Canadian NMR News

contributed by Andrew Lewis (SFU)

SFU Bruker Spectroscopy Facility Opening

The new Bruker Spectroscopy Facility in Simon Fraser University's Department of Chemistry was officially opened on June 27, 2012 by the SFU president Andrew Petter, the president of Bruker Canada Henry Stronks, and Mario Pinto SFU's Vice President, Research. The naming of the Facility recognizes Bruker's ongoing support of faculty, students and advanced scientific endeavors at SFU through equipment donations, in-kind matching, ongoing technical support and training, and highlights a relationship spanning more than 32 years. At the opening, which also celebrated the completion of the $50 M renovation of the Chemistry Department's space in the Shrum Science Center, Dr. Henry Stronks announced the donation of a new Bruker **maXis IMPACT** ultra-high resolution time-of-flight mass
spectrometer valued at more than $400,000, which has just been installed.

SFU was the home of Canada's first 600 MHz NMR spectrometer and is still very well equipped for NMR, currently boasting access to the Bruker solids and liquids 850 MHz NMR system recently installed at UBC in addition to two Bruker cryoprobe-equipped 600 MHz systems, Bruker 400 and 500 MHz multi-receiver spectrometers (all with sample changers), a Bruker 360 MHz microimaging system, plus a customized Bruker 400 MHz wide-bore multireceiver system for solids and micro-imaging having a full complement of high performance r.f. and gradient amplifiers, plus numerous specialized MAS and micro-imaging probes. The Chemistry Department also has three Bruker mass spectrometers, two Bruker EPR systems, and two Bruker x-Ray diffractometers. This equipment is crucial to research undertaken in the Chemistry Department, but it is also used by Biological Sciences, Molecular Biology and Biochemistry, Archaeology, Kinesiology, the Faculty of Health Science, research institutions such as NRC, the Center for Drug Research and Development, governmental agencies, and numerous commercial enterprises.

The Facility Director Dr. Andrew Lewis notes that the new Bruker instruments are already making a huge impact on chemistry related research at SFU, as well as helping to reinvigorate and modernize the Chemistry undergraduate students' experiences through hands-on use. The recently established SFU Bruker Prize in Chemical Spectroscopy is also helping to encourage mastery of the various analytical techniques, thereby fostering and supporting a new generation of experts in spectroscopy.

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**NSERC 2012 Competition Results**

**Discovery Grants**

**Kim Baines** (Western) Low Coordinate Main Group Chemistry: Discovery and Innovation

**Christian Detellier** (Ottawa) Clay minerals based nanohybrid materials

**Gillian Goward** (McMaster) Solid-State Magnetic Resonance Studies of Reaction Mechanisms and Ion Dynamics in Materials for Energy Storage and Conversion

**Pierre Harvey** (Sherbrooke) Donor-acceptor polymers and complexes for photocells and photoinduced H₂-evolution

**Michael Hayden** (Simon Fraser) Frontiers in Nuclear Magnetic Resonance and Magnetic Particle Imaging

**Yining Huang** (Western) Structural Characterization of Nanoporous Materials by Solid-state NMR and Vibrational Spectroscopy

**Peter Macdonald** (Toronto) NMR Lateral Diffusion Measurements in Biomembranes

**Benedict Newling** (New Brunswick) Advances in Magnetic Resonance Imaging (MRI) of Flow

**Suzana Straus** (UBC) Structure and Function of Membrane-Associated Peptides and Proteins

**Discovery Accelerator Supplement**

$120,000 over three years

**Yining Huang** (Western) Structural Characterization of Nanoporous Materials by Solid-state NMR and Vibrational Spectroscopy

**Research Tools and Instruments (RTI)**

**David Bryce** (Ottawa) Single-Crystal NMR Probe for Studies of Weak Interactions and Novel Materials

**Adam Dyker** (New Brunswick) Replacement Console for Varian UNITY 400 NMR Spectrometer

**Paul Hazendonk** (Lethbridge) Solution- and Solid-State 500 MHz Nuclear Magnetic Resonance Facility Upgrade

**David Jakeman** (Dalhousie) A SmartPROBE for NMR studies

**Adrian Schwan** (Guelph) A New Multinuclear Cryoprobe for Nuclear Magnetic Resonance
La moule: nouveau biomatièriaux de pointe?

