

CENTRAL EUROPEAN NMR MEETING

# 27<sup>th</sup> NMR VALTICE

(Biomolecular NMR)

Valtice, Czech Republic

April 22<sup>nd</sup>-25<sup>th</sup>, 2012

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

<b>SUNDAY</b>	<b>APRIL 22, 2012</b>
<b>3:00-6:00 PM</b>	<b>REGISTRATION</b>
<b>6:00 PM</b>	<b>DINNER</b>
<b>7:15 PM</b>	<b>OPENING REMARKS</b> Radek Marek, Jiří Brus
<b>7:25 PM</b>	<b>PETR SEDMERA PRIZE AWARDED BY THE CZECH J. M. MARCI SPECTROSCOPIC SOCIETY</b> Vladimír Sklenář
<b>8:00 PM</b>	<b>GET-TOGETHER PARTY</b>

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### MONDAY APRIL 23, 2012

#### 9:00 AM SESSION 1 – L. ŽÍDEK, Session Chair

9:00 AM STRUCTURAL BIOLOGY BY SOLID-STATE NMR  
Hartmut Oschkinat

9:45 AM THE FILTER EXCHANGE SPECTROSCOPY EXPERIMENT: STUDY OF  
MEMBRANE FLUIDITY  
Pavel Srb, Hana Elicharová, Larisa Starovoytova, Jaroslav Kříž, Hana Sychrová, and  
Jan Lang

10:00 AM STRUCTURE SOLUTION OF NATURAL KILLER CELL RECEPTOR NKR-P1A  
BY NMR AND CHEMICAL CROSS-LINKING  
Josef Chmelik, Daniel Rozbeský, Petr Man, Daniel Kavan, Karel Bezouška, and Petr  
Novák

10:15 AM NMR STUDY OF RNA POLYMERASE DELTA SUBUNIT UNIQUE FOR GRAM-  
POSITIVE BACTERIA  
Veronika Papoušková, Jiří Nováček, Pavel Kadeřávek, Hana Šanderová, Alžběta  
Švenková, Anna Zawadzka-Kazimierczuk, Krzysztof Kazimierczuk, Lukáš Židek,  
Wiktor Koźmiński, Libor Krásný, and Vladimír Sklenář

10:30 AM CONFERENCE PHOTO – IN FRONT OF VALTICE CASTLE  
Radovan Fiala

#### 10:45 AM BREAK

#### 11:15 AM SESSION 2 – H. OSCHKINAT, Session Chair

11:15 AM STRUCTURE OF TDP-43 IN COMPLEX WITH UG-RICH RNA  
Peter J. Lukavsky, Dalia Daujotyte, Fred F. Damberger, and Frédéric H. Allain

11:45 AM NMR STUDIES OF TERNARY CARBOHYDRATE – NAD(H) – CANDIDA  
TENUIS XYLOSE REDUCTASE COMPLEXES  
Micheal Vogl, Regina Kratzer, Bernd Nidetzky, and Lothar Brecker

12:00 STRUCTURE OF MYRISTOYLATED MATRIX PROTEIN OF MASON-PFIZER  
MONKEY VIRUS AND ITS INTERACTION WITH PHOSPHATIDYLINOSITOL  
PHOSPHATES  
Jan Prchal, Pavel Srb, Tomas Ruml, and Richard Hrabal

12:15 PM INFLUENCE OF CYTOSINE METHYLATION ON THE DYNAMICS OF DNA  
DOUBLE-HELIX  
Václav Římal, Helena Štěpánková, and Josef Štěpánek

12:30 PM LUNCH

1:30 PM DIGESTIVE – WINE CROSS-CELLAR

#### 4:30 PM SESSION 3 – E. KLEINPETER, Session Chair

4:30 PM BRUKER – LATEST DEVELOPMENTS  
Pavel Kessler

4:55 PM JEOL – ANALYSIS OF SEMI-SOLID SAMPLES  
Hiroaki Sasakawa

5:15 PM MOLECULAR INTERVENTIONS OF PEPTIDES AND SMALL MOLECULES. A  
STRUCTURAL STUDY  
Sreenivas Reddy Bathula

5:30 PM ANGULAR DEPENDENCE OF <sup>31</sup>P CHEMICAL SHIELDING IN NUCLEIC  
ACIDS  
Jana Přecechtělová, Markéta L. Munzarová, Juha Vaara, Petr Novák, Martin  
Dračinský, and Vladimír Sklenář

