

qNMR Symposium 2018 in Tokyo
- Current Status and Future Prospects for qNMR -

October 31, 2018

FUJIFILM Wako Pure Chemical Corporation Tokyo Principal Office

qNMR Symposium 2018 in Tokyo, Japan

— Current Status and Future Prospects for qNMR —

<Purpose>

A symposium will be held to commemorate the establishment of the qNMR Japan Committee, JC-qNMR, and to foster the existence of the Committee and its activities. The theme will be “Recent Progress and Future Prospects for qNMR”. The symposium is intended to establish a platform for information exchange and educational activities related to qNMR as the next-generation of quantitative analysis, representing the ultimate goal of the committee. Specifically, participants will learn about the latest ISO application and standardization activities, while engaging in an interactive program that will provide an opportunity to utilize and share the research and activities of participants, including brainstorming of ideas for broader dissemination.

<目的>

日本定量 NMR 研究会の設立記念としてシンポジウムを開催し、研究会の存在、及び活動を示します。テーマは設立趣旨の目標でもある、次世代の定量分析を未来につなぐための情報交流・教育活動基盤となることを目指すスタートとしてふさわしい“qNMR の現状と未来を考える”とします。具体的には標準化（ISO 化）や新しいアプリケーションの動向を学びながら、普及のためのアイデアを出し合うなど、参加者の研究・業務に生かす機会となる参加型のプログラムを構成します。

Program

Greetings

Ministry of Economy, Trade and Industry

1. 13:05 - 13:15

“Introduction of qNMR Japan Committee”

Secretary-General

2. 13:15 – 13:45

“Status report on standardization activities”

- Including the prompt report for Inter laboratory comparison study –

Toru Miura (FUJIFILM Wako Pure Chemical Corporation)

3. 13:45 – 14:45

"Calculation, Documentation, and Dissemination of qNMR Data”

Dr. Guido Pauli (University of Illinois at Chicago)

15 minute break

4. 15:00 – 16:00

„Quo Vadis?” The Future of qNMR”

Dr. Bernd Diehl (Spectral Service)

5. 16:00 – 17:30

“Open discussion”

Discussion topic: Next Steps in Moving qNMR Technology forward

Closing address

The program is subject to change without notice.

プログラム (同時通訳付き)

ご挨拶

経済産業省

1. 13時05分～13時15分
日本定量 NMR 研究会について

日本定量 NMR 研究会幹事長

2. 13時15分～13時45分
標準化活動の状況報告 (共同試験速報を含む)

三浦 亨 (富士フイルム和光純薬株式会社)

3. 13時45分～14時45分

"Calculation, Documentation, and Dissemination of qNMR Data"

Dr. Guido Pauli (University of Illinois at Chicago)

休憩 15分

4. 15時～16時00分
„Quo Vadis?“ The Future of qNMR"

Dr. Bernd Diehl (Spectral Service)

5. 16時00分～17時30分

オープンディスカッション

これからの定量 NMR についての提案

(定量 NMR に関するこういうものがあつたらよいな・・・という希望の話)

終了

プログラムは予告なく変更することがあります。あらかじめご了承ください。

Status Report on Activity for International Standardization of qNMR method

Toru Miura

FUJIFILM Wako Pure Chemical Corporation

In 2018, an international summit was held to discuss the international standardization of the qNMR method (qNMR Summit 2018 in Tokyo). The qNMR Summit was first held by the United States Pharmacopoeia (USP) in October 2016, after which the German National Metrological Institute, the Federal Institute for Materials Research and Testing (BAM), held the second summit in March 2017. The qNMR Summit 2018 in Tokyo was attended by many experts and practitioners of the qNMR method worldwide, and lectures and discussions were held over two days. The summit was held as part of efforts to apply the qNMR method under ISO. At the opening meeting with invited experts and observers, an active discussion was held focusing on the ISO draft for qNMR. The ISO draft for qNMR will be continuously considered. Following this, we almost completed the ISO draft in cooperation with experts of the qNMR method around the world. At the present moment, we plan to submit a new work item proposal (NP) to P-member of TC34 (Food products) and to establish a working group (WG) based on the approval from the aforesaid P-member during 2019.

Additionally, in 2018, we conducted an international collaborative study to confirm the international validity of the qNMR method that will help apply the qNMR method under ISO. The participating institutions were as follows: National Institute of Health Sciences (Japan), National Research Institute of Fisheries Science (Japan), National Metrology Institute of Japan (Japan), Japan Food Research Laboratories (Japan), SHIONOGI & CO., LTD (Japan), CHUGAI PHARMACEUTICAL CO., LTD. (Japan), Taisho Pharmaceutical Co., Ltd. (Japan), Institute of Microbial Chemistry (Japan), The United States Pharmacopeial Convention (USA), Baxter Healthcare Corporation (USA), Spectral Service AG (Germany), Roche Diagnostics GmbH (Germany), and Politecnico di Bari (Italy).

In the presentation, I will discuss current status of qNMR method standardization and the results of the collaborative study on qNMR method in detail.

