Speaker Biographies

(Listed alphabetically by last name)
November 17-19, 2020
DRAFT

Prabhakar Achanta, Ph.D.
Postdoctoral Research Associate
College of Pharmacy, University of Illinois at Chicago, USA

Dr. Prabhakar Achanta is a postdoctoral research associate at Prof. Guido Pauli's lab, College of Pharmacy, University of Illinois at Chicago. He has been associated with the group since October 2018. Prior to this role, he worked for about 15 months at a Contract Research Organization in Hyderabad, India in NMR division for structure confirmation and elucidation of synthesized small molecule.

Dr. Achanta did his PhD in Medicinal and Natural Products Chemistry at Kakatiya University, College of Pharmaceutical Sciences, India, during which he isolated few new malabaricanes, a rare class of tricyclic triterpenes.

Dr. Achanta's interests are in Natural Products Drug Discovery and determining purity in pharmaceuticals by NMR. At UIC, he is involved in establishing HiFSA profiles of small molecule therapeutics by deep understanding of their 1H NMR spectra through Full Spin Analysis. He also works towards identifying dentin bio-modifiers from Vitis sps.

Presentation: Day 1 - Quantum Mechanics transforms utility of Benchtop NMR spectrometers in Pharmaceutical Identity Testing

ABSTRACT: Being a quantum mechanical (QM) method, NMR spectra can be interpreted well beyond the level of visual human analysis. Utilizing the QM-based 1HNMR iterative Full Spin Analysis (HiFSA), the understanding of the 1H NMR signals of small molecules can be much enhanced and full coverage be achieved even for complex "multiplets". The QM foundation enables the NMR spectra to be calculated and, thereby, determine chemical shifts (□), coupling constants (J), line widths (□½), line shape and signal intensities with high accuracy. Importantly, such calculations allow us to scale down such NMR spectra to lower magnetic fields such as those (40-100 MHz equivalent) used in modern benchtop instrument. This enables the use of calculated NMR spectra of pharmaceuticals as digital fingerprints, which can be utilized to identify and even quantify APIs using contemporary benchtop NMR spectrometers.

Kristie Adams, Ph.D.
President and CEO
Steelyard Analytics, Inc., USA

Dr. Adams received her Ph.D. in Chemistry from Louisiana State University in 2007. Following a postdoctoral appointment at the National Cancer Institute in Frederick, MD, she accepted a position at the United States Pharmacopeial Convention (USP) in 2011, where her research was focused on developing compendial (q)NMR spectroscopic methods for quality control of medicines, foods, dietary supplements and botanicals. In 2015, Dr. Adams moved to DuPont, where, as a Research Investigator, she utilized (q)NMR spectroscopic methods to deliver critical technical solutions for a broad range of applications across DuPont business units. In 2017, Dr. Adams became the President and CEO of Steelyard Analytics, Inc., a contract NMR spectroscopy laboratory located in the heart of the I-270 biotech corridor in Gaithersburg, MD. Steelyard Analytics is the US daughter company of Spectral Service AG, located in Cologne, Germany. Dr. Adams actively collaborates with the global NMR community, with standards-setting organizations such as AOAC, AOCS and USP, and currently serves as the President of PANIC (Practical Applications of NMR in Industry Conference).

Presentation: Day 3 - Pharmacopeial Applications of qNMR: A Selection of Vignettes
ABSTRACT: forthcoming

Juan Araneda, Ph.D.
Head of Application Chemistry
Nanalysis Corp., Canada

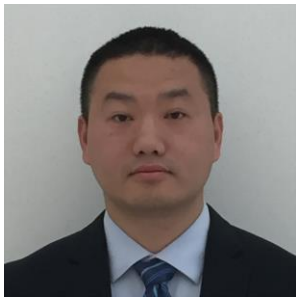
Juan Araneda obtained his M.Sc. and Ph.D. in Chemistry at the University of Calgary in Canada. Shortly after graduation he joined Nanalysis, a manufacturer of low-field, high-resolution benchtop Nuclear Magnetic Resonance (NMR) spectrometers, as an application chemist. Currently he is the Head of Application Chemistry where he focuses on the development of industrial methods to help proliferate the use of benchtop NMR into a variety of industrial applications where NMR Spectroscopy has not been previously used, including forensics, mining, cannabinoid quantification, etc.

