

**2014
the International Year of
Crystallography**

<http://www.iycr2014.org/>

The International Year of Crystallography (**IYCr2014**) is an event promoted in 2014 by the **United Nations** to celebrate the centenary of the discovery of X-ray crystallography and to emphasize the global importance of crystallography in human life. **UNESCO** and the **International Union of Crystallography (IUCr)** are responsible for this event.

The major objectives of the IYCr2014 are:

- to increase public awareness of the science of crystallography and how it underpins most technological developments in our modern society
- to inspire young people through public exhibitions, conferences and hands-on demonstrations in schools
- to illustrate the universality of science
- to intensify the programme Crystallography in Africa and create similar programmes in Asia and Latin America
- to foster international collaboration between scientists worldwide, especially North-South contributions
- to promote education and research in crystallography and its links to other sciences
- to involve the large synchrotron and neutron radiation facilities worldwide in the celebrations of IYCr2014, including the SESAME project set up under UNESCO auspices

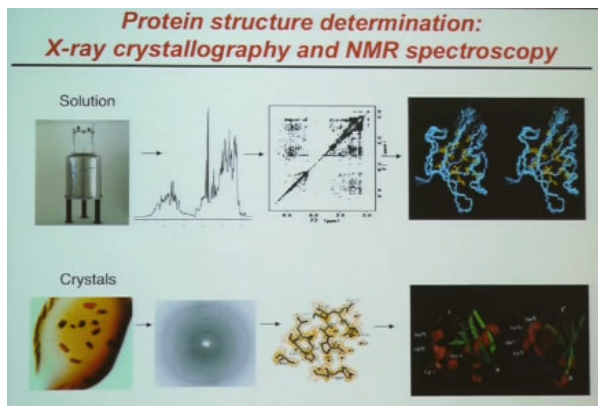
The opening ceremony of the International Year of Crystallography took place in Paris in January 2014. Many activities will follow to celebrate the International Year of Crystallography all over the world. Visit the official **IYCr2014** website for the most recent updates <http://www.iycr2014.org/>

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Seeing is Believing "Viewing the Biological World with X-rays and Magnetic Fields"

The subject of crystallography is dear to many of us working in NMR. Watch these two insightful lectures by **Michael Murphy** and **Lawrence McIntosh** (UBC) on synergy between NMR and X-ray crystallography. The lectures were presented at the *11th Café Scientifique* organized by the Life Sciences Institute at the University of British Columbia.



<http://cafesci.lsi.ubc.ca/2012/11/20/viewing-the-biological-world-with-x-rays-and-magnetic-fields-2/>

<http://tinyurl.com/qabqbs6>

NMR for the masses (ACCN)

A phenomenon of recent years is the fast-paced progress in development of compact bench-top NMR spectrometers which make use of rare-earth permanent magnets and operate in the 40-80 MHz ^1H frequency range.



http://en.wikipedia.org/wiki/Benchtop_NMR_spectrometer

A Calgary-based company **Nanalysis** is one of the world leaders in this field. In early 2014 **Nanalysis** was named the Alberta's Innovator of the Year by *Innovate Calgary*.

<http://www.nanalysis.com/>

Nanalysis is prominently featured in the Winter 2014 issue of *ACCN (L'Actualité chimique canadienne)* the *Canadian Chemical News*.

Roberta Staley "NMR for the masses," *ACCN* January/February 2014.

<http://www.cheminst.ca/magazine/feature-story/nmr-masses>

Recent advances in NMR instrumentation, including compact NMR, have been also highlighted by the RSC's *ChemistryWorld*.

Elisabeth Jeffries "Spinning into focus" *ChemistryWorld*, 9 January 2014.

<http://www.rsc.org/chemistryworld/2014/01/nmr-product-guide>

Sussex Research Laboratories (Ottawa, ON) is a Canadian contract research organization (CRO) which focuses on Carbohydrate & Glycan Synthesis, Glycosylation & GlycoDesign.

<http://www.sussex-research.com/>

An interview with **Brady Clark** (founder and CEO), **Garnet McRae** (director of bioanalytical services), and **Dennis Whitfield** (member of the scientific advisory board) has been recently published in *PharmaTech*. In their interview they discuss the use of modern analytical instrumentation, including NMR and LC-MS/MS, in glycan research.

Cynthia Challener "The Role of NMR and Mass Spectroscopy in Glycan Analysis" *Pharmaceutical Technology* **38** (2014) pp. 52, 54, 62. <http://tinyurl.com/n4m7pfc>

6^{ème} COLLOQUE ANNUEL DU GRASP
6th ANNUAL GRASP SYMPOSIUM



Submitted by Alexey Denisov (Concordia)

Thank you - GRASP Symposium 2013

I would like to thank you all for your participation in our Annual Symposium in November which was a great success again this year with officially 238 participants.

Thank you to our guest speakers for having accepted our invitation, to all of our poster presenters and, of course, to our sponsors and exhibitors for their invaluable support.