Le Code Chastenay is a weekly Quebec television program broadcasted on Télé-Québec and led by Pierre Chastenay, an astronomer at the Montreal Planetarium. The mandate of the program is to popularize research science and technology conducted in Quebec. Earlier this year the show featured an interview with Isabelle Marcotte, Associate Professor at the Department of Chemistry, Université du Québec à Montréal, about their work in NMR structural studies of mussel byssus and development of biomaterials.

To watch the episode (in French) http://tinyurl.com/d8j8up2

VIVA 6 NMR Symposium

The 6th Victoria-Vancouver (VIVA) NMR symposium recently held at Simon Fraser University was a great success. A smaller version of the long-standing MOOT NMR conference, this annual event seeks to bring together people using NMR in the Pacific Northwest, to build and foster an NMR community, and to provide a venue where students rather than professors are encouraged to present their research. As in past years, this event was made possible through the generous financial support of Bruker Canada, Agilent, Cambridge Isotopes Ltd., and the UBC and SFU NMR Facilities. Next year VIVA will be hosted by Chris Barr, the new NMR facility manager at the University of Victoria, on Vancouver Island.

MR Enterprise under siege

Helium gas shortage

Feature article in C&EN "Helium shortage affecting instrument users to extend into 2013" v90/29, p.32-34, July 16, 2012 http://tinyurl.com/ccakg3w

"Low helium supply, high prices affect balloons, MRIs," CBC News, June 18, 2012 http://tinyurl.com/7aok7uc


Deuterium isotope shortage


Helium-3 isotope shortage

"Helium shortage putting medical research up in the air" The Globe and Mail, August 6, 2012 http://tinyurl.com/9cfschc

Petition to "Reclaim the Magnetic Resonance Gordon Research Conference"

Dear Colleagues,

Please see the link below regarding a petition to start a new Gordon Research Conference on "Frontiers of Magnetic Resonance". The short version is that the original Magnetic Resonance GRC was unfortunately cancelled recently due to insufficient attendance over the past several years, perceived by the GRC organizers to be due to the lack of interest in the magnetic resonance community - much more information on this is provided in the link http://www.ipetitions.com/petition/reclaim-the-magnetic-resonance-grc/

If you are supportive of this effort please sign the petition, and also forward to other colleagues in the community whom I may have accidentally left out and who you think may be interested in having the magnetic resonance GRC meeting reinstated. Many thanks.

Best regards,

Christopher Jaroniec, Associate Professor
Ohio State University
http://chemistry.osu.edu/~jaroniec/
Recognition

Recognition: Anthony Mittermaier
reposted from Agilent with permission

Agilent Technologies has announced the winner of the fourth annual Agilent Early Career Professor Award. Dr. Anthony Mittermaier, associate professor of chemistry at McGill University in Montreal, Canada, will receive $50,000 per year for two years in his name, to support his research. Mittermaier joined the faculty in the department of chemistry at McGill in 2005 and has used nuclear magnetic resonance (NMR) spectroscopy in his research to develop an understanding of how the primary amino-acid sequence of a protein determines its dynamic properties. His work has also established links between structural mobility at the microscopic level and functional activity at the macroscopic level.

This year’s award focused on the field of structural biology using NMR, an area of research highly valued by Agilent. To qualify for the award, a professor must make significant contributions to the subset of structural biology that uses NMR techniques to improve understanding of the molecular structure and function of nucleic acids or proteins. Mittermaier’s research has successfully applied molecular biology, mutagenesis methods and NMR to probe the relationship between protein sequences, dynamics and function.

"We are delighted to learn that Agilent has selected our colleague Anthony Mittermaier for this prestigious award," said Professor R. Bruce Lennox, chair of McGill’s department of chemistry. "Professor Mittermaier is a pioneer in recognizing the power of an integrated dynamic and thermodynamic approach to understanding protein behavior. His combined NMR/calorimetry approach to sorting out the coupled protein folding/allostery problem is likely to find widespread application to many protein systems."

"This year, we were fortunate to have another group of impressive candidates," said Jack Wenstrand, director of University Relations at Agilent. "Our winner, Dr. Anthony Mittermaier, has demonstrated the highest level of excellence and skill in structural biology, and we are looking forward to following his innovative research endeavors."

The Agilent Early Career Professor Award is presented annually to recognize and encourage excellence in measurement research. It seeks to establish strong collaborative relationships between Agilent researchers and leading professors early in their careers, as well as to underscore Agilent’s role as a sponsor of university research. More details are available at http://www.agilent.com/univ_relation/profaward/index.shtml

Professor Roderick Wasylishen (University of Alberta) has been awarded one of the highest accolades in the field of solid-state NMR spectroscopy. Rod has been selected as the 2014 Vaughan Lecturer at the Rocky Mountain Conference on Analytical Chemistry.

