



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

Canadian NMR Research News Bulletin #5.4 Fall 2011



Guest Editorial

Kalle Gehring
McGill University

*Harnessing the Power of
Molecular Machines*

Thanks to the NSERC Collaborative Research and Training Experience (**CREATE**) program, an exciting new training opportunity exists for undergraduate and graduate students in the developing field of bionanomachines.

Bionanomachines are submicron scale molecular devices that perform a wide variety of useful tasks. Composed of organic molecules such as sugars, proteins, or nucleic acids, they offer unparalleled advantages in their extremely small size, low production cost, and ease of modification. Bionanomachines already play significant roles in everyday lives, ranging from protein-digesting enzymes in laundry detergents, to improved natural fibers and inexpensive drugs. Biosynthetic medicines, such as insulin, and biomachine-based diagnostic tools are used in healthcare and medicine. In the future, bionanomachines offer the promise of new medical treatments for heart disease and cancer, tools for understanding key biological processes such as cell division or nerve function, and smart materials that respond to external stimuli.

The purpose of this new CREATE Training Program in Bionanomachines (**CTPB**) is to train students in the principles, design and applications of bionanomachines. The program

In This Issue

- 1** Guest Editorial
- 2** Canadian NMR News
- 5** Recognition
- 5** NMR Theses Recently Defended
- 5** On the move
- 6** Upcoming NMR Events
- 6** New MR Books
- 7** NMR Jobs and Vacancies
- 8** Canadian NMR Research Highlights
- 13** Recent NMR Publications
- 19** Contact us

aims to develop creative, versatile and highly skilled experts who can maintain Canada's position as a leader in bionanotechnology. These researchers will also be empowered to drive technological advances and will be capable of building off of their training to pursue careers in a broad variety of domains. The CTPB group consists of researchers at the University of Calgary, University of Saskatchewan, McGill University, Concordia University, Université de Montréal, Université Laval and Université du Québec à Montréal, who focus on different aspects of bionanomachines. Individual areas of expertise are NMR spectroscopy, X-ray crystallography, supramolecular chemistry, biophysics and biomembranes.

A more specific example of work done on bionanomachines is by **Dr. Normand Voyer**, whose group produces artificial ion channels to understand mechanisms of transport and to potentially aid with transport-related diseases such as cystic fibrosis. **Dr. René Roy's** group uses carbohydrates to study antibody-antigen



recognition as it pertains to the treatment of various diseases. In McGill University's Department of Chemistry, the group of **Dr. Hanadi Sleiman** constructs a variety of structures using DNA, which can be used to form nanotubes, or cargo-delivering molecular "cages". At the University of Calgary, **Dr. Peter Tieleman**'s laboratory uses computer simulations to study and model the interaction of lipids with proteins, permitting predictions about drug bioavailability. With his team, **Dr. Kalle Gehring**, the director of the CTPB, studies the structure of proteins and nucleic acids, focusing particularly on understanding the regulation of their interaction. At Concordia University's Department of Chemistry and Biochemistry, **Dr. Christopher Wilds** produces intentionally mutated DNA, in order to study how such mutations can be repaired, and also to gain a better understanding of the diseases these mutants mimic. Combining molecular biology with practical applications is the work of Université Laval's **Dr. Michèle Auger**'s group, which strives to understand and reproduce the biological process of the production of silk webbing by spiders. These are just some of the projects done by members of the CTPB, and there are many other options to choose from.

The CTPB offers two levels of funding: undergraduate and graduate. For undergraduates, 16-week summer research awards of \$5,625 are available at any of the 22 participating laboratories. Graduate CTPB stipends, worth \$20,000 per year for two years, fund graduate studies at the Master's or Doctoral level with a three-month exchange period to promote interdisciplinary training in the rapidly evolving field of bionanomachines. International students are eligible for all CTPB awards.

CTPB graduate applications are due by January 16th, 2012 and undergraduate applications are due by February 15th, 2012. Forms and further details about the programs can be found on the CTPB website at <http://bionano.ca/en> or <http://bionano.ca/fr>

For questions, please contact **Chris von Roretz**, the CTPB Coordinator, at bionano.med@mcgill.ca

Canadian NMR News

Outstanding High School Student Science Awards

Continuing the tradition started three years ago by **André Simpson** and colleagues, the University of Toronto Scarborough has awarded *the UTSC's Outstanding High School Student Science Awards* to six area high school students who wrote the winning essays in science. As part of the visit to the university, the students attended a physics lecture and were able to use equipment in the Nuclear Magnetic Resonance Lab to analyze soft drinks.

This year award was supported by the UTSC department of physical and environmental sciences, Bruker Canada and Pall Life Sciences.

To read the full story:

http://webapps.utsc.utoronto.ca/ose/ose_new_v/article.php?id=3082&cid=1

CFI LOF 2011 Competition Results

Mitsuhiko Ikura (University of Toronto) has been awarded \$795,562 to support the Structural Biology Facility for New Generation Cancer Research

See Dr. Mitsu Ikura speak about his research <http://www.youtube.com/watch?v=i7MNwdSZTxY>

Dmitri Goussev (Wilfrid Laurier University, Waterloo) has received a \$196,533 equipment grant for a new high-resolution nuclear magnetic resonance (NMR) spectrometer for the Chemistry Department.

Read the press release by WLU:

<http://tinyurl.com/cjxaw3>

Trinity Western University (Langley, B.C.) has been awarded a \$398,251 equipment grant for a 400 MHz NMR spectrometer and a mass spectrometer for an Advanced Analytical Laboratory in the recently expanded Neufeld Science Centre.

Read the news story in *Langley Today*:

<http://langleytoday.ca/?p=14522>

Canadian Cancer Society 2011 Research Grants

Cheryl Arrowsmith (Ontario Cancer Institute/PMH) *Structure and function of p53 related proteins* \$430,158 over three years

Julie Forman-Kay (Hospital for Sick Children) *Understanding how multi-site phosphorylation regulates cell cycle* \$397,440 over three years

Lawrence McIntosh (University of British Columbia) *Regulation of ETS transcription factors* \$431,712 over three years

Read the announcement and the complete list of awardees:

<http://tinyurl.com/7c44w9s>

Valerie Booth (Memorial University of Newfoundland) has had her **Tier 2 Canada Research Chair** in Membrane Proteins renewed for five years. Valerie has been also awarded complementary CFI funding under the Leaders Opportunity Fund.

Canada Research Chairs in MR

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

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

A Life in NMR: Interview with Regina Schuck (Agilent)

Regina Schuck is vice president and general manager of Agilent's Research Products Division in the Life Sciences Group. Regina has more than 25 years of experience in NMR and

research MRI. She holds a doctorate in natural sciences from the University of Frankfurt in Germany. Regina speaks with <http://www.spectroscopyNOW.com> about her career in magnetic resonance and her vision and future of MR: <http://tinyurl.com/73g7ljn>

Agilent 101: An Introduction to NMR – a crash course on NMR by Regina Schuck (Agilent) (also available in PDF) http://www.agilent.com/labs/features/2011_101_nmr.html

Submitted by Paul Morris

News from Morris Instruments Inc.

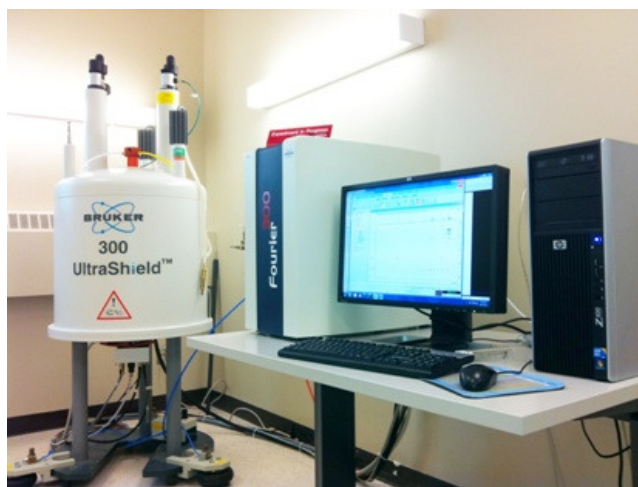
Morris Instruments Inc., based in Ottawa, has brought out a new addition to their line of R.F. Sweeper instruments for probe and coil tuning. The model MX has the same functionality and physical form factor as the lower frequency models, but extends **the tuning range up to 1010 MHz**. The company expects this new model to become increasingly popular as NMR magnets are pushed to ever higher fields.

For more information visit:

<http://morrisinstruments.com/>

Or email:

morris-instruments@rogers.com



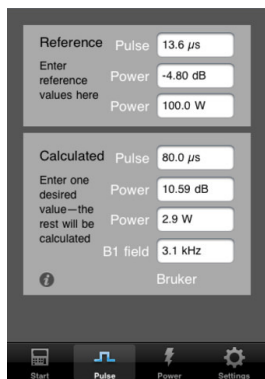
First in Canada: **Bruker Fourier 300** high-resolution compact NMR spectrometer installed in the undergraduate teaching lab, the Department of Chemistry, University of Ottawa (Photo: Glenn Facey) <http://www.science.uottawa.ca/nmr/>

The Russell Varian Prize 2012: 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 reward the initial contribution that laid the ground for the specific technology of great importance in state-of-the-art NMR. It is sponsored by Agilent Technologies and carries a monetary award of 15,000 Euro. The award ceremony will take place at the XXVth ICMRBS in Lyon, August 19-24, 2012, with the winner delivering the Russell Varian Lecture.

