

**CENTRAL EUROPEAN NMR MEETING**

# **25<sup>th</sup> NMR VALTICE**

Valtice, Czech Republic

April 25<sup>th</sup>-28<sup>th</sup>, 2010

## **25<sup>th</sup> NMR Valtice Program**

<b>SUNDAY</b>	<b>APRIL 25, 2010</b>
<b>3:00-6:00 PM</b>	<b>REGISTRATION</b>
<b>6:00 PM</b>	<b>DINNER</b>
<b>7:00 PM</b>	<b>OPENING REMARKS</b> Vladimír Sklenář
<b>7:10 PM</b>	<b>MOLECULAR IMAGING BY IN VIVO MAGNETIC RESONANCE</b> Milan Hájek

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

**MONDAY APRIL 26, 2010**

**9:00 AM SESSION 1 – M. HÁJEK, Session Chair**

9:00 AM TREATMENT OF COHERENCE TRANSFER PATHWAY RECONVERGENCE IN THE SIMULATION OF METABOLITE SPECTRA IN FAST-CYCLED IN-VIVO MR SPECTROSCOPIC IMAGING  
Zenon Starčuk jr.,\* Jana Starčuková

9:15 AM STD NMR OF TERNARY ENZYME-COENZYME-SUBSTRATE COMPLEXES - BINDING STUDIES OF NADH AND NADPH TO CANDIDA TENUIS XYLOSE REDUCTASE  
Michael Vogl,\* Regina Kratzer, Lothar Brecker, Bernd Nidetzky

9:30 AM AUTOMATED SIGNAL DETECTION AND INTEGRAL DETERMINATION - A NEW APPROACH TO ANALYZE (NOT ONLY) IN SITU <sup>1</sup>H NMR MEASUREMENTS  
Lothar Brecker,\* Hyung-Won Koh, Lars Hildebrand, Jan Schlenke, Susanne Felsing, Bernd Reusch

9:45 AM NMR STUDIES OF LIPOSOMES AS DRUG CARRIER SYSTEMS  
Markus Husa,\* Julia Schwarz, Martin Kratzel, Claudia Valenta, Hanspeter Kählig

10:00 AM LC-NMR IN USE  
Jan Sýkora\*

10:15 AM <sup>1</sup>H DETECTED SQSQ EXPERIMENT  
Vratislav Blechta,\* Jan Schraml

**10:30 AM BREAK**

**11:00 AM SESSION 2 – J. JAŻWIŃSKI, Session Chair**

11:00 AM <sup>1</sup>H, <sup>13</sup>C AND <sup>15</sup>N NMR COORDINATION SHIFTS IN Pd(II) AND Pt(II) CHLORIDE COMPLEXES WITH VARIOUS ALKYL AND ARYL DERIVATIVES OF 2,2'-BIPYRIDINE AND 1,10-PHENANTHROLINE  
Tomasz Pawlak,\* Leszek Pazderski, Jerzy Sitkowski, Lech Kozerski, Edward Sztyk

11:15 AM ADDUCTS OF DIAMINES WITH DIMERIC RHODIUM TETRAACETATE-APPLICATION OF <sup>13</sup>C AND <sup>15</sup>N CP-MAS NMR  
Jarosław Jaźwiński, Bohdan Kamieński, Agnieszka Sadlej\*

11:30 AM MULTINUCLEAR NMR STUDY OF SOME ORGANOTIN COMPOUNDS  
Antonín Lyčka,\* Aleš Růžička, Libor Dostál, Roman Jambor

11:45 AM RELATIONS OF NMR, IR AND XRD DATA FOR ORGANOTIN(IV) ZWITTERIONIC COMPLEXES OF MINERAL ACIDS  
Petr Švec, Zdeňka Padělková, Libor Dušek, Antonín Lyčka, Aleš Růžička\*

**12:00 LUNCH**

**2:00 PM SESSION 3 – E. KLEINPETER, Session Chair**

2:00 PM SOLVENT MODELS FOR CALCULATION OF NMR PARAMETERS  
Martin Dračinský,\* Petr Bouř

2:15 PM COMPUTATIONAL STUDIES OF MAGNETIC RESONANCE PROPERTIES IN ENDOHEDRAL FULLERENES  
M. Straka,\* P. Štěpánek, S. Taubert, D. Sundholm, T. Pennanen, J. Vaara, P. Lantto

2:30 PM N-OXIDATION INDUCED CHEMICAL SHIFT IN TERTIARY AMINES – EXPERIMENT AND DFT CALCULATIONS  
Radek Pohl,\* Martin Dračinský, Lenka Slavětínská and Miloš Buděšínský

2:45 PM COMPREHENSIVE STUDY OF THE NMR CHEMICAL SHIFTS FOR 6-HALOPURINES  
Stanislav Standara,\* Kateřina Maliňáková, Radek Marek, Michal Straka and Juha Vaara

3:00 PM QUANTIFICATION OF THE ANISOTROPIC EFFECT IN QUINOXALINY-MONOKETO- AND DIKETO SUBSTITUTED TETRAHYDRODICYCLOPENTADIENE DERIVATIVES  
Anica Lämmermann\*, István Szatmári, Ferenc Fülöp, Erich Kleipeter

