

# NMR Validation

No Need To PANIC

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## Welcome!



Kim Colson & Torsten Schoenberger

Thanks to the efforts of many, we welcome you to the first newsletter for the NMR Validation community. The goal of this newsletter is to keep the community informed of current events and issues in NMR validation and to provide a mechanism by which we can support each other as NMR further expands into regulatory environments. Please join us in making this a valuable resource by sharing your knowledge and experiences for future quarterly newsletters.

We would like to say a quick **thank you** to our wonderful sponsors!



## Practical NMR Validation Teams up with Academia

By Kaylen Obray

*As we progress forward in fostering communication throughout the NMR industry in regards to validation, we are now in collaboration with academia.*



There is a need within the NMR community to **progress forward** in exploring new facets in which we can use analytical techniques to advance our understanding of various systems. One aspect the NMR community hasn't fully encompassed is the validation process which also involves setting reference standards, establishing a common language which directly relates to NMR, communication relating to validation, and much more. After a couple years of discussing **NMR validation within industry**, we have now teamed up with Colorado State University to begin to bring this impending topic to light within the world of academia.

This year, PANIC, with the help of Bruker, has **introduced a scholarship for NMR validation** to provide education in NMR validation through fostering communication and concerns in the NMR community and presentation of

results from our meetings and initiatives. This year the **Bruker Scholarship for Excellence in NMR Validation** was awarded to myself, Kaylen Obray, at Colorado State University (CSU). Along with the familiar names of Kim Colson (Bruker BioSpin), Torsten Schoenberger (Bundeskriminalamt), Kristie Adams (DuPont), and with the help of my mentor, Claudia Boot (CSU), I have begun to build a validation website to further the reach of NMR validation.

I will be attending PANIC 2017, and also helping to organize the validation workshop on **02/24/17!** I look forward to meeting and speaking with all of you and gaining more insight and knowledge into this upcoming topic of NMR Validation. This will not only help the **NMR community**, but also allow us to make improvements to the NMR validation website that will help move this field forward!



Come See us at PANIC  
2017 on February 24 at  
Hilton Head Island!



# NMR Validation Workshop

By Kaylen Obray

*Please join us for the 3rd Annual NMR validation workshop taking place after PANIC on 02/24/2017!*

Please join us for a day of learning, group discussions, short lectures, current developments and much more that revolves around **practical NMR**. This workshop is based around NMR validation, but as we already know this is a vast topic. We will also be focusing on finding a common language that relates to validation and specifically NMR, setting various reference standards, and we are also looking for **YOUR** input. We want to know what you would like to discuss, what is relevant within the community and/or your workplace, and how we can proceed forward.

We have compiled a **survey** (<https://www.surveymonkey.com/r/G3WZZHP>) which we could really use your help in deciding topics to discuss at the upcoming workshop! We want this to be a compilation of thoughts from people representing various industries, government positions, vendors, academia, and more. To make this NMR Validation workshop and website most efficient we need **YOU** to contribute in any way possible. With that we hope that you will attend the **Validation Workshop**, and if you are unable to attend you can still make your presence known by various volunteering and/or sponsorship opportunities!

## Agenda: Validation of NMR Workshop

February 24, 2017

8:00 am Coffee

8:30 Welcome, Progress, Introducing Kaylen Obray, Today's Goals

Kim Colson (Bruker BioSpin)

8:50 Summary of 2016 WW Meetings

Torsten Schoenberger (Bundeskriminalamt)

9:10 "Breakthrough in qNMR literature: announcement of a new handbook"

Bernd Diehl (Spectral Service)

9:35 "qNMR in Pharmacopeial Analysis"

Sitaram Bhavaraju (U.S. Pharmacopeial Convention)

10:00 Discussion

10:15 Break

10:45 NMR Validation Website & Scholar Initiatives

Kaylen Obray (Colorado State University)

11:00 Discussion: Website, Editorial Boards, News, Validation Education

Moderators: Claudia Boot (CSU) and Torsten Schoenberger (Bundeskriminalamt)

