

PANIC NMR 2022 CONFERENCE PROGRAM

(As of Monday, October 17, 2022)



SUNDAY, OCTOBER 16

- 10:00 a.m. to 7:00 p.m. **Registration**
Room: La Jolla Ballroom Foyer
- 1:30 p.m. to 3:30 p.m. **Mestrelab Users Meeting (Refreshments will be Served)**
Room: La Jolla Ballroom E – H
- 4:00 p.m. to 6:00 p.m. **Bruker Users Meeting (Refreshments will be Served)**
Room: La Jolla Ballroom E – H
- 6:00 to 7:30 p.m. **Welcome Reception in the Exhibit Hall with PANIC Exhibitors**
Poster Presentations and Q&A **All Poster Numbers**
Room: La Jolla Ballroom A – D
- 7:30 p.m. **Dinner on Your Own**

MONDAY, OCTOBER 17

- 7:00 a.m. to 5:30 p.m. **Registration**
Room: La Jolla Ballroom Foyer
- 7:30 to 8:30 a.m. **Breakfast on Your Own**
- 8:30 a.m. **PANIC Chairs' Opening Remarks**
Room: La Jolla Ballroom E -- H
- 8:35 to 10:10 a.m. **Session #1: All Molecules, Great and Small**
Session Chairs: Anuji Abraham and Amber Balazs
Room: La Jolla Ballroom E – H
- 8:40 a.m. **HIF-2 inhibitors: Examples of the versatility of NMR in drug discovery**
Speaker: Kevin Gardner, CUNY Advanced Science Research Center
- 9:10 a.m. **Component Quantification in Solids with the Mixture Analysis Using References Method**
Speaker: Dirk Stueber, Merck & Co, Inc.
- 9:40 a.m. **NMR Solution Conformational Analysis and Its Application to Drug Design**
Speaker: Guoyun Bai, Johnson & Johnson

MONDAY, OCTOBER 17 (Continued)

- 10:10 to 10:40 a.m. **Coffee Break in the Exhibit Hall with PANIC Exhibitors**
Room: La Jolla Ballroom A – D
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- 10:40 a.m. to 12:15 p.m. **Session #2: Solid ... Solid as a Rock**
Session Chairs: Ryan Nieuwendaal, Amrit Venkatesh, and Jim DeFelippis
Room: La Jolla Ballroom E – H
- 10:45 a.m. **Practical Aspects of Elucidating Molecular-Level Phenomena in Rechargeable Battery Materials by NMR Spectroscopy: Tips, Tricks, Pitfalls, and Examples**
Speaker: Robert Messinger, The City College of New York
- 11:15 a.m. **Structure and Molecular Dynamics of Semicrystalline Polymers as Explored by Solid State NMR Spectroscopy**
Speaker: Toshikazu Miyoshi, The University of Akron
- 11:45 a.m. **Solid-State Time Domain NMR for Pharmaceutical Analysis**
Speaker: Michael Hanrahan, Kansas Analytical Services
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- 12:15 to 1:15 p.m. **Lunch in the Exhibit Hall with PANIC Exhibitors**
Room: La Jolla Ballroom A – D
- 1:15 to 2:15 p.m. **PANIC Poster Presentations and Q&A **Even Poster Numbers****
Room: La Jolla Ballroom A – D
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- 2:15 to 3:50 p.m. **Session #3: Metabolomics/Mixture analysis: to isolate or not to isolate ... lets go with not!**
Session Chairs: Amy Freund, Laura Castanar Acedo, and Tim Bergeron
Room: La Jolla Ballroom E – H
- 2:20 p.m. **An NMR-based metabolomic view of the natural history of COVID-19 disease**
Speaker: Oscar Millet, CIC bioGUNE
- 2:50 p.m. **GEMSTONE: ultra-selective NMR methods for fast analysis of complex spectra**
Speaker: Mathias Nilsson, University of Manchester
- 3:20 p.m. **Identification and Quantification of Natural and Engineered Metabolites**
Speaker: Brendan Duggan, University of California, San Diego
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- 3:50 to 4:20 p.m. **Coffee Break in the Exhibit Hall with PANIC Exhibitors**
Room: La Jolla Ballroom A – D

MONDAY, OCTOBER 17 (Continued)

4:20 to 5:55 p.m.