**3:15 PM BREAK**

**3:45 PM SESSION 4 – M. HRICOVÍNI, Session Chair**

3:45 PM CONFORMATIONAL STUDY OF CHIRAL CALIX[4]ARENES USING RESIDUAL DIPOLAR COUPLINGS  
Jiří Vlach,\* Hana Dvořáková, Markéta Šimánová and Pavel Lhoták

4:00 PM NMR INVESTIGATION OF GUEST-HOST COMPLEX BETWEEN CHLOROFORM AND CRYPTOPHANE-C  
Zoltán Takács, Mária Šoltéssová,\* Dmytro Kotsyubynsky, Jozef Kowalewski, Jan Lang, Thierry Brotin, Jean-Pierre Dutasta

4:15 PM MOLECULAR DYNAMIC BEHAVIOUR IN WATER/ETHANOL MIXTURES  
Marek Radecki\*

4:30 PM TOKAJ WINE TASTING BY NMR SPECTROSCOPY  
Milan Mazur\*, Lucia Husarikova, Katarina Furdikova, Michal Kalinak, Marian Valko

4:45 PM SNIF – NMR – DETERMINING THE AUTHENTICITY OF WINE  
Pavlna Sečkářová\*, Romana Buchtová, Kamil Kolář, Hana Šimková

**5:00 PM BREAK**

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

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

## TUESDAY APRIL 27, 2010

### 9:00 AM SESSION 5 – W. SCHÖFBERGER, Session Chair

- 9:00 AM STRUCTURE OF BIOLOGICALLY ACTIVE OLIGOSACCHARIDES. THEORY AND EXPERIMENT  
Miloš Hricovíni\*
- 9:15 AM INVESTIGATIONS ON STRUCTURE AND FUNCTION OF A PEPTIDE FROM FROG SKIN  
Ruth Gößler-Schöfberger,\* Lorenz Reith, Alexander Jilek, Wolfgang Schöfberger, Norbert Müller
- 9:30 AM DNA DUPLEX MELTING MONITORED VIA LINESHAPE ANALYSIS OF <sup>1</sup>H NMR SPECTRA  
Václav Římal,\* Helena Štěpánková, Josef Štěpánek
- 9:45 AM BINDING MODE OF PALMATINE TO d(GGAATTGCG).d(CGCAATTCC)  
Jan Novotný,\* Radovan Fiala, Zdeněk Kříž, Radek Marek
- 10:00 AM CONFERENCE PHOTO – IN FRONT OF VALTICE CASTLE  
Radovan Fiala\*

### 10:10 AM BREAK

### 10:30 AM SESSION 6 – L. BRECKER, Session Chair

- 10:30 AM 65 YEARS OF NMR: MILESTONES AND CROSSROADS  
Vladimír Sklenář\*
- 10:50 AM MY 40 YEARS IN NMR  
Josef Dadok\*
- 11:30 AM INITIATING A CHEMIST TO NMR IN CZECHOSLOVAKIA; 50 YEARS AGO AND WHAT FOLLOWED  
Jan Schraml\*
- 11:50 AM THE NMR STORY IN HUNGARY AND IN DEBRECEN  
Gyula Batta\*
- 12:10 PM GLIMPSES OF AND REMARKS ON DEVELOPMENT OF NMR IN AUSTRIA  
Norbert Müller\*
- 12:30 PM HISTORY OF THE NMR VALTICE MEETING  
Miroslav Holík\*

### 12:45 PM LUNCH

### 2:15 PM SESSION 7 – R. HRABAL, Session Chair

- 2:15 PM STRUCTURE DETERMINATION OF THE PERIPLASMIC DOMAIN OF A BACTERIAL MEMBRANE-LOCALIZED TRANSCRIPTION ACTIVATOR BY SOLUTION NMR  
Evelyne Schrank,\* Gabriel Wagner, Vera Fengler, Sarah Tutz, Joachim Reidl and Klaus Zangger
- 2:30 PM SOLUTION STRUCTURE OF THE MEMBRANE ASSOCIATED POLYPEPTIDE FST, TOXIC ANTAGONIST OF THE PAR TOXIN-ANTITOXIN SYSTEM  
Rueckert Hanna Marie,\* Goebl Christoph, Kosol Simone and Zangger Klaus
- 2:45 PM DIFFUSION AND CONVECTION IN PROTEIN NMR  
Marián Grocký,\* Jan Lang
- 3:00 PM CARBON-DETECTED EXPERIMENTS FOR ASSIGNMENT OF PROLINE RICH PROTEINS  
Radovan Fiala,\* Michaela Horníčáková, Lukáš Žídek, and Norbert Müller
- 3:15 PM NMR STUDY OF NATURAL KILLER CELL RECEPTOR NKR-P1A  
Josef Chmelík,\* Daniel Rozbeský, Karel Bezouška
- 3:30 PM BACKBONE MOTIONS OF DELTA SUBUNIT OF RNA POLYMERASE FROM BACILLUS SUBTILIS ON VARIOUS TIME SCALES  
Pavel Kadeřávek,\* Veronika Motáčková

