

**CENTRAL EUROPEAN NMR DISCUSSION GROUPS**

**20<sup>th</sup> NMR VALTICE**

Valtice, Czech Republic

April 4<sup>th</sup>-6<sup>th</sup>, 2005

# 20<sup>th</sup> NMR Valtice Program

**MONDAY APRIL 4, 2005**

**2:00 PM OPENING REMARKS**

Jan Schraml

2:10 PM SMALL LONG-RANGE  $J(^{29}\text{Si}-\text{O}-^{13}\text{C})$  COUPLINGS AS AN  $^{29}\text{Si}$  CHEMICAL SHIFT ASSIGNMENT TOOL.

Jan Sýkora, Vratislav Blechta, Cuřínová Petra, Ludmila Soukupová, Jan Schraml

2:25 PM MULTINUCLEAR NMR STUDY OF TRIORGANOTIN(IV) ESTERS OF 4-KETOPIMELIC ACID.

Jan Chalupa, Jiří Brus, Antonín Lyčka, Jaroslav Holeček, Aleš Růžička

2:40 PM MULTINUCLEAR NMR SPECTROSCOPY APPROACH TO STUDY OF SOLUTION STRUCTURE OF ORGANOTIN(IV) FLUORIDES.

Petr Novák, Zdeňka Padělková, Josef Bareš; Milan Nádvorník, Aleš Růžička, Jaroslav Holeček

2:55 PM  $^{15}\text{N}$  SOLUTION AND SOLID PHASE NMR STUDIES OF 6-MERCAPTOPYRIMIDINES AND THEIR Pd(II), Pt(II) COMPLEXES.

Leszek Pazderski, Iwona Łakomska, Andrzej Wojtczak, Edward Sztyk, Jerzy Sitkowski, Lech Kozerski, Bohdan Kamiński, Wiktor Koźmiński, Jaromír Toušek, Radek Marek

3:10 PM NMR STUDY OF THYMINE-CONTAINING PYRROLIDINE NUCLEOTIDE ANALOGUES.

Radek Pohl, Petr Kočalka, Dominik Rejman and Ivan Rosenberg

3:25 PM TAUTOMERIC EQUILIBRIA OF PURINE DERIVATIVES STUDIED BY LOW-TEMPERATURE NMR SPECTROSCOPY AND QUANTUM CHEMICAL CALCULATIONS.

Pavλίna Sečkářová, Radek Marek, Jaromír Toušek, Michal Hocek, Erkki Kolehmainen, Vladimír Sklenář

3:40 PM NMR STRUCTURE DETERMINATION OF NEW DITERPENE IN SEXUAL GLANDS OF *Nasutitermitinae* (Isoptera, Termitidae).

Miloš Buděšínský, Irena Valterová, Christian Bordereau

3:55 PM NEVER-ENDING STORY OF ERGOT ALKALOIDS: A NMR CONTRIBUTION.

Marek Kuzma, Petr Sedmera, Helena Pelantová, Jiri Faustmann, Ladislav Cvak, Alexandr Jegorov

- 4:10 PM      BREAK**
- 4:30 PM      THE *PUSH-PULL EFFECT* IN SUBSTITUTED OLEFINS – ESTIMATION AND QUANTIFICATION.  
Erich Kleinpeter, Sabrina Klod
- 4:45 PM      POLYMORPHISM OF BILE ACID DERIVATIVES STUDIED BY POWDER AND SINGLE CRYSTAL X-RAY DIFFRACTOMETRY, AND CALCULATED DFT/GIAO AND EXPERIMENTAL <sup>13</sup>C CP/MAS NMR CHEMICAL SHIFTS. PRELIMINARY RESULTS.  
Elina Sievänen, Arto Valkonen, Manu Lahtinen, Suvi Kaikkonen, Erkki Kolehmainen
- 5:00 PM      DETERMINATION OF N-H...N HYDROGEN BOND STRENGTH BY ANALYZING <sup>15</sup>N CHEMICAL SHIFT TENSOR AND ELECTRON DENSITY.  
Radek Marek, Jaromír Toušek, Jiří Brus, Jaromír Marek, Zdeněk Trávníček, Vladimír Sklenář
- 5:15 PM      SELECTIVE MEASUREMENT OF HETERONUCLEAR <sup>1</sup>H-<sup>13</sup>C DIPOLAR COUPLINGS IN MOTIONALLY HETEROGENEOUS SEMICRYSTALLINE POLYMER SYSTEMS.  
Jiří Brus, Martina Urbanová
- 5:30 PM      BREAK**
- 6:00 PM      SOLID STATE <sup>13</sup>C NMR AND DFT QUANTUM-CHEMICAL STUDY OF POLYMER ELECTROLYTE POLY(2-ETHYL-2-OXAZOLINE)/AgCF<sub>3</sub>SO<sub>3</sub>.  
Jiří Spěváček, Jiří Brus, Jiří Dybal, Yong Soo Kang
- 6:15 PM      RELAXATION BEHAVIOUR OF SOLVENT MOLECULES DURING THE PHASE SEPARATION IN POLY(VINYL METHYL ETHER)/WATER/ETHANOL SOLUTIONS.  
Jan Labuta, Lenka Hanyková, Jan Lang, Jiří Spěváček
- 6:30 PM      TIME EFFECT ON THERMOTROPIC PHASE TRANSITION IN AQUEOUS POLYMER SOLUTIONS.  
Larisa Starovoytova, Lenka Hanyková, Jiří Spěváček
- 6:45 PM      SELF-DIFFUSIONAL PROPERTIES OF GENETICALLY ENGINEERED ELASTIN-LIKE MODIFIED POLYPEPTIDES.  
D. Kurková, J. Kříž, J. C. Rodríguez-Cabello, M. Alonso
- 7:00 PM      DINNER**
- 8:00 PM      GET-TOGETHER PARTY IN WINE CELLAR SPONSORED BY VARIAN