For more information:

http://nmr900.ca/nmr_news.html#rvp2012



Attenuator app

Version 1.5 of the popular **Attenuator** app by **Tim Burrow** (University of Toronto) is available for download from iTunes for iPhone, iPod touch and iPad.

Attenuator is a utility for anyone working with radio frequency sources and

needs to know power and voltage after attenuation. You can specify an input voltage (V_{pp} or V_{rms}) and dB of attenuation to get the output voltage, power and attenuation. The impedance can be specified, typically 50 Ohm for most systems. **Added in Version 1.5** for NMR spectroscopists is an option to calculate pulses based on power, in Watts or dB for Agilent and Bruker NMR instruments. This free application is available in English, French, Chinese and Japanese and is sponsored by *Open Technologies*.

To download the **Attenuator** app visit:

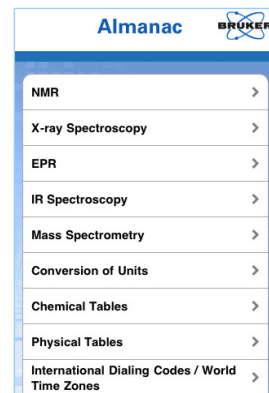
<http://itunes.apple.com/ca/app/attenuator/id367216554>

Tim Burrow

<http://www.chem.utoronto.ca/facilities/nmr/staff.html>

Bruker Almanac app

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. Recently updated **Version 2.0** contains almost all tables of the printed edition including various NMR related data, molecular spectroscopy, x-ray diffraction and mass spectrometry related useful information.

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

You are also invited to visit "**the Resonance**" a new user-oriented website by the Bruker Biospin team to find the latest hardware and software developments, events, tips and tricks, and more <http://www.theresonance.com/>



NMR on Twitter

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

<http://twitter.com/solidstateNMR>

uOttawa NMR by Glenn Facey

<http://twitter.com/uOttawaNMR>

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

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

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

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

Recognition



Brian Sykes, a Distinguished University Professor in the Department of Biochemistry, University of Alberta, has won **the 2010 University of Alberta Cup**. The University Cup is among the highest honors that the University

of Alberta confers on its faculty members. It is awarded in recognition of faculty members who have clearly excelled in both teaching and research. Prof. Sykes was presented with the University Cup at the 2011 **Celebrate!** ceremony, the university's annual celebration of teaching, learning and research, held on September 16, 2011.

Read the news story

<http://tinyurl.com/bwgb8xz>

Photo credit: University of Alberta

Kristopher Ooms (King's University College, Edmonton) won **the 2011 Canadian Society for Chemistry Faculty Advisor Award**. This award is based on a nomination submitted by the Student Chapter recognizing the exceptional performance of their faculty advisor.

Aaron Rossini, a graduate student of Robert Schurko, Windsor, was awarded **the Governor General's Gold Medal** for the highest academic standing at the graduate level among his cohort. *Congratulations, Aaron!*

UWindsor Daily News

<http://tinyurl.com/7bh9ntx>

Bruce Balcom (UNB) is named the Editor of ***New Developments in NMR***, an upcoming in 2012 series of reference books by the Royal Society of Chemistry (RSC) "... that will focus on novel aspects of method and instrumentation development, applications in emerging fields, new techniques and various technologies, fundamentals and theory, the development of new interfaces and important advances being made in many areas of NMR. Special emphasis will be placed on providing comprehensive introductions to the relevant theory to facilitate wider usage of NMR techniques by the chemical community."

<http://www.rsc.org/shop/books/series/91.asp?seriesid=91>

NMR Theses Recently Defended

Zhenghua Nie (McMaster University), August 2011

Supervisors: Profs. Christopher K. Anand and Alex D. Bain

Ph.D. thesis: "Simulation and Optimal Design of Nuclear Magnetic Resonance Experiments"

<http://digitalcommons.mcmaster.ca/opensdissertations/5543/>

External Examiner: Prof. Elliott Burnell (UBC)

Myriam Laneville (Université Laval), October 2011

Supervisor: Prof. Michèle Auger

M.Sc. thesis: "Étude de la structure et des interactions membranaires de différents peptides amyloïdes"

On the move

Alan Wong (a former graduate student of Prof. Gang Wu, Queen's) has recently accepted the 1st-class Charge de Recherche (CR1) position with Centre National de la Recherche Scientifique (CNRS). He will hold the position at CEA-Saclay in France. His current research interests focus on methodology developments: Micro-volume Metabonomic NMR Spectroscopy, Magic-Angle Sample Spinning Magnetic Resonance Imaging and Detection with B1-gradient.

<http://sites.google.com/site/alanwongnmr/home>

Christopher Barr is the new NMR Facility manager in the Department of Chemistry, University of Victoria. At UVic Chris is replacing **Christine Greenwood**, a long-time NMR Facility manager who has recently retired.

To contact Chris Barr:

<http://www.chemistry.uvic.ca/people/staff.php>

Devon Fyson has joined the Bryce lab (uOttawa) as an honours project student.

Mustafa Zeybek has joined the Bryce lab as an Undergraduate Research Opportunity Program (UROP) student.

Upcoming NMR Events

NMR Winter School at CEA Saclay:
Experiment and modelling in Structural NMR

November 28 - December 2, 2011, INSTN -
CEA Saclay, France
<http://www-instn.cea.fr/-2011-Events-.html#NMR>

**High-Throughput Structural Biology (J5) &
Structural Biology of Cellular Processes:
From Atoms to Cells (J6),** Keystone
Symposium

January 22-27, 2012, Keystone, Colorado
<http://www.keystonesymposia.org/>

Biophysical Society 56th Annual Meeting

February 25-29, 2012, San Diego, California
<http://www.biophysics.org/2012meeting>

53rd ENC

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

20th ISMRM Scientific Meeting and Exhibition
of the International Society for Magnetic
Resonance in Medicine

May 5-11, 2012, Melbourne, Australia
<http://www.ismrm.org>

CSC 2012, the 95th Canadian Chemistry
Conference and Exhibition

May 26-30, 2012, Calgary, Alberta, Canada
<http://www.csc2012.ca/>

EUROMAR 2012

July 1-5, 2012, Dublin, Ireland
<http://euromar2012.org>

**54th Rocky Mountain Conference on
Analytical Chemistry**

July 15-19, 2012, Copper Mountain, Colorado
<http://www.rockychem.com/>

ICMRBS 2012 the XXVth International
Conference on Magnetic Resonance in
Biological Systems

August 19-24, 2012, Lyon, France
<http://www.pasteur.fr/infosci/conf/sb/ICMRBS/>

SMASH 2012 Small Molecule NMR Conference
September 9-12, 2012, Providence, Rhode
Island, USA
<http://www.smashnmr.org/>

New MR Books

**NMR Spectroscopy of Polymers:
Innovative Strategies for Complex
Macromolecules**

ACS Symposium Series,
Volume 1077

Editors: **H.N. Cheng, T.
Asakura, A.D. English**
Publisher: ACS, October 2011
Language: English
ISBN: 978-0841226678



<http://dx.doi.org/10.1021/bk-2011-1077>

This ACS *Symposium Series* book includes papers presented at the Symposium "NMR Spectroscopy of Polymers - Innovative NMR Strategies for Complex Macromolecular Systems" which was part of **Pacificchem 2010**, the 2010 International Chemical Congress of Pacific Basin Societies in Honolulu, Hawaii, December 15-20, 2010. Among over 30 contributions on the state-of-the-art NMR spectroscopy in polymers and related systems there are two chapters by Canadian NMR research groups.

P.M. Macdonald, "Diffusion NMR of Polymers in Bicelles," Chapter 14, *NMR Spectroscopy of Polymers: Innovative Strategies for Complex Macromolecules*, Eds. H.N. Cheng, T. Asakura, A.D. English, ACS (2011) pp. 221-250.
<http://dx.doi.org/10.1021/bk-2011-1077.ch014>

H. Thérien-Aubin, Y.J. Wang, and X.X. Zhu, "NMR Imaging and Its Application in the Study of Pharmaceutical Tablets," Chapter 27, *NMR Spectroscopy of Polymers: Innovative Strategies for Complex Macromolecules*, Eds. H.N. Cheng, T. Asakura, A.D. English, ACS (2011) pp. 441-457.
<http://dx.doi.org/10.1021/bk-2011-1077.ch027>

NMR Jobs and Vacancies

Postdoctoral Fellow - Structural Biology of the Ubiquitination Cycle

University of Alberta, Department of Biochemistry

Dr. Leo Spyropoulos invites applications for a Postdoctoral Fellowship in structural biology of the ubiquitination cycle, with a focus on protein NMR spectroscopy. This is a one-year position, with the possibility of extension. Salary will be commensurate with qualifications and experience.

The Department of Biochemistry offers an intensive, collaborative environment for research in structural biology, housing state-of-the-art research facilities, which include high field 600 and 800 MHz NMR spectrometers.

