



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

## Canadian NMR Research News Bulletin #8.2 Spring 2014

### Canadian NMR News

Reposted with permission from  
<http://www.dal.ca/news.html>

#### **Elusive ion evades discovery for decades: Dalhousie NMR facility provides the solid proof**

*Matt Kennedy - April 11, 2014*

The scientific world is one step closer to understanding how nature uses carbon capture to tame poisons, thanks to the discovery of cyanofornate ( $\text{N}\equiv\text{C}-\text{CO}_2^-$ ) a simple but fragile ion involved in the fruit-ripening process that has evaded detection for decades.

The results of the two-year study led by **Jayson Clyburne** of Saint Mary's University and **Heikki Tounonen** of the University of Jyväskylä in Finland, were released last week in *Science*, the world's preeminent scientific journal. Dalhousie's Nuclear Magnetic Resonance Resource (**NMR-3**) facility played a key role in the study.

#### **Saving plants from cyanide with carbon dioxide**

At a time when carbon capture is being looked to as a strategy for managing carbon dioxide emissions caused by humans, the study offers insight into how the natural world handles carbon.

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"Here we have a perfect example of nature taming a poison, and what better way to learn the chemistry of carbon capture than from nature itself?" says Dr. Clyburne, Canada Research Chair in Environmental Science and Materials and professor of Environmental Science and Chemistry at Saint Mary's — and also a Dal alum.

"The fact that cyanofornate was undetected for so long begs the question: What other simple chemistry have we missed?" asks Dr. Tuononen, Academy of Finland research fellow



**Left-to-right:** Luke Murphy, Ulrike Werner-Zwanziger and Jason Clyburne in Dal's NMR lab. (photo by Danny Abriel)

and senior lecturer at the University of Jyväskylä.

Chemists have long been aware of the role that cyanide and carbon dioxide play in fruit ripening, but they've always been observed independent of one another. This study represents the first time scientists have isolated cyanofornate anion ( $\text{N}\equiv\text{C}-\text{CO}_2^-$ ) and explored its structure using crystallography, computational chemistry and spectroscopy. It shows that there's still more to learn about the chemistry of carbon dioxide in cells, and also furthers our understanding of carbon capture.

### Providing the proof

The final proof that Dr. Clyburne and his team had discovered the elusive ion came from **Ulrike Werner-Zwanziger**, adjunct professor (Faculty of Graduate Studies) and solid-state NMR coordinator of the Nuclear Magnetic Resonance Resource (NMR-3) at Dal.

"My contribution to the study was to use solid-state NMR to show that there is a chemical bond between cyanide and carbon dioxide," says Dr. Werner-Zwanziger, a co-author on the study. "Only when we have direct bonding can we get this type of doublet splitting proving the structure of the ion."

Chemists routinely use NMR spectroscopy to study chemical structure of matter in liquids and solids. Located in the Chemistry Building, the NMR-3 facility at Dal is a diverse NMR centre that often acts as a point of collaboration for researchers across the Atlantic Provinces and around the world. Its spectrometers were purchased in part through the Institute for Research in Materials (IRM).

### Learn more: NMR-3 website

<http://www.dal.ca/diff/nmr3.html>

"Taking advantage of our high field solid-state NMR spectrometers and samples prepared by Luke Murphy, a Master of Applied Science candidate at Saint Mary's University, I could determine the coupling mechanism," explains Dr. Werner-Zwanziger.

Also involved in determining the structure was research associate Katherine Robertson (also a Dal alum), in collaboration with Scott Harroun from Christa Brosseau's laboratory at Saint Mary's University.

### Collaborating on a local and global scale

Dr. Werner-Zwanziger says that having the NMR facility in Halifax offers many benefits to the region's research community. The facility has collaborated with scientists in the United States, Brazil, India, Singapore, Europe and beyond.

"We have an outstanding staff of two PhD scientists and instrumentation for liquids and solids ranging from 300 MHz to 700 MHz," says Dr. Werner-Zwanziger. "Our staff is here to support academic and industrial NMR-related research and provide services that include experiment development, data acquisition and interpretation, and assistance to users."

Discoveries like these by Dr. Clyburne and his team of scientists, with the support from the NMR-3 facility and Dr. Werner-Zwanziger at Dal, highlights that nothing happens alone in the world of scientific research.

Story by **Matthew Kennedy** (Dal News)  
Photo by **Danny Abriel** (Dal News)

Reposted with permission from  
<http://www.dal.ca/news/2014/04/11/elusive-ion-evades-discovery-for-decades--dalhousie-nmr-facility.html> <http://tinyurl.com/pmjefx3>

*To learn more about this discovery*

**L.J. Murphy, K.N. Robertson, S.G. Harroun, C.L. Brosseau, U. Werner-Zwanziger, J. Moilanen, H.M. Tuononen, J.A.C. Clyburne**, "A Simple Complex on the Verge of Breakdown: Isolation of the Elusive Cyanofornate Ion," *Science* **344** (2014) 75-78.  
<http://dx.doi.org/10.1126/science.1250808>

**I. Alabugin and R.K. Mohamed**, "A  $\text{CO}_2$  Cloak for the Cyanide Dagger," *Science* **344** (2014) 45-46. (**Science Perspective**)  
<http://dx.doi.org/10.1126/science.1252466>

