

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

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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 Desvaux, 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“**

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TUESDAY MAY 3, 2011

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

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

Jan Schraml, Milan Kurfürst, Vratislav Blechta

9:15 AM ${}^{29}\text{Si}$ 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 ${}^{119}\text{Sn}$ CHEMICAL SHIFT
INVESTIGATIONS OF ORGANOTIN(II) COMPOUNDS

Lies Broeckaert, 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, ${}^{13}\text{C}$, ${}^{15}\text{N}$, ${}^{18}\text{O}$, ${}^{17}\text{O}$ AND NMR CONSUMABLES

Jean-Baptiste Hibon

11:15 AM NMR OF NATURAL PRODUCTS – NOT ONLY A TOOL TO
DETERMINE MOLECULARE 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

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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 Chmelař, 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**