qNMR Workshop/Roundtable

November 17-19, 2020

DRAFT AGENDA (as of November 13) – subject to change

(All times are in Eastern Standard Time, Washington, DC, USA)

DAY 1 (November 17): Understanding qNMR (OPEN) - Webex		
	Welcome and Introductions	
7:00 – 7:30 a.m. EST	7:00 – 7:10 a.m.	Opening: qNMR workshop introductions • **Yang Liu, Ph.D.**, *Incubated Projects Manager, USP*
	7:10– 7:30 a.m.	Welcome Opening: USP Introduction • **Jaap Venema, Ph.D.**, *Executive Vice President & Chief Science Officer, USP*
7:30 – 8:30 a.m.	**Workshop Session I qNMR Applications**	
	7:30 – 7:50 a.m.	qNMR in samples with Protonated Solvents using Benchtop NMR • **Federico Casanova, Ph.D.**, *Chief Executive Officer, Magritek*
	7:50 – 8:10 a.m.	Quantitative 1H-NMR spectroscopy for purity determination using benchtop NMR instruments • **Juan Araneda, Ph.D.**, *Head of Application Chemistry, Nanalysis*
	8:10 – 8:30 a.m.	Implementation of a Benchtop NMR in a Manufacturing Environment • **Travis Gregar, Ph.D.**, *Senior Specialist, 3M*
8:30 – 8:40 a.m.	**Q&A, Break and Coffee Time**	
8:40 – 10:00 a.m.	**Workshop Session II qNMR digital data uses**	
	8:40 – 9:00 a.m.	Compact NMR Spectroscopy: A Versatile Tool for Automated Continuous-Flow Production of Chemicals and Pharmaceuticals • **Klas Meyer, Ph.D.**, *Research Assistant, BAM (Federal Institute for Materials Research and Testing)*

	9:00 – 9:20 a.m.	CRAFT and qNMR • **Krish Krishnamurthy, Ph.D.**, *Founder, Chempacker*
	9:20 - 9:40 a.m.	Quantum Mechanics transforms utility of Benchtop NMR spectrometers in Pharmaceutical Identity Testing • **Prabhakar Achanta, Ph.D.**, *Postdoctoral Research Associate, University of Illinois at Chicago*
	9:40 - 10:00 a.m.	NMR remote analysis for the Food Industry • **Eduardo Nascimento, Ph.D.**, *Field Application Scientist, Bruker BioSpin*
10:00 - 10:10 a.m.	**Q&A**	

DAY 2 (November 18): Validation and qNMR (OPEN) - Webex		
7:00 – 7:05 a.m.	**Opening and Q&A of Day 1**	
7:05 – 8:35 a.m.	**Validation**	
	7:05 – 7:40 a.m.	Analytical chemistry validation and qNMR methods • **Steven Walfish, MBA, M.S.**, *Principal Science & Standards Liaison, USP*
	7:40 – 7:50 a.m.	Q&A
	7:50 – 8:20 a.m.	Proposed Revisions to the USP General Chapters <761> Nuclear Magnetic Resonance Spectroscopy <1761> Applications of Nuclear Magnetic Resonance Spectroscopy • **Dan Sørensen, Ph.D.**, *Regional Regulatory Compliance and Enforcement Officer, Health Canada* • **Christina Miki Szabo, Ph.D.**, *Senior Manager of Research, Baxter Healthcare*
	8:20 – 8:35 a.m.	Q&A
8:35 – 8:45 a.m.	**Break and Coffee Time**	
8:45 – 9:50 a.m.	**qNMR validation in practice**	
	8:45 – 9:15 a.m.	qNMR validation in industry • **Charlotte Corbett, Ph.D.**, *Forensic Drug Chemist, U.S. Drug Enforcement Administration (DEA)*
	9:15 – 9:35 a.m.	Interlaboratory Comparison of benchtop NMR Spectrometers – Purities at 200 and 10 mmol/L • **Michael Maiwald, Ph.D.**, *Head of the Process Analytical Technology Division, BAM (Federal Institute for Materials Research and Testing)*
	9:35 – 9:50 a.m.	qNMR under GxP – Automated End to End Solution • **Fabrice Moriaud, Ph.D.**, *Solutions Development Manager, Bruker BioSpin*
9:50 – 10:00 a.m.	**Q&A**	

DAY 3 (November 19): Roundtable (OPEN) - Webex		
7:00 –9:00 a.m.	**qNMR Applications in pharmacopeias**	
	7:00 – 7:30 a.m.	Measurement of Relative Molar Sensitivity Using the Combination of qNMR and chromatography from the Viewpoint of Regulatory Science • **Naoki Sugimoto, Ph.D.**, *Chief of 2nd Section, Division of Food Additives, National Institute of Health Sciences (NIHS), Japan*
	7:30 – 8:00 a.m.	qNMR in complex drug product quality: from benchtop to high resolution • **Kang Chen, Ph.D.**, *Research Chemist, CDER, U.S. Food & Drug Administration (CDER-FDA)*
	8:00 – 8:30 a.m.	Application of quantitative nuclear magnetic resonance in drug quality control • **Yang Liu, Ph.D.**, *Researcher, National Institutes for Food and Drug Control (NIFDC), China* • **Lan He, Ph.D.**, *Director of Chemical Drug Division, National Institutes for Food and Drug Control (NIFDC), China*
	8:30 – 9:00 a.m.	Pharmacopeial Applications of qNMR: A Selection of Vignettes • **Kristie Adams, Ph.D.**, *President & CEO, Steelyard Analytics, US*
9:00 – 10:00 a.m.	**Roundtable: Panel Discussion** **Moderator**: **Joseph Ray, Ph.D.**, *University of Illinois at Chicago* • Kang Chen, *CDER, U.S. Food & Drug Administration (FDA)* • Charlotte Corbett, *U.S. Drug Enforcement Administration (DEA)* • Helen Corns, *British Pharmacopoeia* • Yang Liu, *National Institutes for Food and Drug Control (NIFDC), China* • Yang Liu, *USP* • Toru Miura, *FUJIFILM-Wako* • Naoki Sugimoto, *National Institute of Health Sciences (NIHS), Japan*	