# 20<sup>th</sup> NMR Valtice Program

**TUESDAY APRIL 5, 2005**

- 8:30 AM APPLICATION OF COGWHEEL PHASE CYCLING IN MULTI-DIMENSIONAL BIO-MOLECULAR NMR.  
Norbert Müller, Wolfgang Schöfberger, Gerhard Zuckerstätter
- 8:45 AM STRUCTURAL REFINEMENT OF PARAMAGNETIC PROTEINS USING  $H_{\alpha}C_{\alpha}$  DIPOLE-DIPOLE AND  $H_{\alpha}$ -CURIE SPIN RELAXATION CROSS-CORRELATION EFFECTS.  
V.N. Sivanandam, Irena Matecko, Lukas Trantirek, Wolfgang Schöfberger, Guido Pintacuda, Norbert Müller
- 9:00 AM STRUCTURE CALCULATION OF THE WILD TYPE MATRIX PROTEIN OF MASON-PFIZER MONKEY VIRUS.  
Jiří Vlach, Jan Lipov, Tomáš Ruml, Richard Hrabal
- 9:15 AM AFFECT OF CYSTEINES ON THE ACTIVITY AND STRUCTURE OF 2 kDa FORM OF M-PMV PROTEASE.  
Richard Hrabal, Helena Bauerová, Aleš Svatoš, Iva Pichová
- 9:30 AM  $^{13}C$ -DETECTED EXPERIMENTS FOR NUCLEIC ACIDS.  
Radovan Fiala
- 9:45 AM SUGAR PUCKER MODULATES THE CROSS-CORRELATED RELAXATION RATES ACROSS THE GLYCOSIDIC BOND IN DNA.  
Vladimír Sychrovsky, Norbert Müller, Bohdan Schneider, Vilko Smrecki, Vladimir Spirko, Jiri Sponer, Lukas Trantirek
- 10:00 AM SOLUTION STRUCTURES OF SMALL MOLECULES FROM RESIDUAL DIPOLAR COUPLINGS.  
Tran N. Pham, David W.H. Rankin, Dušan Uhrín, Tibor Liptaj
- 10:15 AM APPLICATION OF THE MODEL FREE APPROACH TO LOW MOLECULAR WEIGHT SYSTEMS WITH HINDERED INTERNAL ROTATION: CINNAMOYLMESEITYLENE.  
Pavletta Denkova, Valentin Dimitrov, Snezhana Bakalova, Jose Kaneti, Krassimir Danov
- 10:30 AM BREAK**
- 11:00 AM NMR SPECTROSCOPIC TOOLS TO IDENTIFY TRANSITION STATES OF SUBSTRATES IN CHEMICAL AND BIOCATALYSED REACTIONS.  
Lothar Brecker

- 11:15 AM SATURATION TRANSFER DIFFERENCE NMR TO CHARACTERISE BINDING OF SUBSTRATES AND PRODUCTS TO BIOCATALYSTS.  
Catrin Tyl, Lothar Brecker, Grit Straganz, Walter Steiner, Bernd Nidetzky
- 11:30 AM DETERMINATION OF  $^{13}\text{C}$  KINETIC ISOTOPE EFFECTS AT NATURAL ABUNDANCE BY NMR SPECTROSCOPY.  
Marion Kögl, Catrin Tyl, Regina Kratzer, Bernd Nidetzky, Lothar Brecker
- 11:45 AM RECENT RESULTS IN NMR SPECTROSCOPY OF HELICENES.  
D. Šaman, I.G. Stará, I. Starý, P. Sehnal, Z. Alexandrová, J. Míšek
- 12:00 PM NMR AND X-RAY STUDIES OF COUPLING PRODUCTS OF SOME ENAMINONES WITH DIAZONIUM SALTS  
A. Lyčka, P. Šimůnek, M. Pešková, V. Macháček, V. Bertolasi, A. Koloničný
- 12:15 PM PROGRESS IN VARIABLE FIELD NMR RELAXOMETRY.  
S. Sýkora, G.M. Ferrante
- 12:30 PM VARIAN
- 12:50 PM BRUKER
- 1:10 PM LUNCH**
- 2:30 PM CONFERENCE TRIP TO MIKULOV
- 7:00 PM DINNER**
- 8:00 PM MEETING OF THE NMR DISCUSSION GROUPS – REFRESHMENT SPONSORED BY BRUKER AND SCIENTIFIC INSTRUMENT BRNO

