

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

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Practical Applications of NMR in Industry Conference

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Kirsten Skogerson, Monsanto Corporation

Katherine Wu, Albemarle Corporation

Edward Zartler, Quantum Tessera Consulting

MONDAY

7:30 am Registration and Morning Coffee (*La Jolla Ballroom Foyer*)

8:30 **Chairs' Welcome** (*La Jolla Ballroom E-H*)
G. Joseph Ray, Ph.D., Senior Research Scientist, Technology Resources, PCS, Baxter Healthcare
Edward R. Zartler, Ph.D., President & CSO, Quantum Tessa Consulting

SOLIDS/POLYMERS

8:35 **Session Chairs' Remarks**
Jim DeFelippis, The Dow Chemical Company
Michael Davis, Bridgestone Americas Center for Research and Technology

8:45 **Application of Codex to Pressure Sensitive Adhesives**
Mark McCormick, Ph.D., Research Specialist, Corporate Research Analytical Laboratory, 3M

9:15 **Solid-State NMR Study of the Effect of Crosslink Density on Morphology and Local Segmental Mobility in Polyurethane Based Foams**
Daniel Mowery, Ph.D., Research Scientist, Analytical Sciences, The Dow Chemical Company

9:45 **NMR Analysis of Solution Polymers in Industrial R&D**
Brian Antalek, Ph.D., Senior Research Scientist, Analytical Chemistry, Eastman Kodak

10:15 **Coffee Break in the Exhibit Hall with Poster Viewing, Even Numbered Posters** (*La Jolla Ballroom A-D*)

COMPLEX MIXTURES I

10:55 **Session Chair's Remarks**
Kathleen Farley, Pfizer, Inc.

11:05 **nD NMR Spectroscopy of ¹³C-Methylated Humic Substances**
Dusan Uhrin, Ph.D., Reader, Chemistry, University of Edinburgh

11:35 **Solid-State NMR analysis of the Twin-Arginine Translocase**
Torsten H. Walther, Ph.D., Young Investigator Group Leader, Institute of Organic Chemistry, Karlsruhe Institute of Technology (KIT)

12:05 pm **Configurational Analysis of Complex Marine Natural Products, an NMR-Based Computational Approach**
Matthias Koeck, Ph.D., Senior Researcher, Ecological Chemistry, Alred-Wegener-Institut

MONDAY

BRUKER LUNCHEON CO-PRESENTATION

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12:35 **NMR Fingerprinting for Phylogenetics**
Jonathan Ferrier, Ph.D., University of Ottawa

12:50 **InsightMR**
Brian Marquez, Ph.D., Principal Scientist, Bruker Corporation



1:20 **Session Break**

FOOD & AGRICULTURE

2:15 **Session Chair's Remarks**
Gonzalo Hernandez, Vis Magnetica NMR Consulting

2:25 **The Authenticity of Colombian Coffee**
Julien Wist, Ph.D., Assistant Professor, Chemistry Department, Universidad del Valle

2:55 **Effects of Ions on Water Structure: A Low Field ^1H T1 NMR Relaxometry Approach**
Pellegrino Conte, Ph.D., Associate Professor, Dipartimento Scienze Agrarie e Forestali, Università degli Studi di Palermo

3:25 **Applications of NMR Spectroscopy in Olive Oil Analysis**
Emmanuel Hatzakis, Ph.D., NMR Director, Pennsylvania State University

3:55 **Welcome Reception in the Exhibit Hall with Poster Viewing, Odd Numbered Posters (La Jolla Ballroom A-D)**

5:10 **Close of Day**

TUESDAY

- 9:00 am** Morning Coffee in the Exhibit Hall with Poster Viewing, Even Numbered Posters (*La Jolla Ballroom A-D*)
- 10:10** Chairs' Welcome (*La Jolla Ballroom E-H*)
G. Joseph Ray, Ph.D., Senior Research Scientist, Technology Resources, PCS, Baxter Healthcare
Edward R. Zartler, Ph.D., President & CSO, Quantum Tessera Consulting

COMPLEX MIXTURES II

- 10:15** Session Chair's Remarks
Adriana Carvalho de Souza, DSM Biotechnology Center
- 10:25** Quantitative Detection of Nucleic Acid Fragments in a Complex Matrix
Peter P. Lankhorst, DSM Biotechnology Center
- 10:55** Quantitative NMR of Polysaccharides in Complex Food Matrices
Ewoud J.J. van Velzen, Ph.D., Measurement Science, Unilever R&D Vlaardingen
- 11:25** LC/GPC-NMR of Complex Polymer Mixtures
Jian Wu, Ph.D., Research Scientist, Analytical Sciences, Core R&D, The Dow Chemical Company