5:45 PM CORRELATING THE <sup>31</sup>P-NMR PARAMETERS WITH CONFORMATION OF  
NUCLEIC ACIDS  
Ladislav Benda

#### 6:00 PM REFRESHMENT

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

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

### TUESDAY APRIL 24, 2012

#### 10:00 AM SESSION 5 – M. STRAKA, Session Chair

10:00 AM EFFECT OF DEUTERATION ON DYNAMICS OF HYDROGEN BOND ARRAY IN CALIX[4]ARENE  
Lenka Minářová, and Jan Lang

10:15 AM NMR STUDIES OF PURINE DERIVATIVES  
Eliška Procházková, Lucie Čechová, Petr Jansa, Michal Šála, Radim Nencka, and Martin Dračínský

10:30 AM ADDITION OF ACTIVATED METHYLPHOSPHONATE TO CHALCONES – MECHANISM & STEREOCHEMISTRY BY NMR  
Radek Pohl, Stanislav Opekar, and Petr Beier

10:45 AM <sup>7</sup>Li NMR SPECTROSCOPY AS THE TOOL FOR STRUCTURAL EVALUATION OF LITHIUM-SPECTATOR LIGAND COMPLEXES  
Aleš Růžička

11:00 AM ADDUCTS OF RHODIUM(II) TETRATRIFLUOROACETYLATE WITH OXYGENIC LIGANDS: <sup>1</sup>H NMR, <sup>13</sup>C NMR AND DFT STUDIES  
Jaroslav Jaźwiński, Rafał Głazczka

11:15 AM “THROUGH SPACE” *J*-COUPLING BETWEEN HYDROGEN NUCLEI  
M. Dračínský, P. Jansa, and P. Bouř

11:30 AM LUNCH

1:00 PM CONFERENCE TRIP

7:30 PM DINNER

FREE EVENING

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### WEDNESDAY APRIL 25, 2012

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

9:00 AM AUTOMATED SIGNAL DETECTION FOR EVALUATION OF MAGNETIC FIELD HOMOGENITY FROM FOURIER TRANSFORMED <sup>1</sup>H-NMR SPECTRA  
Lothar Brecker, Jan Schlenke, Lars Hildebrand, Susanne Felsing, and Bernd Reusch

9:15 AM INTERPRETATION OF NMR RELAXATION DATA OF FLEXIBLE MOLECULES VIA STOCHASTIC MODELING: A TRISACCHARIDE CASE  
Maria Šoltésová, Mirco Zerbetto, Dmytro Kotsyubynskyy, Jozef Kowalewski, Göran Widmalm, and Antonino Polimeno

9:30 AM RDC OF MUSCLE METABOLITES IN A GEL MODEL  
Karel Bernásek, Marián Grocký, and Jan Lang

9:45 AM APPLICATION OF HCSE PULSE SEQUENCE TO DETECTION OF SMALL SIGNED CARBON-CARBON COUPLING CONSTANTS.  
Vratislav Blechta, Jan Schraml, and Jan Sýkora

10:00 AM EXPLORING NEW <sup>129</sup>Xe CHEMICAL SHIFT RANGES IN EXOTIC HXeY COMPOUNDS: HYDROGEN MORE RELATIVISTIC THAN XENON  
Perttu Lantto, Stanislav Standara, Sebastian Riedel, Juha Vaara, and Michal Straka

10:15 AM BREAK

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

10:45 AM INSIGHTS INTO THE PHARMACEUTICAL CO-CRYSTALS  
Nonappa, Manu Lahtinen, and Erkki Kolehmainen

11:00 AM SOLID-STATE NMR STUDIES OF THERMAL SYNTHESIS OF CYCLIC PEPTIDES  
Magdalena Jaworska, Marek J. Potrzebowski

11:15 AM STUDY OF THERMAL PROCESSES IN THE CRYSTAL LATTICE OF PSEUDO-CYCLIC YAFG TETRAPEPTIDE BY ULTRA-FAST SOLID STATE NMR AND GIPAW CALCULATIONS  
Tomasz Pawlak

11:30 AM INTERPOLATION IN NUMERICAL SIMULATIONS OF NMR SPECTRA OF POWDERS  
Zdeněk Tošner

**11:45 AM JOSEF DADOK PRIZE**  
L. BRECKER, R. FIALA, R. HRABAL, - committee

**12:00 CLOSING REMARKS**

**12:15 PM LUNCH**