

March 4–8, 2018 La Jolla, California  
San Diego Marriott La Jolla

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6th Annual  
**Practical Applications of  
NMR in Industry Conference**

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You are cordially invited to the

### Welcome Reception

in the Exhibit Hall

on Sunday, March 4 from 5:30 to 7:30 pm

*This complimentary reception is the perfect opportunity to casually network 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 Proceedings Link

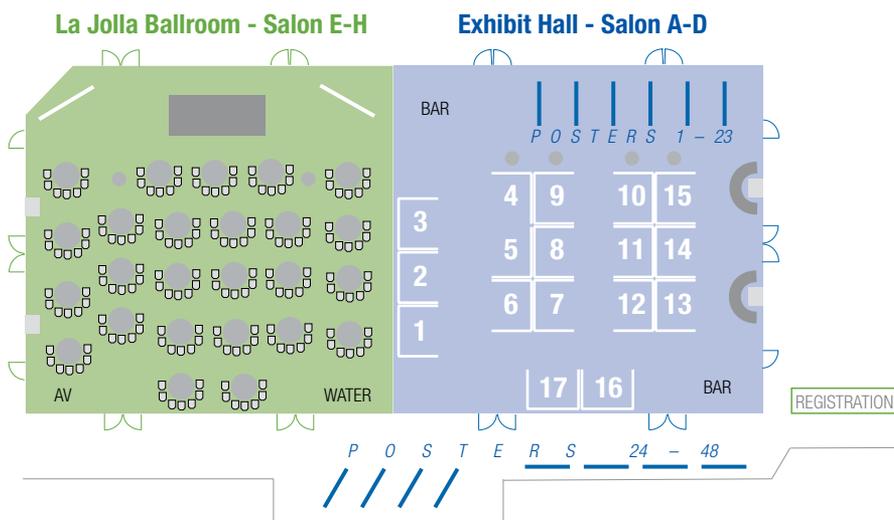
The conference proceedings link is available only to conference attendees.

It gives access to the speaker presentations that have been approved for sharing with the PANIC audience. The page will become accessible after the conclusion of PANIC.

If you attended PANIC and need help with the link, please contact [chair@panicco.org](mailto:chair@panicco.org)

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

## Floor Plan



## Exhibitors

- 1 NanoNord A/S
- 2 Nanalysis Corp
- 3 Revolution NMR LLC/Phoenix
- 4&5 Bruker BioSpin Corp
- 6 Pure Devices GmbH
- 7 Oxford Instruments Inc
- 8 MilliporeSigma
- 9 ACD/Labs
- 10 Cambridge Isotope Laboratories, Inc.
- 11 Magritek Inc.
- 12 Mestrelab Research S.L.
- 13 CortecNet Corp
- 14 Wako Pure Chemical Industries Ltd
- 15 Wilmad LabGloss
- 16 Stelar SRL
- 17 JEOL USA Inc

## Exhibit and Poster Schedule

### Sunday 3.4

5:30 - 7:30 pm Welcome Reception

### Monday 3.5

10:30 - 11:20 am Coffee Break – Odd Posters

4:55 - 6:00 pm Networking Reception – Even Posters

### Tuesday 3.6

10:30 - 11:20 am Coffee Break – Even Posters

4:10 - 5:05 pm Refreshment Break – Odd Posters

6:45 - 7:45 pm Networking Reception – All Posters  
*and last chance to drop off your entries for the Spectrum Contest*

