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5th Annual Practical
Applications of NMR
in Industry Conference



SONESTA RESORT HILTON HEAD ISLAND • HILTON HEAD ISLAND, SC

February 20 – 23, 2017

REGISTER BY JANUARY 6, 2017 AND SAVE UP TO \$150

Please use keycode **NMR F** when registering!

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Additional Educational & Travel Grant provided by Cambridge Isotope Laboratories, Inc.

Join Us in Hilton Head!

Event Pricing

Event Pricing

Advance Registration Discount until January 6, 2017

Conference Only

\$700

Registration after January 6, 2017

\$850

Student Fellowship Program Pricing

Students are required to submit a poster abstract.*

Conference Only

\$400

**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 16, 2016.*

PANICnmr.com

User Meetings

Make plans to arrive in Hilton Head early and attend User Meetings on Monday, February 20, 2017! We're working with Bruker, ACD/Labs and Mestrelab to completely redesign our approach to User Meetings for 2017, to better accommodate our conferees. Registration will be necessary, so stay tuned for more information as the conference date approaches.

Details will be announced as they become available on vendor websites, www.PANICnmr.com, www.nmrvalidation.org and in NMR-related LinkedIn groups (NMR Validation, PANIC).

MONDAY, FEBRUARY 20

- 4:30 pm** Pre-Conference Registration Open
- 5:30** Welcome Reception in the Exhibit Hall with Poster Viewing
- 6:45** End of Day

TUESDAY, FEBRUARY 21

- 8:15 am** Registration & Morning Coffee
- 8:45** Chairs' Welcome
Gonzalo Hernandez, Vis Magnetica NMR Consulting
Kristie M. Adams, Dupont

FORENSICS

- 8:50** Chairperson's Remarks
Torsten Schoenberger, Bundeskriminalamt
- 9:00** Interactive Datahub to Facilitate Identification of Emerging Synthetic Drugs (ESDs)
Aaron Urbas, Ph.D., NIST
- 9:30** The Increasing Need for Structure Elucidation Experts in Forensic Drug Analysis
Charlotte Corbett, Ph.D., DEA
- 10:00** Application of NMR Methods for the Resolution of Forensic Cases at the Swedish National Forensic Center
Simon Dunne, Professor, Swedish National Forensic Center
- 10:30** Coffee Break in the Exhibit Hall with Poster Viewing

POLYMERS

- 11:20** Chairpersons' Remarks
Jim DeFelippis, The Dow Chemical Company
Michael C. Davis, Bridgestone Americas Center for Research and Technology
- 11:30** The Versatility of Liquid State NMR Spectroscopy in Polymer Chemistry and Engineering: An Industrial Perspective
Ard Kolkman, Ph.D., DSM
- 12:00 pm** 2D Quantitative NMR for Large Molecules
Patricia Sepulcri, Ph.D., Sanofi Pasteur Marcy L'Etoile
- 12:30** Field-Cycling NMR Relaxometry as a Versatile Tool of Molecular Rheology
Ernst Roessler, Professor, University of Bayreuth
- 1:00** Luncheon Presentation to be Announced
- 1:45** Session Break
- 2:30** Introduction to Friday's Validation Workshop
Torsten Schoenberger, Bundeskriminalamt

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PHARMACEUTICALS

- 2:45** Chairpersons' Remarks
John Marino, NIST
Carlos Amezcua, Baxter Healthcare Corporation
- 2:55** High-Throughput Analysis of Antibiotics Using Capillary Stop Flow NMR
David Keire, Ph.D., U.S. FDA
- 3:25** Overcoming Challenges with Identification of Ingredients for Counterfeit Drug Investigations
Charles Pathirana, Ph.D., Bristol-Myers Squibb
- 3:55** Water Proton NMR for Noninvasive Pharmaceutical Analysis
Bruce Yu, Professor, University of Maryland
- 4:25** Multi-Attribute Determination Using NMR to Ensure Success
Michael Jones, Ph.D., Pfizer
- 4:55** Light Reception in the Exhibit Hall with Poster Viewing
- 5:45** Transition to Pavilion
- 6:00** Coastal Grill Out Party*
**The Coastal Grill Out Party is complimentary; registration is required. See registration page for details.*
- 9:00** End of Day

