



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

Canadian NMR Research News Bulletin #4.4 Fall 2010



Guest Editorial

**Henry J. Stronks,
Bruker Ltd.**

Dear colleagues, friends,
and valued (potential)
customers:

I'm grateful to the NMR
Bulletin for this
opportunity to write to

you on this happy occasion. As some of you may already know, Bruker is celebrating an important milestone this year, 50 years since the company was founded. Bruker was officially incorporated by **Prof. G. Laukien** on September 7, 1960 and his son, **Dr. Frank Laukien**, rang the opening bell for the NASDAQ stock exchange in New York on September 7, 2010 to celebrate this 50th year of innovation. The Bruker Corporation (NASDAQ: BRKR) has grown to over 4,300 employees worldwide with annual sales in excess of \$1.2 Billion. An excellent overview of the company, its early beginnings and even the answer to the question, "Why the name Bruker?" can be found at:

<http://www.bruker.com/50years.html>

This year also marks the 40th year of incorporation for Bruker Canada, which was incorporated in October, 1970. I would like to state from the outset that rumors of my employment at Bruker during this time period are grossly exaggerated! Of course many of you in Canada will remember **Martin Smith** who headed Bruker Canada for 26 years (since 1976) and was instrumental in establishing Bruker on a strong foundation in Canada. **Dr. Arthur J. Carty**, Director of the newly formed Guelph Waterloo Centre for Graduate Work in Chemistry (GWC²) convinced me to come to Guelph to do a Ph.D. in magnetic resonance. Arthur and Martin were old-time friends (and I am sure they talked!), and after several meetings and conferences, Martin had invited me to interview with Bruker well before my

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scheduled graduation date. I was very fortunate to begin working at Bruker in 1984, beginning in NMR/EPR applications, sales and eventually more managerial roles.

Our legal name in Canada is **Bruker Ltd.** and our business consists of over 30 employees working in various divisions. *Bruker BioSpin* is the magnetic resonance division, covering NMR, MRI and EPR systems. *Bruker Optics* is responsible for FTIR, FTRaman, FTNIR and minispec product lines and *Bruker AXS* handles the X-Ray product lines including XRD, XRF and Single Crystal spectrometers. The *Bruker Daltonics* division is responsible for the mass spectrometer product lines, including Ion Traps, MALDI TOF/TOF, QTOF and FT MS spectrometers. Our newest division is the *Chemical Analysis Division*, which represents the newly acquired product lines from Varian (Agilent) including GC, GC MS, QQQ and ICP/MS. These product lines operate as a subdivision of Bruker Daltonics and are a great compliment and addition to Daltonics series of

mass spectrometers. In Canada, four ex-Varian employees are now working for Bruker Ltd. and we have hired an additional four service people to handle this part of our business. The Bruker Ltd. facility in Milton will become one of the principal North American demo sites for ICP/MS and GC MS, and construction/renovation has already begun in one of our demo bays to create a "clean room" suitable for the stringent demands of extreme sensitivity of the ICP/MS spectrometer.

Additionally, the Bruker Corporation has recently purchased Veeco, a leading company in Atomic Force Microscopy (AFM). This acquisition puts Bruker in a very strong position in this business sector and shows great promise for growth and new technologies for our customer base.

Bruker has grown in so many new and exciting ways by organically expanding our core businesses and also through a series of mergers and acquisitions designed to further strengthen the company as a whole. The landscape of the analytical science marketplace and the life science business has changed dramatically over the past few years, but Bruker is well positioned to lead through its diversity and technical excellence in producing quality and innovative products for the marketplace.

Hardware, software, technology and applications in the end are not the complete solution for our customers. My goal has always been to foster an environment where we can build a community that utilizes common tools to solve scientific problems. We all have something to learn from one another, sharing and contributing ideas/solutions, whether we are interested in small molecules or large proteins, quadrupolar nuclei or spin $\frac{1}{2}$ nuclei, solids NMR or solution NMR. All these approaches are aimed to solving problems using magnetic resonance in fascinating ways and it is incumbent upon all of us to continue to create a positive, unified community to showcase the best we can be. The National Ultrahigh Field NMR Facility for Solids is a good example of the breadth of work that can be accomplished at ultrahigh magnetic fields. Collaborative projects and feedback from our customer base to develop new hardware to solve technically challenging problems also contributes to help all of us to produce the best possible results.

The smaller regional conferences such as **MOOT** and **VIVA** are good examples of not only sharing ideas across an enormous spectrum of research challenges, but also to teach our young researchers how to present and formulate a scientific opinion in a friendly atmosphere and constructive peer reviewed fashion. Organizing and showcasing NMR symposia within the larger context of the Canadian Society for Chemistry is another good example of gathering together to collectively share ideas (and who hasn't enjoyed the Bruker hospitality suite at this event?).

As we reminisce about the past and look into a very bright and exciting future, I would like to thank all of my colleagues at Bruker Ltd. for their continued support, hard work and dedication to serve our customer base. I would also like to thank the Canadian NMR community for your continued support of our products and services. I can assure you that the positive and unified spirit within all aspects of the Canadian NMR community is well recognized on the global stage and I trust that this co-operative venture will continue to develop in the years to come.

I wish everyone a healthy and Happy New Year.

With best regards,

Henry

Canadian NMR News

Outstanding High School Student Science Award winners get to experiment at UTSC

Last year we reported about an important outreach initiative by **André Simpson** and colleagues at the University of Toronto Scarborough aimed at attracting high school students to consider a career in science (*NMR Bulletin #4.1*). Building on the last year's success, the program continued this year with eight high school students receiving a monetary prize, a certificate and a tour of campus. The highlight of the award was an opportunity for students to use first-hand a modern NMR instrument for chemical analysis.

To read the full story and to see the photo gallery of the event

<http://webapps.utsc.utoronto.ca/ose/story.php?id=2323>

Submitted by Igor Moudrakovski (NRC-SIMS)

NMR equipment upgrades at NRC-SIMS

The NRC's Steacie Institute for Molecular Sciences in Ottawa has recently invested in the replacement and upgrading of their NMR instruments to support research in the Functional Materials Program. Among new acquisitions is a Bruker Avance III 500 MHz (11.7 T) NMR spectrometer for solids (pictured) located at the M-40 building on the Montreal Road campus.



