

# The 8<sup>th</sup> International qNMR Summit, Chicago IL, USA

## DAY 1: August 15, 2024

*In-person program: all agenda times are Central Daylight Time (CDT = UTC-5h; Chicago)*

*Online content: 8AM-12PM Chicago; 9 AM-1PM New York; 15-19 Central Europe; 21-1 Beijing and Singapore; 22-2 in Seoul and Tokyo*

| Registration   |   |
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| 07:30 AM to 08:00 AM   | Attendee registration   |
| Welcome  |   |
| 08:00 AM to 08:10 AM   |  <b>Brent Friesen</b> , Dominican University<br> <b>Guido Pauli</b> , University of Illinois at Chicago   |
| 8:10 AM – 9:30 AM Session 1A – Emerging qNMR Approaches with Regulatory Impact |   |
|  | <i>Session Chair: Anton Bzhelyansky, USP</i>  |
| 08:10 AM to 08:30 AM   | Role of qNMR in a regulatory laboratory in the effective control of food, food products, cosmetics and medicines<br> <b>Stephan Walch</b> , Chemical and Veterinary Investigation Offices (CVUA)                                 |
| 08:30 AM to 08:50 AM   | Delivery of SI-traceable qNMR results<br> <b>Steven Westwood</b> , BIPM  |
| 08:50 AM to 09:05 AM   | Application of life cycle approach in the development of a qNMR procedure for ISO 17034 accreditation<br> <b>Toru Miura</b> , FUJIFILM-Wako  |
| 09:05 AM to 09:20 AM   | Application of the life-cycle approach to a qNMR method development, validation, and verification<br> <b>Sunil Paudel</b> , United States Pharmacopeia (USP)   |
| 09:20 AM to 09:30 AM   | <i>Discussion</i>   |
| 9:30 AM – 10:05 AM Session 1B – qNMR in Illicit Drugs Detection                |   |
|  | <i>Session Chair: Anton Bzhelyansky, USP</i>  |
| 09:30 AM to 09:40 AM   | Quantitation with overlapped peak patterns<br> <b>Charlotte Corbett</b> , Drug Enforcement Administration (DEA)  |
| 09:40 AM to 09:50 AM   | Agile forensic and chemical metrology infrastructure to support quantification of new psychoactive substances in Singapore using SI-traceable standards certified by qNMR<br> <b>Ting Lu</b> , Health Sciences Authority (HSA) |
| 09:50 AM to 10:00 AM   | Benchtop NMR analysis of illicit drugs<br> <b>Shallu Verma</b> , University of Canterbury  |
| 10:00 AM to 10:05 AM   | <i>Discussion</i>   |
| 10:05 AM – 10:30 AM Break  |   |
| 10:30 AM – 12:00 PM Session 2 – qNMR Applications – New and Standardized       |   |
|  | <i>Session Chair: Yang Liu, USP</i>   |
| 10:30 AM to 10:50 AM   | Quantitative non-invasive analysis of pharmaceuticals using water proton NMR<br> <b>Marc Taraban</b> , University of Maryland  |
| 10:50 AM to 11:10 AM   | Quantitative solid-state NMR (qSSNMR) for pharmaceutical analysis<br> <b>Yongchao Su</b> , Merck & Co.   |
| 11:10 AM to 11:20 AM   | Development and validation of orthogonal qNMR and HPLC methods for assessment of drug substance: a case study of glutathione<br> <b>Qin Shu</b> , US Food and Drug Administration (FDA)  |
| 11:20 AM to 11:30 AM   | <sup>1</sup> H qNMR-based bioprocess characterization for CHO cell culture<br> <b>Ying-Ting Shi</b> , Zhejiang University  |

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| 11:30 AM to 11:50 AM | Site-specific isotope analysis by NMR spectroscopy<br>🌟 <b>Phuong Mai Le</b> , National Research Council (NRC) |
| 11:50 AM to 12:00 PM | <i>Discussion</i>  |

12:00 PM – 1:30 PM Lunch

1:30 PM – 3:00 PM Workshop 1 – Practical qNMR

*Workshop Details to be Announced*

3:00 PM – 3:30 PM Break

3:30 PM – 5:00 PM Workshop 2 – Education / Outreach

*Workshop Details to be Announced*

5:00 PM Reception and Dinner

## DAY 2: August 16, 2024

*In-person program: all agenda times are Central Daylight Time (CDT = UTC-5h; Chicago)*

*Online content: 8AM-12PM Chicago; 9 AM-1PM New York; 15-19 Central Europe; 21-1 Beijing and Singapore; 22-2 in Seoul and Tokyo*

### Registration

07:30 AM to 08:00 AM Attendee registration

### 8:00 AM – 9:10 AM Session 3A – qNMR Tech – Industry Perspectives

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|----------------------|---|
|                      | <i>Session Chair: Guido Pauli, UIC</i>  |
| 08:00 AM to 08:15 AM | Benchtop qNMR for increased access to industrial Quality Control assays<br>🌟 <b>Matthew Leclerc</b> , Nanalysis                   |
| 08:15 AM to 08:30 AM | Avoiding the human: errors, uncertainties and automation<br>🇬🇧 <b>Iain Day</b> , JEOL-UK  |
| 08:30 AM to 08:45 AM | How to make automated qNMR analysis trustworthy<br>🇩🇪 <b>Matthias Niemitz</b> , NMR Solutions                                     |
| 08:45 AM to 09:00 AM | Automatic qNMR data analysis approach prototype of QMSA-based digital products<br>🇺🇸 <b>Yang Liu</b> , United States Pharmacopeia |
| 09:00 AM to 09:10 AM | <i>Discussion</i>   |