Session #4: Big Trouble in Little Magnets

Session Chairs: Matthew Augustine, Mike Janicke and Gennady Khirich

Room: La Jolla Ballroom E – H

4:25 p.m. **NMR in the chemical warehouse: Development of rapid identification testing procedures with benchtop instrumentation**

Speaker: Jose Napolitano, Genentech Inc.

4:55 p.m. **Benefits of Applying SHARPER Benchtop NMR in Complex Molecules**

Speaker: Claire Dickson, Oxford Instruments

5:25 p.m. **Dual Q, Actively Controlled RF Coil for Improved Signal Detection at Low Magnetic Fields**

Speaker: Karl Stupic, NIST

6:00 p.m.

Dinner on Your Own

TUESDAY, OCTOBER 18

7:00 a.m. to 5:00 p.m.

Registration

Room: La Jolla Ballroom Foyer

7:30 to 8:30 a.m.

Travel Awardee Breakfast (Invitation Only)

Room: Newport Room

8:30 a.m.

PANIC Chairs' Opening Remarks

Room: La Jolla Ballroom E – H

8:35 to 10:10 a.m.

Session #5: Super Session (Part 1): qNMR Advanced Session and Updates, presented by US Pharmacopeia

Session Chairs: Joe Ray, Kristie Adams, and Klas Meyer

Room: La Jolla Ballroom E – H

8:40 a.m. **NMR at USP: Applications in USP-NF (History, General Chapters, Monographs) and USP Reference Standards Evaluation**

Speaker: Edmond Biba, US Pharmacopeia

9:10 a.m. **Proposed revision to the USP NMR General Chapter <761>**

Speaker: Joe Ray, University of Illinois, at Chicago

Toru Miura, FUJIFILM Wako Pure Chemical Corporation

9:40 a.m. **Proposed revision to the USP NMR General Chapter <1761>**

Speaker: Joe Ray, University of Illinois at Chicago

Christina Szabo, Baxter International Inc.

TUESDAY, OCTOBER 18 (Continued)

- 10:10 to 10:40 a.m. **Coffee Break in the Exhibit Hall with PANIC Exhibitors**
Room: La Jolla Ballroom A – D
- 10:40 a.m. to 12:15 p.m. **Session #6: Super Session (Part 2): qNMR Advanced Session and Updates, presented by US Pharmacopeia**
Session Chairs: Joe Ray, Kristie Adams, and Klas Meyer
Room: La Jolla Ballroom E – H
- 10:45 a.m. **Quantitative NMR Determination of PLGAs Molecular Weight and Lactic/Glycolic Ratio**
Speaker: Yixin Ren, US Pharmacopeia
- 11:15 a.m. **A new approach for automated qNMR data analysis**
Speaker: Ben Shapiro, US Pharmacopeia
- 11:45 a.m. **Application of software solution to further develop benchtop NMR as a viable PAT**
Speaker: Jiayu Zhang, The University of British Columbia
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- 12:15 to 1:15 p.m. **Lunch in the Exhibit Hall with PANIC Exhibitors**
Room: La Jolla Ballroom A – D
- 1:15 to 2:15 p.m. **PANIC Poster Presentations and Q&A **Odd Poster Numbers****
Room: La Jolla Ballroom A – D
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- 2:15 to 3:50 p.m. **Session #7: The tough stuff- measuring difficult things in soft materials**
Session Chairs: Sarah Mattler and Jim DeFelippis
Room: La Jolla Ballroom E – H
- 2:20 p.m. **Long-Chain Branch Detection and Quantification in Ethylene-Hexene LLDPE with New ¹³C NMR Pulse Sequences**
Speaker: Zhe Zhou, Dow
- 2:50 p.m. **Monitoring Hydrogel Swelling Using Unilateral NMR**
Speaker: Daniel Gruber, University of Colorado Boulder
- 3:20 p.m. **Speedy and Robust Quantitative Analysis using Generic QA-RINEPT: From Small Molecules to Polymeric Materials**
Speaker: Jianbo Hou, Dow
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- 3:50 to 4:20 p.m. **Coffee Break and Awards Ceremony in the Exhibit Hall with PANIC Exhibitors**
Room: La Jolla Ballroom A – D

