

CENTRAL EUROPEAN NMR MEETING

38th NMR VALTICE

Valtice, Czech Republic

May 18 - 21, 2025

CONFERENCE IS ORGANIZED BY

Central European Institute of Technology (CEITEC)

Masaryk University, Brno

THIS CONFERENCE IS SPONSORED BY

General sponsor:

Bruker

Main sponsor:

Měřicí technika Morava

Other sponsors:

(Alphabetical order)

Amedis

Bluefors

Eurisotop

Jeol

Merck

Rototec-Spintec

Sci-Tech

Zeochem

38th NMR Valtice Program

SUNDAY MAY 18, 2025

**6:30-7:00 PM REGISTRATION – “CHÂTEAU VALTICE”
(GPS: 48.7393206N, 16.7496614E)**

7:00 PM GET-TOGETHER PARTY IN “CHÂTEAU VALTICE”

38th NMR Valtice Program

MONDAY MAY 19, 2025

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

8:50 **OPENING – R. MAREK**

9:00 AM **SESSION 1 – L. BRECKER, Session Chair**

9:00 AM ¹H, ¹³C, ¹⁴N, ¹⁵N, ¹⁹F and ¹⁹⁵Pt NMR STUDY OF SOME
ASYMMETRICALLY SUBSTITUTED DIAZINE DERIVATIVES
Antonín Lyčka

9:15 AM INVESTIGATING STRUCTURAL PARAMETERS VIA ¹⁹⁹Hg NMR
SPECTROSCOPY
Jakub Obuch

9:30 AM SYNTHESIS AND NMR STUDY OF PHOSPHINE AMINOAZOBENZENE
PHOTOSWITCHES
Anna Hruzíková

9:45 AM ³¹P NMR PARAMETERS IN STRUCTURAL ANALYSIS
Eliška Procházková

10:00 AM DYNAMIC NMR: FROM 2-SITE EXCHANGE TO MULTI-SITE
EXCHANGE LINESHAPES AND THEIR ANALYTICAL FORMS
Jan Labuta

10:15 AM USE OF ANALYTICAL FORMS OF LINESHAPES FOR THE ANALYSIS
OF NMR EXCHANGE SPECTRA
Václav Březina

10:30 AM **BREAK**

11:00 AM **SESSION 2 – J. BRUS, Session Chair**

11:00 AM PARAMAGNETIC-ENHANCED SURFACE TRACKING
Jan Blahut

11:15 AM OPTIMAL CONTROL ENABLES EFFICIENT 5QMAS
Andrej Šmelko

- 11:30 AM COMPARISON OF LOW-FIELD NMR RELAXOMETRY AND DSC THERMOPOROMETRY IN CHARACTERIZING POROSITY OF CARBONACEOUS MATERIALS
Eva Kinnertová
- 11:45 AM JEOL NEWS
Imane Senoussaoui
- 12:05 LUNCH – HOTEL KLARET (48.7413239N, 16.7505050E)**
- 2:00 PM SESSION 3 – M. STRAKA, Session Chair**
- 2:00 PM THEORETICAL ANALYSIS OF EPR HYPERFINE COUPLINGS IN $\text{Ru}(\text{acac})\text{Cl}_2(\text{NH}_3)_2$ SYSTEMS
Dora Cidlinská
- 2:15 PM CONTACT NMR SHIFTS IN PARAMAGNETIC HALOGEN BONDED COCRYSTALS
Anagha Sasikumar
- 2:30 PM POSSIBLE APPLICATIONS OF SMALL FOUR-BOND COUPLING CONSTANTS IN STRUCTURAL ANALYSIS
Jana Pavlišová
- 2:45 PM NMR INVESTIGATION OF EXTREMELY STABLE *CIS* FORMS OF PHOTOSWITCHES
Erika Bartůňková
- 3:00 PM CONFORMATIONAL ANALYSIS OF *N,N*-BIS-(β -D-GLUCOPYRANOSYL) ACETAMIDE
Radek Pohl
- 3:15 PM BRUKER NEWS I
Barbara Czarniecki
- 3:35 PM BREAK – Sandwich & Refreshment**
- 4:00 PM SESSION 4 – R. FIALA, Session Chair**
- 4:00 PM VLADIMÍR SKLENÁŘ SCHOLARSHIP AWARDED BY MASARYK UNIVERSITY & MT-M
Radovan Fiala
- 4:30 PM PETR SEDMERA PRIZE AWARDED BY J. M. MARCI SPECTROSCOPIC SOCIETY
Viktor Kanický and Norbert Müller
- 5:10 PM BREAK**