Congratulation to the graduate students and post-docs selected to give an oral presentation. Each of them received a nice certificate and \$100.

And congratulation to the winners of our door prize drawing: **Kevin Chen** (Bose head set provided by *Agilent technologies*), **Irina Gulerez** (iPad mini provided by *GRASP*) and **Sabina Sarvan** (iPad mini provided by *GRASP*).

Feel free to send your comments/suggestions about the event directly to:

E-mail: grasp.med@mcgill.ca

Please, mark your calendar: the 7th Annual GRASP Symposium will be held on Monday, November 24th, 2014. We will look forward to seeing you all again next year.

Kind regards,

Annick Guyot, PhD
GRASP Coordinator

<http://grasp.mcgill.ca>

New Funding announcements


Canada Foundation for Innovation

John R. Evans Leaders Fund

Vladimir Ladizhansky (Guelph) was awarded \$124,091 for advanced equipment for Solid State NMR studies of biomedically important membrane proteins.

http://www.physics.uoguelph.ca/single_news.php?idx=446



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

June 1-5, 2014, Vancouver, B.C., Canada
<http://www.csc2014.ca/>

Solid-state NMR Symposium

Organizers: Suzana Straus (UBC), Carl Michal (UBC), Rob Schurko (Windsor)

Confirmed Invited Speakers:

David Bryce (Ottawa)
Brad Chmelka (UC Santa Barbara)
Yoshitaka Ishii (Uni Illinois Chicago)
Scott Kroeker (Manitoba)
Vlad Ladizhansky (Guelph)
Isabelle Marcotte (UQAM)
Rachel Martin (UC Irvine)
Len Mueller (UC Riverside)

Registration is now open
<http://www.csc2014.ca/registration/registration.html>

ENC 2014 Events

55th ENC March 23-28, 2014, Boston, MA
<http://www.enc-conference.org/>

ACD/Labs NMR Software Symposium
March 23, 2014, Boston, MA
<http://www.acdlabs.com/company/events/eventinfo.php?id=314>

Agilent ENC User Meeting
March 22, 2014, Boston, MA
<http://www.chem.agilent.com/en-US/promotions/Pages/encusermeeting.aspx>

Bruker Pre-ENC NMR Workshops and Breakfast Symposium
March 22-23, 2014, Boston, MA
<http://www.bruker.com/events/enc-2014/enc2014.html>

Cambridge Isotope Laboratories
CIL's 3rd Annual NMR is GOOD but Isotopes Make it Better Contest
<http://www.isotope.com/cil/site/information.cfm?CampaignCode=NMRGOOD>

Submit your entries by March 15th, 2014 !

Mestrelab's Practical Demo
<http://mestrelab.com/events/enc-2014/>



2014 Solid-State NMR Workshop

The 9th Annual Solid-State NMR Workshop organized by the National Ultrahigh-Field NMR Facility for Solids and Bruker Canada will take place in Ottawa later in the Summer. Exact dates will be announced later. Stay tuned!
http://nmr900.ca/news_e.html

On the move

Leigh Spencer (Ph.D. 2014, Goward group, McMaster) is currently working as a postdoctoral fellow at the Hospital for Sick Children (Toronto) in the Mouse Imaging Centre under the supervision of Prof. Brian Nieman.

Sameer Al-Abdul-Wahid (postdoctoral fellow, Kalle Gehring group, McGill) has accepted a position as the NMR/MS Instrumentation Facility Manager in the Department of Chemistry and Biochemistry at Miami University in Oxford, Ohio.
<http://chemistry.muohio.edu/resources/instrumentation>

Bryan Lucier (Ph.D. 2013, Schurko group, Windsor) began a postdoctoral fellowship at Western University under Prof. Yining Huang in January 2014.

Igor Moudrakovski (formerly Senior Research Scientist at NRC, Ottawa/Visiting Scientist at the University of Ottawa) has accepted a position of NMR Scientist at the Max-Planck Institute for Solid State Research in Stuttgart, Germany. <http://www.fkf.mpg.de/en>

Kirk Feindel (Ph.D. 2007, Wasylishen group, Alberta) just started as Associate Professor of MRI and Director of Bioimaging at the Centre for Microscopy, Characterisation and Analysis at the University of Western Australia in Perth.
<http://www.cmca.uwa.edu.au>

Recognition



Lauréate: Michèle Auger

<http://www.youtube.com/watch?v=DFWx9IkiGVQ>

Prof. **Michèle Auger** (Université Laval) has been awarded **the 2013 Prize for best Chair of Undergraduate Studies**.