This new spectrometer is equipped with a wide assortment of probes, including a 1.3 mm ultrahigh-speed MAS Bruker probe, several other MAS and static probes for low-gamma nuclei and for variable-temperature work.



The work-horse of the lab in the past 13 years, the wide-bore solid-state 400 MHz (9.4 T) instrument has been upgraded with a new Avance III console featuring microimaging and

high-power gradient capabilities for diffusion measurements. This instrument is heavily used in gas-hydrate and hydrogen storage research projects.

Other upgrades include a brand-new wide-bore Bruker Avance III 400 MHz instrument for liquid-state NMR research. This instrument is located at the 100 Sussex Drive building.

The physicist helps biologists understand nature

A research profile of **Vladimir Ladizhansky** (Guelph) is published in *The Portico*, the University of Guelph alumni magazine.

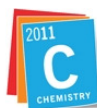
<http://www.uoguelph.ca/theportico/betterplanet/health/>

The Russell Varian Prize 2011: call for nominations

The Russell Varian prize honors the memory of the pioneer behind the first commercial Nuclear Magnetic Resonance spectrometers and co-founder of Varian Associates. The prize is awarded to a researcher based on a single innovative contribution (a single paper, patent, lecture, or piece of hardware) that has proven of high and broad impact on state-of-the-art NMR technology. The prize aims to award the initial contribution that laid the ground for the specific technology of great importance in state-of-the-art NMR. It is sponsored by Varian Inc. and carries a monetary award of 15,000 Euro. The award ceremony will take place at the **EUROMAR 2011** meeting in Frankfurt, Germany, August 21-25, 2011, with the prize winner delivering the Russell Varian lecture.

For more information:

http://nmr900.ca/nmr_news.html#varian



IYC 2011 International Year of Chemistry

International Year of
CHEMISTRY
2011

2011 is the International Year of Chemistry (**IYC**). IYC is a global celebration devoted to chemistry and its role in the well-being of

society. Through events at the local, provincial, national, and international levels, organizers hope to spark enthusiasm for this central science in all people of all ages.

The Chemical Institute of Canada is proud to be leading the Canadian initiative and all CIC members are encouraged to join in the

celebrations in 2011 by holding events of their own or participating in the many events planned throughout the year.

IYC will be promoted in Canada through activities and programs such as a Canadian stamp, the publication of Canadian chemistry milestones, Science Rendezvous, YouTube contest, Chemistry Olympiads, National Chemistry Week, partnerships with developing countries and global experiments. *We are hoping to reach over 500,000 Canadians in our outreach campaign.*

To learn about IYC and how to get involved visit the Canadian IYC website hosted by CIC at <http://www.iyc2011.ca>

Canadian IYC Organizing Committee

Bibliometrics as Weapons of Mass Citation (update)

At the request of several friends and colleagues, we have translated into English a few paragraphs of a paper that appeared a few months ago in *Chimia*. The new version in English can be found at:

<http://www.chimie.ens.fr/Resonance/Bunsen-Magazin-bibliometrics.pdf>

Geoffrey Bodenhausen

Original post

Dear colleagues and friends of the magnetic resonance community.

A recent paper that appeared in *Chimia*, accompanied by a post-face written by **Richard Ernst**, attracted much interest and generated some passionate responses. Since the journal is not widely accessible, I asked the Editor to provide pdf files that you can upload and forward if you wish. Our paper can be found at:

http://www.chimie.ens.fr/Resonance/bibliometrics_1.pdf

The post-face can be uploaded from

http://www.chimie.ens.fr/Resonance/bibliometrics_2.pdf

Sincerely,
Geoffrey Bodenhausen

http://www.chimie.ens.fr/Resonance/geoffrey_bodenhausen.html

NMR on YouTube

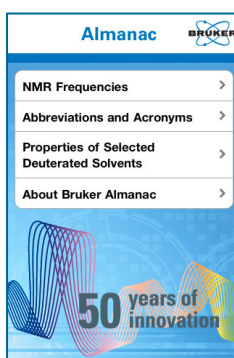
As a clear indication of the growing popularity of NMR spectroscopy it is steadily making its way into social media engines including *YouTube* and the likes. A simple search for "nmr" on *YouTube* in early November brought about nearly 2000 returns (not all of them relevant). One of the most notable is an excellent introductory MR course of eleven videos by **Paul Callaghan**.

Video 1:

<http://www.youtube.com/watch?v=7aRKAXD4dAg>

An interesting Canadian contribution is by **the Institute for Quantum Computing** (Waterloo) offering a basic explanation of quantum computing using nuclear magnetic resonance.

<http://www.youtube.com/watch?v=ppXcQIi5I20>



Bruker Almanac for iPhone/iPod touch

Published annually for over three decades, **Bruker Almanac** has been a tradition in Bruker's history, providing useful information to many scientists around the world. This almanac is now available as a free application for iPhone/iPod

touch/iPad that can be downloaded from the iTunes store. The current version of the Bruker Almanac App contains several handy tables of useful NMR information.

<http://itunes.apple.com/ca/app/almanac/id367770786>

To download the complete **Bruker Almanac 2010** as a PDF file with scientific tables and charts and Bruker product guide visit www.bruker.com/almanac

Another NMR-related App is from **Tim Burrow** (University of Toronto). His recently updated **Attenuator** utility calculates attenuation values:
<http://itunes.apple.com/ca/app/attenuator/id367216554>

NMR Theses Recently Defended

Congratulate your students here!

Qian Liu (Department of Biochemistry, McGill), June 2010
Supervisor: Kalle Gehring
Ph.D. thesis "Structural Insights into Apoptotic Regulation by BCL-2 Family"

Aaron Rossini (University of Windsor), September 2010
Supervisor: Robert Schurko
Ph.D. thesis: "Characterization of Inorganic Catalysts and Materials by Solid-State NMR"

Peter Pallister (Carleton University), September 2010
Supervisor: John Ripmeester
M.Sc. thesis: "Study of Local Environment and Nuclear Interactions in Magnesium and Sulfur Containing Materials by ^{25}Mg and ^{33}S Solid-State Nuclear Magnetic Resonance Spectroscopy and First-Principles Calculations"

Recognition

Myrna Simpson, Professor of environmental chemistry at the University of Toronto Scarborough, has received **the 2010 Environmental Sciences Award** jointly offered by the Society of Environmental Toxicology and Chemistry (SETAC) and the Royal Society of Chemistry. This award recognizes early to midcareer scientists who have accomplished and published outstanding contributions that have advanced the understanding or development of environmental systems, technologies, methodologies or other relevant research in the environmental sciences.

