

CENTRAL EUROPEAN NMR MEETING

23rd NMR VALTICE

Valtice, Czech Republic

April 20th-23rd, 2008

23rd NMR Valtice Program

SUNDAY APRIL 20, 2008

3:30-6:30 PM REGISTRATION

7:00 PM OPENING REMARKS
Jan Schraml

7:00 PM GET-TOGETHER PARTY

23rd NMR Valtice Program

MONDAY APRIL 21, 2008

9:00 AM SESSION 1 – E. KLEINPETER, Session Chair

9:00 AM RDCS IN NMR STRUCTURE ELUCIDATION OF SMALL MOLECULES
Dusan Uhrin*

9:30 AM TAUTOMERS OF NEUTRAL AND PROTONATED PYRIMIDINE
DERIVATIVES WITH SP³ HYBRIDIZED CARBON ATOM IN POSITION
5
M. Dračinský*, M. Buděšínský, A. Holý

9:45 AM TAUTOMERISM AND REACTIVITY OF TOPOTECAN UNDER
VARIOUS CONDITIONS
Karolina Hyz*, Wojciech Bocian, Jerzy Sitkowski, Elżbieta Bednarek, Robert
Kawęcki, Lech Kozerski

10:00 AM NMR STUDY OF TAUTOMERIC FORMS OF KINETIN AND
KINETINRIBOSIDE DERIVATIVES
Radka Novotná*, Igor Popa, Zdeněk Trávníček

10:15 AM CONFORMATIONAL CHANGES OF INDOLE DERIVATIVES UPON
ANION INTERACTION
Damjan Makuc*, Janez Plavec

10:30 AM BREAK

11:00 AM SESSION 2 – V. SYCHROVSKÝ, Session Chair

11:00 AM SPATIAL MAGNETIC PROPERTIES OF TRISANNELATED BENZENES
AND CYCLOBUTADIENE DIANION DERIVATIVES SUBJECTED TO
AROMATICITY
Erich Kleinpeter* and Andreas Koch

11:15 AM ³¹P CHEMICAL SHIFT TENSORS IN NUCLEIC ACIDS FROM THE
QUANTUM CHEMISTRY POINT OF VIEW
Jana Přecechtělová*, Petr Padrta, Markéta L. Munzarová, Vladimír Sklenář

11:30 AM TOWARDS CALCULATIONS OF CHEMICAL SHIFTS AT
EXPERIMENTAL CONDITIONS
Michal Straka*, Perrtu Lantto, Juha Vaara, Stefan Taubert

11:45 AM ¹³C CHEMICAL SHIFT TENSORS IN REGIOISOMERS OF
N-SUBSTITUTED ADENINES
Kateřina Maliňáková*, Stanislav Standara, Radek Marek

12:00 PM CARBON-CARBON SPIN-SPIN COUPLINGS IN ENAMINONE SYSTEM
Marta Bugaj*, Krystyna Kamieńska-Trela, Jerzy Sitkowski

12:15 PM LUNCH

2:00 PM SESSION 3 – J. JAŽWIŃSKI, Session Chair

2:00 PM REARRANGEMENT OF 9b-HYDROXY-IMIDAZO[4,5-c]QUINOLINE-2,4-
DIONES TO SPIROINDOLINONES
Antonín Lyčka*, Antonín Klásek, Aleš Růžička, Ivan Mikšík

2:15 PM HIGH RESOLUTION MAGIC ANGLE SPINNING NMR IN ORGANOTIN
CATALYSIS
R. Willem*, V. Pinoie, K. Poelmans, M. Biesemans

2:30 PM COUPLING CONSTANTS IN CHELATED ORGANOTIN COMPOUNDS
Petr Svec, Josef Bares, Zdenka Padelkova, Ales Ruzicka*

2:45 PM ADDUCTS OF CHIRAL AMINES AND AZIRIDINES WITH
RHODIUM(II) TETRAACYLATES – ¹H, ¹³C AND ¹⁵N NMR STUDIES
Agnieszka Sadlej*, Jarosław Jaźwiński

3:00 PM ¹H, ¹³C AND ¹⁵N NMR COORDINATION SHIFTS IN Au(III), Pd(II) AND
Pt(II) CHLORIDE COMPLEXES WITH PHENYLPYRIDINES
L. Pazderski*, J. Sitkowski, J. Toušek, L. Kozerski, E. Szyk

3:15 PM ERROR SOURCES IN QUANTITATIVE EPR SPECTROSCOPY
M. Mazur*

3:30 PM BREAK

4:00 PM SESSION 4 – J. BRUS, Session Chair

4:00 PM NMR SPECTRA PROCESSING, VERIFICATION AND ELUCIDATION:
CHALLENGES AND CURRENT PROGRESS
Stanislav Sýkora*, Carlos Cobas

