

**CENTRAL EUROPEAN NMR MEETING**

# **39<sup>th</sup> NMR VALTICE**

Valtice, Czech Republic

May 17 - 20, 2026

# 39<sup>th</sup> NMR Valtice Program

**SUNDAY      MAY 17, 2026**

**6:00-6:30 PM    REGISTRATION – “VALTICKÉ PODZEMÍ“  
(GPS: 48.7396283N, 16.7502150E)**

**6:30 PM          GET-TOGETHER PARTY IN “VALTICKÉ PODZEMÍ”**

# 39<sup>th</sup> NMR Valtice Program

**MONDAY MAY 18, 2026**

**8:30-8:50**      **REGISTRATION „CENTRUM EXCELENCE“ (GPS: 48.7411942N, 16.7485308E)**

**8:50**            **OPENING – R. MAREK**

**9:00 AM**        **SESSION 1 – A. RATHNER, Session Chair**

9:00 AM        MODERN TRENDS IN MRI  
Vít Herynek

10:00 AM        CHEMICAL SHIFT IMAGING ON BIOMOLECULAR CONDENSATES  
Manuel Baumgartner

10:15 AM        RESIDUE-RESOLVED LIQUID-STATE HYPERPOLARIZED NMR OF  
PEPTIDE CONDENSATE SURFACES  
Denis Kurzbach

10:30 AM        DNA FOLDING INTERMEDIATES REVEALED BY DISSOLUTION  
DYNAMIC NUCLEAR POLARIZATION  
Milan Zachrdla

10:45 AM        CONFERENCE PHOTO I  
Radovan Fiala

**10:50 AM**      **BREAK**

**11:15 AM**      **SESSION 2 – R. POHL, Session Chair**

11:15 AM        TUNABLE OLFACTORY PEPTIDES FOR SENSITIVE DETECTION OF  
CHEMICAL AGENTS  
Adriana Rathner

11:30 AM        SELF-ASSEMBLY OF SILAFFIN R5 DERIVED PEPTIDES PROBED VIA  
NMR GUIDED MOLECULAR DYNAMICS SIMULATIONS  
Benjamin Bernrieder

11:45 AM        STRUCTURAL STUDIES OF BIOACTIVE SUPRAMOLECULAR  
COMPLEXES  
Ondřej Jurček

12:00            JEOL NEWS  
Imane Senoussaoui

- 12:20 LUNCH – HOTEL KLARET (48.7413239N, 16.7505050E)**
- 2:15 PM SESSION 3 – O. JURČEK, Session Chair**
- 2:15 PM pH INFLUENCE ON SUPRAMOLECULAR ASSEMBLIES  
Karolina Štandová
- 2:30 PM <sup>31</sup>P AND <sup>15</sup>N NMR TOOLBOX FOR STRUCTURAL ANALYSIS OF CYCLIC PHOSHAZENES  
Lucie Černá
- 2:45 PM SYNERGISTIC INSIGHTS INTO CYCLODEXTRIN — PFAS COMPLEXATION THROUGH NMR, ITC, AND QM CALCULATIONS  
Christopher Hobbs
- 3:00 PM CALCULATION AND ANALYSIS OF PSEUDOCONTACT NMR SHIFTS IN TRANSITION-METAL COMPOUNDS AND THEIR SUPRAMOLECULAR COMPLEXES  
Viliam Volko
- 3:15 PM TRACKING Ag<sup>+</sup> COORDINATION BY <sup>109</sup>Ag NMR: FROM MONOMERIC TO TRIMERIC SILVER – CARBORANE ADDUCTS  
Michal Straka
- 3:30 PM NMR-BASED STRUCTURE ELUCIDATION AND BIOACTIVITY PROFILING OF THE SECONDARY METABOLITES FROM PENTAS SPECIES  
Emanuel Mahambo
- 3:45 PM BRUKER NEWS  
Barbara Czarniecki, Frank Schumann
- 4:05 PM BREAK – Sandwich & Refreshment**
- 4:30 PM SESSION 4 – R. FIALA, Session Chair**
- 4:30 PM VLADIMÍR SKLENÁŘ SCHOLARSHIP AWARDED BY M<sub>t</sub>M & CEITEC  
Michaela Wimmerová, Felix Holáň, Radovan Fiala
- THE ROAD TOWARDS <sup>1</sup>H HOTSPOT MRI  
Martin Orságh
- 5:00 PM PETR SEDMERA PRIZE AWARDED BY THE CZECH J. M. MARCI SPECTROSCOPIC SOCIETY  
Norbert Müller, Viktor Kanický
- NMR CHALLENGE  
Martin Dračínský

**5:40 PM**

**BREAK**

**6:45 PM**

**CONFERENCE PHOTO II (GPS: 48.7401189N, 16.7567156E)**  
Radovan Fiala

**7:00-9:00 PM**

**BRUKER EVENING: “SALON VÍN ČESKÉ REPUBLIKY“**  
**(GPS: 48.7395478N, 16.7557453E)**

# 39<sup>th</sup> NMR Valtice Program

**TUESDAY MAY 19, 2026**

**9:00 AM      SESSION 5 – Z. TOŠNER, Session Chair**

9:00 AM      INVESTIGATION OF  $^{17}\text{O}$  –  $^1\text{H}$  PAIR INVOLVED IN STRONG HYDROGEN  
BOND USING RESPDOR  
Erika Bartůňková