<http://webapps.utsc.utoronto.ca/ose/story.php?id=2377>

André Simpson, Professor of chemistry at the University of Toronto Scarborough, has been awarded **the Principal's Award for Faculty Research**.

André is also a recipient of **the 2010 Royal Society of Chemistry Joseph Black Award** "for his original research in the area of NMR spectrometry and especially its direct application to multiphase mixtures."

Read the research profile of André Simpson "Using groundbreaking technology to uncover the truth about soil"

<http://webapps.utsc.utoronto.ca/ose/story.php?id=2316>

Hiyam Hamaed (University of Windsor) has been awarded **the Governor General's Gold Medal** as the top graduate student in her cohort. Hiyam did her Ph.D. in solid-state NMR under the supervision of Robert Schurko. While working on her Ph.D. project "Solid-state NMR spectroscopy of unreceptive nuclei in inorganic and organic systems" Hiyam was a frequent user of the 900 NMR Facility in Ottawa.
Congratulations with the Gold Medal, Hiyam!

Read a feature story about Hiyam in the University of Windsor's *Daily News*
<http://tinyurl.com/38843jx>

On the move

Submitted by Irene Kwan (Queen's)

Dr. Alan Wong, a former graduate student of **Gang Wu**, visited Queen's University in Kingston on August 16, 2010. Alan presented a seminar to the Department of Chemistry entitled "*Unconventional approaches to high-resolution NMR spectroscopy and imaging*" to highlight his recent applications of slow-MAS technique to NMR spectroscopy and MRI. Alan is now with the French Atomic Energy Commission (C.E.A.), Saclay, France. At the end of his visit, the Wu group had a wonderful dinner at a local Greek restaurant.



left to right: Gang, David, Kathy, Irene, Mohammad, Parisa, Jen, Fabricia, and Alan. Picture taken by Jeff.

On the move (cont'd)

Submitted by Glenn Facey (Ottawa)

The NMR Facility at the University of Ottawa welcomes a new member, **Dr. Andy Lo**, formerly a post-doc in David Bryce's lab. Andy replaced **Cheryl McDowall** as the NMR Facility technician on August 23. Cheryl left her post as NMR technician in order to pursue full time graduate studies in September with Natalie Goto. The NMR Facility thanks Cheryl for her years of dedicated service and wishes her well in her studies.

Reposted from <http://www.chemistry.mcmaster.ca>

NMR Applications Specialist at McMaster

I am pleased to announce that **Dr. Dan Sørensen** has accepted the department's offer as the NMR Applications Specialist. Dr. Sørensen will take up the position previously occupied by **Dr. Don Hughes** prior to his untimely death. Dr. Sørensen will take up this position in early January 2011.

Those of you had the opportunity to attend Dr. Sørensen's seminar on September 17 will know what he has accomplished and will understand why I am extremely pleased to announce his acceptance of our offer.

Dr. Sørensen obtained his PhD in Denmark in 2002 and moved to Canada to take up a position at a now-defunct start-up company in Montreal that specialized in the isolation of bio-active natural products. In 2004 Dr. Sørensen moved to Merck-Frosst and oversaw the NMR lab then the combination of the NMR lab and mass spectrometry facility within the company. He is a first-class high resolution NMR spectroscopist. Chemists with this type of expertise are very hard to find and in big demand.

The imminent closure of the Merck-Frosst research labs provided us with the opportunity to hire Dr. Sørensen.

Brian McCarry, Chair
Chemistry & Chemical Biology
McMaster University

Upcoming NMR Events

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

2010 MRS Fall Meeting

November 29 - December 3, 2010, Boston, MA
Abstracts for technical symposia are available
http://www.mrs.org/s_mrs/sec.asp?CID=27791&DID=332879



Pacifichem 2010 The International Chemical Congress of Pacific Basin Societies

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

Frontiers of NMR in Biology Keystone Symposium

January 8-13, 2011, Big Sky, MT
<http://www.keystonesymposia.org/>



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

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



Biophysical Society 55th Annual Meeting

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

52nd ENC

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



19th ISMRM — Scientific Meeting and Exhibition of the International Society for Magnetic Resonance in Medicine

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



CSC 2011, the 94th Canadian Chemistry Conference and Exhibition

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

Magnetic Resonance Gordon Research Conference

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

EUROMAR 2011

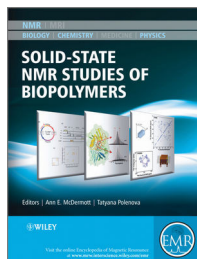
August 21-25, 2011, Frankfurt, Germany
<http://euromar2011.org/>

7th Alpine Conference on Solid-State NMR

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

New Books

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



Solid State NMR Studies of Biopolymers

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

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

Wiley: "The field of solid state NMR of biological samples has blossomed recently, requiring new practitioners in industry and academia to have fundamental understanding of this technology. Discussed are Solid State NMR methods for studying structure dynamics and ligand-binding in biopolymers as well as RF pulse sequences for various applications, including not only a systematic catalog but also a discussion of theoretical tools for analysis of pulse sequences. Including practical examples of biochemical applications, this dependable EMR handbook thoroughly examines a field sure to expand in the years ahead."

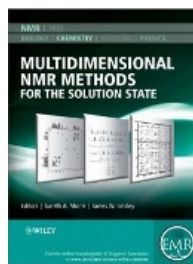
Canadian contributions

V. Ladizhansky, "Dipolar-Based Torsion Angle Measurements for Protein Structure Determination," Chapter 14, *Solid-State NMR Studies of Biopolymers (EMR Books)*, Eds. A.E.

