

CENTRAL EUROPEAN NMR MEETING

37th NMR VALTICE

Valtice, Czech Republic

May 19 - 22, 2024

37th NMR Valtice Program

SUNDAY MAY 19, 2024

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

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

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MONDAY MAY 20, 2024

- 8:30-9:00** **REGISTRATION „CENTRUM EXCELENCE“ (GPS: 48.7411942N, 16.7485308E)**
- 9:00** **OPENING – R. MAREK**
- 9:10 AM** **SESSION 1 – D. KURTZBACH, Session Chair**
- 9:10 AM NEW VISTAS FOR EPR AND ITS RELATION TO NMR
Gunnar Jeschke
- 10:00 AM PHOTOCATALYTICALLY-ASSISTED GENERATION OF TRANSIENT
RADICALS — EPR CASE STUDY EXAMPLES
Ján Tarábek
- 10:15 AM PARAMAGNETIC MOLE UNVEILS METALLACARBORANE
AGGREGATION SECRETS
P. Matějčíček, R. Fernandez-Alvarez, J. Blahut, Z. Tošner, B. Hleli, Ž. Medoš, P.
Orgin, T. Urbič, M. Bešter-Rogač
- 10:30 AM THROUGH-BOND MECHANISM OF LIGAND HYPERFINE COUPLING
J. Novotný, M. Munzarová, Radek Marek
- 10:45 AM CONFERENCE PHOTO I
Radovan Fiala
- 10:55 AM** **BREAK**
- 11:30 AM** **SESSION 2 – G. JESCHKE, Session Chair**
- 11:30 AM APPLICATIONS OF DISSOLUTION DNP FOR FAST REAL-TIME
MONITORING
Denis Kurtzbach
- 12:00 HYPERPOLARIZED NUCLEAR OVERHAUSER ENHANCEMENT OF
METHYL GROUPS
Milan Zachrdla, E. Turhan, P. Vasos, D. Kurtzbach
- 12:15 NEW PROTON-DETECTED INADEQUATE (PDI) EXPERIMENTS WITH
HSQC ARTIFACT SUPPRESSION AND A STRATEGY FOR
IDENTIFICATION OF ¹H-¹³C FOUR-BOND CORRELATIONS
J. Sakas, Dušan Uhrín, O. W. Sørensen
- 12:30** **LUNCH – HOTEL KLARET (48.7413239N, 16.7505050E)**

- 2:30 PM SESSION 3 – D. UHRÍN, Session Chair**
- 2:30 PM YELLOW TWIG (NAUCLEA ORIENTALIS): IN SITU ¹H NMR TO STUDY STRICTOSAMIDE DEGLUCOSYLATION AS A KEY STEP IN ALKALOID BIOSYNTHESIS
Weerasak Songoen, F. Traxler, J. Schinnerl, L. Brecker
- 2:45 PM CONFORMER SELECTION OF N-LACTOSYLACETAMIDE DERIVATIVE BY GALECTIN-3
Nina Habanová, J. Zýka, J. Choutka, J. Angulo, R. Pohl
- 3:00 PM INTERACTION OF MONOFUNCTIONAL PLATINUM COMPOUNDS WITH DNA
Aliaksandra Kursit, S. S. Paul, P. Podbevšek, J. Novotný, R. Marek
- 3:15 PM JEOL NEWS 2024
Ahmed Dhifaoui
- 3:30 PM BRUKER NEWS 2024
Pavel Kessler
- 3:55 PM BREAK – Sandwich & Refreshment**
- 4:30 PM SESSION 4 – R. FIALA, Session Chair**
- 4:30 PM PETR SEDMERA PRIZE AWARDED BY THE CZECH J. M. MARCI SPECTROSCOPIC SOCIETY
Radovan Fiala
- 5:10 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)**

