

CENTRAL EUROPEAN NMR MEETING

31st NMR VALTICE

Valtice, Czech Republic

April 24-27, 2016

31st NMR Valtice Program

SUNDAY APRIL 24, 2016

3:00-6:00 PM REGISTRATION

6:00 PM DINNER

7:30 PM OPENING REMARKS
Radek Marek

7:40 PM PETR SEDMERA PRIZE AWARDED BY THE CZECH J. M. MARCI
SPECTROSCOPIC SOCIETY
Viktor Kanický, Vladimír Sklenář

8:30 PM EURISO-TOP GET-TOGETHER PARTY

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MONDAY APRIL 25, 2016

9:00 AM SESSION 1 – J. BRUS, Session Chair

9:00 AM USING NMR TO CHARACTERISE DYNAMICS AND DISORDER IN
MOLECULAR SOLIDS
Paul Hodgkinson

9:45 AM MULTI-OBJECTIVE SOLID-STATE NMR
Matthias Bechmann, Matthias Guggenberger

10:00 AM THEORETICAL ANALYSIS OF ¹³C RELAXATION IN CO₂ ADSORBED IN
DMOF-1
Mikuláš Peksa, Sareeya Burrekaew, Rochus Schmid, Frank Stallmach,
Jan Lang

10:15 AM CONFERENCE PHOTO
Radovan Fiala

10:30 AM BREAK

11:15 AM SESSION 2 – P. HODGKINSON, Session Chair

11:15 AM COMBINED NMR AND DFT STUDIES ON THE COMPLEXATION
CHEMISTRY OF LAPPERT'S Sn(II) DIAMIDE
Rudolph Willem, Lies Broeckert, Jan Turek, Aleš Růžička, Frank de Proft

11:30 AM GIANT ¹³C AND ²⁹Si NMR CHEMICAL SHIFTS IN TI(I) AND Pb(II)
COMPOUNDS
Jan Vicha, Radek Marek, Michal Straka

11:45 AM PLATINUM PRODRUGS FOR ENCAPSULATION WITH MACROCYCLIC
CARRIERS
Jan Chyba, Karolina Wawrocka, Radek Marek

12: 00 ISOCYTOSINE TAUTOMER EQUILIBRIUM CONTROL VIA
INTERMOLECULAR HYDROGEN BONDING
Radek Pohl, Martin Dračinský

- 12:15** **LUNCH**
- 2:15 PM** **SESSION 3 – M. BECHMANN, Session Chair**
- 2:15 PM INVESTIGATION OF CROSSLINKING IN POLY(VINYL)ALCOHOL
HYDROGELS BY CP-MAS ¹³C NMR SPECTROSCOPY
Jan Vícha, Lukáš Münster, Ivo Kuřitka
- 2:30 PM ²H CHEMICAL SHIFT IMAGING OF PHASE TRANSITION IN
POLYACRYLAMIDE NETWORK
Karel Bernášek, Lenka Hanyková, Jan Lang
- 2:45 PM MEASUREMENT OF CARBON-CARBON COUPLINGS BETWEEN
CHEMICALLY EQUIVALENT NUCLEI
Vratislav Blechta, Tomáš Strašák, Jan Sýkora
- 3:00 PM THE QUEST FOR SENSITIVITY
Zdeněk Tošner
- 3:15 PM ON A CERTAIN TYPE OF TENSORIAL TRANSFORMATIONS
Jiří Czernek
- 3:30 PM** **BREAK**
- 4:15 PM** **SESSION 4 – SPONSORS, E. SIEVÄNEN, Session Chair**
- 4:15 PM BRUKER
Pavel Kessler
- 4:45 PM JEOL
Michal Maloň
- 5:05 PM ICE WINE AND STRAW WINE TASTING BY NMR SPECTROMETER
Milan Mazúr, Michal Kaliňák, Marián Valko
- 5:30 PM** **REFRESHMENT IN HUBERTUS**
- 7:00-9:00 PM** **SCIENTIFIC INSTRUMENTS BRNO EVENING:
VISIT OF “SALON VÍN ČESKÉ REPUBLIKY“**

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TUESDAY APRIL 26, 2015

9:30 AM SESSION 5 – M. STRAKA, Session Chair

9:30 AM ELECTRON DENSITY “PUSH-PULL” EFFECT ON
5-NITROSOPYRIMIDINES (EPR SPECTROELECTROCHEMICAL, NMR
AND DFT STUDY)
Jan Tarábek, Eliška Procházková, Martin Dračínský, Lucie Čechová,
Zlatko Janeba

9:45 AM PARAMAGNETIC RUTHENIUM METALLODRUGS: EXPERIMENT AND
THEORY
Jan Novotný, Martin Sojka, Marek Nečas, Radek Marek

