1ˢᵗ NMReDATA symposium, 26.9.2019 Porto, Portugal

Relevance of the NMReDATA Initiative in chemistry

9:00   *Forewords on the NMReDATA Initiative, Damien Jeannerat*
9:15   Jonathan Bisson, University of Illinois Chicago, USA
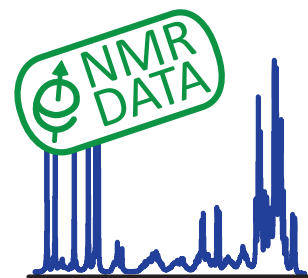   *What can we do with RAW NMR data and spin parameters*
10:00 Wolfgang Robien, University of Vienna, Austria
     A few remarks on wrong structures in the literature
10:20 Nils Schloerer, University of Cologne, Germany
     Teaching NMR data handling, electronic assignment and CASE at the university

10:40-11:00 Coffee Break

Available software and tools relevant to the NMReDATA Initiative

11:00 Stefan Kuhn, De Montfort University, Leicester, UK
     NMReDATA software and nmrshiftdb2
11:20 Pavel Kessler, Bruker Biospin, Germany
     Bruker implementation of NMReData
11:40 Mitcheell Maestre-Martinez, Mestrelab, Spain
     Mnova meets NMReData: automation workflows and new opportunities
12:00 Dimitris Argyropoulos, ACD/Labs, Canada
     Implementing the NMReDATA format into your workflows using
     ACD/Labs software
12:20 Sina Kazemi, SIGNALS, Germany
     LOGS - a natural fit for NMReData

12:40-13:30 Lunch Break

Further development of NMReDATA

13:30 Robert Hanson, St. Olaf College, Northfield, MN, 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
13:50 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
14:10 Jean-Marc Nuzillard, University of Champagne Ardenne, France
     NMReDATA file validation through Computer-Assisted Structure Elucidation
14:30 Damien Jeannerat, University of Geneva, Switzerland
     Validation of NMReDATA by spectral simulation
14:50 Tomas Lebl, St Andrews University, UK
     NOMAD - NMR Online Management and Datastore

15:10 - 15:40 Coffee break

Round table discussion : Future version of the format and admistration of the NMReDATA Initiative

15:40   *Discussion of open issues with the format*
     Structure, funding and organisation of the NMReDATA Initiative
16:20 Acknowledgements and closing remarks

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