The Vaughan lecture series is named in honour of Robert W. Vaughan (1941-1979), an extraordinary scholar and leader in solid-state NMR.

To learn more about the award and to see the list of past Vaughan Lecturers visit the RMCAC website. http://www.rockychem.com/honors/vaughan-lecturer.html

Professor Lewis Kay (University of Toronto) has been named the University Professor, the highest honour awarded to a University of Toronto faculty member.

Read the full story at the UofT News "Changing the way we look at molecules. Globally renowned chemists recognized." http://news.utoronto.ca/changing-way-we-look-molecules
Recognition (continued)

contributed by Andrew Lewis (SFU)

**SFU Bruker Prize in Chemical Spectroscopy**

Linus Chiang from Dr. Tim Storr’s group is the winner of the 2012 SFU Bruker Prize in Chemical Spectroscopy. His publication "Radical Localization in a Series of Symmetric Ni(II) Complexes with Oxidized Salen Ligands" has been accepted for publication in *Chemistry - A European Journal*. The prize recognizes Chemistry graduate students at Simon Fraser University who use cutting-edge techniques, develop new experimental methods, or perform detailed theoretical analyses of spectroscopic data to solve chemical problems. Thanks in part to generous support from Bruker Canada, Linus receives $1,000 towards conference expenses. The prize was presented by the president of Bruker Canada Dr. Henry Stronks at the recent celebration marking the official opening of the SFU Bruker Spectroscopy Facility.

Past winners include Monica Szczepina (2010), Jefferson Chan (2010), Brinda Prasad (2011) and Mike Webb (2011). For further details see: [www.chemistry.sfu.ca/teaching/scholarships/Brukerprize](http://www.chemistry.sfu.ca/teaching/scholarships/Brukerprize)

reposted from [http://www.chem.ubc.ca](http://www.chem.ubc.ca)

Associate Professor Suzana Straus (UBC Chemistry) was recently awarded a Marie Curie International Incoming Fellowship. These awards, granted by the European Commission, are designed to attract top-class researchers to work and undertake research in Europe with the ultimate goal of developing mutually-beneficial research cooperation between Europe and Canada.

Dr. Straus is conducting research at the Institut Laue Langevin, a world-renowned neutron research facility located in Grenoble, France. The Marie Curie IIF will enable her to study the mechanism of action of lipopeptide antibiotics, the interaction of lipopeptides with bacterial membrane components, and the assembly of filamentous bacteriophage. She will learn about a range of techniques such as small angle neutron scattering, neutron reflectivity, and diffraction methods.

**NMR Theses Recently Defended**

**Irene Kwan** (Queen's University) June 25, 2012

Supervisor: Prof. Gang Wu

**Ph.D. thesis:** "Structural Elucidation of Guanosine Self-Assemblies Using Spectroscopic and Computational Methods"

External Examiner: Prof. Glenn Penner (University of Guelph)

[http://qspace.library.queensu.ca/handle/1974/7295](http://qspace.library.queensu.ca/handle/1974/7295)

**Jonathan Guimond-Tremblay** (Université Laval), 2012

Supervisor: Jean-François Paquin

Co-supervisor: Michèle Auger

**M.Sc. thesis:** "Synthèse et propriétés d'analogues monofluorés de la 1,2-dimyristoyl-sn-glycéro-3-phosphocholine: Vers la création de nouvelles sondes topologiques membranaires"

[http://archimede.bibl.ulaval.ca/archimede/meta/28670](http://archimede.bibl.ulaval.ca/archimede/meta/28670)

**Andre Sutrisno** (University of Western Ontario), April 2012

Supervisor: Prof. Yining Huang

**Ph.D. thesis:** "Solid-State Nuclear Magnetic Resonance Spectroscopy of Low-Gamma Quadrupolar Nuclei in Inorganic Materials"

External Examiner: Prof. Darren Brouwer (Redeemer University College)

[http://ir.lib.uwo.ca/etd/460/](http://ir.lib.uwo.ca/etd/460/)
On the move

**Irene Kwan**, after successfully defending her Ph.D. thesis in the Gang Wu group (Queen's), Irene has taken up an analytical chemist position at Apotex in Toronto.

**Becky Chapman** (Ph.D., 2012, Bryce group, Ottawa) has taken up a position at the Council of Canadian Academies (CCA) in Ottawa. The CCA is an independent, not-for-profit corporation that supports science-based, expert assessments to inform public policy development in Canada.

