

March 3-7, 2019 Hilton Head Island, SC  
Sonesta Resort

# PANIC

7th Annual  
**Practical Applications of  
NMR in Industry Conference**



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You are cordially invited to the

### Welcome Reception

on Sunday, March 3 from 6:00 to 8:00 pm

*This complimentary reception is the perfect opportunity to network casually with other delegates, exhibitors, sponsors, poster presenters, and speakers in an informal setting.*

*Cocktails and light hors d'oeuvres will be served.*

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# Leadership

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# Conference Information

## Conference Proceedings Link

Please use the link below to access copies of the speaker presentations that have been submitted and approved for sharing with the PANIC audience.

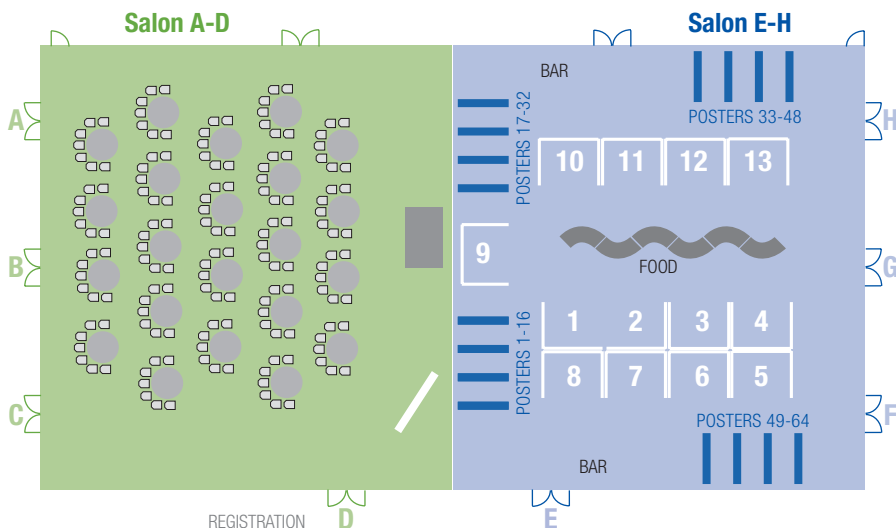
This page will not be accessible until after the conclusion of PANIC.

Link: [www.panicmr.com/panic-2019-proceedings](http://www.panicmr.com/panic-2019-proceedings)

Password: PAN1C7proc5 (Hint: PANIC 7 proceedings)

If you are looking for a specific set of slides that is not on the site, please contact the speaker directly for more information.

## Floor Plan - Santee Ballroom



## Exhibit and Poster Schedule

### Monday March 4

- 10:15 – 11:15 am Coffee Break  
Odd Posters
- 4:55 – 6:55 pm Networking Reception  
Even Posters

### Tuesday March 5

- 10:15 – 11:15 am Coffee Break  
Even Posters
- 5:10 – 7:10 pm Networking Reception  
Odd Posters

### Wednesday March 6

- 10:45 – 11:45 am Coffee Break  
All Posters

## Exhibitors

- |                      |                            |
|----------------------|----------------------------|
| 1&2 JEOL             | 8 Bruker                   |
| 3 Nanalysis Corp     | 9 MR Resources             |
| 4 Wilmad LabGlass    | 10 ACD/Labs                |
| 5 FUJI FILM Wako     | 11 Magritek Inc.           |
| 6 Oxford Instruments | 12 Mettler Toledo          |
| 7 CortecNet          | 13 Mestrelab Research S.L. |