*ChemistryWorld*: Isolation of cyanofornate suggests new carbon capture approaches, **Simon Hadlington**, April 7, 2014  
<http://www.rsc.org/chemistryworld/2014/04/isolation-cyanofornate-suggests-new-carbon-capture-approaches>  
<http://tinyurl.com/nmy7h5n>

*C&EN News of the Week*: Cyanofornate structure could aid efforts to trap carbon dioxide, **Celia Henry Arnaud**, April 7, 2014  
<http://cen.acs.org/articles/92/i14/Cyanofornate-Structure-Aid-Efforts-Trap.html>  
<http://tinyurl.com/nbcrsry>

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**C-CRAFT** - the University of Lethbridge launches *the Canadian Centre for Research in Advanced Fluorine Technologies*

<http://www.uleth.ca/unews/article/university-launches-c-craft-advancing-science-fluorine-chemistry> <http://tinyurl.com/o2pcbxo>

<http://www.uleth.ca/research/canadian-centre-research-advanced-fluorine-technologies-c-craft> <http://tinyurl.com/o58ck3q>

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### **UNB spinoff Green Imaging Technologies declares dividends**

A University of New Brunswick (UNB) spinoff company that provides nuclear magnetic resonance (NMR) solutions for the oil and gas sector has celebrated nearly a decade of growth by declaring dividends for the first time.

<http://blogs.unb.ca/newsroom/2014/02/03/unb-spinoff-green-imaging-technologies-declares-dividends/> <http://tinyurl.com/lsezvzv>

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### **MOOT 2014 - First Announcement**

Dear colleagues,

On behalf of the organizing committee we would like to invite you to attend the 27<sup>th</sup> edition of the MOOT NMR Symposium which this year will take place in Montréal, **October 18<sup>th</sup>-19<sup>th</sup>, 2014**. Please mark your calendars! The meeting will be held at **the Université du Québec à Montréal (UQAM)** in the heart of the city center. We will provide more details about the conference via e-mail as they become available. The official 27<sup>th</sup> MOOT website will be online shortly.

If you have any questions, comments or suggestions, please E-mail us at email: [marcotte.isabelle@uqam.ca](mailto:marcotte.isabelle@uqam.ca)

We look forward to seeing you in October!

**MOOT XXVII Organizing Committee**  
Alexandre Arnold and Isabelle Marcotte

Département de Chimie  
Université du Québec à Montréal  
C.P. 8888, Succ. Centre-Ville  
Montréal (Québec) H3C 3P8  
<http://www.nanoqam.uqam.ca/professeur.php?id=5&lang=fr>


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**2014  
the International Year of  
Crystallography**

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

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 **IUCr XXIII Congress and General Assembly of the International Union of Crystallography**

August 5-12, 2014, Montréal, Québec  
<http://www.iucr2014.org/>

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### **4<sup>th</sup> SMARTER meeting on NMR and Crystallography**

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

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**Crystallography at 100**  
*Science's Special Issue*

7 March 2014

Vol. 343, Issue 6175

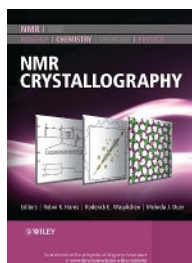
<http://www.sciencemag.org/site/special/crystallography/>

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**Colin R. Groom and Frank H. Allen**, "The Cambridge Structural Database in Retrospect and Prospect" *Angewandte Chemie International Edition* **53** (2014) pages 662-671. **(review)**

<http://dx.doi.org/10.1002/anie.201306438>

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### **NMR Crystallography**

Robin K. Harris (Editor)  
Roderick E. Wasylshen (Editor)  
Melinda J. Duer (Editor)  
**Hardcover:** 520 pages  
**Publisher:** Wiley; January 2010

**Language:** English

**ISBN:** 978-0470699614

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

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

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## Recognition

Prof. **Isabelle Marcotte** (Université du Québec à Montréal) has been awarded the **2014 UQAM Young Researcher Award by the Faculty of Science**

*UQAM:* Le Prix relève récompense un ou une jeune professeur(e) dont les débuts en recherche sont prometteurs. Arrivée à l'UQAM en 2006, Isabelle Marcotte a rapidement monté un programme d'envergure internationale sur la résonance magnétique nucléaire (RMN) des systèmes biologiques, appliqué en particulier à l'étude des membranes biologiques et des fibres naturelles. La RMN est l'une des principales techniques utilisées par les chimistes pour caractériser et reconnaître la structure moléculaire. La professeure Marcotte s'en sert pour étudier l'interaction de peptides et de médicaments avec les membranes lipidiques qui entourent les cellules. Elle fait partie des rares chercheurs dans le monde à utiliser la RMN sur des cellules vivantes.

Isabelle Marcotte utilise la RMN pour comprendre l'agencement moléculaire des fibres biologiques. Elle s'est penchée notamment sur celle du byssus de la moule – un déchet de l'aquaculture. Son programme de recherche consiste à déterminer par RMN la structure du byssus de manière à pouvoir valoriser cette fibre par la fabrication de biomatériaux. Ce projet aux retombées prometteuses a été reconnu par la revue *Québec Sciences* comme l'un des 50 défis à relever d'ici 2050. La chercheuse est maintenant considérée comme la spécialiste des études de biomatériaux par RMN au Canada et se positionne comme une étoile montante sur la scène internationale.