- 11:55** ASPECT IMAGING LUNCHEON PRESENTATION
NMR NO LIMITS
Tali Cohen, Director, NMR Division, Aspect Imaging
Uri Rapoport, Founder, President & CEO, Aspect Imaging

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- 12:40 pm** Session Break

PETROCHEMICAL/REFINERY

- 1:35** Session Chair's Remarks
Katherine Wu, Albermarle Corporation
Michael C. Davis, Bridgestone Americas Center for Research and Technology
- 1:45** NMR Applications in Petrochemical Industry
Maziar Sardashti, Ph.D., Principal Scientist Lead, Analytical Sciences, Phillips 66
- 2:15** *In situ* NMR Reveals Water Can Dramatically Increase or Suppress Zeolite-Catalyzed Alkane C-H Bond Activation
Jeffery White, Ph.D., Professor, Chemistry, Oklahoma State University
- 2:45** PLS Modeling of the Petroleum Cut 13C NMR Spectra to Predict a Complex Property of Base Oil
Marion Lacoue-Negre, Ph.D., Research Engineer, Products Characterization, IFP Energies Nouvelles

TUESDAY

3:15 Refreshment Break in the Exhibit Hall with Poster Viewing, Odd Numbered Posters (La Jolla Ballroom A-D)

BENCHTOP (LOW RES)

3:55 Session Chair's Remarks

John Edwards, Process NMR Associates, LLC

4:05 An Orthogonal Study of Applied NMR Spectroscopy for Process QA/QC of an Oligosaccharide-Based Food Ingredient

Lee Madsen II, Ph.D., Director, Research & Development, ISOThrive, LLC

4:35 Detection and quantification of adulterants in dietary supplements with a low-field bench-top 1H NMR spectrometer

Myriam Malet-Martino, Ph.D., University Professor, Chemistry, Paul Sabatier University

5:05 The Power of Variable Field Spin-Relaxation

Robert G. Bryant, Ph.D., Commonwealth Professor, Emeritus, Chemistry, University of Virginia

5:35 Networking Reception in the Exhibit Hall with Poster Viewing, All Posters (La Jolla Ballroom A-D)

6:35 Close of Day

WEDNESDAY

8:00 am Morning Coffee (*La Jolla Ballroom Foyer*)

8:30 Chairs' Welcome (*La Jolla Ballroom E-H*)

G. Joseph Ray, Ph.D., Senior Research Scientist, Technology Resources, PCS, Baxter Healthcare
Edward R. Zartler, Ph.D., President & CSO, Quantum Tessa Consulting

UNIQUE APPLICATIONS

8:35 Session Chair's Remarks

Molly Bohlen, Procter & Gamble

8:45 HCNMBC: A New Method for Identification of Nitrogen Heterocycles via Natural Abundance ¹³C-¹⁵N Coupling

Steve Cheatham, Ph.D., NMR Spectroscopist, Analytical, DuPont Crop Protection

9:15 NMR Measurement of Molecular Dynamics to Characterize Material Structure and Transport Function: Microrheology of Colloids and Phase Transitions in Polymers

Joseph Seymour, Ph.D., Professor, Chemical and Biological Engineering, Montana State University

9:45 Quantitative Studies of Fast Reactions with a Novel Thermostatted Micro-Reactor NMR Probe Head

Erik von Harbou, Ph.D., Assistant Professor, Laboratory of Engineering Thermodynamics, University of Kaiserslautern

10:15 Coffee Break in the Exhibit Hall with Poster Viewing, Even Numbered Posters (*La Jolla Ballroom A-D*)

QNMR/QUANTITATION

10:50 Session Chairs' Remarks

John Marino, NIST

Kristie M. Adams, The United States Pharmacopeial Convention

11:00 Model-Free Quantitative Component Analysis by Solid State NMR Using the Direct Exponential Curve Resolution Algorithm

Dirk Stueber, Ph.D., Associate Principal Scientist, MRL, Merck

11:30 qNMR forever – reference material metrology at high pressures and high purities

Michael Maiwald, Ph.D., Head, Division, Process Analytical Technology, BAM Federal Institute for Materials Research and Testing

12:00 pm Top of the Traceability Chain: NIST Primary Standard Reference Materials for qNMR