Ce prix vise à reconnaître la qualité des interventions et le rôle clé du directeur de programme quant au développement de la formation et à l'encadrement des étudiants. Il valorise les pratiques exemplaires de gestion pédagogique et leur rôle de premier plan dans la qualité des programmes et leur développement continu.

https://www.bsp.ulaval.ca/reconnaissance/prix_12_13/prix_12_13.php

Citation (PDF)

https://www.bsp.ulaval.ca/reconnaissance/prix_12_13/documents/Profil_2013_Auger.pdf

Prof. **Roderick Wasylshen** (University of Alberta) will present **the 2014 Vaughan Lecturer** at the 56th Annual Rocky Mountain Conference on Magnetic Resonance which will take place **July 13-17, 2014**, Copper Mountain, Colorado.

The conference registration and abstract submission is now open

<http://www.rockychem.com/>

Prof. **David Bryce** (Ottawa) has been awarded the **2014 Keith Laidler Award**.

Sponsored by the Chemical Institute of Canada, Physical, Theoretical and Computation Chemistry Division, the Keith Laidler Award is presented to a scientist residing in Canada who has made a distinguished contribution to the field of physical chemistry while working in Canada, recognizing early achievement in his/her independent research career.

<http://www.cheminst.ca/awards/csc-awards/keith-laidler-award>

NMR Theses Recently Defended

Eve Gagné (Université Laval) November 2013

Supervisor: Prof. Michèle Auger

Co-supervisors: Prof. Michel Guertin and Prof. Patrick Lagüe

M.Sc. thesis: "Études spectroscopiques de l'interaction entre des membranes modèles et une hémoglobine tronquée"

Tara Leigh Spencer Noakes (McMaster University) Spring 2014

Supervisor: Prof. Gillian Goward

Ph.D. Chemistry: "Multinuclear NMR Spectroscopy Methods for the Study of Structure and Dynamics in Solid-State Electrolytes for Lithium Ion Batteries"

<http://digitalcommons.mcmaster.ca/opensdissertations/8627/>

Jun Xu (University of Western Ontario) December 2013

Supervisor: Prof. Yining Huang

Ph.D. Chemistry: "Multinuclear Solid-State Nuclear Magnetic Resonance Spectroscopy of Microporous Materials"

<http://ir.lib.uwo.ca/etd/1752/>

John E.C. Wren (University of Manitoba) January 15, 2014

Supervisor: Prof. Scott Kroeker

Ph.D. Chemistry: "Application of Nuclear Magnetic Resonance to the Study of Nuclear Waste Relevant Molybdates at Ambient and High Temperatures"

<http://mspace.lib.umanitoba.ca/handle/1993/23235>

Piotr Garbacz (University of Warsaw) December 2013

Supervisors: Prof. Karol Jackowski (Warsaw), Prof. Roderick Wasylshen (Alberta)

Ph.D. Chemistry: "NMR Studies of Magnetic Shielding in Gaseous Hydrogen and Solid Iridium Hydrides"

<http://depotuw.ceon.pl/handle/item/433>

Brian Lucier (University of Windsor) September 2013

Supervisor: Prof. Robert Schurko

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

<http://scholar.uwindsor.ca/etd/4909/>

NMR Events

55th ENC March 23-28, 2014, Boston, MA
<http://www.enc-conference.org/>


RSC NMR Discussion Group, Spring Meeting 2014 "NMR in Structural Biology"

April 10-11, 2014, University of Cambridge,
Department of Chemistry, UK
<http://www-keeler.ch.cam.ac.uk/NMRDG/index.html>

FoodMR 2014 XII International Conference on
the Applications of Magnetic Resonance in Food
Science: Defining Food by Magnetic Resonance

May 20-23, 2014, Cesena, Italy
<http://www.foodmr.org>



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Isabelle Marcotte (UQAM)
Rachel Martin (UC Irvine)
Len Mueller (UC Riverside)

Registration is now open

<http://www.csc2014.ca/registration/registration.html>

AMPERE NMR School

June 22-28, 2014, Zakopane, Poland
<http://www.staff.amu.edu.pl/~school/>

EUROMAR 2014

June 29 - July 3, 2014, Zürich, Switzerland
<http://www.euromar2014.org/>

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

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

**Solution and solid-state NMR of
paramagnetic molecules** EMBO Practical
Course

July 13-19, 2014, Sesto Fiorentino, Italy
<http://events.embo.org/14-paramagnetism/>

**Multidimensional NMR in structural
biology**, EMBO Practical Course

August 10-15, 2014, Joachimsthal, Germany
<http://www3.mpibpc.mpg.de/groups/griesinger/training/embo2014/>

ICMRBS 2014, the XXVIth International
Conference on Magnetic Resonance in
Biological Systems

August 24-29, 2014, Dallas, Texas
<http://icmrbs2014.org/>

**4th SMARTER meeting on NMR and
Crystallography**

September 1-4, 2014, Durham University, UK
<http://www.ccpnc.ac.uk/smarter4/>

**SMASH 2014 Small Molecule NMR
Conference**

September 7-10, 2014, Atlanta, Georgia, USA
<http://www.smashnmr.org/>

 **MOOT XXVII NMR Symposium**

Fall 2014, Montreal, Quebec
<http://www.mootnmr.org>

 **7th Annual GRASP Symposium**

November 24, 2014, McGill University,
Montréal, QC, Canada
<http://grasp.mcgill.ca/english/symposium/symposium.html>

