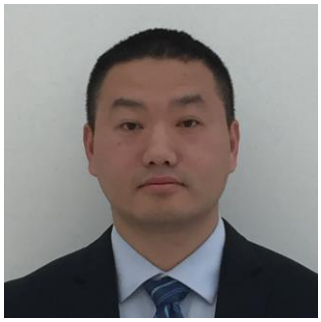
Speaker Biographies

(Listed alphabetically by last name)
November 16-18, 2021



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 research the quality of complex drug products.

Presentation: Day 1 - High Resolution ^{19}F qNMR Reveals Mass-balanced Drug Phase Distribution in Oil-in-Water Nano-Emulsion Formulations

高分辨率 ^{19}FqNMR 揭示了水包油纳米乳液制剂中质量平衡的药物相分布

ABSTRACT: An oil-in-water (o/w) nano-emulsion (NE) is composed of oil globules stabilized by surfactant and dispersed in an aqueous phase. Nano-emulsions are used to formulate hydrophobic active pharmaceutical ingredient (API) and typically allow higher dosage strengths and better content uniformity. One knowledge gap for NE drug products is the lack of information about API phase distribution in the oil (o), surfactant (s) and water (w) phases, challenging to measure non-invasively in emulsions, especially for an API in (s) phase, the interface between the dispersed phase (o) and the continuous phase (w). Here, high resolution 19F quantitative NMR (qNMR) spectroscopy was applied directly on a NE drug product (DP) with difluprednate (DFPN) as the API. Specifically, the resolved chemical shifts of the F28 nucleus in DFPN depended on the type of shielding molecules in each phase. The integration of F28 peaks robustly yielded mass-balanced quantitative distribution of 1.8%, 35% and 59% per label claim (LC), for (w), (s) and (o) phases, respectively. Furthermore, the dilution dependent F28 peak line-broadening was characteristic of dynamic exchange between NE and micro-emulsion (ME) globules, suggesting that API availability could be quickly achieved using an o/w NE formulation.

Lei Chen
Chief Pharmacist
Chinese Pharmacopeia, China

Lei, chief pharmacist, works in the General Chapters, Excipients and Packaging Division of Chinese Pharmacopoeia, mainly engaged in the management of pharmaceutical excipients and pharmaceutical packaging standards in the Chinese Pharmacopoeia.

陈蕾，主任药师，现任职于国家药典委员会通则辅料包材处，主要从事《中国药典》药用辅料和药包材标准的管理工作。

Presentation: Day 2 - Considerations of applying NMR in the quality control of pharmaceutical excipients – ChP perspective

中国药典对核磁共振在药用辅料质量控制中应用的考量

Andrew Coy, Ph.D.
CEO, Magritek Limited, New Zealand

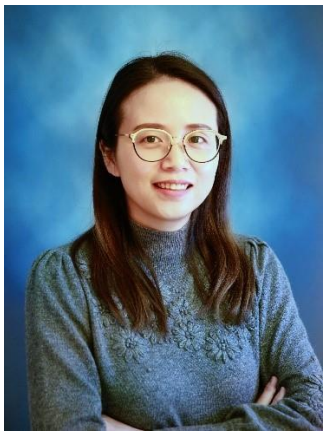
Dr Andrew Coy is the CEO of Magritek since its inception in 2004. He has a PhD in Physics from Massey University in New Zealand where he worked on pulsed field gradient NMR with Professor Sir Paul Callaghan. Andrew has led Magritek from its foundation as a University spin out company to its current position as a highly successful manufacturer and the global leader in Benchtop NMR Spectroscopy with the family of 90 MHz, 80 MHz and 60 MHz Spinsolve NMR spectrometers. Andrew is a 2011 Sir Peter Blake Emerging Leader and was a member of the team that won the 2010 Prime Minister's Science Prize in New Zealand.

Presentation: Day 2 - Latest developments in qNMR and Benchtop NMR spectroscopy

定量核磁及台式核磁仪最新进展

ABSTRACT: The sensitivity and resolution of Benchtop NMR spectrometers has been steadily improving over the years as more and more powerful magnets and electronics are made available. A key feature of Benchtop NMR spectrometers is the ability to deploy them at the point of need where the chemist is working. Quantitative NMR methods (qNMR) work very well on Benchtop NMR as long as the spectrometer has sufficient performance for the application being addressed. In this presentation we will show a number of applications and examples of qNMR methods, including on the new Spinsolve 90 MHz and Multi X spectrometers. We will also show how high performance solvent suppression can enable more applications on samples measured without preparation in a deuterated solvent increasing the ease of use and versatility of these spectrometers. The importance of method reproducibility and automation will also be presented along with the need for automatic nuclei switching featured on the new Multi X combined with an autosampler and one click qNMR software implementation.

随着越来越多强大的磁铁和电子设备的出现，桌面核磁共振波谱仪的灵敏度和分辨率在过去几年中稳步提高。桌面核磁共振波谱仪的一个关键特征是它能够在化学普通实验室运行工作。桌面核磁共振波谱仪有足够的性能可以让定量 NMR 方法（qNMR）在桌面 NMR 上应用得非常好。在本演示中，我们将展示一些 qNMR 方法的应用和示例，包括新的 Spinsolve 90 MHz 和多 X 波谱仪。我们还将展示高性能溶剂抑制如何能够在无氘代溶剂样品上实现更多应用，从而增加波谱仪的易用性和多功能性。新的 Multi-X 仪器结合自动取样器结合，实现方法再现性和自动化应用，自动切换不同核的检测，以及一键式 qNMR 软件实现定量分析，也将在本次演示中介绍。



Huiwen Deng, M.Sc.
Pharma Business Development Manager
Bruker BioSpin, China

Huiwen has a MSc in Radiophysics from East China Normal University, and she studied metabolism NMR and other liquid/solid NMR technology in Shanghai Key Laboratory of Magnetic Resonance. She worked in Wuxi AppTec for 5 years, becoming proficient in structure elucidation. In the next 5 years, she worked in DSM Nutritional Products, and developed multiple qNMR methods to assist process research and authenticity identification. Then she worked in China Novartis Institutes for Biomedical Research for 3 years, and established NMR based fragment screening and optimization methods to support innovative drug discovery. She joined Bruker in 2020 as Pharma business development manager, responsible for magnetic resonance products promotion in pharmaceutical industry.