The successful applicant will be employed primarily to study the structure, dynamics, interactions, and kinetics of proteins and enzymes of the ubiquitination cycle, with an emphasis on determining the molecular basis underlying the recognition of polyubiquitin chains as well as the enzymatic catalysis of ubiquitin chain elongation. Experience with general biochemistry, protein expression and purification, protein NMR spectroscopy, protein structure determination, molecular dynamics simulations, enzyme kinetics, and familiarity with computer programming and software (UNIX, Linux, Mathematica) is an asset. Responsibilities of the postdoctoral fellow include coordinating and completing research projects, training and mentoring graduate students, participating in research discussions, and working closely and cooperatively with other members of the Department involved in structural biology. The postdoctoral fellow will be expected to participate fully in research, publication, and dissemination activities.

Qualified candidates will have a recent Ph.D. in protein NMR spectroscopy or a closely related field. Applications will be accepted from candidates who will complete their doctoral degree within one year. Information about this position can be obtained by contacting **Dr. Leo Spyropoulos**

leo.spyropoulos@ualberta.ca

Applicants should send a letter of application, a curriculum vitae, and an example of published

research to Dr. Leo Spyropoulos by e-mail, or by regular mail:

Dr. Leo Spyropoulos
Department of Biochemistry
Room 416, Medical Sciences Bldg.,
University of Alberta
Edmonton, Alberta, T6G 2H7
Canada

The University of Alberta welcomes diversity and encourages applications from all qualified women and men, including persons with disabilities, members of visible minorities, and Aboriginal persons.

Additional Information:

Department of Biochemistry:
<http://www.biochem.ualberta.ca>

Postdoctoral Fellows Office:
<http://www.postdoc.ualberta.ca>

the Spyropoulos lab:
<http://www.bionmr.ualberta.ca/~lspy/index.html>

Postdoctoral Opening: Solid-State NMR Investigation of Battery Materials Brown University, Providence, RI

A joint postdoctoral position is available at Brown University between the Department of Chemistry and the School of Engineering. The research project supported by the US Department of Energy is to investigate battery materials using solid-state NMR techniques including ^{129}Xe NMR. The successful candidate will benefit from strong collaborations between Chemistry and Engineering. Interested applicants should have a Ph.D. in Chemistry, Physics, Engineering, or a related discipline with an emphasis on solid-state NMR spectroscopy. Previous NMR experiences and expertise in one or more of the following areas are highly desirable: solid-state NMR spectroscopy, NMR instrumentation, electrochemistry, battery, ^{129}Xe NMR, materials synthesis and characterization.

Inquiries and applications should be directed by email to **Dr. Li-Qiong Wang**

li_qiong_wang@brown.edu

Applications should include a CV, brief description of research interests, and contact information for references.

Brown University situated on the College Hill in the historically and culturally rich city of Providence is a leading Ivy League institute

with distinctive undergraduate and graduate academic programs.

Brown University is an equal opportunity employer with a strong commitment to seeking diversity in its workforce.

Additional Information:

Brown University
<http://www.brown.edu/>

Department of Chemistry
<http://chemistry.brown.edu/>

School of Engineering
<http://www.brown.edu/academics/engineering/>

Dr. Li-Qiong Wang
<http://www.chem.brown.edu/people/facultypage.php?id=1263922649>

Metropolitan Museum of Art/University of Delaware

Postdoctoral position

The Metropolitan Museum of Art and the Department of Chemistry and Biochemistry of the University of Delaware have an immediate opening for a postdoctoral fellow to participate in a collaborative project funded by the Cultural Heritage Science Program of the National Science Foundation. The project involves making and characterizing model compounds and systems related to the stability of oil paintings, primarily using solid-state ^{13}C and ^{207}Pb NMR spectroscopy, as well as other techniques, to identify reactions of lead-containing pigments with the polymer matrix.

http://nmr900.ca/nmr_jobs.html#udmma

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

MetaboHunter

D. Tulpan, S. Léger, L. Belliveau, A. Culf, M. Cuperlovic-Culf, "MetaboHunter: an automatic approach for identification of metabolites from ^1H -NMR spectra of complex mixtures," *BMC Bioinformatics* **12** (2011) 400. (**open access**)
<http://dx.doi.org/10.1186/1471-2105-12-400>

Background One-dimensional ^1H -NMR spectroscopy is widely used for high-throughput characterization of metabolites in complex biological mixtures. However, the accurate identification of individual compounds is still a challenging task, particularly in spectral regions with higher peak densities. The need for automatic tools to facilitate and further improve the accuracy of such tasks, while using increasingly larger reference spectral libraries becomes a priority of current metabolomics research.

Results We introduce a web server application, called MetaboHunter, which can be used for automatic assignment of ^1H -NMR spectra of metabolites. MetaboHunter provides methods for automatic metabolite identification based on spectra or peak lists with three different search methods and with possibility for peak drift in a user defined spectral range. The assignment is performed using as reference libraries manually curated data from two major publicly available databases of NMR metabolite standard measurements (HMDB and MMCD). Tests using a variety of synthetic and experimental spectra of single and multi metabolite mixtures show that MetaboHunter is able to identify, in average, more than 80% of detectable metabolites from spectra of synthetic mixtures and more than 50% from spectra corresponding to experimental mixtures. This work also suggests that better scoring functions improve by more than 30% the performance of MetaboHunter's metabolite identification methods.

Conclusions MetaboHunter is a freely accessible, easy to use and user friendly ^1H -NMR-based web server application that provides efficient data input and pre-processing, flexible parameter settings, fast and automatic metabolite fingerprinting and results visualization via intuitive plotting and compound peak hit maps. Compared to other published and freely accessible metabolomics tools, MetaboHunter implements three efficient methods to search for metabolites in manually curated data from two reference libraries.

<http://www.nrcbioinformatics.ca/metabohunter/>

"Anarchy in the proteome" - interview with Julie Forman-Kay

Julie Forman-Kay (Hospital for Sick Children) speaks about her research in disordered proteins in a podcast interview to *the Chemistry World*. Available for download at *Chemistry World Podcast*, August 2011, "6.05-13.00 Julie Forman-Kay reveals that disordered, unfolded proteins are much more functional and much more common than previously thought".

<http://www.rsc.org/chemistryworld/podcast/2011/CWpodcastAug11.asp>

Part of this interview is also featured in the printed August 2011 issue of the *Chemistry World* (subscription required): **M. Gross** "Anarchy in the proteome", *Chemistry World*, August 2011, Volume 8, No 8, p.42-45.

<http://www.rsc.org/chemistryworld/issues/2011/August/index.asp>



Encyclopedia of Magnetic Resonance: new entries

G. Wu "Oxygen 17 NMR Studies of Organic and Biological Molecules", *Encyclopedia of Magnetic Resonance* (2011).

<http://dx.doi.org/10.1002/9780470034590.emrstm1212>

D.I. Hoult "Magnetic Resonance with Conducting and High-Dielectric Samples", *Encyclopedia of Magnetic Resonance* (2011).

<http://dx.doi.org/10.1002/9780470034590.emrstm1182>

Paper in *Angewandte Chemie*

E. MacDonald, L. Doyle, N. Burford, U. Werner-Zwanziger, and A. Decken, "Stannylphosphonium Cations," *Angewandte Chemie International Edition* (2011) online.

<http://dx.doi.org/10.1002/anie.201105370>



R.T. McKay, "How the 1D-NOESY suppresses solvent signal in metabonomics NMR spectroscopy: An examination of the pulse sequence components and evolution," *Concepts in Magnetic Resonance Part A* **38A** (2011) 197–220.

<http://dx.doi.org/10.1002/cmra.20223>

Progress in NMR Spectroscopy



J.L. Kitevski-LeBlanca and R.S. Prosser, "Current Applications of ^{19}F NMR to Studies of Protein Structure and Dynamics," *Progress in Nuclear Magnetic Resonance Spectroscopy* (2011) online. **(Invited Review)**

<http://dx.doi.org/10.1016/j.pnmrs.2011.06.003>

G. Wu and J. Zhu "NMR studies of alkali metal ions in organic and biological solids," *Progress in Nuclear Magnetic Resonance Spectroscopy* (2011) online. **(Invited Review)**

<http://dx.doi.org/10.1016/j.pnmrs.2011.06.002>

L.A. O'Dell "Direct Detection of Nitrogen-14 in Solid-State NMR Spectroscopy," *Progress in Nuclear Magnetic Resonance Spectroscopy* **59** (2011) 295-318. **(Invited Review)**

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

A.D. Bain and B. Berno, "Liouvillians in NMR: the Direct Method Revisited," *Progress in Nuclear Magnetic Resonance Spectroscopy* **59** (2011) 223-244. **(Invited Review)**

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

NMR papers in *Nature*

J.R. Bothe, E.N. Nikolova, C.D. Eichhorn, J. Chugh, A.L. Hansen and H.M. Al-Hashimi, "Characterizing RNA dynamics at atomic resolution using solution-state NMR spectroscopy," *Nature Methods* **8** (2011) 919–931. **(Review)**

<http://dx.doi.org/10.1038/nmeth.1735>

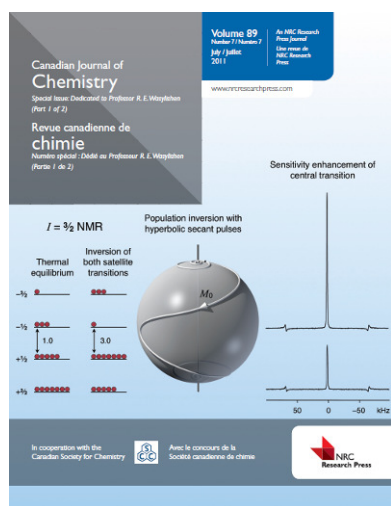
G. Bouvignies, P. Vallurupalli, D.F. Hansen, B.E. Correia, O. Lange, A. Bah, R.M. Vernon, F.W. Dahlquist, D. Baker & L.E. Kay, "Solution structure of a minor and transiently formed state of a T4 lysozyme mutant," *Nature* **477** (2011) 111–114.