**Cory Widdifield** (Ph.D, 2012, Bryce group, Ottawa) has taken up a postdoctoral fellowship under the supervision of Lyndon Emsley at the CRMN in Lyon, France.

**Luke O’Dell** joined NRC Canada in Ottawa as a Research Associate in October 2009, working under Dr. Chris Ratcliffe and Dr. Andreas Brinkmann on a number of projects including the development of $^{14}$N methods, applications of optimal control theory and DFT calculations for quadrupolar nuclei, and high-pressure magic angle spinning NMR. On August 1st Luke started a new position as a Senior Lecturer at Deakin University (Victoria, Australia) where he will continue to pursue his current research interests as well as teaching and building his own research group. [http://deakin.edu.au/](http://deakin.edu.au/)

The 900 NMR Facility News

**NMR Facility Annual Report 2011-2012**

Dear NMR Facility Users:

we are preparing our 2011-2012 Annual Report and we would like to receive the following information from you by the August 25th deadline:

1) a brief progress report for each of your research projects. Please prepare a separate report for each project, regardless of whether the project has ended or not. Each report should illustrate for non-NMR specialists major project findings and should normally not exceed one-two pages (text and figures) (preferably MS Word format, or an ASCII text + figures separately). Selected progress reports will be included in the printed version of the Annual Report [http://nmr900.ca/annual_e.html](http://nmr900.ca/annual_e.html)

2) 2011-2012 research publications featuring results from the 900 instrument (published, accepted, submitted)

3) 2011-2012 Honor theses, Ph.D. theses and similar works by your students using the 900 results (please indicate name of the student, department, title of thesis, date of the defence)

4) any other relevant information you may consider useful including in our report

Let me know if any questions, and thank you for your contribution!

On behalf of the Facility Steering Committee, Victor Terskikh

Email: terskikhv@nrc-cnrc.gc.ca

**2010-2011 Annual Report**

the 2010/11 Annual Report of the 900 NMR Facility is available for download at [http://nmr900.ca/annual_e.html](http://nmr900.ca/annual_e.html)
25th MOOT NMR Minisymposium

We are pleased to announce that the 25th MOOT NMR Minisymposium will be held at Université Laval in Quebec City on October 20-21, 2012.

Registration for the 25th MOOT is now open. Please visit the MOOT web site for information about registration and the banquet.

The deadline for registration is October 1st (August 20th if you have dietary requirements)

http://nmr.ulaval.ca/moot/registration.html

The talks and poster session will be held in Pavillon Alexandre-Vachon at Université Laval.

The banquet will be held at the Morrin Centre in historical old Quebec City. This is the site of the city’s first prison, built over 200 years ago, as well as the site of the Morrin College from 1862-1902. http://nmr.ulaval.ca/moot/location.html

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

We are looking forward to seeing you in Quebec City in October.

Michèle Auger et Stéphane Gagné

25th MOOT NMR Minisymposium
October 20-21, 2012
Université Laval
Québec City
http://www.mootnmr.org

5ème COLLOQUE ANNUEL DU GRASP
5th ANNUAL GRASP SYMPOSIUM

November 19, 2012, 8:00am - 6:30pm
McGill New Residence Hall
3625 Avenue du Parc
Montréal, QC, H2X 3P8
514-398-3471

Dear Colleagues,

Drs. Kalle Gehring and Albert Berghuis would like to invite you to take part in the fifth scientific symposium of GRASP (Groupe de Recherche Axé sur la Structure des Protéines).

Outstanding international speakers - Gregory Petsko, Wolfgang Peti, Frank Sicheri, Anne-Claude Gingras, Paul de Koninck, Brian Sykes - poster sessions, exhibitors and short talks will be presented at this auspicious event, demonstrating the affluence of structural biology research in Quebec.

Registration is free, thanks to our very generous sponsors, but you need to register if you want your abstract to be selected for an oral presentation and/or your abstract title to be printed in the booklet. Registration is not yet open, but is coming soon!