邓惠文，制药市场拓展经理，布鲁克拜厄斯宾

惠文是华东师范大学无线电物理学硕士，在上海市磁共振重点实验室从事体外组织代谢和其他固液核磁共振的应用研究。她在药明康德新药开发有限公司工作了 5 年，从事小分子核磁共振分析工作，积累了大量结构解析经验。随后 5 年她在帝斯曼（中国）营养产品部，负责营养品工艺研发以及天然产物提取创新项目的分析工作，期间建立了多种定量核磁分析方法辅助工艺研发以及产品真实性鉴定。之后她在诺华（中国）生物医学研究中心工作的 3 年中，负责肿瘤和肝脏项目的药物早期研发至临床前阶段的分析工作，建立了基于片段的核磁共振筛选及优化方法助力先导化合物的发现。2020 年初惠文加入布鲁克（中国），担任制药市场拓展经理一职，负责磁共振相关产品在中国制药市场的推广工作。

Presentation: Day 2 - NMR Landscape from Benchtop to Ultra High Field

从台式到超高场的核磁共振应用格局

ABSTRACT: Nuclear magnetic resonance spectroscopy is an ideal analytical technique that allows for non-invasive and non-destructive plus quantitative analytical investigations into molecular structure, dynamic processes and chemical reactions etc. Bruker is the industry leader in the manufacturing of unique high-performance magnetic resonance instruments. The Ultra-high field NMR (1.1/1.2 GHz) is one of the only analytical technologies that allow for advanced research on structural functional biology of proteins and protein complexes including intrinsically disordered proteins (IDPs). The Fourier 80, an easy-to-use, compact benchtop system with high-performance has been designed for the highest data quality and stability. Quantification is required in the drug discovery, development, and manufacturing. Inherently quantitative, NMR enable rapid and straightforward quantification of solids and liquids without the need of method development or response factor calculations. Bruker has a suite of tools designed to simplify workflow and enhance productivity to check the concentration of ligands for screening, measure the potency of APIs, determine in-situ yields, quantify polymorph and amorphous form, or check the filling of your vials and syringes. And now efficient analytical request management with instrument time optimization, in a GxP environment, is also possible for qNMR, and for NMR in general, from 1.2 GHz all the way down to 80 MHz, increasing the mainstream adoption of the technique. Bruker-Mestrelab new tools for potency/purity determination streamline this process with a fully automatic workflow from experiment submission to report, making it the ideal solution for both experts and non-experts.

核磁共振是一种理想的分析技术，它可以对分子结构、动态过程和化学反应等进行非侵入性、非破坏性且定量的分析研究。布鲁克是制造高性能磁共振谱仪的行业领导者。AVANCE NEO 1.1 和 1.2 GHz 超高场 NMR 系统可用于蛋白质和蛋白质复合物（包括固有无序蛋白）的功能结构生物学研究。而简单易用的 80 MHz 的 Fourier 台式波谱仪，具有出色的线型、高分辨率和灵敏度，可以保证最高的数据质量和稳定性。定量分析在药物发现、研发与生产阶段是必不可少的。由于核磁具有天生的定量性，可以对固液体化合物进行快速且直接的定量而无需方法的开发或

响应因子的计算。布鲁克开发了一系列解决方案，旨在简化工作流程和提高生产力，在检查筛选配体的浓度，测定 API 的含量，确定反应的产率，定量多晶型/无定形态，以及非接触式称重等应用中发挥着重要的作用。而现在高效的分析请求管理与仪器时间优化也可用于 qNMR，不论是 在 1.2 GHz 超高场还是 80 MHz 低场核磁谱仪上均可实现，并可在 GxP 环境下工作，增加了该技术更广泛的应用范围。布鲁克与 Mestrelab 共同开发的用于含量/纯度测定的新工具简化了工作流程，实现了从实验提交到最终报告的工作流程全自动化，对核磁专家和非专家们都不失为理想之选。

Xiaojuan Deng, Ph.D.
Team leader of the composition analysis department
The Analysis and Testing Center of Tianjin University, China

Dr. Deng graduated from Tianjin University with a bachelor's, master's and PhD in Chemical Engineering, Pharmaceutical Science and Materials Science, respectively. Now as a senior engineer, she is the team leader of the composition analysis department, the Analysis and Testing Center of Tianjin University. During the long-term responsibility in instrument management and related education of NMR, she has published more than 20 papers in journals including Trends in Analytical Chemistry, Chemical Engineering Journal and Food Chemistry etc., and has obtained four authorized invention patents. She headed a number of projects such as the National Natural Science Foundation of China, the independent innovation fund of Tianjin University and the educational reform project. She has also participated in the formulation of a qNMR industry standard. She teaches the Laboratory Exercise in Instrumental Analysis, Material Engineering Practice for students, and is responsible for the construction of liquid NMR online training system. As the first person to complete, she won a youth award of science and technology award of China Association for Instrumental Analysis (CAIA) in 2017.

邓小娟, 天津大学分析测试中心成分分析室负责人，高级工程师，于天津大学化工学院、药学院、材料学院分别获得本硕博学位。任职以来主要负责核磁等大型仪器的管理维护及相关教学培训等工作。近年来发表论文二十余篇，其中以第一作者在 Trends in Analytical Chemistry，Chemical Engineering Journal，Food Chemistry 等期刊发表多篇 SCI 论文，获得授权发明专利四项，主持国家自然科学基金青年基金、天津大学自主创新基金、教改项目等多项课题研究，参与一项定量核磁行业标准的制定。承担仪器分析的实验室体验、材料工程实践等课程中核磁部分的教学，负责液体核磁线上培训体系的建设。作为第一完成人获得 2017 年度中国分析测试协会科学技术（CAIA）奖青年奖一项。

Presentation: Day 2 - (q)NMR education in Tianjin University

（定量）核磁基础教学实践——以天津大学为例

ABSTRACT: With the development of NMR technology and the requirement of advanced scientific research, quantitative NMR is increasingly used in supporting technical innovation. It is also necessary for current NMR education to keep pace with the times and constantly update content of the courses. This presentation will introduce the exploration of qNMR education in Tianjin University, including the overview of NMR education, development and some application examples of qNMR in teaching.