*Santee Ballroom, Salon D Foyer*

## Onsite Registration Hours

**Saturday, March 2**

3:00 pm – 7:00 pm

**Sunday, March 3**

7:00 am – 7:00 pm

**Monday, March 4**

7:00 am – 6:00 pm

**Tuesday, March 5**

7:00 am – 5:30 pm

**Wednesday, March 6**

7:00 am – 5:30 pm

**Thursday, March 7**

7:00 am – 1 pm

## March 3 Sunday

*Santee Ballroom, Salon A-D*

### Users' Meetings

**7:30 Continental Breakfast  
and Networking**

**8:00 – 11:00 ACD/Labs**

**11:00 – 11:30 Break**

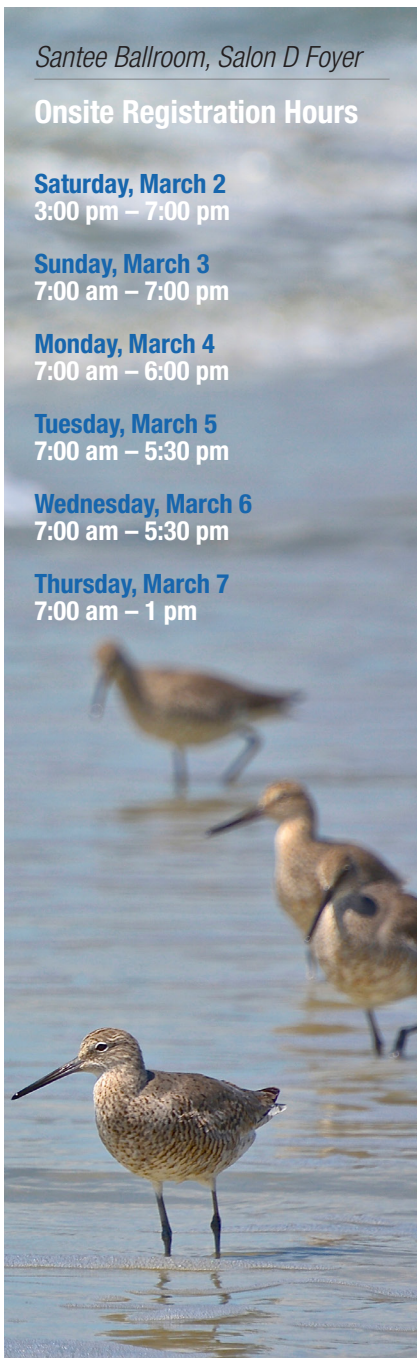
**11:30 – 2:30 Mestrelab  
including lunch**

**2:30 – 3:00 Break**

**3:00 – 6:00 Bruker**

*6:00–8:00*

**Welcome Reception for  
PANIC 2019**



## March 4 Monday Morning

8:30 Santee Ballroom, Salon A-D

### PNIC Chair's Welcome

8:35 Santee Ballroom, Salon A-D

### Session 1

#### NMR Applications in Food and Agriculture

J. Marino, J. Warren  
*Chairs*

#### 8:35 Opening Remarks

#### 8:45 Using Single Sided NMR Relaxometry for Process Control in Real Factory Environments

##### Matthew Augustine

*University of California, Davis*

#### 9:15 The Potato Skin: Protective Barrier, Burdensome Industrial Waste, Useful Antioxidant or Inspiration for Materials Design?

##### Ruth E. Stark

*City College of New York*

K. Dastmalchi, S. Chatterjee, A. Kligman,  
V. C. Phan, O. Serra, M. Figueras

#### 9:45 NMR-based Multiparametric Characterization of Foodstuffs: The Pros Without the Cons of Targeted Analyses Applied to Food Safety

##### Erwann Hamon

*Aerial*

L. Fougy, V. Stahl, R. Recht

10:15 – 11:15 Santee Ballroom,  
Salon E-H

### Poster Viewing with Coffee Break (odd numbers)

11:15 Santee Ballroom, Salon A-D

### Session 2

#### Pharmaceutical NMR Applications: Topics in Drug Discovery and Characterization

K. Sackett  
*Chair*

#### 11:15 Opening Remarks

#### 11:25 Discovery and Characterization of Small Molecule Fragments that Bind and Inhibit the Ubiquitin Specific Protease 7 (USP7)

##### Paola Di Lello

*Genentech*

T. Crawford, K. Deshayes, J. Drobnick,  
J. Drummond, J. Ernst, M. Kwok, C. Ly,  
T. Maurer, J. Murray, C. Ndubaku, R. Pastor,  
L. Rouge, V. Tsui, R. Zhao, K. Zobel, I. Wertz

