Conference Agenda

Session Overview

Date: Sunday, 06/July/2025

9:30 - 11:45	**JEOL breakfast seminar** Location: **Tulindberg Hall**
11:30 - 15:30	**Bruker lunch symposium** Location: **Tulindberg Hall** Lunch 11:30-12:30, Symposium 12:30 -15:30
16:00 - 19:00	**Opening and prize ceremonies** Location: **Madetoja Hall** Hostess: Anu Kantola
19:00 - 21:00	**Welcome reception** Location: **Pohjankartano lobby** Welcome reception by the City of Oulu

Date: Monday, 07/July/2025

8:45 - 10:15

Plenary 1
Location: **Madetoja Hall**
Chair: Juha Vaara

8:45 - 9:30

Fractals and Polymer Upcycling: Imaging, Spectroscopy, Relaxometry, Diffusometry

Jeffrey Reimer

9:30 - 10:15

Magnetic Resonance and Integrative Structural Biology, Outside and Inside Mammalian Cells

Tatyana Polenova, Angela Gronenborn, Caitlin Quinn, Kumar Tekwani Movellan, Changmiao Guo, Roman Zadorozhnyi, Somayeh Zeinalilathori, Jochem Struppe, Daniel Banks, James Kempf

10:15 - 10:45

Coffee
Location: **Music Center and Pohjankartano lobbies**

10:45 - 12:45

Parallel 1: BioNMR
Location: **Madetoja Hall**
Chair: Perttu Permi

10:45 - 11:15

Intrinsically disordered regulators of endocytosis - an integrated NMR/single molecule fluorescence approach

Sigrid Milles

11:15 - 11:35

Long-lived coherences in the direct dimension to follow redox kinetics of antioxidants in cells

Aude Sadet, Elena Ionita, Ioana Fidel, Cristina Stavarache, Mihai Ciubotaru, Dennis Kurzbach, Paul Vasos

11:35 - 11:40

Unraveling the side-chain dynamics of the protein kinase p38ɣ through Ultrafast High-Resolution Relaxometry (UHRR)

Ana Paula Aguilar Alva, Lucas Siemons, Ulric le Paige, Philippe Pelupessy, Guillaume Bouvignies, Nicolas Wolff, Florence Cordier, Jorge Garibay, Agnès Glemot, Philip Wurm, Jean-Max Tyburn, Fabien Ferrage

11:40 - 11:45

Distinct mechanisms of allosteric modulation at the β1-adrenergic receptor

Thomas H. Harman, Timothy Noel, Andrew J. Y. Jones, Graham Ladds, Daniel Nietlispach

11:45 - 11:50

Isoleucine Side Chains as Reporters of Conformational Freedom in Protein Folding Studied by DNP-Enhanced NMR

Leonardo Levorin, Nina Becker, Boran Uluca-Yazgi, Luis Gardon, Mirko Kraus, Philipp Neudecker, Lothar Gremer, Henrike Heise

Parallel 2: Benchtop and low field
Location: **Tulindberg Hall**
Chair: Camilla Terenzi

10:45 - 11:15

New directions in ultralow-field NMR

Michael C D Tayler

11:15 - 11:35

Live magnetic observation of parahydrogen hyperpolarization dynamics

James Eills, Morgan W. Mitchell, Irene Marco Rius, Michael C. D. Tayler

11:35 - 11:40

New developments in high-pressure low-field NMR spectroscopy

Johannes Denninger, Sergio Alejandro Ortiz Restrepo, Anton Duchowny, Koen Linssen, Alina Adams

11:40 - 11:45

Benchtop DNP on Varying 1H Spins Quantities Towards Broad Range Sample Hyperpolarization

Charlotte Bocquelet, Ewoud Vaneeckhaute, Arianna Actis, Nathan Rougier, Huu-Nghia Le, Laurent Veyre, Chloe Thieuleux, James Kempf, Arthur Pinon, Quentin Stern, Sami Jannin

11:45 - 11:50

Towards quantitative analysis of complex mixtures with benchtop spectroscopy using SABRE hyperpolarisation

Bono O. Jimmink, Mattia Negroni, Arno P.M. Kentgens, Marco Tessari

11:50 - 11:55

Benchtop NMR analysis of illicit drugs

Shallu Verma, James A. Robinson, Ben Bogun, Daniel J. Holland

Parallel 3: Hyperpolarisation
Location: **Pohjankartano Hall**
Chair: Mikko Kettunen

10:45 - 11:15

Exploring Xe Exchange Kinetics for Molecular Host Systems in HyperCEST NMR

Leif Schröder

11:15 - 11:35

Diamond DNP at 3.4 T and 7 T

Daphna Shimon

11:35 - 11:40

Systematic study of hyperpolarization with hybrid polarizing solids – moving towards pure hyperpolarized solutions after dissolution-dynamic nuclear polarization

Ekaterina V. Pokochueva, Nghia H. Le, Sylvie Guibert, Chloé Gioiosa, Quentin Stern, James Tolchard, Charlotte Bocquelet, Olivier Cala, Matthieu Cavailles, Laurent Veyre, Otto Mankinen, Ville-Veikko Telkki, Chloé Thieuleux, Sami Jannin

11:40 - 11:45

Nitroxide-Doped Solid Matrices: a New DNP MAS NMR Approach to Polarize Sensitive Surfaces

Salah-Eddine Akrial, Nghia Le, Judith Schlagnitweit, Soleyah Houget, Teresa Insinna, Gille Casano, Laurent Veyre, Clémant Camp, David Gajan, Olivier Ouari, Chloé Thieuleux, Anne Lesage

11:45 - 11:50

SCREAM-DNP for Site-Specific Polarization Transfer to Heteronuclei and Ring Puckering Dynamics