10:00 AM MOLECULAR MOVEMENTS OF LANTHANIDE(III) COMPLEXES WITH
MACROCYCLIC LIGANDS
Jan Blahut, Petr Hermann, Jan Kotek, Zdeněk Tošner

10:15 AM DESIGN OF SMART DELIVERY SYSTEMS FOR ANTICANCER
METALLODRUGS
Martin Novák, Petra Munzarová, Jan Chyba, Radek Marek

10:30 AM BREAK

11:15 AM SESSION 6 – J. SÝKORA, Session Chair

11:15 AM 10 YEARS OF NUCLEAR SPIN NOISE RESEARCH AT JKU
Norbert Müller

11:30 AM DYNAMICS EFFECTS OF SPIN NOISE NMR
Victor Rodin, Matthias Bechmann, Stephan Ginthör, Norbert Müller

11:45 AM NMR AEROSOLOMICS: NOVEL METHOD FOR ORGANIC AEROSOL
ANALYSIS
Štěpán Horník, Jaroslav Schwarz, Jan Sýkora

12:00 POSSIBILITIES OF BENCHTOP NMR IN TEACHING ORGANIC
CHEMISTRY AT UNIVERSITY LEVEL
Juho Itoniemi, Elina Sievänen

12:15 **STUDYING THE BINDING NATURE OF INTERMEDIATE UDP-XYL-4O**
Claudia Puchner, Thomas Eixelsberger, Lothar Brecker, Bernd Nidetzky

12:30 LUNCH

1:30 PM FREE AFTERNOON – DISCUSSIONS

6:00 PM DINNER

7:30 PM CONCERT IN BAROQUE THEATER – Nostalgia Quartet

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WEDNESDAY APRIL 27, 2016

9:00 AM SESSION 7 – K. KUBÍČEK, Session Chair

9:00 AM STRUCTURAL BASIS FOR TRANSCRIPTION TERMINATION COUPLED
TO mRNA PROCESSING/DEGRADATION

Tomasz Kabzinski, Jana Laláková, Andrea Fořtová, Karel Kubíček, Štěpánka
Vaňáčková, Richard Štefl

9:15 AM INTERACTION OF RETROVIRAL MATRIX PROTEINS
WITH LIPOSOMES

Tomáš Kroupa, Jan Prchal, Tomáš Ruml, Richard Hrabal

9:30 AM STRUCTURAL CHARACTERIZATION OF β -CELL DIFFERENTIATION
FACTOR NKX6.1

Vojtěch Duchoslav, Pavel Srb, Rozálie Hexnerová, Irena Sieglová, Milan
Fábry, Václav Veverka

9:45 AM PROBING THE RECEPTOR SPECIFICITY BY SAMPLING THE
CONFORMATIONAL SPACE OF INSULIN-LIKE GROWTH FACTOR II C
DOMAIN

Rozálie Hexnerová, Květoslava Křížková, Milan Fábry, Kateřina Kedrová,
Michaela Collinsová, Pavel Srb, Zdeněk Tošner, Jiří Jiráček, Lenka Žáková,
Václav Veverka

10:00 AM HOW CAN NMR BE USEFUL FOR THE ASSESSMENT OF THE
ANTIDIABETIC THERAPY EFFECTIVENESS?

Martina Bugáňová, Helena Pelantová, Martina Holubová, Blanka Šedivá,
Blanka Železná, Lenka Maletínská, Jaroslav Kuneš, Martin Haluzík, Marek
Kuzma

10:15 AM COMBINING LIGAND AND PROTEIN PERSPECTIVES IN FRAGMENT-
BASED DRUG DISCOVERY

Lukáš Vrzal, Dominika Chalupská, Evžen Bouřa, Radim Nencka,
Hana Dvořáková, and Václav Veverka

10:30 AM BREAK – SPONSORED BY EURISO-TOP

11:15 AM SESSION 8 – V. VEVERKA, Session Chair

11:15 AM A "RED THREAD" THROUGH THE GREEN WORLD
OF THE GENUS *PSYCHOTRIA L.*
Lothar Brecker, Johann Schinnerl, Andreas Berger, Karin Valant-Vetschera

11:30 AM COMPARISON OF QUANTITATION METHODS FOR METABOLOMICS
Michal Kaliňák, Martin Kopčík

11:45 AM INTERACTION OF HOMODIMERIC PROTEIN WITH DIAMAGNETIC
AND PARAMAGNETIC INHIBITOR: HIV PROTEASE AND
CARBORANES
Pavel Srb, Michal Svoboda, Ladislav Benda, Ján Tarábek, Klára Šašková, Jan
Konvalinka, Václav Šícha, Václav Veverka

12:00 JOSEF DADOK PRIZE
L. Brecker, R. Fiala, J. Schraml

12:15 CLOSING REMARKS

12:30 LUNCH