<http://www.actualites.uqam.ca/2014/4473-prix-recherche-faculte-sciences-mateescu-marcotte>

<http://tinyurl.com/mzr3lqd>

**Maiwenn Beaugrand** (PhD student, Marcotte group, UQAM) has received the "**Personnalité Facultaire**" prize from the UQAM Faculty of Science

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## 55<sup>th</sup> ENC Student Travel Awards

Following the long tradition, ENC has awarded **2014 Student Travel Stipends** to support students attending the 55<sup>th</sup> ENC Conference held March 23-28, 2014 in Boston, Massachusetts. The stipends were provided by the ENC, the Suraj P. Manrao Science Foundation, and by the generous contributions of sponsors. Among awardees there were several Canadian recipients, including

**Kevin Burgess** (University of Ottawa)

**Donald Gagne** (INRS-Institut Armand-Frappier)

**Marie-Laurence Tremblay** (Dalhousie University)

**Shu Han** (University of British Columbia)

<http://www.enc-conference.org>

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Prof. **Gang Wu** (Queen's) has accepted an invitation to join the Editorial Board of *Solid State Nuclear Magnetic Resonance* (Elsevier).



**David Bryce** (University of Ottawa) has been promoted to the rank of **Full Professor**.

*Congratulations, Dave!*

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## NMR Theses Recently Defended

**Patrick Szell** (University of Ottawa)

Supervisor: Prof. David Bryce

**B.Sc. (Honours) thesis:** "Probing Non-Covalent Interactions with NMR"

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**Rosha Teymoori** (University of Alberta) March 7, 2014

Supervisor: Prof. Roderick Wasylshen

**Ph.D. Chemistry:** "Solid-State Nuclear Magnetic Resonance and Computational Investigations of Half-Integer Quadrupolar Nuclei"

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## On the move

Bruker Ltd.

April 8, 2014



Dear Valued Customers,

I am writing to inform you that **Thomas Buser** has accepted the position of **Head of NMR Installations**, effective August 1, 2014. His new role will be based out of our factory location in Fällanden, Switzerland. Switzerland is where Thomas began his career with Bruker 25 years ago and this role necessitates an exciting move "back home" for Thomas and his family. Over the years, Thomas has held various roles and has always shown our customers a passion for detail, conviction for quality, strong work ethic and an ability to advocate on your behalf. We are very fortunate that he will continue his good service to both Bruker and our global customer base.

Please join me in congratulating Thomas and we wish him much success in his new role.

Thank you,

Sincerely

Dr. Henry J. Stronks  
President, Bruker Ltd.

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**Andre Sutrisno** (Ph.D. 2012, Huang group, Western), formerly a postdoctoral fellow with Andre Simpson at the University of Toronto Scarborough, will be heading south in June 2014 as he has accepted a position of Solid-state NMR Spectroscopist in the School of Chemical Sciences at the University of Illinois at Urbana-Champaign

<http://www.scs.illinois.edu/nmr/>

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**Jun Xu** (Ph.D. 2013, Huang group, Western) will begin a postdoctoral fellowship at University of California, Berkeley under Prof. Jeffrey Reimer in June 2014.

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## NMR Software

contributed by David Bryce (Ottawa)

### EFGShield, version 4.0

*New version of EFGShield with GUI now available for Gaussian, CASTEP, and ADF files*



"EFGShield" is our software for the parsing and analysis of shielding and EFG data from Gaussian output files. Thanks to the work of my students **Nuiok Dicaire** and **Fred Perras**, I am pleased to announce that a new and improved version of EFGShield with a GUI is now available. There are many advantages to the new version. Most importantly, CASTEP and ADF output files can now be used in addition to Gaussian files.

The program now runs with a graphical user interface (GUI) rather than the old command line prompt. It runs under modern versions of Windows and also works in Windows emulators we have tested. The new and improved version offers many advantages compared to previous versions including:


- can now read magnetic shielding and electric field gradient output for Gaussian, ADF, and CASTEP software
- GUI functionality
- much easier to find and load files with long path names
- easier to save output files where you want them
- see results summary directly in the program window without having to open the output files
- can view results summary for different atoms and for different output files without having to restart the program
- updated quadrupole moments

New version of **EFGShield** is available for download from the "Software" link in the menu on the left on our webpage  
<http://mysite.science.uottawa.ca/dbryce/>

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## NMR Events

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

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

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### 2014 Finnish NMR symposium

June 4-6, 2014, Pikku-Syöte, Finland  
<http://nmrsymposium.fi/2014/index.php>

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### AMPERE NMR School

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

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### EUROMAR 2014

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

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### NMRCM 2014 NMR in Condensed Matter

July 7-11, 2014, St. Petersburg, Russia  
<http://nmr.phys.spbu.ru/nmrcm/>

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### "New Frontiers in Biophysics"

British Biophysical Society, biennial meeting  
July 9-11, 2014, Warwick, U.K.  
<http://britishbiophysics.org.uk/>

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### 56<sup>th</sup> 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>

