



Fifth International qNMR Summit
October 2-3, 2019
USP Meetings Center, Rockville, MD USA

Agenda

DAY ONE: October 2, 2019

- 8:00 – 8:30 a.m.** **Registration & Coffee**
- 8:30 – 9:00 a.m.** **Welcome and Introductions¹**
- 8:30 – 8:40 a.m. Welcome
 Renee Stake, *Manager, Meetings & Marketing, USP*
- 8:40 – 8:50 a.m. Welcome – Fifth International qNMR Summit
 Gabriel Giancaspro, *VP Dietary Supplements & Herbal Medicines, USP*
- 8:50 – 9:00 a.m. Introduction: qNMR Advancements and Persisters
 Guido Pauli, *Director, Center for Natural Products Research (CENAPT)*
- 9:00 – 10:30 p.m.** **Morning Session I – qNMR Methodology¹**
- Moderated by: Guido Pauli, *CENAPT*
- 9:00 – 9:30 a.m. CRAFT – qNMR in Time-Domain, a New Paradigm
 Krish Krishnamurthy, *Applications Scientist, ChemPacker*
- 9:30 – 10:00 a.m. Solutions for Automated Data Integrity and Integration
 Tucker Rubino, *Lab Weighing Market Manager, Mettler-Toledo*
- 10:00 – 10:30 a.m. External Standardization in qNMR
 Yuzo Nishizaki, *Researcher, Division of Food Additives, NIHS*
- 10:30 – 11:00 a.m.** **Morning Break**

¹ Session open to public Webex.

- 11:00 – 12:00 p.m.** **Morning Session II – qNMR Methodology**
- Moderated by: José Napolitano, *AbbVie*
- 11:00 – 11:15 a.m. Discussion from Morning Session I
- 11:15 – 12:00 p.m. The Five Most Well-Known Secrets of Quantitation by NMR
Matthias Niemitz, *CEO, NMR Solutions*
Guido Pauli, *Director, CENAPT*
- 12:00 – 1:00 p.m.** **Lunch**
- 1:00 – 2:30 p.m.** **Afternoon Session I – qNMR Applications**
- Moderated by: José Napolitano, *AbbVie*
- 1:00 – 1:20 p.m. Quantitative ¹H NMR Study Case: Ticagrelor Related Compound A
Sitaram Bhavaraju, *NMR Team Lead, USP*
- 1:20 – 1:40 p.m. qNMR in the Analysis of Anti-Sense Oligonucleotides (ASOs)
Rasika Phansalkar, *Research Chemist, Biogen*
- 1:40 – 2:00 p.m. Peak Purity in qNMR: Towards Solving the Challenge of Chronically Impure
Proanthocyanidins Signals
Joo-Won Nam, *Assistant Professor, Yeungnam University*
- 2:00 – 2:20 p.m. Public qNMR Resources: validNMR, NMR Wiki, qNMR.org
Kristie Adams, *CEO, Steelyard Analytics*
- 2:20 – 2:30 p.m. Discussion
- 2:30 – 3:00 p.m.** **Afternoon Break**
- 3:00 – 4:00 p.m.** **Afternoon Session II – qNMR Applications**
- Moderated by: Guido Pauli, *CENAPT*
- 3:00 – 3:20 p.m. qNMR Challenges and Limitations
Charlotte Corbett, *Special Testing and Research Laboratory, DEA*
- 3:20 – 3:40 p.m. Improving Comparability in Organic Chemical Measurement: qNMR at NIST
Aaron Urbas, *Research Chemist, Chemical Sciences Division, NIST*
- 3:40 – 4:00 p.m. Sodium NMR – an Exercise in Industrial Validation
Joseph Ray, *Adjunct Professor, University of Illinois at Chicago*

