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Second Annual **Practical**
Applications of NMR
in Industry Conference

Hilton Charlotte University Place | Charlotte, North Carolina



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Student Pricing	\$395*
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Registration after January 10, 2014	\$850

**Students are required to submit a poster abstract for review and approval.
This discounted registration rate is for Student delegates only. Poster
abstracts must be submitted by December 20, 2013.*

Additional registration details

Each registration includes all conference sessions, posters and exhibits,
food functions, and access to the conference proceedings link.

Sessions Include

Biological NMR
Complex Mixtures
Low Volume/Low Resolution
Materials
Nutraceuticals
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Pharmaceutical NMR
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Quantitation
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Workshops:

Methods Validation
Data Management
Future of NMR

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Please use **keycode NMR F** when registering

MONDAY, FEBRUARY 3

7:00 am Registration and Morning Coffee

8:00 Co-Chair's Welcome

G. Joseph Ray, Baxter Healthcare and Daron I. Freedberg, FDA

COMPLEX MIXTURES I

8:05 Session Chair's Remarks

Molly P. Bohlen, The Procter and Gamble Company

8:10 Targeted and Non-Targeted NMR Analysis in Food Surveillance

Yulia Monakhova, Ph.D., CVUA Karlsruhe

8:40 NMR in Metabolomics: Characterizing Metabolites in Complex Environments

Rafael Brüscheiler, Ph.D., Ohio Research Scholar, Department of Chemistry and Biochemistry, Ohio State University and College of Medicine

9:10 Structure Determination of Fragrance and Flavor Ingredients in Mixtures

Jing Li, Ph.D., Senior Research Investigator, International Flavors and Fragrances

9:40 Networking Coffee Break

POLYMERS

10:10 Session Chair's Remarks

Jim DeFelippis, The Dow Chemical Company

10:15 Analyses of Polyolefins by Temperature-Gradient NMR Spectroscopy

Frank Malz, Ph.D., Manager, Structure Elucidation Group, Fraunhofer Institute for Structural Durability and System Reliability

10:45 ¹³C NMR on Chain Microstructure of Polymers

Guangxin Lin, Ph.D., Analytical Chemist, Innovative Plastics, SABIC

11:15 NMR Spectroscopy Characterization of Silicone Polymers and Fluids used in Electronic Components

Todd M. Alam, Department of Electronic, Optical and Nanostructured Materials, Sandia National Laboratories

11:45 BRUKER LUNCHEON PRESENTATION:
Complete Molecular Confidence: The Most
Convenient and Powerful Software Suite for NMR
Data Analysis on the Fly

Till Kühn, Ph.D., NMR Application & Product Manager, Bruker BioSpin

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GETTING MORE WITH LESS: LOW VOLUME/LOW RESOLUTION NMR

1:15 pm Session Chairs' Remarks

Kirsten Skogerson, Monsanto and John Marino, NIST

1:20 NMR for Non-NMR Spectroscopists: How to Gain More with Lower Resolution

Maria V.S. Elipe, Ph.D., NMR Leader, Structure Elucidation, Analytical R&D, Amgen, Inc.

1:50 Integration of Capillary NMR into a Multidisciplinary Approach for Characterization of Trace Components in Mixtures

Dave Detlefsen, Ph.D., Co-Founder, Novatia

2:20 Pushing NMR to the Nanoscale: Progress and Challenges

Daniel Rugar, Ph.D., Manager, Nanoscale Studies, Almaden Research Center, IBM

2:50 Refreshment Break in the Exhibit Hall with Poster Viewing

NUTRACEUTICALS

3:20 Session Chair's Remarks

Kristie M. Adams, The United States Pharmacopeial Convention

3:25 Improved Techniques for Mixture Analysis

David Russell, Ph.D., Applications Scientist, Research Products Group, Agilent Technologies

3:55 NMR-Based Authentication of Nutraceuticals, Herbal Supplements, and Food Additives: Economic- and Efficacy-Driven Adulteration of Aloe Vera, Herbal Erectile Dysfunction Supplements, and Acacia Gum