#### 11:55 Identifying Pharmaceutical Salt and Co-crystals using <sup>1</sup>H Solid State NMR

##### Heather Frericks Schmidt

*Pfizer*

S. Luthra, I. Samardjiev

#### 12:25 Use of NMR for Measuring Critical Quality Attributes for Oil-in-Water Emulsion Drug Products

##### Sharadraj Patil

*FDA*

D. Keire, K. Chen



## March 4 Monday Afternoon

*1:00–2:30 Outside weather permitting*

### Networking Lunch

Discounted lunch ticket in registration packet

*2:30–2:45 Santee Ballroom, Salon A-D*

### Announcements – CRO Questionnaire and Introduction of Valid NMR Fellow

F. Delaglio and T. Schoenberger

*2:45 Santee Ballroom, Salon A-D*

### Session 3

#### Analysis of Materials by Magnetic Resonance

M. Davis, A. Abraham  
*Chairs*

#### 2:45 Opening Remarks

#### 2:55 NMR and Industrial Glass Research

**Randall E. Youngman**  
*Corning Incorporated*

#### 3:25 A New Tool for Solid-State NMR – a Computational Platform to Predict and Display Spectra for Inorganic Solids

**Sophia Hayes**  
*Washington University*  
S. Dwaraknath, K. Persson, H. Sun

#### 3:55 Quantitative Solid-State and Solution NMR Applications in Chemical and Nanoscale Metrology

**Andreas Brinkman**  
*National Research Council Canada*

#### 4:25 Role of Deuterium NMR in Solving the Mystery of the Mechanism of Phillips Catalyst

**Masud Monwar**  
*Chevron Phillips  
Chemical Company*  
C. Cruz, J. Barr, M. McDaniel

*4:55–6:55 Santee Ballroom, Salon E-H*

#### Poster Viewing with Reception (even numbers)

*6:55*

#### End of Day

## March 5 Tuesday Morning

8:30 Santee Ballroom, Salon A-D

### **PANIC Chair's Welcome**

8:35 Santee Ballroom, Salon A-D

#### **Session 4**

### **NMR Applications in the Energy Sector**

K. Wu  
*Chair*

#### **8:35 Opening Remarks**

#### **8:45 High-Spatial-Resolution NMR Scanner for Reservoir Characterization**

##### **Stacey Althaus**

*Aramco Services Company*  
J-H. Chen, G. Eppler, Y. Zhao

#### **9:15 Nondestructive Battery Diagnostics with MRI**

##### **Alexej Jerschow**

*New York University*  
M. Mohammadi, E. Silletta, A. Ilott

#### **9:45 Magnetic Resonance Multiphase Flowmeter: Flow Characterization in the Upstream Oil and Gas Industry**

##### **Lucas Cerioni**

*Krohne New Technologies*  
R. Tromp, S. Luik, O. Bousche, M. Zoeteweyj,  
J. Hogendoorn

10:15–11:15 Santee Ballroom,  
Salon E-H

### **Poster Viewing with Coffee Break (even numbers)**

11:15 La Jolla Ballroom, Salon A-D

#### **Session 5**

### **New Tools for Complex Mixtures**

B. Mayer, M. Janicke  
*Chairs*

#### **11:15 Opening Remarks**

#### **11:25 Simplifying the Analysis of Mixtures: New NMR Methods and Software**

##### **Laura Castañar Acedo**

*University of Manchester*

#### **11:55 Fast Quantitative 2D NMR Methods for the Analysis of Complex Mixtures at High and Medium Magnetic Field**

##### **Patrick Giraudeau**

*University of Nantes*

#### **12:25 Enabling Practical Applications of Low and Ultra-Low-Field NMR via Hyperpolarization**

##### **Meghan Halse**

*University of York*



## March 5 Tuesday Afternoon

1:00–2:30

**Lunch** Sponsored by 

### **CRAFT for Delta NMR Software: Time Domain NMR Data Analysis for Practical Applications**

Takanori Komatsu  
*JEOL*

2:30 *Santee Ballroom, Salon A-D*

### **Session 6**

#### **Contract NMR Measurement Services: A Panel Discussion**

F. Delaglio  
*Chair*

#### **2:30 Opening Remarks**

**CRO Panelists**

**Ruth Steele**

*Janssen Research and Development*

**Alan Gibbs**

*Janssen Research and  
Development*

**Ted Turner**

*Spectral Data Services*

**Khalid Thakur**

*Chemtos*

3:30 *Santee Ballroom, Salon A-D*

### **Session 7**

#### **Monitoring Manufacturing Processes with NMR**

C. Amezcua  
*Chair*

#### **3:30 Opening Remarks**

#### **3:40 How Online NMR Spectroscopy Accelerates Chemical Process Development and Manufacturing – From Automated Spectral Analysis to Integrated NMR Micro Reactors**

**Michael Maiwald**

*Bundesanstalt für Materialforschung und  
-prüfung (BAM)*

S. Kern, M. Bornemann, S. Guhl, L. Wander,  
K. Meyer, A. Paul

#### **4:10 Towards Improved Process Monitoring by Overhauser DNP**

**Raphael Kircher**

*University of Kaiserslautern*  
K. Munnemann, H. Hasse

#### **4:40 NMR and Mass Spectroscopy Go Mobile: Using NMR and MS as Process Analytical Technologies at the Fume Hood**

**Mark Milton**

*Takeda Pharmaceuticals*  
W. Lee, M. Zell

5:10 – 7:10 *Santee Ballroom, Salon E-H*

#### **Poster Viewing with Reception (odd numbers)**

7:10

### **End of Day**

## March 6 Wednesday Morning

8:30 Santee Ballroom, Salon A-D

### PANIC Chair's Welcome

8:35 Santee Ballroom, Salon A-D

### Session 8

#### Healthier Living Through NMR

J. DeFelippis, M. Bohlen  
Chairs

#### 835 Opening Remarks

#### 8:45 NMR Metabolite Resonance Signature Predicts ER+/HER2 Metastatic Breast Cancer Patient Response to CDK4/6 Inhibitors