Presentation: Day 1 - Quantitative 1H-NMR spectroscopy for purity determination using benchtop NMR instruments
ABSTRACT: Nuclear Magnetic Resonance (NMR) is an extremely powerful technique that is frequently used throughout pharmaceutical research to identify new compounds, assess purity, and characterize/optimize chemical reactions. Although considerably less prevalent, it has also been established as a powerful technique for routine quantitative analysis. In this context, benchtop NMR has emerged as a complementary NMR technology with which to increase the accessibility and reach of NMR to includes research and QA/QC laboratories, as well as expand the user base. In this talk, we showcase several applications of benchtop NMR instruments in purity determination.

Federico Casanova, Ph.D.
Chief Executive Officer
Magritek, Germany

Federico is a specialist in the development of hardware and methodologies for portable and desktop NMR systems. He got his PhD in physics in 2001 in Cordoba, Argentina and move to Germany with an Alexander von Humboldt fellowship to join the group of Prof. Blümich at the RWTH University in Aachen. After two years as a postdoctoral fellow he remained at the RWTH as project leader where he worked on several projects in basic and applied research areas related to mobile and benchtop NMR. He has published over 50 papers in different scientific journals, has contributed to 10 book chapters, has edited a book on single-sided NMR, and is inventor of 8 patents. As a reviewer he has refereed a large number of papers for more than 10 different journals in the area of magnetic resonance, magnetic resonance imaging, and applied chemistry and physics. During his time at the university he acquired considerable experience developing solutions for in-line application of NMR working in close collaboration with different partners in industry. He is one of the founders of Magritek and is member of its board of directors. Since 2012 works as the CEO of the German office of Magritek.

Presentation: Day 1 - qNMR in samples with Protonated Solvents using Benchtop NMR
ABSTRACT: Quantification by NMR of analytes in liquid formulations presents big challenges due to the strong spectral signatures from the protonated solvents typically used in the production process. In order to achieve the required accuracy in this type of sample, solvent suppression techniques are a powerful option. In this presentation, we describe the implementation and use of qNMR with solvent suppression on the Spinsolve ULTRA as an easy-to-use, compact and inexpensive tool to perform routine analysis. Examples include the quantification of components present in excipient mixtures down to millimolar concentrations. Furthermore, it is shown that this technique can even be applied for online-quantification, which is demonstrated on an example of a glucose fermentation using yeast.



Kang Chen, Ph.D.
Research Chemist
U.S. Food & Drug Administration (FDA-CDER), USA

Kang Chen graduated with PhD in chemistry from New York University. He had been at NIH as a postdoc and staff scientist, developing NMR methods to study protein structure and dynamics. In 2014 he moved to the US Food and Drug Administration's Center for Drug evaluation and Research (CDER) where he develops NMR methods to assess the quality of complex drugs including peptide, proteins, nano emulsions etc.

Panelist: Day 3 - Roundtable Panel Discussion

Presentation: Day 3 - qNMR in complex drug product quality: from benchtop to high resolution
ABSTRACT: The qNMR application in complex drug product quality research is discussed. Chemical assay examples are for quantification of API in complex formulation using beach-top low field instrument and measurement of API release from nanoparticle. More extended qNMR studies are quantification of DOSY and kinetics results on complex drug products.

Charlotte Corbett, Ph.D.
Forensic Drug Chemist
U.S. Drug Enforcement Administration (DEA), USA

Charlotte Corbett has worked as a forensic drug chemist for 18 years. She has specialized in nuclear magnetic resonance (NMR) for the past eight years. The U.S. Drug Enforcement Administration utilizes NMR for purity determination, structure differentiation, identification, and structure elucidation. DEA continues to simplify quantitation through automation.

Panelist: Day 3 - Roundtable Panel Discussion

Presentation: Day 2 - qNMR validation in industry
ABSTRACT: The US Drug Enforcement Administration analyzes various materials for the presence and amount of controlled substances. qNMR is used to quantitate multiple compounds with simple sample preparation and automated processing. A general method is validated for each instrument. Specific analyte, solvent and internal calibrant methods are validated separately. Upon sample analysis, blank and quality control samples are included. qNMR has become a convenient method with integrated assessment of reliability.

