

**CENTRAL EUROPEAN NMR MEETING**

**32<sup>nd</sup> NMR VALTICE**

**Valtice, Czech Republic**

**April 23-26, 2017**

Edited by: Jan Novotný and Radek Marek, Masaryk University, Brno

Printed by: Stuaire, s.r.o.

ISBN 978-80-86441-49-8

# **CONFERENCE IS ORGANIZED BY**

**Central European Institute of Technology (CEITEC)**

**Masaryk University, Brno**

# **THIS CONFERENCE IS SPONSORED BY**

## **General sponsor:**

BRUKER

## **Main sponsors:**

Armar Chemicals

Euriso-Top

## **Other sponsors:**

(Alphabetical order)

Chemstar

CortecNet

Jeol

Lach-Ner

Magritek

Merck

Měřicí technika Morava

Mesbach Energy

SciTech

# 32<sup>nd</sup> NMR Valtice Program

**SUNDAY      APRIL 23, 2017**

**3:00-6:00 PM    REGISTRATION**

**6:00 PM          DINNER**

**7:30 PM          OPENING REMARKS**  
Radek Marek

**7:40 PM          PETR SEDMERA PRIZE AWARDED BY THE CZECH J. M. MARCI  
SPECTROSCOPIC SOCIETY**  
Viktor Kanický, Radovan Fiala

MULTIPLE CELLULAR PROTEINS INTERACT WITH LEDGF/p75  
THROUGH A CONSERVED UNSTRUCTURED CONSENSUS MOTIF  
(*Nat. Commun.*, **2015**, 6:7968)

Petr Tesina, Kateřina Čermáková, Magdalena Hořejší, Kateřina Procházková,  
Milan Fábry, Subhalakshmi Sharma, Frauke Christ, Jonas Demeulemeester,  
Zeger Debyser, Jan De Rijck, Václav Veverka, Pavlína Řezáčová

**8:30 PM          EURISO-TOP EVENING**

# 32<sup>nd</sup> NMR Valtice Program

**MONDAY APRIL 24, 2017**

**9:00 AM SESSION 1 – J. NOVOTNÝ, Session Chair**

9:00 AM NMR STUDIES OF TETRAHELICAL DNA STRUCTURES AND THEIR DYNAMIC TRANSFORMATIONS  
Janez Plavec

9:45 AM NMR STUDY OF BASE-MODIFIED G-QUADRUPLEXES  
Kateřina Peterková, Jan Novotný, Radek Marek

10:00 AM NMR STUDY OF d(CCCGAGA) i-MOTIF STRUCTURE  
Aleř Novotný, Jan Novotný, Radovan Fiala, Radek Marek

10:15 AM CONFERENCE PHOTO  
Radovan Fiala

**10:30 AM BREAK**

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

11:00 AM HEDGEHOG IN THE CAGE: CAN WE FIND THE PARAMAGNETIC INHIBITOR SITE USING PROTEIN NMR, QUANTUM MECHANICS AND MOLECULAR DYNAMICS SIMULATIONS?  
Pavel Srb, Michal Svoboda, Ladislav Benda, Klára řařková, Jan Konvalinka, Václav řícha, Václav Veverka

11:15 AM BIOCHEMICAL AND STRUCTURAL CHARACTERIZATION OF THE BUDDING YEAST PROTEIN YLR455W  
Ibidolapo Atinuke Adekoya, Kateřina řermáková, Marcela Mádlíková, Norbert Müller, Václav Veverka

11:30 AM INTERACTION OF MASON-PFIZER MONKEY VIRUS ENV PROTEIN WITH ITS MATRIX PROTEIN  
Jan Prchal, Tomáš Kroupa, Tomáš Ruml, Richard Hrabal

11:45 AM NMR INTERACTION STUDIES OF NOVEL ANTIMICROBIAL PEPTIDES WITH BACTERIAL PROTEINS  
Maria Bräuer, Michal Kamenicky, Kathrin Volk, Kamil Önder, Norbert Müller

12:00 TARGETING PROTEIN-PROTEIN INTERACTIONS: A HOT TOPIC IN ANTIBIOTICS DISCOVERY  
Michal Kamenicky, Maria Bräuer, Kathrin Volk, Kamil Önder, Christian Klein, Norbert Müller