##### Elizabeth O'Day

*Olaris Therapeutics, Inc*  
J. Warner

#### 9:15 Establishing SI-traceable NMR Relaxometry for Use in Quantitative MRI Biomarker Validation

##### Karl Stupic

*National Institute of Standards and  
Technology*  
M. Boss, K. Keenan, S. Russek

#### 9:45 Fingertip Assessment of Cardiometabolic Health Using Compact NMR

##### Vipulkumar Patel

*Texas Tech University Health Sciences  
Center*  
D. Cistola

10:15 Santee Ballroom, Salon A-D

### Awards Ceremony

#### Poster Awards, Presentation of Travel Grant Winners and Spectrum Contest Award Winners

J. Marino, P. Giraudeau, J. Cort, M. Davis

10:45–11:45 Santee Ballroom,  
Salon E-H

### Poster Viewing with Coffee Break (all posters)

11:45 Santee Ballroom, Salon A-D

### Session 9

#### Using NMR to Help the Environment

S. M. Cabral de Menezes  
Chair

#### 11:45 Opening Remarks

#### 11:55 Tailoring Ionic Liquid Materials for CO<sub>2</sub> Capture: A Rational Contribution from NMR

##### Marta Corvo

*New University of Lisbon*  
J. Dupont, S. Einloft, E. Cabrita

#### 12:25 New Pathways in Green Chemistry: What Can Solid-State NMR Spectroscopy Tell Us About Mechanochemistry?

##### Robert Schurko,

*University of Windsor*  
A. Peach, C. O'Keefe, S. Holmes, J. Gemus,  
C. Vojvodin, C. Mottillo, T. Friš i

## March 6 Wednesday Afternoon

1:00–2:30

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**Lunch** On your own

2:30 *Santee Ballroom, Salon A-D*

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### Session 10

#### NMR for National Security and Forensics

J. Cort, J. Warren  
*Chairs*

#### 2:30 Opening Remarks

#### 2:40 Nuclear Magnetic Resonance at Low to Ultra-Low Magnetic Fields for Signature Detection of Chemical Warfare Agents and Emerging Threat Materials

**Robert F. Williams**

*Los Alamos National Laboratory*  
M. Espy, T. Erkkila, M. Janicke, D. Kaseman,  
P. Magnelind, R. Michalczyk, P. Nath,  
T. Nelson, J. Schmidt, S. Widgeon,  
A. Urbaitis, J. Yoder

#### 3:10 Forensic Analysis of Petrol by High Field NMR

**Yanita Yankova Yankova**

*Eurofins Forensics Services*  
M. Cole, A. Hossain

#### 3:40 Nuclear Magnetic Resonance Spectroscopy of Radioactive Solids and Liquids: Methods and Applications

**Herman Cho**

*Pacific Northwest National Laboratory*

4:10

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### Quick Break



4:25 *Santee Ballroom, Salon A-D*

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### Session 11

#### Spectacular qNMR Applications

T. Schoenberger  
*Chair*

#### 4:25 Opening Remarks

#### 4:35 Quantitative NMR for Measurement of Sodium in Solutions

**G. Joseph Ray**

*Baxter International*

#### 5:05 NMR as a Powerful Alternative for Complexometric Titration to Analyze Metal Ions Qualitatively and Quantitatively

**Elina Zailer**

*Spectral Service AG*  
B. Diehl, K. Kraus

#### 5:35 A Practical Application of CRAFT Processing for the Quantitation of Trace Impurities in Biologics-Based Drugs

**Ken Skidmore**

*Genentech*  
G. Khirich

6:05 *Santee Ballroom, Salon A-D*

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### PANIC Chair's Closing Remarks

6:15

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### End of PANIC 2019

## March 7 Thursday

8:15–5:30 Santee Ballroom, Salon A-D

### Validation Workshop

8:15 Coffee available

#### 8:30 Welcome – Opening Statements

Torsten Schoenberger (BKA) &  
Michael Maiwald (BAM)

#### 8:50 Presentation: “Quality by Design (QbD) principles applied to NMR methods”

Ian Clegg (Bruker Biospin Inc.)