Helen Corns
Principal Pharmacopoeial Scientist
British Pharmacopoeia (BP), UK

I am a Principal Pharmacopoeial Scientist at the British Pharmacopoeia (BP) responsible for 2 of the BP Expert Advisory Groups on Medicinal Chemicals (EAGs MC1 and MC2). In this role I have been looking at how new/enhanced analytical technologies are evaluated for adoption in the BP. I am an analytical chemist by training, which has included identification and quantification of illicit drugs using NMR, along with a variety of other analytical techniques. I hold a BSc(Hons) in Chemistry from the University of Leeds.

Panelist: Day 3 - Roundtable Panel Discussion

Travis Gregar, Ph.D.
Senior Specialist
3M, USA

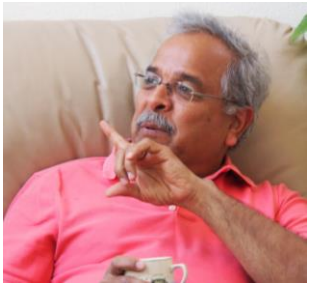
Travis Gregar attended Arizona State University where he earned his BA Ed in Chemical Education and the University of Arizona where he earned his PhD in Organic Chemistry. He has been working for 3M in the Corporate Research Analytical Lab since 2000.

Presentation: Day 1 - Implementation of a Benchtop NMR in a Manufacturing Environment
ABSTRACT: Traditional analytical measurements in a manufacturing setting requires simple, repeatable, and easy to perform tests with minimal effort. With the introduction of low field NMR units, new analytical methods are now possible to both replace some of the traditional methods as well as implement new procedures to help increase throughput, reduce risk, and line down time in the factory setting.

Lan He, Ph.D.
Director of Chemical Drug Division
National Institutes for Food and Drug Control (NIFDC), China

Professor Lan He has long been engaged in drug chemistry, drug analysis and drug quality control research. Her research area includes: new fluorescent probe to detect intracellular and extracellular NO, quantitative nuclear magnetic resonance and ambient mass spectrometry. She organized the editing and publishing of the first series of China's spectrum handbook for chemical reference materials. She published more than 80 articles in Nature, PNAS, Chem. Comm., Angew., Chem. Int. Ed., Org. Lett. and J. Am. Chem. Soc. Etc. She also won 27 invention patents and 4 provincial and ministerial level science and technology awards.

Presentation (presented by colleague Yang Liu, NIFDC): Day 3 - Application of quantitative nuclear magnetic resonance in drug quality control
ABSTRACT: See abstract under Yang Liu, NIFDC.



Krish Krishnamurthy, Ph.D.
Founder
Chempacker LLC, USA

Krish Krishnamurthy received his Ph.D. in Synthetic Organic Chemistry and his NMR research career started with his post-doctoral tenure with Prof. (late) George Olah. He explored NMR applications in the study of structure and dynamics of carbocation intermediates. He spent next three decades between Pharma and vendor (Varian) labs pursuing research in pulse sequence development in small molecule NMR. He is currently an independent researcher focusing on time-domain data processing. He is the recipient of 2018 James Shoolery award (SMASH conference) in recognition of his life-time contribution to the field of small molecule NMR.

Presentation: Day 1 - CRAFT and qNMR
ABSTRACT: CRAFT is an unconventional data processing tool. Unlike conventional tools that work in frequency domain, CRAFT processes the data in time domain1. Phase and baseline corrections and a requirement of minimum peak separation is a unchallenged prerequisite for accurate quantification in conventional frequency domain analysis. CRAFT redefines overlap, phase-correction and baseline correction. We present examples of qNMR results based on CRAFT 1D analysis and demonstrate its validation and benefits. Quantitative of 2D nmr analysis is an emerging analytical tool2. Analysis of 2D data by CRAFT presents unique opportunity for 2D qNMR. Example preliminary results of 2D qNMR by CRAFT will also be presented.
References:
1. K. Krishnamurthy, Magn. Reson. Chem., 2013, 51, 821-829
2. R. Crouch, T. Bergeron, M. Frey and A. Krishnaswami, Poster presented at SMASH 2018

Yang Liu, Ph.D.
Researcher
National Institutes for Food and Drug Control (NIFDC), China

Dr. Yang Liu received his Ph.D. from University of Maryland, College Park. After a year at NIH, he joined National institutes for food and drug control (NIFDC) at Beijing, China. He engaged in drug quality related work for more than ten years, and is responsible for the registration and inspection of chemical drugs, retesting and standardization of chemical reference substances and assessing identification and purity of chemical reference substances.