### Wednesday 3.7

10:30 to 11:30 am Coffee Break – All Posters

*La Jolla Ballroom, Foyer area*

## Onsite Registration Hours

**Saturday, March 3**  
3:00 pm – 7:00 pm

**Sunday, March 4**  
7:00 am – 5:30 pm

**Monday, March 5**  
7:00 am – 6:00 pm

**Tuesday, March 6**  
7:00 am – 5:30 pm

**Wednesday, March 7**  
7:00 am – 4:30pm

**Thursday, March 8**  
7:00 am – 1:00 pm

## 3.4 Sunday

*7:30–5:30 La Jolla Ballroom, Salon E-H*

### Users' Meetings

**7:30 Coffee, Continental Breakfast, and Networking**

**8:30 Mestrelab**

**11:00 Break**

**11:15 Bruker (Lunch provided)**

**2:00 Afternoon refreshments and Break**

**2:30 ACD/Labs**

**5:30 End of Users' Meetings**

*5:30 La Jolla Ballroom, Salon E-H*

### Welcome Reception for PANIC 2018



## 3.5 Monday Morning

8:45 *La Jolla Ballroom, Salon E-H*

### Chair Welcome

8:50 *Salon E-H*

### Session 1

#### A Foodie's Guide to NMR: Safety, Quality & Authenticity

M. P. Bohlen, J. P. Marino  
*Chairs*

#### 8:50 Opening Remarks

9:00 **1. Quality assurance of foods and functional ingredients using quantitative NMR methods.**

**I. Burton**, F. Berrue, C. Martinez-Farina

9:30 **2. High-field NMR for the analysis of scotch whisky.**

**W. Kew**, I. Goodall, D. Uhrin

10:00 **3. Get the control about the pathway to Rebaudioside M – identification by 2D NMR spectroscopy of the unknowns after semi-preparative HPLC isolation.**

**S. Gosiewska**, B. Ozalp, O. Schouten, R. van der Hoeven, P. Lankhorst, A. Carvalho de Souza

10:30–11:20 *La Jolla Ballroom, Salon A-D & Foyer*

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

11:20 *La Jolla Ballroom, Salon E-H*

### Session 2

#### qNMR: Every Atom Counts!

T. Schoenberger  
*Chair*

#### 11:20 Opening Remarks

11:30 **4. Quantitative NMR using low gamma quadrupolar nuclei.**

**J.M. Hook**, D. Lawes

12:00 **5. Automation of qNMR in an industrial environment.**

**S. Garms**

12:30 **6. Steelyard method – An innovative *ab initio* quantification.**

**B. Diehl**



## 3.5 Monday Afternoon

1:00–2:30 *La Jolla Ballroom,  
Salon E-H*

**Lunch** Sponsored by 

### Automated qNMR analysis, its necessity and the proposal from JEOL

**Takako Suematsu** (JEOL)

2:30–2:45 *La Jolla Ballroom, Salon E-H*

### Introduction of the ValidNMR Fellow, Elina Zailer

T. Schoenberger  
*Chair*

2:45 *La Jolla Ballroom, Salon E-H*

### Session 3

### NMR in the Pharmaceutical Industry: Applications to Drug Design, Manufacturing & Structural Fingerprinting

C. A. Amezcuca  
*Chair*

### 2:45 Opening Remarks

### 2:55 7. Impacting drug design using Residual Dipolar Couplings.

**K.A. Farley**, R.R. Gil, Y. Che, D. Anderson,  
C. Limberakis, V. Shanmugasundaram

### 3:25 8. Integrating NMR methods further into process R&D and manufacturing at AbbVie.

**J. G. Napolitano**

### 3:55 9. 2D NMR HOS fingerprints of monoclonal antibody therapeutics: Benchmarking acquisition and chemometric methods through an international inter-laboratory study.

**R. G. Brinson**, L.W. Arbogast, F. Delaglio,  
J.P. Marino

### 4:25 10. Chemometric methods to quantify 1D and 2D NMR spectral differences among similar protein therapeutics.

**K. Chen**, J. Park, F. Li, S. Patil, D.A. Keire

4:55–6:00 *La Jolla Ballroom,  
Salon A-D & Foyer*

### Poster Viewing with Reception (even numbers)

6:00

### End of Day

## 3.6 Tuesday Morning

7:30 *Los Angeles Room*

### Travel Grant Awardee Breakfast

8:45 *La Jolla Ballroom, Salon E-H*

### Chair Welcome

8:50 *La Jolla Ballroom, Salon E-H*

#### Session 4

### Challenges in Polymer Characterization: NMR has Solutions

J. DeFelippis  
*Chair*

#### 8:50 Opening Remarks

9:00 **20. Dipolar based time domain NMR techniques and their use for the characterization of industrial relevant materials.**

**E. Azevedo**, T.B. Moraes

9:30 **21. Characterization of network structural motifs in siloxane elastomers using magnetic resonance.**