Biophysical Society 59th Annual Meeting

February 7-11, 2015, Baltimore, Maryland
<http://www.biophysics.org/2015meeting>



Biophysical Society of Canada - Travel Awards and Mixer

PANIC 2015 Practical Applications of NMR in Industry Conference

February 11-13, 2015, La Jolla, CA
<http://www.panicnmr.com/>



CSC 2015 the 98th Canadian Chemistry Conference and Exhibition
"Chemistry in a Sustainable World"

June 13-17, 2015, Ottawa, ON, Canada
<http://www.csc2015.ca/>

ISMAR 2015 19th International Society of Magnetic Resonance Conference

August 16-21, 2015, Shanghai, China
<http://ismar2015.ecnu.edu.cn/>
<http://www.ismar.org/>

9th Alpine Conference on Solid-State NMR

September 13-17, 2015, Chamonix Mont-Blanc, France
<http://www.alpine-conference.org>



Pacifichem 2015 The International Chemical Congress of Pacific Basin Societies

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

> NMR Spectroscopy of Polymers and Biobased Materials (#12)

> Advances in Biological Solid-State NMR (#120) Michèle Auger, co-chair

> Biomolecular Structure and Dynamics: Recent Advances in NMR (#181) Mitsuhiro Ikura, co-chair

<http://www.pacifichem.org/symposiadesc2015/>



ISMAR 2017 20th International Society of Magnetic Resonance Conference

July 23-28, 2017, Québec City, Québec, Canada
<http://www.ismar.org/>

News from the Publishers



Canadian Journal
of **Chemistry**

January 6, 2014
Ottawa, ON

Canadian Journal of Chemistry Best Paper Award

<http://www.cdnsciencepub.com/news-and-events/press-releases/CJC-Best-Paper-Award.aspx>

The *Canadian Journal of Chemistry* (CJC) and its publisher, Canadian Science Publishing (CSP), are pleased to announce the new CJC Best Paper Award.

This new award will annually recognize the "best paper" published in the CJC in the preceding year, by a scientist residing in Canada.

The winner will present an award lecture at the Canadian Society for Chemistry (CSC)'s annual Canadian Chemistry Conference and Exhibition, with the first award to be presented in 2015. The winner will also give a sponsored lecture at one or two Canadian universities. In addition, the award-winning paper will be made open access and fully available to the public.

"We feel this award is a great opportunity to recognize outstanding work published in our journal, while helping to support our research community and further disseminate research in chemistry in Canada. This award has been in development for a while, in conjunction with CSP and the CSC. We are very pleased to see it come to fruition," said **Dr. Yining Huang**, Senior Editor of the CJC.

Nominations will be made by the journal's Editorial Board from the papers published in the previous year (between January and December). Canadian corresponding authors who are interested in applying for the award should submit their work to the CJC at <http://mc06.manuscriptcentral.com/cjc-pubs>

and indicate at time of submission that they would like the manuscript to be considered for the award nomination. The authors should also indicate their intention in the cover letter.

Authors do not need to be a member of the Chemical Institute of Canada to apply, but must hold a professional appointment as an

independent researcher in academia, government, or industry in Canada at the time of nomination.

For full terms of reference and more information, please visit <http://www.nrcresearchpress.com/page/cjc/award>

About the *Canadian Journal of Chemistry*

Published since 1929, this monthly journal reports current research findings in all branches of chemistry. It includes the traditional areas of analytical, inorganic, organic, and physical-theoretical chemistry and newer interdisciplinary areas such as materials science, spectroscopy, chemical physics, and biological, medicinal and environmental chemistry. Articles describing original research and reviews are welcome.

About Canadian Science Publishing

Canadian Science Publishing is an independent, not-for-profit scholarly publisher dedicated to serving the needs of researchers and their communities. The NRC Research Press journals are Canadian Science Publishing's flagship suite of award-winning international publications. We publish 16 titles under this imprint, many in continuous publication since 1929, including the *Canadian Journal of Chemistry*.

MRC the new *Magnetic Resonance in Chemistry*

Wiley: It is with great pleasure that we introduce the new look of *Magnetic Resonance in Chemistry* (MRC) into the community.

Together with this updated design, the editors have taken the opportunity to modernise and to develop the content and editorial structure of our journal to better serve the research needs of our authors and readers. As an editorial board, we recognise that the research trajectory of our community extends beyond the previous moniker of our brand and this rebranding is an endeavour to extend our scope into these developing research horizons.