随着核磁技术的发展和前沿科研的需求，定量核磁共振技术的应用范围越来越广泛，相关核磁教学课程也有必要与时俱进，不断更新教学方法和内容。本主题报告将以天津大学为例，介绍（定量）核磁基础教学实践与人才培养的一些探索，包括核磁教学实践现状，定量核磁教学内容的持续改进与一些典型案例分析等。

Yukihiro Goda, Ph.D.
Director General of National Institute of Health Sciences (NIHS), Japan

Dr. Yukihiro Goda graduated from the University of Tokyo in 1980 and earned his PhD from the Department of Pharmaceutical Sciences, the University of Tokyo in 1985. From 1986, he was a Researcher and Senior Researcher at the Division of Food Additives of the National Institute of Health Sciences (NIHS) and in 1996 became the Section Chief of the Division of Foods. In 2001, he was promoted to the Head of the Division of Pharmacognosy, Phytochemistry and Narcotics, and in 2013, he became the Head of the Division of Drugs, NIHS. From 2018 to 2020 he was the Deputy Director General of NIHS. Presently Dr. Goda is the Director General of NIHS. His expertise includes regulatory science of pharmaceuticals, natural medicines, illegal drugs, food colorants, borderline products between foods and drugs, and natural product chemistry. Throughout his career, Dr. Goda has published more than 450 research papers. Since 2008, he has been actively promoting the development and standardization of quantitative NMR, particularly in the area of natural products of the Japanese Pharmacopoeia (JP). Owing to Dr. Goda's efforts, JP included qNMR in the section of crude drugs since 2012. Thirty-seven monographs utilizing qNMR are listed in the 18th Edition of JP. Since 2002 Dr. Yukihiro Goda had been the Chair of the Expert Committee of Natural Medicines and in 2014 became the Chair of the Expert Committee of Chemical Drugs in the Japanese Pharmacopoeia. Currently, he is the Chair of the JP Standing Committee.

Presentation: Day 1 - Introduction of the Committee for the Development of qNMR Technology in Japan (qNMR-J)

日本定量核磁技术发展委员会

ABSTRACT: The Committee for the Development of qNMR Technology in Japan (qNMR-J) was established on October 31, 2018, to carry out activities for the advancement and dissemination of quantitative methods using NMR (qNMR). qNMR has recently been utilized to determine the absolute amounts of organic molecules with metrological traceability since signal intensity is directly proportional to the number of each nucleus in a molecule. qNMR for determining the purity or content of chemicals has been adopted into the official standards such as the Japanese Pharmacopoeia and the Specifications and Standards for Food Additives. In addition, the general rules for qNMR have been standardized in the Japanese Industrial Standards (JIS). qNMR will indeed become one of the general methods for quantitation that any researcher or practitioner accepts and will also be utilized in various fields if we continue the active collaboration through activities such as infrastructure development, information exchanges, facility tours, and personal networking, and the standardization and harmonization of the methodology related to qNMR. In our view, qNMR-J has been established to serve as a window for accessing and disseminating information inside and outside Japan and to become a foundation for free and open information exchange and educational activity to support the next-generation quantitative analysis. In this presentation, I will introduce the qNMR-J, focusing on the activities conducted so far.

Lan He, Ph.D.
Director of Chemical Drug Division
Institute for Chemical Drug Control
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: Day 1 - Application of qNMR in Drug Quality Control

定量核磁在药品质量控制中的应用

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 application of proton qNMR in characterizing the assay and impurity of APIs; application of 19F qNMR in characterizing fluoro-containing APIs and application of 13C qNMR in characterizing long chain fatty-acids.

Yong Jiang, Ph.D.
Professor
Dean of Department of Natural Medicines Chemistry
School of Pharmaceutical Sciences
Peking University, China

Dr. Yong Jiang currently acts as the full professor and the dean of Department of Natural Medicines Chemistry, School of Pharmaceutical Sciences, Peking University. She received her Ph.D. from Peking University in 2003. Then she worked as a postdoctoral fellow in The Institut de Recherche Pierre Fabre, France. Her major research interests focus on the studies of the effective components, mechanisms, and quality control of traditional Chinese medicines. She has authored 200+ papers in the international peer-reviewed journals, such as Adv Sci, Med Res Rev, Org Lett, Anal Chem, Lab on Chip, J Biol Chem, J Nat Prod. She has been authorized for 30 patents. She was the second winner of a Second-Class Prize of the State Scientific and Technological Progress Award. She was elected into the projects of “National Science Fund for Distinguished Young Scholars” and “New Century Excellent Talent in University from Ministry of Education of China.” She serves as the editorial board member for the journals such as Acta Pham Sin B, Pharmacol Res, Chem Biodivers, and so forth.

姜勇，北京大学药学院新体制长聘教授、博士生导师、天然药物学系主任，国家自然科学基金首批优秀青年基金获得者、教育部新世纪优秀人才。兼任国家野生植物保护协会肉苁蓉保育委员会秘书长、中国仪器仪表学会药物质量分析与过程控制分会常务理事，北京药学会药物分析专委会副主任委员，北京中医药学会临床合理用药评价专业委员会副主任委员等；Acta Pham Sin B，Pharmacol Res, Chin Chem Lett，Chem Biodivers, 药学学报、中国中药杂志等杂志编委、青年编委。 研究方向为中药、天然药物活性成分与作用机制，中药质量控制与评价研究。先后

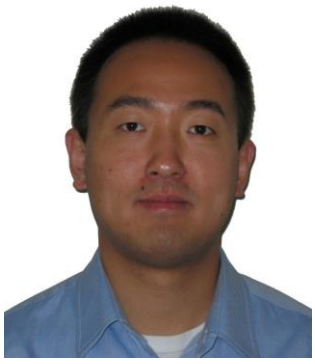
主持国家重点研发计划、国家重大新药创制专项、国家自然科学基金等课题 20 余项；共发表研究论文 280 余篇，其中 SCI 论文 200 篇；申请授权专利 30 项；负责参与了 10 余项创新药物研发，获得新药证书 2 个；建立的 20 余项标准被《中国药典》及国家药品标准收载；研究成果获得了国家科技进步二等奖 1 项以及省部级科技奖励 9 项。