**A.M. Sawvel**, S.C. Chinn, M. Gee, A. Maiti, H. Mason, R.S. Maxwell, J.P. Lewicki

10:00 **22. Relaxation and diffusion filtration in polymers: Residual monomers quantitation and complex chemical mixture analysis.**

**T. Zhuang**

10:30–11:20 *La Jolla Ballroom, Salon A-D & Foyer*

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

11:20 *La Jolla Ballroom, Salon E-H*

#### Session 5

### As it Happens: Process Monitoring by NMR

J. A. Surface  
*Chair*

#### 11:20 Opening Remarks

11:30 **14. Redefining peak overlap - reaction monitoring by CRAFT (Complete Reduction to Amplitude Frequency Table) using low-field NMR system.**

**K. Krishnamurthy**, D.J. Russell

12:00 **15. Reaction monitoring of silane hydrolysis via NMR and vibrational spectroscopy.**

**D. Eldred**, X. Chen

12:30 **16. Earth's field NMR to detect spilled oil released under ice.**

**M.S. Conradi**, E. Fukushima, S. Altobelli, N. Sowko

## 3.6 Tuesday Afternoon

1:00–2:30 La Jolla Ballroom, Salon E-H

**Lunch** Sponsored by 

### Moving NMR out of the Basement

Kim Colson (Bruker), Anna Codina (Bruker),  
Maria Silva Elipe (Amgen, Inc.)

2:30 La Jolla Ballroom, Salon E-H

### Session 6

#### Small Field – Big Impact: Applications of Low Field & Time Domain Spectroscopy in Industry

J. Warren  
*Chair*

#### 2:30 Opening Remarks

#### 2:40 17. Quantitative analysis of complex natural mixtures with benchtop NMR.

**Y. Matviychuk**, J. Yeo, D.J. Holland

#### 3:10 18. Compact NMR for metabolic health monitoring and disease prevention.

**D.P. Cistola**

#### 3:40 19. Field-cycling NMR and its application to study molecular dynamics.

**M. Hofmann**, B. Kresse, E. Rössler

4:10–5:05 La Jolla Ballroom,  
Salon A-D & Foyer

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

5:05 La Jolla Ballroom, Salon E-H

### Session 7

#### NMR in the Oil Industry: A Role from Upstream to Downstream

S. C. Menezes, K. Wu  
*Chairs*

#### 5:05 Opening Remarks

#### 5:15 11. NMR in extreme environments. **N.J. Heaton**

#### 5:45 12. Zooming in on heterogeneous catalysts and their catalysed reactions using magic angle spinning solid-state NMR.

K. Houben, A. Lucini Paioni, D. Mance,  
J. van der Zwan, A. Dutta Chowdhury,  
S. Chung, R. Danisi, B.M. Weckhuysen,  
**E.T. Vogt**, M. Baldus

#### 6:15 13. Elucidating structural characteristics of renewable products from a two-step ex situ hydropyrolysis vapor upgrading process by one- and two- dimensional NMR spectroscopy.

**J. Lai**, L. Zhang, K. Gong

6:45–7:45 La Jolla Ballroom,  
Salon A-D & Foyer

### Poster Viewing with Reception (all posters)

## 3.7 Wednesday Morning

8:45 *La Jolla Ballroom, Salon E-H*

### Chair Welcome

8:50 *La Jolla Ballroom, Salon E-H*

### Session 8

#### Nukes, Nerve Agents, and Narcotics: NMR for National Security

J. R. Cort, B. P. Mayer  
*Chairs*

#### 8:50 Opening Remarks

#### 9:00 23. NMR spectroscopic investigation of plastic bonded high explosives.

H. Mason, J.S. Vaughn, A. Gash

#### 9:30 24. Multinuclear NMR monitoring of decontamination chemistries of bulk chemical agents and simulants.

T.M. Alam, M.K. Kinnan

#### 10:00 25. Using NMR to combat the opioid crisis.

B.N. Brewer, S.W. Wheasler

10:30–11:30 *La Jolla Ballroom, Salon A-D & Foyer*

### Poster Viewing with Coffee Break

11:30 *La Jolla Ballroom, Salon E-H*

### Session 9

#### Non-Uniform Sampling for (Faster) Fun and Profit: a Tutorial

F. Delaglio, D. Rovnyak  
*Chairs*

1:00–2:30 *La Jolla Ballroom, Salon E-H*

### Lunch

## 3.7 Wednesday Afternoon

2:30–2:55 *La Jolla Ballroom, Salon E-H*

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

M. Bohlen  
*Chair*

2:55 *La Jolla Ballroom, Salon E-H*

#### Session 10

#### Solid-State NMR & DNP

A. Abraham  
*Chair*

#### 2:55 Opening Remarks

3:05 **26. DNP enhanced solid-state NMR spectroscopy for the characterization of pure and formulated pharmaceuticals.**