Katrice Lippa, Ph.D., Scientific Advisor, Chemical Sciences Division, NIST

WEDNESDAY

- 12:30 Lunchtime Discussion Forum: ‘What will the future of NMR look like without Agilent/Varian?’**
 After acquiring Varian Instruments only four years ago, Agilent’s sudden announcement to shut down its NMR division in October of 2014 has left only two major commercial vendors of high-field NMR systems worldwide: Bruker and JEOL. While much of the immediate discussion surrounding Agilent’s decision has been justly focused on its impact on Varian/Agilent NMR customers, we feel that we should engage the NMR community as a whole. Towards this goal, we will be holding a lunchtime forum, led by a panel of experts from industry, academia and government, which will focus on the broader implications of Agilent’s decision on the future of NMR research.
 We are hoping for a lively and engaging discussion and aim to produce a short white paper that will be posted on the PANIC website, representing a consensus summary of the opinions of PANIC 2015 attendees.

- 1:15 Session Break**

CHEMOMETRICS

- 2:10 Session Chair’s Remarks**
Kirsten Skogerson, Monsanto Corporation
- 2:20 NMR Metabolomics: Practical Issues and Common Problems**
Robert Powers, Department of Chemistry, University of Nebraska, Lincoln
- 2:50 2D NMR-Based Metabolomics Uncovers Interactions between Conserved Biochemical Pathways in the Model Organism *Caenorhabditis elegans***
Yevgeniy Izrayelit, Ph.D., Postdoctoral Fellow, Engineering, Brown University
- 3:20 Parameterization of 1-D and 2-D NMR Relaxation Measurements for Understanding Complex Multiphase Mixtures**
Charles Eads, Ph.D., Research Fellow, Corporate Functions Analytical, The Procter & Gamble Co.
- 3:50 Refreshment Break in the Exhibit Hall with Poster Viewing, Odd Numbered Posters & Last Chance for Viewing (La Jolla Ballroom A-D)**

NMR/REGULATORY

- 4:20 Session Chair’s Remarks**
Darón Freedberg, CBER, FDA
- 4:30 Specificity of NMR Methods**
Christina Szabo, Ph.D., Senior Research Scientist, R&D, Baxter Healthcare Corporation
- 5:00 Very High Similarity of the Three-Dimensional Structure of Recombinant Protein Therapeutics by NMR at Natural Abundance**
Yves Aubin, Ph.D., Research Scientist, Biologics and Genetic Directorate, Health Canada
- 5:30 Close of Day**

THURSDAY

8:00 am Morning Coffee (*La Jolla Ballroom Foyer*)

8:30 Chairs' Welcome (*La Jolla Ballroom E-H*)
G. Joseph Ray, Ph.D., Senior Research Scientist, Technology Resources, PCS, Baxter Healthcare
Edward R. Zartler, Ph.D., President & CSO, Quantum Tessera Consulting

NMR IN HEALTH/DIAGNOSTICS

8:35 Session Chair's Remarks
David Cistola, University of North Texas Health Science Center, Fort Worth

8:45 Simultaneous NMR Assessment of Inflammation Status and Cardiovascular and Diabetes Risk in a Real World Clinical Laboratory Setting
James Otvos, Ph.D., Adjunct Professor of Molecular and Structural Biochemistry, North Carolina State University; Adjunct Professor of Medicine, University of North Carolina, Chapel Hill; CSO, LipoScience, Inc.

9:15 Liposcale: A Novel Advanced Lipoprotein Test based on 2D Diffusion-Ordered 1H NMR Spectroscopy
Roger Mallol, Ph.D., CEO, Biosfer Teslab

9:45 Developing a First Trimester Diagnostic Tool and Therapy for Preeclampsia Using NMR
Jonathan Ferrier, Ph.D., Postdoctoral fellow, Chronic Disease Program, OHRI, The Ottawa Hospital

10:15 Networking Coffee Break (*La Jolla Ballroom Foyer*)

FORENSICS

10:45 Session Chair's Remarks, Poster Awards Announced and Spectrum Contest Answer Revealed with Prizes Awarded
Torsten Schoenberger, Bundeskriminalamt

10:55 Forensic Applications of NMR at Lawrence Livermore National Laboratory: Biomedical Forensic Analysis and the Organization for the Prohibition of Chemical Weapons
Brian Mayer, Ph.D., Research Chemist, Forensic Science Center, Lawrence Livermore National Laboratory

11:25 NMR at Customs: A New Weapon in the Fight Against Tax Evasion and Unknown Substances
Martin Berkheij, Ph.D., Scientist, Dutch Customs Laboratory

11:55 Fully Automated Quantitative NMR at DEA
Patrick Hays, Senior Research Chemist, DEA Special Testing and Research Laboratory