12:15 Lunch

1:00 "Validation of multivariate NMR methods: case studies of heparin and lecithin"

Yulia Monakhova (Spectral Service)

1:25 Discussion

1:40 Workshop (Topics Determined based on Survey)

Moderators: tbd

3:15 Break

3:30 Government Perspective (speaker tbd)

4:00 Wrap-Up Discussion: "What we've learned, setting our path forward and plans for next year"

Kim Colson (Bruker Biospin) and Torsten Schoenberger (Bundeskriminalamt)

4:45 Close of Validation Workshop



## NMR Validation

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Come Visit Us At...

[www.validnmr.com](http://www.validnmr.com) (Will be live 01/16/17)  
<https://www.linkedin.com/groups/8482840>



# International NMR Interlaboratory

## Comparison

By Vito Gallo

*A new International NMR Interlaboratory Comparison organized by Innovative Solutions!*

I warmly invite you to participate to the **new International NMR Interlaboratory Comparison** organized by Innovative Solutions. For details, please visit [www.innovative-solutions.it](http://www.innovative-solutions.it)

This comparison is organized and funded by **Innovative Solutions S.r.l.** in the framework of the project "Recupero del Germoplasma Viticolo Pugliese" (Re.Ge.Vi.P.), "Progetti Integrati per la Biodiversità" – P.S.R. FEASR 2014-2020, Misura 10.2.1 "Progetti per la conservazione e valorizzazione delle risorse genetiche in agricoltura" – Trascinamento della Mis. 214 Az. 4 sub az. a) del PSR 2007-2013.

Since 2012, with the aim to encourage the use of qNMR in official methods, Innovative Solutions embarked on the organization of NMR inter-laboratory comparisons (NMR-ILCs) according to ISO/IEC 17043:2010 and reference normative therein. NMR-ILCs provide objective standards for individual laboratories, allow them to **compare analytical results** from different laboratories and represent a way to check the quality and the accuracy of the analytical job.

### Contact Information

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[www.innovative-solutions.it](http://www.innovative-solutions.it)

# Volunteer and Sponsorship Opportunities

By Kaylen Obray

## P & B

We would like to personally thank PANIC & Bruker for being our largest contributors to the Validation Workshop this year! With this help provided by PANIC & Bruker we are able to make this Validation Workshop free to anyone who wishes to further their knowledge about practical NMR!

As mentioned previously within this newsletter, we want to gain not only **community awareness** about the need for NMR Validation, but also would like to gain support from our fellow colleagues. We would like to solicit **volunteer and sponsorship opportunities** which would benefit this cause. Volunteer options have been listed on our survey which can be found at (<https://www.surveymonkey.com/r/G3WZZHP>), and they consist of many possible options. We have the need for note takers and leaders for group discussions during our **Validation Workshop**. We also are looking for help to reach out to possible companies and academic institutions for sponsorships and also prospective attendees for the workshop. Other volunteer options revolve around the **Validation Website** which consist of consulting with Kaylen, the "website master", and input on the "wiki" editorial boards. There are also more ways to contribute, and we would love your support!

We would also be pleased to accept any **sponsorships from vendors or other organizations**. We are currently receiving help from PANIC & Bruker BioSpin, but we are always looking more possibilities to get NMR Validation on the map! With your sponsorship your company and/or institution will be featured both here in the newsletter and on the Validation NMR website. Please see below for contact information regarding both volunteer and sponsorship opportunities.

### Contact Information

**Volunteer:** Kaylen Obray <kaylen@validnmr.com>  
**Sponsorship:** Jim DeFelippis <treasurer@panicco.org>

## Events

*Keep up to date on the our communities progress towards NMR validation!*



**NMR Validation Website Goes LIVE!**

Please follow the link to our NMR Validation website! Our hope is to make this a community-based website!



**NMR Validation Workshop**

Please join us for a day of learning and sharing ideas in hope to solve difficult topics within our



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