TUESDAY, OCTOBER 18 (Continued)

- 4:20 to 5:55 p.m. **Session #8: PANIC 10th Anniversary Session (We are 10!)**
Session Chairs: Kristie Adams and Sarah Mattler
Room: La Jolla Ballroom E – H
- 4:25 p.m. **Impacting Drug Design using NMR Solution Conformations**
Speaker: Kathleen Farley, Pfizer
- 4:55 p.m. **Tackling a Tripartite Glycan Conundrum: Flexibility/Sparse Structural Data/Signal Resolution**
Speaker: Darón Freedberg, FDA
- 5:25 p.m. **Rapid NMR Method for the Assignment of Regioisomers in Monosubstituted 1,2,3-Thiadiazoles**
Speaker: Carlos Amezcua, FMC
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- 6:00 to 7:00 p.m. **PANIC 10-Year Anniversary Happy Hour**
- 7:00 p.m. **Dinner on Your Own**

WEDNESDAY, OCTOBER 19

- 7:00 a.m. to 2:00 p.m. **Registration**
Room: La Jolla Ballroom Foyer
- 7:30 to 8:30 a.m. **Breakfast on Your Own**
- 8:30 a.m. **Opening Remarks**
Room: La Jolla Ballroom E – H
- 8:35 to 10:10 a.m. **Session #9: Proteins, Peptides, Genes/Vaccines – With our Magnets Now You're Seen**
Session Chairs: Kelly Sackett, Gennady Khirich, and Anuji Abraham
Room: La Jolla Ballroom E – H
- 8:40 a.m. **NMR Characterization of Polyphosphorylation Reactions in Low Complexity Domain Proteins**
Speaker: Peter Mirau, Air Force Research Labs
- 9:10 a.m. **Water proton nuclear magnetic resonance for vaccine and gene therapy product characterizations**
Speaker: Marc Taraban, University of Maryland
- 9:40 a.m. **Facilitated structure verification of therapeutic peptides from 2D heteronuclear maps acquired at natural abundance**
Speaker: Subrata Mishra, US Pharmacopeia

WEDNESDAY, OCTOBER 19 (Continued)

10:10 to 10:25 a.m.

Coffee Break

Room: La Jolla Ballroom Foyer

10:25 a.m. to 12:00 p.m.

Session #10: MR in Chemistry: A Few of Our Favorite Things

Session Chairs: Gennady Khirich, Amber Balazs, and John Cort

Room: La Jolla Ballroom E – H

10:30 a.m. **Applied pKa Determination via NMR to Aid Surfactant Understanding**

Speaker: Jackie Thomas, Procter & Gamble

11:00 a.m. **LED-NMR: A Practical Tool for Shining Light on Photochemical Reactions**

Speaker: Mikhail Reibarkh, Merck & Co, Inc.

11:30 a.m. **Reference-free Quantitative NOE and the Structural Value of Two-bond (2JCH) Coupling Constants for Configurational Analysis of Small Molecules**

Speaker: Roberto Gil, Carnegie Mellon University

12:00 p.m.

Lunch

Room: La Jolla Ballroom Foyer

12:15 to 1:50 p.m.

Session #11: Bayes'ed and (Un)Confused: Using Bayesian Statistics and Prior Knowledge to Understand NMR Data and Make Decisions

Session Chairs: Frank Delaglio and Mark Dixon

Room: La Jolla Ballroom E - H

12:20 p.m. **Belief, Decision, and Bayes**

Speaker: Hamid Eghbalnia, UConn Health

12:50 p.m. **When is a peak, a peak?**

Speaker: Colin Kinz-Thompson, Rutgers University - Newark

1:20 p.m. **Back to basics – S/N, resolution and lineshape in time-domain analysis**

Speaker: Krish Krishnamurthy, Chempacker LLC

1:50 p.m.