12:25 pm Closing Remarks
G. Joseph Ray, Ph.D., Senior Research Scientist, Technology Resources, PCS, Baxter Healthcare
Edward R. Zartler, Ph.D., President & CSO, Quantum Tessera Consulting

12:30 Close of PANIC 2015

Sponsor & Exhibitor Company Descriptions

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The Metabolomics Society

843.762.8865 (Treasurer) | www.metabolomicsociety.org

The Metabolomics Society is the international association dedicated to promoting metabolomics, the comprehensive study of small molecules in biological systems and how they respond to stimuli such as disease or genetic modification. It is an independent, non-profit organization, founded in 2004. The Society currently has more than 700 members across 20 countries.

Nanalysis Corp.

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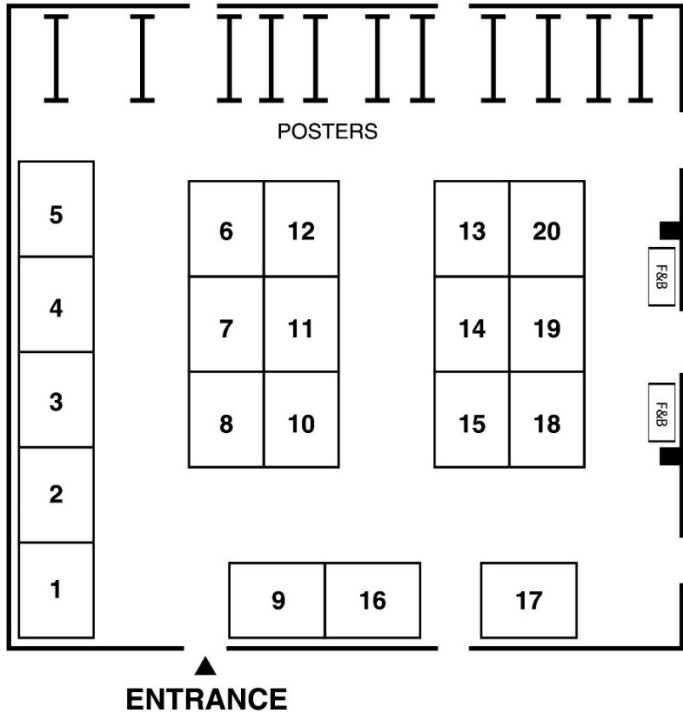
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Exhibit and Poster Schedule and Floor Plan

(La Jolla Ballroom A-D)

<u>Monday</u>	
10:15-10:55am	Coffee Break, <i>Even Numbered Posters</i>
3:55-5:10pm	Welcome Reception, <i>Odd Numbered Posters</i>
<u>Tuesday</u>	
9:00-10:10am	Morning Coffee, <i>Even Numbered Posters</i>
3:15-3:55pm	Refreshment Break, <i>Odd Numbered Posters</i>
5:35-6:35pm	Networking Reception, <i>All Posters</i>
<u>Wednesday</u>	
10:15-10:50am	Coffee Break, <i>Even Numbered Posters</i>
3:50-4:20pm	Refreshment Break, <i>Odd Numbered Posters & Last chance to drop off your entry for the Spectrum Contest</i>



Company	Booth #
Advanced Chemistry Development (ACD/Labs)	12
Anasazi Instruments, Inc.	4
ASPECT IMAGING	1&9
Bruker Corporation	8
Chemomx Inc.	11
HTS-110 Ltd	10
JEOL USA, Inc.	2
LEAP Technologies	15
Magritek	14
Mestrelab Research, S.L.	5
Nanalysis Corp.	19
New Era Enterprises, Inc.	17
Oxford Instruments	6
Quantum Design, Inc.	3
Sigma-Aldrich	7
Silantes GmbH	20
Stelar s.r.l.	16

Poster Presenters
(La Jolla Balroom A-D)

Presenting Monday through Wednesday

BAM Federal Institute for Materials Research and Testing

- 1 Klaus Rademann; Michael Maiwald; and Klas Meyer: *High-Pressure qNMR Studies of Fluids and Gases*
- 2 Clément Laurain; Klas Meyer; Andrea Paul; Dirk Engel; Gisela Guthausen; Matthias Kraume; Michael Maiwald; and Nicolai Zientek: *Automated Data Evaluation and Modeling of Simultaneous 19F-1H Medium Resolution NMR Spectra for Online Reaction Monitoring*