Presentation: Day 2 - Quality analysis of traditional Chinese medicines based on qHNMR

基于 qHNMR 的中药质量分析

ABSTRACT: The quality of traditional Chinese medicine (TCM) is closely related to its chemicals contained, but complex and diverse ingredients are existed in TCM, which makes the quality control being difficult and a bottleneck in the process of modernization and globalization of TCMs. NMR technique is a versatile technology, which was mainly used to resolve the structures of compounds, but in recent years, it has been widely used for the metabolomics and traditional herbal medicine quality analysis. qNMR is an unbiased detection tool, which can detect all the metabolites in a single run, and make the compounds with different structural types, polarities and molecular weights present in a same spectrogram. This method has also the advantages of simple sample preparation process, fast detection process, high stability, good reproducibility and sample easy to recycle, which are particularly suitable for the detection of TCMs with the complex constitution. Moreover, this technology does not need the references of the determined components, which supplies a solution for the problem of reference scarcity in the quantitative analysis of TCMs. In this paper, we used Dictamni Cortex, Magnoliae Officinalis Cortex, Vignae Semen, Cistanches Herba, and Cinnamomi Cortex as samples to illustrate the application of qHNMR technology in the quantitative and qualitative analysis of TCMs.

中药的质量和它所含的化学成分具有密切关系，但是中药成分复杂、结构多样，使得中药的质量控制一直是一个难题，也是中药现代化和国际化的一个瓶颈。NMR 是一个通用技术，原来主要用于化合物的结构鉴定，但近些年已经越来越广泛用于中药和植物药的质量分析和代谢组学分析。qNMR 是一项无偏向的检测技术，能够在一次检测中检测所有的代谢物，使得不同结构类型、不同极性、不同分子量的化合物都能在一张谱图呈现出来。这项技术还具有简单的样品处理、快速的分析过程、稳定和重现性好、样品易回收等特点，适合于含有复杂化学成分的中药分析。另外，这项技术不需要待测物标准品，为中药定量分析中对照品缺乏的难题提供了一种新的解决方案。本文，我们将以白鲜皮、功劳木、赤小豆、肉苁蓉、肉桂等为例，介绍 qHNMR 在中药定性和定量分析中的应用。



Jie Liu, M.Sc.
Associate Director, Scientific Affairs
USP, China

Mr. Liu graduated from Lanzhou University majored in organic chemistry and obtained his master's degree on medicinal chemistry from Chinese Academy of Medical Sciences. He joined USP-China in 2008 and his current role in scientific affairs is to grow USP scientific voice and presence globally. He has extensive experience in the areas of food fraud mitigation, dietary supplement standards and regulations, nitrosamine risk assessment, and analytical procedure lifecycle. He's coauthored over 10 peer-reviewed articles and patents, and has been invited to present in numerous conferences. Prio to USP, Jie was a medicinal chemist in Celera and Novartis.

Moderator: Day 2

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

Dr. Yang Liu is quantitative NMR (qNMR) expert and Incubated Projects Manager in USP's Product Quality & Analytical Method Department. Dr. Liu collaborates with scientific experts to bring more qNMR applications into USP, including high-field and benchtop qNMR applications, development of computer-aid methodologies, and compendial qNMR applications. Dr. Liu is a guest scientist at the National Institute of Standards and Technology (NIST), concentrating on the evaluation of benchtop (q)NMR instrumentation pharmacopeial and forensic applications. Dr. Liu is working with the USP qNMR Expert Panel for updating General Chapters <761> and <1761>. Dr. Liu as USP expert, has been also invited by ISO Working Group (ISO/TC 34, WG 24), in reviewing ISO/DIS24583, qNMR standards. Dr. Liu's scientific expertise includes qNMR method development and validation for measurement. He has published over 20 peer-reviewed articles and has been an invited speaker or workshop organizer for numerous scientific conferences.

Moderator: Day 3

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

Toru Miura is a principal scientist of Functional Materials Research Laboratories within FUJIFILM Wako Pure Chemical Corporation. He has been with FUJIFILM Wako Pure Chemical Corporation 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 Certified Reference Materials using mass balance, freezing point depression method and quantitative NMR (qNMR). He is a working group member of the Japanese Pharmacopeia herbal medicine and chemical pharmaceutical related to qNMR methodology, a 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 Expert Panel for qNMR to develop revisions of USP NMR General Chapters <761> and＜1761＞.

Presentation: Day 1 - Practice of Life Cycle Approach to Method Validation for QNMR Analytical Procedure

USP <761> 核磁共振通则中引入生命周期方法用于定量核磁方法验证

ABSTRACT: USP General Chapters ⟨761⟩ Nuclear Magnetic Resonance Spectroscopy and ⟨1761⟩ Applications of Nuclear Magnetic Resonance Spectroscopy are currently being revised by the quantitative nuclear magnetic resonance (qNMR) Expert Panel. One major purpose of this revision is to align with the proposed new USP General Chapter: The Analytical Procedure Lifecycle <1220>, which is aligned with Analytical Quality by Design (AQbD) concepts and offers a lifecycle approach to method validation, method transfer and verification of analytical procedures. In this presentation, I will discuss the outline of the practice of life cycle approach to method validation for qNMR analytical procedure, focusing on the concepts of Analytical Target Profile (ATP), Quality Risk Management (QRM), instrument qualification and evaluation of measurement uncertainty.

Jeff Moore, Ph.D.
Senior Director, Scientific Affairs & Strategy
USP, USA

Dr. Jeff Moore is the head of Scientific Affairs & Strategy at US Pharmacopeia. He holds a PhD in food chemistry from the University of Maryland and a BS from Michigan State University. He leads a team of scientists responsible for growing USP scientific voice and presence globally and led USP's COVID-19 treatments initiative in 2020. He is the author of the most cited manuscript on food fraud and led the development of USP's Food Fraud Database in 2012. He has extensive experience in the areas of risk-based systems approaches to food safety, food authenticity testing, non-targeted testing, food fraud mitigation, food chemical safety, and international food additive regulations. He serves on the EU-China SAFE and EU Food Integrity advisory boards and University of Maryland's Global Leadership Council. He has authored more than 30 manuscripts in peer reviewed journals and book chapters. Prior to joining USP Jeff was a research scientist at Nestlè.