Panelist: Day 3 - Roundtable Panel Discussion

Presentation (presenting on behalf of Lan He, NIFDC): Day 3 - Application of quantitative nuclear magnetic resonance in drug quality control

ABSTRACT: Quantitative nuclear magnetic resonance (qNMR) is a powerful tool in measuring drug content because of its high speed, sensitivity and precision. This method has been widely utilized in chemical drug quality control within National Institutes for Food and Drug Control (NIFDC), China.
Our study includes several fields:
1) Application of proton qNMR in characterizing the assay of chemical reference substances
2) Application of 19F qNMR in characterizing fluoro-containing APIs and drug products
3) Application of 13C qNMR in characterizing long chain fatty-acids

Yang Liu, Ph.D.
Incubated Projects Manager, Product Quality & Analytical Methods
United States Pharmacopeia (USP), USA

Yang Liu received the Ph.D. degree from University of Illinois at Chicago, College of Pharmacy, where he worked with Professor Guido Pauli, and studied quantitative NMR (qNMR), countercurrent chromatography, and eutectic phenomenon in natural products.

Dr. Liu is experienced in qNMR applications, including identification and quantification of natural products, synthetic APIs, and natural/synthetic polymers. As USP Global Fellow in 2017, he has worked on a project about reference standard determinations using qNMR and development of digital NMR reference standards in Prof. Pauli's lab. In 2018, he has transited the project to USP Rockville campus, and been honored as USP qNMR Fellow. In 2019, he was invited to be a guest scientist at the National Institute of Standards and Technology (NIST), to evaluate benchtop (q)NMR instrument as pharmacopeial technology.

Presentation: Day 1 - Opening: qNMR workshop introductions

Panelist: Day 3 - Roundtable Panel Discussion

Michael Maiwald, Ph.D.
Head of the Process Analytical Technology Division
Bundesanstalt für Materialforschung und -prüfung (BAM), Germany

Dr. Michael Maiwald is physico-chemist. He graduated from Ruhr-University Bochum, Germany, in 1994. In 2012 his habilitation (post-doctoral lecturing qualification) followed at Technical University Kaiserslautern, Germany. Since 2008 he is head of the division Process Analytical Technology at Bundesanstalt für Materialforschung und -prüfung (BAM) in Berlin, Germany. BAM is a senior scientific and technical Federal institute with responsibility to Federal Ministry for Economic Affairs and Energy. Previously, he was research associate and group leader at central services analytics at Merck KGaA, Darmstadt, Germany. His research activities are in the field of quantitative online NMR spectroscopy, other analytical online methods, chemometrics, and sensor automation concepts. He works actively in different industrial, scientific, and standardization working groups.

Presentation: Day 2 - Interlaboratory Comparison of benchtop NMR Spectrometers – Purities at 200 and 10 mmol/L

ABSTRACT: Due to its advantages of being a direct comparison method, quantitative NMR spectroscopy (qNMR) becomes more and more popular in industry. While conventional high-field NMR systems are often associated

with high investment and operational costs, the upcoming market of permanent-magnet based benchtop NMR systems show a considerable option for a lot of applications. The mobility of these systems allows to bring them more closely to the real production environment, e.g. for at-line quality control.

In this work we present an interlaboratory comparison study investigating the qNMR performance of state-of-the-art benchtop NMR spectrometers. Therefore, BAM prepared two samples of a mixture of NMR reference standards tetramethylbenzene (TMB) and tetrachloronitrobenzene (TCNB) at concentration levels of 200 mM and 10 mM. These “ready-to-use” samples were sent to participant laboratories, which performed analysis on their benchtop NMR equipment of different vendors and fields from 43 to 80 MHz. Raw data was reported back and further investigated by using different data analysis methods at BAM.

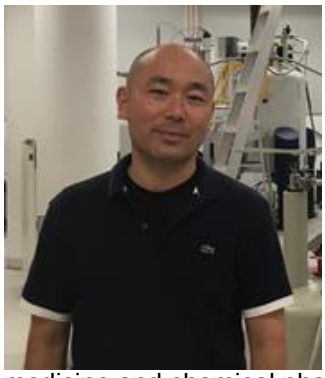
After this very first qNMR comparison study of benchtop NMR spectrometers show promising results, following studies are planned to cover more parts of the qNMR process, e.g. sample preparation and weighing, but also data analysis, as commonly done in similar studies for high-field NMR spectroscopy in industry and metrology.

