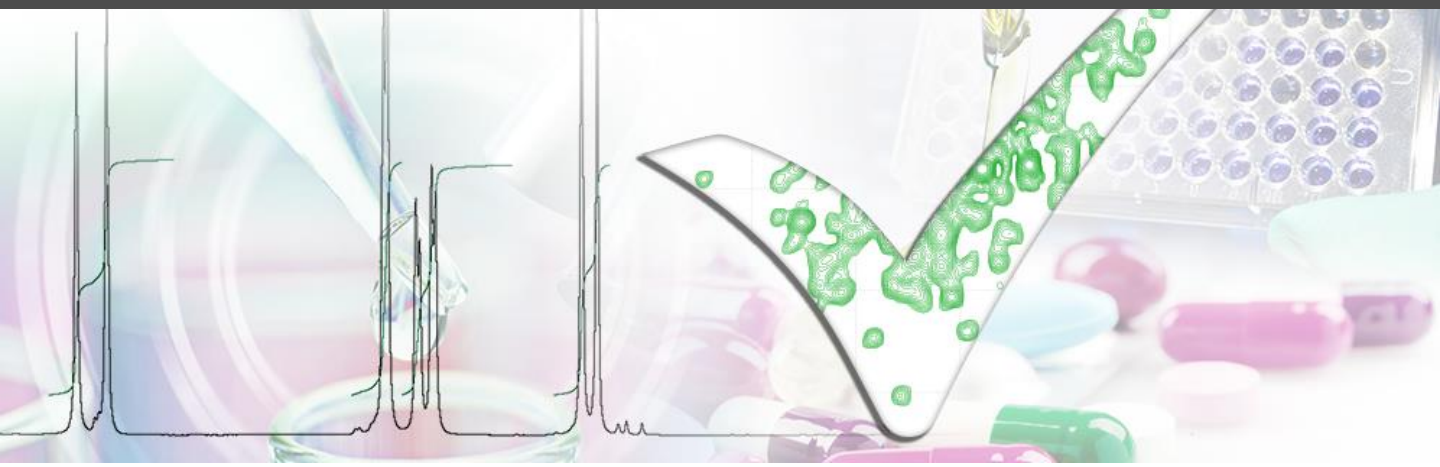
VOL. 13 I Sept 2021

NMR VALIDATION

No Need to PANIC



Overview of the Newsletter

- ValidNMR Webinar #3
- USP qNMR Summit 2021
- ValidNMR Forum
- ValidNMR @ PANIC 2021

- ValidNMR Webinars -

We are delighted to introduce our schedule of regular webinars that showcase qNMR topics. In March 2021 we started a new online webinar series - free of charge - to share information, knowledge and research results with the community **to empower you**!

Therefore, we would like to ask you:

- Which topics are of interest for you?
- How often should a ValidNMR webinar be organized per year?
- Do you want to attend live, or do you want to have only access to recorded webinars?
- Are you interested in giving a webinar?
- From your perspective, who should present a webinar?

Email us via committee@validnmr.com or answer via our online survey

SURVEY

https://www.surveymonkey.de/r/9S8QD2R

Webinar #3

Sponsor Talk: Lab Management, qNMR and GxP

Speaker: Dr. Fabrice Moriaud, Bruker

Dr Moriaud described an enterprise software solution for any spectrum acquisition. Billed as a "request-to-result management solution" which manages the full work flow, from sample submission to report receipt. Results and analysis metadata are kept in a database. This can work with IS-qNMR, adhering to data integrity principles. Screen shots were shown of the web-based sample acquisition procedure, interacting with ICON-NMR. Processing and qNMR analysis is handled by Mestrenova, with all its functionality. An example report was shown for qNMR using an internal standard. The databased raw data can be accessed. Metadata are kept (Request details). An audit trail is maintained, and digital signatures supported. The system is described as scalable from a single lab to a global solution. This is a Mestrelab-Bruker collaboration. Finally, Bruker's 80 MHz benchtop NMR with CTC sample changer was described.