Presentation: Day 2 - The qNMR Method in the Remdesivir Toolkit and beyond

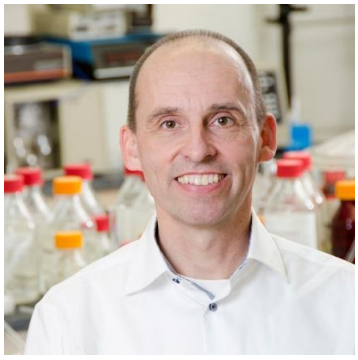
定量核磁在 USP 瑞德西韦方法中的应用及展望

ABSTRACT: This presentation will provide an overview of USP's recently published Methods to Assist in Detecting Falsified Remdesivir with a focus on lessons learned from the qNMR method development and validation work.

Kevin Moore, Ph.D.
Senior Manager, Pharmacopeial Collaboration
USP, USA

Dr. Moore currently holds the position of Sr. Manager, Pharmacopeial Collaboration at the United States Pharmacopeia. Dr. Moore's primary function is to manage technical, scientific and strategic aspects related to USP's harmonization and collaborative activities with global pharmacopeias. Specific roles include managing USP's technical activities in the Pharmacopeial Discussion Group (PDG), coordinating standard development with individual pharmacopeias for scientific collaboration, collaborating with WHO through the International Meeting of the World Pharmacopeias, and supporting ICH initiatives through USP's observer status to the ICH Assembly. Previously, Dr. Moore worked for USP as a Scientific Liaison and Manager for Pharmacopeial Harmonization in the Excipients Group. Dr. Moore has nearly 20 years' experience in the fields of Compendial Science and Pharmaceutical Analytical Support. Dr. Moore holds a Ph.D. in Inorganic Chemistry from the University of Pennsylvania and a B.S. in Chemistry and Biology from LeMoyne College.

Moderator: Day 1



Guido Pauli, Dr. rer. nat., FAPA
Norman R. Farnsworth Professor of Pharmacognosy
Department of Pharmaceutical Sciences
Director, Pharmacognosy Institute
Associate Director, Institute for Tuberculosis Research
University of Illinois at Chicago, UIC College of Pharmacy, USA

Trained as a pharmacist with specialization in pharmaceutical analysis, Dr. Pauli holds a doctoral degree (Dr. rer. nat.) in pharmacognosy. He is currently the Norman R. Farnsworth Professor of Pharmacognosy, Director of the Pharmacognosy Institute, and Associate Director of the Institute for Tuberculosis Research (ITR) at the University of Illinois at Chicago College of Pharmacy. His basic and translational research project involve bioactive natural products (NPs) from diverse sources, particularly plants and actinomycetes, NP technologies, dietary supplements, clinical and dental intervention materials, drug discovery, the NAPRALERT database, and institutional training programs. Main research interests encompass bioanalytical methodology and interdisciplinary evaluation of plant-derived natural health products, anti-TB hit-to-lead development, dental biomodifiers, and pharmaceutical analysis. He has pioneered the development of innovative approaches including quantitative NMR and countercurrent separation, to advance rigor and reproducibility as well as identification of bioactive principles, respectively. Dr. Pauli seeks to enhance the understanding of natural products as health products and sources of new drugs. He is dedicated to the advancement of pharmacopoeial methods through volunteer work at the United States Pharmacopoeia (USP), where he serves as Chair of the Non-botanical Dietary Supplements Expert Committee and the Modernization of Analytical Methods Joint Subcommittee. His academic track record includes mentoring of 20 Ph.D. students, 27 postdocs, 17 visiting scientists, and ongoing international collaborations. His 250+ peer-reviewed publications have received 10,000+ citations (Scopus) and earned an h-index of 51 in Scopus and 63 in Google Scholar.

Presentation: Day 1: Advancement and Persistence in quantitative NMR (qNMR)

定量核磁发展及远景

ABSTRACT: Since George Hanna at the U.S. FDA started pioneering the development of modern quantitative NMR (qNMR) in mid-1980s, the method has grown into a universal, highly capable, and metrology-quality technique with wide applications, well beyond pharmaceutical and chemical analysis. Two subsequent “waves” of foundational work in Europe, U.S., Australia, and Japan until the early-2010s laid the scientific ground for a modern toolbox of qNMR methods. The quasi-exponentially growing qNMR literature as well as often publicly inaccessible proprietary data provide strong experimental evidence for the favorable performance of NMR as a primary analytical tool.
This presentation summarizes both recent key advancements in qNMR methodology and aspects that persistent as inconsistencies, difficult questions, and challenges for further qNMR development. On the advancement side, covered topics involve achievable qNMR uncertainties, experimental evidence, and community building, which provide strong collective support for qNMR as a quantitative analytical technique. Topic related to persistence involve naming and terminology, analytical complexity, reproducibility, and long-term habits in qNMR.
The overarching goal of this presentation will be to provide both global perspectives and detailed examples for the current standing of qNMR as well as for needs and opportunities for its further development.

Chen Peng, Ph.D.
Vice President of Business Development for North America and Asia
Mestrelab Research S.L., USA

Dr. Chen Peng is the Vice President of Business Development for North America and Asia since he joined Mestrelab Research S.L. in May 2008. He got his B.Sc. in Organometallic Chemistry from Wuhan University, China. He obtained his PhD from the Shanghai Institute of Organic Chemistry with a dissertation work on computer-assisted structure elucidation for organic compounds and natural products using 1D and 2D NMR data. He did post-doctoral research work on selective excitation NMR spectroscopy in Prof Geoffrey Bodenhausen's group in the National High Magnetic Field Laboratory (Tallahassee, FL). He had worked as the main developer of NMR-SAMS, the first commercial software product for structure elucidation, in Spectrum Research, based on his PhD work. He also worked as a senior software product developer for Felix in Molecular Simulation Inc (Accelrys). He worked as a senior software developer and product manager for NMR related tools in the KnowItAll software package of Bio-Rad Informatics. Since his tenure in Mestrelab, Chen enjoys traveling between states/countries to present Mnova to universities and companies onsite or at tradeshows. He also brings back feedback and custom development projects to the Development Group. Occasionally he jumps on writing Mnova scripts for customers with special needs, and actually a few of those scripts were further developed to Mnova plugins such as qNMR and Screen.

