

CENTRAL EUROPEAN NMR MEETING

30th NMR VALTICE

Valtice, Czech Republic

April 19-22, 2015

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30th NMR Valtice Program

SUNDAY APRIL 19, 2015

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

STRUCTURE OF FRAMEWORK ALUMINUM LEWIS SITES AND
PERTURBED ALUMINUM ATOMS IN ZEOLITES AS DETERMINED
BY $^{27}\text{Al}\{^1\text{H}\}$ REDOR (3Q) MAS NMR SPECTROSCOPY AND
DFT/MOLECULAR MECHANICS
Jiří Dědeček

8:30 PM EURISO-TOP GET-TOGETHER PARTY

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MONDAY APRIL 20, 2015

9:30 AM SESSION 1 – G. BATTA, Session Chair

9:30 AM NMR SPECTROSCOPY AS SOLE METHOD? - A CONCERTED
ANALYSIS IN THE FIGHT AGAINST TOOTH LOSS
Lothar Brecker

9:45 AM MAPPING OF GLYCOSAMINOGLYCANS IN CARTILAGE BY
CHEMICAL EXCHANGE SATURATION TRANSFER MRI
Vladimir Mlynarik, Štefan Zbýň, Siegfried Trattnig

10:00 AM TRICHODERMA ATROVIRIDE IN ANAEROBIOSIS
Michal Kaliňák

10:15 AM COMPARISON OF DIFFERENT ANTIDIABETIC INTERVENTIONS ON
THE DEVELOPMENT OF URINAL METABOLIC PROFILE IN MICE
MODEL OF OBESITY
Martina Bugáňová, Helena Pelantová, Marek Kuzma, Jiří Anýž, Daniel
Novák, Blanka Železná, Lenka Maletínská, Martin Haluzík

10:30 AM CONFERENCE PHOTO
Radovan Fiala

10:45 AM BREAK

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

11:15 AM FRAGMENT-BASED APPROACH IN DRUG DISCOVERY
Lukáš Vrzal, Hana Dvořáková, Václav Veverka

11:30 AM CHARACTERIZATION OF DCL-1, A C-TYPE LECTIN LIKE RECEPTOR
Eliška Pospíšilová, Zdeněk Kukačka, Josef Chmelík, Daniel Kavan, Petr
Novák

11:45 AM TOWARDS STRUCTURAL CHARACTERIZATION OF INSULIN LIKE
GROWTH FACTOR II ANALOGUES
Rozálie Hexnerová, Květoslava Křížková, Lenka Žáková, Milan Fábry,
Kateřina Kedrová, Michaela Collinsová, Zdeněk Tošner, Jiří Jiráček and
Václav Veverka

- 12: 00 CYTOSINE METHYLATION STABILIZES ALL BASE PAIRS IN A SHORT DNA DUPLEX
Vaclav Římal, Ondřej Socha, Helena Štěpánková, Josef Štěpánek
- 12:15 DETERMINATION OF M-PMV CAPSID PROTEIN C-TERMINAL DOMAIN STRUCTURE
Jan Prchal, Tibor Fuzik, Pavel Ulbrich, Tomas Ruml, Richard Hrabal
- 12:30 LUNCH**
- 2:30 PM SESSION 3 – R. POHL, Session Chair**
- 2:30 PM PARAMAGNETIC NMR OF RUTHENIUM DRUGS
Jan Novotný, Martin Sojka, Marek Nečas, Radek Marek
- 2:45 PM EXPERIMENTAL DETERMINATION OF STRUCTURAL PARAMETERS IN SELECTED POLYCYCLIC AROMATIC COMPOUNDS
Martin Dračínský, Ivana Císařová, Tomáš Strašák, Jan Storch, Jan Sýkora
- 3:00 PM ‘PLANAMERISM’: A NOVEL STEREOCHEMICAL PHENOMENON?
Eliška Procházková, Lucie Čechová, Ivana Císařová, Zlatko Janeba and Martin Dračínský
- 3:15 PM MEASUREMENT AND CALCULATION OF COMPLEXATION CONSTANTS OF VERY WEAK AND VERY STRONG COMPLEXES
Petra Cuřínová, Jan Storch, Jaroslav Žádný, Petr Velíšek, Martin Bernard, Tomáš Klejch, Pavel Lhoták, Milan Bernauer
- 3:30 PM MAIN GROUP METAL COMPLEXES CONTAINING AMIDINATE AND GUANIDINATE(1- OR 2-) LIGANDS; A PLAYGROUND FOR NMR SPECTROSCOPY
Jana Nevoralová, Emílie Riemlová, Michal Bílek, Barbora Hloušková, Zdenka Růžičková, Tomáš Chlupatý, Aleš Růžička
- 3:45 PM BREAK**
- 4:15 PM SESSION 4 – SPONSORS, M. HRICOVINI, Session Chair**
- 4:15 PM BRUKER
Pavel Kessler
- 4:45 PM JEOL
Michal Maloň, Keisuke Okayama
- 5:30 PM REFRESHMENT**
- 7:00-9:00 PM SCIENTIFIC INSTRUMENTS BRNO EVENING:
VISIT OF “SALON VÍN ČESKÉ REPUBLIKY“**