#### 9:10 Presentation: “Validation of Software”

Carlos Amezcua (Baxter International)

#### 9:30 Presentation: “Good Weighing Practice (GWP) for accurate qNMR sample preparation”

Tucker Rubino (Mettler-Toledo GmbH)

9:50 Break

#### 10:10 Workshop Session #1: Design of Analytical Procedures

##### (A) Establish an Analytical Target Profile (ATP)

Session Leader: José G. Napolitano (AbbVie)

##### (B) Identify the Critical Quality Attributes of qNMR

Session Leader: Dan Sorensen (Eurofins Alphora)

##### (C) Plan the Analytical Instrument Qualification

Session Leader: Christoph Freudenberger (Bruker Biospin Inc.)

#### 11:40 Presentation: “ValidNMR Website and Wiki”

Kristie Adams (Steelyard Analytics)

12:00 Lunch

#### 1:00 Presentation: “Tackling ‘dark’ uncertainty in SI traceable qNMR analysis of peptides and glycans”

Cailean Clarkson (LGC)

#### 1:20 Workshop Session #2: Verification of Analytical Procedures

##### (D) Plan the Analytical Control Strategy and Verification

Session Leader: Torsten Schoenberger (BKA)

##### (E) Experimental Factors to Consider for Generation of a qNMR Method Validation Protocol

Session Leader: Joe Ray (Baxter International)

##### (F) Use of Statistical Tools for Evaluation of Measurement Uncertainty

Session Leader: Michael Maiwald (BAM)

#### 2:50 Open Forum – Q&A, Discussions

Kristie Adams (Steelyard Analytics)

#### 3:15 The Workshop Adjourns – Closing Statements

Torsten Schoenberger (BKA) &  
Michael Maiwald (BAM)

#### 3:30 ValidNMR Business Meeting

ValidNMR committee members  
(open to observers and interested parties)

#### 5:30 The ValidNMR Business Meeting Adjourns

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**Booth 10**

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Booths 1 and 2

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Booth 13

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**Booth 3**

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Nanalysis manufactures benchtop Nuclear Magnetic Resonance (NMR) spectrometers aimed at proliferating the use of NMR in qualitative and quantitative chemical applications – including pharma, petrochemicals, and process control, etc.. The NMRReady-60 is compact, multinuclear, 60 MHz award-winning spectrometers. For more information please visit [www.nanalysis.com](http://www.nanalysis.com).



## **National Institute of Standards and Technology**

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# Sponsors & Exhibitors



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**Booth 6**

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- P1.** Interaction of Beta-2-Adrenoceptor Ligands with Dodecyl Phosphocholine Detergent Micelles  
**Charles Babu, Novartis**, B. Wang, A. Graboski
- P2.** Bayesian Framework for Efficient Quantitative Analysis of Arrayed NMR Experiments  
**Daniel J. Holland, University of Canterbury**, Y. Matviychuk, E. Steimers, A. Friebe, E. von Harbou, K. Münnemann
- P3.** NMR-based Metabolomics for Classification and Characterization of Tea Extracts  
**Congmei Cao, Herbalife**, H. Ma, S. Babajanian, Q. Gao, Y. Zhang, P. Chang, G. Swanson
- P4.** Nicotine and Its Effect on Degradation in Electronic Cigarettes by  $^1\text{H}$  NMR  
**Anna Duell, Portland State University**, D. Peyton
- P5.** Analysis of a Coating Solution in a Manufacturing Environment Using Benchtop NMR  
**Paul Bowyer, Magritek Inc.**, T. Gregar
- P6.** Integrating Benchtop NMR Into an Industrial Environment: Opportunities and Challenges  
**Paul Bowyer, Magritek Inc.**, H. Robert
- P7.** MR Microimaging and Spectroscopy in Consumer Products Research  
**Nicole Westrick, (Presented by: Jackie Thomas and Carrie Furnish), Procter and Gamble**, D. Maltbie, T. Dicolandrea
- P8.** Determination of LDPE Content in LDPE/LLDPE Blends via  $^{13}\text{C}$  NMR Method  
**Masud Monwar, Chevron Phillips Chemical Company LP**, Y. Yu
- P9.** A Computational Approach to Simulate NMR Data from Digital Porous Media  
**Everton Lucas de Oliveira, Instituto de Fisica de Sao Carlos**, T. Bonagamba, A. Araujo-Ferreira, W. Trevizan, V. de França Machado, B. Coutinho Camilo dos Santos
- P10.** Benchtop NMR Spectroscopy Enables in-situ Studies of Phase Equilibria and Batch Distillation  
**Anne Friebe, Technical University of Kaiserslautern**, K. Münnemann, E. von Harbou, H. Hasse
- P11.** Quantification of Fast Flow NMR Measurements by Modeling of Magnetization Build-Up  
**Anne Friebe, Technical University of Kaiserslautern**, E. von Harbou, K. Münnemann, H. Hasse
- P12.** Chemometric Workflows for 2D NMR  
**Bryan Hanson, DePauw University**