<http://dx.doi.org/10.1038/nature10349>

T. Wu, H. Mayaffre, S. Krämer, M. Horvatic, C. Berthier, W.N. Hardy, R. Liang, D.A. Bonn and M.-H. Julien, "Magnetic-field-induced charge-stripe order in the high-temperature superconductor $\text{YBa}_2\text{Cu}_3\text{O}_y$," *Nature* **477** (2011) 191–194.

<http://dx.doi.org/10.1038/nature10345>

Special Issue Dedicated to Professor R.E. Wasylishen



Canadian Journal of Chemistry, Volume 89, Number 7 (2011) (part 1 of 2)
<http://www.nrcresearchpress.com/toc/cjc/89/7>

Tribute: Professor Roderick E. Wasylishen
Un hommage à Roderick E. Wasylishen
David Bryce, Gang Wu, Yining Huang, *Canadian Journal of Chemistry*, 2011, 89:xi-xvi,
<http://dx.doi.org/10.1139/v11-067>

Improvements in MR imaging of solids through gradient waveform optimization
Marco L.H. Gruwel, Peter Latta, Boguslaw Tomanek
Canadian Journal of Chemistry, 2011, 89:729-736, <http://dx.doi.org/10.1139/v11-022>

Measurement and calculation of ^{13}C chemical shift tensors in α -glucose and α -glucose monohydrate
Darren H. Brouwer, Kevin P. Langendoen, Quentin Ferrant
Canadian Journal of Chemistry, 2011, 89:737-744, <http://dx.doi.org/10.1139/v11-017>

Zero-mode TEM parallel-plate resonator for high-resolution thin film magnetic resonance imaging
Ziheng Zhang, Andrew E. Marble, Rodney P. MacGregor, Jonathan Martin, Haijiang Wang, Bruce J. Balcom
Canadian Journal of Chemistry, 2011, 89:745-753, <http://dx.doi.org/10.1139/v11-018>

A multinuclear solid-state magnetic resonance and GIPAW DFT study of anhydrous calcium chloride and its hydrates
Cory M. Widdifield, David L. Bryce
Canadian Journal of Chemistry, 2011, 89:754-763, <http://dx.doi.org/10.1139/v11-009>

Exact calculation of the response of a quadrupolar nucleus to radio frequency irradiation
T. Leigh Spencer, Gillian R. Goward, Alex D. Bain
Canadian Journal of Chemistry, 2011, 89:764-769, <http://dx.doi.org/10.1139/v11-024>

NMR crystallography – Three polymorphs of phenobarbital
Anuji Abraham, David C. Apperley, Thomas Gelbrich, Robin K. Harris, Ulrich J. Griesser
Canadian Journal of Chemistry, 2011, 89:770-778, <http://dx.doi.org/10.1139/v11-011>

Quadrupolar central transition (QCT) and ^{13}C NMR competition studies of metal ion binding to ovotransferrin
Jillian A. Saponja, Hans J. Vogel
Canadian Journal of Chemistry, 2011, 89:779-788, <http://dx.doi.org/10.1139/v11-019>

A ZORA-DFT and NLMO study of the one-bond fluorine–X indirect nuclear spin-spin coupling tensors for various VSEPR geometries
Frédéric A. Perras, David L. Bryce
Canadian Journal of Chemistry, 2011, 89:789-802, <http://dx.doi.org/10.1139/v10-172>

A natural abundance solid-state ^{25}Mg NMR study of layered magnesium phosphates
Jianfeng Zhu, Yining Huang
Canadian Journal of Chemistry, 2011, 89:803-813, <http://dx.doi.org/10.1139/v10-171>

[Pt@Pb₁₂]²⁻ – A challenging system for relativistic density functional theory calculations of ^{195}Pt and ^{207}Pb NMR parameters
Boris Le Guennic, Jochen Autschbach
Canadian Journal of Chemistry, 2011, 89:814-821, <http://dx.doi.org/10.1139/v11-054>

A solid-state $^{35/37}\text{Cl}$ NMR study of a chloride ion receptor and a GIPAW-DFT study of chlorine NMR interaction tensors in organic hydrochlorides
Rebecca P. Chapman, Jennifer R. Hiscock, Philip A. Gale, David L. Bryce
Canadian Journal of Chemistry, 2011, 89:822-834, <http://dx.doi.org/10.1139/v10-177>

Nuclear magnetic resonance and mass spectrometry studies of 2',3',5'-O-triacetylguanosine self-assembly in the presence of alkaline earth metal ions (Ca²⁺, Sr²⁺, Ba²⁺)

Irene C.M. Kwan, Yi-Min She, Gang Wu
Canadian Journal of Chemistry, 2011, 89:835-844, <http://dx.doi.org/10.1139/v10-179>

Deposition of gold nanoparticles on organo-kaolinite – Application in electrocatalysis for carbon monoxide oxidation

Sadok Letaief, Wendy Pell, Christian Detellier
Canadian Journal of Chemistry, 2011, 89:845-853, <http://dx.doi.org/10.1139/v11-028>

Investigation of the disorder of dibromo- and dichloromethane in their tri-*ortho*-thymotide clathrates using X-ray diffraction and solid-state ²H NMR spectroscopy

Glenn A. Facey, Ilia Korobkov
Canadian Journal of Chemistry, 2011, 89:854-862, <http://dx.doi.org/10.1139/v10-178>

Solid-state ²⁰⁷Pb nuclear magnetic resonance studies of adducts of 1,10-phenanthroline with lead(II) halides

Alicia Glatfelter, Shi Bai, Olga Dmitrenko, Dale L. Perry, Scott E. Van Bramer, Cecil Dybowski
Canadian Journal of Chemistry, 2011, 89:863-869, <http://dx.doi.org/10.1139/v10-176>

Phosphorus-31 and vanadium-51 solid-state nuclear magnetic resonance spectroscopy of β-vanadyl phosphate – Effects of homo- and heteronuclear spin-spin, electrostatic, and paramagnetic interactions

Klaus Eichele, Arnd-Rüdiger Grimmer
Canadian Journal of Chemistry, 2011, 89:870-884, <http://dx.doi.org/10.1139/v11-025>

Phase transformation of calcium phosphates in the presence of glutamic acid

Tim W.T. Tsai, Wei-Ya Chen, Yao-Hung Tseng, Jerry C.C. Chan
Canadian Journal of Chemistry, 2011, 89:885-891, <http://dx.doi.org/10.1139/v11-032>

Estimating internuclear distances between half-integer quadrupolar nuclei by central-transition double-quantum sideband NMR spectroscopy

Andreas Brinkmann, Mattias Edén
Canadian Journal of Chemistry, 2011, 89:892-899, <http://dx.doi.org/10.1139/v11-020>

Separation of nematic and smectic-A potential effects on solute ordering in a series of binary 6OCB–8OCB mixtures

E. Elliott Burnell, Ronald Y. Dong, Adrian C.J. Weber, Xuan Yang, Anand Yethiraj
Canadian Journal of Chemistry, 2011, 89:900-908, <http://dx.doi.org/10.1139/v11-027>

Resonance assignments and secondary structure analysis of dynein light chain 8 by magic-angle spinning NMR spectroscopy

Shangjin Sun, Andrew H. Butterworth, Sivakumar Paramasivam, Si Yan, Christine M. Lightcap, John C. Williams, Tatyana Polenova
Canadian Journal of Chemistry, 2011, 89:909-918, <http://dx.doi.org/10.1139/v11-030>

Multinuclear solid-state NMR of square-planar platinum complexes – Cisplatin and related systems

Bryan E.G. Lucier, Alex R. Reidel, Robert W. Schurko
Canadian Journal of Chemistry, 2011, 89:919-937, <http://dx.doi.org/10.1139/v11-033>

Canadian Journal of Chemistry, Volume 89, Number 9 (2011) (part 2 of 2)
<http://www.nrcresearchpress.com/toc/cjc/89/9>

Diffusion NMR and bicelle morphology

Peter M. Macdonald, Ronald Soong
Canadian Journal of Chemistry, 2011, 89:1021-1035, <http://dx.doi.org/10.1139/v11-038>

A multinuclear NMR and quantum chemical study of solid trimethylammonium chloride

Glenn H. Penner, Renee Webber, Luke A. O'Dell
Canadian Journal of Chemistry, 2011, 89:1036-1046, <http://dx.doi.org/10.1139/v11-034>