Speech Title : „Quo Vadis?” The Future of qNMR

Prof. Dr. Bernd W.K. Diehl, Spectral Service AG, Cologne, Germany

The use of a NMR instrument in a manner of and in competition to a balance is derived and illustrated. A comparison between the abilities of micro and ultra micro balances for qNMR experiments will be discussed. The function of a qNMR measurement for “weighing” sugar granules and Peptides below 1 mg is validated and compared. The influence of proper experimental design for qNMR experiments is demonstrated at the results of Interlaboratory comparison

The power of a quantum mechanical balance by the first time use of heteronuclear referencing of qNMR methods is demonstrated at several examples. Further to organic compounds inorganic cations such as Ca^{2+} , Mg^{2+} , Sr^{2+} , Ba^{2+} , Pb^{2+} , Be^{2+} , Sn^{2+} and Zn^{2+} can be analyzed indirectly by ^1H NMR spectroscopy after being complexed with unselective reagents such as EDTA, DTPA or DOTA. The examinations show that NMR spectroscopy is a powerful alternative for complexometric reactions which are conventionally used to indicate the endpoint of a titration by means of a colored complex. The new technique enables the quantification of even low amounts of metals ions below 1 ppm, exemplarily for Pb^{2+} . The quantitation of non-sensitive nuclei like K^+ , or sulfur in SO_4^{2-} can be boosted by indirect measurement of different classical precipitation methods by ^{55}Co and ^1H NMR spectroscopy.

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Biography (free format)

BIOGRAPHICAL INFORMATION



Name: Prof. Dr. Bernd W. K. Diehl, 14.08.1960

Married, 4 Children

Education: Dr. rer. nat, Dipl. Chemist, Philipps University Marburg 1988 in Organic Chemistry and NMR Spectroscopy

Employment: Bayer Research Center, 1988 until 1990, head of NMR Spectroscopy

1990 founder and CEO of Spectral Service AG, Cologne, Germany

2017 founder Steelyard Analytics Inc., Manassas, U.S.

2017 Guest professorship in Chicago

2018 Professor University of Applied Science Bonn-Rhein-Sieg

Lectureships:

Universities of Marburg and Bonn, NMR Spectroscopy (1998 – 2000),

Since 2013 University of Applied Science Bonn-Rhein-Sieg: NMR Spectroscopy

Since 2015 University of Würzburg: Mass Spectrometry

Associations Membership:

President of I.L.P.S. (International Lecithin and Phospholipid Society)

Chair of AOCS (American Oil Chemist Society) Phospholipid Division,

Member of ACS, GDCh, DGF, Euro Fed Lipids, Nordic Lipidforum

Calculation, Documentation, and Dissemination of qNMR Data

Speaker's name and affiliation

Dr. Guido F. Pauli

PCRPS & CENAPT, University of Illinois at Chicago College of Pharmacy, 833 S. Wood St., Chicago, IL 60612 (U.S.A.)

Abstract/Content

This symposium contribution seeks to answer **three major questions** associated with the current status and further development of quantitative NMR (qNMR). **(i)** How are qNMR data generated and reported? **(ii)** What is more challenging: qNMR experimental methodology, or its calculation, documentation, and dissemination (“CD₂”? **(iii)** Is qNMR repeatable and reproducible given the way its CD₂ is practiced today? Taking into account the current qNMR knowledge base, evidence will be reviewed and presented to address **five key hypotheses**:

(Hyp#1) calculation and documentation in qNMR is currently under-developed, and the Dissemination of qNMR outcomes is driven by outdated mechanisms.

(Hyp#2) Integration is the most popular quantitative measure in qNMR, but also most complex in terms of CD₂, compared to existing alternative methods.

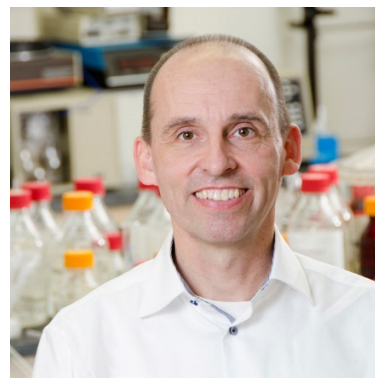
(Hyp#3) qNMR outcomes need adequate quantitative reporting tools and raw qNMR data reporting can lead the ongoing movement towards FAIR data sharing.

(Hyp#4) Quantum Mechanics are the roots of (q)NMR, and QM-qNMR combines analytical specificity with efficient CD₂ workflows.

(Hyp#5) qNMR has excellent repeatability, but only mixed reproducibility and high activation energy for global adoption - both for mainly CD₂ reasons.

Referring to outcomes from our own qNMR research, answers will be developed to can potentially guide the development of CD₂ efforts in qNMR research and method development.

Guido F. Pauli. 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 Program for Collaborative Research in the Pharmaceutical Sciences (PCRPS), 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, NP technologies (CENAPT), botanical dietary supplements (Botanical Center), clinical and dental intervention materials, drug discovery, the NAPRALERT database, and institutional training programs. Main research interests encompass the metabolomic analysis of natural health products, botanicals, anti-TB hit-to-lead development, dental biomodifiers, and pharmaceutical analysis. He has expertise in the development of analytical methods and innovative approaches, including quantitative NMR and countercurrent separation. Dr. Pauli seeks to address challenges posed by nature's metabolomic variation and enhance the understanding of natural products as health products and sources of new drugs. His academic track record includes mentoring of 18 Ph.D. students, 20 postdocs, 15 visiting scientists, and international collaborations particularly in China and Europe. His ~200 peer-reviewed publications have an h-index of 44 (Scopus).



Guido F. Pauli, Dr. rer. nat., FAPA

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qNMR Japan Committee,

JC-qNMR