9:15 AM      OPTIMAL CONTROL DERIVED PULSE SEQUENCE FOR MIXING OF  
HOMO-NUCLEAR ( $\text{C}\beta$ - $\text{C}\alpha$ ) SPINS – APPLICATIONS IN PROTEIN  
ASSIGNMENTS  
Vinay Ganapathy

9:30 AM      OPTIMAL CONTROL SELECTIVE PULSES FOR RELIABLE  
HETERONUCLEAR CONNECTIVITY MEASUREMENTS  
Andrej Šmelko

9:45 AM      ACCURATE SIMULATION AND INTERPRETATION OF BENCHTOP  
NMR SPECTRA WITH HQSPECTRUM  
Manuel Hodecker

10:00 AM      MACHINE LEARNING FOR PREDICTIONS OF NMR PARAMETERS  
Ema Chaloupecká

10:15 AM      BLUEFORS NEWS - HELIUM MANAGEMENT  
Julien Jousset

10:30 AM      MAGRITEK NEWS

**10:45 AM      BREAK – sponsored by Měřicí technika Morava**

**11:15 AM      SESSION 6 – M. DRAČÍNSKÝ, Session Chair**

11:15 AM      NUCLEAR MAGNETIC DIPOLE MOMENTS FROM AB INITIO  
CALCULATIONS AND NMR EXPERIMENTS: RECENT ADVANCES  
Andrej Hurajt

11:30 AM      FROM MD SIMULATIONS TO ACCURATE  $^{203}\text{Ti}$  AND  $^{205}\text{Ti}$  NUCLEAR  
MAGNETIC DIPOLE MOMENTS  
Martin Žňava

11:45 AM      PROPAGATION OF HEAVY-ATOM EFFECTS IN LIGAND NMR  
Daniel Blasco

- 12:00      MULTISPIN OPTIMAL CONTROL FOR PROTON-DETECTED  
BIOMOLECULAR SOLID-STATE NMR  
Zdeněk Tošner
- 12:15      MERCK NEWS - DEUTERIUM AND CARBON-13 KEY ISOTOPES FOR  
NMR-SPECTROSCOPY  
Matthias Schulze
- 12:35 PM      LUNCH IN KLARET (48.7413239N, 16.7505050E)**
- 2:30 PM      BRUKER WORKSHOP
- 3:15 PM      FREE DISCUSSIONS**

# 39<sup>th</sup> NMR Valtice Program

**WEDNESDAY MAY 20, 2026**

**9:00 AM      SESSION 7 – A. LYČKA, Session Chair**

9:00 AM      MEASUREMENT OF LONG-RANGE  $^1\text{H}$ - $^{13}\text{C}$  SCALAR COUPLING  
CONSTANTS FOR DETERMINATION OF CONFORMATION AND  
RELATIVE CONFIGURATION OF MOLECULES BY NMR METHODS  
Daria Lavryshchieva

9:15 AM      INVESTIGATION OF LONG-RANGE  $^4J$  AND  $^5J$  COUPLINGS IN  
AROMATIC AND BICYCLIC SYSTEMS  
Jana Pavlišová

9:30 AM      LIGHT-INDUCED ISOMERIZATION AND OXIDATION IN  
PHOSPHINOAMINO-SUBSTITUTED AZOBENZENES  
Anna Pospíšilová

9:45 AM       $^{13}\text{C}$  ATTACHED PROTON TEST EXPERIMENT IN AN ANISOTROPIC  
NMR ANALYSIS  
Eliška Procházková

10:00 AM      UNDERSTANDING pNMR SHIFTS IN TETREL RADICALS: EFFECTS OF  
SPIN – ORBIT COUPLING AND BOND COVALENCY  
Anagha Sasikumar

**10:15 AM      BREAK**

**10:45 AM      SESSION 8 – P. SRB, Session Chair**

10:45 AM      INSIGHTS INTO COMPOSITION-DRIVEN KINETICS OF  
RESORCINOL – FORMALDEHYDE POLYCONDENSATION BY LOW-  
FIELD NMR RELAXOMETRY  
Eva Kinnertová

11:00 AM       $^{14}\text{N}$ - $^1\text{H}$  COHERENCE TRANSFER VIA OPTIMAL CONTROL  
Jan Blahut

11:15 AM      REVISED MOLECULAR STRUCTURES AND THEIR FOOTPRINTS IN  
LITERATURE AND IN AI BASED SEARCHES  
Lothar Brecker

11:30 AM      APPLICATIONS OF THE DEEP LEARNING MODEL SHIFTML3 TO  
POLYMORPHIC SYSTEMS  
Jiří Czernek



|                 |                                                                       |
|-----------------|-----------------------------------------------------------------------|
| <b>11:45 AM</b> | <b>JOSEF DADOK PRIZE</b><br><u>Lothar Brecker &amp; Radovan Fiala</u> |
| <b>11:55 AM</b> | <b>CLOSING REMARKS, VALTICE 2026</b><br><u>Radek Marek</u>            |
| <b>12:00</b>    | <b>LUNCH IN KLARET (48.7413239N, 16.7505050E)</b>                     |