For more information: **Editorial** "MRC the new *Magnetic Resonance in Chemistry*" *Magnetic Resonance in Chemistry* **52** (2014) 1–2. <http://dx.doi.org/10.1002/mrc.4033>



eMagRes: Retirement of Professor Robin Harris

At the end of 2013 **Professor Robin Harris** will retire from his position as co-Editor in Chief of **eMagRes**. The success of *eMagRes*, and its predecessor the *Encyclopedia of Magnetic Resonance*, has largely been down to Robin's high level of attention to detail and dedication to the publication, with many years of co-ordinating the Editorial Board and assisting the Wiley editorial team in reminding authors of their promise to deliver.

The *eMagRes* team at **Wiley** are enormously grateful for the time and effort that Robin has put into the publication over the years; it has been an honour to work with an Editor who is so enthusiastic about the publication.

Robin's role as Editor-in-Chief, since his appointment in February 1993, has seen him orchestrate multiple large-scale works for the *eMagRes* publication:

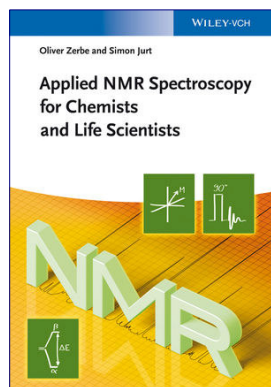
- The original print, 9-volume *Encyclopedia, Encyclopedia of Magnetic Resonance*
- Six Handbooks in the *eMagRes* series
- The second, 10-volume, print edition of the *Encyclopedia of NMR*
- Quarterly online updates to *eMagRes* since 2007

Following his retirement as co-Editor-in-Chief Robin will join the International Advisory Board as its Chairman. As part of this role Robin will continue to provide valuable advice to ensure the future success of *eMagRes*.

Following Robin's retirement **Professor Roderick Wasylishen** will become the sole Editor-in-Chief for the topics relating to NMR in *eMagRes*. We wish Rod every success in his role as Editor-in-Chief.

The **Wiley eMagRes** Team
<http://onlinelibrary.wiley.com/book/10.1002/9780470034590/>

New NMR Books



Applied NMR Spectroscopy for Chemists and Life Scientists

Authors: Oliver Zerbe and Simon Jurt

Paperback: 548 pages
Language: English
Publisher: Wiley-VCH (January 13, 2014)
ISBN: 978-3527327744

<http://www.amazon.com/dp/3527327746>

<http://www.amazon.ca/dp/3527327746>

Wiley: From complex structure elucidation to biomolecular interactions - this application oriented textbook covers both theory and practice of modern NMR applications.

Part one sets the stage with a general description of NMR introducing important parameters such as the chemical shift and scalar or dipolar couplings.

Part two describes the theory behind NMR, providing a profound understanding of the involved spin physics, deliberately kept shorter than in other NMR textbooks, and without a rigorous mathematical treatment of all the physico-chemical computations.

Part three discusses technical and practical aspects of how to use NMR. Important phenomena such as relaxation, exchange, or the nuclear Overhauser effects and the methods of modern NMR spectroscopy including multidimensional experiments, solid state NMR, and the measurement of molecular interactions are the subject of part four.

The final part explains the use of NMR for the structure determination of selected classes of complex biomolecules, from steroids to peptides or proteins, nucleic acids, and carbohydrates.

For chemists as well as users of NMR technology in the biological sciences.

Table of contents

<http://ca.wiley.com/WileyCDA/WileyTitle/productCd-3527327746.html>

Advances in Biological Solid-State NMR

Proteins and Membrane-Active Peptides

Editors: Frances Separovic and Akira Naito

Hardcover: 384 pages

Language: English

Publisher: RSC (March 30, 2014)

ISBN: 978-1849739108



<http://www.amazon.com/dp/1849739102>

<http://www.amazon.ca/dp/1849739102>

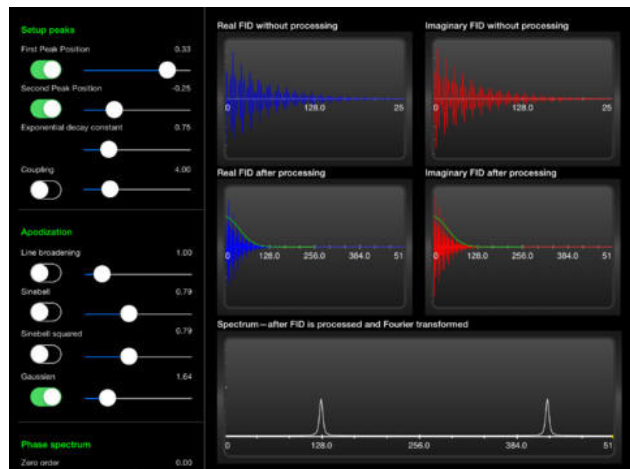
RSC: The complexity and heterogeneity of biological systems has posed an immense challenge in recent years. An increasingly important tool for obtaining molecular and atomic scale information on a range of large biological molecules and cellular components is solid-state NMR. This technique can address fascinating problems in structural biology, including the arrangement of supramolecular complexes and fibril formation in relation to molecular folding, misfolding and aggregation. *Advances in Biological Solid-State NMR* brings the reader up to date with chapters from international leaders of this growing field, covering the most recent developments in the methodology and applications of solid-state NMR to studies of membrane interactions and molecular motions. A much needed discussion of membrane systems is detailed alongside important developments in in situ analysis. Topics include applications to biological membranes, membrane active peptides, membrane proteins, protein assemblies and in-cell NMR. This exposition of an invaluable technique will interest those working in a range of related spectroscopic and biological fields. A basic introduction invites those interested to familiarise themselves with the basic mathematical and conceptual foundations of solid-state NMR. A thorough and comprehensive discussion of this promising technique follows, which will be essential reading for those working or studying at postgraduate level in this exciting field.