- P13.** The Structure of Asphaltene Aggregates Investigated by Solution and Solid State NMR  
**Paul Hazendonk, University of Lethbridge**, Y. Ratna, M. Gerken
- P14.** Can We Use TD-NMR for the Quality Characteristics of Soft Candies?  
**Mecit Oztop, Middle East Technical University**, E. Ates, E. Ozvural
- P15.** Magnetic Field Effect on Electrochemical Reactions Monitored in-situ by High Field NMR Spectrometers  
**Carlos Lobo, Instituto de Quimica de Sao Carlos**, B. Gomes, P. da Silva, E. Danieli Magritek, M. Carmo, S. Benders, B. Blümich, L. Colnago
- P16.** Use of Inductively Coupled Coils for Electrochemistry-NMR Coupling  
**Carlos Lobo, Instituto de Quimica de Sao Carlos**, B. Gomes, H. Bouzouma, E. Danieli, B. Blümich, L. Colnago
- P17.** Getting Ahead of the Game: Complete Analysis of New Psychoactive Substances  
**Eduardo Nascimento, Bruker**
- P18.** Towards Accurate Uncertainty Estimation in Model-based Analysis of NMR Data  
**Yevgen Matviychuk, University of Canterbury**, E. Steimers, E. Kessler, E. von Harbou, K. Münnemann, D. Holland
- P19.** NMR and the Materials Genome Initiative  
**Ryan Nieuwendaal, NIST**, E. Anderson, V. Witherspoon, C. Soles, D. DeLongchamp, D. Reid, J. de Pablo
- P20.** Reaction Monitoring using Quantitative NMR (qNMR) and Process Analytical Technology (PAT)  
**Toru Miura, FUJIFILM Wako**
- P21.** Applications of atomic magnetometers in NMR and MRI  
**Igor Savukov, LANL**, Y. Kim
- P22.** Facile Smart LF-NMR Relaxometer for Monitoring of Food Product's Oxidation  
**Zeev Wiesman, Ben Gurion University of the Negev**
- P23.** Site-Specific Natural Abundance Isotope Fractionation NMR  $^{13}\text{C}/^{12}\text{C}$  Ratios (SNIF-NMR) as High Fidelity Chemical Attribution Signatures for Chemical Threat Agents  
**Robert Williams, LANL**, R. Michalczuk, M. Alvarez, Z. Li
- P24.** Using Predicted  $^{13}\text{C}$  NMR Spectra with Open Resources for Structure Dereplication of Natural Products  
**Arvin Moser, ACD/Labs**, D. Argyropoulos, S. Golotvin, T. Chilczuk, T. Niedermeyer

- P25.** A New Method for the Reliable Detection of  $^{13}\text{C}$  Multiplets of Fluorine Containing Compounds  
**Dimitris Argyropoulos, ACD/Labs,** S. Golotvin, R. Pol, V. Mikhailenko
- P26.** Application of NMR in the Surveillance of Drug Products: Two Recent Case Studies  
**Qin Shu, US Food and Drug Administration,** J. Yang, P. Chitranshi, D. Willett, M. Karfunkle, J. Rodriguez, D. Keire
- P27.** Use of High Resolution 2D NMR Methods to Characterize Physicochemical Liabilities of Monoclonal Antibodies  
**Subhabrata Majumder, Pfizer,** A. Saati, S. Philip, L. Marzilli, J. Rouse, M. Jones, A. Alphonse Ignatius
- P28.** WIFI-NMRS: Inductive Coupling and Flow for Increased NMR Sensitivity  
**Guillaume Carret, Cortecnet,** P. Berthault, T. Berthelot
- P29.** qHNMR of Tetrahydrocannabinol (THC) in Edibles and Plant Materials  
**Charlotte Corbett, DEA,** E. Guest
- P30.** Detection and Determination of Adulterants in Aloe vera Using NMR  
**Isaac Lee, Herbalife,** Q. Gao, J. Vo, H. Ma, P. Purohit, V. Zarraga, P. Chang, G. Swanson
- P31.** Block-Copolymer Micelles for Tunable Cargo Delivery: Structure, Dynamics and Molecular Partitioning Investigated by NMR Diffusometry  
**Xiuli Li, Virginia Tech,** L. Madsen, B. Kidd, T. Cooksey, M. Robertson
- P32.** Developing a Direct NMR Method to Measure Chemical Exchange in Aqueous Systems  
**Samantha Miller, Colorado State University,** N. Levinger, B. Wiebenga-Sanford
- P33.** High-Accuracy Analysis of Gas-Phase Mixtures by  $^1\text{H}$  NMR: Application to Vapor-Liquid Equilibrium of Refrigerant Mixtures  
**Jason Widegreen, NIST,** C. Suiter, M. McLinden, T. Bruno
- P34.** New Insights on Drug Location inside Crystalline  $\gamma$ -Cyclodextrin MOFs by Solid-State NMR Spectroscopy and Molecular Modeling  
**Charlotte Martineau-Corcoss, University of Versailles,** R. Gref, L. Xue, M. Porcino, A. Zenacker, M. Menendez, J. Zhang
- P35.** Water Flow-NMR—A Prospective Contact-Free In-Line Analytical Tool for Continuous Biomanufacturing  
**Marc B. Taraban, University of Maryland,** K. Briggs, Y. Yu
- P36.** Development of Certified Reference Materials (CRM) for Quantitative Nuclear Magnetic Resonance (qNMR) as ampuled solutions  
**Alexander Rueck, Sigma-Aldrich,** R. Rigger, C. Hellriegel, K. Breitruck, M. Obkircher