自 2008 年 5 月加入 Mestrelab Research S.L. 以来，彭琛博士一直担任北美和亚洲业务发展副总裁。他获得武汉大学金属有机化学学士学位，并获得上海有机化学研究所博士学位，博士论文工作是使用 1D 和 2D NMR 数据对有机化合物和天然产物进行计算机辅助结构解析。在国家强磁场实验室（佛罗里达州塔拉哈西）的 Geoffrey Bodenhausen 教授课题组从事选择性激发核磁共振谱博士后研究工作。 基于他博士期间的工作，他曾在 Spectrum Research 担任 NMR-SAMS（第一个用于结构解析的商业软件产品）的主要开发人员。他还在 Molecular Simulation Inc (Accelrys) 担任 Felix 的高级软件产品开发人员。他曾在 Bio-Rad Informatics 的 KnowItAll 软件包中担任 NMR 相关工具的高级软件开发人员和产品经理。 自从在 Mestrelab 任职以来，彭博士在各州/国家之间现场或展会上向大学和公司展示 Mnova 并将反馈带回给开发团队。偶尔他也会为有特殊需求的客户编写 Mnova 脚本，其中一些脚本被进一步开发为 Mnova 插件，例如 qNMR 和 Screen。

Presentation: Day 2 - From Requests to Results: Recent Progresses on the Development of MDrive for qNMR

从需求到结果：qNMR 软件 MDrive 开发的最新进展

ABSTRACT: In order to further improve the efficiency of the analytical chemistry, we have been developing MDrive, a web-based solution that can be integrated into GxP or non-GxP informatics environment to provide semi/fully automated workflows for sample submission and recording or request of analytical services. Mdrive also allows administrating instruments, managing experiments and SOPs, automating acquisition and processing, visualizing the results, and storing the raw data and reports for legacy, compliancy or further re-use. This talk will focus on its application to automated qNMR analysis, using the Mnova qNMR software tools to compute the concentration or purity of samples, in a GxP environment where compliance tools such as audit trail and signature are provided.

为了进一步提高分析化学的效率，我们一直在开发 MDrive，一种基于网络的解决方案，可以集成到 GxP 或非 GxP 环境下，为样品提交和记录提供半/全自动工作流程分析服务。 Mdrive 还允许管理仪器、管理实验和 SOP、自动化采集和处理、可视化结果以及存储原始数据和报告以供留存、合规或重复使用。 本报告将重点介绍其在自动化 qNMR 分析中的应用，在 GxP 环境中使用 Mnova qNMR 软件工具计算样品的浓度或纯度，其提供的合规性工具，例如审计跟踪和签名。

Wenbin Shen
Director of the Analysis and Testing Center
China Pharmaceutical University, China

Shen Wenbin, graduated from the Chemistry Department of Nanjing University in 1987, majoring in organic chemistry. He is currently the director of the Analysis and Testing Center of China Pharmaceutical University, Associate Research Fellow. The chairman of the Nuclear Magnetic Resonance Professional Committee of Jiangsu Analysis and Testing Association. He has been engaged in nuclear magnetic resonance testing and research since work, mainly including nuclear magnetic resonance qualitative (structural elucidation of known and unknown compounds, and impurities) and quantitative nuclear magnetic resonance work (API standardization and content determination of impurity reference materials, etc.), as well as pharmaceuticals and organic compound structure analysis. As the main contributor, completed the 2010 edition of Chinese Pharmacopoeia appendix "NMR method" (implemented in October 2010); meanwhile complied the NMR method operating procedures. Annotated pharmacopoeia appendix "NMR method" has been completed based on hands on experience.

沈文斌，1987 年毕业于南京大学化学系，专业有机化学。现任中国药科大学分析测试中心主任，江苏省分析测试协会核磁共振专业委员会主任委员，副研究员。工作以来一直从事核磁共振测试和研究工作，主要包括核磁共振定性（已知、未知化合物、杂质的结构确认）和核磁共振定量工作（API 的标化及杂质对照品的含量测定等），以及药物、有机化合物的结构分析工作等。作为主要起草者，完成了 2010 版中国药典附录“核磁共振法”（国内首次上药典，2010 年 10 月起实施）；同时完成了核磁共振法操作规程，并结合个人多年核磁共振操作实践的应用基础上，完成了药典附录“核磁共振法”的注释工作。

Presentation: Day 2 - NMR Standards in Chinese Pharmacopeia and knowledge sharing of qNMR technology

中国药典核磁共振法及定量核磁共振实验经验交流

ABSTRACT: The contents of nuclear magnetic resonance in Chinese Pharmacopoeia. The effect of choosing internal standard, solvent, peaks to be quantified, and the baseline on the results in quantitative NMR experiment.
中国药典中有关核磁共振的内容. 定量核磁共振实验中关于内标的选择、溶剂的选择、定量峰的选择，以及基线对实验结果的影响.

Baoning Su, Ph.D.
Vice president and head of Core Analytical Services
WuXi AppTec, China

Dr. Baoning Su is served as vice president and head of Core Analytical Services of WuXi AppTec. The team has around one thousand state-of-the-art analytical and purification instruments and over 700 research scientists located in Shanghai, Tianjin, Wuhan, Qidong and Chengdu, China. Core Analytical Services of WuXi AppTec provides comprehensive analytical, purification and structure identification services to domestic and international clients. Prior to join WuXi AppTec, Dr. Su has worked as Research Investigator and Senior Research Investigator at Bristol-Myers Squibb with impurity/degradant isolation and identification as major responsibilities. Dr. Su received his Ph.D degree from Lanzhou University in 1998. After that, he has worked several years in University of Tokushima, University of Illinois at Chicago, and The Ohio State University. Dr. Su has published over 70 peer-reviewed research articles.