John Edwards, Ph.D., Process NMR Associates

4:25 Fishing in the Multiplet Pond: HiFSA-Based qHNMR of Natural Products and Pharmacopeial Materials

Guido Pauli, Ph.D., Associate Professor, Medicinal Chemistry and Pharmacognosy, College of Pharmacy, University of Illinois, Chicago

4:55 **WORKSHOP: METHODS VALIDATION**

Moderated by: Carlos Amezcua, Ph.D., Structural Elucidation Group, Baxter Healthcare

Timothy L. Shelbourn, Research Scientist, Small Molecule Design and Development, Eli Lilly and Company

Torsten Schoenberger, Forensic Science Institute of the Federal Criminal Police Office (BKA), Germany

Michele Derider, Ph.D., Molecular Structure and Spectroscopy Group, Catalent Pharma Solutions

5:55 Welcome Reception in the Exhibit Hall with Poster Viewing

6:55 Close of Day 1

TUESDAY, FEBRUARY 4

8:00 am Co-Chair's Remarks

G. Joseph Ray, Baxter Healthcare and Daron I. Freedberg, FDA

BIOLOGICAL/PHARMACEUTICAL NMR

8:05 Session Chair's Remarks

Carlos Amezcua, Baxter Healthcare

8:10 BioNMR without Labeled Protein - Applications in Pharmaceutical Industry

Alfred Ross, Ph.D., Head, Project NMR Work Group, F. Hoffmann-La Roche Basel

8:40 Characterization of Formulated Monoclonal Antibodies by ¹H NMR

Leszek Poppe, Ph.D., Principal Scientist, Molecular Structure and Characterization, Amgen

9:10 NMR in the Characterization and Quality Control of Polysaccharide-Based Vaccines

Chris Jones, Ph.D., National Institute for Biological Standards and Control (NIBSC)

9:40 Coffee Break in the Exhibit Hall with Poster Viewing

QUANTITATION

10:10 Session Chair's Remarks

Torsten Schoenberger, Forensic Science Institute of the Federal Criminal Police Office (BKA), Germany

10:15 The Swiss Army Knife for Quantitative NMR: Creation of a Universal NMR Reference Standard

Bernd W.K. Diehl, Ph.D., CEO, Spectral Service AG

10:45 Comparison of ¹³C Quantitation Results on Different NMR Spectrometer/Probe Configurations

Catherine Quinn, Research Associate, Structure Elucidation Group, Baxter Healthcare

11:15 ¹H NMR Quantification of Major Saccharides in Açai Raw Materials: A Comparison of the Internal Standard Methodology with the Absolute Intensity qNMR Method

Angela I. Calderón, Ph.D., Assistant Professor, Department of Pharmacal Sciences, Auburn University School of Pharmacy

**11:45 AGILENT LUNCHEON PRESENTATION:
CRAFT – An Automated Deconvolution
Tool for Complex NMR Spectra**

Krish Krishnamurthy, Ph.D., Applications Fellow, Research Products Division,
Agilent Technologies

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COMPLEX MIXTURES II

1:15 pm Session Chair's Remarks

Kathleen Farley, Pfizer, Inc.

1:20 Metabolomics in Aquaculture

Dan Bearden, Ph.D., Lead NMR Scientist, Chemical Sciences Division, National
Institute of Standards and Technology (NIST)

1:50 Challenges Faced and Benefits Realized in Moving Applications from High-Field NMR to Low-Field (Permanent Magnet) NMR Systems, to Support Nutritional Manufacturing Operations

Marti Bergana, Ph.D., Principal Research Scientist & Section Manager,
Abbott Nutrition

