Second Annual Practical Applications of NMR in Industry Conference
Hilton Charlotte University Place | Charlotte, North Carolina
February 3 – 5, 2014

REGISTER BY NOVEMBER 8 AND SAVE UP TO $200

Event Pricing

Student Pricing $395*
Early Registration Discount until November 8, 2013 $650
Advance Registration Discount until January 10, 2014 $750
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
- Online/At Line NMR
- Pharmaceutical NMR
- Polymers
- Quantitation
- Solid State & Imaging
- Structure Elucidation
- Unique Applications

Workshops:
- Methods Validation
- Data Management
- Future of NMR

reg@healthtech.com
P: 781.972.5400 or Toll-free in the U.S. 888.999.6288
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 Manokhova, Ph.D., CVUA Karlsruhe

8:40 NMR in Metabolomics: Characterizing Metabolites in Complex Environments
Rafael Bruschweiler, 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 Kuhn, Ph.D., NMR Application & Product Manager, Bruker BioSpin

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 Pharmacopoeial 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

10:55 Improved Quantitation with 1H NMR
Leszek Poppe, Ph.D., Principal Scientist, Molecular Structure and Characterization, Amgen

11:15 1H NMR Quantification of Major Saccharides in Açaí 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

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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 & CEO, Quantum Tessera Consulting
Kristie M. Adams, Ph.D., Senior Principal Scientist, Quantum Tessera Consulting

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 J. 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 Amezgua, 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)

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 J. Freedberg, FDA

4:50 Close of PANIC
Sponsorship & Exhibit Opportunities

**PREMIER SPONSOR: LUNCHEON WORKSHOP—1 LEFT!**
- 30-minute podium presentation (plus 15 minutes for Q&A)
- Boxed-style lunch for all conference attendees (125-150 expected)
- Logo and luncheon workshop promotion on the event website, conference proceedings, program guide and on-site signage (contingent of meeting marketing deadlines)
- One 8’x10’ exhibit space
- Two (2) full access conference registrations for your staff (in addition to speaker)
- 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 physical mailing usage

**SPONSORSHIP FEE: $15,000**

**CORPORATE SPONSOR**
Benefits include ONE of the following options:
- Tote Bags
- Lanyards – SOLD
- Exhibit Hall Reception
- One 8’x10’ exhibit space
- Two (2) full access conference registrations for your staff
- Logo on the event website, conference proceedings, program guide and on-site signage (contingent of meeting marketing deadlines)
- 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 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

**CURRENT SPONSORS & EXHIBITORS** As of 9/27/13
- Advanced Chemistry Development, Inc. (ACD/Labs)
- Agilent Technologies
- Aspect Imaging
- Bruker Biospin
- Doty Scientific
- HTS-110
- JEOL USA, Inc.
- Mestrelab Research, S.L.
- One Resonance Sensors, LLC
- Oxford Instruments

**EDUCATIONAL AND OR TRAVEL GRANT SPONSORS** As of 9/27/13
- Cambridge Isotope Labs
- Monsanto
- National Institute of Standards & Technology (NIST)

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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).

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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**

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Hotel & Travel Information

**CONFERENCE VENUE AND HOTEL:**
Hilton Charlotte University Place
8629 JM Keynes Drive
Charlotte, NC 28262
Phone: 704-547-7444

**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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