

CENTRAL EUROPEAN NMR MEETING

26th NMR VALTICE

(Solid-state NMR)

Valtice, Czech Republic

May 1st-4th, 2011

26th NMR Valtice Program

SUNDAY **MAY 1, 2011**

3:00-6:00 PM **REGISTRATION**

6:00 PM **DINNER**

7:00 PM **OPENING REMARKS**
Radek Marek, Jiří Brus

7:10 PM **PETR SEDMERA PRIZE AWARDED BY THE CZECH J. M. MARCI
SPECTROSCOPIC SOCIETY**
Viktor Kanický

INTERACTION OF HYDRONIUM IONS WITH ELECTRON-DONOR
LIGANDS: NMR AND THEORETICAL STUDY
(*J. Phys. Chem. A*, **2009**, *113*, 5896-5905)
Jaroslav Kříž

8:00 PM **GET-TOGETHER PARTY ON INVITATION BY NCBR**
Vladimír Sklenář

26th NMR Valtice Program

MONDAY MAY 2, 2011

9:00 AM SESSION 1 – R. MAREK, Session Chair

9:00 AM DIPOLAR NMR FOR THE STUDY OF COMPLEX POLYMER DYNAMICS AT HIGH AND LOW RESOLUTION
Kay Saalwächter

9:45 AM SUPRAMOLECULAR STRUCTURE OF PULPS BY CP-MAS ¹³C NMR AND ITS RELATION TO ACCESSIBILITY AND REACTIVITY
P. Wollboldt, G.Zuckerstätter, H. K.Weber, H.Sixta

10:00 AM NMR CRYSTALLOGRAPHY IN PHARMACEUTICAL RESEARCH
J. Brus, J. Czernek, M. Urbanova, L. Kobera, O. Policianova

10:15 AM CONFERENCE PHOTO – IN FRONT OF VALTICE CASTLE
Radovan Fiala

10:30 AM BREAK

11:00 AM SESSION 2 – K. SAALWÄCHTER, Session Chair

11:00 AM APPLICATIONS OF SOLID STATE NMR SPECTROSCOPY IN STRUCTURAL STUDIES OF ORGANIC AND BIOORGANIC COMPOUNDS
Marek J. Potrzebowski

11:30 AM NMR STUDIES OF ORGANOGELS DERIVED FROM BILE ACID-L-METHIONINE METHYL ESTER CONJUGATES
Virpi Noponen, Nonappa, Arto Valkonen, Manu Lahtinen, Hannu Salo, Erkki Kolehmainen, Elina Sievänen

11:45 AM SOLID STATE NMR CHARACTERIZATION OF PHYTOSTEROL CONJUGATES AND THEIR COMPONENTS
Erkki Kolehmainen, Nonappa, Hana Svobodová, Ondřej Jurček, Kari Ahonen, Satu Ikonen, Zdeněk Wimmer

12:00 NMR CHEMICAL SHIFT TENSORS IN PURINES
Kateřina Maliňáková, Lucie Novosadová, Martin Babinský, Radek Marek

12:15 PM LUNCH

1:15 PM DIGESTIVE - CHÂTEAU WINE CELLAR

3:00 PM SESSION 3 – M. J. POTRZEBOWSKI, Session Chair

3:00 PM SOLID-STATE NMR OF CELLULOSIC MATERIALS
G. Zuckerstätter, G. Schild, N. Terinte, C. Schuster, T. Roeder, P. Wollboldt, H. K. Weber, H. Sixta

3:15 PM NMR OF ORGANICALLY COATED SILICON NANOCRYSTALS
Jan Lang, Kateřina Kůsová, Ondřej Cibulka, Ivan Pelant

3:30 PM NMR CRYSTALLOGRAPHY: CALCULATIONS OF SOLID-STATE NMR PARAMETERS OF ISOCYTOSINE AND SESQUITERPENE LACTONES
Martin Dracinsky, Urszula Rychlewska, Petr Jansa, Kari Ahonen, Miloš Buděšínský