Talk #1: 2H SOLCOR: A novel tool for reducing volume variation as a source of error in external standard quantitative NMR

Speaker: Jason Ewanicki, Pfizer

Tube to tube volume difference presents a challenge in obtaining accurate external standard quantitative NMR (esqNMR) results. Deuterium (2H) is easily observable, intrinsically quantitative, present in all samples, free of interfering signals, insensitive to probe tune/match and sample saltiness. These properties make 2H SOLCOR (2H observed SOLvent CORrected) an ideal tool for volume correction whenever difference exist between reference standard and analyte, such as esqNMR. We demonstrate a technique where 2H peak integrals from the solvent are used as a universal internal standard to correct volume variations in NMR tubes, thereby improving the accuracy and precision of esqNMR method This simple yet effective technique is described in this talk. Practical considerations for successful implementation are investigated. 2H SOLCOR can be applied anywhere esqNMR is used, including where precious samples need to be accurately quantified for qualification as an authentic analytical standard. The technique also lends itself to accurate quantitation in situations where sample treatment is necessary. Paper

Talk #2: Community-built calibration systems for the development of non-targeted NMR methods

Speaker: Prof. Vito Gallo, Technical University of Bari, Italy

In recent years, non-targeted analysis by Nuclear Magnetic Resonance spectroscopy (NMR) has being experienced an increasing number of applications. Among the possible application, non-targeted NMR has been focused with particular attention to food quality control and fraud detection.[1] The strong power of non-targeted NMR methods resides in the possibility to provides, for a given sample, statistically equivalent signals in spite of using spectrometers that are different in hardware features.[2]

Nevertheless, to date, no internationally agreed guidelines are available to regulate the procedures for non-targeted NMR analyses over different laboratories. Moreover, no official analytical parameters have been established so far to determine the repeatability and reproducibility of the applied protocols in this field. We recently provided some contributions to this research area by organizing inter-laboratory comparisons and elaborating the huge amount of collected data. A particular focus was dedicated to evaluating the reproducibility of the NMR analyses performed through different spectrometers and by many operators, by developing common calibration lines and validated classification models.[3,4] The effect of processing of data was investigated towards the development of more efficient chemometric analysis.[5] Nevertheless, the variability induced by the operator during the preparation of the NMR sample is still understudied.

In this presentation, as part of a collaborative research project, this aspect was taken under deep investigation. Thus, 65 samples of tomato collected from different Italian regions were subjected to the same strict analytical protocol encompassing the sample preparation and the subsequent NMR analysis. Such a protocol was performed by two different operators and utilizing two diverse spectrometers. The study provided useful insights into the effect of variations in the sample preparation, the protocol of analysis, and the processing of data on the reproducibility of the results. The results will be presented with the final goal to provide a methodological pipeline to assess the reproducibility of NMR data produced by different spectrometers and to create a community-built calibration system enabling identification of unknown sample by suitable NMR based classification systems.

[1] M. Bevilacqua, et al. TrAC 2017, 96, 42-51.

[2] Gallo V, et al. Anal. Chem. 2015, 87, 6709-6717

[3] Ragone R, et al. Food Chem. 2020, 332, 127339

[4] Gallo V, et al. Food Anal. Methods 2020, 13, 530–541.

[5] Musio B, et al. Talanta 2020, 214, 120855

- USP qNMR Summit 2021 -

Summary Agenda George Hanna Award qNMR Summit Pre-Reads

Register Now

USP qNMR Summit 2021

October 5, 2021—October 7, 2021
7:00 AM-5:00 PM ET

Virtual Workshop - WebEx

USP is convening the 6th International qNMR Summit (October 5th to 7th, 2021), the foremost colloquium of the qNMR practitioners. The Summit will examine the state of qNMR and address challenges of adopting qNMR as an analytical technique, review development of practical qNMR validation guidelines, and explore potential implications of qNMR implementation in industrial, contract laboratory and regulatory settings. The Summit will survey the latest advances and developments in the field, including those of instrumentation, data acquisition and management and novel applications. The Summit will work toward consolidating ongoing efforts and map out directions in which the field is progressing. The Summit is co-sponsored by the Center for Natural Products Technologies (CENAPT) at the University of Illinois at Chicago, a leading institution advancing qNMR and supplying trained cadre to the industrial, academic and government research laboratories. To find information on past qNMR Summits, please visit http://www.qnmrsummit.com/