View contents and Chapter 1 (free access)

<http://pubs.rsc.org/en/Content/eBook/978-1-84973-910-8>

NMR apps

Learn NMR FID is a free interactive app for iPad written by **Tim Burrow** (University of Toronto) to allow students explore basic NMR acquisition and processing concepts

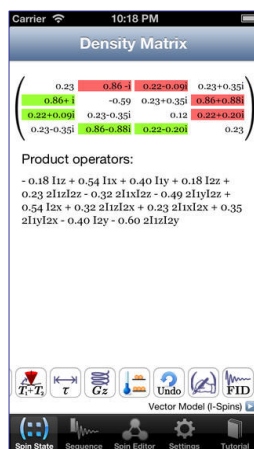


To download **Learn NMR FID** app visit:
<http://itunes.apple.com/us/app/learn-nmr-fid/id785450176>

Let Tim know if you have any suggestions or ideas to improve his app
<http://www.learnnmr.com/>

Another recent app by **Tim Burrow** is the **Attenuator app** for iPhone, iPad, and iPod which will be useful for anyone working with radio frequency sources and needs to know power and voltage after attenuation.

To download the **Attenuator** app visit:
<http://itunes.apple.com/ca/app/attenuator/id367216554>



Insensitive app is written by **Klaus Boldt** (University of Melbourne).

Insensitive simulates the quantum mechanical models that are used to describe NMR experiments. The vector model, density matrix and product operators of an ensemble of up to four spins-1/2 and two spin types are visualized. Each step from the first

radiofrequency pulse to the acquisition of the spectrum can be manipulated. Features include selective pulses, weak and strong coupling, dipolar relaxation, gradients, cartesian and

spherical product operator basis, phase correction, pulse sequence recording and a comprehensive tutorial. To download **Insensitive** visit:

<http://itunes.apple.com/ca/app/insensitive/id385275424>

Insensitive is intended for education or self education in NMR at an intermediate level. It does not teach how to interpret spectra, but rather focuses on the visualization of textbook NMR theory. Free Mac OS X version of **Insensitive** is available for download at

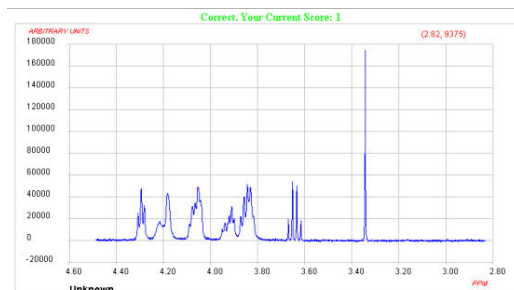
<http://www.chemie.uni-hamburg.de/nmr/insensitive>

For more background information about **Insensitive** and to cite

Klaus Boldt "Simulating spin dynamics in NMR with a new computer program intended for education: Inensitive" *Concepts in Magnetic Resonance Part A* **38** (2011) 17–24.
<http://dx.doi.org/10.1002/cmr.a.20203>

The Spectral Game is a web-based game where players try to match molecules to various forms of interactive spectra including ^1H and ^{13}C NMR spectra, Mass spectra, Infrared, NIR and UV-Vis spectra, and Raman spectra. Each correct selection earns the player one point and play continues until the player supplies an incorrect answer. Try it today!

<http://www.spectralgame.com/>



Click on the molecule that corresponds to the spectrum. Hit F11 to enlarge browser window.
No spectrum? Spectrum reversed? **FLAG IT!**
No spectrum? Something wrong with the spectrum? Comment. (opens in new window)

For more information

J.-C. Bradley, R.J. Lancashire, A.S. Lang and A.J. Williams "The Spectral Game: leveraging Open Data and crowdsourcing for education" *Journal of Cheminformatics* **1** (2009) 9. (**Open Access**)

<http://dx.doi.org/10.1186/1758-2946-1-9>

NMR Jobs and Vacancies

Two Graduate Positions, Environmental NMR Center, University of Toronto

Two Graduate Positions in the "Development of In-vivo NMR Spectroscopy to Understand Environmental Stress" in the Environmental NMR Center at the University of Toronto, Canada

Professor Andre Simpson is looking for graduate students for Sept 2014.