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

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

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### 22<sup>nd</sup> IUPAC International Conference on Physical Organic Chemistry

August 10-15, 2014, Ottawa, ON, Canada  
<http://events.science.uottawa.ca/icpoc22/welcome.html>

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

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

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### ICMRBS 2014, the XXVI<sup>th</sup> International Conference on Magnetic Resonance in Biological Systems

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

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### 4<sup>th</sup> SMARTER meeting on NMR and Crystallography

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

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### SMASH 2014 Small Molecule NMR Conference

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

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### MOOT XXVII NMR Symposium

October 18-19, 2014, Université du Québec à Montréal, Montréal, QC, Canada  
<http://www.mootnmr.org>

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### 2014 Industrial Chemistry Conference

November 12-14, 2014, Edmonton, Alberta, Canada  
<http://www.cic2014.ca/>

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### 7<sup>th</sup> Annual GRASP Symposium

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

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### Biophysical Society 59<sup>th</sup> Annual Meeting

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

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 Biophysical Society of Canada - Travel Awards and Mixer

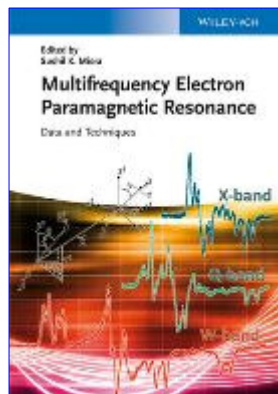
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### PANIC 2015 Practical Applications of NMR in Industry Conference

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

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## New MR Books



### Multifrequency Electron Paramagnetic Resonance: Data and Techniques

Sushil K. Misra (Editor)

Hardcover: 320 pages  
Publisher: Wiley  
May 2014  
Language: English  
ISBN: 978-3527412228

<http://ca.wiley.com/WileyCDA/WileyTitle/productCd-3527412220.html>  
<http://www.amazon.com/dp/3527412220>  
<http://www.amazon.ca/dp/3527412220>

**Wiley:** This handbook is aimed to deliver an up-to-date account of some of the recently developed experimental and theoretical methods in EPR, as well as a complete up-to-date listing of the experimentally determined values of multifrequency transition-ion spin Hamiltonian parameters by Sushil Misra, reported in the past 20 years, extending such a listing published by him in the Handbook on Electron Spin Resonance, volume 2. This extensive data tabulation makes up roughly 60% of the book's content. It is complemented by the first full compilation of hyperfine splittings and g-factors for aminoxyl (nitroxide) radicals since 197 by Larry Berliner, a world expert on spin labeling, helping to identify and interpret substances and processes by means of EPR techniques. The book also includes coverage of the recently developed experimental technique of rapid-scan EPR by Sandra Eaton and Gareth Eaton, and a thorough review of computational modeling in EPR by Stefan Stoll, author of Easy Spin.

#### Table of contents

<http://ca.wiley.com/WileyCDA/WileyTitle/productCd-3527412220.html>

See also **Multifrequency Electron Paramagnetic Resonance: Theory and Applications**, edited by **Sushil K. Misra**  
Hardcover, 1056 pages, Wiley-VCH; 2011  
ISBN: 978-3527407798

<http://www.amazon.com/dp/3527407790>  
<http://www.amazon.ca/dp/3527407790>

## Advances in Biological Solid-State NMR

### Proteins and Membrane-Active Peptides

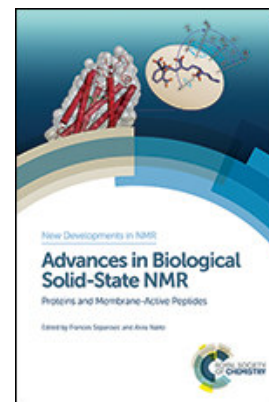
**Editors:** Frances Separovic and Akira Naito

**Hardcover:** 384 pages

**Language:** English

**Publisher:** RSC (March 30, 2014)

**ISBN:** 978-1849739108

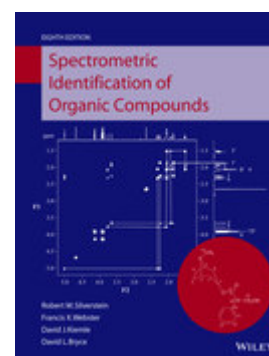


<http://www.amazon.com/dp/1849739102>  
<http://www.amazon.ca/dp/1849739102>

## Spectrometric Identification of Organic Compounds, 8<sup>th</sup> Edition

**Robert M. Silverstein,**  
**Francis X. Webster,**  
**David Kiemle,**  
**David L. Bryce**

Paperback: 462 pages  
Publisher: Wiley;  
September 2014  
Language: English  
ISBN: 978-0470616376



<http://ca.wiley.com/WileyCDA/WileyTitle/productCd-EHEP001779.html>  
<http://www.amazon.com/dp/0470616377>  
<http://www.amazon.ca/dp/0470616377>

**Wiley:** First published over 40 years ago, this was the first text on the identification of organic compounds using spectroscopy. This text is now considered to be a classic. The key strength of this text is the extensive set of real-data problems. Even professional chemists use these spectra as reference data. Spectrometric Identification of Organic Compounds is written by and for organic chemists, and emphasizes the synergistic effect resulting from the interplay of the spectra. This book is characterized by its problem-solving approach with extensive reference charts and tables.