For information about this symposium, please send an email grasped@mcgill.ca or visit http://grasp.mcgill.ca/english/conferences/conferences.html

Sincerely,

The organizing committee:

Kalle Gehring, GRASP Director
Albert Berghuis, GRASP Co-Director
Annick Guyot, GRASP Coordinator

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

August 19-24, 2012, Lyon, France
http://www.pasteur.fr/infosci/conf/sb/ICMRBS/
NMR Events (continued)

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

**SMARTER 3 Conference**
September 10-13, 2012, Versailles, France

**IV Ibero-American NMR Meeting**
September 25-28, 2012, University of Aveiro, Portugal
http://www.spq.pt/eventos/iberoanmr2012/

**VIIth Symposium “Nuclear Magnetic Resonance in Chemistry, Physics and Biological Sciences”**
September 26-28, 2012, Warsaw, Poland
http://www.icho.edu.pl/SympNMR2012/home.html

**CSChE 2012,** the 62nd Canadian Chemical Engineering Conference
October 14-17, 2012, Vancouver, BC, Canada
http://www.csche2012.ca

**PANIC “Practical Applications of NMR in Industry Conference”**
October 15-17, 2012, Chicago, IL
https://m360.casss.org/event.aspx?eventID=42925

**MOOT XXV NMR Symposium**
October 20-21, 2012, Université Laval, Quebec City
http://www.mootnmr.org

**5th Annual GRASP Symposium**
November 19, 2012, McGill University, Montréal, QC, Canada
http://grasp.mcgill.ca/english/conferences/conferences.html

**Frontiers of NMR in Biology**
Keystone Symposium
January 13-18, 2013, Snowbird, Utah, U.S.
http://www.keystonesymposia.org/index.cfm?enweb.Meeting.Program&meetingId=1181

**54th ENC**
April 14-19, 2013, Asilomar, Pacific Grove, California
http://www.enc-conference.org/

**18th Triennial ISMAR Conference**
May 19-24, 2013, Rio de Janeiro, Brazil
http://www.ismar2013.net/
Registration will open September 21st, 2012

**CSC 2013,** the 96th Canadian Chemistry Conference and Exhibition
May 26-30, 2013, Québec, Québec, Canada
http://www.csc2013.ca/

**Computational Aspects of Metabolomic NMR**
Gordon Research Seminar
June 1-2, 2013 Mount Snow Resort West Dover, VT

**Computational Aspects of Biomolecular NMR**
Gordon Research Conference
June 2-7, 2013 Mount Snow Resort West Dover, VT
http://www.grc.org/programs.aspx?year=2013&program=bionmr

**7th Annual VIVA NMR Symposium**
June 2013, University of Victoria, Victoria B.C.

**EUROMAR 2013**
June 30 – July 5, 2013, Hersonissos, Crete, Greece
http://euromar2013.org/

**8th Alpine Conference** on Solid-State NMR
September 8-12, 2013, Chamonix Mont-Blanc, France
http://www.alpine-conference.org

**SMASH 2013** Small Molecule NMR Conference
September, 2013, Santiago de Compostela, Spain
http://www.smashnmr.org/
Wiley: Many important materials do not contain spin-1/2 nuclei traditionally investigated by NMR spectroscopy and secondly, dissolving solid materials in a solvent may be impossible or may destroy the integrity of the material. All these obstacles can be overcome by NMR experiments at high-magnetic field strengths and investigating the properties of quadrupolar nuclei.

This Handbook gives an up-to-date account of NMR of quadrupolar nuclei in the solid state. Each chapter of the Handbook has been prepared by an expert who has made significant contributions to our understanding and appreciation of the importance of NMR studies of quadrupolar nuclei in solids.

The text is divided into three Parts:
A) Basic Principles of Quadrupolar NMR
B) Advanced Solid-State NMR Techniques to Investigate Quadrupolar Nuclei
C) Applications Involving NMR Studies of Quadrupolar Nuclei in Solids.

The first section provides the reader with the background necessary to appreciate the challenges in acquiring and interpreting NMR spectra of quadrupolar nuclei in solids. The second section presents cutting-edge techniques and methodology for employing these spectroscopic techniques to investigate quadrupolar nuclei in solids. The final section explores applications of solid-state NMR studies of solids ranging from investigations of biological samples to porous materials, catalysts, geological samples and high-temperature superconductors.

All these articles will be published on EMR:

Wiley: Many important materials do not contain spin-1/2 nuclei traditionally investigated by NMR spectroscopy and secondly, dissolving solid materials in a solvent may be impossible or may destroy the integrity of the material. All these obstacles can be overcome by NMR experiments at high-magnetic field strengths and investigating the properties of quadrupolar nuclei.