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TUESDAY APRIL 21, 2015

9:30 AM SESSION 5 – R. WILLEM, Session Chair

9:30 AM “IN VINO VERITAS - IN VINO SANITAS”
Milan Mazúr, Michal Kaliňák, Marián Valko

9:45 AM RDC CROSS-CORRELATION IN MULTIPLE DEGREES OF
ORIENTATION AFTER SCALING USING QUADRUPOLEAR SPLITTING
OF THE DEUTERIUM SIGNAL
Michal Šoral, Jana Doháňošová, Tibor Liptaj

10:00 AM NUMERICAL OPTIMAL CONTROL INSPIRES ANALYTIC SOLUTIONS
Zdeněk Tošner

10:15 AM GRADIENT ECHO IN SPIN-NOISE EXPERIMENTS
Victor Rodin, Norbert Müller

10:30 AM SYMMETRY-BASED PULSE SEQUENCES AND GENETIC
ALGORITHMS
Matthias Bechmann

10:45 AM BREAK

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

11:15 AM Ordering and Dynamics of CO₂ in Metal-Organic Framework
Zn₂(BDC)₂(DABCO)
Mikuláš Peksa, Frank Stallmach, Rochus Schmid, Jan Lang

11:30 AM UNRAVELING IN SITU THE CHEMICAL STRUCTURES OF
POLYOXOMOLYBDATE BASED AMPHIPHILIC NANO-HYBRIDS IN
AQUEOUS SOLUTIONS BY ³¹P DOSY NMR AND MOLECULAR
MECHANICS
Pavletta Shestakova, Gregory Absillis, Francisco J. Martin-Martinez,
Frank De Proft, Rudolph Willem, Tatjana N. Parac-Vogt

11:45 AM UNUSUAL ¹J(^{1/2}H-¹⁴N) COUPLINGS IN HR-MAS NMR SPECTRA OF
POLY(ACRYLAMIDE) BASED DOUBLE NETWORK HYDROGELS
Pavletta Shestakova, Rudolph Willem, Elena Vassileva

- 12:00 POWDER NMR CRYSTALLOGRAPHY OF NEW POLYANHYDRIDE
INJECTABLE MICROBEAD FORMULATIONS OF DECITABINE
J. Brus, J. Czernek, M. Husak, M. Hrubý, P. Švec
- 12:15 “INVISIBLE” CONFORMERS OF A DISULFIDE PROTEIN
Gyula Batta, Adám Fizil, Zoltán Gáspári, Teréz Barna and Florentine Marx
- 12:30 LUNCH**
- 2:30 PM CONFERENCE TRIP – MIKULOV**
- 6:00 PM DINNER IN MIKULOV**
- 9:30 PM BUS MIKULOV - VALTICE**

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WEDNESDAY APRIL 22, 2015

9:30 AM SESSION 7 – E. KLEINPETER, Session Chair

9:30 AM CONFORMATIONAL DYNAMICS OF DOTA-LIKE Eu(III) COMPLEX
Jan Blahut, Petr Hermann, Jan Kotek, Zdeněk Tošner

9:45 AM TOWARDS MECHANISM OF COBALT-MEDIATED
CYCLOISOMERISATION OF YNEDINITRILES
Sergei Chercheja, Jiří Klívar, Andrej Jančařík, Jiří Rybáček, Simon Salzl,
Ján Tarábek, Lubomír Pospíšil, Jana Vacek Chocholoušová, Jaroslav Vacek,
Radek Pohl, Ivana Císařová, Ivo Starý, Irena G. Stará

10:00 AM CALIBRATION OF pNMR CALCULATIONS ON Ru(III) COMPOUND
Sophia Bazzi, Jan Vícha, Jan Novotný, Radek Marek

10:15 AM BREAK – SPONSORED BY EURISO-TOP

10:45 AM SESSION 8 – C. FOROUTAN-NEJAD, Session Chair

10:45 AM MODELING PARAMAGNETIC NMR SHIFTS IN COMMP-12 PROTEIN
Ladislav Benda, Jiří Mareš, Giacomo Parigi, Claudio Luchinat, Martin Kaupp,
Juha Vaara

11:00 AM DFT CALCULATIONS OF STRUCTURE AND NMR PARAMETERS IN
HEPARIN TRISACCHARIDE
Miloš Hricovíni

11:15 AM NUCLEAR DELOCALISATION OF HYDROGEN ATOMS IN STRONG
HYDROGEN BONDS
Martin Dračínský, Eliška Procházková, Lucie Čechová, Zlatko Janeba

11:30 AM JOSEF DADOK PRIZE

11:45 AM CLOSING REMARKS

12:00 LUNCH