Solid-state nuclear magnetic resonance (NMR) spectroscopy reveals distinctive protein dynamics in closely related spider silks

Isabelle Cloutier, Jérémie Leclerc, Thierry Lefèvre, Michèle Auger
Canadian Journal of Chemistry, 2011, 89:1047-1054, <http://dx.doi.org/10.1139/v11-036>

Water molecular reorientation in ice and tetrahydrofuran clathrate hydrate from lineshape analysis of ¹⁷O spin-echo NMR spectra

Yong Ba, John A. Ripmeester, Christopher I. Ratcliffe
Canadian Journal of Chemistry, 2011, 89:1055-1064, <http://dx.doi.org/10.1139/v11-040>

The refocused discrimination induced by variable amplitude minipulses (DIVAM) experiment – Improved domain selection in semicrystalline fluoropolymers by ^{19}F solid state NMR spectroscopy

Tony Montana, Paul Hazendonk, Philip Wormald, Dinu Iuga

Canadian Journal of Chemistry, 2011, 89:1065-1075, <http://dx.doi.org/10.1139/v11-043>

High-field multinuclear solid-state nuclear magnetic resonance (NMR) and first principle calculations in MgSO_4 polymorphs

Peter J. Pallister, Igor L. Moudrakovski, John A. Ripmeester

Canadian Journal of Chemistry, 2011, 89:1076-1086, <http://dx.doi.org/10.1139/v11-044>

Obtaining accurate chemical shifts for all magnetic nuclei (^1H , ^{13}C , ^{17}O , and ^{27}Al) in tris(2,4-pentanedionato- O,O') aluminium (III) – A solid-state NMR case study

Alan Wong, Mark E. Smith, Victor Terskikh, Gang Wu

Canadian Journal of Chemistry, 2011, 89:1087-1094, <http://dx.doi.org/10.1139/v11-046>

^2H double- and zero-quantum filtered NMR spectroscopy for probing the environments of water in Nafion

Jesse R. Vanderveen, Mark A. Blackburn, Kristopher J. Ooms

Canadian Journal of Chemistry, 2011, 89:1095-1104, <http://dx.doi.org/10.1139/v11-045>

Structural analysis of lanthanum-containing battery materials using ^{139}La solid-state NMR

Leigh Spencer, Eric Coomes, Eric Ye, Victor Terskikh, Adam Ramzy, Venkataraman Thangadurai, Gillian R. Goward

Canadian Journal of Chemistry, 2011, 89:1105-1117, <http://dx.doi.org/10.1139/v11-049>

Reconnaissance of diverse structural and electronic environments in germanium halides by solid-state ^{73}Ge NMR and quantum chemical calculations

Brandon J. Greer, Vladimir K. Michaelis, Victor V. Terskikh, Scott Kroeker

Canadian Journal of Chemistry, 2011, 89:1118-1129, <http://dx.doi.org/10.1139/v11-052>

Sensitivity enhancement in MAS NMR of half-integer quadrupolar nuclei using sideband selective double-frequency sweeps

M. Goswami, P.J.M. van Bentum, A.P.M. Kentgens

Canadian Journal of Chemistry, 2011, 89:1130-1137, <http://dx.doi.org/10.1139/v11-053>

A ^1H NMR study of the fatty acid distribution in developing flax bolls before and after a cooking treatment

Christopher W. Kirby, Jason L. McCallum, Bourlaye Fofana

Canadian Journal of Chemistry, 2011, 89:1138-1142, <http://dx.doi.org/10.1139/v11-057>

^{129}Xe and ^2H nuclear magnetic resonance (NMR) of xenon and deuterated-chloroform solutes in a thermotropic biaxial nematic liquid crystal

P. Tallavaara, A.M. Kantola, J. Jokisaari, T. Meyer, D.A. Wilson, G.H. Mehl

Canadian Journal of Chemistry, 2011, 89:1143-1149, <http://dx.doi.org/10.1139/v11-062>

An improved scheme for the calculation of NMR chemical shifts in periodic systems based on gauge including atomic orbitals and density functional theory

Dmitry Skachkov, Mykhaylo Krykunov, Tom Ziegler

Canadian Journal of Chemistry, 2011, 89:1150-1161, <http://dx.doi.org/10.1139/v11-050>



Participants of the ICASS 2009 NMR symposium in honour of Rod Wasylshen (August 2009, Kingston, ON). Photo credit: Irene Kwan

Recent NMR Publications

most recent NMR publications by Canadian research groups as they appear on <http://www.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

E.E. Burnell, R.Y. Dong, A.C.J. Weber, X. Yang, A. Yethiraj, "Separation of nematic and smectic-A potential effects on solute ordering in a series of binary 6OCB–8OCB mixtures," *Canadian Journal of Chemistry* **89** (2011) 900-908. **(Special Issue)**
<http://dx.doi.org/10.1139/v11-027>

Dalhousie University

E. MacDonald, L. Doyle, N. Burford, U. Werner-Zwanziger, and A. Decken, "Stannylphosphonium Cations," *Angewandte Chemie International Edition* (2011) online.
<http://dx.doi.org/10.1002/anie.201105370>



J.L. MacDonald, U. Werner-Zwanziger, B. Chen, J.W. Zwanziger, D. Forgeron, "A ^{43}Ca and ^{13}C NMR Study of the Chemical Interaction Between Poly(ethylene-vinylacetate) and White Cement During Hydration," *Solid State Nuclear Magnetic Resonance* **40** (2011) 78-83.
<http://dx.doi.org/10.1016/j.ssnmr.2011.07.001>

NRC-IMB, Halifax

K.H. Soanes, J.C. Achenbach, I.W. Burton, J.P.M. Hui, S.L. Penny, and T.K. Karakach, "Molecular characterization of zebrafish embryogenesis via DNA microarrays and multi-platform time course metabolomics studies," *J. Proteome Res.* **10** (2011) 5102–5117.
<http://dx.doi.org/10.1021/pr2005549>

Agriculture and Agri-Food Canada, Charlottetown

C.W. Kirby, J.L. McCallum, B. Fofana, "A ^1H NMR study of the fatty acid distribution in developing flax bolls before and after a cooking treatment," *Canadian Journal of Chemistry* **89** (2011) 1138-1142. **(Special Issue)**
<http://dx.doi.org/10.1139/v11-057>

University of New Brunswick

I.V. Mastikhin, A. Arbabi, B. Newling, A. Hamza, A. Adair, "Magnetic resonance imaging of velocity fields, the void fraction and gas dynamics in a cavitating liquid," *Experiments in Fluids* (2011) in press.
<http://dx.doi.org/10.1007/s00348-011-1209-9>

O. Petrov and I. Furó, "A study of freezing-melting hysteresis of water in different porous materials. Part II: Surfactant-templated silicas," *Physical Chemistry Chemical Physics* **13** (2011) 16358-16365.
<http://dx.doi.org/10.1039/c1cp21902b>

H. Han, M. Ouellette, B. MacMillan, F. Goora, R. MacGregor, D. Green, B.J. Balcom, "High pressure magnetic resonance imaging with metallic vessels," *Journal of Magnetic Resonance* **213** (2011) 90-97.
<http://dx.doi.org/10.1016/j.jmr.2011.09.001>

H. Han and B.J. Balcom, "Magnetic resonance imaging inside cylindrical metal containers with an eddy current self-compensated method," *Meas. Sci. Technol.* **22** (2011) 115501.
<http://dx.doi.org/10.1088/0957-0233/22/11/115501>

O.V. Petrov, B.J. Balcom, "Two-dimensional T_2 distribution mapping in porous solids with phase encode MRI," *Journal of Magnetic Resonance* **212** (2011) 102-108.
<http://dx.doi.org/10.1016/j.jmr.2011.06.018>

F. Marica, S.A.B. Jofré, K.U. Mayer, B.J. Balcom, T.A. Al, "Determination of Spatially-Resolved Porosity, Tracer Distributions and Diffusion Coefficients in Porous Media Using MRI Measurements and Numerical Simulations," *Journal of Contaminant Hydrology* **125** (2011) 47-56.
<http://dx.doi.org/10.1016/j.jconhyd.2011.04.008>

NRC-IIT, Moncton


D. Tulpan, S. Léger, L. Belliveau, A. Culf, M. Cuperlovic-Culf, "MetaboHunter: an automatic approach for identification of metabolites from ^1H -NMR spectra of complex mixtures," *BMC Bioinformatics* **12** (2011) 400.
<http://dx.doi.org/10.1186/1471-2105-12-400>

Université Laval

R. Guillet-Nicolas, J.-L. Bridot, Y. Seo, M.-A. Fortin, F. Kleitz, "Enhanced Relaxometric Properties of MRI "Positive" Contrast Agents Confined in Three-Dimensional Cubic Mesoporous Silica Nanoparticles," *Advanced Functional Materials* (2011) online.
<http://dx.doi.org/10.1002/adfm.201101766>

P.-Y. Savard, R. Daigle, S. Morin, A. Sebilo, F. Meindre, P. Lagüe, M. Guertin, and S.M. Gagné, "Structure and Dynamics of Mycobacterium tuberculosis Truncated Hemoglobin N: Insights from NMR Spectroscopy and Molecular Dynamics Simulations," *Biochemistry* (2011) accepted.
<http://dx.doi.org/10.1021/bi201059a>