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All these articles will be published on EMR:

Solid State NMR: Basic Principles & Practice

David C. Apperley (Author), Robin K. Harris (Author), Paul Hodgkinson (Author)

Hardcover: 280 pages
Language: English
Publisher: Momentum Press, June 2012
ISBN: 978-1606503508
http://www.amazon.com/dp/1606503502/
http://www.amazon.ca/dp/1606503502/

Encyclopedia of NMR
(2nd edition)

Roderick E. Wasylishen (Editor)
Robin K. Harris (Editor)

Hardcover: 6240 pages
Language: English
ISBN: 978-0470058213
Publisher: Wiley, October 2012
http://www.amazon.com/dp/0470058218/
http://www.amazon.ca/dp/0470058218/

Encyclopedia of Magnetic Resonance: NMR, Second Edition captures every aspect of the interdisciplinary nature of magnetic resonance and provides the most complete and up-to-date source in the field. The articles are presented in alphabetical order and the wide use of cross references make it easy to find the appropriate information. With more than 50% new and updated articles, the Second Edition features a full focus on all aspects of NMR and includes NMR of Biomolecules and NMR of Solids. All articles are published online on the Encyclopedia of Magnetic Resonance.
NMR Software

contributed by David Bryce (Ottawa)

**QUEST – QUadrapolar Exact SofTware**

**QUEST** is a new program for the exact simulation of solid-state NMR spectra of quadrupolar nuclei in stationary powdered samples which employs diagonalization of the combined Zeeman-quadrupolar Hamiltonian. The program may be used to simulate NMR spectra over the full regime of Larmor and quadrupolar frequencies, which encompasses scenarios ranging from high-field NMR to nuclear quadrupole resonance (NQR, where the Larmor frequency is zero) and does not make use of approximations when treating the quadrupolar interaction. The program, which uses a graphical user interface, also incorporates chemical shift anisotropy and non-coincident chemical shift and quadrupolar tensor frames. QUEST can be used to simulate static NMR and NQR spectra with any relative size of the Zeeman and quadrupolar interactions and correctly predicts the appearance of “forbidden” or “overtone” NMR as well as NQR transitions.

**QUEST version 1.1.1** is now available for download on the software page at

http://mysite.science.uottawa.ca/dbryce/

Updates include optional Boltzmann population effects, an interactive cursor, spin-3 nuclides, vertical scaling, variable coil angle for all spins, and more!

QUEST is described in an article just published in *Solid State Nuclear Magnetic Resonance* (2012).


http://dx.doi.org/10.1016/j.ssnmr.2012.05.002

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**ACD/Spectrus Processor Review**

In early 2012 Advanced Chemistry Development, Inc., (ACD/Labs) released ACD/Spectrus Processor, an all-in-one, multi-technique analytical data processing and chemical characterization tool for synthetic chemists.

http://www.acdlabs.com/products/adh/spectrusprocessor/

Professor **Eugene Kwan** of Harvard University reviewed the software and shares his impressions in this article for the *Journal of Chemical Information and Modeling*.

Looking specifically at the NMR capabilities of the software he discusses the ease of multiplet analysis (integration and determination of coupling constants), automatic generation of multiplet reports, and the capability for working with series of spectra and using ACD/NMR predictors in teaching.

**E. Kwan**: "A CD/Spectrus Processor is a commercial suite of programs for the analysis of NMR, MS, optical, and chromatographic data. Many readers are likely familiar with an earlier version of the program, ACD/NMR Processor, which only handled NMR data and is still freely available to academics. ACD/Spectrus Processor is a newer, commercial version of this software that is much more user-friendly. This review is restricted to the NMR-related capabilities of ACD/Spectrus Processor and an associated program, ACD/NMR Predictor."


http://dx.doi.org/10.1021/ci300249w

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**NMR Tools for Origin 8.5.x, 8.6**


**Features:** Import 1D & 2D data (FID or spectrum), MacNMR, NTNMR, FIDCSI, XWINNMR, MSL, CMXW, Spinsight, VNMR and more.

**1D processing** (either dimension), Baseline correction, left|right shift, apodize, zero fill, FT, IFT, Hadamard transform, phase adjust, SNR and more.

**2D processing**, Transpose, slice selection, coaddition, phase cycling and more.
The Bruker Dynamics Center

Bruker Biospin's Dynamics Center (DC) is a new, standalone program for fitting relaxation and diffusion NMR parameters for both small molecules (solids and liquids) and for biological samples. The small molecules part (the General Dynamics Center) requires only a TopSpin license and can be used for analysing $T_1$, $T_2$, $T_1\rho$, DOSY (using ILT or DOSY transform), REDOR, and CP buildup experiments, while the Protein Dynamics Center requires a separate license and can be used to fit heteronuclear NOE, $T_1$, $T_2$, $T_1\rho$, exchange, and NOE/$T_1$/T_2 data.