Florian Taube, Max Gierth, Björn Corzilius

11:50 - 11:55

NMR masers: from single mode DNP hyperpolarization at 1.2K

	11:50 - 11:55 **Backbone resonance assignment of large intrinsically disordered proteins** Paulina Bartosińska-Marzec, Sonja Knödlstorfer, Thomas Schwarz, Karin Ledolter, Wiktor Koźmiński, Robert Konrat, Anna Zawadzka-Kazimierczuk **11:55 - 12:15** **Combining NMR and AlphaFold to identify new partner protein binding motifs in intrinsically disordered proteins** Elise Delaforge, Thibault Orand, Maud Tengo, Andrés Palencia, Malene R. Jensen **12:15 - 12:45** **NMR sheds light on the DNA binding mechanism of multi-zinc finger proteins** Thibault Viennet, Maolu Yin, Stuart Orkin, Haribabu Arthanari	**11:55 - 12:15** **Toward a more accessible NMR metabolomics with ultra-resolved methods to enhance the performance of compact NMR** Jonathan Farjon, Joris Mandral, Jean-Nicolas Dumez, Patrick Giraudeau **12:15 - 12:45** **Rethinking Brownstein and Tarr in Biological Porous Media** Kathryn Anderssen	**to multimode masers in solution through electronic control of radiation feedback.** Vineeth Francis Thalakottoor Jose Chacko, Alain Louis-Joseph, Daniel Abergel **11:55 - 12:15** **Symmetry-Based Pulsed DNP and EPR Sequences** Zhenfeng Pang, Giuseppe Sicoli, Benoit Driesschaert, Jean-Paul Amoureux, Hervé Vezin, Kong Ooi Tan **12:15 - 12:45** **SABRE of pyruvate: Linking catalyst design to spin and exchange dynamics** Gabriele Stevanato
12:45 - 13:45	**JEOL lunch workshop** Location: **Tulindberg Hall**	**Lunch** Location: **Music Center and Pohjankartano lobbies**	
13:45 - 15:45	**Posters: Odd-numbered posters** Location: **Pohjankartano lobby**		
15:45 - 17:45	**Parallel 4: Materials** Location: **Madetoja Hall** Chair: Bernhard Bluemich **15:45 - 16:15** **STABILITY OF MOF IN PRESENCE OF WATER: NEW INSIGHTS FROM HIGH-FIELD SOLID-STATE NMR** Athulya Nadol, Florian Venel, Raynald Giovine, Jessica Špačková, Thomas-Vavier Métro, Danielle Laurencin, Christel Gervais, Christophe Volkringer, Olivier Lafon, Frédérique Pourpoint **16:15 - 16:35** **NMR of endofullerenes and endofullerides** George Razvan Bacanu, Murari Soundararajan, Geoffrey Paul McNulty, Vijyesh K. Vyas, Keisuke Matsui, Naoya Yoshikane, Mark C. Walkey, Elisabeth S. Marsden, Gabriela Hoffman, Sally Bloodworth, Francesco Giustiniano, Karel Kouřil, Marina Caravetta, Kosmas Prassides, Richard J. Whitby, Malcolm H. Levitt **16:35 - 16:40** **Degradation Assessment and Conservation Monitoring of Waterlogged Archeological Wood by Multimodal and Multiparametric NMR Methods** Elisa Villani, Valeria Stagno, Liisa	**Parallel 5: EPR** Location: **Tulindberg Hall** Chair: Olav Schiemann **15:45 - 16:15** **Effects of methyl groups in proteins on electron spin echo decay** Gunnar Jeschke **16:15 - 16:35** **Pulsed EPR and DNP at 94 GHz** Thierry Dubroca, Ilya Litvak, Chiemeka Korrigan Amadi **16:35 - 16:40** **High Field EPR Investigation of ^{13}C DNP Mechanisms of P1 Centers in Diamond** Orit Nir-Arad, David H. Shlomi, Eyal Laster, Nurit Manukovsky, Alexander B. Fialkov, Ilia Kaminker **16:40 - 16:45** **Sensitivity increase & 2D Deconvolution of ENDOR spectra with chirp pulses** Julian Alexander Stropp, Nino Wili, Daniel Klose **16:45 - 16:50** **Analysing the architecture of PTBP1-RNA biomolecular condensates with pulsed EPR** Olga Vojtíšková, Yinan Ni, Sergei Kuzin, Frédéric Allain, Gunnar	**Parallel 6: Small molecules and pharmaceuticals** Location: **Pohjankartano Hall** Chair: Tuulia Tynkkynen **15:45 - 16:15** **Shining light on polyaspartates: Novel photoresponsive alignment media for structure elucidation** Rimjhim Hossain, Christina Thiele **16:15 - 16:35** **19F MAS DNP Enhanced NMR Spectroscopy of Drug Molecules** Judith Schlagnitweit, Annabelle Peyronnet, David Gajan, Martins Balodis, Guido Pintacuda, Olivier Ouari, Anne Lesage **16:35 - 16:40** **Fast and flow-compatible 3D diffusion NMR** Yuliia Horbenko, Jérémy Marchand, Aurélie Bernard, Patrick Giraudeau, François-Xavier Felpin, Jean-Nicolas Dumez **16:40 - 16:45** **Interplay between polymer dynamics and dynamic reaction networks** Dawei Qi, Xuncheng Shi, Caihong Lin, Jianwei Li **16:45 - 16:50**

Ivancic, Ville-Veikko Telkki, Magdalena Broda, Silvia Capuani, Otto Mankinen

16:40 - 16:45

Optimally Controlled NMR in Electrochemistry: Surface-Selective Measurements above Conductive Materials

Armin Johannes Römer, Johannes Florian Kochs, Michael Schatz, Matthias Streun, Sven Jovanovic, Simone Swantje Köcher, Josef Granwehr

16:45 - 16:50

Close-up of a key step in the elaboration of a new phase change material : Solvent – Cellulose Interactions Studied by Pulse Field Gradient NMR

Djibril Rouzaud, Philippe Bazin, Arnaud Travert, Cassandre Kouvatas

16:50 - 16:55

Characterization of Reclaimed Old Wood using 3 point flexure test and Solid-State NMR

Nametso Linda Moumakwa, Mark John Hughes

16:55 - 17:15

Time-dependent diffusion power spectra and correlated exchange in entangled polymers

Sophia N. Fricke, Velencia Witherspoon, Jeremy Demarteau, Brett A. Helms, Jeffrey A. Reimer

