

CENTRAL EUROPEAN NMR MEETING

24th NMR VALTICE

Valtice, Czech Republic

April 26th-29th, 2009

24th NMR Valtice Program

SUNDAY APRIL 26, 2009

3:30-6:30 PM REGISTRATION

7:00 PM DINNER

8:00 PM OPENING REMARKS
Jan Schraml

8:10 PM LEDNICE-VALTICE AREA
Lucie Krejzová, Eva Horsáková

24th NMR Valtice Program

MONDAY APRIL 27, 2009

9:00 AM SESSION 1 – V. SKLENÁŘ, Session Chair

- 9:00 AM MASS SPECTROMETRY IS NOT NMR RIVAL
Vladimír Havlíček*
- 9:30 AM INTERACTION OF THE N-TERMINAL MYRISTIC ACID WITH MATRIX PROTEIN FROM MASON-PFIZER MONKEY VIRUS
Jan Prchal*, Jiri Vlach, Tomas Ruml, Richard Hrabal
- 9:45 AM DIFFUSION AND TITRATION DATA ANALYSIS REVEAL OLIGOMERIZATION OF MASON PFIZER MONKEY VIRUS MATRIX PROTEIN
Pavel Srb*, Jiří Vlach, Jan Prchal, Marián Grocký, Jan Lang, Richard Hrabal and Tomáš Ruml
- 10:00 AM STRUCTURAL STUDY OF AN RNA POLYMERASE SUBUNIT UNIQUE FOR GRAM-POSITIVE BACTERIA
Veronika Motáčková*, Hana Šanderová, Jiří Nováček, Lukáš Žídek, Vladimír Sklenář, Libor Krásný
- 10:15 AM MAGE (MELANOMA-ASSOCIATED ANTIGEN) DOMAIN STRUCTURAL STUDIES USING NMR
Sreenivas Reddy Bathula*, Jan Paleček, Lukáš Žídek, and Vladimír Sklenář
- 10:30 AM BREAK**
- 11:00 AM SESSION 2 – M. BUDĚŠÍNSKÝ, Session Chair**
- 11:00 AM ¹³C CHEMICAL SHIFTS – STRUCTURE RELATIONSHIPS IN NUCLEIC ACIDS
Petr Novák, Vladimír Sklenář, and Radovan Fiala*
- 11:15 AM BINDING MODE OF PROTOBERBERINE ALKALOIDS TO d(AAGAATTCTT)₂
Martin Babinský*, Radovan Fiala, Zdeněk Kříž, Radek Marek
- 11:30 AM ³¹P CHEMICAL SHIFT ANISOTROPY TENSORS IN [d(CGGAATTCGCG)]₂. A MOLECULAR DYNAMICS AND DENSITY FUNCTIONAL STUDY.
J. Precechtelova*, P. Novak, M.L. Munzarova, M. Kaupp, and V. Sklenar
- 11:45 AM SPIN NOISE: NON-LINEAR EFFECTS
Norbert Müller*, Alexej Jerschow, Martin Nausner, Vilko Smrecki, Judith Schlagnitweit

12:00 LUNCH

2:00 PM SESSION 3 – V. G. MALKIN, Session Chair

- 2:00 PM INTERPRETATION OF NMR SPIN-SPIN COUPLINGS: METHODOLOGY AND EXAMPLES
Olga L. Malkina*
- 2:30 PM CARBON-CARBON SPIN-SPIN COUPLINGS IN ARYL ENAMINOKETONES AND THEIR THIOANALOGUES. EXPERIMENT AND THEORY
M. Bugaj*, P. Baran, K. Kamieńska-Trela, A. Krówczyński
- 2:45 PM J(CC) COUPLINGS IN SUBSTITUTED BEZENES
Z. Biedrzycka, A. Dąbrowski and K. Kamieńska-Trela*
- 3:00 PM SMALL ²⁹Si-¹³C COUPLINGS AND THEIR SIGNS FOR ANY SPIN SYSTEM AT NATURAL ABUNDANCE
Vratislav Blechta* and Jan Schraml
- 3:15 PM NMR STUDY AND THEORETICAL CALCULATIONS OF ROTATIONAL BARRIERS IN NEW 8-SUBSTITUTED DERIVATIVES OF PROTOBERBERINE ALKALOIDS
Lukáš Maier*, Tomáš Šolomek, Zdeněk Kříž, Radek Marek
- 3:30 PM BREAK**
- 4:00 PM SESSION 4 – K. KAMIEŃSKA-TRELA, Session Chair**
- 4:00 PM STD-DOSY: A METHOD TO SIMPLIFY AND ANALYZE MULTI-COMPONENT ENZYME/SUBSTRATE SYSTEMS?
Markus Kramer* and Erich Kleinpeter
- 4:15 PM OPTIMIZATION OF SAMPLE PREPARATION FOR DIFFERENTIATION OF ACTAEA SPECIES BY ¹H-NMR SPECTROSCOPY
Sonja Prinz*, Judith Singhuber, Antje Huefner, Oliver Donath, Hans-Peter Kaehlig, Johannes Saukel, Ming Zhu, Brigitte Kopp
- 4:30 PM ¹H NMR SPECTROSCOPY AS TOOL TO FOLLOW CHANGES IN THE FATTY ACIDS OF FISH OILS
Lothar Brecker*, Catrin E. Tyl, Karl-Heinz Wagner
- 4:45 PM NMR SPECTROSCOPY OF COMPLEX LIQUID MIXTURES SAMPLE PRE-CONCENTRATION, YES OR NO?
Milan Mazúr*, Michal Kaliňák, Katarína Furdíková, Marián Valko
- 5:00 PM BREAK**
- 7:00-9:00 PM SCIENTIFIC INSTRUMENTS BRNO EVENING:
VISIT OF "SALON VÍN ČESKÉ REPUBLIKY"**

