

# Swedish NMR meeting 2022, October 4-6

Wallenberg Conference Center, Medicinaregatan 20A, Göteborg

[www.gu.se/nmr/english/events/swedish-nmr-meeting-2022](http://www.gu.se/nmr/english/events/swedish-nmr-meeting-2022)

## ----- Tuesday October 4 -----

11.00 – 12:00 Registration, poster mounting  
12.00 – 13.00 Lunch served at Lyktan  
13.00 – 13.10 **Opening & Welcome** (Göran Karlsson, Director of SwedNMR)

13.15 – 14.00 **New Developments in Small Molecule NMR: From Fast-Pulsing 2D Experiments to Flexibility Determination Using Partially Aligned Samples**  
Burkhard Luy, Karlsruhe Institute of Technology

### Session 1 “Small molecules”, Chair: Mattias Hedenström

14.00 – 14.30 **Expanding the Boundaries of Characterising Weak Interactions in Dilute Solutions**  
Mate Erdelyi, Uppsala University

14.30 – 15.00 Coffee

15.00 – 16.00 **Selected presentations, 3x20 minutes**

Substrate binding and protonation states at the active-site of a nickel superoxide dismutase-derived metallopeptide: implications for the mechanism of superoxide degradation

Daniel Tietze, University of Gothenburg

**In-Cell Quantification of Drugs by MAS DNP NMR**

Staffan Schantz, AstraZeneca and the University of Gothenburg

**Characterization of a new rotenoid from the leaves of *Millettia oblata* ssp. *teitensis***

Ivan Kiganda, University of Nairobi and Uppsala University

16.00 – 16.30 **Isotopically labelled carbohydrates for NMR studies of protein-carbohydrate interactions**  
Gustav Nestor, Swedish University of Agricultural Sciences

16.30 – 18.00 **Bruker user meeting (I)**

**Welcome** (Dick Sandström)

**Magnet and Probe Updates** (Andrew Gibbs)

**Developments in Metabolomics NMR** (Claire Canet)

**News and Updates on Recent Bio-NMR Experiments and TopSpin Features** (Maksim Mayzel)

18.00 - 20.30 Informal mixer & Poster session

## ----- Wednesday October 5 -----

### Session 2 “BioNMR (I)”, Chair: Vladislav Orekhov

08.30 – 09.15 **Expanding the molecular basis for sugar recognition in the malarial sugar transporter**  
David Drew, Stockholm University

09.15 – 10.15 **Selected presentations, 3x20 minutes**

**Structural basis of substrate recognition and allosteric activation of the pro-apoptotic mitochondrial HtrA2 protease**

Emelie Aspholm, University of Gothenburg

**Unravelling Bcl-2 proteins' functioning at mitochondrial membrane level**

Gerhard Gröbner, Umeå University

**The MYC oncoprotein directly interacts with its chromatin cofactor PNUTS to recruit PP1 phosphatase**

Alexandra Ahlner, Linköping University

10.15 – 10.45 Coffee

10.45 – 11.15 **The tale of loop-mutations: How a natural variant of the SARS-CoV-2 nucleocapsid protein enables detailed studies of the full-length protein by solution NMR spectroscopy**  
Irena Matečko-Burmann, University of Gothenburg

11.15 – 12.15 **Selected presentations 3 x 20 minutes**

**Novel NMR Assignment strategy for large proteins with IDPs**

Peter Agback, Swedish University of Agricultural Sciences

*In-situ* characterization of the bacterial outer membrane protein A

Johannes Thoma, University of Gothenburg

*HR MAS NMR-based metabolomics – prostate cancer as case*

Ilona Dudka, Umeå University

12.30 – 13.30 Lunch served at Lyktan

**Session 3**      **“BioNMR (II)”, Chair: Göran Karlsson**

13.30 – 14.00 *Through hardship to the multidimensional NMR and back again*

Vladislav Orekhov, University of Gothenburg

14.00 – 15.00 **Selected presentations 3 x 20 minutes**

*SUN: Band-Selective Suppression of Unwanted Signals in Complex Mixtures*

Elin Alexandersson, Swedish University of Agricultural Sciences

*Metabolomics as a readout of the genotype*

Anders Malmendal, Roskilde University

*Water transport in paper-based packaging materials and other examples of MRI and NMR in chemical engineering*

Diana Bernin, Chalmers University of Technology

15.00 – 16.30 Coffee, poster session and/or visit at the Swedish NMR Centre

16.30 – 17.00 *Automated metabolite quantitation by <sup>1</sup>H-NMR*

Hanna Eriksson Röhnisch, Swedish University of Agricultural Sciences

17.00 – 18.00 **Bruker user meeting (II)**

*Game Changing Sensitivity Enhancement with the CPMAS CryoProbe (Alia Hassan)*

*Benchtop NMR Updates (Jens Chr. Madsen)*

*Service News (Nils Nyberg)*

18.30 – 21.00 Meeting Dinner at Restaurant Lyktan

----- **Thursday October 6** -----

08.30 – 09.15 *How NMR spectroscopy can help close the phosphate cycle*

Ulla Gro Nielsen, University of Southern Denmark

**Session 4**      **Solids and Materials NMR, Chairs: Tobias Sparrman & Sergei Dvinskikh**

09.15 – 10.15 **Selected presentations 3 x 20 minutes**

*Studying modified cellulose materials using DNP-NMR spectroscopy*

Hampus Karlsson, Chalmers University of Technology

*The right answer for the right reason: towards reliable predictions of paramagnetic NMR shifts*

Aleksander Jaworski, Stockholm University

*Hydrogen bonding in bulk and nanoconfined ionic liquid crystals*

Sergei Dvinskikh, Royal Institute of Technology

10.15 – 10.45 Coffee

10.45 – 11.15 *The fate of Li ions in the carbon electrodes of Li-ion batteries*

Istvan Furo, Royal Institute of Technology

11.15 – 12.15 **Selected presentations 3 x 20 minutes**

*A first peek at the Nordic Algae Cell Wall Structure*

Tobias Sparrman, Umeå University

*Multi-scale structural investigations of protein materials*

Christofer Lendel, Royal Institute of Technology

*MAS DNP NMR for Pharmaceutical Formulation Characterization*

Arthur C. Pinon, University of Gothenburg

12.30 – 13.30 Lunch served at Lyktan

13.30 – 14.15 *Solid-State NMR of Pharmaceuticals and Plant Cell Walls*

Steven Brown, Warwick University

14.15 – 14.30 Closing remarks (tba)

Scientific committee: SwedNMR module groups & Mattias Hedenström, Sergei Dvinskikh, Vladislav Orekhov, Göran Karlsson.

Local committee: C. Persson, A. Pedersen, U. Brath, D. Malmodin, A. Pinon, Z. Takacs, Göran Karlsson, Swedish NMR Centre