17:15 - 17:45

The Return of Symmetry-Based Pulse Sequences

Urvashi Heramun, Mohamed Sabba, M. Bonifac Legrady, Chloe Gioiosa, Quentin Stern, Sami Jannin, Malcolm H. Levitt

Jeschke, Maxim Yulikov

16:50 - 16:55

Enabling EPR measurements in cells utilising reductively stable spin labels

Yannik Limbach, Caspar Heubach, Olav Schiemann, Bela Bode

16:55 - 17:15

Tracing host-pathogen interactions through pulse dipolar EPR spectroscopy – pathogen surface protein interaction with host tissue

Katrin Ackermann, Laura Remmel, Bela Ernest Bode

17:15 - 17:45

Exploring Organic Photovoltaics from the Spin Perspective with EPR and EDMR

Claudia Tait, Jack Palmer, Lorenzo Catini

Fully automated analysis of photo-CIDNP NMR spectra for fast fragment screening

Giulia Fischetti, Nicolas Schmid, Matthias Bütikofer, Félix Torres, Andreas Henrici, Dirk Wilhelm

16:50 - 16:55

NMR of H2@C70 & 2(H2)@C70 Endofullerenes in a Magnetically Aligned Liquid Crystal Solution

Geoffrey P McNulty, George R Bacanu, Vijyesh K Vyas, Murari Soundararajan, Stéphane Rols, Richard J Whitby, Malcolm H Levitt

16:55 - 17:15

Enantiomeric discrimination of pharmaceutical ingredients by NMR in chiral weakly orienting media

Vincent Chiapolino, François-Marie Moussallieh, Philippe Lesot, Boris Gouilleux

17:15 - 17:45

Ultrahigh-resolution NMR spectroscopy

Ralph Adams

17:45 - 18:15 — **Coffee**
Location: **Music Center and Pohjankartano lobbies**

18:15 - 19:00 — **Plenary 2**
Location: **Madetoja Hall**
Chair: Isabella Felli

18:15 - 19:00

Animal Detected Magnetic Resonance

Peter Hore

20:00 - 23:00 — **Bruker night**
Location: **Nallikari restaurant**

Date: Tuesday, 08/July/2025

8:45 - 10:15

Plenary 3
Location: **Madetoja Hall**
Chair: Chantal Tax

8:45 - 9:30

RNA dynamics and its impact on function

Katja Petzold, Emma R. Andersson, Alan Chen

9:30 - 10:15

From NMR of tissue samples to Metabolic MRI in patients

Dennis Klomp

10:15 - 10:45

Coffee
Location: **Music Center and Pohjankartano lobbies**

10:45 - 12:45

Parallel 7: Liquid-state methods
Location: **Madetoja Hall**
Chair: Petrik Galvosas

10:45 - 11:15

NMR transport studies in battery electrolytes – ion transport mechanisms and ion-ion correlations

Monika Schönhoff

11:15 - 11:35

NMR relaxation and diffusion study of liquid phase separations in confinement

Siegfried Stapf, Niklas Siebert, Carlos Mattea, Bulat Gizatullin, Anam Sara, Christian Dressler

11:35 - 11:40

Real-time NMR Investigation of Electrolyte Degradation in Aqueous Organic Redox Flow Batteries

Kawarpal Singh, Clare Grey

11:40 - 11:45

Lithium-ion motional behavior under confinement: An NMR study of Carbon aerogel

Surya Parkash, Samanwita Pal

11:45 - 11:50

A new method to extract couplings between prochiral methylene protons with very close chemical shifts

Elisa Norzagaray, James R.D. Montgomery, Davy Sinnaeve

11:50 - 11:55

Robust bilinear rotations and HUGE-BIRD

Yannik Tomas Woordes, Tony Reinsperger, Burkhard Luy

11:55 - 12:15

Ultrafast Laplace NMR for biomaterials

Otto Mankinen, Katja Tolkkinen, Chang Qi, Atte Lepistö, Antti

Parallel 8: EPR
Location: **Tulindberg Hall**
Chair: Marilena Di Valentin

10:45 - 11:15

Following Conformational Changes in Cas13a with PELDOR

Olav Schiemann, Maria Vicino, Catrin Allar, Benjamin Kaupp

11:15 - 11:35

NV Centers Based Hyperpolarization of Local and Bulk 13C Nuclei in Diamond at 7 and 14 T

Ilia Kaminker

11:35 - 11:40

94 GHz chirp and phase-modulated EPR experiments for spin dynamics analysis and ENDOR spectroscopy

Marvin Lenjer, Nino Wili, Fabian Hecker, Marina Bennati

11:40 - 11:45

The peptides within R5-templated silica particles resemble a condensed phase with liquid-like properties

Dörte Brandis, Giulia Mollica, Dennis Kurzbach

11:45 - 11:50

RNA-binding proteins undergoing Liquid-Liquid Phase Separation – Towards building a conformational ensemble using DEER

Elise Komarczuk, Maria Escura Pérez, Laura Galazzo, Maxim Yulikov, Frédéric Allain, Gunnar Jeschke

11:50 - 11:55

Combining Orientation selective Light-Induced Pulsed Dipolar Spectroscopy with Molecular Dynamics

Giulia Da Ros, Daniele Panariti, Ghejli Kullolli, Arnau Bertran,

Parallel 9: Solid-state methods
Location: **Pohjankartano Hall**
Chair: Anne Lesage

10:45 - 11:15

Fast magic-angle spinning rates and deuteration facilitate proton detected solid-state NMR spectroscopy to study the cell walls of pathogenic fungi

Alons Lends, Alvis Zvirgzdins, Ats Kaldma, Jana Petkus, Ago Samoson

11:15 - 11:35

DNP surface-enhanced 17O MQMAS and D-HOMCOR of 17O labeled metal oxides

Hiroki Nagashima, Julien Trébosc, Olivier Lafon, Jean-Paul Amoureux

11:35 - 11:40

The role of formate mobility for adaptive hydrogenation catalysts probed by solid-state NMR spectroscopy

Yufei Wu, Yuyan Zhang, Julius Schlüter, Henrik Walschus, Maria Fyta, Walter Leitner, Alexis Bordet, Thomas Wiegand