Applications to both the Department of Chemistry (MSc or PhD)

<http://www.chem.utoronto.ca/grad/>

and Environmental Science (PhD only)

<http://www.uts.utoronto.ca/~physsci/phd/>

are now being accepted.

Canadian students wanting to complete a PhD are preferred. International students cannot be accepted through the Chemistry program, but may be considered through the Environmental Science PhD program under exceptional circumstances.

Students interested in these positions can contact

E-mail: andre.simpson@utoronto.ca

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

Research Project Description

Present environmental policies are set primarily on the basis of acute toxicity of individual chemical species, however, additional molecular-level information is desperately needed to help understand risks associated with sub-lethal toxicity of individual compounds and mixtures. This includes understanding: the toxic mode of action, bioaccumulation, biotransformation, excretion and contaminant binding *in-vivo*. This is stressed in an report "Toxicity Testing in the 21st Century" (EPA) which states "*The new paradigm should facilitate evaluating the susceptibility of different life-stages, understanding the mechanisms by which toxicity occurs, and considering the risks of concurrent, cumulative exposure to multiple and diverse chemicals*".

Nuclear Magnetic Resonance (NMR) is one of the most powerful tools in modern research and unlike most analytical approaches can be

applied *in-vivo*. Comprehensive Multiphase (CMP) NMR spectroscopy (a novel NMR technology co-developed between my research group and Bruker) permits the full range of solid, gel and liquid NMR experiments to be performed on an intact samples. As such CMP-NMR holds the potential study of *all bonds* in *all phases* to be studied and differentiated *in-situ* in unaltered samples. CMP-NMR has yet to be applied *in-vivo* but is ideal for unravelling the fate, interactions and reactivity of contaminants *in-vivo* as well as identifying any structural changes in the organism. In addition, static NMR flow studies (i.e. organism in a tube supplied with food and oxygen) provide a complimentary low stress environment to study an organism's metabolic response.

This research will combine CMP-NMR and static flow NMR to provide an ideal framework that permits the direct correlation between the *in-vivo* fate/reactivity of the contaminant and the organism's metabolic response to the stressor. The resulting information is important to answering key questions such as: What is the toxic-mode-of-action of the contaminant and the biochemical pathways disturbed?; When bound, is a contaminant still toxic?; Does permanent binding/sequestration of the contaminant occur *in-vivo*?; Do more toxic or highly reactive (for example radicals) biotransformation products form?; Are metabolic perturbations permanent or do the organisms fully recover?; Can sub-lethal levels of numerous contaminants produce a synergistic toxic effect?; How do environmental conditions affect these processes? Answers to these questions are critical for setting meaningful and realistic environmental policies regarding contaminant-levels but are in large part impossible or very challenging to answer using standard acute toxicity tests which are currently the most common practice.

This proposed research will impact many areas. CMP-NMR will be developed for the first time *in-vivo* (in any field) and as it holds the potential for *all bonds* in *all phases* to be studied and differentiated it likely represents a key future tool to understand biological processes in general. Second, this research will improve the fundamental understanding of aquatic toxicity. By simultaneously measuring contaminant behavior and the metabolic stress response from the organism it should be

possible to explain why and how certain chemicals (and mixtures) are toxic and how this varies with environmental conditions.

Ph.D. Position in Structural Biology, Institut de Biologie Structurale, Grenoble, France
http://nmr900.ca/nmr_jobs.html#IBS

Solid-State NMR Postdoctoral Position, Pacific Northwest National Laboratory, Richland, WA, U.S.
http://nmr900.ca/nmr_jobs.html#pnpl

Tenure Track Academic Position in Sustainable Chemistry, Memorial University of Newfoundland
<http://www.mun.ca/chem/news.php?id=2954>

Three small molecule **NMR spectroscopist** positions at Merck, New Jersey. U.S.
http://nmr900.ca/nmr_jobs.html#Merck

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- Victor Tersikh** @nmr900 · 1h
NMRCM 2014, 11th International Symposium and Summer School, July 7-11, 2014, Saint-Petersburg, Russia nmr.phys.spbu.ru/nmrcm/
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Technician in Nuclear Magnetic Resonance - Lancaster University - [jobs.ac.uk](http://jobs.ac.uk/job/AIG349/tec...)
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Chemical Institute of Canada Career Site
<http://niche.workopolis.com/frontoffice/enterSeekerHomeAction.do?sitecode=pl56>

Academic jobs at Canadian universities AUCC)
http://oraweb.aucc.ca/pls/ua/ua_re

Wiley Job Network: Search Healthcare, Science, and Academic Jobs
<http://www.wileyjobnetwork.com/>