WEDNESDAY, FEBRUARY 22

- 8:15 am** Morning Coffee
- 8:45** Chairs' Welcome
Gonzalo Hernandez, Vis Magnetica NMR Consulting
Kristie M. Adams, Dupont
- STRUCTURE ELUCIDATION AND COMPLEX MIXTURES**
- 8:50** Chairperson's Remarks
David Cistola, University of North Texas Health Science Center
- 9:00** CLIP-COSY: Rapid Acquisition of COSY-Type Correlation Spectra with In-Phase Signal Character
Lukas Kaltschnee, Ph.D., NIH
- 9:30** Marine Natural Products as a Challenge for an NMR-Based Structure Elucidation
Matthias Köck, Ph.D., Alfred-Wegener Institute
- 10:00** The NIST Metabolomics Data Quality Initiative: qMet
Dan Bearden, Ph.D., NIST
- 10:30** Coffee Break in the Exhibit Hall with Poster Viewing

PETROLEUM AND PETROCHEMISTRY

- 11:20** Chairpersons' Remarks
Sonia Maria Menezes, Petrobras Brazil
Katherine Wu, Albemarle Corporation
- 11:30** NMR Spectroscopy and Calculus of the Average Molecular Parameters of Crude Oils and Fractions
Juan Carlos Poveda Jaramillo, Professor, Universidad Industrial de Santander
- 12:00 pm** Supporting Development of New Refining Technologies Using Simple and Quick NMR Methodologies
Ajit Pradhan, Ph.D., Chevron Energy Technology Company
- 12:30** Research and Development in Oil and Porous Media NMR
Tito J. Bonagamba, Professor, Universidade de Sao Paulo
- 1:00** Luncheon Presentation to be Announced

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FOOD AND AGRICULTURE

2:30 Chairperson's Remarks

Adriana Carvalho de Souza, DSM Biotechnology Center

2:40 Rapid and Quantitative Assessment of Early Lipid Oxidation in Food Emulsions During Shelf-Life by Nuclear Magnetic Resonance

Donny Merckx, Unilever

3:10 Investigation of Egg Yolk Lipids with NMR

Svenja Ackermann, Chemical and Veterinary Investigation Office, CVUA Karlsruhe

3:40 Several NMR Applications for the Analysis of Foods and Dietary Supplements

Clark Ridge, Ph.D., U.S. FDA

4:10 Refreshment Break in the Exhibit Hall with Poster Viewing

PLANT PRODUCTION/PROBLEM SOLVING

5:05 Chairperson's Remarks

J. Andrew Surface, PPG Industries, Inc.

5:15 NMR Spectroscopy as a Tool for Process Development and Optimization

Erik von Harbou, Professor, University of Kaiserslautern

5:45 Plant Support Using NMR

Sarah Mattler, Ph.D., Exxon Mobil Chemical Company

6:15 Compact NMR Spectroscopy for Sustainable and Flexible Production of High Quality Chemical Products

Simon Kern, BAM

6:45 Networking Reception in the Exhibit Hall with Poster Viewing

7:45 End of Day

THURSDAY, FEBRUARY 23

8:15 am Morning Coffee

8:45 Chairs' Welcome

Gonzalo Hernandez, Vis Magnetica NMR Consulting

Kristie M. Adams, Dupont

SOLIDS/DNP

8:50 Chairperson's Remarks

Michael C. Davis, Bridgestone Americas Center for Research and Technology

9:00 From Traditional Small Molecules to Novel Liquid Crystal Formulations in Drug Development: A Solid-State NMR Journey

Anuji Abraham, Ph.D., Bristol-Myers Squibb

9:30 Dynamic Nuclear Polarization (DNP) Enhanced Solid-State NMR Investigations of Pharmaceuticals

Yongchao Su, Ph.D., Merck Research Laboratories

10:00 Structural Investigation of Organic Materials by Solid-State Dynamic Nuclear Polarization Nuclear Magnetic Resonance Spectroscopy

Stephane Viel, Professor, Aix-Marseille University

10:30 Coffee Break in the Exhibit Hall with Poster Viewing

LOW-FIELD/BENCHTOP

11:30 Chairperson's Remarks

Kathleen Farley, Pfizer, Inc.