Klas Meyer, Ph.D.
Research Assistant
Bundesanstalt für Materialforschung und -prüfung (BAM), Germany

Klas received his Ph.D. in Analytical Chemistry from Humboldt Universität zu Berlin in 2017 for the work on “High-pressure NMR spectroscopy” in gas mixtures and process applications. The experimental work was performed in the Process Analytical Technology group of Michael Maiwald at Bundesanstalt für Materialforschung und -prüfung (BAM). After that he joined Magritek GmbH in Aachen as Application Scientist for Benchtop NMR spectrometers. Since end of 2018 he returned to BAM responsible for the research fields of quantitative NMR spectroscopy (qNMR) and process spectroscopy.

Presentation: Day 1 - Compact NMR Spectroscopy: A Versatile Tool for Automated ContinuousFlow Production of Chemicals and Pharmaceuticals

ABSTRACT: Chemical companies must find new paths to successfully survive in a changing environment. The potential of digital technologies belongs to these. Flexible and modular chemical plants can produce various high-quality products using multi-purpose equipment with short downtimes between campaigns and reduce time to market for new products. Intensified continuous production plants allow for difficult to produce compounds. Therefore, fully automated “chemical” process control along with real-time quality control are prerequisites to such concepts and thus should be based on “chemical” information. The advances of a fully automated NMR sensor were exploited, using a given pharmaceutical lithiation reaction as an example process within a modular pilot plant. A commercially available benchtop NMR spectrometer was integrated to the full requirements of an automated chemical production environment such as, e.g., explosion safety, field communication, and robust evaluation of sensor data. It was thereof used for direct loop advanced process control and real-time optimization of the process. NMR appeared as preeminent online analytical tool and allowed using a modular data analysis tool, which even served as reliable reference method for further PAT applications. In future, such fully integrated and intelligently interconnecting “smart” systems and processes can speed up the high-quality production of specialty chemicals and pharmaceuticals.



Toru Miura, Ph.D.
Laboratory Manager of Functional Materials Research Laboratories
FUJIFILM Wako Pure Chemical Corporation, Japan

Toru Miura is Laboratory Manager of Functional Materials Research Laboratories within FUJIFILM Wako Pure Chemical Corporation, and responsible for development of Certified Reference Material (CRM), and NMR related products including qNMR calibration standard and deuterated solvents. He has been with FUJIFILM Wako since 2011. Prior to joining FUJIFILM Wako, he worked as a researcher of the National Metrology Institute of Japan (NMIJ), mainly focusing on development of test conditions for purity determination with 1H qNMR using internal calibration methodology. He is a sub-committee member of the Japanese Pharmacopeia herbal medicine and chemical pharmaceutical related to Quantitative Nuclear Magnetic Resonance (qNMR), drafting committee member for the Japanese Industrial Standard (JIS) K 0138 (General Rules for Quantitative Nuclear Magnetic Resonance Spectroscopy) and an expert of WG24 on qNMR established in ISO/TC34 (Food products). Since 2020, he serves as a member of the United States Pharmacopeia (USP) Expert Panel for qNMR to develop revisions of USP General Chapters <761> and＜1761＞.

Event Moderator: Day 2

Panelist: Day 3 - Roundtable Panel Discussion

Fabrice Moriaud, Ph.D.
Solutions Development Manager
Bruker BioSpin, Biotech Pharma (BPH), Switzerland

Fabrice Moriaud, Ph.D. has extensive experience in leading the development of solutions for the Pharma industry. He is a chemist by training and has an academic background in EPR and NMR.

Presentation: Day 2 - qNMR under GxP – Automated End to End Solution
ABSTRACT: There are many available quantitative NMR methods depending on the application. The most popular ones are those used to calculate potency or purity and concentration. Potency determination by internal standard is used primarily during the stages of drug development due to its low accuracy error. During drug development and manufacturing, when working under GxP, it is critical to comply with 21CFRp11 and the principles of data integrity.

Here, we present a qNMR solution, designed with GxP in mind, with full traceability from initial question to result and detailed control over users and their rights. The software is web-based and can be operated by a variety of users, experts, and non-experts in NMR. Structured around a database, it enables data integrity and management of qNMR methods. These methods are typically designed by method developers, approved by method verifiers and deployed to the laboratory scientists. Efficient analytical request management with instrument time optimization, in a GxP environment, is now also possible for qNMR, and NMR in general, increasing the mainstream adoption of the technique.