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<http://ca.wiley.com/WileyCDA/WileyTitle/productCd-EHEP001779.html>

## NMR Jobs and Vacancies

### NMR Facility Research Associate, University of Toronto

Faculty / Division: Faculty of Arts and Science  
Department: Chemistry  
Specialty: Nuclear Magnetic Resonance (NMR) Spectroscopy  
Campus: St. George Campus  
Principal Investigator: Professor Robert Batey

**Description:** The NMR Facility has undergone a recent expansion and now has a total of ten NMR spectrometers, ranging in field strength from 200 to 700 MHz. Some of the systems are used in a walk-up fashion, while sample changers are used to facilitate most of the routine NMR acquisitions. The Facility has both Agilent/Varian and Bruker spectrometers with cryogenically cooled probes, solids probes, and a wide range of liquids probes. The NMR Facility is a team-oriented environment whose staff currently includes two Ph.D.-level scientists, and two support technicians.

We are seeking a PhD-level Research Associate to join the CSICOMP NMR facility in the Department of Chemistry at the University of Toronto. The incumbent will be under the general direction of the Facility Manager and will provide scientific and technical support services, with a focus on solid state and small-molecule solution state NMR spectroscopy. Specifically, the incumbent will be responsible for, or assist with, the following principal duties in the facility: implementing NMR experiments, client services, instrument maintenance, teaching and training, and developing operational workflow within the lab. The incumbent will also be expected to take a lead role in the implementation of solid state NMR at the facility.

**Qualifications:** MINIMUM: The candidate must have demonstrated proficiency in the field of NMR spectroscopy as indicated by peer-reviewed publication and / or conference presentations. The candidate must also possess a working knowledge of solution state NMR techniques, including basic calibrations.

- A working knowledge of solid state NMR techniques and the related NMR instrumentation is preferred.
- Familiarity with common spectrometer and magnet maintenance, such as cryogen fills, is preferred
- Teaching and training experience is preferred

**EDUCATION:** The candidate should possess a Ph.D. or equivalent experience in the fields of chemistry, physics, or biochemistry.

**EXPERIENCE:** - Two or more years experience in an NMR laboratory environment with at least one year

- of experience maintaining NMR instrumentation
- Advanced knowledge of 1D and 2D solution state and solid state NMR techniques, including sample preparation, methodology and interpretation
- Ability to troubleshoot technical problems related to the spectrometers, associated hardware, and software. This includes operating system (i.e. Linux) maintenance and management
- Proficiency with computers systems and vendor-packaged software for NMR data acquisition and clerical duties (e-mail, word processing, etc.)
- Experience handling cryogenics, compressed gases, dewars, and gas cylinders

**SKILLS:** - Strong communication and interpersonal skills, as the incumbent will often be the first point of contact for regular and new facility users

- Above average concentration and ability to plan for and organize work flow in a multitasking customer focused environment with changing priorities and frequent interruptions
- Proficiency with word processing and spreadsheet software
- Experience with Unix and/or is Linux preferable, but not necessary

**OTHER:** - Experience with NMR sample preparation, including the manipulation of solvents and chemicals

- Familiarity with common solution and solid state NMR methods and interpretation
- Familiarity with electronic test equipment (e.g. oscilloscopes, digital multimeters, etc.)
- Familiarity with NMR spectrometers and associated hardware including automatic sample changers

All qualified candidates are encouraged to apply; however, Canadians and permanent residents will be given priority. The University of Toronto is strongly committed to diversity within its community and especially welcomes applications from visible minority group members, women, Aboriginal persons, persons with disabilities, members of sexual minority groups, and others who may contribute to the further diversification of ideas.

Employee Group: Research Associates  
Appointment Type: Limited Term, Term: One year  
term FTE: 100%  
Anticipated Start Date: July 1st, 2014  
Schedule: Full-time  
Salary: Minimum: \$40,920 Maximum: \$76,725  
Job Posting: May 7, 2014  
Job Closing Date: We will begin reviewing application on 30 days after the posting date; however, the position will remain open until filled.

**Please apply to:**  
Professor Robert Batey  
Chair, Department of Chemistry  
University of Toronto  
email: [chair@chem.utoronto.ca](mailto:chair@chem.utoronto.ca)



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## Graduate student position, the University of Guelph, Guelph, Ontario

We are seeking highly motivated PhD students to work in the protein NMR group at the University of Guelph. Our group is broadly interested in membrane protein structure. Our main research tool is magic angle spinning solid state NMR, but we also used other complementary biochemical, biophysical and computational methods. The research will be conducted at the University of Guelph NMR Centre, which is equipped with an array of solid-state NMR spectrometers at field strengths from 500 MHz to 800 MHz, and with a recently installed Dynamic Nuclear Polarization spectrometer. This gives us the unique ability to probe atomic level details of molecular structure, dynamics, and interactions. The specific project will deal with protein-lipid and protein-water interactions, with emphasis on the methodological aspect.

For examples of our work, see our recent publications:

<http://www.nature.com/nmeth/journal/v10/n10/full/nmeth.2635.html>  
<http://pubs.acs.org/doi/abs/10.1021/ja411633w>

The candidates must have a degree in chemistry, physics or biochemistry.

