

CENTRAL EUROPEAN NMR DISCUSSION GROUPS

21st NMR VALTICE

Valtice, Czech Republic

April 23rd-26th, 2006

21st NMR Valtice Program

SUNDAY APRIL 23, 2006

3:30-6:30 PM REGISTRATION

7:00 PM DINNER

8:00 PM OPENING REMARKS
Jan Schraml, Norbert Müller, Vladimír Sklenář

8:15 PM THE ANALYSIS OF STABLE ISOTOPES BY IRMS AND SNIF-NMR.
J. Mazáč

9:00 PM MEETING OF THE NMR DISCUSSION GROUPS.

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MONDAY APRIL 24, 2006

9:00 AM SESSION 1

9:00 AM RECENT RESULTS USING SATURATION TRANSFER DIFFERENCE
NMR TO CHARACTERIZE ENZYME-SUBSTRATE BINDING.
Lothar Brecker*, Renate Auer, Sandra Schwarz, Bernd Nidetzky

9:15 AM CONFORMATIONAL AND BIOLOGICAL STUDIES OF
PENTAPEPTIDES CONTAINING TWO DEHYDROAMINO ACID
RESIDUES.
R. Latajka*, M. Jewginski, M. Pawelczak, M. Makowski and P. Kafarski

9:30 AM A MOTIONAL ANALYSIS OF MATRIX PROTEINS OF MASON-PFIZER
MONKEY VIRUS.
Pavel Srb*, Jan Lang, J.Lipov, J. Vlach V. Veverka, T. Ruml and R.Hrabal

9:45 AM A SINGLE-POINT MUTATION OF M-PMV MATRIX PROTEIN CAUSES
REORIENTATION OF PROTEIN DOMAINS AND CHANGES THE
PHENOTYPE OF THE VIRUS.
Jiří Vlach*, Jan Lipov, Václav Veverka, Jan Lang, Pavel Srb, Tomáš Ruml and
Richard Hrabal

10:00 AM HYDROGEN BOND INFLUENCE ON CSA IN MODEL PEPTIDE.
Shen Liang,* Ji Hong-Fang, Vilko Smrečki, Norbert Müller

10:15 AM BREAK

10:45 AM SESSION 2

10:45 AM A SIMPLE APPROACH FOR SIGNAL-TO-NOISE ENHANCEMENT IN
NMR SPECTRA BY AUTOMATIC CORRECTION OF SPIKES IN THE
TAIL OF THE FID.
Nikolay G. Vassilev

11:00 AM OPTIMIZATION OF CPMG SPIN ECHO EXPERIMENT FOR
DETERMINATION OF CHEMICAL EXCHANGE.
Kateřina Vágnerová*, Jan Lang

- 11:15 AM COMBINED USE OF COMPLETE LINESHAPE ANALYSIS OF 1D SPECTRA SUBJECTED TO REFERENCE DECONVOLUTION AND LINEAR PREDICTION, 1D-SELECTIVE-EXSY AND 2D-EXSY SPECTRA FOR THE STUDY OF CHEMICAL EXCHANGE.
Pavletta Denkova* and Valentin Dimitrov
- 11:30 AM COGWHEEL PHASE CYCLING IN COMMON TRIPLE RESONANCE EXPERIMENTS FOR THE LIQUID PHASE.
Gerhard Zuckerstaetter* and Norbert Mueller
- 11:45 AM DETECTING NUCLEAR SPIN NOISE.
Alexej Jerschow, Norbert Müller*, and Gerhard Zuckerstätter
- 12:00 LUNCH**
- 2:00 PM SESSION 3**
- 2:00 PM REVERSIBLE FORMATION OF DIMER OF TETRA ISONICOTINAMIDE DERIVATIVE OF CALIX[4]ARENE.
Hana Dvořáková*, Jan Lang, Pavel Lhoták
- 2:15 PM ¹⁵N CHEMICAL SHIFT OF META AND PARA SUBSTITUTED BENZONITRILES.
Žáček, Schraml
- 2:30 PM NMR SPECTROSCOPY OF PURINE DERIVATES AS POTENTIAL DRUGS OF NEURODEGENERATIVE DISEASES.
Tomáš Bartl*, Radek Marek, Luděk Beneš
- 2:45 PM N-ALKYLPURINE DERIVATIVES AS MODEL SYSTEMS OF PURINE TAUTOMERS: STUDY OF SUBSTITUTION EFFECTS ON SOLUTION-STATE NMR PARAMETERS.
Kateřina Maliňáková*, Zuzana Zacharová, Stanislav Standara, Jaromír Toušek, Michal Hocek, Vladimír Sklenář and Radek Marek
- 3:00 PM AN ANOMALOUS COURSE OF THE REDUCTION OF 2-3-OXO-3,4-DIHYDROQUINOXALIN-2-YLBENZENE DIAZONIUM SALT. A REINVESTIGATION.
Antonín Lyčka*, Iveta Fryšová, Jan Slouka
- 3:15 PM QUANTIFICATION OF THE PUSH-PULL EFFECT IN TOLANES C ALSO A RE-EVALUATION OF FACTORS AFFECTING THE ¹³C CHEMICAL SHIFTS OF CARBON ATOMS OF THE CC TRIPLE BOND.
Erich Kleinpeter* and Anja Schulenburg
- 3:30 PM BREAK**

4:00 PM SESSION 4

4:00 PM DETECTION OF POLYMORPHIC FORMS BY MEANS OF SOLID-STATE
NMR SPECTROSCOPY.