37th NMR Valtice Program

TUESDAY MAY 21, 2024

9:15 AM SESSION 5 – J. CZERNEK, Session Chair

9:15 AM LOW-FIELD NMR RELAXOMETRY – TOOL FOR CHARACTERIZATION
OF CARBONACEOUS MATERIALS POROSITY
Eva Kinnertová, P. Kopčan, V. Slovák

9:30 AM NMR-CHALLENGE.COM: EXPLORING THE MOST COMMON
MISTAKES IN NMR ASSIGNMENTS
Zuzana Osifová, O. Socha, M. Dračínský

9:45 AM EXPLORING THE IMPACT OF ALIGNMENT MEDIA ON RDC
ANALYSIS OF ³¹P-BASED COMPOUNDS
Markéta Christou, L. Tučková, H. Kocek, A. Růžička, M. Straka, E.
Procházková

10:00 AM OXFORD INSTRUMENTS NEWS
Chris Mason

10:20 AM BREAK – Měřicí technika Morava

10:45 AM SESSION 6 – L. TRANTÍREK, Session Chair

10:45 AM NMR SIGNAL ASSIGNMENT FROM A STRUCTURAL VIEWPOINT
Jiří Czernek, M. Urbanová, J. Brus

11:00 AM DYNAMICS OF HOST-GUEST COMPLEXES AND NMR SHIFTS
Jakub Jakubec, S. S. Paul, P. Jurček, J. Novotný, P. Kulhánek, R. Marek

11:15 AM MARGITEK - WORKSHOP

12:00 LUNCH IN KLARET (48.7413239N, 16.7505050E)

2:00 PM FREE DISCUSSIONS

37th NMR Valtice Program

WEDNESDAY MAY 22, 2024

- 9:00 AM SESSION 7 – J. SÝKORA, Session Chair**
- 9:00 AM NMR METHODS FOR THE STRUCTURE ELUCIDATION OF ISOTOPICALLY-LABELLED DISINFECTION BY-PRODUCTS
Nicholle G. A. Bell, D. Uhrín, J. Sakas, R. York, E. Kitson, A. R. Smith
- 9:15 AM EXPLORING LIMITS OF MQMAS EFFICIENCY BY OPTIMAL CONTROL THEORY
Andrej Šmelko, Z. Tošner
- 9:30 AM NMR CRYSTALLOGRAPHY OF DOTAM COMPLEXES: HIGH-RESOLUTION ULTRA-WIDELINE ¹⁹⁹Hg NMR SPECTROSCOPY OF CHLOROMERCURATE POLYANIONS
Jakub Obuch, L. Kobera, J. Brus, P. Hermann
- 9:45 AM ³¹P NMR PARAMETERS FOR STEREOCHEMICAL ANALYSIS OF DOPO DERIVATIVES
Anna Hruzíková, A. Ešnerová, L. Tučková, I. Císařová, A. Růžička, O. Baszczyński, E. Procházková
- 10:00 AM SUPRAMOLECULAR ASSEMBLIES BETWEEN PLATINUM(II) COMPOUNDS AND CUCURBIT[8]URIL
Shib S. Paul, J. Novotný, R. Marek
- 10:15 AM BREAK**
- 10:45 AM SESSION 8 – Z. TOŠNER, Session Chair**
- 10:45 AM NMR STUDY OF DIIMINOISOINDOLES, PROMISING LIGANDS FOR COORDINATION CHEMISTRY
Eliška Procházková, S. Majerová, A. Růžička
- 11:00 AM ¹⁷O NMR STUDY OF AZO-HYDRAZO TAUTOMERISM
Antonín Lyčka
- 11:15 AM ¹⁴N THE HOLY GRALE FOR OPTIMAL CONTROL
Jan Blahut, M. Dračínský
- 11:30 AM JOSEF DADOK PRIZE**
Lothar Brecker & Radovan Fiala
- 11:45 AM CLOSING REMARKS**
Radek Marek
- 12:00 AM LUNCH IN KLARET (48.7413239N, 16.7505050E)**