11:40 - 11:45

Deeper insight into supramolecular hydrogel structure and dynamics through the combined use of solid-state, liquid-state and relaxometry NMR

Corentin Boulogne, Jeremy Morere, Paul Hoschtettler, Marie-Christine Averlant-Petit, Emmanuelle Bignon, Loïc Stefan, Sabine Bouguet-Bonnet, Carole Gardiennet

11:45 - 11:50

Investigating structural parameters via ^{199}Hg NMR spectroscopy

Jakub Obuch, Libor Kobera, Jiří Brus, Petr Hermann

11:50 - 11:55

	Raasakka, Sarah Mailhiot, Mateusz Urbańczyk, Christian Hilty, Ville-Veikko Telkki 12:15 - 12:45 **Shining the light on Diffusion NMR. The Time-Resolved Diffusion NMR for studying photochemical reactions** Mateusz Urbańczyk, Marek Czarnota, Farwa Khalid, Chunchesh Malangi Gajendramurthy	Christiane Timmel, Marina Gobbo, Alberta Ferrarini, Marilena Di Valentin, Alice Bowen 11:55 - 12:15 **Triplet Excitons in Carbon Nitride Photocatalysts** Arianna Actis, Michele Melchionna, Giacomo FIlippini, Paolo Fornasiero, Maurizio Prato, Mario Chiesa, Enrico Salvadori 12:15 - 12:45 **Advances in oscillator-based magnetic resonance** Jens Anders, Michal Kern, Bernhard Blümich, Klaus Lips	**Concentration-Dependent Mechanisms of Melittin-Induced Membrane Destabilization: An Interdisciplinary Approach** Andrea Chacón Calderón, Pavel Zelenovskii, Márcio Soares, Ellen C. Wrobel, Osvaldo N. Oliveira Jr., Daniel Pereira, Luís Mafra, Mariana Sardo, Ildefonso Marín-Montesinos, Ana Barros-Timmons 11:55 - 12:15 **Structures and Dynamics of Self-Assembled and Membrane-Bound Tau from Solid-State NMR** Mei Hong 12:15 - 12:45 **Development of MAS solid-state NMR methods and applications to the structural characterization of amyloid fibrils** Bernd Reif
12:45 - 13:45	**Lunch** Location: Music Center and Pohjankartano lobbies		
13:15 - 14:15	**Magritek lunch workshop** Location: Tulindberg Hall		
13:45 - 15:45	**Posters: Even-numbered posters** Location: Pohjankartano lobby		
15:45 - 16:45	**Tutorial 1: Magnetic Resonance tutorial** Location: Madetoja Hall Chair: Perttu Hilla 15:45 - 16:45 **Solid-State NMR Techniques for Efficient Protein Structure Determination** Mei Hong	**CCPN Workshop** Location: Class room B114	
16:45 - 17:45	**Tutorial 2** Location: Madetoja Hall Chair: Perttu Hilla **Multidimensional diffusion-relaxation correlation NMR and MRI** Daniel Topgaard	**CCPN Workshop** Location: Class room B114	
17:45 - 18:15	**Coffee** Location: Music Center lobby		
18:15 - 19:00	**Plenary 4** Location: Madetoja Hall Chair: Alexander Barnes 18:15 - 19:00 **New applications of magnetic resonance and DNP NMR methods to study interfaces and complex oxides in lithium batteries** Clare Grey		
19:00 - 20:30	**JEOL music night** Location: Madetoja Hall		

Date: Wednesday, 09/July/2025

8:45 - 10:15

Plenary 5
Location: **Madetoja Hall**
Chair: Patrick Giraudeau

8:45 - 9:30

Magnetic resonance at nanoscale enabled by diamond spin qubits

Fedor Jelezko

9:30 - 10:15

Exploring the properties of photogenerated multi-spin systems by transient EPR spectroscopy

Sabine Richert

10:15 - 10:45

Coffee
Location: **Music Center and Pohjankartano lobbies**

10:45 - 12:45

Parallel 10: BioNMR
Location: **Madetoja Hall**
Chair: Oscar Millet

10:45 - 11:15

The dynamic chaperone network in the endoplasmic reticulum

Sebastian Hiller, Anna Leder, Guillaume Mas

11:15 - 11:35

Exploiting bacterial OMVs as tools for the in-situ characterization of proteins

Björn Burmann

11:35 - 11:40

Combined solution- and MAS NMR reveal a locally unfolded state of the bacteriophage tail tube that prevents premature assembly

Undina Guillerm, Yong Wang, Charles-Adrien Arnaud, Claudine Darnault, Kresten Lindorff-Larsen, Cécile Breyton, Paul Schanda

11:40 - 11:45

Efficient NMR methods to characterize therapeutic antibodies at atomic resolution.

Béatrice Vibert, Faustine Henot, Arthur Giraud, Sarra Dbira, Rida Awad, Elodie Crublet, Lionel Imbert, Oriane Frances, Camille Doyen, Jérôme Boisbouvier

11:45 - 11:50

Expression And NMR Characterization Of Labelled P-domains Of Emerging Norovirus

Siyu Lin, Henry Flatau, Ileana Zeravica, Rebecca Calamandrei, Linda Cerofolini, Jesus Angulo, Cristina Nativi, Marco Fragai

11:50 - 11:55

NMR Reveals a Cryptic SH2 Binding Motif in the Disordered Region of Src

Parallel 11: Single-molecule/NV, BioNMR and Hyperpolarisation
Location: **Tulindberg Hall**
Chair: Igor Koptyug
Talk of C. Degen will be given by K. Herb.