### 9:10 AM – 9:45 AM Session 3B – qNMR Capability Building

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|                      | <i>Session Chair: Guido Pauli, UIC</i>  |
| 09:10 AM to 09:20 AM | A collaborative study on platform <sup>1</sup> H quantitative NMR method: towards capacity building for novices<br>🇨🇳 <b>Jing Zhang</b> , WuXi AppTec |
| 09:20 AM to 09:30 AM | NMRXiv: a fair, open-source, and consensus-driven -- NMR data repository and computational platform<br>🇩🇪 <b>Chandu Nainala</b> , University of Jena  |
| 09:30 AM to 09:40 AM | www.nmrium.org: Revolutionizing NMR spectral processing with a web-based application<br>🇨🇪 <b>Luc Patiny</b> , Zakodium                               |
| 09:40 AM to 09:50 AM | <i>Discussion</i>   |

9:50 AM – 10:00 AM Break

10:00 AM – 11:05 AM Session 4A – qNMR Applications – APIs and Purity

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|                      | <i>Session Chair: Shao-Nong Chen, UIC</i>  |
| 10:00 AM to 10:20 AM | Quantification of halo-acetic acids in solutions using relative molar sensitivity obtained by qNMR/chromatography<br>🇯🇵 <b>Taichi Yamazaki</b> , National Metrology Institute of Japan (AIST)                  |
| 10:20 AM to 10:35 AM | Fast <sup>31</sup> P qNMR method for accurate oligonucleotide API assay in formulation<br>🇺🇸 <b>Jiayi Li</b> , US Food and Drug Administration (FDA)   |
| 10:35 AM to 10:45 AM | Investigating the stability of Valeriana-type iridoid glycosides by qNMR<br>🇰🇷 <b>Trung Huy Ngo</b> , Yeungnam University  |
| 10:45 AM to 10:55 AM | Absolute purity determination of pharmaceuticals using quantitative <sup>31</sup> P- AND <sup>19</sup> F-NMR and Method Validation<br>🇯🇵 <b>Nahoko Uchiyama</b> , National Institute of Health Sciences (NIHS) |
| 10:55 AM to 11:05 AM | <i>Discussion</i>  |

11:05 AM – 12:00 PM Session 4B – qNMR Applications – Specialized

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|                      | <i>Session Chair: Shao-Nong Chen, UIC</i>  |
| 11:05 AM to 11:20 AM | Roadmap to Consistent qNMR in the pharmaceutical industry<br>🇺🇸 <b>Michele DeRider</b> , Catalent Pharma Solutions   |
| 11:20 AM to 11:35 AM | Identification by HSQC and quantification by qHNMR Innovate pharmacopeial amino acid analysis<br>🇺🇸 <b>Daniela Rebolgar</b> , University of Illinois at Chicago                            |
| 11:35 AM to 11:45 AM | Application of deconvolution for qNMR purity assessment of pyributicarb containing similar structural impurities<br>🇯🇵 <b>China Okamoto</b> , National Metrology Institute of Japan (AIST) |
| 11:45 AM to 11:55 AM | Enhancing TCM pharmaceutical process characterization through <sup>1</sup> H-qNMR assisted with chemometrics<br>🇨🇳 <b>Jiayu Yang</b> , Zhejiang University                                 |
| 11:55 AM to 12:05 PM | <i>Discussion</i>  |

12:05 PM – 1:30 PM Lunch

1:30 PM – 3:00 PM Workshop 3 – Lifecycle Approach to qNMR Method Development

*Workshop Details to be Announced*

3:00 – 3:20 PM Break

3:20 PM – 4:00 PM Digital Posters / Flash Presentations

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|----------------------|---|
|                      | <i>Session Chair: Daniela Rebolgar, UIC</i>   |
| 03:20 PM to 03:30 PM | Development of a synthetic fecal metabolite calibration solution<br>🇺🇸 <b>Aaron Urbas</b> , National Institute of Standards and Technology  |
| 03:30 PM to 03:40 PM | Fecal metabolome profiles differ among uncastrated Nelore males belonging to distinct selection lines<br>🇧🇷 <b>Luisa Almeida</b> , University of São Paulo                                    |
| 03:40 PM to 03:50 PM | Validation of relative quantitative benchtop NMR procedure for polysaccharide branching: comparison of different procedure validation approaches<br>🇺🇸 <b>Ping He</b> , Baxter Healthcare Co. |
| 03:50 PM to 04:00 PM | <i>Discussion</i>   |

4:00 PM – 4:50 PM General Discussion – What is Needed to Move qNMR Forward?

4:50 PM – 5:00 PM Concluding Remarks

5:00 PM Post-Summit Dinner