Applications are accepted to both

the Department of Physics  
<http://www.physics.uoguelph.ca>

or Biophysics Interdepartmental Group  
<https://www.uoguelph.ca/biophysics/welcome-biophysics>

For more information contact

### Dr. Vladimir Ladizhansky

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

<http://www.physics.uoguelph.ca/~vladimir/>

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## Postdoctoral position in solid-state NMR of pharmaceuticals, University of Windsor

A PDF position is available in the Schurko group at the University of Windsor (Windsor, Ontario) with starting dates between May 2014 - September 2014. The PDF will be in charge of conducting research and managing a project area involving SSNMR of pharmaceutical compounds, related materials and nanoparticles. We are equipped with 400 MHz and 500 MHz SSNMR spectrometers, pXRD and scXRD equipment, wet lab spaces (including glove boxes) and fantastic shared computational resources. We also have access to high field (800, 900 MHz) NMR spectrometers. The PDF candidate should have extensive background in solid-state NMR. The position starts with a one-year contract, with option to extend to second and third years via mutual agreement of the PDF and the PI. Please contact me for more information.

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<http://www.uwindsor.ca/schurko>

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Victor Terskikh @nmr900 · 3h  
Agilent workshop at 2014 RMC "Targeting Environmental, Agricultural, and Plant Science with Solid-state NMR" July 12 events.signup4.com/NSF-RCNworkshop  
Details



Victor Terskikh @nmr900 · May 16  
Important development in  $^{43}\text{Ca}$  solid-state NMR, Cory Widdifield, Igor Moudrakovski and David Bryce (uOttawa) @PCCP [pubs.rsc.org/en/Content/Art...](http://pubs.rsc.org/en/Content/Art...)

### DrugBank 4.0

**V. Law, C. Knox, Y. Djoumbou, T. Jewison, A.C. Guo, Y. Liu, A. Maciejewski, D. Arndt, M. Wilson, V. Neveu, A. Tang, G. Gabriel, C. Ly, S. Adamjee, Z.T. Dame, B. Han, Y. Zhou and D.S. Wishart** "DrugBank 4.0: shedding new light on drug metabolism" *Nucleic Acids Research* **42** (2014) D1091-D1097. (**open access**) <http://dx.doi.org/10.1093/nar/gkt1068>

**Abstract:** DrugBank (<http://www.drugbank.ca>) is a comprehensive online database containing extensive biochemical and pharmacological information about drugs, their mechanisms and their targets. Since it was first described in 2006, DrugBank has rapidly evolved, both in response to user requests and in response to changing trends in drug research and development. Previous versions of DrugBank have been widely used to facilitate drug and *in silico* drug target discovery. The latest update, DrugBank 4.0, has been further expanded to contain data on drug metabolism, absorption, distribution, metabolism, excretion and toxicity (ADMET) and other kinds of quantitative structure activity relationships (QSAR) information. These enhancements are intended to facilitate research in xenobiotic metabolism (both prediction and characterization), pharmacokinetics, pharmacodynamics and drug design/discovery. For this release, >1200 drug metabolites (including their structures, names, activity, abundance and other detailed data) have been added along with >1300 drug metabolism reactions (including metabolizing enzymes and reaction types) and dozens of drug metabolism pathways. Another 30 predicted or measured ADMET parameters have been added to each DrugCard, bringing the average number of quantitative ADMET values for Food and Drug Administration-approved drugs close to 40. **Referential nuclear magnetic resonance and MS spectra have been added for almost 400 drugs** as well as spectral and mass matching tools to facilitate compound identification. This expanded collection of drug information is complemented by a number of new or improved search tools, including one that provides a simple analyses of drug–target, –enzyme and –transporter associations to provide insight on drug–drug interactions.

**In the news:** *University of Montreal scientists discover molecular details of kissing disease virus attacks*

<http://www.nouvelles.umontreal.ca/udem-news/news/20140410-scientists-discover-molecular-details-of-kissing-disease-virus-attacks.html> <http://tinyurl.com/onpwn2y>

**P.R. Chabot, L. Raiola, M. Lussier-Price, T. Morse, G. Arseneault, J. Archambault, J.G. Omichinski**, "Structural and Functional Characterization of a Complex between the Acidic Transactivation Domain of EBNA2 and the Tfb1/p62 Subunit of TFIIH," *PLoS Pathogenes* **10** (2014) e1004042. <http://dx.doi.org/10.1371/journal.ppat.1004042>

### **Journal of Magnetic Resonance**

special "JMR Perspectives" issue:  
*Foresights in Biomolecular Solution-State NMR Spectroscopy*  
Volume 241, pp. 1-170 (April 2014)

<http://www.sciencedirect.com/science/journal/10907807/241>

**Lewis E. Kay, Lucio Frydman**, "A special "JMR Perspectives" issue: Foresights in biomolecular solution-state NMR spectroscopy – from spin gymnastics to structure and dynamics," *Journal of Magnetic Resonance* **241** (2014) 1-2. (**Editorial**) <http://dx.doi.org/10.1016/j.jmr.2014.01.010>

### **Journal of Medicinal Chemistry**

special thematic issue:  
*Hepatitis C Virus (HCV) Therapies*  
Volume 57, issue 5,  
pp. 1625-2166 (March 13, 2014)