### 3:45 PM BREAK

### 4:15 PM SESSION 8 – R. FIALA, Session Chair

- 4:15 PM NON-UNIFORM SAMPLING, CARBON DETECTION AND HIGH DIMENSIONALITY AS MEANS OF IMPROVING RESOLUTION FOR ASSIGNMENT OF DISORDERED PROTEINS  
Jiří Nováček, Veronika Motáčková, Anna Zawadzka, Krzysztof Kazimierczuk, Wiktor Koźmiński, Lukáš Žídek, Vladimír Sklenář
- 4:30 PM INTERACTION OF M-PMV MATRIX PROTEIN WITH PHOSPHATIDYLINOSITOL  
Jan Prchal,\* Jiri Vlach, Tomas Ruml, Richard Hrabal
- 4:45 PM BRUKER  
Pavel Kessler\*
- 5:15 PM LACH-NER, PURE CHEMICALS AND SPECIALIZED SERVICES  
Jiří Vokál\*
- 5:30 PM BREAK
- 6:00 PM DINNER
- 7:00 PM FREE EVENING

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

**WEDNESDAY APRIL 28, 2010**

**9:00 AM SESSION 9 – J. SCHRAML, Session Chair**

- 9:00 AM NMR DIFFUSION MEASUREMENTS IN POROUS MEDIA  
Mikuláš Peksa,\* Milan Kočířk, Jan Lang
- 9:15 AM HIGH-PRESSURE NMR: A TOOL FOR TIN-CATALYSED ORGANIC  
CARBONATES SYNTHESIS FROM CARBON DIOXIDE AND  
ALCOHOLS  
Laurent Plasseraud,\* Michel Picquet and Gabor Laurency
- 9:30 AM SOLID STATE NMR STUDIES OF SELF-ASSEMBLED SOFT  
MATERIALS  
Nonappa,\* Manu Lahtinen, Babita, Erkki Kolehmainen
- 9:45 AM PHASE SEPARATION IN AQUEOUS SOLUTIONS OF POLY(N-  
ISOPROPYLMETHACRYLAMIDE)/POLY(N-VINYLCAPROLACTAM)  
MIXTURES  
Hana Kouřilová,\* Lenka Hanyková, Jiří Spěvák
- 10:00 AM BEHAVIOUR OF WATER DURING TEMPERATURE-INDUCED PHASE  
SEPARATION IN POLY(VINYL METHYL ETHER)/D<sub>2</sub>O SOLUTIONS  
Jiří Spěvák,\* Lenka Hanyková, Jan Labuta
- 10:15 AM BIODEGRADATION OF ORGANIC POLLUTANS FORMALDEHYDE,  
METHANOLE AND FORMATE PRESENT IN CLOUDS: CONTRIBUTION  
TO ATMOSPHERIC CHEMISTRY  
Slavomira Husarova,\* Pierre Amato, Martine Sancelme, Maria Matulova and  
Anne-Marie Delort
- 10:30 AM ADVANCES IN THE NMR BASED CHARACTERIZATION OF WOOD  
AND WOOD PRODUCTS  
Gerhard Zuckerstaetter,\* Petra Wollboldt, Gabriele Schild, Hedda K. Weber  
and Herbert Sixta
- 10:45 AM BREAK**
- 11:15 AM SESSION 10 – D. ŠAMAN, Session Chair**
- 11:15 AM NMR NOISE  
Norbert Müller,\* Martin Nausner, Judith Schlagnitweit, Vilko Smrecki,  
Alexej Jerschow
- 11:30 AM THREE-DIMENSIONAL NMR SPECTROSCOPY OF ORGANIC  
MOLECULES  
Maria Misiak\* and Wiktor Koźmiński
- 11:45 AM ATROPINE – NEW INSIGHTS INTO AN OLD MOLECULE  
Matthias Heydenreich,\* Andreas Koch, Larissa V. Schmietendorf, Erich  
Kleinpeter

- 12:00 CARBON-CARBON SPIN-SPIN COUPLINGS <sup>n</sup>J(CC) VS. MOLECULAR  
GEOMETRY IN 3-HALOGENOACRYLIC ACIDS AND THEIR METHYL  
ESTERS. EXPERIMENT AND THEORY  
Marta Bugaj,\* Krystyna Kamińska-Trela
- 12:15 PM NMR BASED STRUCTURE DETERMINATION OF ALKALOIDS  
ISOLATED FROM PLANTS OF THE GENUS PSYCHOTRIA L.  
(RUBIACEAE)  
Hannes Faßhuber,\* Martin Bernhard, Andreas Berger, Johann Schinnerl,  
Wolfgang Robien, Harald Greger, Lothar Brecker
- 12:30 PM NMR STUDY OF BRANCHED ARABINAN OBTAINED FROM SUGAR  
BEET FIBER BY QUATERNIZATION UNDER ACIDIC CONDITIONS  
Iveta Uhliaríková\* and Ivan Šimkovic
- 12:45 PM JOSEF DADOK PRIZE**
- 12:55 PM CLOSING REMARKS**
- 13:00 PM LUNCH**