Closing Remarks

Room: La Jolla Ballroom E - H



PANIC NMR 2022 CONFERENCE POSTER PRESENTATIONS

(As of Monday, October 17, 2022)

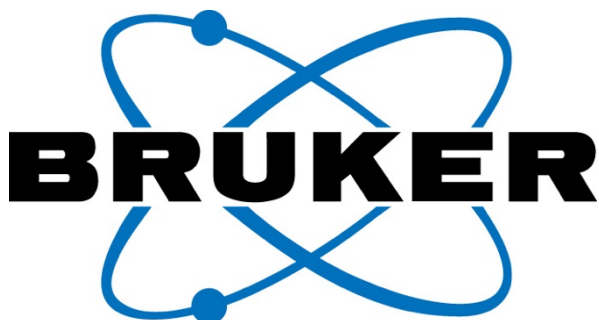
- Poster 1. **Quantification of Lithium using Lithium-7 qNMR**
Juan Araneda
- Poster 2. **Practical aspects of ^{13}C qNMR**
Adolfo Botana
- Poster 3. **Application of Quality by Design principles to the development qNMR methods**
Christoph Freudenberger
- Poster 4. **Developing Next Generations of Polyolefins for Sustainability Assisted by Solid-State NMR**
Navin Kafle
- Poster 5. **Molecular Interaction of Caffeine and Chlorogenic Acid in Coffea arabica Whole Coffee Cherries Extracts by NMR Spectroscopy**
Diganta Kalita
- Poster 6. **Detection of Degradation in Polymers for Carbon Capture Applications**
Maxwell Marple
- Poster 7. **Using Single-Sided NMR to Monitor the Curing of 3D Printed Resin**
Michele Martin
- Poster 8. **Compact NMR Spectroscopy in the field: A Versatile PAT Tool for Production of Specialty Chemicals**
Klas Meyer
- Poster 9. **Searching Libraries of Known Structures for Dereplication: Benefits and Requirements**
Arvin Moser
- Poster 10. **NMR Tools for the Assessment of Antibody-Drug Candidates Aggregation State**
Pablo Trigo Mourino
- Poster 11. **Programming the Intensity of Small Molecule Signals in Complex Formulations Through Bespoke Non- Uniform Sampling Schedules**
Ben Reiner

- Poster 12. **wNMR analytics of biologics: IPC or release analytics done in seconds!**
Maximiian Hartl, Dinah Funke
- Poster 13. **Flow NMR and its application in process monitoring and drug development**
Aritra Sarker
- Poster 14. **Variable Temperature Low-Field TD NMR—Novel Applications to Emulsion Drug Products**
Marc Taraban
- Poster 15. **Elucidations of Complex Chemical Reactions of Carbon Fiber Precursors by Sensitivity Enhanced Solid-state NMR**
Toshikazu Miyoshi
- Poster 16. **Predicting Stability of Lyophilized Protein Formulations using Solid State NMR**
Cole Tower
- Poster 17. **Exploring the Correlation of LF NMR Relaxation with the Composition Based Glass Transition**
Siran Sultan Uguz
- Poster 18. **Automation and Additive Manufacturing Techniques in the ssNMR Maker Space**
Jose Uribe
- Poster 19. **Quantitative Comparison of ¹³C Spectra Acquired Using a New Adiabatic Anti-Ring Pulse Sequence to the Conventional Inverse-Gated Decoupling Single Pulse Experiment**
Joseph Vasquez
- Poster 20. **Automated Quantitation of Taste Active Metabolites in Wine**
Flynn Watson
- Poster 21. **Characterization of Mitochondrial PolgD257A Mutant Mouse using NMR Metabolomics**
Qiuwel Xu
- Poster 22. **Towards the development of rapid, automated identification tests for neat organic liquids using benchtop NMR instrumentation.**
Yicheng (Cassie) Yang
- Poster 23. **Interleaved Magnetoencephalography and Magnetic Resonance Imaging with Multichannel Atomic Magnetometers**
Young Jin Kim
- Poster 24. **Relationship between water-holding capacity and T2 parameters in poultry breast meat**
Hong Zhuang

*We look forward to seeing you at PANIC 2023 in Nashville!
March 12 – 15, 2023*

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(As of Thursday, October 13, 2022)



Mestrelab Research



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