

CENTRAL EUROPEAN NMR DISCUSSION GROUPS

22nd NMR VALTICE

Valtice, Czech Republic

April 15th-18th, 2007

22nd NMR Valtice Program

SUNDAY APRIL 15, 2007

3:30-6:30 PM REGISTRATION

7:00 PM DINNER

8:00 PM OPENING REMARKS
Jan Schraml, Norbert Müller

8:15 PM VARIAN EVENING

22nd NMR Valtice Program

MONDAY APRIL 16, 2007

9:00 AM SESSION 1 - R. FIALA, Session Chair

9:00 AM NEW EDITED / FILTERED *STD* AND *DOSY* EXPERIMENTS IN AQUEOUS SOLUTION AND BIOMOLECULAR APPLICATIONS

Gyula Batta*, Katalin E. Kövér, Patrick Groves, Angeles Canales, Jesús Jiménez-Barbero

9:15 AM LIMITS OF ACCURACY OF RNA DYNAMICS STUDIED BY MODEL FREE ANALYSIS OF C-13 RELAXATION

Pavel Kadeřávek*, Radovan Fiala

9:30 AM THEORETICAL NMR STUDY OF WATSON-CRICK/SUGAR EDGE RNA BASE PAIR FAMILY

Z. Vokáčová*, J. Šponer, V. Sychrovský

9:45 AM NMR INVESTIGATIONS ON OLIGONUCLEOTIDE-PORPHYRIN COMPLEXES

M. Haeubl*, M. Nausner, L. Trantírek, V. Smrečki, N. Müller and W. Schoefberger

10:00 AM RESIDUAL DIPOLAR COUPLINGS FROM STRETCHED POLYACRYLAMIDE GEL. EXPERIENCE AND APPLICATIONS.

Jiří Vlach, Jan Prchal, Richard Hrabal

10:15 AM BREAK

10:45 AM SESSION 2 - G. BATTA, Session Chair

10:45 AM STRUCTURE OF BOMBYX MORI CHEMOSENSORY PROTEIN 1 IN SOLUTION

Séverine Jansen, Josef Chmelík*, Lukáš Žídek, Petr Padrta, Petr Novák, Jean-François Picimbon, Christer Löfstedt and Vladimír Sklenář

11:00 AM CARBONYL CARBON RELAXATION RATES MEASUREMENT IN MATRIX PROTEINS OF M-PMV

Pavel Srb*, Marian Grocký, Jan Lang, Jiří Vlach, Jan Prchal, Tomáš Ruml, Richard Hrabal

11:15 AM DESIGN OF NEW NMR EXPERIMENTS BY MEANS OF OPTIMAL CONTROL THEORY

Zdenek Toner

- 11:30 AM RECENT PROGRESS IN SPIN NOISE SPECTROSCOPY
Norbert Mueller*, Alexej Jerschow
- 11:45 AM PERSPECTIVES OF PASSIVE AND ACTIVE MAGNETIC RESONANCE
IN ASTRONOMY
Stanislav Sykora
- 12:00 LUNCH**
- 2:00 PM SESSION 3 - L. BRECKER, Session Chair**
- 2:00 PM LC-NMR METHOD FOR ANALYSIS OF FREE FATTY ACIDS IN
NATURAL OILS
Sykora J.,* Sovová H., Kurfürst M., Schraml J.
- 2:15 PM LC-NMR OF POLYSILOXANES
Blechta V., Sýkora J., Kurfurst M., Schraml J.*
- 2:30 PM COUPLING CONSTANTS $^2J(^{29}\text{Si}-\text{O}-^{29}\text{Si})$ IN MODEL OLIGOMERIC
SILOXANES
Milan Kurfurst*, Jan Schraml
- 2:45 PM INEPT-INADEQUATE IN ^{29}Si NMR
Vratislav Blechta*, Jan Schraml
- 3:00 PM BREAK**
- 3:30 PM SPONSORS - R. HRABAL, Session Chair**
- 3:30 PM VARIAN
- 4:15 PM SIB, BRUKER
- 5:00 PM BREAK**
- 7:00 PM DINNER**
- 8:00 PM SCIENTIFIC INSTRUMENTS BRNO EVENING**

22nd NMR Valtice Program

TUESDAY APRIL 17, 2007

9:00 AM SESSION 4 – E. KOLEHMAINEN, Session Chair

9:00 AM THE RING CURRENT EFFECT OF FULLERENES
E. Kleinpeter*, S. Klod, A. Koch

9:15 AM STEREOCHEMICAL ANALYSIS OF NAPHTH[1,2-E][1,3]OXAZINO[4,3-A][1,3]ISO-QUINOLINE AND NAPHTH[2,1-E][1,3]OXAZINO[4,3-A][1,3]ISOQUINOLINE DERIVATIVES
Matthias Heydenreich*, Andreas Koch, István Szatmári, Ferenc Fülöp and Erich Kleinpeter