4:30 PM SIB, BRUKER

5:00 PM NMRtec

5:15 PM VARIAN

5:30 PM BREAK

6:00 PM DINNER

**7:00-9:00 PM SCIENTIFIC INSTRUMENTS BRNO EVENING:
VISIT OF “SALON VÍN ČESKÉ REPUBLIKY”**

23rd NMR Valtice Program

TUESDAY APRIL 22, 2008

9:00 AM SESSION 5 – W. SCHÖFBERBER, Session Chair

- 9:00 AM DOSY AND DIFFUSION MEASUREMENT IN MODERN NMR
Marc-André Delsuc*
- 9:30 AM MULTIPLEX PHASE CYCLING IN THE LIQUID STATE
Gerhard Zuckerstätter*, Norbert Müller
- 9:45 AM TOWARDS MULTI-PURPOSE NMR EXPERIMENTS
Judith Schlagnitweit*, Gerhard Zuckerstätter, Norbert Müller
- 10:00 AM NMR EXPERIMENT DESIGN BY OPTIMAL CONTROL:
ALTERNATIVE ALGORITHMS FOR REDUCING RF POWER
Zdeněk Tosner*, Ivan I. Maximov, Niels Chr. Nielsen
- 10:15 AM THE VISUALIZATION OF INSULIN AGGREGATION
Anna Tarnowska*, Wojciech Bocian, Jerzy Sitkowski, Elzbieta Bednarek,
Robert Kawęcki, Lech Kozerski
- 10:30 AM STUDY OF PREPARATION AND CHARACTERIZATION OF WATER
SOLUBLE GOLD NANOPARTICLES BY NMR
Pavel Rezanka*, Pavel Zvatora, Jakub Rak, Vladimír Kral
- 10:45 AM **BREAK**
- 11:15 AM SESSION 6 – L. BRECKER, Session Chair
- 11:15 AM NMR ANALYSIS OF AEROSOL PARTICLES
Jan Sýkora*
- 11:30 AM REORGANIZATION PROCESSES DURING THE THERMOTROPIC
PHASE TRANSITIONS IN AQUEOUS POLYMER SOLUTIONS OF
POLYMER MIXTURES
L. Starovoytova*, J. Kriz
- 11:45 AM ¹³C AND ¹⁵N CPMAS NMR STUDIES OF POLYMORPHS AND
SOLVATES OF LITHOCHOLYL(*N*-2-AMINOETHYL)AMIDE
Babita Behera, Arto Valkonen, Manu Lahtinen, Minna Tolonen, Elina
Sievänen, Reijo Kauppinen, and Erkki Kolehmainen*
- 12:00 PM MEASUREMENT OF RELATIVE SIGNS OF ²⁹Si-¹³C COUPLINGS
Vratislav Blechta *, Jan Schraml

- 12:15 PM DIHYDROXAMIC ACIDS AGAIN
Schraml J*, Cigler P.
- 12:30 PM PROBING THE FLEXIBILITY OF INTERNAL ROTATION IN
SILYLATED PHENOLS WITH THE NMR SCALAR COUPLING
CONSTANTS
Sychrovský*, Benda, Prokop, Blechta, Schraml, Špirko
- 12:45 PM **LUNCH**
- 2:00 PM BUS TO MIKULOV – English speaking group
- 2:30 PM BUS TO MIKULOV – Czech speaking group
- 7:00 PM **DINNER**
- 8:00 PM **FREE EVENING**

23rd NMR Valtice Program

WEDNESDAY APRIL 23, 2008

9:00 AM SESSION 7 – G. BATTA, Session Chair

- 9:00 AM DNA BINDING STUDIES OF ANTI-TUMOR AGENTS: NMR, FLUORESCENCE, DOCKING AND MOLECULAR MODELING APPROACHES
Prateek Pandya and Surat Kumar*
- 9:30 AM ¹³C RELAXATION STUDY OF RNA DYNAMICS: APPLICATION TO UUCG HAIRPIN LOOP
Pavel Kadeřávek*, Radovan Fiala
- 9:45 AM CAN CROSS-CORRELATION EFFECTS BE MEASURED IN A DIPEPTIDE ?
Lorenz Reith*, Ladislav Benda, Jaroslav Sebestik, Milos Budesinsky, Vladimir Sychrovsky, Norbert Müller
- 10:00 AM STD-NMR SPECTROSCOPY TO STUDY INFLUENCES OF CO-SUBSTRATES, CO-ENZYMES, AND ENZYME MODIFICATIONS ON SUBSTRATE BINDING TO BIOCATALYSTS
Lothar Brecker*, Regina Kratzer, Christiane Goedl, Alexandra Schwarz, Michael Vogl, Bernd Nidetzky
- 10:15 AM METABOLISM OF TRICHODERMA VIRIDE THROUGH NMR
Kaliňák Michal*, Ondřejková Agáta, Liptaj Tibor
- 10:30 AM BREAK**
- 11:00 AM SESSION 8 – D. UHRÍN, Session Chair**
- 11:00 AM PAF AND AFP: TWO ANTIFUNGAL PROTEINS. JUST THE LETTERS?
G. Batta*, S. Sándor, Z. Gáspári, T. Barna, K. E. Kövér, É. Leiter, I. Pócsi, U. Binder, B. Sarg, L. Kaiserer, H. Lindner and F. Marx
- 11:15 AM EXPRESSION AND NMR INVESTIGATION ON RECOMBINANT PSBQ PROTEIN
Michaela Hornicakova*, Wolfgang Schöfberger, Norbert Müller, Jaroslava Ristvejova, Ivana Kuta, Rüdiger Ettrich
- 11:30 AM FUNCTIONAL AND STRUCTURAL STUDY OF MUTANTS OF MATRIX PROTEIN FROM MASON-PFIZER MONKEY VIRUS WHICH AFFECT BUDDING
Jan Prchal*, Michal Doležel, Jiří Vlach, Jan Lipov, Tomáš Ruml, Richard Hrabal

- 11:45 AM MASON-PFIZER MONKEY VIRUS MATRIX PROTEIN: MONOMER OR OLIGOMER?
Pavel Srb*, Marian Grocký, Jiří Vlach, Jan Prchal, Jan Lipov, Jan Lang, Tomáš Ruml and Richard Hrabal
- 12:00 PM TEMPERATURE DENATURATION OF LIPID TRANSFER PROTEIN I STUDIED BY NMR AND DIFFERENTIAL SCANNING CALORIMETRY
Jitka Žídková*, Michaela Matejková, Lukáš Žídek, Michaela Wimmerová, and Vladimír Sklenář
- 12:15 PM CLOSING REMARKS**
- 12:30 PM LUNCH**