Eduardo Nascimento, Ph.D.
Field Application Scientist – AIC (Applied, Industrial & Clinical MR Market Division)
Bruker BioSpin Corp., USA

Eduardo Nascimento holds a doctoral degree in Chemistry with experience in NMR-based metabolomics of biofluids and food. As a Research Associate worked on the development of analytical methods for red meat and beer analysis using HPLC-SPE-NMR and matrix-assisted DOSY. In 2013 joined Bruker do Brazil as an Application Engineer responsible for NMR installation, training, and customer support. Since 2016, he is working as a Field Application Scientist responsible for pre- and post-sales activities focused on TD-NMR and Screener systems (FoodScreener and IVDr) at Bruker BioSpin in the United States.

Presentation: Day 1 - NMR remote analysis for the Food Industry
ABSTRACT: The FoodScreener system, a 400 MHz NMR standardized platform, provides quantitative and statistical analysis for the Food Industry (Juice, Wine, and Honey). In this presentation, the concept behind the quantitative remote analysis will be described. From sample preparation to pdf report, a handful of standard operation procedures are employed which guarantees identical spectra acquisition. More than 50 parameters are quantified and delivered to the customer in less than 20 minutes (Wine-Profiling). The method was developed under ISO-17025 accreditation and extensive validation protocols. Some examples showing how qNMR is applied in the Food Industry will be shown.

G. Joseph Ray, Ph.D.
Adjunct Professor
University of Illinois at Chicago, USA

Dr. Ray received his PhD from Carnegie Mellon in 1968 and after a postdoc at The Ohio State University joined the NMR laboratory at Amoco/British Petroleum.in 1970. In 200, he joined the NMR laboratory at Baxter healthcare and in 2018 joined Professor Guido Pauli's group at UIC. He has used NMR essentially every type of NMR experiment including multinuclear, multidimensional, high-resolution, and solid-state to characterize petroleum, polymers, catalyst, other organics and biologically important systems. Emphasis has been on the quantitative and qualitative analysis of gases, liquids and solids. Both 1D and 2D NMR techniques were developed and used to solve structure - property relationships for diverse business groups including organics, fuels, polyesters, polyolefins, catalysts, zeolites, and biotech related materials. He was a founding member and first President of PANIC Inc, is a member of ValidNMR and is currently Chair of the current USP Quantitative Nuclear Magnetic Resonance Expert Group that is rewriting Chapters <761> and 1761.

Event Moderator: Day 3

Dan Sørensen, Ph.D.
Regional Regulatory Compliance and Enforcement Officer
Health Canada

Dr. Dan Sorensen graduated from University of Copenhagen, Denmark, in 2002 with a PhD in chemistry. The same year, he moved to Canada to continue natural products research and work on discovery of novel antibiotics and anticancer drugs as a Research Scientist at Ecopia Biosciences Inc. in Montréal, Québec.

In 2004, he joined the Merck Frosst Centre for Therapeutic Research, where he held a position as a Senior Research Chemist and conducted research in medicinal chemistry and drug metabolism, primarily structural characterization by NMR, and eventually managed the NMR and LC-MS facility in the medicinal chemistry department.

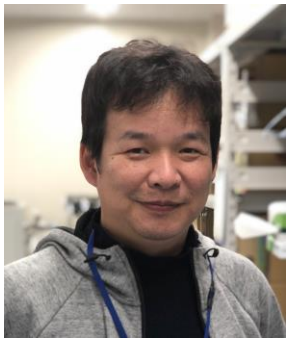
After the Merck Frosst site closure at the end of 2010, he moved to Hamilton, Ontario, to assume a position as an NMR Application Specialist at McMaster University. He took on additional responsibility as a GMP Quality Manager and facilitated the creation of a GMP-compliant NMR contract testing laboratory at McMaster.
In 2017, he went on to work as an Analytical Team Leader and NMR Specialist at Eurofins CDMO Alphora Inc. and was in charge of design, development and validation of analytical procedures for quality control in API manufacturing.

Dr. Sorensen was also an Adjunct Research Professor at Carleton University from 2008 to 2017 and has always been keen on sharing knowledge through coaching, mentoring and workshops.