**A.J. Rossini**

3:35 **27. Chemical systems monitoring of catalysis to extremophiles is enabled by high pressure – high temperature MAS-NMR.**

**D.W. Hoyt**, E.D. Walter, H.S. Mehta, J.A. Sears, L. Qi, A. Chamas, S.L. Scott

4:05 **28. To Klystron or not to Klystron?**

**B. O'Hare**

4:35 **29. Magic angle spinning NMR for structural analysis of pharmaceuticals and biological assemblies.**

J. Struppe, C. Quinn, M. Lu, M. Wang, S. Sarkar, M. Rosay, I. Sergeev, W.E. Maas, A.M. Gronenborn, **T.E. Polenova**

5:05 *La Jolla Ballroom, Salon E-H*

### Closing Comments and Announcements

5:15

### End of PANIC 2018



## 3.8 Thursday

8:00–5:00 La Jolla Ballroom, Salon E

### Validation Workshop

Kim Colson & Torsten Schoenberger  
*Chairs*

8:00 Coffee is served

8:20 **Welcome – Opening Statements**

Kim Colson (Bruker) &  
Torsten Schoenberger (Bundeskriminalamt)

#### Session 1

8:50 **Lightning talk: “Quality Improvement in qNMR Spectroscopy”**

Elina Zailer (Spectral Service)

9:00 **Presentation: “qNMR Method Validation Following the USP 1210 Chapter, Statistical Tools for Procedure Validation”**

Carlos Amezcua (Baxter International Inc.)

9:20 **Workshop Session #1**

**(A) ValidNMR Wiki**

Kristie Adams (Steelyard Analytics)

**(B) Required Validation Parameters**

Stefan Garms (Lonza)

10:20 **Workshop debriefing**

(Session leaders)

10:30 Break

#### Session 2

11:00 **Lightning talk: “Meeting the requirements of FDA, ISO, GxP”**

Bernd Diehl (Spectral Service)

11:10 **Presentation: “Validation Strategy using Lifecycle and Quality Risk Management”**

Dan Sorensen  
(Eurofins | Alphora Research Inc.)

11:30 **Workshop Session #2**

**(C) Data integrity**

Carlos Amezcua (Baxter International Inc.)

**(D) Protocols / Education**

Elina Zailer (Spectral Service)

12:30 **Workshop debriefing**

(Session leaders)

12:40 Lunch

#### Session 3

1:30 **Lightning talk: “A new realization of SI for organic chemical measurement: NIST PS1”**

Michael Nelson (National Institute of Standards and Technology)

1:40 **Presentation: “The Nuts and Bolts of qNMR”**

Ian Burton (NRC)

2:00 **Workshop Session #3**

**(E) Uncertainty Analysis**

Michael Nelson (National Institute of Standards and Technology)

**(F) Reference Materials**

Kevin Millis (Cambridge Isotope Laboratories)

3:00 **Workshop debriefing**

(Session Leaders)

3:10 Break

3:30 **Presentation: “Novel Proficiency Testing Scheme for  $^1\text{H}$ ,  $^{31}\text{P}$  and  $^{19}\text{F}$  quantitative Nuclear Magnetic Resonance (qNMR)”**

Markus Obkircher (Merck KGaA)

4:00 **Open Forum**

Kim Colson (Bruker) &  
Torsten Schoenberger (Bundeskriminalamt)

5:00 **Closing Statements**

Kim Colson (Bruker) &  
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- P3.** Already producing or still calibrating? – Advances of model-based data evaluation concepts for quantitative online NMR spectroscopy.  
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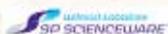
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