2:20 Assessing Atropisomer Axial Chirality in Drug Discovery and Development

Steven R. LaPlante, Ph.D., Co-Founder, NMX Solutions

2:50 Refreshment Break in the Exhibit Hall with Poster Viewing

ONLINE/AT LINE NMR

3:20 Session Chair's Remarks

John Edwards, Process NMR Associates, LLC

3:25 A Compact, Portable 4.7 T Driven NMR System for Reaction Monitoring

Mark Zell, Ph.D., Senior Principal Scientist & Technical Leader, Structure
Elucidation Group, Pfizer

3:55 NMR Well Logging and Downhole Fluid Characterization

Martin Hürlimann, Ph.D., Scientific Advisor, Schlumberger-Doll Research

4:25 Characterizing a Hydrogenation Reaction: *In situ* NMR and Mechanistic Modeling

Jonas Buser, NMR Structural Characterization Group, Eli Lilly and Company

4:55 WORKSHOP: FUTURE OF NMR

Moderated by: Edward Zartler, Ph.D., President & CSO, Quantum Tessera
Consulting

Kristie M. Adams, Ph.D., NMR Spectroscopist, Research & Development
Laboratory, The United States Pharmacopeial Convention

Bernd W.K. Diehl, Ph.D., CEO, Spectral Service AG

Chris Jones, Ph.D., National Institute for Biological Standards and Control
(NIBSC)

5:55 Refreshment Break in the Exhibit Hall with Poster Viewing

6:55 Close of Day 2

WEDNESDAY, FEBRUARY 5

8:10 am Co-Chair's Remarks

G. Joseph Ray, Baxter Healthcare and Daron I. Freedberg, FDA

UNIQUE APPLICATIONS

8:15 Session Chair's Remarks

Edward Zartler, Quantum Tessera Consulting

8:20 Automated Metabolite Analysis for Clinical Diagnostic Applications

Tom O'Connell, Ph.D., Senior Director, Research & Development, LipoScience

8:50 HR-MAS NMR as a Direct Tool for the Analysis of Viscous Materials

Martina Vermathen, Ph.D., Principal Investigator, Department of Chemistry &
Biochemistry, University of Berne, Switzerland

9:20 How Polarization Transfer Techniques and 2D NMR can be used for Isotopic Analysis at Natural Abundance

Serge Akoka, Ph.D., Professor, Analytical Chemistry, University of Nantes, France

9:50 Coffee Break in the Exhibit Hall with Poster Viewing

STRUCTURE ELUCIDATION

10:20 pm Session Chair's Remarks

Gonzalo Hernandez, NMR Consultant

10:25 Recent Advances in ADEQUATE and Covariance Processing: A New Paradigm in Structure Elucidation

Gary E. Martin, Ph.D., Senior Principal Scientist, Merck Research Laboratories

10:55 Structural Analysis of Rigid and Flexible Small Organic Molecules Assisted by Residual Dipolar Couplings

Roberto R. Gil, Ph.D., Research Professor and Director, NMR Laboratory,
Department of Chemistry, Carnegie Mellon University

11:25 NMR with Multiple Receivers

Ēriks Kupče, Ph.D., DrHab, Principal Scientist, BrukerBioSpin

11:55 Luncheon Presentation (Sponsorship Opportunity Available)
or Lunch on Your Own

1:25 pm WORKSHOP: DATA MANAGEMENT

Moderated by: Kathleen Farley, Pfizer, Inc.

Bruce A. Johnson, Ph.D., Founder & President, One Moon Scientific, Inc.

Carlos Amezcua, Ph.D., Structural Elucidation Group, Baxter Healthcare

Molly P. Bohlen, Principal Researcher, Fabric and Home Care Analytical

Sciences, The Procter and Gamble Company

2:25 Networking Refreshment Break

MATERIALS

Session Chairs: Edward Zartler, Quantum Tessera Consulting

John Edwards, Process NMR Associates, LLC

2:45 Solid-State NMR Utility in API and Formulation Process Development

Robert Wenslow, Ph.D., Vice President, Business Development, Crystal
Pharmatech Co., Ltd.