For more information, contact Robin Stein (robin.stein@bruker.ca), Martine Monette (martine.monette@bruker.ca), or Joseph Weiss (joseph.weiss@bruker.ca).

The programs can be downloaded for Windows or Linux machines by logging into http://www.bruker-biospin.com and clicking on Service & Support > NMR > Software Downloads > Dynamics Center (for either Windows or Linux) (Fig.1). Tutorials with data are also available from this page, as is a link to license request forms.

Using the Dynamics Center

Both parts of the DC are organized into methods (such as $T_1$ or hetero NOe), each of which has several nodes, or steps to follow, which have to be gone through in order. The manual is available under Help>Manual. Data to be analyzed with the DC should be processed up to the point where the relaxation/dynamics dimension is to be analyzed, so for example, an $xf2$ should be done for pseudo-2D data such as small molecule $T_1$ analysis.

Peak picking is done using any of several options: automatically, using threshold-based peak picking, or from a previous assignment, either in the form of a peaklist file from a 1D spectrum or, for proteins, from a BMRB or XEASY file. Parameters such as mixing times, variable counter times, or incremented gradient strengths are read in from TopSpin without further processing needed, and if a standard Bruker pulse program is used, DC knows what sort of functional form is needed for the analysis of dynamics data (under the Analysis tab). After fitting, the fit curves can be viewed simultaneously with the spectra (Fig.3).

Figure 1. Downloading DC and tutorials from the Bruker website http://www.bruker-biospin.com

Figure 2. The Bruker Dynamics Center, showing the General Dynamics tab.
Protein Dynamics Center

The principles of use of the protein dynamics center are similar to those of the general dynamics center, but data viewing possibilities is more powerful (2D data can be overlaid) and peak assignments from BMRB or XEASY files can be displayed on the spectra.

**Figure 6.** The file browser for the Dynamics Center and a slice of a 3D dataset showing residue assignments.

**Figure 7.** T1rho analysis using the Protein Dynamics Center.

**Figure 8.** T1 analysis using the Protein Dynamics Center.
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<thead>
<tr>
<th>Position</th>
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<th>Details</th>
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<tr>
<td>Postdoctoral Position in MRI of batteries</td>
<td>New York University</td>
<td>Immediate Opening for a Postdoc position on a joint project between New York University (Alexej Jerschow) and Stony Brook University (Clare Grey) <a href="http://nmr900.ca/nmr_jobs.html#nyu">http://nmr900.ca/nmr_jobs.html#nyu</a></td>
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<tr>
<td>Experimental Officer in Nuclear Magnetic Resonance</td>
<td>University of York, UK</td>
<td><a href="http://nmr900.ca/nmr_jobs.html#uy">http://nmr900.ca/nmr_jobs.html#uy</a></td>
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<tr>
<td>NMR Postdoctoral Positions</td>
<td>University of Pennsylvania</td>
<td><a href="http://nmr900.ca/nmr_jobs.html#bionmr">http://nmr900.ca/nmr_jobs.html#bionmr</a></td>
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<td>Postdoctoral position</td>
<td>Florida State University &amp; NHMFL</td>
<td><a href="http://nmr900.ca/nmr_jobs.html#fsu">http://nmr900.ca/nmr_jobs.html#fsu</a></td>
</tr>
<tr>
<td>Tenure-track faculty position in Inorganic Chemistry</td>
<td>University of Western Ontario, London, ON</td>
<td><a href="http://nmr900.ca/nmr_jobs.html#uwo">http://nmr900.ca/nmr_jobs.html#uwo</a></td>
</tr>
<tr>
<td>Two postdoctoral Research Associate positions</td>
<td>University of Wisconsin-Madison</td>
<td><a href="http://nmr900.ca/nmr_jobs.html#nmrfam">http://nmr900.ca/nmr_jobs.html#nmrfam</a></td>
</tr>
<tr>
<td>Tenure-track faculty position in Inorganic or Materials Chemistry</td>
<td>University of Alberta</td>
<td><a href="http://nmr900.ca/nmr_jobs.html#ua6">http://nmr900.ca/nmr_jobs.html#ua6</a></td>
</tr>
<tr>
<td>Listings of NMR jobs and vacancies</td>
<td>Canadian NMR Jobs</td>
<td><a href="http://nmr900.ca/nmr_jobs.html">http://nmr900.ca/nmr_jobs.html</a></td>
</tr>
<tr>
<td></td>
<td>AMPERE mailing list</td>
<td><a href="https://listes.sc.univ-paris-diderot.fr/sympa/info/nmr">https://listes.sc.univ-paris-diderot.fr/sympa/info/nmr</a></td>
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</table>
Canadian NMR Research Highlights