Jaroslav Havlíček

4:15 PM NMR STUDY OF DISTAMYCIN DERIVATIVES.

Foltýnová J.*, Tkadlecová M., Král V.

4:30 PM ONE STRUCTURAL CHANGE – BIG CONFORMATIONAL
DIFFERENCES. AN ISOMER OF FK-506.

Petr Sedmera*, Ladislav Cvak, Alexandr Jegorov, Jan Čejka, and Bohumil
Kratochvíl

4:45 PM BEHAVIOR OF THE NOYORI'S CATALYST UNDER TRANSFER
HYDROGENATION CONDITIONS STUDIED BY NMR.

Marek Kuzma*, Helena Pelantová, Petr Sedmera, Petr Kačer, Helena Šiklová,
Libor Červený

5:00 PM RADIAL AND LONGITUDINAL PROFILES OF SIGNAL INTENSITY OF
A SINGLE TE102 RECTANGULAR CAVITY. THREEDIMENSIONAL
SURFACE PLOT FOR A POINTLIKE SAMPLE.

Milan Mazur

5:45 PM DINNER

**7:00-9.30 PM SCIENTIFIC INSTRUMENTS BRNO EVENING: VISIT OF “SALON
VÍN ČESKÉ REPUBLIKY“**

21st NMR Valtice Program

TUESDAY APRIL 25, 2006

9:00 AM SESSION 5

9:00 AM EFFECTS OF TRANSIENT ISCHEMIA ON RAT BRAIN ENERGY METABOLISM ASSESSED BY IN VIVO ³¹P MRS.
Bačiak L.*, Horecký J., Vančová O., Kašparová S.

9:15 AM NEONATAL RAT BRAIN ANOXIA DETERMINED BY IN VIVO ³¹P MR SPECTROSCOPY.
Ladislav Bačiak, Ivo Juránek, Michal Kaliňák*, Michal Dubovický, Svatava Kašparová

9:30 AM PROTON MAGNETIC RESONANCE SPECTROSCOPY OF THE FRONTAL WHITE MATTER IN SCHIZOPHRENIA: PREVIEW AND PRELIMINARY REPORT.
J. Dragašek, M. Bittšanský*, P. Jankovič, M. Drímalová, D. Dobrota

9:45 AM BREAK

10:15 AM SPONSORS

10:15 AM VARIAN

11:00 AM BRUKER

11:45 AM LUNCH

12:45 PM VISIT OF CROSS CELLAR

7:00 PM DINNER

8:00 PM VARIAN EVENING: PARTY IN WINE CELLAR

21st NMR Valtice Program

WEDNESDAY APRIL 26, 2006

9:00 AM SESSION 6

9:00 AM INTERFACE NMR AND ORGANOTIN CATALYSIS.
Rudolph Willem*, Vanja Pinoie, Kevin Poelmans, Monique Biesemans, Ingrid Verbruggen, Gaëlle Deshayes, Philippe Degee, Philippe Dubois

9:15 AM ONE BOND $^1J(^{119}\text{Sn}-^{117/119}\text{Sn})$ COUPLING CONSTANTS IN 1,1,2,2-TETRATBUTYL DISTANNANE DERIVATIVES.
Jan Sykora,* Katharina Decker, Michaela Flock and Frank Uhlig

9:30 AM TIN-119 CHEMICAL SHIFT DANCE IN C,N-CHELATED COMPOUNDS.
Zdeňka Padělková, Josef Bareš, Aleš Růžička*

9:45 AM ^{57}Fe NMR STUDY OF MAGNETIC DOMAIN WALLS IN YTTRIUM IRON GARNET.
K. Kouril*, J.Kohout, H. Stepankova, J. Englich, V. Chlan

10:00 AM LC NMR OF COMMERCIAL PRODUCT.
Vratislav Blechta*, Jan Sýkora, Milan Kurfürst, and Jan Schraml

10:15 AM BREAK

10:45 AM SESSION 7

10:45 AM NMR PARAMETERS IN RNA MOLECULES AND THEIR CORRELATION WITH MOLECULAR STRUCTURE.
Zuzana Vokáčová*, Bohdan Schneider and Vladimír Sychrovský

11:00 AM THE EFFECT OF CHEMICAL SHIFT TENSOR ASYMMETRY ON RELAXATION BEHAVIOR OF BASE CARBONS IN NUCLEIC ACID.
Pavel Kadeřávek*, Radovan Fiala

11:15 AM THEORETICAL STUDY OF THE EFFECTS OF DNA STACKING INTERACTIONS ON THE NMR CHEMICAL SHIFTS.
David Reha*, Vladimír Sklenar

11:30 AM SPIN-STATE SELECTIVE ^{13}C -DETECTED EXPERIMENTS FOR MEASURING SCALAR AND DIPOLAR COUPLINGS IN NUCLEIC ACID BASES.
Radovan Fiala

11:45 AM CLOSING REMARKS
Jan Schraml