McDermott and T. Polenova, Wiley (2010) pp. 273-284.
<http://dx.doi.org/10.1002/9780470034590.emrstm1153>

M. Auger, "Structural and Dynamics Studies of Lipids by Solid-State NMR", Chapter 27, *Solid-State NMR Studies of Biopolymers (EMR Books)*, Eds. A.E. McDermott and T. Polenova, Wiley (2010) pp. 463-472.
<http://dx.doi.org/10.1002/9780470034590.emrstm1100>

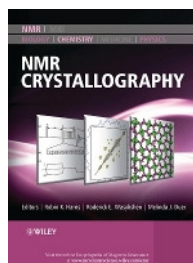
Table of Contents and **Google preview** are available at Wiley
<http://www.wiley-vch.de/publish/en/books/ISBN978-0-470-72122-3>



Multidimensional NMR Methods for the Solution State

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

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



NMR Crystallography

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

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

NMR Jobs and Vacancies

University of Toronto Scarborough

Postdoctoral Research Associate in multiphase NMR Spectroscopy

Environmental NMR Centre, Department of Chemistry, University of Toronto at Scarborough, Toronto, Ontario, Canada

Project Description: This is a unique opportunity to develop a novel area of NMR spectroscopy termed Comprehensive Multiphase NMR spectroscopy (CMP NMR). The position is for 1 year, and may be extended to 18 months depending on budget. The candidate will join a

team working on the development of CMP NMR.

CMP NMR is a new area of NMR spectroscopy that incorporates solid-state, semi-solids (HR-MAS) and solution-state NMR. The candidate will work with a range of unique hardware prototypes to study intact natural samples that have solid, gel and liquid components (samples may include plants, soils, sediments, tissue/bone etc.) thereby eliminating the need for drying or pre-treatment. This research aims to differentiate molecular structures in various natural phases and more importantly, to permit the study of the chemistry and transport between phases and across key interfaces by NMR spectroscopy for the first time. The successful candidate will have excellent opportunities to publish in a diverse range of disciplines.

The project will be carried out in close collaboration with Bruker BioSpin and will involve: 1) fundamental development of the technique and preliminary applications in a range of disciplines; and 2) development of applications in environmental chemistry. Environmental applications will focus on understanding the molecular processes behind soil/sediment contamination. The costs associated with the clean-up of contaminated sites in the European Union and the United States is on the order of 1.4 trillion euro. However, current remediation strategies target only the soluble fraction of soil leaving a considerable soil-bound component, that has been linked to a variety of illnesses. Remediation of this "sequestered" fraction is presently impossible as the chemical components of soil that strongly bind contaminants as-well as the molecular mechanisms that hold the contaminants to the soil are not known. CMP-NMR will provide a detailed insight at the molecular-level of the processes that cause contaminants to be entrapped in the soil matrix and describe the complete binding environment of the contaminant in unaltered natural samples. The results of this project will contribute directly to the development of novel soil remediation strategies.

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 interesting in to learn all areas of NMR spectroscopy. The candidate must be open minded and willing to work with very complex environmental samples. 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, micro-imaging, and hyphenated (2D-HPLC-SPE-NMR-MS(Q-q-TOF) NMR spectrometers.

The candidate should have an interest in environmental chemistry and/or willingness to learn key issues in this field.

Application

Candidates should send a complete C.V. including a publication list, a one page statement outlining their suitability and their interest in the position. Candidates should arrange to have 2-3 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
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
Canada

or e-mailed as a PDF attachment to

E-mail: andre.simpson@utoronto.ca

<http://www.utoronto.ca/~asimpson/>

We are looking to fill the position immediately and applications will be considered as they are received. We would like to fill the position and have the candidate start by Jan 1st 2011 at the absolute latest. Candidates that can start immediately will be given preference.

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

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

Advances in Biological NMR

Marta Oleszczuk and **Brian Sykes** (Alberta) attended the Joint EUROMAR 2010 - 17th ISMAR Conference in Florence, Italy in early July 2010. They summarized their observations on the current state of biological NMR in this perspective in the *Journal of Magnetic Resonance*.

M. Oleszczuk, B.D. Sykes, "Advances in Biological NMR circa WWMR 2010 in Florence," *Journal of Magnetic Resonance* **207** (2010) 1-7. <http://dx.doi.org/10.1016/j.jmr.2010.09.015>

NMR in vaccine research

Yves Aubin (Health Canada) and colleagues have published an article in *BioPharm International* describing NMR approaches in characterizing polysaccharide vaccines, including some advanced influenza, meningococcal and pneumococcal vaccines.

Y. Aubin, C. Jones, and D.I. Freedberg, "Using NMR Spectroscopy to Obtain the Higher Order Structure of Biopharmaceutical Products," *BioPharm International Supplements*, August 2010.

This article is available at <http://tinyurl.com/375uems>

Two NMR papers in PNAS

P.A. Chong, H. Lin, J.L. Wrana, and J.D. Forman-Kay, "Coupling of tandem Smad ubiquitination regulatory factor (Smurf) WW domains modulates target specificity," *Proc. Natl. Acad. Sci. USA* **107** (2010) 18404-18409. <http://dx.doi.org/10.1073/pnas.1003023107>

H. Ghasriani, T. Ducat, C.T. Hart, F. Hafizi, N. Chang, A. Al-Baldawi, S.H. Ayed, P. Lundström, J.A.R. Dillon, and N.K. Goto, "Appropriation of the MinD protein-interaction motif by the dimeric interface of the bacterial cell division regulator MinE," *Proc. Natl. Acad. Sci. USA* **107** (2010) 18416-18421. <http://dx.doi.org/10.1073/pnas.1007141107>

NMR paper in Science

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>

This research article by **Lewis Kay** (University of Toronto) and colleagues is also accompanied by the *Science Perspective*

H.M. Al-Hashimi, "Exciting Structures", *Science* **329** (2010) 1295-1296. <http://dx.doi.org/10.1126/science.1195571>

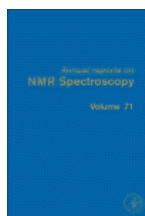
NMR paper in Nature

A.M. Ruschak, T.L. Religa, S. Breuer, S. Witt and L.E. Kay, "The proteasome antechamber maintains substrates in an unfolded state," *Nature* **467** (2010) 868-871. <http://dx.doi.org/10.1038/nature09444>

NMR paper in Nature Structural & Molecular Biology

E. Matta-Camacho, G. Kozlov, F.F. Li and K. Gehring, "Structural basis of substrate recognition and specificity in the N-end rule pathway," *Nature Structural & Molecular Biology* **17** (2010) 1182-1187. <http://dx.doi.org/10.1038/nsmb.1894>

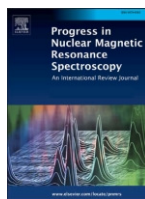
Annual Reports on NMR Spectroscopy



John A. Weil, "Magnetic Resonance of Systems with Equivalent Spin-1/2 Nuclides," *Annual Reports on NMR Spectroscopy* **71** (2010) 1-34.