<http://pubs.acs.org/toc/jmcmar/57/5>

*Contributions from the Departments of Chemistry and Biological Sciences, Boehringer Ingelheim (Canada) Ltd., Laval, Quebec, Canada*

**S.R. LaPlante, H. Nar, C.T. Lemke, A. Jakalian, N. Aubry, and S.H. Kawai**, "Ligand Bioactive Conformation Plays a Critical Role in the Design of Drugs That Target the Hepatitis C Virus NS3 Protease," *J. Med. Chem.* **57** (2014) 1777–1789. <http://dx.doi.org/10.1021/jm401338c>

**S.R. LaPlante, P. Forgione, C. Boucher, R. Coulombe, J. Gillard, O. Hucke, A. Jakalian, M.-A. Joly, G. Kukulj, C. Lemke, R. McCollum, S. Titolo, P.L. Beaulieu, T.**

**Stammers**, "Enantiomeric atropisomers inhibit HCV polymerase and/or HIV matrix: Characterizing hindered bond rotations and target selectivity," *J. Med. Chem.* **57** (2014) 1944-1951.

<http://dx.doi.org/10.1021/jm401202a>

**S.R. LaPlante, A. Padyana, A. Abeywardnae, P.R. Bonneau, M. Cartier, R. Colombe, A. Jakalian, J. Jones, X. Li, S. Liang, G. McKercher, P.W. White, Q. Zhang, and S.J. Taylor**, "Integrated Strategies for Identifying Leads that Target the NS3 Helicase of the Hepatitis C Virus," *J. Med. Chem.* **57** (2014) 2074-2090.

<http://dx.doi.org/10.1021/jm401432c>

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#### NMR paper in *Science*

**L.J. Murphy, K.N. Robertson, S.G. Harroun, C.L. Brosseau, U. Werner-Zwanziger, J. Moilanen, H.M. Tuononen, J.A.C. Clyburne**, "A Simple Complex on the Verge of Breakdown: Isolation of the Elusive Cyanofolate Ion," *Science* **344** (2014) 75-78.

<http://dx.doi.org/10.1126/science.1250808>

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#### Two NMR papers in *Nature* titles

**S. Bastos-Aristizabal, G. Kozlov, K. Gehring**, "Structure of the substrate-binding b' domain of the Protein disulfide isomerase-like protein of the testis," *Nature Scientific Reports* **4** (2014) 4464. **(open access)**

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**C.M. Crudden, J.H. Horton, I.I. Ebraldize, O.V. Zenkina, A.B. McLean, B. Drevniok, Z. She, H.-B. Kraatz, N.J. Mosey, T. Seki, E.C. Keske, J.D. Leake, A. Rousina-Webb, G. Wu**, "Ultra stable self-assembled monolayers of N-heterocyclic carbenes on gold," *Nature Chemistry* **6** (2014) 409-414. (highlighted in *C&EN News of the Week*)

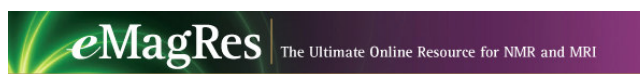
<http://dx.doi.org/10.1038/nchem.1891>

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**M.P. Latham, A. Sekhar, L.E. Kay**, "Understanding the mechanism of proteasome 20S core particle gating," *Proc. Natl. Acad. Sci. USA* **111** (2014) 5532-5537.

<http://dx.doi.org/10.1073/pnas.1322079111>



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<http://dx.doi.org/10.1002/9780470034590.emrstm1338>

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**R.M. Epand, K. D'Souza, B. Berno, M. Schlame**, "Membrane Curvature Modulation of Protein Activity Determined by NMR," *Biochimica et Biophysica Acta (BBA) - Biomembranes* (2014) online. **(Review)**

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**D.L. Bryce, J. Viger-Gravel**, "Solid-State NMR Study of Halogen-Bonded Adducts," *Topics in Current Chemistry* (2014) online. **(Invited Review)**

[http://dx.doi.org/10.1007/128\\_2014\\_542](http://dx.doi.org/10.1007/128_2014_542)

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**D.A. Marvin, M.F. Symmons, S.K. Straus**, "Structure and assembly of filamentous bacteriophages," *Progress in Biophysics and Molecular Biology* **114** (2014) 80-122.

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**D.E. Spratt, H. Walden, G.S. Shaw**, "RBR E3 ubiquitin ligases: new structures, new insights, new questions," *Biochemical Journal* **458** (2014) 421-437. **(Review)**

<http://dx.doi.org/10.1042/BJ20140006>

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**F.A. Perras and D.L. Bryce**, "Boron-Boron J Coupling Constants are Unique Probes of Electronic Structure: A Solid-State NMR and Molecular Orbital Study," *Chemical Science* **5** (2014) 2428-2437. **(Edge Article)**

<http://dx.doi.org/10.1039/c4sc00603h>

## 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.

### Memorial University of Newfoundland

**I. Marcotte and V. Booth** <sup>2</sup>H Solid-State NMR Study of Peptide–Membrane Interactions in Intact Bacteria" **Chapter 24** in *Advances in Biological Solid-State NMR: Proteins and Membrane-Active Peptides*, RSC Publishing (2014) 459-475.  
<http://dx.doi.org/10.1039/9781782627449-00459>

