T. Murphy, and B.P. Kelleher, "Tracking the fate of microbially sequestered carbon dioxide in soil organic matter," *Environ. Sci. Technol.* (2013) online.
http://dx.doi.org/10.1021/es3050696

D. Courtier-Murias, A.J. Simpson, C. Marzadori, G. Baldoni, C. Ciavatta, J.M. Fernández, E.G. López-de-Sá, C.Plaza, "Unraveling the long-term stabilization mechanisms of organic materials in soils by physical fractionation and NMR spectroscopy," *Agriculture, Ecosystems & Environment* **171** (2013) 9-18.
http://dx.doi.org/10.1016/j.agee.2013.03.010

M.J. Smith, B.G. Neel, and M. Ikura, "NMR-based functional profiling of RASopathies and oncogenic RAS mutations," *Proc. Natl. Acad. Sci. USA* **110** (2013) 4574-4579.
http://dx.doi.org/10.1073/pnas.1218173110

R. Rosenzweig, S. Moradi, A. Zarrine-Afsar, J.R. Glover, L.E. Kay, "Unraveling the Mechanism of Protein Disaggregation Through a ClpB-DnaK Interaction," *Science* **339** (2013) 1080-1083.
http://dx.doi.org/10.1126/science.1233066

V. Tugarinov and L.E. Kay, "Estimating Side-Chain Order in [U-^{2}H; $^{13}CH_3$]-Labeled High Molecular Weight Proteins from Analysis of HMQC/HSQC Spectra," *J. Phys. Chem. B* **117** (2013) 3571–3577.
http://dx.doi.org/10.1021/jp401088c

G.M. Findlay, M.J. Smith, F. Lanner, M.S. Hsiung, G.D. Gish, E. Petsalaki, K. Cockburn, T. Kaneko, H. Huang, R.D. Bagshaw, T. Ketela, M. Tucholska, L. Taylor, D.D. Bowtell, J. Moffat, M. Ikura, S.S.C. Li, S.S. Sidhu, J. Rossant, T. Pawson, "Interaction Domains of Sos1/Grb2 Are Finely Tuned for Cooperative Control of Embryonic Stem Cell Fate," *Cell* **152** (2013) 1008–1020.
http://dx.doi.org/10.1016/j.cell.2013.01.056

P. Vallurupalli, L.E. Kay, "Probing Slow Chemical Exchange at Carbonyl Sites in Proteins by Chemical Exchange Saturation Transfer NMR Spectroscopy," *Angewandte Chemie International Edition* **52** (2013) 4156–4159.
http://dx.doi.org/10.1002/anie.201209118

A.L. Hansen, G. Bouvignies, L.E. Kay, "Probing slowly exchanging protein systems via ^{13}Cα-CEST: monitoring folding of the Im7 protein," *Journal of Biomolecular NMR* **55** (2013) 279-289.
http://dx.doi.org/10.1007/s10858-013-9711-4

F.J. Amador, P.B. Stathopulos, M. Enomoto, M. Ikura, "Ryanodine Receptor Calcium Release Channels: Lessons from structure-function studies," *FEBS Journal* (2013) online. **(Review)**
http://dx.doi.org/10.1111/febs.12194

M.T. Mazhab-Jafari, C.B. Marshall, P.B. Stathopulos, Y. Kobashigawa, V. Stambolic, L.E. Kay, F. Inagaki, and M. Ikura, "Membrane-dependent modulation of the mTOR activator Rheb: NMR observations of a GTPase tethered to a lipid-bilayer nanodisc," *J. Am. Chem. Soc.* **135** (2013) 3367–3370.
http://dx.doi.org/10.1021/ja312508w

U.H.N. Dürr, R. Soong, A. Ramamoorthy, "When detergent meets bilayer: birth and coming of age of lipid bicelles," *Progress in Nuclear Magnetic Resonance Spectroscopy* **69** (2013) 1-22. **(Invited Review)**
http://dx.doi.org/10.1016/j.pnmrs.2013.01.001

Brock University

D. Marquardt, J.A. Williams, N. Kucerka, J. Atkinson, S.R. Wassall, J. Katsaras, and T.A. Harroun, "Tocopherol activity correlates with its location in a membrane: A new perspective on the anti-oxidant Vitamin E," *J. Am. Chem. Soc.* (2013) online.
http://dx.doi.org/10.1021/ja312665r

D. Hurem, A.G. Moiseev, R. Simionescu, and T. Dudding, "A Detailed NMR and DFT Based Study of the Sakurai-Hosomi-Yamamoto Asymmetric Allylation Reaction," *J. Org. Chem.* **78** (2013) 4440-4445.
http://dx.doi.org/10.1021/jo400451u

