

North Jersey ACS NMR Topical Group 2020 Virtual NMR Symposium

Oct 20th, 2020

More information available on our website: <https://www.njacs.org/nmr-mtg>

Link to the webinar:

<https://merck.webex.com/merck/onstage/g.php?MTID=ebda26df40a7eb1530bd22b6c00fdbbe2>

Password: NJACS-2020

The Symposium is **FREE** of charge

Session 1 (8.00-10.50am EST)

Yulan Wang
Singapore Phenome Center

Ruth M. Gschwind
University of Regensburg

Gareth Morris
University of Manchester

Vladislav Y. Orekhov
University of Gothenburg

Session 2 (11:10am–1.10pm EST)

Isabella Felli
University of Florence
Alexandre Bonvin
Utrecht University
Teresa Carlomagno
Leibniz University of Hannover

Session 3 (2.00-4.00pm EST)

Robert Schurko
National High Magnetic Field Laboratory

Robin de Graaf
Yale University

Daniel Raftery
University of Washington

Session 4 (4.20-5.40pm EST)

William Gerwick
University of California, San Diego

Till Maurer
Merck & Co.

Keynote session (5:40–6.40pm)

Maurizio Pellecchia
University of California, Riverside

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Session 1 (8:00-10:50am EST)

Session Chair: **István Pelczar**, Princeton University

8:00 – 8:10 am Opening remarks by **Justyna Sikorska**, Chair of NJACS NMR Topical Group

8:10 – 8:50 am **Yulan Wang**, Singapore Phenome Center

Detection of metabolic reprogramming associated with HBV infection using metabonomics

8:50 – 9:30 am **Ruth M. Gschwind**, University of Regensburg

NMR as mechanistic tool in photocatalysis

9:30 – 10:10 am **Gareth Morris**, University of Manchester

Ultraclean pure shift NMR?

10:10 – 10:50 am **Vladislav Y. Orekhov**, University of Gothenburg

Fast NMR: solving a puzzle with most of the parts missing

10:50 – 11:10 am “Coffee” break

Session 2 (11:10-2:00 pm EST)

Session Chair: **Gaetano T. Montelione**, RPI

11:10 – 11:50 am **Isabella C. Felli**, University of Florence

Intrinsically disordered proteins by NMR: what can ¹³C direct detection can tell us?

11:50 – 12:30 pm **Alexandre M.J.J. Bonvin**, Utrecht University

Integrative modelling of biomolecular complexes

12:30 – 1:10 pm **Teresa Carlomagno**, Leibniz University of Hannover

High molecular-weight complexes in the regulation of gene expression: a view by integrative structural biology

1:10 – 2:00 pm “Lunch” break

Session 3 (2:00-4:20 pm EST)

Session Chair: **Mark McCoy**, Merck & Co.

2:00 – 2:40 pm **Robert W. Schurko**, National High Magnetic Field Laboratory

Mechanochemical Synthesis of Active Pharmaceutical Ingredients and their Characterization with New NMR Crystallographic Methods based on Solid-State NMR of Quadrupolar Nuclei

2:40 – 3:20 pm **Robin de Graaf**, Yale University

Deuterium Metabolic Imaging (DMI), a novel MR-based method to map metabolism in 3D

3:20 – 4:00 pm **Daniel Raftery**, University of Washington

How Quantitative NMR Enables New Metabolomics Methods

4:00 – 4:20 pm “Coffee” break

Session 4 (4:20-7:00 pm EST)

Session Chair: **Luciano Mueller**, Bristol-Myers Squibb

4:20 – 5:00 pm **William Gerwick**, University of California, San Diego

Accelerated Identification of Natural Products using Small Molecule Accurate Recognition Technology (SMART) 2.1

5:00 – 5:40 pm **Till Maurer**, Merck & Co.

Discovery and characterization of active small molecule ligands targeting the function of ubiquitin specific protease USP7 by a catalytic site independent mechanism

Keynote Presentation

5:40 – 6:40 pm **Maurizio Pellecchia**, University of California, Riverside

NMR-based screening of combinatorial libraries to target protein-protein interactions with reversible or covalent agents

6:40 – 7:00 pm Closing remarks by **Bradley Falk**, Co-chair of NJACS NMR Topical Group