Dr. Sorensen recently (2020) became as a GMP Inspector at Health Canada and serves on the USP qNMR Expert Panel as an individual expert; not a Government Liaison.

Co-Presentation with Christina Szabo: Day 2 - Proposed Revisions to the USP General Chapters <761> Nuclear Magnetic Resonance Spectroscopy, <1761> Applications of Nuclear Magnetic Resonance Spectroscopy

ABSTRACT: USP General Chapters <761> and <1761> are currently being revised by an Expert Panel. Since the last revision in 2013 there has been a surge in the utilization of NMR as a quantitative tool to determine purity of organic compounds and the composition of mixtures and there is an urgent need to provide current guidance on the use of qNMR for applications within scope of the USP. The purpose of this stimuli article is to propose the adoption of quantitative NMR (qNMR) as a measurement method that is consistent with the already established principles and guidance framework of metrology – the science of measurement and its application. The concepts of Analytical Target Profile (ATP) and Target Measurement Uncertainty (TMU) are introduced as the principal benchmarks to be used for validation of analytical procedures based on qNMR. A holistic understanding of the measurement procedure and system that accounts for uncertainty contributions from specified sources can be used to qualify the NMR instrument and qNMR method using Certified Reference Materials (CRMs) and thus simplify the validation of the final compound-specific analytical procedure. For example, linearity, a traditional method performance characteristic, can be verified as part of the NMR instrument operational qualification (OQ) and may not have to be verified as part of the qNMR method qualification.



Naoki Sugimoto, Ph.D.
Chief of 2nd Section, Division of Food Additives
National Institute of Health Sciences (NIHS), Japan

Dr. Naoki Sugimoto received Ph.D. in Pharmacy from Kanazawa University in 1997 and then joined the National Institute of Health Sciences (NIHS) in Japan. His research has been the structure determination of natural compounds and the development of new quantitative methods for regulatory sciences. He has engaged in the development of qNMR and firstly realized the idea of using qNMR to improve analytical data accuracy in Japan's Specifications and Standards for Food Additives (JSFA) and Japanese Pharmacopeia (JP). His institute stipulated many analytical standards used qNMR for the purity determinations in these Japanese official documents. He was one of the experts to standardized JIS K0138 (qNMR) and is now involved in the international standardization of qNMR as an expert for ISO/TC34/WG24 (qNMR).

Panelist: Day 3 - Roundtable Panel Discussion

Presentation: Day 3 - Measurement of Relative Molar Sensitivity Using the Combination of qNMR and chromatography from the Viewpoint of Regulatory Science
ABSTRACT: The reference materials of target analytes for accurate quantifications have still lacked. This inescapable situation causes a problem in regulatory science. To solve this problem, we designed a new chromatographic analysis technique using relative molar sensitivity (RMS) and using arbitrary reference instead of using each reference material of the analyte. RMS is a coefficient of target analyte relative to an arbitrary reference. The offline combination of 1H qNMR spectroscopy and chromatography plays a role in determining the RMSs of any kinds of analytes to a reference standard cheaply available in the reagent markets. Using this technique, if the accurate RMSs can be determined beforehand, any analytes can be quantified by chromatography with the RMSs and an arbitrary reference. In this presentation, I would like to introduce;

- Advantage of Combination of chromatography and 1H qNMR
- Determination of relative molar sensitivity (RMS)
- Development of reference-free quantification method using RMS
- Application of single-reference chromatography with RMS for regulatory science

Christina Szabo, Ph.D.
Senior Manager of Research
Baxter Healthcare, USA

Dr. Christina Szabo is currently Senior Manager of Research at Baxter Healthcare. She has been aligned with the Renal Care business of Baxter since 2018 and leads Renal R&D Analytical Chemistry and Stability. Prior to that she was Director of Research of Advanced Chemistry and Investigations in the Corporate Analytical Center of Excellence that supported investigations and changes to existing products and development of new products for all of Baxter's businesses by application of Nuclear Magnetic Resonance and Mass Spectrometry, Extractables and Leachables, and Elemental Impurities. She had also completed a half-year rotation in Global Regulatory Affairs. Her research started in the area of natural products while studying at the University of Hawai'i, where she isolated compounds and elucidated structures of bioactive components in marine organisms. During her graduate studies at the University of Illinois at Urbana-Champaign she probed relationships between local protein conformations and NMR properties using quantum chemistry and experimental NMR. This then led to further computational studies in the area of rational drug design and quantitative structure activity relationships. Her experience has grown to include structure elucidation of peptides, proteins, polysaccharides and small organic molecules, and analytical method validation. One of Dr. Szabo's areas of particular interest is to work on approaches that are compliant with regulations and streamlined in a scientifically justified manner. She aims to apply her background in science and experience in industry in ways that will ultimately benefit patients and public health.