9:30 AM NMR SPECTROSCOPIC DIFFERENTIATION OF NORMAL AND ACI-ERGOT PEPTIDE ALKALOIDS AND THEIR 12'-ALKOXY DERIVATIVES
Helena Pelantová*, Petr Sedmera, Ladislav Cvak, Josef Stuchlík, and Alexandr Jegorov

9:45 AM EXPLORING FUNCTIONALIZED PORPHYRINES WITH QUANTUM MECHANICAL CALCULATION
Martin Nausner*, Norbert Müller, Martin Häubl, Susanne Schürz, Wolfgang Schöfberger

10:00 AM SOLUTION STRUCTURE OF SOME BISBENZYLISOQUINOLINE ALKALOIDS CALCIUM COMPLEXES BY NMR SPECTROSCOPY
Ioana Stanculescu*, Cristina Mandravel, Roger Dommissé

10:15 AM BREAK

10:45 AM SESSION 5 – E. KLEINPETER, Session Chair

10:45 AM NMR STUDY OF REARRANGEMENTS OF IMIDAZO[4,5-C]QUINOLIN-2,4-DIONES
Antonín Lyčka* and Antonín Klásek

11:00 AM ¹H, ¹³C, ¹⁵N NMR COORDINATION SHIFTS IN Pd(II) AND Pt(II) CHLORIDE COMPLEXES WITH METHYL AND PHENYL DERIVATIVES OF 2,2'-BIPYRIDINE AND 1,10-PHENANTHROLINE
L. Pazderski, J. Sitkowski, J. Toušek, R. Marek, L. Kozerski, E. Szlyk

- 11:15 AM CONFORMATIONAL ANALYSIS AND NH-TAUTOMERISM OF MESO-(1,3)-DITHIANYL SUBSTITUTED PORPHYRINS STUDIED BY NMR SPECTROSCOPY AND MOLECULAR MODELLING
Philipp Wacker*, Katja Dahms, Mathias O. Senge, Erich Kleinpeter
- 11:30 AM ¹³C CP/MAS CHARACTERIZATION OF *N*-LITHOCHOLYL-L-(CYSTEINE ETHYL ESTER)-CAPPED GOLD NANOPARTICLES
Erkki Kolehmainen*, Virpi Noponen, Shreedhar Bhat, Elina Sievänen
- 11:45 AM LUNCH**
- 1:30 PM BUS TO LEDNICE – English speaking group
- 2:15 PM BUS TO LEDNICE – Czech speaking group
- 7:00 PM DINNER**
- 8:00 PM MEETING OF THE NMR DISCUSSION GROUPS**

22nd NMR Valtice Program

WEDNESDAY APRIL 18, 2007

9:00 AM SESSION 6 - W. SCHOEFBERGER, Session Chair

9:00 AM NOVEL BIOMARKER FOR MONITORING ALZHEIMER'S DISEASE
³¹P MRS STUDY OF CREATINE KINASE ACTIVITY IN THE RAT
BRAIN.

S. Kašparová, L. Bačiak*, N. Žilka, M. Novák, S. Zbýň, J. Horecký, and T. Liptaj

9:15 AM IN VIVO ³¹P MRS STUDY OF THE RAT BRAIN METABOLISM AND
EFFECT OF SIMVASTATIN ON CEREBRAL ACTIVITY UNDER
HYPERCHOLESTEROLEMIA CONDITION

K. Kačmarská, A. Adameová, L. Bačiak, T. Liptaj, M. Kuželová, S. Kašparová.

9:30 AM NEW INSIGHT INTO AN OLD PROBLEM – IN SITU NMR OF ACETYL
GROUP MIGRATION IN GLYCOSYL ACETATE / ACETYLGLUCOSE.

Lothar Brecker*, Marek Mahut, Alexandra Schwarz, Bernd Nidetzky

9:45 AM A TIN CYLINDRICAL SAMPLE POSITIONED IN/OUT OF THE CENTRE
OF BRUKER RECTANGULAR CAVITY

Milan Mazur*, Petra Boanská, and Marian Valko

10:00 AM SEGMENTAL DYNAMICS IN POLYMER NANOCOMPOSITES AS SEEN
BY SOLID-STATE NMR

Jiri Brus*, Martina Urbanova

10:15 AM BREAK

10:45 AM SESSION 7 - J. BRUS, Session Chair

10:45 AM POLYMORPHIC PURITY & SOLID-STATE NMR SPECTROSCOPY

Jaroslav Havlíček, Josef Jirman

11:00 AM PHASE TRANSITION IN WATER-ETHANOL POLYMER SOLUTIONS
STUDIED BY NMR METHODS. CONONSOLVENCY EFFECT.

Hana Kourilova*, Lenka Hanykova

11:15 AM PHASE SEPARATION OF TEMPERATURE SENSITIVE POLYMER
SYSTEMS: INFLUENCE OF ADDITIVES

L. Starovoytova

11:30 AM SOLID-STATE NMR STUDIES OF POLYSACCHARIDE SYSTEMS

Jiří Spěváček*, Jiří Brus

11:45 AM **CLOSING REMARKS**
Radek Marek, Jan Schraml

12:00 **LUNCH**