10:45 - 11:15

Optical detection of single defect spins in diamond

Christian Degen

11:15 - 11:35

Switching off a GPCR: different facets of receptor desensitization studied at atomic resolution

Arnelle Löbbert, Nils Lorz, Philip Rößler, Alvar D. Gossert

11:35 - 11:40

High-precision spectroscopy of a single 93Nb nuclear spin in solid

Zhiyuan Will Huang, Jaime Travesedo, Nicholas Thill, James O'Sullivan, Louis Pallegoix, Philippe Goldner, Patrice Bertet, Emmanuel Flurin

11:40 - 11:45

SimOS: A Python Framework for Simulations of Optically Addressable Spins

Laura A. Völker, John M. Abendroth, Christian L. Degen, Konstantin Herb

11:45 - 11:50

Structural transition from closed to open for the Influenza A M2 proton channel as observed by proton-detected solid-state NMR

Swantje Mohr, Caspar Schattenberg, Tillmann Utesch, Henry Sawczyc, Veniamin Chevelkov, Sascha Lange, Jacek Kozuch, Han Sun, Adam Lange

11:50 - 11:55

Suitability of Various Cryptophane-A Derivatives for Gadolinium Detection in

Parallel 12: Theory and computation
Location: **Pohjankartano Hall**
Chair: Perttu Lantto

10:45 - 11:15

Exploiting NMR Crystallography for the Study of Disorder in Phosphate-Based Frameworks

Sharon Ashbrook

11:15 - 11:35

Equivariant Neural Networks Reveal How Host–Guest Interactions Shape Xenon NMR Chemical Shift in Porous Organic Cages

Ouail Zakary, Perttu Lantto

11:35 - 11:40

Nuclear spin-state transport in nonlinear kinetic processes

Anupama Acharya, Madhukar Said, Sylwia J. Barker, Marcel Utz, Bruno Linclau, Ilya Kuprov

11:40 - 11:45

Atomistic structures of early-stage prenucleation clusters by hyperpolarized NMR-validated, quantum mechanical calculations

Christopher Pötzl, Ertan Turhan, Christel Gervais, Thierry Azaïs, Dennis Kurzbach

11:45 - 11:50

MOLDETR: A CHEMISTRY-INFORMED DEEP LEARNING MODEL FOR NEXT-GENERATION ANALYSIS OF MOLECULAR SPECTRA

Nicolas Schmid, Marc Wanner, Giulia Fischetti, Andreas Henrici, Mohsen Meshkian, Simon Bruderer, Rudolf M. Füchslin, Bjoern Heitmann, Jan Dirk Wegner, Roland K.O. Sigel, Dirk Wilhelm

11:50 - 11:55

Instrumental distortions in quantum optimal control

	Alejandro Fernández, Andras Lang, Marga Gairí, Maria Teresa González, Miquel Pons **11:55 - 12:15** **Metabolite partitioning into biomolecular condensates mimics organic solvent behaviour** Virgínia Casablancas-Antràs, James T. Eaton, Ben R. Naylor, Charles J. Buchanan, Abigail Turner, Spencer J. Anthony-Cahill, Andrew J. Baldwin **12:15 - 12:45** **Cross-correlated relaxation experiments for studying protein structure and dynamics** Anna Zawadzka-Kazimierczuk, Paulina Bartosińska-Marzec, Irene Ceccolini, Clemens Kauffmann, Bartłomiej Banaś, Andreas Beier, Daniel Braun, Julian Holzinger, Wiktor Koźmiński, Robert Konrat	**Solution using 129Xe HyperCEST Spectroscopy** Hannah Louise Gerbeth, Jabadurai Jayapaul, Patrick Werner, Leif Schröder **11:55 - 12:15** **Towards a nanodiamond-based plateform for room temperature hyperpolarization** Rémi Blinder, Yuliya Mindarava, Martin Korzeczek, Alastair Marshall, Felix Glöckler, Steffen Nothelfer, Alwin Kienle, Christian Laube, Wolfgang Knolle, Christian Jentgens, Viatcheslav Agafonov, Valery Davydov, Martin Plenio, Fedor Jelezko **12:15 - 12:45** **Quantum sensing with diamond nitrogen vacancy centers** Ania Bleszynski	Uluk Rasulov, Ilya Kuprov **11:55 - 12:15** **SLEEPY: Simple simulation of relaxation and dynamics in NMR** Albert Andrew Smith-Penzel, Kai Zumpfe **12:15 - 12:45** **Fast and Highly Resolved NMR: Photo-CIDNP and super resolution NMR** Roland Riek
12:45 - 13:45	**Lunch** Location: **Music Center and Pohjankartano lobbies**		
13:45 - 15:45	**Posters: All posters** Location: **Pohjankartano lobby**		
15:45 - 17:45	**Parallel 13: Hyperpolarisation** Location: **Madetoja Hall** Chair: Vladimir Zhivonitko **15:45 - 16:15** **High-field optically induced NMR hyperpolarization in solids** Lyndon Emsley **16:15 - 16:35** **Hyperpolarizing porous polymer matrices for MAS DNP** Johanna Guazzelli, Marie Juramy, Théo El Daraï, Léo Gazzetta, Samuel F. Cousin, Damien Montarnal, Sami Jannin, Trang Phan, Didier Gigmes, Giulia Mollica **16:35 - 16:40** **Field-dependent 15N Relaxation and Chemically Induced Deceleration of Nuclear Spin Relaxation (CIDER)** Josh Philipp Peters, Charbel Assaf, Arne Brahms, Kolja Them, Mirco Gerdsen, Rainer Herges, Jan-Bernd Hövener, Andrey N. Pravdivtsev **16:40 - 16:45** **J-coupling interactions and Hydrogen/Ligand Exchange in SABRE Systems** Charbel D. Assaf, Oleg G. Salnikov, Vladimir Zhivonitko, Xin Gui, Anna P. Yi, Simon B. Duckett, Eduard Chekmenev, Alexander A. Auer, Igor V. Koptyug, Jan-bernd Hövener, Andrey N. Pravdivtsev	**Parallel 14: Metabolomics** Location: **Tulindberg Hall** Chair: Mateusz Urbańczyk **15:45 - 16:15** **Adapting parahydrogen hyperpolarization for metabolomics applications** Kerti Ausmees, Kärolin Kork, Claudia Kallaste, Indrek Reile **16:15 - 16:35** **Hyperpolarization and deuterium NMR enable real-time in vitro metabolomics: yeast and intestinal organoids case study** Josh P. Peters, Hang Xiang, Fatima Anum, Farhad Haj Mohamad, Charbel Assaf, Philip Rosenstiel, Stefan Schreiber, Jan-Bernd Hövener, Konrad Aden, Andrey Pravdivtsev **16:35 - 16:55** **Ultrafast Correlation Spectroscopy with multi-solvent suppression for the analysis of wine** Pia S. Mayer, Jérémy Marchand, Marine P.M. Letertre, Jean-Nicolas Dumez, Søren B. Engelsen, Patrick Giraudeau **16:55 - 17:15** **Pure Shift NMR: A Robust and General Method for Determining Quantitative Metabolic Profiles in Biofluids** Nicolas Giraud	**Parallel 15: Materials** Location: **Pohjankartano Hall** Chair: Guido Pintacuda **15:45 - 16:15** **Approaches for operando Nuclear Magnetic Resonance of rechargeable batteries** Raphael Praud, Ludivine Afonso de Araujo, Khashayar Bagheri, Beas Roy, Vincent Sarou-Kanian, David Sicsic, Michael Deschamps, Elodie Salager **16:15 - 16:35** **CO_2 Speciation in Amine-Modified Porous Silicas for Direct Air Capture by DNP Enhanced Solid-State NMR** Ildefonso Marín-Montesinos, Márcio Soares, Salah-Eddine Akrial, David Gajan, Mariana Sardo, Anne Lesage, Luís Mafra **16:35 - 16:40** **Classification and Identification of Facet- and Edge-Specific γ-Al2O3 Surface Sites from 1H/27Al NMR Cross-Signatures and DFT Modelling** Domenico Gioffrè, Pierre Florian, Thomas Pigeon, Pascal Raybaud, Céline Chizallet, Christophe Copéret **16:40 - 16:45** **INVESTIGATING DYNAMIC PROCESSES IN MOLECULAR CHARGE CARRIERS BY MEANS OF NMR**