Canadian NMR Research Highlights

Protein Ensemble Database

M. Varadi, S. Kosol, P. Lebrun, E. Valentini, M. Blackledge, A.K. Dunker, I.C. Felli, J.D. Forman-Kay, R.W. Kriwacki, R. Pierattelli, J. Sussman, D.I. Svergun, V.N. Uversky, M. Vendruscolo, D. Wishart, P.E. Wright and P. Tompa, "pE-DB: a database of structural ensembles of intrinsically disordered and of unfolded proteins," *Nucleic Acids Research* **42** (2014) D326-D335. (**Open Access**)
<http://dx.doi.org/10.1093/nar/gkt960>

Abstract: The goal of pE-DB (<http://pedb.vib.be>) is to serve as an openly accessible database for the deposition of structural ensembles of intrinsically disordered proteins (IDPs) and of denatured proteins based on **nuclear magnetic resonance spectroscopy**, small-angle X-ray scattering and other data measured in solution. Owing to the inherent flexibility of IDPs, solution techniques are particularly appropriate for characterizing their biophysical properties, and structural ensembles in agreement with these data provide a convenient tool for describing the underlying conformational sampling. **Database entries consist of** (i) primary experimental data with descriptions of the acquisition methods and algorithms used for the ensemble calculations, and (ii) the structural ensembles consistent with these data, provided as a set of models in a Protein Data Bank format. PE-DB is open for submissions from the community, and is intended as a forum for disseminating the structural ensembles and the methodologies used to generate them. While the need to represent the IDP structures is clear, methods for determining and evaluating the structural ensembles are still evolving. The availability of the pE-DB database is expected to promote the development of new modeling methods and leads to a better understanding of how function arises from disordered states.

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

One of the authors of this important work **Julie Forman-Kay** (Hospital for Sick Children) had discussed her research in disordered proteins in a podcast interview with *the Chemistry*

World in 2011. This podcast is 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 was also featured in the printed August 2011 issue of the *Chemistry World* (subscription required):

M. Gross "Anarchy in the proteome", *Chemistry World* **8** (2011) 42-45.

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

Israel Journal of Chemistry
Special Issue in Celebration of
Prof. Shimon Vega's 70th Birthday

Volume 54, Issue 1-2
pp. 1-221 (February, 2014)

<http://onlinelibrary.wiley.com/doi/10.1002/ijch.v54.1/2/issuetoc>

free access to all papers in this issue

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M.J. Smith, M. Ikura, "Integrated RAS signaling defined by parallel NMR detection of effectors and regulators," *Nature Chemical Biology* **10** (2014) 223-230.

<http://dx.doi.org/10.1038/nchembio.1435>

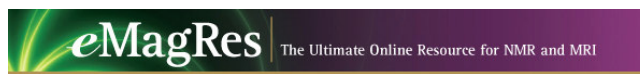
P.B. Stathopoulos, R. Schindl, M. Fahrner, L. Zheng, G.M. Gasmir-Seabrook, M. Muik, C. Romanin & M. Ikura, "STIM1/Orai1 coiled-coil interplay in the regulation of store-operated calcium entry," *Nature Communications* **4** (2013) 2963.

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L. Shia and L.E. Kay, "Tracing an allosteric pathway regulating the activity of the HslV protease," *Proc. Natl. Acad. Sci. USA* (2014) online.

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A. Sutrisko, A.J. Simpson, "Metals in the Environment," *eMagRes* **2** (2013) 467-476.

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(Review)

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<http://dx.doi.org/10.1016/B978-0-12-800185-1.00001-2>



NMR research could help oilsands

Lethbridge Herald highlights recent research on asphaltenes by **Paul Hazendonk** and colleagues from the University of Lethbridge. <http://lethbridgeherald.com/news/local-news/2013/12/13/research-could-help-oilsands/>

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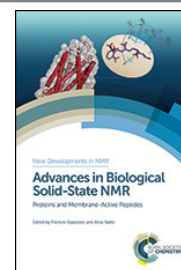
Editorial in Magnetic Resonance in Medicine

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Advances in Biological Solid-State NMR Proteins and Membrane-Active Peptides

Editors: Frances Separovic and Akira Naito
RSC Publishing, 2014

<http://dx.doi.org/10.1039/9781782627449>



Sherry S.W. Leung and Jenifer Thewalt "Deuterium NMR of Mixed Lipid Membranes" Chapter 10 in *Advances in Biological Solid-State NMR: Proteins and Membrane-Active Peptides*, RSC Publishing (2014) 180-199. <http://dx.doi.org/10.1039/9781782627449-00180>

Matthieu Fillion, Normand Voyer and Michèle Auger "Membrane Interactions of Amphiphilic Peptides with Antimicrobial Potential: A Solid-State NMR Study" Chapter 11 in *Advances in Biological Solid-State NMR: Proteins and Membrane-Active Peptides*, RSC Publishing (2014) 200-213. <http://dx.doi.org/10.1039/9781782627449-00200>

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Recent NMR Publications

Most recent NMR publications by Canadian research groups as they appear on <http://nmr900.ca> website. This list should not be considered complete. Let us know of your recent publications as they become available.

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