3:45 PM PREDICTING THE CHEMICAL SHIELDING OF CRYSTALLINE FORMS OF PEPTIDES
Jiří Czernek

4:00 PM RELATIVISTIC DFT STUDY OF NMR CHEMICAL SHIFTS FOR SELECTED Pt(II), Pd(II) AND Au(III) COMPLEXES
Tomasz Pawlak, Markéta L. Munzarová, Leszek Pazderski, Radek Marek

4:15 PM BREAK

4:45 PM SESSION 4 – J. SCHRAML, Session Chair

4:45 PM THE INFLUENCE OF TUNING, MATCHING AND CABLE LENGTHS ON NMR NOISE SPECTRA
Norbert Müller, Judith Schlagnitweit, Michaela Horničáková, Martin Nausner, Alexej Jerschow, Eli Bendet-Taicher, Hervé Desvieux, Steven W. Morgan, Vilko Smrečki

5:00 PM GEOMETRICAL INTERPRETATIONS OF THE GENERALIZED ORDER PARAMETERS
Pavel Srb, Jan Lang, Richard Hrabal

5:15 PM OPTIMIZING *HYDRONMR* FOR APPLICATION ON SMALL MOLECULES
M. Šoltesová, J. Lang

5:30 PM DETECTION OF SIGNED HOMONUCLEAR COUPLINGS BETWEEN LOW ABUNDANT NUCLEI
V. Blechta, J. Schraml

5:45 PM RECENT PROGRESS IN NUMERICAL SIMULATIONS OF SPIN DYNAMICS OF LARGE SYSTEMS
Z. Tošner

6:00 PM EFFICIENT INDIRECT QUADRATURE DETECTION BY MULTIPLEX PHASE CYCLING
Judith Schlagnitweit, Michaela Horničáková, Gerhard Zuckerstätter, Norbert Müller

6:15 PM REFRESHMENT

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

26th NMR Valtice Program

TUESDAY MAY 3, 2011

9:00 AM SESSION 5 – E. KOLEHMAINEN, Session Chair

9:00 AM EMPIRICAL AND NOT-SO-EMPIRICAL CORRELATIONS HOLDING FOR $^2J(^{29}\text{Si}-\text{O}-^{29}\text{Si})$ COUPLINGS IN INDUSTRIALLY IMPORTANT SILOXANES
Jan Schraml, Milan Kurfürst, Vratislav Blechta

9:15 AM ^{29}Si NMR IN PHENYLSILANE POLYMER ANALYSIS
Jiří Pinkas, Vratislav Blechta, Jindřich Karban, Jan Sýkora

9:30 AM NMR STUDY OF SOME ORGANOMETALIC CHALCOGENIDES
Antonín Lyčka, Libor Dostál, Roman Jambor, Aleš Růžička, Frank de Proft

9:45 AM NMR PARAMETERS OF TIN(II) COMPLEXES AND ORGANOMETALLICS
Tomáš Chlupatý, Aleš Růžička

10:00 AM THEORETICAL AND EXPERIMENTAL ^{119}Sn CHEMICAL SHIFT INVESTIGATIONS OF ORGANOTIN(II) COMPOUNDS
Lies Broeckert, Frank De Proft, Ales Ruzicka, Monique Biesemans, Rudolph Willem

10:15 AM BRUKER
Pavel Kessler

10:35 AM BREAK

11:00 AM SESSION 6 – E. KLEINPETER, Session Chair

11:00 AM CORTECNET: YOUR PARTNER FOR STABLE ISOTOPES, LABELLED COMPOUNDS: D, ^{13}C , ^{15}N , ^{18}O , ^{17}O AND NMR CONSUMABLES
Jean-Baptiste Hibon

11:15 AM NMR OF NATURAL PRODUCTS – NOT ONLY A TOOL TO DETERMINE MOLECULAR STRUCTURES
Lothar Brecker, Johann Schinnerl, Harald Greger, Karin M. Valant-Vetschera

11:30 AM NMR STUDY OF HELQUATS
Radek Pohl, David Šaman, Vojtěch Svoboda, Louis Adriaenssens, Jan Vávra, Lukáš Severa, Filip Teplý