<http://dx.doi.org/10.1016/B978-0-08-089054-8.00001-0>

Progress in NMR Spectroscopy



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* (2010) online. **(Invited Review)**

<http://dx.doi.org/10.1016/j.pnmrs.2010.09.001>

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.

Dalhousie University

X. Zhang, J.W. Zwanziger, "Design and Applications of an *in situ* Electrochemical NMR Cell," *Journal of Magnetic Resonance* (2010) online.
<http://dx.doi.org/10.1016/j.jmr.2010.10.013>

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

University of New Brunswick

J.C. García-Naranjo, I.V. Mastikhin, B.G. Colpitts and B.J. Balcom, "A unilateral magnet with an extended constant magnetic field gradient," *Journal of Magnetic Resonance* (2010) accepted.
<http://dx.doi.org/10.1016/j.jmr.2010.09.018>

O. Petrov and I. Furó, "A study of freezing-melting hysteresis of water in different porous materials. Part I: Porous silica glasses," *Microporous and Mesoporous Materials* (2010) accepted.
<http://dx.doi.org/10.1016/j.micromeso.2010.08.012>

H. Han, B.J. Balcom, "Magnetic resonance imaging inside metallic vessels," *Measurement Science & Technology* **21** (2010) 103001.
<http://dx.doi.org/10.1088/0957-0233/21/10/103001>

H. Han, D. Green, M. Ouellette, R. MacGregor, B.J. Balcom, "Non-Cartesian sampled centric scan SPRITE imaging with magnetic field gradient and $B_0(t)$ field measurements for MRI in the vicinity of metal structures," *Journal of Magnetic Resonance* **206** (2010) 97-104.
<http://dx.doi.org/10.1016/j.jmr.2010.06.012>

Université Laval

S. Morin, C.M. Clouthier, S. Gobeil, J.N. Pelletier and S.M. Gagné, "Backbone resonance assignments of an artificially engineered TEM-1/PSE-4 Class A β -lactamase chimera," *Biomolecular NMR Assignments* **4** (2010) 127-130.
<http://dx.doi.org/10.1007/s12104-010-9227-8>

M. Auger, "Structural and Dynamics Studies of Lipids by Solid-State NMR ", Chapter 27, *Solid-State NMR Studies of Biopolymers (EMR Books)*, Eds. A.E. McDermott and T. Polenova, Wiley (2010) pp. 463-472.
<http://dx.doi.org/10.1002/9780470034590.emrstm1100>

McGill University

G. Kozlov, S. Bastos-Aristizabal, P. Määttänen, A. Rosenauer, F. Zheng, A. Killikelly, J.-F. Trempe, D.Y. Thomas and K. Gehring, "Structural Basis of Cyclophilin B Binding by the Calnexin/Calreticulin P-domain," *Journal of Biological Chemistry* **285** (2010) 35551-35557. (*JBC's Paper of the Week*)
<http://dx.doi.org/10.1074/jbc.M110.160101>

E. Matta-Camacho, G. Kozlov, F.F. Li and K. Gehring, "Structural basis of substrate recognition and specificity in the N-end rule pathway," *Nature Structural & Molecular Biology* **17** (2010) 1182-1187.
<http://dx.doi.org/10.1038/nsmb.1894>

Université de Montréal

Z.-K. Cui, G. Bastiat, M. Lafleur, "Formation of Fluid Lamellar Phase and Large Unilamellar Vesicles with Octadecyl Methyl Sulfoxide/Cholesterol Mixtures," *Langmuir* **26** (2010) 12733-12739.
<http://dx.doi.org/10.1021/la100749k>

S. Morin, C.M. Clouthier, S. Gobeil, J.N. Pelletier and S.M. Gagné, "Backbone resonance assignments of an artificially engineered TEM-1/PSE-4 Class A β -lactamase chimera," *Biomolecular NMR Assignments* **4** (2010) 127-130.
<http://dx.doi.org/10.1007/s12104-010-9227-8>


NRC-SIMS

R. Flacau, C.I. Ratcliffe, S. Desgreniers, Y. Yao, D.D. Klug, P. Pallister, I.L. Moudrakovski and J.A. Ripmeester, "Structure and dynamics of ammonium borohydride," *ChemComm* (2010) online. (part of a themed web-based issue **Hydrogen**)
<http://dx.doi.org/10.1039/c0cc03297b>


J.-W. Lee, H. Lu, I.L. Moudrakovski, C.I. Ratcliffe, and J.A. Ripmeester, "Thermodynamic and Molecular-Scale Analysis of New Systems of Water-Soluble Hydrate Formers + CH₄," *J. Phys. Chem. B* **114** (2010) 13393–13398.
<http://dx.doi.org/10.1021/jp106466s>

R. Alizadeh, J.J. Beaudoin, L. Raki, V. Terskikh, "C–S–H/polyaniline nanocomposites prepared by in situ polymerization", *J Mater Sci* (2010) in press.
<http://dx.doi.org/10.1007/s10853-010-4918-1>

J.M. Taylor, R.K. Mah, I.L. Moudrakovski, C.I. Ratcliffe, R. Vaidhyanathan, and G.K.H. Shimizu, "Facile Proton Conduction via Ordered Water Molecules in a Phosphonate Metal-Organic Framework", *J. Am. Chem. Soc.* **132** (2010) 14055–14057.
<http://dx.doi.org/10.1021/ja107035w>

 **L.A. O'Dell and I. Moudrakovski,** "Testing the Sensitivity Limits of ³³S NMR: An Ultra-wideline Study of Elemental Sulfur," *Journal of Magnetic Resonance* (2010) online.
<http://dx.doi.org/10.1016/j.jmr.2010.08.022>

S. Alavi, T.K. Woo, A. Sirjoosingh, S. Lang, I. Moudrakovski, J.A. Ripmeester, "Hydrogen Adsorption and Diffusion in p-tert-Butylcalix[4]arene: An Experimental and Molecular Simulation Study", *Chemistry – A European Journal* **16** (2010) 11689–11696.
<http://dx.doi.org/10.1002/chem.201000589>