### Dalhousie University

**E.L. Zodrow, J.A. D'Angelo, U. Werner-Zwanziger, B. Chen**, "Hair-trichomes-files, and spectrochemistry of *Macroneuropteris scheuchzeri* (Basal Cambrian, Sydney Coalfield, Canada)," *Paleontographica, Abt. B: Palaeobotany - Paleophytology* **290** (2014) 141-153. <http://www.schweizerbart.de/>

**L.J. Murphy, K.N. Robertson, S.G. Harroun, C.L. Brosseau, U. Werner-Zwanziger, J. Moilanen, H.M. Tuononen, J.A.C. Clyburne**, "A Simple Complex on the Verge of Breakdown: Isolation of the Elusive Cyanofolate Ion," *Science* **344** (2014) 75-78.  
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**B.E. Kennedy, V.G. LeBlanc, T.M. Mailman, D. Fice, I. Burton, T.K. Karakach, B. Karten**, "Pre-Symptomatic Activation of Antioxidant Responses and Alterations in Glucose and Pyruvate Metabolism in Niemann-Pick Type C1-Deficient Murine Brain," *PLoS ONE* **8** (2013) e82685.  
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**A.S. Culf, M. Čuperlović-Culf, D.A. Léger, A. Decken**, "Small Head-to-Tail Macrocyclic  $\alpha$ -Peptoids," *Org. Lett.* **16** (2014) 2780-2783.  
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Resonance Imaging: Profiling and Local T2 measurement," *Measurement Science and Technology* **25** (2014) 035004.  
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**M. Fillion, M. Noël, A. Lorin, N. Voyer, M. Auger**, "Investigation of the mechanism of action of novel amphipathic peptides: Insights from solid-state NMR studies of oriented lipid bilayers," *Biochimica et Biophysica Acta (BBA) - Biomembranes* (2014) accepted.  
<http://dx.doi.org/10.1016/j.bbamem.2014.01.029>

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**M. Beaugrand, A.A. Arnold, J. Hénin, D.E. Warschawski, P.T.F. Williamson, and I. Marcotte**, "Lipid Concentration and Molar Ratio Boundaries for the Use of Isotropic Bicelles," *Langmuir* (2014) accepted.  
<http://dx.doi.org/10.1021/la5004353>

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**P.R. Chabot, L. Raiola, M. Lussier-Price, T. Morse, G. Arseneault, J. Archambault, J.G. Omichinski,** "Structural and Functional Characterization of a Complex between the Acidic Transactivation Domain of EBNA2 and the Tfb1/p62 Subunit of TFIIH," *PLoS Pathogenes* **10** (2014) e1004042.  
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 **C.M. Widdifield, I. Moudrakovski, and D.L. Bryce,** "Calcium-43 Chemical Shift and Electric Field Gradient Tensor Interplay: A Sensitive Probe of Structure, Polymorphism, and Hydration," *PCCP* **16** (2014) accepted.  
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 **F.A. Perras, D.L. Bryce,** "Theoretical Study of Homonuclear J Coupling Between Quadrupolar Spins: Single-Crystal, DOR, and J-Resolved NMR," *Journal of Magnetic Resonance* **242** (2014) 23–32.  
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**Pauli**, "2D NMR Barcoding and Differential Analysis of Complex Mixtures for Chemical Identification: The *Actaea* Triterpenes," *Anal. Chem.* **86** (2014) 3964–3972.  
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### Queen's University

**C.M. Crudden, J.H. Horton, I.I. Ebraldize, O.V. Zenkina, A.B. McLean, B. Drevniok, Z. She, H.-B. Kraatz, N.J. Mosey, T. Seki, E.C. Keske, J.D. Leake, A. Rousina-Webb, G. Wu**, "Ultra stable self-assembled monolayers of N-heterocyclic carbenes on gold," *Nature Chemistry* **6** (2014) 409–414. (highlighted in *C&EN News of the Week*)  
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**C.C. Cummins, C. Huang, T.J. Miller, M.W. Reintinger, J.M. Stauber, I. Tannou, D. Tofan, A. Toubaei, A. Velian, and G. Wu**, "The Stannylphosphide Anion Reagent Sodium Bis(triphenylstannyl) Phosphide: Synthesis, Structural Characterization, and Reactions with Indium, Tin, and Gold Electrophiles," *Inorganic Chemistry* **53** (2014) 3678–3687.  
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**K.A. Gelato, M. Tauber, M.S. Ong, S. Winter, K. Hiragami-Hamada, J. Sindlinger, A. Lemak, Y. Bultsma, S. Houlston, D. Schwarzer, N. Divecha, C.H. Arrowsmith, W. Fischle**, "Accessibility of Different Histone H3-Binding Domains of UHRF1 Is Allosterically Regulated by Phosphatidylinositol 5-Phosphate," *Molecular Cell* (2014) online.  
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**B.A. Cottrell, M. Gonsior, S.A. Timko, A.J. Simpson, W.J. Cooper**, "Photochemistry of marine and fresh waters: A role for copper-dissolved organic matter ligands," *Marine Chemistry* (2014) accepted.  
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### McMaster University

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