11:45 AM EXPERIMENTAL DETERMINATION OF MECHANISMS OF HYDROGEN BOND FLIP-FLOP IN CALIX[4]ARENE
Lenka Minářová, Jan Lang

12:00 SUPRAMOLECULAR COMPLEXES OF DISULFONATED DERIVATIVES OF 9,10-DIPHENYLANTHRACENE AND CORRESPONDING ENDOPEROXIDES WITH CYCLODEXTRINS
Lenka Slavětínská, Jiří Mosinger, Martin Dračinský

12:15 PM NMR AND COMPUTATIONAL STUDY OF SUPRAMOLECULAR COMPLEXES
Martin Babinský, Petr Kulhánek, Viktor Kolman, Vladimír Šindelář, Radek Marek

12:30 PM LUNCH

1:30 PM VISIT OF VALTICE CHÂTEAU

2:30 PM FREE ACTIVITIES

7:00 PM DINNER

8:00 PM FREE EVENING

26th NMR Valtice Program

WEDNESDAY MAY 4, 2011

9:00 AM SESSION 7 – M. BUDĚŠÍNSKÝ, Session Chair

9:00 AM PHOSPHORUS CHEMICAL SHIFTS IN B-DNA:
THE DEPENDENCE ON BACKBONE TORSION ANGLES STUDIED BY
COMBINED MD/DFT CALCULATIONS

Jana Přecechtělová, Petr Novák, Markéta L. Munzarová, Martin Kaupp,
Vladimír Sklenář

9:15 AM BACKBONE ASSIGNMENT OF THREE CLFB BINDING SERINE-RICH
PEPTIDES AT NATURAL ISOTOPE ABUNDANCE

Maria Theresia Pöschko, Michaela Horničáková, Judith Schlagnitweit, Kamil
Önder, Norbert Müller

9:30 AM INCREASE OF CONFORMATIONAL ENTROPY FAVORS BINDING OF
ADAR2 DSRBM2 AT RNA MISMATCHES

Josef Pasulka, Florian C. Oberstrass, Jaroslav Koca, Frederic H.-T. Allain,
Richard Stefl

9:45 AM RECOGNITION OF TRANSCRIPTION TERMINATION SIGNAL BY THE
NUCLEAR POLYADENYLATED RNA BINDING (NAB)3 PROTEIN

Fruzsina Hobor, Roberto Pergoli, Karel Kubicek, Dominika Hrossova,
Veronika Bacikova, Michal Zimmermann, Josef Pasulka, Ctirad Hofr,
Stepanka Vanacova, Richard Stefl

10:00 AM STRUCTURAL STUDY ON MYRISTOYLATED M-PMV MATRIX
PROTEIN

Jan Prchal, Tomas Ruml, Richard Hrabal

10:15 AM BREAK

10:45 AM SESSION 8 – A. LYČKA, Session Chair

10:45 AM INTERACTION of 1,2-DIMETHOXYETHANE WITH WATER: NMR, IR,
AND DFT STUDY

Jaroslav Kříž, Jiří Dybal

11:00 AM UTILIZATION OF TD-NMR FOR HETERO-PHASE POLYMER STUDIES

Josef Chmelář, Hana Hajová, Juraj Kosek

11:15 AM NMR STUDY OF NEW CYANOBACTERIAL CYCLIC PEPTIDES
CAUSING CYTOTOXIC EFFECT VIA CELL MEMBRANE
PERMEABILIZATION

Pavel Hrouzek, Helena Pelantová, Marek Kuzma, Jan Černý, Petr Novák,
Radovan Fišer, Petr Šimek, Dalibor Štys, Alena Lukešová, Jiří Kopecký

11:30 AM NMR STUDY OF RALSTONIA SOLANACEARUM LECTIN
INTERACTIONS

Peter Bystrický, Karel Kubíček, Marie Pokorná, Radovan Fiala, Michaela
Wimmerová

11:45 AM STRUCTURE OF THE HUMAN PROGRAMMED CELL DEATH 1
RECEPTOR AND IMPLICATIONS FOR IMMUNE MODULATION BY
LIGAND BINDING

Václav Veverka

12:00 JOSEF DADOK PRIZE

R. WILLEM, M. J. POTRZEBOWSKI, R. FIALA - committee

12:15 PM CLOSING REMARKS

12:30 PM LUNCH