



qNMR Summit 2023

March 29-31, 2023

NH Hotel, Santiago de Compostela

qnmrsummit2023.org

Conference Schedule

WEDNESDAY, March 29 — Morning

09:00 — 10:00 **Registration**

10:00 — 10:10 **Welcome Day 1**

10:10 — 10:50 **Session 1 — Quality Assurance**

Session chair: Ulrike Holzgrabe

10:10 — The Use of qNMR for the Characterisation of European Pharmacopoeia Reference Standards

Matthias Weber, EDQM, Straßbourg, France

10:30 — Quantification and Identification by Community-Built NMR Analytical Systems

Vito Gallo, Politecnico di Bari, Italy

10:50 — 11:45 **Coffee / Posters / Exhibitors**

11:45 — 13:05 **Session 2 — Pharma I**

Session chair: Jose Napolitano

11:45 — The Key Role of ^{19}F qNMR in Human Absorption, Distribution, Metabolism and Excretion Studies of Nirmatrelvir: A Faster Route to Emergency Use Authorization

Greg Walker, Pfizer USA

12:05 — Applications of qNMR in the pharmaceutical industry

David Longmire, AstraZeneca UK

12:25 — Quantitative NMR tools in lyotropic liquid crystals to determine the enantiopurity of a chiral active pharmaceutical ingredient

Boris Gouilleux, Institut de Chimie Moléculaire et des Matériaux d'Orsay, France

12:45 — Bacterial and mammalian metabolomic profiling using spatially resolved qNMR techniques

Trey Koev, University of East Anglia, UK

13:05 — 13:45 **Session 3 — Flash Presentations**

Session chair: TBA

13:45 — 15:00 **Light lunch / Posters / Exhibitors**

WEDNESDAY, March 29 — Afternoon

15:00 — 15:40

Session 4 — Forensics

Session chair: Torsten Schoenberger

15:00 — Building an innovative database for the simultaneous identification and quantification of Novel Psychedelic Substances via benchtop NMR

Steffen Breinlinger / Rafael Sacramento, Kykeon Analytics Ltd

15:20 — I FED MY BENCHTOP NMR ECSTASY TABLETS - 3,4-Methylenedioxymethamphetamine Quantification via Benchtop ¹H qNMR Spectroscopy

Anca Frinculescu, King's College London, UK

15:40 — 16:15

Session 5 — Keynote Speaker

Introduction: Mike Bernstein

15:40 — qNMR of Biopolymers using Stimulated Echo Pulsed Field Gradients

Bernd Diehl, Spectral Service, Germany

18:00 — 19:15

Guided tour of the Old Town

20:00 —

Tapas Tour

Thursday, March 30 — Morning

09:00 — 09:10 **Welcome Day 2**

09:10 — 10:10 **Session 6 — Polymers**

Session chair: Bernd Diehl

09:10 — Benchtop NMR vs High Field NMR: Multivariate Calibration and Calibration transfer for Molecular Weight Analysis of Lignin

René Burger, Bonn-Rhein-Sieg University of Applied Sciences (Germany)

09:30 — ^{13}C solid-state NMR applied to the characterization of high-molecular weight polymers: Sevelamer as a case study

Jose Ignacio Lopez Sanchez, Universidad Internacional de La Rioja (UNIR), Spain

09:50 — Tackling uncertainty in SI traceable qNMR analysis of complex samples

Cailean Clarkson, LGC (UK)

10:10 — 10:45 **Coffee / Posters / Exhibitors**

10:45 — 11:45 **Session 7 — Pharma II**

Session chair: Peter Howe

10:45 — Development of an externally calibrated qNMR workflow for small-molecule pharmaceutical R&D

Jose Napolitano, Genentech, USA

11:05 — Rapid pKa measurements, ion-binding analysis and other 'titrations' using ^1H chemical shift imaging techniques

Matthew Wallace, University of East Anglia, UK

11:25 — Enzymatic assays in a single NMR tube: using imaging NMR to extract Michaelis Menten enzymatic parameters

Serena Monaco, University of East Anglia, UK

11:45 — 11:50 **Short break**

- 11:50 — 12:50 **Session 8 — Experimental Optimization**
Session chair: Nadine Peez

11:50 — The challenges of performing qNMR with multiple pulse experiments
Howard Foster, Manchester University, UK

12:10 — Similarity calculations and differential NMR as alternative for multivariate data analysis
Jan Schripsema, Universidade Estadual do Norte Fluminense, Brazil

12:30 — Practical aspects of ¹³C qNMR
Adolfo Botana, JEOL, UK

12:50 — 13:00 “qNMR – the handbook” — a new resource

Thursday, March 30 — Afternoon

- 13:00 — 14:30 **Light lunch / Exhibitors / Posters**
- 14:30 — 15:30 **Session 9 — Automation**
Session chair: Michael Maiwald