- P37.** Use of CRAFT for Automatic 1D and 2D Quantification with Batch Analysis  
**Ronald Crouch, JEOL-USA, M. Borchers, T. Komatsu, K. Krishnamurthy**
- P38.** Certification of Marine Toxins by Quantitative NMR at the Highest Metrological Level  
**Markus Obkircher, Millipore Sigma**
- P39.** Interlaboratory Comparison of Benchtop NMR Spectrometers – Purities at 200 and 10 mmol/L  
**Klas Meyer, Bundesanstalt für Materialforschung und -prüfung (BAM), C. Peters, M. Maiwald**
- P40.** Quantification of Natural Products in Herbal Supplements by a Combined 1D and 2D qNMR Approach  
**Puong Mai Le, National Research Council Canada, C. Milande, E. Martineau, P. Giraudeau, J. Farjon**
- P41.** Tackling ‘Dark’ Uncertainty in SI Traceable qNMR Analysis of Peptides and Glycans  
**Cailean Clarkson, LGC**
- P42.** Flexible Automation with Compact NMR Instruments  
**Simon Kern, Bundesanstalt für Materialforschung und -prüfung (BAM), L. Wander, K. Meyer, S. Guhl, A. Mukkula, M. Holtkamp, M. Salge, C. Fleischer, N. Weber, R. King, S. Engell, A. Paul, M. Remelhe, M. Maiwald**
- P43.** Toward an NMR-based Monitoring of Coffee Origin? An industrial Case-Study  
**Raphael Recht, Aeriël, L. Febvay, D. Aoudé-Werner, V. Viraswami, H. This, E. Hamon**
- P44.** Fast, Accurate and Precise Automated Gravimetric Sample Preparation Applied to NMR-based Authenticity Control of Honey and Olive Oil  
**Nutsima Schnell, Mettler Toledo, P. Weinelt, G. Hofmann, B. Schuetz, A. Steck**
- P45.** Detection and Structural Characterization of Ultra-weak Biomolecular Interactions Using Lanthanides  
**Madeleine Strickland, National Institutes of Health, A. Opina, L. Ehrlich, S. Watanabe, R. Swenson, O. Vasalatiy, C. Carter, N. Tjandra**
- P46.** The Automated Assignment of Carbohydrate Spectra via NMR Spectroscopy  
**Elaine K. Adair, University of Edinburgh, D. Uhrin**
- P47.** A Versatile Expression and Purification Method for Isotopically Labeled  $\beta$ -Amyloid Family  
**Bharat Somireddy Venkata, The University of Chicago, J. Zerweck, P. Moore, S. Meredith**
- P48.** Single Pulse NQR for Broad Resonance Lines  
**Thai Ly, CSIRO Mineral Resources, R. Yong, J. Daniels, D. Miljak**