16:45 - 16:50

Glucose as a Versatile Glassing Agent for Hyperpolarizing Key Metabolites in Biological Studies

Léa Gutiérrez, Mehdi Soussi-Therond, Charles Bretot, Karen Dos Santos, Aiky Razanahoera, Daniel Abergel, Véronique Baud, Nicolas Giraud, Mathieu Baudin

16:50 - 16:55

Monitoring pyruvate to lactate conversion in biological solutions at low magnetic fields

Charlotte Von Petersdorff-Campen, Gonzalo Gabriel Rodriguez, Maria Daniela Santi, Josef Elsaßer, Stefan Glöggler

16:55 - 17:15

Achieving strong polarization of 13C nuclei at high concentrations with parahydrogen

Vitaly Kozinenko, Bogdan Rodin, Leonard Schraff, Laurynas Dagys, Zumrud Ahmadova, Martin Korzeczek, Martin Plenio, Ilai Schwartz, Stephan Knecht

17:15 - 17:45

Elucidating Biomolecular Interactions using Hyperpolarization by Parahydrogen and Dynamic Nuclear Polarization

Nirmalya Pradhan, Oindrila Biswas, Ashes Roy, Pierce Pham, Olivia Chatterjee, Anshul Gautam, Ratnamala Mandal, Chang Qi, Christian Hilty

17:15 - 17:45

New frontiers in NMR metabolomics: integrating more sensitive and resolved NMR into the metabolomics workflow

Marine Letertre

SPECTROSCOPY AND DIFFERENTIAL SCANNING CALORIMETRY

Weronika Wrembel, Zbigniew Fojud

16:45 - 16:50

95Mo MAS SSNMR of grafted molecular complexes at ultra-high field (28.2 T)

Celine Moussa, Olivier Lafon, Julien Trebosc, Andrew Rankin, Mostafa Taoufic, Regis Gauvin, Laurent Delevoye

16:50 - 16:55

Exploiting 17O Solid-State NMR Spectroscopy of Catalysts and Porous Solids

Jonathan M. Keys, Ben L. Griffiths, Nicole L. Kelly, Daniel M. Dawson, Ming-Feng Hsieh, Chia-Hsin Chen, Stephen P. Day, Sharon E. Ashbrook

16:55 - 17:15

Pushing the Frontiers of Performance Polymers with Fast-MAS Proton NMR and DFT

Akshay Kumar, Arno Kentgens

17:15 - 17:45

Solution-State NMR and Biomineralization: Watching Minerals Form in Real Time with Hyperpolarization, AI, and Fractals

Dennis Kurzbach

17:45 - 18:15	**Coffee** Location: **Music Center and Pohjankartano lobbies**
18:15 - 19:00	**Plenary 6** Location: **Madetoja Hall** Chair: Claudia Avalos **18:15 - 19:00** **Reinventing dissolution Dynamic Nuclear Polarization (by accident and ignorance)** Sami Jannin
20:00 - 21:00	**Group walking and running** Location: **Toripolliisi, market square**

Date: Thursday, 10/July/2025

8:45 - 10:15

Plenary 7
Location: **Madetoja Hall**
Chair: Rina Rosenzweig

8:45 - 9:30

Solid-state NMR of viral (membrane) proteins

Anja Böckmann

9:30 - 10:15

From Hyperpolarization Chemistry to Quantum Oscillators: Rethinking What Nuclear Magnetic Resonance Can Be

Danila Barskiy

10:15 - 10:45

Coffee
Location: **Music Center and Pohjankartano lobbies**

10:45 - 12:45

Parallel 16: Theory and computation
Location: **Madetoja Hall**
Chair: Krzysztof Kazimierczuk

10:45 - 11:15

SimpNMR – a tool for ab initio assisted paramagnetic NMR analysis

Jon Kragskow, Ernest Borysenko, James Whipham, Elizaveta Suturina

11:15 - 11:35

Pulse Sequence Engineering using Single-Spin Vector Effective Hamiltonians

José P. Carvalho, Anders B. Nielsen, David L Goodwin, Nino Wili, Niels Chr. Nielsen

11:35 - 11:40

Rela2x: Analytic and automatic NMR relaxation theory

Perttu Hilla, Juha Vaara

11:40 - 11:45

Optimal Control Pulses for Ultrawide Bandwidth NMR Using Seedless

Jack Bercovici, Abigail L. Turner, Ben G. Davis, Andrew J. Baldwin

11:45 - 11:50

Magnetstein: Web Application for Quantitative NMR Mixture Analysis

Antoni Moszyński, Antoni Goldstein, Barbara Domżał, Michał Startek, Anna Gambin, Krzysztof Kazimierczuk