J. Leclerc, T. Lefèvre, F. Pottier, L.-P. Morency, C. Lapointe-Verreault, S.M. Gagné, M. Auger, "Structure and pH-induced alterations of recombinant and natural spider silk proteins in solution," *Biopolymers* (2011) online.
<http://dx.doi.org/10.1002/bip.21717>

 **I. Cloutier, J. Leclerc, T. Lefèvre, and M. Auger,** "Solid-State NMR Spectroscopy Reveals Distinctive Protein Dynamics in Closely-Related Spider Silks," *Canadian Journal of Chemistry* **89** (2011) 1047-1054. **(Special Issue)**
<http://dx.doi.org/10.1139/v11-036>

McGill University

R. Soudy, A. Gill, T. Sprules, A. Lavasanifar, and K. Kaur, "Proteolytically Stable Cancer Targeting Peptides with High Affinity for Breast Cancer Cells," *J. Med. Chem.* **54** (2011) 7523-7534.
<http://dx.doi.org/10.1021/jm200750x>

A.C.Y. Fan, G. Kozlov, A. Hoegl, R.C. Marcellus, M.J.H. Wong, K. Gehring and J.C. Young, "Interaction between the human mitochondrial import receptors Tom20 and Tom70 in vitro suggests a chaperone displacement mechanism," *Journal of Biological Chemistry* **286** (2011) 32208-32219.
<http://dx.doi.org/10.1074/jbc.M111.280446>


Université de Montréal


H. Thérien-Aubin, Y.J. Wang, and X.X. Zhu, "NMR Imaging and Its Application in the Study of Pharmaceutical Tablets," Chapter 27, *NMR Spectroscopy of Polymers: Innovative Strategies for Complex Macromolecules*, Eds. H.N. Cheng, T. Asakura, A.D. English, ACS (2011) pp. 441-457.
<http://dx.doi.org/10.1021/bk-2011-1077.ch027>


Y.J. Wang, E. Assaad, P. Ispas-Szabo, M.A. Mateescu, X.X. Zhu, "NMR imaging of chitosan and carboxymethyl starch tablets: Swelling and hydration of the polyelectrolyte complex," *International Journal of Pharmaceutics* **419** (2011) 215-221.
<http://dx.doi.org/10.1016/j.ijpharm.2011.08.008>

University of Ottawa

S. Letaief, J. Leclercq, Y. Liu and C. Detellier, "Single kaolinite nanometer layers prepared by an in situ polymerization - exfoliation process in presence of ionic liquids," *Langmuir* (2011) accepted.
<http://dx.doi.org/10.1021/la203492m>

 **J. Viger-Gravel, I. Korobkov, and D.L. Bryce,** "Multinuclear Solid-State Magnetic Resonance and X-ray Diffraction Study of Some Thiocyanate and Selenocyanate Complexes Exhibiting Halogen Bonding," *Cryst. Growth Des.* **11** (2011) 4984-4995.
<http://dx.doi.org/10.1021/cg200889y>

 **F.A. Perras and D.L. Bryce,** "Residual Dipolar Coupling Between Quadrupolar Nuclei Under Magic-Angle Spinning and Double-Rotation Conditions," *Journal of Magnetic Resonance* **213** (2011) 82-89.
<http://dx.doi.org/10.1016/j.jmr.2011.08.043>

 **L. Spencer, E. Coomes, E. Ye, V. Terskikh, A. Ramzy, V. Thangadurai, and G. Goward,** "Structural Analysis of Lanthanum-Containing Battery Materials Using ¹³⁹La Solid-State NMR," *Canadian Journal of Chemistry* **89** (2011) 1105-1117. **(Special Issue)**
<http://dx.doi.org/10.1139/v11-049>

NRC-SIMS, Ottawa



D. Bardelang, K. Udachin, D.M. Leek, J.C. Margeson, G. Chan, C.I. Ratcliffe, and J.A Ripmeester,

"Cucurbit[n]urils (n = 5 to 8): A Comprehensive Solid State Study," *Crystal Growth and Design* (2011) ASAP.
<http://dx.doi.org/10.1021/cg201173j>

Y. Ba, J.A. Ripmeester, C.I. Ratcliffe,
"Water molecular reorientation in ice and tetrahydrofuran clathrate hydrate from lineshape analysis of ^{17}O spin-echo NMR spectra," *Canadian Journal of Chemistry* **89** (2011) 1055-1064. **(Special Issue)**
<http://dx.doi.org/10.1139/v11-040>

V. Tersikh, A.R. Kermode, "In vivo nuclear magnetic resonance metabolite profiling in plant seeds," *Methods in Molecular Biology* **773** (2011) 307-318.
http://dx.doi.org/10.1007/978-1-61779-231-1_18

V. Tersikh, K. Müller, A.R. Kermode, G. Leubner-Metzger, "In Vivo ^1H NMR Microimaging During Seed Imbibition, Germination, and Early Growth," *Methods in Molecular Biology* **773** (2011) 319-327.
http://dx.doi.org/10.1007/978-1-61779-231-1_17



P.J. Pallister, I.L. Moudrakovski, J.A. Ripmeester, "High-field multinuclear solid-state nuclear magnetic resonance (NMR) and first principle calculations in MgSO_4 polymorphs," *Canadian Journal of Chemistry* **89** (2011) 1076-1086. **(Special Issue)**
<http://dx.doi.org/10.1139/v11-044>



G.H. Penner, R. Webber, L.A. O'Dell, "A multinuclear NMR and quantum chemical study of solid trimethylammonium chloride," *Canadian Journal of Chemistry* **89** (2011) 1036-1046. **(Special Issue)**
<http://dx.doi.org/10.1139/v11-034>



L.A. O'Dell and C.I. Ratcliffe, " ^{14}N magic angle spinning overtone NMR spectra," *Chemical Physics Letters* **514** (2011) 168-173.
<http://dx.doi.org/10.1016/j.cplett.2011.08.030>

NRC-IBS, Ottawa

E. Altman, V. Chandan, J. Li, E. Vinogradov, "A re-investigation of the lipopolysaccharide structure of *Helicobacter pylori* strain Sydney (SS1)," *FEBS Journal* **278** (2011) 3484-3493.
<http://dx.doi.org/10.1111/j.1742-4658.2011.08270.x>

Queen's University

J. Zhu, T. Kurahashi, H. Fujii and G. Wu, "Solid-state ^{17}O NMR and computational studies of terminal transition metal oxo compounds," *Chemical Science* (2011) online. **(Edge Article)**
<http://dx.doi.org/10.1039/C1SC00725D>

G. Wu "Oxygen 17 NMR Studies of Organic and Biological Molecules", *Encyclopedia of Magnetic Resonance* (2011).
<http://dx.doi.org/10.1002/9780470034590.emrstm1212>

G. Wu, Z. Gan, I.C.M. Kwan, J.C. Fettinger, and J.T. Davis, "High Resolution ^{39}K NMR Spectroscopy of Bio-organic Solids," *J. Am. Chem. Soc.* (2011) ASAP.
<http://dx.doi.org/10.1021/ja2052446>

I.C.M. Kwan, Y.-M. She, G. Wu, "Nuclear magnetic resonance and mass spectrometry studies of 2',3',5'-O-triacetylguanosine self-assembly in the presence of alkaline earth metal ions (Ca^{2+} , Sr^{2+} , Ba^{2+})," *Canadian Journal of Chemistry* **89** (2011) 835-844. **(Special Issue)**
<http://dx.doi.org/10.1139/v10-179>

University of Toronto

P. Vallurupalli, G. Bouvignies, and L.E. Kay, "Increasing the Exchange Time-Scale That Can Be Probed by CPMG Relaxation Dispersion NMR," *J. Phys. Chem. B* (2011) ASAP.
<http://dx.doi.org/10.1021/jp209610v>

J.R. Bothe, E.N. Nikolova, C.D. Eichhorn, J. Chugh, A.L. Hansen and H.M. Al-Hashimi, "Characterizing RNA dynamics at atomic resolution using solution-state NMR spectroscopy," *Nature Methods* **8** (2011) 919-931. **(Review)**
<http://dx.doi.org/10.1038/nmeth.1735>

H. Sun, L.E. Kay, and V. Tugarinov, "An Optimized Relaxation-Based Coherence Transfer NMR Experiment for the Measurement of Side-Chain Order in Methyl-Protonated, Highly Deuterated Proteins," *J. Phys. Chem. B* (2011) accepted.
<http://dx.doi.org/10.1021/jp209049k>

M. Seino, W. Wang, J.E. Lofgreen, D.P. Puzzo, T. Manabe, and G.A. Ozin, "Low-k Periodic Mesoporous Organosilica with Air Walls: POSS-PMO," *J. Am. Chem. Soc.* **133** (2011) 18082–18085.
<http://dx.doi.org/10.1021/ja2080136>

P.M. Macdonald, "Diffusion NMR of Polymers in Bicelles," Chapter 14, *NMR Spectroscopy of Polymers: Innovative Strategies for Complex Macromolecules*, Eds. H.N. Cheng, T. Asakura, A.D. English, ACS (2011) pp. 221-250.
<http://dx.doi.org/10.1021/bk-2011-1077.ch014>