11:40 Nondestructive Materials Testing and Reaction Monitoring with Compact NMR Instruments

Bernhard Blümich, Professor, RWTH Aachen University

12:10 pm Advanced Methods in TD-NMR Relaxometry: Applications in Agriculture and Food Products

Luiz Colnago, Ph.D., EMBRAPA Instrumentacao

12:40 ¹⁹F and ¹H TD-NMR Prospective Applications in Quantitation and Qualitative Analysis for Small and Large Molecule Pharmaceuticals

Maria Victoria Silva Elipse, Ph.D., Amgen

1:10 Luncheon Presentation (Sponsorship Opportunity Available) or Enjoy Lunch on Your Own

1:55 Session Break

2:40 Poster Awards & Spectrum Contest Winners Announced

Poster awards provided by MRC/Wiley

DATA PROCESSING AND ANALYSIS TOOLS

2:55 Chairperson's Remarks

Kristie M. Adams, Dupont

3:05 Non-Uniform Sampling for All: More Spectral Quality, Less Measurement Time

Frank Delaglio, Ph.D., IBBR, NIST

3:35 NMR Mixture Analysis Using Machine Learning

Paul Coote, Ph.D., Harvard Medical School

4:05 Using R to Make Sense of NMR Datasets

Bryan Hanson, Professor, DePauw University

4:35 Discussion

4:55 End of PANIC 2017

Save the date for the Third Annual Validation Workshop at PANIC!

Please join us on Friday, February 24, 2017 for a day-long workshop dedicated to current developments in validation of NMR methods. This interactive workshop will consist of several short lectures on key aspects of (q)NMR method validation, updates on recent developments in the field, and opportunities for collaborative exchange of ideas.

Don't miss the opportunity to be part of this (most) promising movement for practical NMR!

Attendance is free, but registration is necessary. As the conference date approaches, keep an eye out for additional information, posted at www.PANICnmr.com, www.nmrvalidation.org and in NMR-related LinkedIn groups (NMR Validation, PANIC).

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 16, 2016**.

Reasons you should present your research poster at this conference:

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

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 4th 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 **December 16, 2016**

Current Sponsors, Exhibitors & Educational Support Sponsors (as of August 30, 2016)

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Sponsorship & Exhibit Opportunities

► **PREMIER SPONSOR:** Includes 30-minute luncheon presentation with an additional 15 minutes for Q&A – Only TWO opportunities remaining!

Sponsorship Fee: \$15,000

► **CORPORATE SPONSOR:** Includes choice of branding item!

Sponsorship Fee: \$10,000

► **CORPORATE SUPPORT SPONSOR**

Sponsorship Fee: \$8,500

► **COASTAL GRILL OUT PARTY SPONSOR**

The host hotel is located directly on the beach and features an open-air pavilion overlooking the pool area. In an effort to encourage extended networking hours, we're thinking a dinner reception in the Pavilion with music and dancing on Tuesday evening. The open-air pavilion does have a roof in case of inclement weather. The reception would be open to all conference participants: conference delegates, speakers, exhibitors and sponsors. We are looking for sponsors to help us cover the cost for the reception/music etc.

Sponsorship Fee: \$5,000

► **STUDENT EDUCATIONAL & TRAVEL GRANT SPONSOR**

PANIC provides a limited number of student travel grants for Ph.D. students and post-doctoral fellows who present posters at the 5th 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 are required to email a letter 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 and the applicant's CV.

With branding ~ Sponsorship Fee: \$1,500

Without branding ~ Sponsorship Fee: \$900

► **EXHIBIT BOOTH: 8' x 10' exhibit space**

Early Rate (before September 23, 2016): \$3,495

Standard Rate: \$3,795

For additional information regarding sponsorship and exhibit opportunities, please contact:

Carolyn Benton

Business Development Manager

781-972-5412

cbenton@healthtech.com

Hotel & Travel Information

Conference Venue and Hotel:

Sonesta Resort Hilton Head Island
130 Shipyard Drive
Hilton Head Island, SC 29928
Phone: 843-842-2400

Reservations: Go to the travel page of PANICnmr.com

Discounted Room Rate: \$159 single rate / \$179 double rate, plus \$10.00 resort fee*

(single rate includes breakfast for one and double rate includes breakfast buffet for two & complimentary guestroom Wi-Fi)

Discounted Cut-off Date: January 23, 2017

 **Book Early! Plan Your Trip to Hilton Head, South Carolina**

PANICnmr.com

reg@healthtech.com

P: 781.972.5400 or Toll-free in the U.S. 888.999.6288

Please use keycode **NMR F** when registering