 **L.A. O'Dell and C.I. Ratcliffe,** "Ultra-wideline ¹⁴N NMR spectroscopy as a probe of molecular dynamics," *Chemical Communications* **46** (2010) 6774–6776.
<http://dx.doi.org/10.1039/c0cc01902j>


NRC-ICPET


N. Li, D.W. Shin, D.S. Hwang, Y.M. Lee, and M.D. Guiver, "Polymer Electrolyte Membranes Derived from New Sulfone Monomers with Pendent Sulfonic Acid Groups," *Macromolecules* (2010) ASAP.
<http://dx.doi.org/10.1021/ma102107a>

N. Du, G.P. Robertson, I. Pinnau, and M.D. Guiver, "Polymers of Intrinsic Microporosity with Dinaphthyl and Thianthrene Segments," *Macromolecules* **43** (2010) 8580–8587.
<http://dx.doi.org/10.1021/ma101930x>

University of Ottawa

H. Ghasriani, T. Ducat, C.T. Hart, F. Hafizi, N. Chang, A. Al-Baldawi, S.H. Ayed, P. Lundström, J.A.R. Dillon, and N.K. Goto, "Appropriation of the MinD protein-interaction motif by the dimeric interface of the bacterial cell division regulator MinE," *Proc. Natl. Acad. Sci. USA* **107** (2010) 18416–18421.
<http://dx.doi.org/10.1073/pnas.1007141107>

 **A.Y.H. Lo, T. Jurca, D.S. Richeson, and D.L. Bryce,** "Multinuclear Solid-State Magnetic Resonance Study of In⁺ and Ag⁺ in Neutral Weakly Coordinating Environments," *J. Phys. Chem. Lett.* **1** (2010) 3078–3084.
<http://dx.doi.org/10.1021/jz101241r>

 **C.M. Widdifield and D.L. Bryce,** "Solid-State ¹²⁷I NMR and GIPAW DFT Study of Metal Iodides and their Hydrates: Structure, Symmetry, and Higher-Order Quadrupole-Induced Effects," *Journal of Physical Chemistry A* **114** (2010) 10810–10823.
<http://dx.doi.org/10.1021/jp108237x>

S. Alavi, T.K. Woo, A. Sirjoosingh, S. Lang, I. Moudrakovski, J.A. Ripmeester, "Hydrogen Adsorption and Diffusion in p-tert-Butylcalix[4]arene: An Experimental and Molecular Simulation Study", *Chemistry – A European Journal* **16** (2010) 11689–11696.
<http://dx.doi.org/10.1002/chem.201000589>

Queen's University

F. Sauriol, J.F. Sonnenberg, S.J. Chadder, A.F. Dunlop-Briere, M.C. Baird, P.H.M. Budzelaar, "Remarkable Reactions and Intermediates in Titanocene(IV) Chemistry: Migratory Insertion Reactions of 2,2-Disubstituted-1-alkenes, Intramolecular 1,5-sigma Bond Metathesis via epsilon-Agostic Interactions, and a Rare Example of a beta-Agostic Alkyltitanocene Complex," *J. Am. Chem. Soc.* **132** (2010) 13357–13370.
<http://dx.doi.org/10.1021/ja104526v>



J. Zhu, J.Y.C. Lau, and G. Wu, "A Solid-State ^{17}O NMR Study of L-Tyrosine in Different Ionization States: Implications for Probing Tyrosine Side Chains in Proteins," *Journal of Physical Chemistry B* **114** (2010) 11681–11688.
<http://dx.doi.org/10.1021/jp1055123>



J. Zhu, E. Ye, V. Terskikh, and G. Wu, "Solid-State ^{17}O NMR Spectroscopy of Large Protein-Ligand Complexes," *Angewandte Chemie International Edition* **49** (2010) 8399–8402. **(Cover Article)**
<http://dx.doi.org/10.1002/anie.201002041>

University of Toronto

S. Ko, G.B. Kang, S.M. Song, J.-G. Lee, D.Y. Shin, J.-H. Yun, Y. Sheng, C. Cheong, Y.H. Jeon, Y.-K. Jung, C.H. Arrowsmith, G.V. Avvakumov, S. Dhe-Paganon, Y.J. Yoo, S.H. Eom, and W. Lee, "Structural Basis of E2-25K/UBB+1 Interaction Leading to Proteasome Inhibition and Neurotoxicity," *Journal of Biological Chemistry* **285** (2010) 36070–36080.
<http://dx.doi.org/10.1074/jbc.M110.145219>

J. Chan, H. Yamazaki, N. Ishiyama, M.-D. Seo, T.K. Mal, T. Michikawa, K. Mikoshiba, and M. Ikura, "Structural Studies of Inositol 1,4,5-Trisphosphate Receptor COUPLING LIGAND BINDING TO CHANNEL GATING," *Journal of Biological Chemistry* **285** (2010) 36092–36099.
<http://dx.doi.org/10.1074/jbc.M110.140160>

P.A. Chong, H. Lin, J.L. Wrana, and J.D. Forman-Kay, "Coupling of tandem Smad ubiquitination regulatory factor (Smurf) WW

domains modulates target specificity," *Proc. Natl. Acad. Sci. USA* **107** (2010) 18404–18409.
<http://dx.doi.org/10.1073/pnas.1003023107>

A.M. Ruschak, A. Velyvis, L.E. Kay, "A simple strategy for ^{13}C , ^1H labeling at the Ile-y2 methyl position in highly deuterated proteins," *Journal of Biomolecular NMR* **48** (2010) 129–135.
<http://dx.doi.org/10.1007/s10858-010-9449-1>

A.M. Ruschak, T.L. Religa, S. Breuer, S. Witt and L.E. Kay, "The proteasome antechamber maintains substrates in an unfolded state," *Nature* **467** (2010) 868–871.
<http://dx.doi.org/10.1038/nature09444>

J.-X. Lu, S. Sharpe, R. Ghirlando, W.-M. Yau, R. Tycko, "Oligomerization state and supramolecular structure of the HIV-1 Vpu protein transmembrane segment in phospholipid bilayers," *Protein Science* **19** (2010) 1877–1896.
<http://dx.doi.org/10.1002/pro.474>

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* (2010) in press. **(Invited Review)**
<http://dx.doi.org/10.1016/j.pnmrs.2010.09.001>