J.R. McKelvie, D.M. Wolfe, M.A. Celejewski, M. Alaee, A.J. Simpson, M.J. Simpson, "Metabolic responses of *Eisenia fetida* after sub-lethal exposure to organic contaminants with different toxic modes of action," *Environmental Pollution* **159** (2011) 3620-3626.
<http://dx.doi.org/10.1016/j.envpol.2011.08.002>

J.S. Clemente, A.J. Simpson, M.J. Simpson, "Association of specific organic matter compounds in size fractions of soils under different environmental controls," *Organic Geochemistry* **42** (2011) 1169-1180.
<http://dx.doi.org/10.1016/j.orggeochem.2011.08.010>

V. Kanelis, P.A. Chong, J.D. Forman-Kay, "NMR spectroscopy to study the dynamics and interactions of CFTR," *Methods in molecular biology* **741** (2011) 377-403.
http://dx.doi.org/10.1007/978-1-61779-117-8_25

Y. Powder-George, J. Frank, R.S. Ramsewak and W.F. Reynolds, "The Use of Coupled HSQC Spectra to Aid in Stereochemical Assignments of Molecules with Severe Proton Spectral Overlap," *Phytochemical Analysis* (2011) online.
<http://dx.doi.org/10.1002/pca.1354>

A.L. Hansen, L.E. Kay, "Quantifying millisecond time-scale exchange in proteins by CPMG relaxation dispersion NMR spectroscopy of side-chain carbonyl groups," *Journal of Biomolecular NMR* **50** (2011) 347-355.
<http://dx.doi.org/10.1007/s10858-011-9520-6>

G. Bouvignies, P. Vallurupalli, D.F. Hansen, B.E. Correia, O. Lange, A. Bah, R.M. Vernon, F.W. Dahlquist, D. Baker & L.E. Kay, "Solution structure of a minor and transiently formed state of a T4 lysozyme mutant," *Nature* **477** (2011) 111–114.
<http://dx.doi.org/10.1038/nature10349>

P.M. Macdonald, R. Soong, "Diffusion NMR and bicelle morphology," *Canadian Journal of Chemistry* **89** (2011) 1021-1035. **(Review) (Special Issue)**
<http://dx.doi.org/10.1139/v11-038>

A.J. Baldwin, H. Lioe, C.V. Robinson, L.E. Kay, J.L.P. Benesch, "alfaB-crystallin polydispersity is a consequence of unbiased quaternary dynamics," *Journal of Molecular Biology* **413** (2011) 297-309.
<http://dx.doi.org/10.1016/j.jmb.2011.07.016>

A.J. Baldwin, G.R. Hilton, H. Lioe, C. Bagneris, J.L.P. Benesch, L.E. Kay, "Quaternary dynamics of alfaB-crystallin as a direct consequence of localised tertiary fluctuations in the C-terminus," *Journal of Molecular Biology* **413** (2011) 310-320.
<http://dx.doi.org/10.1016/j.jmb.2011.07.017>

McMaster University

B.L. Ellis, T.N. Ramesh, L.J.M. Davis, G.R. Goward, and L.F. Nazar, "Structure and Electrochemistry of Two-Electron Redox Couples in Lithium Metal Fluorophosphates Based on the Tavorite Structure," *Chem. Mater.* (2011) ASAP.
<http://dx.doi.org/10.1021/cm201773n>

L.J.M. Davis, B. Ellis, T.N. Ramesh, L.F. Nazar, A.D. Bain, and G.R. Goward, "⁶Li 1D EXSY NMR Spectroscopy: A New Tool for Studying Lithium Dynamics in Paramagnetic Materials Applied to Monoclinic Li₂V(PO₄)F," *J. Phys. Chem. C* **115** (2011) 22603–22608.
<http://dx.doi.org/10.1021/jp2059408>

A.D. Bain, M. Baron, S.K. Burger, V.J. Kowalewski, M.B. Rodriguez, "Interconversion Study in 1,4-Substituted Six-Membered Cyclohexane-Type Rings. Structure and Dynamics of trans-1,4-Dibromo-1,4-dicyanocyclohexane," *J. Phys. Chem. A* **115** (2011) 9207-9216.
<http://dx.doi.org/10.1021/jp205375f>

University of Guelph

M.E. Ward, L. Shi, E.M.R. Lake, S. Krishnamurthy, H. Hutchins, L.S. Brown, and V. Ladizhansky, "Proton Detected Solid-State NMR Reveals Intramembrane Polar Networks in a Seven-Helical Transmembrane Protein Proteorhodopsin," *J. Am. Chem. Soc.* **133** (2011) 17434–17443.

<http://dx.doi.org/10.1021/ja207137h>



G.H. Penner, R. Webber, L.A. O'Dell,

"A multinuclear NMR and quantum chemical study of solid trimethylammonium chloride," *Canadian Journal of Chemistry* **89** (2011) 1036–1046. **(Special Issue)**

<http://dx.doi.org/10.1139/v11-034>

S. Wang, L. Shi, I. Kawamura, L.S. Brown, and V. Ladizhansky, "Site-Specific Solid-State NMR Detection of Hydrogen-Deuterium Exchange Reveals Conformational Changes in a 7-Helical Transmembrane Protein," *Biophysical Journal* **101** (2011) L23–L25.

<http://dx.doi.org/10.1016/j.bpj.2011.06.035>

University of Waterloo

J. Zhang, C.A. Ryan, R. Laflamme, J. Baugh, "Coherent control of two nuclear spins using the anisotropic hyperfine interaction," *Phys. Rev. Lett.* **107** (2011) 170503.

<http://dx.doi.org/10.1103/PhysRevLett.107.170503>

O. Moussa, J. Baugh, C.A. Ryan, R. Laflamme, "Demonstration of sufficient control for two rounds of quantum error correction in a solid state ensemble quantum information processor," *Physical Review Letters* **107** (2011) 160501.

<http://dx.doi.org/10.1103/PhysRevLett.107.160501>

J. Hassan, H. Peemoeller, "Analysis of ^2H NMR spectra of water molecules on the surface of nano-silica material, MCM-41: Deconvolution of the signal into a Lorentzian and a powder pattern line shapes," *Physica B: Condensed Matter* (2011) online.

<http://dx.doi.org/10.1016/j.physb.2011.10.023>

G. Passante, O. Moussa, D.A. Trottier, and R. Laflamme, "Experimental detection of nonclassical correlations in mixed-state

quantum computation," *Phys. Rev. A* **84** (2011) 044302.

<http://dx.doi.org/10.1103/PhysRevA.84.044302>

J. Zhang, D. Gangloff, O. Moussa, and R. Laflamme, "Experimental quantum error correction with high fidelity," *Phys. Rev. A* **84** (2011) 034303.

<http://dx.doi.org/10.1103/PhysRevA.84.034303>

L.J.M. Davis, B. Ellis, T.N. Ramesh, L.F. Nazar, A.D. Bain, and G.R. Goward, " ^6Li 1D EXSY NMR Spectroscopy: A New Tool for Studying Lithium Dynamics in Paramagnetic Materials Applied to Monoclinic $\text{Li}_2\text{V}(\text{PO}_4)\text{F}$," *J. Phys. Chem. C* **115** (2011) 22603–22608.

<http://dx.doi.org/10.1021/jp2059408>

University of Western Ontario

L. Zhang, J. Bates, D. Chen, H.-Y. Nie, and Y. Huang, "Investigations of Formation of Molecular Sieve SAPO-34," *J. Phys. Chem. C* **115** (2011) 22309–22319.

<http://dx.doi.org/10.1021/jp208560t>

M. McCallum, G.S. Shaw and C. Creuzenet, "Characterization of the dehydratase WcbK and the reductase WcaG involved in GDP-6-deoxymanno-heptose biosynthesis in *Campylobacter jejuni*," *Biochem. J.* **439** (2011) 235–248.

<http://dx.doi.org/10.1042/BJ20110890>

A. Rezvanpour, L. Santamaria-Kisiel and G.S. Shaw, "The S100A10-annexin A2 complex provides a novel asymmetric platform for membrane repair," *Journal of Biological Chemistry* **286** (2011) 40174–40183.

<http://dx.doi.org/10.1074/jbc.M111.244038>

B.R. Dempsey and G.S. Shaw, "Identification of Calcium-Independent and Calcium-Enhanced Binding Between S100B and the Dopamine D2 Receptor," *Biochemistry* **50** (2011) 9056–9065.

<http://dx.doi.org/10.1021/bi201054x>

University of Windsor



B.E.G. Lucier, A.R. Reidel, R.W. Schurko, "Multinuclear solid-state NMR

of square-planar platinum complexes — Cisplatin and related systems," *Canadian Journal of Chemistry* **89** (2011) 919–937. **(Special Issue)**

<http://dx.doi.org/10.1139/v11-033>

P.B. Chatterjee, O. Goncharov-Zapata, L.L. Quinn, G. Hou, H. Hamaed, R.W. Schurko, T. Polenova, and D.C. Crans, "Characterization of Noninnocent Metal Complexes Using Solid-State NMR Spectroscopy: o-Dioxolene Vanadium Complexes," *Inorg. Chem.* **50** (2011) 9794–9803.

