



1st NMReDATA Symposium

Following the SMASH 2019 conference

26. September 2019

Porto, Portugal

Program

Feature presentation:

Jonathan Bisson, University of Illinois Chicago, USA: What can we do with RAW NMR data and spin parameters

Short contributions:

Stefan Kuhn, De Montfort University, Leicester, UK: NMReDATA software and nmrshiftdb2

Tomas Lebl, St Andrews University, UK: NOMAD - NMR Online Management and Datastore

Jean-Marc Nuzillard, University of Champagne Ardenne, France: NMReDATA file validation through Computer-Assisted Structure Elucidation

Wolfgang Robien, University of Vienna, Austria: A few remarks on wrong structures in the literature

Damien Jeannerat, NMReDATA Initiative, Switzerland: Validation of NMReDATA by spectral simulation

Angel Herráez, University of Alcalá, Spain: NMReDATA J_reader: an HTML interface for displaying the contents of NMReDATA files, molecular structure, NMR data and spectra

Nils Schloerer, University of Cologne, Germany: Teaching NMR data handling, electronic assignment and CASE at the university

Robert Hanson, St. Olaf College, Northfield, USA: Putting it all together: Fully automated NMR spectrometer, web-based analysis, and spectral simulation with 2D/3D structure correlation for first-year organic chemistry

Pavel Kessler, Bruker Biospin, Germany, Bruker: Implementation of NMReData

Carlos Cobas, Mestrelab, Spain: Mnova meets NMReData: automation workflows and new opportunities

Dimitris Argyropoulos, ACD/Labs, Canada: Implementing the NMReDATA format into your workflows using ACD/Labs software

Sina Kazemi, SIGNALS, Germany: LOGS - a natural fit for NMReData

Information

<https://nmredata.org/wiki/Symposium2019>

Registration: <https://bit.ly/2XFAHFW>

Contact: symposium2019@nmredata.org

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