- P49.** Accelerating Chemical Process Development and Manufacturing – Design and Validation of an Integrated NMR Micro Mixer  
**Martin Bornemann, Bundesanstalt für Materialforschung und -prüfung (BAM),** S. Kern, N. Jurtz, M. Kraume, M. Maiwald
- P50.** Characterizing Dynamic Allosteric Changes in Antibody-Antigen Interactions  
**Gaohua Liu, Nexomics Biosciences, Inc.,** A. Gibbs, R. Steele, J. Liang, T. Yang, G. Montelione, R. Xiao
- P51.** See SIERRA and SMILE: Removal of Excipient Peaks in  $^1\text{H}$ ,  $^{13}\text{C}$  Spectra of Protein Therapeutics at Natural Isotopic Abundance by Selective Suppression of Spin Pairs Augmented by Signal Modeling and Subtraction  
**Frank Delaglio, NIST,** J. Marino, L. Arbogast, J. Ying
- P52.** Method Development and qNMR Analysis of Medical Cannabis and CBD Products  
**Kristie M. Adams, Steelyard Analytics, Inc.,** E. Zailer, A. Formes, B. Diehl
- P53.** Interrogation of Teflon® AF by  $^{19}\text{F}$  2D PASS NMR  
**Micheal C. Davis, Chemours,** P. Brothers
- P54.** Reducing NMR Tube Volume Variation, a Source of Error in External qNMR, by Implementation of  $^2\text{H}$  Experiment  
**Jason Ewanicki, Pfizer,** W. Wang
- P55.** Innovative Capabilities at the EMSL User Facility to Support the Study of Materials and Biosystems with NMR Spectroscopy  
**John R. Cort, Pacific Northwest National Laboratory,** S. Burton, Y. Chen, E. Eder, M. Froehlike, K. Sung Han, D. Hoyt, W. Kew, A. Lipton, H. Mehta, T. Palazzo, J. Sears Jr., E. Walter, N. Washton, A. Wong, R. Young
- P56.** Multi-exponential T2 Relaxometry Analysis Based on a New Denoising and Modified MDL/Matrix Pencil Algorithms  
**Santiago Ponte, Vadim Zorin, Carlos Cobas, Mestrelab Research** Stanislav Sykora, Ester Maria Vasini, Maria Silva Elipse
- P57.** Mgears - Mnova General Enterprise Automation Rapid Solution  
**Santiago Dominguez, Irakusne Lopez, Agustin Barba, Esther Vaz, Pablo Monje, Mestrelab Research**











# GUESS THE SPECTRA

YES, THERE ARE TWO PUZZLES THIS YEAR!

## PUZZLE 1

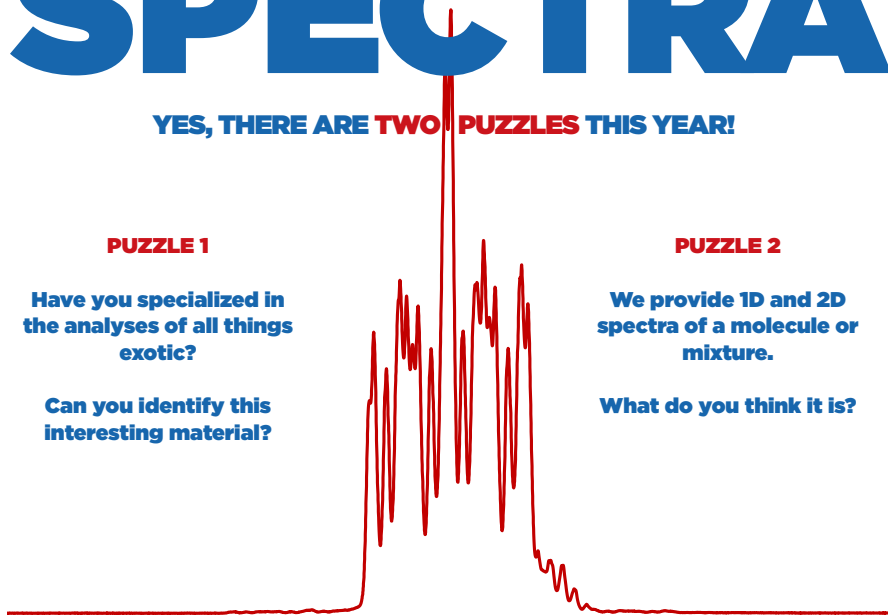
Have you specialized in the analyses of all things exotic?

Can you identify this interesting material?

## PUZZLE 2

We provide 1D and 2D spectra of a molecule or mixture.

What do you think it is?



# WIN PRIZES

## FIRST PRIZE: A NEST THERMOSTAT

Saving energy is a beautiful thing. Winning the spectral contest is pretty cool, too!

## SECOND PRIZE: A \$100 VISA CARD

Drop your entries before **TUESDAY, MARCH 5 AT 7:10 PM**

The answers will be revealed—and prizes awarded—**WEDNESDAY, MARCH 6 AT 10:15 AM**

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