**Cover article in Nature Chemistry**


http://dx.doi.org/10.1038/nchem.1354

This work has been highlighted in ACCN *Canadian Chemical News*, July/August, 2012, page 12, "Wheels on the MOF go round and round" [http://www.accn.ca/index.php?ci_id=3477&la_id=1](http://www.accn.ca/index.php?ci_id=3477&la_id=1)

For more background information see *uWindsor Daily News*, June 18, 2012 “Chemists break new ground in molecular machine research" [http://tinyurl.com/csyh6p8](http://tinyurl.com/csyh6p8)

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**NMR paper in Angewandte Chemie**


http://dx.doi.org/10.1002/anie.201203547

This work has been highlighted in *Chemical & Engineering News*, June 18, 2012, Volume 90, Issue 25, page 32, Science and Technology Concentrates, "Zinc Dianion Drives Cross-Coupling" [http://cen.acs.org/articles/90/i25/Zinc-Dianion-Drives-Cross-Coupling.html](http://cen.acs.org/articles/90/i25/Zinc-Dianion-Drives-Cross-Coupling.html)

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**Biochemistry and Cell Biology**

special issue on lactoferrin
guest-edited by Nidia León-Sicairos
(Autonomous University of Sinaloa, México)
and Hans Vogel (University of Calgary)

volume 90 (2012) issue 3

http://www.nrcresearchpress.com/toc/bcb/90/3


http://dx.doi.org/10.1139/o2012-020


http://dx.doi.org/10.1139/o2012-016


http://dx.doi.org/10.1139/o11-057

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**NMR for Quantum Computing**


http://dx.doi.org/10.1038/ncomms1860

Donor Spins in a $^{28}$Si "Semiconductor Vacuum”,” *Science* **336** (2012) 1280-1283. [http://dx.doi.org/10.1126/science.1217635](http://dx.doi.org/10.1126/science.1217635)

The latter work by the Mike Thewalt group from SFU and their colleagues from Germany and UK has been highlighted in the *Science* Perspective


Review article in *Chest*


Review in *Annual Reports on NMR Spectroscopy*

W.F. Reynolds, D.C. Burns, "Getting the Most Out of HSQC and HMBC Spectra," *Annual Reports on NMR Spectroscopy* **76** (2012) 1-21. [Review] [http://dx.doi.org/10.1016/B978-0-12-397019-0.00001-7](http://dx.doi.org/10.1016/B978-0-12-397019-0.00001-7)

Review in *Methods*


Review in *the Journal of Chemical Ecology*


NMR paper in *PNAS*


Edge article in *Chemical Science*


Encyclopedia of Magnetic Resonance: new entries


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


Dalhousie University


NRC, Halifax


University of New Brunswick


Université Laval


Université de Sherbrooke / INRS-Institut Armand-Frappier


McGill University


Université de Montréal


University of Ottawa


NRC, Ottawa


Queen's University


York University


University of Toronto


**Apotex, Toronto**


**Brock University**


**University of Guelph**


**University of Waterloo**


University of Western Ontario


University of Windsor


University of Regina


University of Saskatchewan


University of Alberta


University of Calgary


University of Alberta


http://dx.doi.org/10.3762/bjoc.8.130

http://dx.doi.org/10.1021/pr300487s

http://dx.doi.org/10.1139/o2012-021

http://dx.doi.org/10.1021/pr201274r

University of British Columbia
C.M. Stevens, M. Okon, L.P. McIntosh, M. Paetzel, "$^1$H, $^{13}$C and $^{15}$N resonance assignments and peptide binding site chemical shift perturbation mapping for the Escherichia coli redox enzyme chaperone DmsD," Biomolecular NMR Assignments (2012) online. 
http://dx.doi.org/10.1007/s12104-012-9408-8

http://dx.doi.org/10.1021/jp305064x

http://dx.doi.org/10.1016/j.str.2012.04.014

Simon Fraser University
http://dx.doi.org/10.1126/science.1217635

Natural Resources Canada, Victoria
http://dx.doi.org/10.1139/x2012-076

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