# 20<sup>th</sup> NMR Valtice Program

**WEDNESDAY APRIL 6, 2005**

- 8:30 AM PLANAR SAMPLE GEOMETRY IN MAGNETIC RESONANCE SPECTROSCOPY.  
Milan Mazúr
- 8:45 AM FULLY AUTOMATIC FIRST-ORDER MULTIPLY ANALYSIS (FAFOMA).  
Nikolay G. Vassilev
- 9:00 AM NMR SPECTROSCOPIC AND COMPUTATIONAL INVESTIGATIONS ON TRIMETHYLSILYL- SUBSTITUTED GROUP 14 ELEMENT ALKALI DERIVATIVES.  
R. Fischer, J. Fischer, M. Flock, J. Baumgartner, C. Marschner, F. Uhlig
- 9:15 AM (<sup>1</sup>H-<sup>29</sup>Si) gHMQC LC NMR EXPERIMENT  
Vratislav Blechta, Jan Sýkora, Jiří Hetflejš, Stanislav Šabata and Jan Schraml
- 9:30 AM CONFORMATIONAL STUDY OF CALIX[4]PHYRINS.  
Hana Dvořáková, Markéta Bernátková, Bruno Andrioletti, Vladimír Král, Petr Bouř
- 9:45 AM FLIP-FLOP MOTION OF CIRCULAR HYDROGEN BOND ARRAY IN THIALCALIX[4]ARENE.  
Jan Lang, Kateřina Šetková, Veronika Deckerová, Pavel Lhoták, Jiří Czernek
- 10:00 AM SELECTIVE RECEPTORS FOR AN ION PAIR BASED ON CALIX[4]ARENE.  
Petra Cuřínová, Jan Budka, Gu Rong, Wim Dehaen, Jan Schraml
- 10:15 AM INVESTIGATION OF CATION COMPLEXATION BY MACROCYCLIC ETHERS USING <sup>13</sup>C NMR SPIN-LATTICE DIPOLAR RELAXATION TIME MEASUREMENTS.  
Matthias Heydenreich, Çakıl Erk, Erich Kleinpeter
- 10:30 AM BREAK**
- 11:00 AM SOLID STATE NMR SPECTROSCOPY OF THE ADENOSINE- 5'-TRIPHOSPHATE-DISODIUM AND QUANTUM MECHANICS CALCULATIONS.

Wolfgang Schoefberger, Karunesh Arora, Rajeev Kumar, Wen Ling, Alexej Jerschow

- 11:15 AM <sup>57</sup>Fe NMR IN PURE AND SUBSTITUTED MAGNETITE.  
H. Štěpánková, E. Gamaliy, V. Chlan, J. Kohout, J. English, P. Novák,  
V. A. M. Brabers
- 11:30 AM HYPERFINE INTERACTIONS IN LUTETIUM IRON GARNET –  
EXPERIMENT AND THEORY.  
V. Chlan<sup>a</sup>, H. Štěpánková<sup>a</sup>, P. Novák<sup>b</sup>, J. English<sup>a</sup>, D. Nižňanský
- 11:45 AM CREATINE KINASE ACTIVITY IN THE RAT BRAIN UNDER  
CONDITION CHRONIC HYPERTENSION: AN ANIMAL MODEL  
S. Kašparová, L. Bačiak, V. Mlynárik, Š. Zbýň, V. Belan, T. Liptaj
- 12:00 PM 1-H/13-C HETERONUCLEAR POLARISATION TRANSFER (INEPT) IN  
HUMAN CALF MUSCLE  
Albrecht I. Schmid, Ewald Moser, Martin Krssak, Michael Roden
- 12:15 PM DOES GABA HAVE A DIFFERENT ROLE IN *TRICHODERMA VIRIDE*  
AND *SACCHAROMYCES CEREVISIAE*?  
Michal Kaliňák, Katarína Majerníková, Tibor Liptaj, Ludovít Varečka
- 12:30 AM HIGH SPATIAL RESOLUTION SPECTROSCOPIC IMAGING OF  
INTRAMYOCYELLULAR LIPIDS IN HUMAN CALF MUSCLE  
M. Chmelík, S. Gruber, E. Moser, M. Roden
- 12:45 PM **CLOSING REMARKS**  
Jan Schraml