苏保宁博士现任药明康德副总裁，核心分析部负责人。部门在上海/天津/武汉/启东/成都五地拥有近千台各类国际一流的大型分析分离仪器，700 余位研发人员，为内外部客户提供药物研发过程中所需

的全方位分析分离及结构鉴定服务。在加盟药明康德前苏保宁博士就职于美国施贵宝，先后担任研究员及高级研究员，主要从事原料药和制剂中杂质和降解产物的分析、分离和结构鉴定。苏保宁博士 1998 年毕业于兰州大学化学系，获化学博士学位。毕业后曾在德岛大学，伊利诺伊州大学芝加哥分校和俄亥俄州立大学学习工作，在行业期刊发表了 70 余篇科研论文。

Presentation: Day 2 - Application of qNMR in drug discovery and development

定量核磁在药物研发中的应用

ABSTRACT: Purity determination using QNMR technique has been widely used in recent years. The most significant advantages of QNMR are a reference standard of analyte itself is not needed, less sample is needed and fast turnaround time. This presentation will introduce the principle and operation workflow of QNMR, and more importantly, will use actual example to demonstrate the application of QNMR in drug discovery and development.

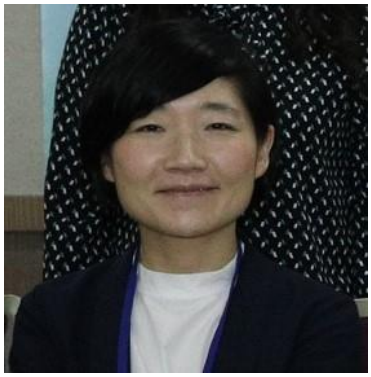
近些年来，利用定量核磁技术对化合物的纯度进行标定得到了越来越广泛的应用。定量核磁的最大优点是无需自身对照品、化合物用量少和分析速度快。本讲座将详细介绍定量核磁技术的原理、操作流程，并用实际案例分享该技术在药物研发中的应用。

Geoff Tsen, Ph.D.
Vice President and Region Manager
USP, China

Geoff Tsen, Ph.D., is Vice President and Region Manager, Greater China. In this role, he is responsible for leading strategic development and advancing public health through USP's quality standards. As General Manager of USP- China, Dr. Tsen focuses on operational units including Global Laboratory Operations, Science and Pharmacopeial Education as well as customer development and external affairs.
Dr. Tsen started his professional career in 1997 as a Ph.D. research scientist at Tufts University Medical Center in Boston, followed by nearly six years in commercial sales and marketing at Bio-Rad, a global life sciences and in vitro diagnostic player, based in Massachusetts and California.
In 2006, Dr. Tsen served in McKinsey & Company as a management consultant, focusing on strategy, operations and organizational structure within the healthcare sector including the top 10 global pharmaceuticals companies. He has held leadership roles at Becton Dickinson with its pre-analytical portfolio, and the Biopharmaceuticals Group of Pall, a worldwide leader in filtration and purification technologies. Most recently, he served as a principle consultant at Ernst & Young, China's strategy and operations group, specializing in healthcare and life sciences.
Dr. Tsen holds a Ph.D. degree in molecular and cellular biology from The Ohio State University, a MBA degree from University of Chicago Booth School of Business, and a B.S. degree from Fudan University.

Presentation: Day 3 – Building qNMR Scientific Community in China Pharma Industry

建立药品领域的定量核磁科学交流社区



Nahoko Uchiyama, Ph.D.
Section Chief, Division of Pharmacognosy, Phytochemistry and Narcotics
National Institute of Health Sciences (NIHS), Japan

I received my Ph.D. in Pharmaceutical Sciences from Kyoto University, Japan in 2004. After completing my Ph.D., I worked as Junior Assistant Professor at the Department of Pharmacognosy, Faculty of Pharmaceutical Sciences, Doshisha Women's College of Liberal Arts in Kyoto (Japan). In 2006, I moved to National Institute of Health Sciences (NIHS) in Tokyo, Japan as Researcher in the Narcotics Section of the Pharmacognosy, Phytochemistry and Narcotics Division, and was promoted to Senior Researcher at the same Division in 2009. I investigated chemical analysis of abused drugs, especially designer drugs. Since 2016, I have been working as Section Chief in the Pharmacognosy Section of the same Division of NIHS. My current research is mainly focused on chemical evaluation of herbal medicines along with chemical analysis of unregulated drugs and counterfeit medicines. I am also contributing to the development of Japanese Pharmacopoeia (JP) standards for crude drugs and Kampo extracts as a member of JP expert committee on crude drugs.

Presentation: Day 1 - Utilization of qNMR for assay in Japanese pharmacopoeia
定量核磁在日本药典中的应用

ABSTRACT: Quantitative NMR (qNMR) was implemented in the Japanese Pharmacopoeia (JP) since the release of JP16 Supplement II published in 2014. This presentation details the following topics: 1) Nineteen reagents evaluated by qNMR as the HPLC reference standards in the assay of crude drug section; 2) development of the optimal preparation method for qNMR of hygroscopic reagents; 3) utilization of relative molar sensitivity (RMS) coupled with qNMR and HPLC for assay of perillaldehyde, an unstable compound in Perilla Herb; 4) qNMR description in the guideline for drafting the JP; 5) a comparison of descriptions related to qNMR among the three pharmacopoeias (JP, USP, EP). 6) utilization of 31P-qNMR absolute determination method as a further approach in qMNR for organophosphorus pharmaceuticals.