14:30 — QNMR For Busy People - Automation and Quantification
David Williamson, Mestrelab, Spain

14:50 — T₁ determination for qNMR - do it fast
Reiner Kerssebaum/Torsten Schoenberger, Bruker/BKA

15:10 — Multi-nuclei quantification with benchtop NMR using external standards
Jürgen Kolz, Magritek, Germany

15:30 — 16:05 **Session 10 — Keynote Speaker**
Introduction: Mike Bernstein

Similarity calculations and differential NMR for the evaluation and improvement of qNMR parameters
Jan Schripsema, Universidade Estadual do Norte Fluminense, Brazil

20:00 — **Conference Dinner**
HOSTAL DE LOS REYES CATÓLICOS

Friday, March 31 — Morning

09:00 — 09:10 **Welcome Day 3**

09:10 — 10:10 **Session 11 — Food**

Session chair: Vito Gallo

09:10 — Application of NMR Spectrometry in Food Control
Jan Teipel, CVUA Karlsruhe

09:30 — A real-life assessment for reproducibility in NMR metabolomics

Calin Deleanu, Romanian Academy, Bucharest, Romania

09:50 — Analysis of the metabolic profile of cysts and nauplius of *Artemia salina* using similarity calculations and differential NMR

Ronald dos Santos Merlim, Universidade Estadual do Norte, Brazil

10:10 — 10:45 **Coffee / Posters / Exhibitors**

10:45 — 12:05 **Session 12 — Mixed Applications**

Session chair: Klas Meyer

10:45 — qNMR of Li-ion batteries

Nadine Peez, Spectral Service, Germany

11:05 — The use of quantitative NOEs for the simultaneous determination of the relative configuration and conformation of small organic molecules using the floating chirality restrained DG/DDD approach

Matthias Köck, Alfred Wegener Institut, Germany

11:25 — Pulse Length Based Concentration Determination (PULCON) for accurate quantification of multi-nuclear operando FlowNMR data without internal standards

Adam Khan, University of Bath, UK

11:45 — Quantification of Lithium in Brines Using Benchtop NMR Spectroscopy

Juan Araneda, Nanalysis, Canada

12:05

Concluding remarks
End of Meeting

Posters

- P1 Determining water content by NMR
Peter Howe, AstraZeneca, UK
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- P2 Holistic analysis of herbicide formulations with nuclear magnetic resonance, similarity calculations and differential NMR
Thaís Ruy Aiolfi, Denise Dagnino, Jan Schripsema, Universidade Estadual do Norte, Brazil
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- P3 Analysis of the metabolic profile of cysts and nauplius of *Artemia salina* using similarity calculations and differential NMR
Ronald dos Santos Merlim, Universidade Estadual do Norte, Brazil
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- P4 Uncovering the reaction pathways of Polyethyleneterephthalate (PET) depolymerization under neutral hydrolysis – Use of qNMR for Process Optimization
Antonio Jaime-Azuara, Thomas Helmer Pedersen and Reinhard Wimmer, Aalborg University, Denmark
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- P5 Rapid Continuous Cell Metabolomic Profiling by Chemical Shift Imaging NMR
*Trey Koev^{*1}, Hannah Harris², Fred Warren² and Matthew Wallace¹, 1. NMR Group, School of Pharmacy, University of East Anglia, Norwich Research Park, NR4 7TJ; 2. Food Innovation and Health, Quadram Institute Bioscience, Norwich Research Park, NR4 7UQ*
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- P6 Rapid pKa measurements, ion-binding analysis and other 'titrations' using ¹H chemical shift imaging techniques
Matthew Wallace, University of East Anglia
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- P7 Enzymatic assays in a single NMR tube: using imaging NMR to extract Michaelis Menten enzymatic parameters
Serena Monaco, Matthew Wallace - School of Pharmacy, University of East Anglia, Norwich, UK*
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- P8 Software package TotalXMR to support quantification of total content of X-nucleus from TD data
Stan Sýkora, Extra Byte
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- P9 Combining NMR and Artificial Intelligence to Improve Food Identification: Insights from a Pilot Project with the Central Inspectorate of Quality Protection and Fraud Repression (ICQRF, part of the Italian Ministry of Agriculture)
*Maurizio Triggiani,^{a,b} Biagia Musio,^{a,b} Stefano Todisco,^a Marica Antonicelli,^a Maria Trisolini,^b Piero Mastroilli,^{a,b} Mario Latronico,^{a,b} Stefania Carpino,^c Vincenzo Di Martino,^c Laura Gambino,^c Vito Gallo^a,
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