6:45 PM **CONFERENCE PHOTO (GPS: 48.7401189N, 16.7567156E)**
Radovan Fiala

7:00-9:00 PM **BRUKER EVENING: “SALON VÍN ČESKÉ REPUBLIKY“**
(GPS: 48.7395478N, 16.7557453E)

38th NMR Valtice Program

TUESDAY MAY 20, 2025

9:00 AM SESSION 5 – M. DRAČÍNSKÝ, Session Chair

9:00 AM ON THE NMR PARAMETERS OF VARIOUS CONFIGURATIONS OF
COVALENT ORGANIC FRAMEWORKS
Jiří Czernek

9:15 AM FROM FLUORINATED METHANES TO SYNTHETIC CATHINONES – A
SEARCH FOR OPTIMAL DFT LEVEL FOR NMR PARAMETERS
PREDICTION
Natalina Makieieva

9:30 AM ON THE LINK BETWEEN SPIN-ORBIT RELATIVITY AND
MAGNETICALLY INDUCED CURRENT DENSITIES IN HEAVY-ATOM
HYDRIDES
Daniel Santana Blasco

9:45 AM $^1J(^{13}\text{C}-^{14}\text{N})$ COUPLINGS: WELL KNOWN, BUT RARELY DETECTED
Lothar Brecker

10:00 AM BLUEFORS NEWS: LIQUID HELIUM MANAGEMENT SOLUTIONS
Julien Jousset

10:20 AM BREAK – Měřicí technika Morava

10:45 AM SESSION 6 – E. PROCHÁZKOVÁ, Session Chair

10:45 AM STRUCTURAL BASIS OF BIS-QUINOLINIUM SCAFFOLDS BINDING
TO QUADRUPLEX-DUPLEX HYBRIDS FROM PIM1 ONCOGENE
Anirban Ghosh

11:00 AM BINDING OF ARALKYL-THIODIGALACTOSIDES TO HUMAN
GALECTIN-3: INSIGHTS FROM SATURATION TRANSFER
DIFFERENCE NMR AND MOLECULAR DOCKING
László Bence Farkash

11:15 AM SUPRAMOLECULAR STRUCTURE AND DYNAMICS OF
GLYCOPEPTIDE ANTIBIOTICS BY NMR: EREMOMYCIN AND
ORITAVANCIN
Réka Pálma Erdei

11:30 AM BRUKER NEWS II
Pavel Kessler

11:50 LUNCH IN KLARET (48.7413239N, 16.7505050E)

1:45 PM BRUKER WORKSHOP

3:00 PM FREE DISCUSSIONS

38th NMR Valtice Program

WEDNESDAY MAY 21, 2025

9:00 AM SESSION 7 – R. HRABAL, Session Chair

9:00 AM STEREOCHEMISTRY IN THE SYNTHESIS OF CALLUNENE, A
NATURAL COMPOUND WITH ANTIPARASITIC EFFECTS
Petra Cuřínová

9:15 AM PROBING THE MULTI-SUBSITE BINDING POCKET
OF GALECTIN-3 VIA ¹⁹F NMR SPECTROSCOPY
Nina Habanová

9:30 AM NMR STRUCTURE ELUCIDATION OF UNKNOWN NATURAL
PRODUCTS ISOLATED FROM MICROSCOPIC FUNGI
Lucie Černá

9:45 AM STRUCTURAL AND STEREOCHEMICAL IDENTIFICATIONS OF
RARELY FOUND FLAVAN-BENZOFURANS FROM *ARTOCARPUS*
LACUCHA USING NMR AND MOLECULAR MODELING
Weerasak Songoen

10:00 AM BREAK

10:30 AM SESSION 8 – J. BLAHUT, Session Chair

10:30 AM A CUP OF TEA OR COFFEE
Teobald Kupka

10:45 AM CHASING EXOTIC MOLECULES WITH ¹⁰⁹Ag NMR
Michal Straka

11:00 AM A “MICROSCOPE” FOR EPR DATA SOFTWARE PACKAGE FOR R
STATISTICAL LANGUAGE TO PROCESS AND ANALYZE EPR DATA
AND SPECTRA IN CHEMISTRY
Ján Tarábek

11:15 AM PERSPECTIVES OF PRESERVATION OF EQUIVALENT PATHWAYS IN
MULTIDIMENSIONAL SOLID-STATE NMR
Zdeněk Tošner

11:30 AM JOSEF DADOK PRIZE
Lothar Brecker & Radovan Fiala

11:40 AM CLOSING REMARKS, VALTICE 2026
Radek Marek

11:45 AM LUNCH IN KLARET (48.7413239N, 16.7505050E)