



October 5 – 7, 2021

DAY 1: Tuesday, October 5	
(All times are Eastern Daylight Time, Washington, DC, USA)	
Welcome and Introductions	
TIME (EDT)	PRESENTATION
7:00 – 7:10 am	Welcome Kayla White, <i>USP (USA)</i>
7:10 – 7:20 am	Opening: USP Introduction Michael Levy, <i>USP (USA)</i>
7:20 – 7:30 am	Opening: CENAPT/UIC Introduction Guido Pauli, <i>UIC (USA)</i>
Session I: Pharmacopeial qNMR Updates	
Moderator: Anton Bzhelyansky, <i>USP (USA)</i>	
7:30 – 8:00 am	Newly updated USP General Chapters <761> and <1761> Lucy Botros, <i>USP (USA)</i>
8:00 – 8:20 am	Practice of Lifecycle in Method Validation Toru Miura, <i>FUJIFILM-Wako Pure Chemical Corporation (Japan)</i>
8:20 – 8:40 am	Utilization of qNMR for assay in Japanese pharmacopoeia Nahoko Uchiyama, <i>National Institute of Health Sciences (Japan)</i>
8:40 – 8:50 am	Q&A
8:50 – 9:00 am	Break
Session II: Inaugural George Hanna qNMR Award Ceremony	
Moderator: Anton Bzhelyansky, <i>USP (USA)</i>	
9:00 – 9:30 am	George Hanna Award: Concept, Intentions, Parameters Ad Bax, <i>National Institutes of Health (USA)</i> and qNMR Summit Organizers
9:30 – 9:40 am	Break

Session III: qNMR, a Primary Analytical Method	
Moderator: Michael Nelson, <i>NIST</i> (USA)	
9:40 – 10:00 am	Quantitative Analysis of Heparin in Heparinoid Unfractionated Raw Materials Bernd Diehl, <i>Spectral Service</i> (Germany)
10:00 – 10:20 am	Recent qNMR Applications in Metrology Bruno Garrido, <i>National Institute of Metrology Standardization</i> (Brazil)
10:20 – 10:40 am	Benchtop NMR for Forensic Drug Analysis Aaron Urbas, <i>National Institute of Standards and Technology</i> (USA)
10:40 – 10:50 am	Q&A
10:50 – 11:00 am	Day 1 Closing Remarks The qNMR Summit Organizers

DAY 2: Wednesday, October 6	
(All times are Eastern Daylight Time, Washington, DC, USA)	
Session I: qNMR Education	
Moderator: Yang Liu, <i>USP</i> (USA)	
TIME (EDT)	PRESENTATION
10:00 – 10:30 am	Teaching Basics of ¹H-qNMR in Life Sciences Holger Stark, <i>Heinrich Heine University Düsseldorf</i> (Germany) Aleksandra Zivkovic, <i>Heinrich Heine University Düsseldorf</i> (Germany)
10:30 – 10:35 am	Q&A
Session II: New Horizons in qNMR	
Moderator: Yang Liu, <i>USP</i> (USA)	
10:35 – 10:55 am	Quantitative 2D NMR Methods for Complex Mixtures Patrick Giraudeau, <i>University of Nantes</i> (France)
10:55 – 11:15 am	Quantum Mechanical Analysis Matthias Niemitz, <i>NMR Solutions</i> (Finland)
11:15 – 11:35 am	Exploring Concepts in qNMR with Monte Carlo Simulations: Facts, Fiction, and a Few Surprises Gennady Khirich, <i>Genentech</i> (USA)
11:35 – 11:55 am	Micro qNMR - Certification of Marine Toxins Markus Obkircher, <i>Millipore Sigma / Merck KGaA Darmstadt</i> (Germany)
11:55 am – 12:10 pm	Q&A
12:10 – 12:20 pm	Break
Session III: qNMR Industrial and Quality Applications	
Moderator: Kristie Adams, <i>Steelyard Analytics</i> (USA)	

12:20 – 12:40 pm	High Resolution ¹⁹F qNMR Reveals Mass-Balanced Drug Phase Distribution in Oil-in-Water Nano-Emulsion Formulations Kang Chen, FDA CDER (US)
12:40 – 1:00 pm	Assurance of qNMR Results by Use of Suitable qNMR Standards, Performance Qualification, and Proficiency Testing Alexander Rück, Millipore Sigma / Merck KGaA Darmstadt (Germany)
1:00 – 1:20 pm	Simplification of NMR Workflows by Standardization Using the ²D Integral of Deuterated Solvents as Applied to Aloe vera Preparations Yulia Monakhova, Spectral Service (Germany)
1:20 – 1:40 pm	The qNMR Method in the Remdesivir Toolkit and Beyond Jeff Moore, USP (USA)
1:40 – 1:50 pm	Q&A
1:50 – 2:00 p.m.	Day 2 Closing Remarks The qNMR Summit Organizers

DAY 3: Thursday, October 7

(All times are Eastern Daylight Time, Washington, DC, USA)

Session I: qNMR in Pharmacy, Industry, and Regulatory

Moderator: Christina Szabo, Baxter (USA)

TIME (EDT)	PRESENTATION
1:00 – 1:20 pm	Development of a Quantitative Performance Qualification Standard Anna Codina, Bruker BioSpin (UK)
1:20 – 1:40 pm	Plain ¹H NMR Analysis Streamlines the Quality Control of WHO Essential Medicines Prabhakar S. Achanta, University of Illinois at Chicago (USA)
1:40 – 1:45 pm	Q&A

Session II: qNMR Capacity Building

Moderator: Christina Szabo, Baxter (USA)

1:45 – 2:05 pm	Current Use and Opportunities for qNMR in Regulatory and Industrial Laboratories. What are the Differences? Stephan Walch, CVUA (Germany)
2:05 – 2:25 pm	qNMR Stimuli: Observations & Opportunities Guido Pauli, CENAPT & Pharmacognosy Institute, UIC (USA)
2:25 – 2:30 pm	Q&A
2:30 – 2:40 pm	Break

Session III: qNMR in Pharmaceutical Development

Moderator: Charlotte Corbett, Drug Enforcement Administration (USA)

2:40 – 3:00 pm	Use of qNMR in Reference Standards Development
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	Ravi Reddy, <i>USP</i> (USA)
3:00 – 3:20 pm	Weighing the Unweighable Sample: The Transformative Role of qNMR in the Discovery of New Medicines Greg Walker, <i>Pfizer</i> (USA)
3:20 – 3:40 pm	The Impact of qNMR in Small-Molecule Pharmaceutical R&D Jose Napolitano, <i>Genentech</i> (USA)
3:40 – 3:50 pm	Q&A
3:50 – 4:00 pm	Break
Session IV: Panel Discussion	
Moderator: Charlotte Corbett, <i>Drug Enforcement Administration</i> (USA)	
4:00 – 4:50 pm	Panel Discussion: Gennady Khirich, Matthias Niemitz, John Price, Holger Stark, Stephan Walch, Gregory Walker
4:50 – 5:00 pm	Summit Closing Remarks

Preliminary