Event Moderator: Day 1

Co-Presentation with Dan Sørensen: Day 2 - Proposed Revisions to the USP General Chapters <761> Nuclear Magnetic Resonance Spectroscopy, <1761> Applications of Nuclear Magnetic Resonance Spectroscopy

ABSTRACT: USP General Chapters <761> and <1761> are currently being revised by an Expert Panel. Since the last revision in 2013 there has been a surge in the utilization of NMR as a quantitative tool to determine purity of organic compounds and the composition of mixtures and there is an urgent need to provide current guidance on the use of qNMR for applications within scope of the USP. The purpose of this stimuli article is to propose the adoption of quantitative NMR (qNMR) as a measurement method that is consistent with the already established principles and guidance framework of metrology – the science of measurement and its application. The concepts of Analytical Target Profile (ATP) and Target Measurement Uncertainty (TMU) are introduced as the principal benchmarks to be used for validation of analytical procedures based on qNMR. A holistic understanding of the measurement procedure and system that accounts for uncertainty contributions from specified sources can be used to qualify the NMR instrument and qNMR method using Certified Reference Materials (CRMs) and thus simplify the validation of the final compound-specific analytical procedure. For example, linearity, a traditional method performance characteristic, can be verified as part of the NMR instrument operational qualification (OQ) and may not have to be verified as part of the qNMR method qualification.

Jaap Venema, Ph.D.
Executive Vice President and Chief Science Officer
United States Pharmacopeia (USP), USA

Jaap Venema, Ph.D., Executive Vice President and Chief Science Officer (CSO) for USP, leads the organization's scientific strategy and development of quality standards for medicines, dietary supplements, food ingredients and healthcare practice. Dr. Venema oversees implementation of the USP Science Quality Framework, which grounds quality standards development in pharmaceutical science to increase public trust in medicines. He guides exploration of emerging technologies that may inform future quality standards; serves as Chair of USP's Council of Experts; and oversees collaborations with other pharmacopeial and scientific groups. With more than 25 years' experience in global research and development, as well as academic research, Dr. Venema previously served in scientific leadership positions at Solvay and AbbVie (formerly Abbott Laboratories). A native of the Netherlands, Dr. Venema earned a master's degree in Chemistry from the Free University of Amsterdam, and a Ph.D. in Biochemistry and Molecular Biology from Leiden University in the Netherlands.

Presentation: Day 1 - Opening: USP Introduction

Steven Walfish, MBA, M.S.
Principal Science & Standards Liaison
United States Pharmacopeia (USP), USA

Mr. Walfish is Principal Science & Standards Liaison at United States Pharmacopeia (USP) responsible for the Statistics Expert Committee. Prior to this role Mr. Walfish was Principal Statistician at Becton Dickinson in Franklin Lakes, NJ responsible for supporting continuous improvement efforts and process development for worldwide operations. Mr. Walfish has held roles at GE Healthcare, Human Genome Sciences and Chiron. Steven was President of Statistical Outsourcing Services, a consulting company that provides statistical analysis and training to the FDA regulated industries.

Mr. Walfish brings over 30 years of industrial expertise in the development and application of statistical methods for solving complex business issues. Steven has experience applying statistical methods to analytical method verification and validation and stability analysis.

Mr. Walfish holds a Bachelors of Arts in Statistics from the University of Buffalo, Masters of Science in Statistics from Rutgers University and an Executive MBA from Boston University.

Presentation: Day 2 - Analytical chemistry validation and qNMR methods

ABSTRACT: The objective of this talk is to get the qNMR community to think about how validation and qualification fits the USP validation paradigm. USP has published in PF two new chapters on qNMR. This talk supports the proposed USP <761> and <1761> chapters with a focus on USP <1225> and <1220>. Emphasis will be on the validation parameters such as accuracy and precision in light of the qNMR technology.