Jaap Venema, Ph.D.
Executive Vice President & Chief Science Officer
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 – Welcome Opening
定量核磁研讨会开幕致辞

Xinyi Xu, Ph.D.
Deputy Chief Pharmacist
Division of General Chapters, Excipients and Packaging
Chinese Pharmacopeia, China

Dr. Xu is working in the General Chapters, Excipients and Packaging Division of the Chinese Pharmacopoeia, mainly engaged in the development and coordination of the technical requirements for physical and chemical analysis of the Chinese Pharmacopoeia volume IV. Responsible for and participated in a number of projects initiated by Ministry of Science and Technology, National Natural Science Foundation of China, and Chinese Pharmacopoeia, etc., participated in the compilation of 5 books, published more than 20 papers in domestic and international journals, and applied 3 national invention patents. Dr. Xu is a member of the Molecular Pharmacognosy Committee of the Chinese Society of Integrated Traditional Chinese and Western Medicine, and member of the Expert Committee of the Chinese Medical Education Association.
徐昕怡，博士，副主任药师，现任职于国家药典委员会通则辅料包材处，主要从事《中国药典》四部理化分析通用技术要求的制定和协调工作。负责并参与科技部、国家自然科学基金委员会、国家药典委员会等多项课题，参与编著书籍 5 部，在国内外期刊发表论文 20 余篇，获得国家发明专利授权 3 项。现任中国中西医结合学会分子生药学专业委员会青年委员，中国医药教育协会专家委员会药学专家库专家。

Presentation: Day 2 - Chinese Pharmacopoeia General Chapter 0441 Nuclear Magnetic Resonance Spectroscopy — Revisions to add qNMR technology
《中国药典》通则 0441 核磁共振波谱法—定量核磁技术的增修订

Wei Zhang
Associate researcher
Division of Chemical Metrology and Analytical Science
National Institute of Metrology (NIM), China

Wei ZHANG is an associate researcher in the Division of Chemical Metrology and Analytical Science, National Institute of Metrology, P.R. China (NIM). Wei ZHANG was graduated from China pharmaceutical University in 2000, and received bachelor's degree in pharmaceutical Analysis. Since 2001, he has been engaged in the research of NMR for determination of organic compounds. He worked in NIM focusing on the applications of qNMR (quantitative nuclear magnetic resonance), LC (liquid chromatography) and MS (mass spectrometry) for research of purity and solution certified reference materials (CRMs). He is the first researcher in NIM to use qNMR as one of the main quantitative methods for the development of certified purity reference materials, and has been successfully developed a batch of national primary certified reference materials such as Sudan red and Acrylamide. He extends the scope of accurate value assignment of qNMR from high purity sample to low purity sample by establishing new approaches such as ISRC (internal standard recovery correction)-HPLC-qNMR method. He has participated in 12 international comparisons, organized by CCQM, for purity assessment of organic compounds using qNMR, and all the results are consistent with the reference values in international comparison. He has been engaged in the study the performance evaluation methods of nuclear magnetic resonance spectrometer, and completed the first National Calibration Specification for Superconducting Pulsed Fourier Transform Nuclear Magnetic Resonance Spectrometers（JJF1448-2014）as the first author. He was engaged in the research on qNMR applications at a visiting researcher in the Bureau International des Poids et Measures (BIPM) in 2016, and 2018, respectively. He has published 32 papers including 16 SCI papers. He received one national science and technology progress award, and four provincial-ministerial awards.

张伟是中国计量科学研究院化学计量与分析所副研究员，2000 年毕业于中国药科大学药物分析专业，获学士学位。2001 年开始从事有机化合物核磁定值研究工作。他致力于定量核磁，液相色谱和质谱等技术应用于纯度和溶液有证标准物质的研究。 他在国内首次将定量核磁作为主要定值方法之一应用于有证纯度标准物质的研制，成功研制了苏丹红，丙烯酰胺等一批国家一级纯度标准物质。他建立了内标回收率校正(ISRC)-液相色谱-定量核磁（HPLC-qNMR）等新方法，将定量核磁的定值范围从高纯度样品扩展到低纯度样品。他参加 CCQM（国际物质咨询委员会）组织的有机化合物纯度比对，负责并完成定量核磁比对 12 项，比对结果均取得国际等效一致。他研究核磁共振谱仪的性能评价方法，并作为第一起草人完成了我国 2014 年颁布的第一部超导傅里叶变换核磁共振谱仪计量校准规范（JJF1448-2014）。他分别于 2016 年和 2018 年在国际计量局（Bureau International des Poids et Measures(BIPM)）从事定量核磁应用方面的研究工作。他发表论文 32 篇其中 SCI 论文 16 篇，获得奖励有国家科技进步二等奖一项省部级科技进步奖 4 项。

Presentation: Day 2 - qNMR in Metrology

定量核磁在计量中的应用

ABSTRACT: Quantitative nuclear magnetic resonance (qNMR) is an important method to assess the purity of organic compounds. The results of organic compounds by qNMR are affected by many factors, including the preparation of samples, the quantitative parameters of NMR, the data processing, and CRMs (certified reference materials) used as internal standards. The chosen of certified reference materials with reliable values is a prerequisite to get accurate result by qNMR. We have developed a series of CRMs for qNMR as internal standard, and the values of these internal standards can be traceble to the primary CRM benzoic acid in NIM. The CRM benzoic acid in NIM has been cross-validated with qNMR internal standards in BIPM, and therefore the value of benzoic acid in NIM can be internationally recognized accordingly. For the samples with lower purity, especially the compounds having molecular weight larger than 500 Da, qNMR has a risk of error for the purity assessment, because the peaks corresponding impurities are difficult to be completely separated from the peak of major component. We developed four new methods to overcome this problem.

定量核磁（qNMR）是评估有机化合物纯度的重要方法，在化学计量中广泛用于测定有机化合物的纯度。有机化合物的核磁定量结果会受到多个因素的影响，样品的配制，定量参数的设定，数据处理软件的使用，以及是否使用有证标准物质作为内标。而是否使用量值可靠的有证标准物质作为内标是核磁定量结果准确的前提条件，中国计量院研发了系列有证标准物质用于核磁定量，这些内标的量值都可被溯源到中国计量院的国家基准标准物质苯甲酸上。中国计量院的苯甲酸与国际计量局的系列核磁内标进行交叉验证，从而使国家计量院苯甲酸的量值得到国际间的互认。 对于分子量高于 500 的低纯度有机化合物定量核磁的定值存在着风险，因为杂质峰很可能与主组分的峰没有完全分离。我们开发了四种新方法来解决这个问题。