3:15 Insights into Molecular Packing of Semicrystalline P3HT by Variable Temperature ¹H Relaxation and ¹³C Solid-State NMR Measurements

Ryan Nieuwendaal, National Institute of Standards and Technology (NIST)

SOLID STATE & IMAGING

Session Chair: Yves Aubin, Health Canada

3:45 Solid State NMR: A Multi-Function Tool in Pharmaceutical Development, much more than a "Phase Meter"

George B. Crull, Ph.D., Leader, Solid State Spectroscopy Group, Material
Science, Drug Product Science and Technology, Bristol-Myers Squibb

4:15 New Methods for Solid-State NMR of Active Pharmaceutical Ingredients: Bulk, Polymorphic and Dosage Forms

Rob Schurko, Ph.D., Professor, Department of Chemistry and Biochemistry,
University of Windsor

4:45 Closing Remarks

G. Joseph Ray, Baxter Healthcare and Daron I. Freedberg, FDA

4:50 Close of PANIC

Sponsorship & Exhibit Opportunities

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- 30-minute podium presentation (plus 15 minutes for Q&A)
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- One 8'x10' exhibit space
- Two (2) full access conference registrations for your staff (in addition to speaker)
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 - Additional full conference registrations available at a discount for your staff (limit of 5)
 - 50-word company description in the Program & Exhibits Guide
 - Pre- & post-conference attendee lists for one-time usage

Sponsorship fee: \$10,000

► CORPORATE SUPPORT SPONSOR

- One (1) full access conference registration for your staff
- Logo on the event website, conference proceedings, program guide and on-site signage (contingent of meeting marketing deadlines)
- 50-word company description in the Program & Exhibits Guide
- Additional full conference registrations available at a discount for your staff (limit of 5)
- Post-conference attendee list for one-time usage

Sponsorship fee: \$8,500 (includes exhibit space)

Without Exhibit Space: \$5,000

► EXHIBIT BOOTH SPACE

- Booth space (8'D x 10'W)
- Two (2) full access conference registrations for your staff (booth and session access)
- Corporate URL link on conference proceedings
- 50-word company description in the Program & Exhibits Guide

Exhibit fee: \$3,795

For additional information (including Educational Grant Sponsorships), contact:

Carolyn Benton – Business Development Manager

781-972-5412 | cbenton@healthtech.com

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Present a Poster

PANIC encourages all delegates to gain further exposure by presenting their work in the poster sessions. To secure a poster board and inclusion in the conference materials, your abstract must be submitted, approved and your registration paid in full by December 20, 2013.

Register online, or by phone, fax or mail. Please indicate that you would like to present a poster. Once your registration has been fully processed, we will send an email with a unique link and instructions for submitting your abstract using our online abstract submission tool.

Reasons you should present your research poster:

- Your poster will be exposed to our international delegation
- Your poster abstract will be published in our conference materials
- Your research will be seen by industry leaders

Note: Posters should be portrait orientation, with maximum dimensions of 36 inches wide (3 feet) by 48 inches high (4 feet).

Student Travel Grants

PANIC is pleased to provide a limited number of student travel grants for Ph.D. students and post-doctoral fellows who present posters at the 2nd annual Practical Applications of NMR in Industry Conference (PANIC). Ph.D. students or post-doctoral fellows conducting research with professors in Industry or at universities throughout the world are eligible.

Applicants should email a letter to grants@panicnmr.com requesting consideration for the grant, along with the following documents:

- Two letters of recommendation. At least one of these letters should be from the applicant's advisor or supervisor
- A PDF version of poster abstract
- The applicant's CV

Submissions for travel grants must be received by November 29, 2013

Hotel & Travel Information

CONFERENCE VENUE AND HOTEL:

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Discounted Room Rate: \$160* s/d *Room Rate includes Breakfast daily in hotel restaurant and Internet in guestroom

Discounted Room Rate Cut-off Date: January 3, 2014

Please visit the hotel page of our conference website to make your reservations online or call the hotel directly to reserve your sleeping accommodations. Rooms are limited, so please book early.

For additional travel information, including flight and car rental discounts, visit PANICnmr.com

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