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TUESDAY APRIL 28, 2009

9:00 AM SESSION 5 – J. BRUS, Session Chair

- 9:00 AM NMR STUDIES OF XYLOSE REDUCTASE CATALYZED TRANSFORMATIONS
Michael Vogl*, Regina Kratzer, Bernd Nidetzky, Lothar Brecker
- 9:15 AM REORGANIZATION PROCESSES DURING THE THERMOTROPIC PHASE TRANSITIONS IN AQUEOUS POLYMER SOLUTIONS OF POLYMER MIXTURES
L. Starovoytova*, J. Kriz
- 9:30 AM NMR STUDY OF TEMPERATURE-INDUCED PHASE TRANSITION IN SOLUTIONS OF POLY(N-ISOPROPYLMETHACRYLAMIDE/ACRYLAMIDE) COPOLYMERS
Julie Brülllová*, Hana Kouřilová, Lenka Hanyková
- 9:45 AM STRUCTURE DETERMINATION OF OLIGOMERIC SILOXANES
Milan Kurfürst* and Jan Schraml
- 10:00 AM SOLID STATE NMR STUDIES OF BILE ACIDS: DETECTION, ISOLATION AND STRUCTURAL INVESTIGATION OF POLYMORPHS
Nonappa*, Manu Lahtinen, Satu Ikonen, Erkki Kolehmainen and Reijo Kauppinen
- 10:15 AM BEHAVIOR OF HOMONUCLEAR SPIN PAIR DURING CPMG PULSE SEQUENCE
Zdeněk Tošner*, Antonín Škoch

10:30 AM BREAK

11:00 AM SESSION 6 – J. JAŽWIŃSKI, Session Chair

- 11:00 AM NMR HARDWARE AND NEW ELECTRONICS: A BOAT IN A HURRICANE
Stanislav Sykora*
- 11:15 AM BRUKER, SIB
Pavel Kessler*
- 11:45 AM ACROS ORGANICS PRODUCTS BY LACH-NER COMP.
Oldřich Malíček*

12:00 CORTECNET
Jean Baptiste Hibon*

12:15 PM LUNCH

1:30 PM CONFERENCE TRIP

7:30 PM DINNER

8:00 PM FREE EVENING

24th NMR Valtice Program

WEDNESDAY APRIL 29, 2009

9:00 AM SESSION 7 – E. KLEINPETER, Session Chair

9:00 AM ¹⁵N NMR SPECTRA – APPLICATION OF “OLD-FASHIONED” DIRECT DETECTION

Antonín Lyčka*, Svatopluk Zeman, Štěpán Frebort, Numan Almonasy

9:15 AM NMR STUDIES ON ADDUCTS OF DIRHODIUM(II) TETRAACYLATES WITH THE MULTIFUNCTIONAL LIGANDS

Jarosław Jaźwiński, Rafał Głazeczka*, Monika Kamińska

9:30 AM LIGAND EXCHANGE AND THE CONFIGURATION OF THE NITROGENOUS CENTRE IN ADDUCTS OF CHIRAL AMINES WITH RHODIUM(II) TETRAACYLATE

Jarosław Jaźwiński, Agnieszka Sadlej*

9:45 AM TAXANES: NEW MEMBERS AND NEW REACTIONS

Marek Kuzma*, Petr Sedmera, Ladislav Cvak, Jiří Maleček, Miroslav Petrákovič, and Alexandr Jegorov

10:00 AM FK-506 AND ITS CONGENERS

Petr Sedmera*, Ladislav Cvak, Pavel Blatný, and Alexandr Jegorov

10:15 AM STRUCTURAL STUDIES OF HOMOISOFLAVONOIDS

Elina Sievänen*, Jaromír Toušek, Radek Marek

10:30 AM BREAK

11:00 AM SESSION 8 – A. LYČKA, Session Chair

11:00 AM PEROXIDASE-CATALYZED FORMATION OF (DEOXY)GUANOSINE ADDUCTS BY SUDAN I

Martin Dračinský*, Marcela Semanská, Josef Cvačka, Václav Martínek, Marie Stiborová

11:15 AM STABILITY OF NOVEL REAGENTS FOR INTRODUCTION OF URACIL AND THYMINE MONITORED BY NMR

Radek Pohl* and Dominik Rejman

11:30 AM NMR AND THEORETICAL INVESTIGATIONS OF HYDROGEN BONDING IN 1,3-AMINO- α / β -NAPHTHOL DERIVATIVES

Anica Lämmermann*, István Szatmári, Ferenc Fülöp, Erich Kleipeter

11:45 AM COMPLEXATION PROPERTIES OF THE NEW CALIX[4]ARENE – BASED RECEPTORS

Petra Cuřínová*, Jan Budka, Markéta Budková, Markéta Zajícová, Romana Pálková, Jan Sýkora, Pavel Lhoták, Ivan Stibor

12:00 SIZE OF ETHANOL MOLECULAR CLUSTERS FROM DIFFUSION MEASUREMENTS AND CALCULATIONS

Mária Šoltéssová*, Ladislav Benda, Jiří Czernek, Jan Lang

12:15 PM CLOSING REMARKS

12:30 PM LUNCH