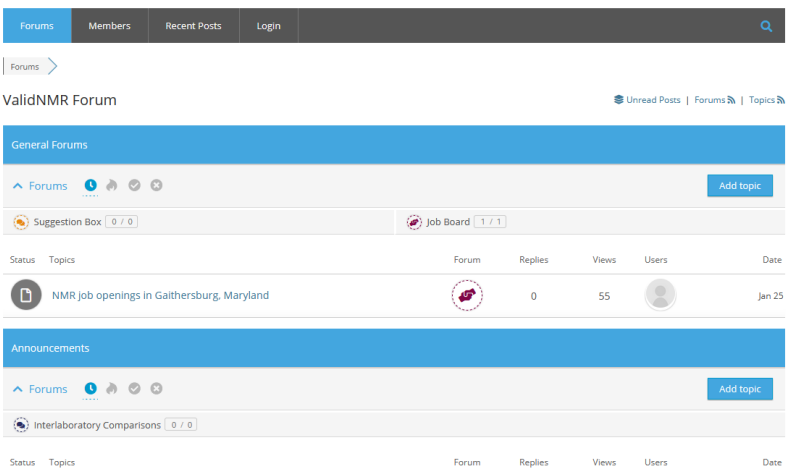
Date: October 5-7, 2021

- October 5th, 2021, 7 am -11 am EDT
- October 6th, 2021, 10 am – 2 pm EDT
- October 7th, 2021, 1 pm – 5 pm EDT

Cost: Free

- ValidNMR Forum! -

Our idea is to increase the knowledge sharing by preparing a forum where you, the NMR specialists, have the chance to ask questions, to send response and answers to the community and to share your experiences.



Access Forum

- ValidNMR @ PANIC 2021 -
October 17-20, Nashville, TN

"PANIC is truly a unique conference experience! This must-attend conference provides a superior educational event for industrial, regulatory, government, and academic scientists seeking to learn about and discuss applications of NMR to pharmaceuticals, polymers, petroleum, food/agriculture, and plant production that are rarely discussed at other NMR meetings.

This remarkable conference affords its participants with the unique opportunity to broaden their knowledge, exchange ideas about the latest technologies, and engage in dynamic conversations with peers and partners from around the world."

TUESDAY, OCTOBER 19

8:30 a.m.	ValidNMR Workshop Welcome **ValidNMR Session #1 (Keynote Lecture):** **"Setting Standards: Revision of USP general chapters <761>/<1761>" ,** Dan Sorensen, USP
9:15 a.m.	**ValidNMR Session #2 (Open Forum — Sli.do assisted): "What does 'Quality' mean to you?"** Klas Meyer, BAM & Kristie Adams, Steelyard
9:45 a.m.	**ValidNMR Session #3: "Laboratory accreditation as a reliable indicator of technical competence for testing, calibration and measurement organizations – An introduction to ISO/IEC 17025 using the example of qNMR spectroscopy.",** Michael Maiwald, BAM
10:10 a.m.	Exhibit Hall Open, Poster (Even) Presentations and Coffee Break
11:10 a.m.	**ValidNMR Session #4: "Fundamentals of quality measurement; traceability, validation, and uncertainty.",** Mike Nelson, NIST
11:40 a.m.	**ValidNMR Session #5: "Accreditation ISO 17025 Authenticity and Quality Control of Food, including statistical methods, flexibility.",** Birk Schütz, Bruker
12:10 p.m.	**ValidNMR Session #6 (Open Forum — Sli.do assisted): "Open Q+A / Ask us anything",** Klas Meyer, BAM & Kristie Adams, Steelyard

Register

- Thank you to our Sponsors! -

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Practical Applications of NMR in Industry Conference PANIC

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Want to be featured in the next ValidNMR newsletter?

The deadline for submissions and contributions to the next newsletter is December 20, 2021.
Please contact us at committee@validnmr.com!