11:50 - 11:55

FAIRSpec-Ready Spectroscopic Data Collections - Enabling FAIR publication of spectral data

Mark Archibald, Ian Bruno, Stuart Chalk, Antony N. Davies, Robert M. Hanson, Stefan Kuhn, Robert J. Lancashire, Henry S. Rzepa

11:55 - 12:15

Parallel 17: Hardware
Location: **Tulindberg Hall**
Chair: Elina Sievänen

10:45 - 11:15

Methods and Instruments for High-Field MAS DNP toward Intracellular Structural Biology

Yoh Matsuki

11:15 - 11:35

42 Tesla Miniature Magnet

Pin-Hui {Sabrina} Chen, Chukun Gao, Nicholas Alaniva, James Ellison, Snædís Björgvinsdóttir, Edward Saliba, Yanhui Hu, Ioannis Pagonakis, Alexander Däpp, Ronny Gunzenhauser, Michael Urban, Jasmin Schönzart, Alexander Barnes

11:35 - 11:40

Development of a combined 329 GHz/500 MHz EPR/NMR/DNP system

Jan Dubský, Oleksii Laguta, Petr Drexler, Radovan Fiala, Ladislav Křenek, Petr Neugebauer

11:40 - 11:45

Sliding-sample DNP cryostat for thermal-swing applications

Nathan Rougier, Ewoud Vaneeckhaute, Yang Wang, Charlotte Bocquelet, Quentin Stern, Roberto Melzi, James Kempf, Sami Jannin

11:45 - 11:50

Low-field dynamic nuclear polarization for the investigation of batteries

Vera Michaela Barysch, Beatrice Wolff, Matthias Streun, Peter Jakes, Peter Philipp Maria Schleker, Josef Granwehr

11:50 - 11:55

Bridging the Funding Gap: An Open-Design 30 GHz EPR Spectrometer for Advanced DEER Applications

Parallel 18: Solid-state methods
Location: **Pohjankartano Hall**
Chair: Göran Karlsson

10:45 - 11:15

Optimizing Pulse Sequences Based on Effective Hamiltonians

Matthias Ernst

11:15 - 11:35

Structure and dynamics in filamentous phage life cycle

Amir Goldbourt

11:35 - 11:40

Beyond boundaries: ultrafast MAS at 160 kHz and high-resolution proton-detected NMR

Claire Ollier, Zhiyu Sun, Sara Medina Gomez, Eloïse Béhuré, Adrienn Rancz, Kristof Grohe, Lukas Becker, Frank Engelke, Sebastian Wegner, Tatyana Polenova, Tanguy Le Marchand, Guido Pintacuda

11:40 - 11:45

1H–87Rb Double Resonance NMR to Detect the Incorporation of Formamidinium into Rb-based Non-perovskite Phases

Ummugulsum Gunes, Michael Allan Hope, Yuxuan Zhang, Likai Zheng, Lukas Pfeifer, Michael Grätzel, Lyndon Emsley

11:45 - 11:50

Probing the backbone and binding sites of light responsive diamagnetic Zinc protoporphyrin and semi-artificial peptide scaffold by MAS NMR.

Padmaja Kar, Huub Groot

11:50 - 11:55

Beware of the structure: Phosphorus Dynamics in Post-

	SIMPSON++: Simulations and time propagation for large spin-systems David L. Goodwin, Zdeněk Tošner, Niels Chr. Nielsen **12:15 - 12:45** **Protein NMR assignment by isotope pattern recognition** Uluk Rasulov, Harrison K. Wang, Thibault Viennet, Maxim A. Droemer, Srđan Matosin, Sebastian Schindler, Zhen-Yu J. Sun, Luca Mureddu, Geerten W. Vuister, Scott Robson, Haribabu Arthanari, Ilya Kuprov	Hugo Karas, Daniel Klose, Stefan Stoll, Gunnar Jeschke **11:55 - 12:15** **A parallel line probe for spatially selective electrochemical NMR spectroscopy** Ruipeng Luo, Hans Janssen, Arno Kentgens, Evan Wenbo Zhao **12:15 - 12:45** **Increasing NMR sample throughput** Jan Korvink, Neil MacKinnon, Mazin Jouda, Dario Mager, Ronald Kampmann, Sagar Wadhwa	**Synthetically Modified NU-1000 MOF in the presence of water – Insights from Advanced NMR Spectroscopy** Jennifer Theissen, Elien Derveaux, Robert Mateo Narváez Adams, Sander Smeets, Nick Gys, Rob Ameloot, Wouter Marchal, Peter Adriaensens **11:55 - 12:15** **Calcium-Mediated Inactivation of the MthK Potassium Channel: Insights from Solid-State NMR and MD Simulations** Carl Öster, Reinier de Vries, Wojciech Kopec, Bert de Groot, Adam Lange **12:15 - 12:45** **Molecular dynamics, sparse isotope labeling, and 19F: Towards site-specificity in DNP-enhanced biomolecular MAS NMR** Björn Corzilius
12:45 - 13:45	**Lunch** Location: **Music Center and Pohjankartano lobbies**		
13:45 - 15:45	**Parallel 19: Liquid-state methods** Location: **Madetoja Hall** Chair: Anne Selent **13:45 - 14:15** **Decoding Order and Disorder in Proteins by NMR Spectroscopy** Roberta Pierattelli **14:15 - 14:35** **Precise vicinal J-couplings to determine rotamer populations in aliphatic chains by spin-chain zero-quantum spectroscopy** Kirill Sheberstov, Dmitry Cheshkov, Dmitry Sinitsyn, Geoffrey Bodenhausen **14:35 - 14:40** **What is my reaction intermediate? Resolving individual spectra in real-time NMR reaction monitoring** Nouran A. Hamed, Marshall Smith, Alexander P. Golovanov, Ralph W. Adams, Gareth A. Morris, Mathias Nilsson **14:40 - 14:45** **Water-detected NMR reveals novel insights into disease-associated RNA condensates** Johannes Schmoll, Mihajlo Novakovic, Frédéric Allain **14:45 - 14:50** **Structural and Dynamic Insights into the Loss of Activity of Tolaasin I, an**	**Parallel 20: Paramagnetic NMR** Location: **Tulindberg Hall** Chair: Matthias Ernst **13:45 - 14:15** **The revolving power of fast magic-angle spinning** Guido Pintacuda **14:15 - 14:35** **Paramagnetic materials: challenges and opportunities for solid-state NMR** Jonas Koppe, Gabriel Balavoine, Wassilios Papawassiliou, Md Ashraful Islam, Christophe Copéret, Guido Pintacuda, Andrew J Pell **14:35 - 14:40** **Bridging experiments with theory: computational solid-state NMR insight into a paramagnetic iron catalyst** Gabriel Balavoine, José Pedro Albuquerque de Carvalho, Kevin J. Sanders, Gwendal Kervern, Florian Allouche, Christophe Copéret, Guido Pintacuda, Andrew J. Pell **14:40 - 14:45** **A deep look into structure and interaction of cyclic and linear peptides based on EF-hand motifs with various lanthanides** Yulia Perevedentseva, Nikolai Klishin, Ruslan Nedielkov, Heiko M. Möller **14:45 - 14:50** **What can we learn about spin-crossover complexes using**	**Parallel 21: MRI** Location: **Pohjankartano Hall** Chair: Miika Nieminen **13:45 - 14:15** **Flow characteristics of periodic porous media using double rotation-modulated gradient diffusion NMR** Daniel Clarke, Daniel Topgaard **14:15 - 14:35** **Hyperpolarized 129Xe Uptake Dynamics in Porous Media and Polymeric Dissolved Phase for Industrial Catalysis and Clinical Applications.** Max Filkins, Stefano Collins, Guilhelm J. Collier, Graham Norquay, Jim M. Wild, Sean P. Rigby, Galina E. Pavlovskaya, Thomas Meersmann **14:35 - 14:40** **Ligand Screening Beyond T1ρ: Reducing the Protein Consumption by One Order of Magnitude with the PEARLScreen Experiment** Nils Lorz, Barbara Czarniecki, Sandra Loss, Benno Meier, Alvar D. Gossert **14:40 - 14:45** **High Throughput in NMR: Rapid Sample Analysis using Localised Spectroscopy** Marie C. Harder, Felicia Cilanov, Alvar D. Gossert, Robin A. de Graaf, Arno P. M. Kentgens