J.C. D'eon, A.J. Simpson, R. Kumar, A.J. Baer, S.A. Mabury, "Determining the molecular interactions of perfluorinated carboxylic acids with human sera and isolated human serum albumin using nuclear magnetic resonance spectroscopy," *Environmental Toxicology and Chemistry* **29** (2010) 1678–1688.
<http://dx.doi.org/10.1002/etc.204>

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>

N. Fatemi, D.M. Korzhnev, A. Velyvis, B. Sarkar and J.D. Forman-Kay, "NMR Characterization of Copper-binding Domains 4–6 of ATP7B," *Biochemistry* **49** (2010) 8468–8477.
<http://dx.doi.org/10.1021/bi1008535>

X. Feng, A.J. Simpson, E.G. Gregorich, B. Elberling, D.W. Hopkins, A.D. Sparrow, P.M. Novis, L.G. Greenfield, M.J. Simpson, "Chemical Characterization of Microbial-Dominated Soil Organic Matter in the Garwood Valley, Antarctica," *Geochimica et Cosmochimica Acta* **74** (2010) 6485-6498.
<http://dx.doi.org/10.1016/j.gca.2010.08.019>

R. Muhandiram and L.E. Kay "3D HMQC-NOESY, NOESY-HMQC, and NOESY-HSQC," Chapter 25, *Multidimensional NMR Methods for the Solution State (EMR Books)*, Eds. G.A. Morris and J.W. Emsley, Wiley (2010) pp. 335-350.
<http://dx.doi.org/10.1002/9780470034590.emrstm0563>

McMaster University

N. Vasdev, M.D. Moran, H.M. Tuononen, R. Chirakal, R.J. Suontamo, A.D. Bain and G.J. Schrobilgen, "NMR Spectroscopic Evidence for the Intermediacy of XeF_3^- in XeF_2/F^- Exchange, Attempted Syntheses and Thermochemistry of XeF_3^- Salts, and Theoretical Studies of the XeF_3^- Anion", *Inorganic Chemistry* **49** (2010) 8997-9004.
<http://dx.doi.org/10.1021/ic101275m>

A.D. Bain "COSY: Quantitative Analysis," Chapter 13, *Multidimensional NMR Methods for the Solution State (EMR Books)*, Eds. G.A. Morris and J.W. Emsley, Wiley (2010) pp. 167-176.
<http://dx.doi.org/10.1002/9780470034590.emrstm0095>

A.D. Bain, C.K. Anand, Z. Nie, "Exact Solution to the Bloch Equations and Application to the Hahn Echo", *Journal of Magnetic Resonance* **206** (2010) 227-240.
<http://dx.doi.org/10.1016/j.jmr.2010.07.012>

University of Guelph

S. Hughes and S.P. Graether, "Cryoprotective mechanism of a small intrinsically disordered dehydrin protein," *Protein Science* (2010) accepted.
<http://dx.doi.org/10.1002/pro.534>


S.N. Patel and S.P. Graether, "Increased flexibility decreases antifreeze protein activity," *Protein Science* (2010) accepted.
<http://dx.doi.org/10.1002/pro.516>

V. Ladizhansky, "Dipolar-Based Torsion Angle Measurements for Protein Structure Determination," Chapter 14, *Solid-State NMR Studies of Biopolymers (EMR Books)*, Eds. A.E. McDermott and T. Polenova, Wiley (2010) pp. 273-284.
<http://dx.doi.org/10.1002/9780470034590.emrstm1153>

M.A.M. Ahmed, V.V. Bamm, G. Harauz, V. Ladizhansky, "Solid-State NMR Spectroscopy of Membrane-Associated Myelin Basic Protein—Conformation and Dynamics of an Immunodominant Epitope," *Biophysical Journal* **99** (2010) 1247-1255.
<http://dx.doi.org/10.1016/j.bpj.2010.06.022>


University of Western Ontario

H.W. Nesbitt, G.M. Bancroft, G.S. Henderson, R. Ho, K.N. Dalby, Y. Huang, Z. Yan, "Bridging, non-bridging and free (O^{2-}) oxygen in $\text{Na}_2\text{O-SiO}_2$ glasses: An X-ray Photoelectron Spectroscopic (XPS) and Nuclear Magnetic Resonance (NMR) study," *Journal of Non-Crystalline Solids* (2010) online.
<http://dx.doi.org/10.1016/j.jnoncrysol.2010.09.031>

 **Z. Yan, C.W. Kirby, and Y. Huang,** "Characterization of the gel phases formed in the synthesis of microporous gallophosphate, cloverite," *Journal of Materials Chemistry* **20** (2010) 10200-10210.
<http://dx.doi.org/10.1039/c0jm02670k>

University of Windsor

A.W. MacGregor, L.A. O'Dell, R.W. Schurko, "New Methods for the Acquisition of Ultra-Wideline Solid-State NMR Spectra of Spin-1/2 Nuclides," *Journal of Magnetic Resonance* (2010) accepted.
<http://dx.doi.org/10.1016/j.jmr.2010.10.011>

 **A.J. Rossini, I. Hung and R.W. Schurko,** "Solid-State $^{47/49}\text{Ti}$ NMR of Titanocene Chlorides," *J. Phys. Chem. Lett.* **1** (2010) 2989-2998.
<http://dx.doi.org/10.1021/jz1012017>

A.J. Rossini, H. Hamaed, R.W. Schurko, "The Application of Frequency Swept Pulses for the Acquisition of Nuclear Quadrupole Resonance Spectra," *Journal of Magnetic Resonance* **206** (2010) 32-40.
<http://dx.doi.org/10.1016/j.jmr.2010.05.018>

University of Manitoba



V.K. Michaelis and S. Kroeker, ⁷³Ge Solid-State NMR of Germanium Oxide

Materials: Experimental and Theoretical Studies," *Journal of Physical Chemistry C* (2010) ASAP.

<http://dx.doi.org/10.1021/jp1071082>

C. Martineau, V.K. Michaelis, S. Schuller, S. Kroeker, "Liquid-liquid phase separation in model nuclear waste glasses: A solid-state double-resonance NMR study," *Chemistry of Materials* **22** (2010) 4896–4903.