M. Roux, E. Sternin, V. Bonnet, C. Fajolles, and F. Djedaini-Pilard, "Dynamic Lipid Lateral Segregation driven by Lauryl Cyclodextrin Interactions at the Membrane Surface," *Langmuir* **29** (2013) 3677–3687.
http://dx.doi.org/10.1021/la304524a

McMaster University

T.L. Spencer, L.A. O'Dell, I.L. Moudrakovski, and G.R. Goward, "Dynamics of Ag^+ Ions in $RbAg_4I_5$ Probed Indirectly Via ^{87}Rb Solid-State NMR," *Journal of Physical Chemistry C* **117** (2013) online.
http://dx.doi.org/10.1021/jp3125928

T.R. Field and A.D. Bain, "Dynamical theory of spin relaxation," *Phys. Rev. E* **87** (2013) 022110.
http://dx.doi.org/10.1103/PhysRevE.87.022110

T.L. Spencer, G.R. Goward, A.D. Bain, "Complete Description of the Interactions of a Quadrupolar Nucleus with a Radiofrequency Field. Implications for Data Fitting," *Solid State Nuclear Magnetic Resonance* (2013) accepted.
http://dx.doi.org/10.1016/j.ssnmr.2013.03.002

L.J.M. Davis, G.R. Goward, "Differentiating Lithium Ion Hopping Rates in Vanadium Phosphate versus Vanadium Fluorophosphate Structures Using 1D ^{6}Li Selective Inversion NMR," *J. Phys. Chem. C* **117** (2013) 7981–7992.
http://dx.doi.org/10.1021/jp310790g

A.D. Bain, "NMR quadrupole liouvillians for arbitrary spin: Exact symbolic expressions and perturbation solutions," *Concepts in Magnetic Resonance Part A* **42A** (2013) 45–58.
http://dx.doi.org/10.1002/cmr.a.21259

Z.-Q. Zhu, M.Q. Salih, E. Fynn, A.D. Bain, and C.M. Beaudry, "The Garuganin and Garugamblin Diarylether Heptanoids: Total Synthesis and Determination of Chiral Properties Using Dynamic NMR," *J. Org. Chem.* **78** (2013) 2881–2896.
http://dx.doi.org/10.1021/jo400157d

Redeemer University College

D.H. Brouwer, S. Cadars, J. Eckert, Z. Liu, O. Terasaki, B.F. Chmelka, "A general protocol for determining the structures of molecularly ordered but non-crystalline silicate frameworks," *J. Am. Chem. Soc.* **135** (2013) 5641–5655.
http://dx.doi.org/10.1021/ja311649m

D.H. Brouwer, "Structure solution of network materials by solid-state NMR without knowledge of the crystallographic space group," *Solid State Nuclear Magnetic Resonance* **51-52** (2013) 37-45.
http://dx.doi.org/10.1016/j.ssnmr.2013.01.003

University of Guelph

S. Emami, Y. Fan, R. Munro, V. Ladizhansky, L.S. Brown, "Yeast-expressed human membrane protein aquaporin-1 yields excellent resolution of solid-state MAS NMR spectra," *Journal of Biomolecular NMR* **55** (2013) 147-155.
http://dx.doi.org/10.1007/s10858-013-9710-5

University of Waterloo

B. Alipanahi, N. Krislock, A. Ghodsi, H. Wolkowicz, L. Donaldson, M. Li, "Determining protein structures from NOESY distance constraints by semidefinite programming," *Journal of Computational Biology* **20** (2013) 296-310.
http://dx.doi.org/10.1089/cmb.2012.0089

S. Sokolenko, R. McKay, E.J.M. Blondeel, M.J. Lewis, D. Chang, B. George, M.G. Aucoin, "Understanding the variability of compound quantification from targeted profiling metabolomics of 1D-^{1}H-NMR spectra in synthetic mixtures and urine with additional insights on choice of pulse sequences and robotic sampling," *Metabolomics* (2013) online.
http://dx.doi.org/10.1007/s11306-013-0503-3

University of Western Ontario

L. Zhang, D. Chen, H.-Y. Nie, Y. Huang, "A Study of the Formation of Microporous Material SAPO-37," *Microporous and Mesoporous Materials* **175** (2013) 147–156.
http://dx.doi.org/10.1016/j.micromeso.2013.03.026

J. Xu, V.V. Terskikh, and Y. Huang, "Resolving Multiple Non-Equivalent Metal Sites in Magnesium-Containing Metal-organic Frameworks by Natural Abundance ^{25}Mg Solid-State NMR," *Chemistry - A European Journal* **19** (2013) 4432–4436. **(Cover Article)**
http://dx.doi.org/10.1002/chem.201300113