	antimicrobial cyclic lipopeptide. Durga Prasad, Niels Geudens, Benjamin Kovacs, Jose C. Martins, Monica Höfte **14:50 - 14:55** **Shaping of the selectivity profile of single-scan ultraselective NMR experiments** Armand Régheasse, Margherita Bazzoni, Rituraj Mishra, Patrick Giraudeau, Aurélie Bernard, Jean-Nicolas Dumez **14:55 - 15:15** **ShimNet: the data-driven deep learning approach to post-acquisition improvement of NMR spectra distorted by magnetic field inhomogeneity** Sylwia Jopa, Marek Bukowicki, Alexandra Shchukina, Przemysław Olbratowski, Krzysztof Kazimierczuk **15:15 - 15:45** **A Preclinical Low-Field MRI scanner for Multimodal Imaging: Photon detected-MRI and beyond** Dimitrios Sakellariou	**solid-state NMR?** Wassilios Papawassiliou, Jonas Koppe, Märker Katharina, Gabriel Balavoine, José P. Carvalho, Subhradip Paul, Guido Pintacuda, Grace G. Morgan, Gaël de Paëpe, Andrew J. Pell **14:50 - 14:55** **Fluoride coordination to Ln(III) complexes: probing anion-anion binding with low and high-Resolution NMR** Marco Ricci, Lorenzo Risolo, Daniela Lalli, Carlos Platas Iglesias, Mauro Botta **14:55 - 15:15** **Room-Temperature Overhauser DNP on luminescent poly-TTM radical films with engineered electron delocalization** Yao Fu, Petri Murto, Craig Yu, Hugo Bronstein, Clare Grey **15:15 - 15:45** **Lanthanoid tags for biomolecular NMR** Pascal Rieder, Feng-Jie Wu, Philip Rößler, Stephan Grzesiek, Alvar Gossert, Daniel Häussinger	**14:45 - 14:50** **Development of an MRI methodology for polymeric films by ex-situ solid-state NMR with a needle-like ferromagnet** Natsuki Kawabata, Naoki Asakawa **14:50 - 14:55** **High-Resolution NMR and MRI Characterization of Catalytic Reactor in Gas-Phase Enabled by Hollow Alumina Supports** Elizaveta S. Kononenko, Ivan V. Skovpin, Dudari B. Burueva, Larissa M. Kovtunova, Vladimir N. Rogozhnikov, Kristina I. Shefer, Alexey N. Salanov, Igor V. Koptyug **14:55 - 15:15** **The role and properties of lignin for bio-based carbon fibers** Diana Bernin, Feryal Guerroudj, Leandro Cid Gomes, Jenny Bengtsson **15:15 - 15:45** **Compression-Induced Microstructure in Osteoarthritic Cartilage: Insights from micro-MRI and Sodium MQF Spectroscopy** Galina Pavlovskaya, Katie Mutyambizi, Haniya Mohamed, Thomas Meersmann
15:45 - 16:15	**Coffee** Location: **Music Center lobby**		
16:15 - 17:15	**Closing ceremony** Location: **Madetoja Hall**		
17:15 - 18:45	**Plenary 8** Location: **Madetoja Hall** Chair: Marcel Utz **17:15 - 18:00** **Structural basis of the indirect inhibition of apoptosis by Bcl-xL** Enrica Bordignon **18:00 - 18:45** **Miniature 40 Tesla Magnets, Pulsed DNP and EPR with Gyrotrons, Electric MAS, and In-Cell DNP** Alexander Barnes		
20:00	**Conference dinner** Location: **Radisson Blu Hotel, Restaurant Toivo**		