<http://dx.doi.org/10.1021/cm1006058>

S. Kroeker, C.S. Higman, V.K. Michaelis, N.B. Svenda, S. Schuller, "Precipitation of Mixed-Alkali Molybdates During HLW Vitrification", in *Scientific Basis for Nuclear Waste Management XXXIV*, edited by K.L. Smith, S. Kroeker, B. Uberuaga, K.R. Whittle (*Mater. Res. Soc. Symp. Proc. Volume 1265*, Warrendale, PA, 2010), 1265-AA03-03.

<http://dx.doi.org/10.1557/PROC-1265-AA03-03>

NRC-IBD

O.B. Ijare, T. Bezabeh, N. Albiin, I.C.P. Smith, "Magnetic resonance spectroscopy of bile in the detection of cholangiocarcinoma," *Journal of Hepatology*, (2010) in press.

<http://dx.doi.org/10.1016/j.jhep.2010.08.039>

S. Varma, M.N.A. Eskin, R. Bird, B. Dolenko, J. Raju, O.B. Ijare, T. Bezabeh, "Potential of Magnetic Resonance Spectroscopy in Assessing the Effect of Fatty Acids on Inflammatory Bowel Disease in an Animal Model," *Lipids* **45** (2010) 843–854.

<http://dx.doi.org/10.1007/s11745-010-3455-7>

University of Alberta

S. Szeto, S. Reinke, B.D. Sykes, and B.D. Lemire, "Mutations in the *Saccharomyces cerevisiae* Succinate Dehydrogenase Result in Distinct Metabolic Phenotypes Revealed Through ¹H-NMR-Based Metabolic Footprinting," *J. Proteome Res.* (2010) accepted.

<http://dx.doi.org/10.1021/pr100880y>

M. Oleszczuk, B.D. Sykes, "Advances in Biological NMR circa WWMR 2010 in Florence," *Journal of Magnetic Resonance* **207** (2010) 1-7.
<http://dx.doi.org/10.1016/j.jmr.2010.09.015>

S.N. Reinke, X. Hu, B.D. Sykes, B.D. Lemire, "Caenorhabditis elegans diet significantly affects metabolic profile, mitochondrial DNA levels, lifespan and brood size," *Molecular Genetics and Metabolism* **100** (2010) 274-282.

<http://dx.doi.org/10.1016/j.ymgme.2010.03.013>

T.T. Nakashima and R.E.D. McClung "Heteronuclear Shift Correlation Spectroscopy," Chapter 22, *Multidimensional NMR Methods for the Solution State (EMR Books)*, Eds. G.A. Morris and J.W. Emsley, Wiley (2010) pp. 289-304.

<http://dx.doi.org/10.1002/9780470034590.emrstm0209>

University of Calgary

R. Schicho, A. Nazyrova, R. Shaykhutdinov, G. Duggan, H.J. Vogel and M. Storr, "Quantitative metabolomic profiling of serum and urine in DSS-induced ulcerative colitis of mice by ¹H NMR spectroscopy," *J. Proteome Res.* (2010) accepted.

<http://dx.doi.org/10.1021/pr100547y>

E.S. Kadantsev and T. Ziegler, "First-principles calculation of parameters of electron paramagnetic resonance spectroscopy in solids", *Magnetic Resonance in Chemistry* (2010) online. (**Invited Article, Special Issue**)

<http://dx.doi.org/10.1002/mrc.2655>

J.M. Taylor, R.K. Mah, I.L. Moudrakovski, C.I. Ratcliffe, R. Vaidhyanathan, and G.K.H. Shimizu, "Facile Proton Conduction via Ordered Water Molecules in a Phosphonate Metal-Organic Framework", *J. Am. Chem. Soc.* **132** (2010) 14055-14057.

<http://dx.doi.org/10.1021/ja107035w>

D.I. Chan, B.C.H. Chu, C.K.Y. Lau, H.N. Hunter, D.M. Byers, H.J. Vogel, "NMR solution structure and biophysical characterization of vibrio harveyi acyl carrier protein A75H effects of divalent metal ions," *Journal of Biological Chemistry* **285** (2010) 30558-30566.

<http://dx.doi.org/10.1074/jbc.M110.128298>



Q. Li and V. Thangadurai, "A comparative 2 and 4-probe DC and 2-probe AC electrical conductivity of novel co-doped $Ce_{(0.9-x)}RE_xMo_{0.1}O_{(2.1-0.5x)}$ (RE=Y, Sm, Gd; $x = 0.2, 0.3$)," *Journal of Materials Chemistry* **20** (2010) 7970-7983.
<http://dx.doi.org/10.1039/c0jm01324b>

M.L. Workentine, J.J. Harrison, A.M. Weljie, V.A. Tran, P.U. Stenroos, V. Tremaroli, H.J. Vogel, H. Ceri, R.J. Turner, "Phenotypic and metabolic profiling of colony morphology variants evolved from *Pseudomonas fluorescens* biofilms," *Environmental Microbiology* **12** (2010) 1565-1577.
<http://dx.doi.org/10.1111/j.1462-2920.2010.02185.x>

University of British Columbia

C.A. Michal, "Defeating Radiation Damping and Magnetic Field Inhomogeneity with Spatially Encoded Noise," *Chem.Phys.Chem.* (2010) online.
<http://dx.doi.org/10.1002/cphc.201000527>

H.G. Yoon, S.W. Kang, R.Y. Dong, A. Marini, K.A. Suresh, M. Srinivasarao, S. Kumar, "Nematic biaxiality in a bent-core material," *Physical Reivew E* **81** (2010) 051706.
<http://dx.doi.org/10.1103/PhysRevE.81.051706>

J.T.J. Cheng, J.D. Hale, J. Kindrachuk, H. Jessen, M. Elliott, R.E.W. Hancock, S.K. Straus, "Importance of Residue 13 and the C-Terminus for the Structure and Activity of the Antimicrobial Peptide Aurein 2.2," *Biophysical Journal* **99** (2010) 2926-2935.
<http://dx.doi.org/10.1016/j.bpj.2010.08.077>

M. Wieczorek, H. Jessen, J. Kindrachuk, W.R.P. Scott, M. Elliott, K. Hilpert, J.T.J. Cheng, R.E.W. Hancock and S.K. Straus, "Structural Studies of a Peptide with Immune Modulating and Direct Antimicrobial Activity," *Chemistry & Biology* **17** (2010) 970-980.
<http://dx.doi.org/10.1016/j.chembiol.2010.07.007>

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