University of Saskatchewan

M.S. Afifi, R.S. Farag, I.A. Shaaban, L.D. Wilson, W.M. Zoghaib, T.A. Mohamed, "Infrared and NMR spectra, tautomerism, vibrational assignment, normal coordinate analysis, and quantum mechanical calculations of 4-amino-5-pyrimidinecarbonitrile," *Spectrochimica Acta Part A: Molecular and Biomolecular Spectroscopy* (2013) accepted.
http://dx.doi.org/10.1016/j.saa.2013.04.004

University of Alberta

M.R. Richards, Y. Bai, T.L. Lowary , "Comparison between DFT- and NMR-based conformational analysis of methyl galactofuranosides," *Carbohydrate Research* (2013) accepted.
http://dx.doi.org/10.1016/j.carres.2013.03.030

S.E. Pineda-Sanabria, I.M. Robertson, M.X. Li, B.D. Sykes, "Interaction between the regulatory domain of cardiac troponin C and the acidosis-resistant cardiac troponin i A162H," *Cardiovascular Research* **97** (2013) 481-489.
http://dx.doi.org/10.1093/cvr/cvs348

I.M. Robertson, S.E. Pineda-Sanabria, B.D. Sykes, "Approaches to protein-ligand structure determination by NMR spectroscopy: Applications in drug binding to the cardiac regulatory protein troponin C," *Biophysics and Structure to Counter Threats and Challenges, NATO Science for Peace and Security Series B: Physics and Biophysics* (2013) Chapter 8, 121-134.
http://dx.doi.org/10.1007/978-94-007-4923-8_8

S. Sokolenko, R. McKay, E.J.M. Blondeel, M.J. Lewis, D. Chang, B. George, M.G. Aucoin, "Understanding the variability of compound quantification from targeted profiling metabolomics of 1D-^{1}H-NMR spectra in synthetic mixtures and urine with additional insights on choice of pulse sequences and robotic sampling," *Metabolomics* (2013) online.
http://dx.doi.org/10.1007/s11306-013-0503-3

University of Calgary

D. Bartusika, B. Tomanek, "Detection of ^{19}F-Labeled Biopharmaceuticals in Cell Cultures with Magnetic Resonance," *Advanced Drug Delivery Reviews* (2013) online. http://dx.doi.org/10.1016/j.addr.2013.04.010

E.F. Haney, A.P. Petersen, C.K. Lau, W. Jing, D.G. Storey, H.J. Vogel, "Mechanism of Action of Puroindoline Derived Tryptophan-rich Antimicrobial Peptides," *Biochimica et Biophysica Acta (BBA) - Biomembranes* **1828** (2013) 1802–1813. http://dx.doi.org/10.1016/j.bbamem.2013.03.023

B. Mickiewicz, H.J. Vogel, H.R. Wong and B.W. Winston, "Metabolomics as a Novel Approach for Early Diagnosis of Pediatric Septic Shock and its Mortality," *Am. J. Respir. Crit. Care Med.* **187** (2013) 967-976. http://dx.doi.org/10.1164/rccm.201209-1726OC

University of Lethbridge

F. Faghihi, N. Mohammadi, P. Hazendonk, "The effect of rigid polymeric particles addition on the local dynamic heterogeneity and the ultrasound attenuation of butyl acrylate-methyl methacrylate copolymers," *Polymer* **54** (2013) 3038-3046. http://dx.doi.org/10.1016/j.polymer.2013.03.037

E. Sosińska, R. Przybylski, P. Hazendonk, Y.Y. Zhao, J.M. Curtis, "Characterisation of non-polar dimers formed during thermo-oxidative degradation of β-sitosterol," *Food Chemistry* **139** (2013) 464-474. http://dx.doi.org/10.1016/j.foodchem.2013.01.053

University of British Columbia

M.L. Ludwiczek, I. D'Angelo, G.N. Yalloway, J.A. Brockerman, M. Okon, J.E. Nielsen, N.C. J. Strynadka, S.G. Withers, and L.P. McIntosh, "Strategies for Modulating the pH-Dependent Activity of a Family 11 Glycoside Hydrolase," *Biochemistry* **52** (2013) online. http://dx.doi.org/10.1021/bi400034m

Simon Fraser University

B. Prasad, D.J. Mah, A.R. Lewis, E. Plettner, "Water Oxidation by a Cytochrome P450: Mechanism and Function of the Reaction," *PLoS ONE* **8** (2013) e61897. http://dx.doi.org/10.1371/journal.pone.0061897

Contact us

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