- 4:00 – 4:45 p.m. Afternoon Session III – qNMR Pioneers ²**
- Moderated by: Guido Pauli, *CENAPT*
- 4:00 – 4:15 p.m. The Pioneering qNMR Work of George M. Hanna at FDA
Guido Pauli, *Professor, UIC / CENAPT*
- 4:15 – 4:25 p.m. Working with George
Cesar Lau-Cam, *Professor, St. John's University*
- 4:25 – 4:35 p.m. Establishing a qNMR CRO Business
Bernd Diehl, *CEO, Spectral Service*
- 4:35 – 4:45 p.m. USP George Hanna qNMR Award Announcement
Michael Levy, *VP Research & Innovation, USP*
- 4:45 – 5:00 p.m. Wrap-Up Discussion: Key Topics from Day 1**
- 5:10 – 5:30 p.m. Transportation to the Cambria Hotel Rockville**
- 6:30 – 8:30 p.m. Reception and Dinner**

DAY TWO: October 3, 2019

- 8:00 – 8:30 a.m. Registration & Coffee**
- 8:30 – 10:00 a.m. Morning Session I – Invited Talks**
- Moderated by: Guido Pauli, *CENAPT*
- 8:30 – 8:50 a.m. The New Dimensions of Quantum Mechanical Spectral Analysis (QMSA)
Pekka Laatikainen, *Spin Discoveries*
- 08:50 – 09:25 a.m. Universal Calibrator Suite for the Widespread Application of qNMR in
Analytical Laboratories
Gustavo Martos, *Organic Programme, BIPM*
- 09:25 – 10:00 a.m. Multinuclear NMR, Chirality, and Holistic Quality Analysis
Bernd Diehl, *CEO, Spectral Service*
- 10:00 – 10:30 a.m. Morning Break**
- 10:30 – 12:00 p.m. Morning Session II – Selected Abstracts ²**
- Moderated by: José Napolitano, *AbbVie*
- 10:30 – 11:05 a.m. Proficiency Testing to Improve Your qNMR Laboratory Performance
Markus Obkircher, *Head of Reference Materials R&D, MilliporeSigma*

² Session open to public Webex

11:05 – 11:40 a.m.	Good Weighing Practice for Accurate qNMR Sample Preparation Klaus Fritsch, <i>Manager Compliance, Mettler-Toledo</i>
11:40 – 12:00 p.m.	Application of Quality by Design Principles to the Development of qNMR Methods Christoph Freudenberger, <i>NMR Application Scientist, Bruker Biospin</i>
12:00 – 1:00 p.m.	Lunch
1:00 – 2:00 p.m.	Afternoon Session I – qNMR and Regulations <ul style="list-style-type: none">Moderated by: José Napolitano, <i>AbbVie</i>
1:00 – 1:20 p.m.	General Rules for Quantitative NMR spectroscopy (JIS K 0138:2018) Toru Miura, <i>Research Chemist, FUJIFILM Wako Pure Chemical Corporation</i>
1:20 – 1:45 p.m.	Progress in Proposal of an ISO Standard for Purity Assessment by qNMR Takeshi Saito, <i>Chief Senior Researcher, NMIJ/AIST</i>
1:45 – 2:00 p.m.	Updates and Future Vision of qNMR at U.S. Pharmacopeia Yang Liu, <i>Science Fellow, Research & Innovation, USP</i>
2:00 – 2:30 p.m.	Afternoon Break
2:30 – 5:00 p.m.	Afternoon Session II – qNMR and the Future of Measurement <ul style="list-style-type: none">Moderated by: Guido Pauli, <i>CENAPT</i>
2:30 – 3:00 p.m.	qNMR in a Contract Development and Manufacturing Organization Dan Sorensen, <i>Analytical Team Leader, Eurofins CDMO Alphora Research</i>
3:00 – 5:00 p.m.	Panel Discussion
5:00 – 5:15 p.m.	qNMR Summit Wrap-Up Discussion
5:15 – 5:30 p.m.	Next Steps
5:30 p.m.	Summit Concludes