Bristol-Myers Squibb Company

- 3 Colleen Mcnaney; Yingzi Wang; Dieter Drexler; Mike Reily; and Stella Huang: *Monitoring Stability of Reference Standard Solution for Neurotransmitters by Q-NMR*

Bruker UK Limited

- 4 Peter Gierth; Chris Stapleton; Andrew Kirkham; Julia Smith; Nicola Tonge; Nora Kouris; Brian L. Marquez; Andrew Gibbs; and Anna Codina: *Getting Ahead of the Game - NMR Solutions for the Complete Analysis of New Psychoactive Substances*

City College of New York

- 5 Ranajeet Ghose; Hsin Wang; and Benjamin Reed: *Solution NMR Studies on Vaccinia Virus Topoisomerase 1B*

Drug Enforcement Administration (DEA)

- 6 Patrick A. Hays and Charlotte A. Corbett: *NMR Applications at the Drug Enforcement Administration*

Embrapa Instrumentation

- 7 Amanda Becceneri; Márcia Cominetti; Luiz Colnago; and Roberta Manzano Maria: *Metabolic Profile Analysis of Cancer Cell by HR-MAS NMR*

Genentech, Inc.

- 8 Nick Magarian; Kate Lee; Kunal Nagpal; Yung-Hsiang Kao; and Kenneth Skidmore: *Use of a CPMG Method to Validate Single-Use Equipment in the Purification Processes of Biological Therapeutics*

Impact Analytical

- 9 Arthur Ferruzzi: *Determination of Activated PEG Content in a Cellulosic Substrate by 1H NMR Assay*

JEOL Resonance, Inc.

- 10 Junko Hosoe; Naoki Sugimoto; Yuko Yamada; Toru Miura; Masako Hayakawa; Hiroki Suzuki; Takao Katsuhara; Hiroaki Nishimura; Yuichi Kikuchi; Tadatoshi Yamashita; Yukihiro Goda; and Takako Suematsu: *Application of AQARI (Accurate Quantitative NMR with Internal Substance) to the Reagents in the Crude Drug Section of the Japanese Pharmacopoeia*

LGC

- 11 Michael Nelson; Adam LeGresley; and Fahmina Fardus: *Calibration and Measurement Uncertainty in Quantitative HSQC Experiments*

Poster Presenters

Louisiana State University

- 12 K. Wu; T. Ray; J. A. Surface; S. Jenkins-Bounds; and Larry Simeral: *RECAMP with NMR*

Massachusetts Institute of Technology

- 13 Tuo Wang; Mei Hong; Yong Bum Park; Daniel J. Cosgrove; and Paul White: *Water–Polysaccharide Interactions in the Primary Cell Wall of Arabidopsis thaliana from Spin Diffusion Solid-State NMR*

Merck & Co., Inc.

- 14 Gary E. Martin; R. Thomas Williamson; and James H. Small: *Structure Elucidation Strategies to Interrogate Low-Level Oxidative Drug Metabolites Utilizing Pure Shift and Novel Scalar-Coupled Pulse Sequences*

National Institute of Health Sciences, Japan

- 15 Kyoko Sato; Naoki Sugimoto; Atsuko Tada; Hiroshi Akiyama; and Takashi Ohtsuki: *Absolute Quantification of Analytical Standard for Food Additive by ¹H Quantitative NMR*

National Institute of Standards and Technology

- 16 Luke Arbogast; Robert Brinson; and John P. Marino: *Application of NMR Spectral Fingerprinting for Structure Assessment of Monoclonal Antibody Therapeutics*
- 17 Chad Snyder; Dean Delongchamp; and Ryan Nieuwendaal: *Details on Measuring Crystallinity in Poly(3-hexylthiophene) from Solid-State NMR and DSC*

Novo Nordisk A/S

- 18 Joan Malmstrøm: *Quantification of Silicone Oil and Its Degradation Products in Aqueous Pharmaceutical Formulations by [¹H]-NMR Spectroscopy*
- 19 Henrik Olsen and Joan Malmstrøm: *Validation of Quantitative [¹H]-NMR Spectroscopy Methods Used for Determination of the Main Compound or Trace Impurities*

Pfizer, Inc.

- 20 Fiona Lin; Chenghua Deng; Peter Li; Vilo Pavliak; Nathan Lacher; Michael T. Jones; and Kelly Sackett: *NMR as an Analytical Tool in Identifying and Quantifying Conjugation in Glycoconjugate Vaccines*
- 21 Raman Sharma: *Assessing the Effects of Background Contaminants on the Interpretation and Quantitation of 1D and 2D NMR Spectra of Drug Metabolites Isolated from Biological Matrices*

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