<http://dx.doi.org/10.1021/ic200046k>

University of Manitoba

A.J. Lussier, F.C. Hawthorne, P.M. Aguiar, V.K. Michaelis, S. Kroeker, "Elbaite-liddicoatite from Black Rapids Glacier, Alaska," *Periodico di Mineralogia* **80** (2011) 57-73.

<http://dx.doi.org/10.2451/2011PM0005>

NRC-IBD, Winnipeg

D.I. Hoult "Magnetic Resonance with Conducting and High-Dielectric Samples", *Encyclopedia of Magnetic Resonance* (2011).

<http://dx.doi.org/10.1002/9780470034590.emrstm1182>

University of Saskatchewan

Z. Li, Y. Pan, "First-principles study of boron oxygen hole centers in crystals: Electronic structures and nuclear hyperfine and quadrupole parameters," *Physical Review B - Condensed Matter and Materials Physics* **84** (2011) 115112.

<http://dx.doi.org/10.1103/PhysRevB.84.115112>

University of Alberta

T. Jewison, C. Knox, V. Neveu, Y. Djoumbou, A.C. Guo, J. Lee, P. Liu, R. Mandal, R. Krishnamurthy, I. Sinelnikov, M. Wilson and D.S. Wishart, "YMDB: the Yeast Metabolome Database," *Nucl. Acids Res.* (2011) online.

<http://dx.doi.org/10.1093/nar/gkr916>

K.P. Santo, M. Berjanskii, D.S. Wishart, M. Stepanova, "Comparative analysis of essential collective dynamics and NMR-derived flexibility profiles in evolutionarily diverse prion proteins," *Prion* **5** (2011) 188-200.

<http://dx.doi.org/10.4161/pri.5.3.16097>

R.T. McKay, "How the 1D-NOESY suppresses solvent signal in metabonomics NMR spectroscopy: An examination of the pulse

sequence components and evolution," *Concepts in Magnetic Resonance Part A* **38A** (2011) 197–220.

<http://dx.doi.org/10.1002/cmr.a.20223>

R. Perez-Pineiro, T.C. Bjorndahl, M.V. Berjanskii, D. Hau, L. Li, A. Huang, R. Lee, E. Gibbs, C. Ladner, Y.W. Dong, A. Abera, N.R. Cashman and D.S. Wishart, "The prion protein binds thiamine," *FEBS Journal* **278** (2011) 4002–4014.

<http://dx.doi.org/10.1111/j.1742-4658.2011.08304.x>

K. Campbell, K.J. Ooms, M.J. Ferguson, P.J. Stang, R.E. Wasylshen, R.R. Tykwinski, "Shape-persistent macrocycles — Self-assembly reactions and characterization by hyperpolarized ^{129}Xe NMR spectroscopy," *Canadian Journal of Chemistry* **89** (2011) 1264-1276.

<http://dx.doi.org/10.1139/v11-077>

O. Julien, S. Chatterjee, T.C. Bjorndahl, B. Sweeting, S. Acharya, V. Semchenko, A. Chakrabartty, E.F. Pai, D.S. Wishart, B.D. Sykes, and N.R. Cashman, "Relative and Regional Stabilities of the Hamster, Mouse, Rabbit, and Bovine Prion Proteins toward Urea Unfolding Assessed by Nuclear Magnetic Resonance and Circular Dichroism Spectroscopies," *Biochemistry* **50** (2011) 7536-7545.

<http://dx.doi.org/10.1021/bi200731e>

University of Calgary

O. Rekdal, B.E. Haug, M. Kalaaji, H.N. Hunter, I. Lindin, I. Israelsson, T. Solstad, N. Yang, M. Brandl, D. Mantzilas and H.J. Vogel, "The relative spatial positions of tryptophan and cationic residues in helical membrane-active peptides determines their cytotoxicity," *Journal of Biological Chemistry* (2011) online.

<http://dx.doi.org/10.1074/jbc.M111.279281>

L. Truong, V. Thangadurai, "Soft-chemistry of garnet-type $\text{Li}_{5+x}\text{Ba}_x\text{La}_{3-x}\text{Nb}_2\text{O}_{12}$ ($x = 0, 0.5, 1$): Reversible H^+/Li^+ ion-exchange reaction and their X-ray, ^7Li MAS NMR, IR, and AC impedance spectroscopy characterization," *Chemistry of Materials* **23** (2011) 3970-3977.

<http://dx.doi.org/10.1021/cm2015127>

G.E. Duggan, D.S. Hittel, C.C. Hughey, A. Weljie, H.J. Vogel, J. Shearer,

"Differentiating short- and long-term effects of diet in the obese mouse using ^1H nuclear magnetic resonance metabolomics," *Diabetes Obesity & Metabolism* **13** (2011) 859-862.
<http://dx.doi.org/10.1111/j.1463-1326.2011.01410.x>

J.G.M. Bolscher, M.J. Oudhoff, K. Nazmi, J.M. Antos, C.P. Guimaraes, E. Spooner, E.F. Haney, J.J.G. Vallejo, H.J. Vogel, W. van't Hof, H.L. Ploegh, E.C.I. Veerman, "Sortase A as a tool for high-yield histatin cyclization," *FASEB Journal* **25** (2011) 2650-2658.
<http://dx.doi.org/10.1096/fj.11-182212>



L. Spencer, E. Coomes, E. Ye, V. Terskikh, A. Ramzy, V. Thangadurai, and G. Goward, "Structural Analysis of Lanthanum-Containing Battery Materials Using ^{139}La Solid-State NMR," *Canadian Journal of Chemistry* **89** (2011) 1105-1117. (Special Issue)
<http://dx.doi.org/10.1139/v11-049>

D. Skachkov, M. Krykunov, T. Ziegler, "An improved scheme for the calculation of NMR chemical shifts in periodic systems based on gauge including atomic orbitals and density functional theory," *Canadian Journal of Chemistry* **89** (2011) 1150-1161. (Special Issue)
<http://dx.doi.org/10.1139/v11-050>

University of Lethbridge

P. Chaudhary, R.A. Shank, T. Montana, J.T. Goettel, N.A. Foroud, P. Hazendonk and F. Eudes, "Hydrogen-Bonding Interactions in T-2 Toxin Studied Using Solution and Solid-State NMR," *Toxins* **3** (2011) 1310-1331.
<http://dx.doi.org/10.3390/toxins3101310>

A.H. Karoyo, A.S. Borisov, L.D. Wilson, P. Hazendonk, "Formation of Host-Guest Complexes of beta-Cyclodextrin and Perfluorooctanoic Acid," *J. Phys. Chem. B* **115** (2011) 9511-9527.
<http://dx.doi.org/10.1021/jp110806k>

T. Montana, P. Hazendonk, P. Wormald, D. Iuga, "The refocused discrimination induced by variable amplitude minipulses (DIVAM) experiment — Improved domain selection in semicrystalline fluoropolymers by ^{19}F solid state nuclear magnetic resonance spectroscopy," *Canadian Journal of Chemistry* **89** (2011) 1065-1075. (Special Issue)
<http://dx.doi.org/10.1139/v11-043>

University of British Columbia

S.J. Baturin, M. Okon, L.P. McIntosh, "Structure, dynamics, and ionization equilibria of the tyrosine residues in *Bacillus circulans* xylanase," *Journal of Biomolecular NMR* **51** (2011) 379-394.
<http://dx.doi.org/10.1007/s10858-011-9564-7>

T. Wu, H. Mayaffre, S. Krämer, M. Horvatic, C. Berthier, W.N. Hardy, R. Liang, D.A. Bonn and M.-H. Julien, "Magnetic-field-induced charge-stripe order in the high-temperature superconductor $\text{YBa}_2\text{Cu}_3\text{O}_y$," *Nature* **477** (2011) 191-194.
<http://dx.doi.org/10.1038/nature10345>

E.E. Burnell, R.Y. Dong, A.C.J. Weber, X. Yang, A. Yethiraj, "Separation of nematic and smectic-A potential effects on solute ordering in a series of binary 6OCB-8OCB mixtures," *Canadian Journal of Chemistry* **89** (2011) 900-908. (Special Issue)
<http://dx.doi.org/10.1139/v11-027>

Simon Fraser University

M.G. Szczepina, D.W. Bleile, J. Müllegger, A.R. Lewis and B.M. Pinto, "WaterLOGSY NMR Experiments in Conjunction with Molecular-Dynamics Simulations Identify Immobilized Water Molecules That Bridge Peptide Mimic MDWNMHA to Anticarbhydrate Antibody SYA/J6," *Chemistry - A European Journal* **17** (2011) 11438-11445.
<http://dx.doi.org/10.1002/chem.201101464>

M.G. Szczepina, D.W. Bleile, and B.M. Pinto, "Investigation of the Binding of a Carbohydrate-Mimetic Peptide to its Complementary Anticarbhydrate Antibody by STD-NMR Spectroscopy and Molecular-Dynamics Simulations," *Chemistry - A European Journal* **17** (2011) 11446-11455.
<http://dx.doi.org/10.1002/chem.201100222>

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