**12:15 LUNCH**

- 2:00 PM      SESSION 3 – V. SKLENÁŘ, Session Chair**
- 2:00 PM      FROM PROTEIN SEQUENCE TO NMR STRUCTURE IN A MATTER OF DAYS USING CHAINS/ROSETTA  
Thomas Evangelidis, Jiří Nováček, Nikolaos G. Sgourakis, Konstantinos Tripsianes
- 2:15 PM      STRUCTURAL CHARACTERIZATION OF PROTEIN KINASE ASK1 AND ITS INTERACTION WITH THIOREDOXIN  
Katarína Pšenáková, Václav Veverka, Rozálie Hexnerová, Pavel Srb, Salome Kylarová, Veronika Obsilová, Tomáš Obsil
- 2:30 PM      ABBREVIATION PARADISE: THE TAZ2 (CBP) TAD (C/EBPB) INTERACTION  
Rozálie Hexnerová, Maria Miller, Václav Veverka
- 2:45 PM      STRUCTURAL BASIS FOR OVERLAP OF LEDGF/P75 AND HRP-2 IN MLL LEUKEMIA  
Kateřina Čermáková, Sara El Ashkar, Marcela Madlíková, Rozálie Hexnerová, Lukáš Vrzal, Pavel Srb, Zeger Debysers, Jan De Rijck, Pavlína Řezáčová, Václav Veverka
- 3:00 PM      NMR IN TO STUDY CASCADE REACTIONS – STATE OF THE ART AND FORECAST  
Patricia Wildberger, Martin Pfeiffer, Bernd Nidetzky, Lothar Brecker
- 3:15 PM      THE EFFECTS OF DIET AND MICROBIOTA ON THE FECAL METABOLOME IN MICE  
Martina Bugáňová, Helena Pelantová, Miloslav Kverka, Štěpán Coufal, Tomáš Hudcovic, Marek Kuzma
- 3:30 PM      FILTER-EXCHANGE DIFFUSION NMR SPECTROSCOPY: A POWERFUL METHOD FOR INVESTIGATION OF WATER TRANSPORT THROUGH PLASMA MEMBRANE IN YEASTS  
Mária Šoltéssová, Hana Elicharová, Pavel Srb, Michal Růžička, Larisa Starovoytova, Hana Sychrová, Jan Lang
- 3:45 PM      BREAK**
- 4:30 PM      SESSION 4 – R. HRABAL, Session Chair**
- 4:30 PM      CZECH INFRASTRUCTURE FOR INTEGRATIVE STRUCTURAL BIOLOGY  
Vladimír Sklenář
- 4:50 PM      BRUKER NEWS 2017  
Pavel Kessler
- 5:10 PM      NEW JEOL NMR PRODUCTS FOR 2017  
Michal Maloň
- 6:00 PM      DINNER**
- 7:30-9:00 PM      BRUKER EVENING:  
VISIT OF “SALON VÍN ČESKÉ REPUBLIKY“**

# 32<sup>nd</sup> NMR Valtice Program

**TUESDAY APRIL 25, 2017**

**9:00 AM      SESSION 5 – J. JAZWINSKI, Session Chair**

9:00 AM      CALCULATION OF BINDING CONSTANTS OF DIASTEREOMERIC  
COMPLEXES

Petra Cuřínová, Martin Jakubec, Jan Storch, Roman Holakovský

9:15 AM      POTENTIAL PLATINUM ANTICANCER DRUGS AND THEIR  
INTERACTION WITH MACROCYCLES

Karolina Wawrocka, Jan Chyba, Radek Marek

9:30 AM      BINDING STUDY OF POTENTIAL RUTHENIUM METALLODRUGS  
AND MACROCYCLIC CARRIERS BY USING NMR SPECTROSCOPY

Petra Munzarová, Martin Novák, Jan Chyba, Radek Marek

9:45 AM      NMR STUDIES OF CHOLESTEROL AND CYCLODEXTRINS

Karolína Kučáková, Bohumil Dolenský

10:00 AM      MRI STUDY OF TEMPERATURE RESPONSIVE HYDROGEL  
NETWORKS BASED ON *N*-ISOPROPYLACRYLAMIDE

Karel Bernášek, Lenka Hanyková, Jan Lang

10:15 AM      *d*-ELEMENT RELAXATION AGENTS FOR <sup>19</sup>F-MRI: CHEMISTRY AND  
PHYSICS TOWARD *IN VIVO* APPLICATION

Jan Blahut, Jan Kotek, Zdeněk Tošner, Karel Bernášek, Jan Lang, Vít Herynek,  
Andrea Gálisová, Carlos Platas-Iglesias, Danuta Kruk, Petr Hermann

10:30 AM      DETERMINATION OF THE ORBITAL AND PARAMAGNETIC  
CONTRIBUTIONS TO THE <sup>1</sup>H AND <sup>13</sup>C NMR CHEMICAL SHIFTS OF  
RUTHENIUM(III) COMPLEXES

Lukáš Jeremias, Jan Novotný, Michal Repiský, Stanislav Komorovský, Radek  
Marek

10:45 AM      INTERPRETING THE NMR SPECTRA OF PARAMAGNETIC Ru(III)  
COMPLEXES

David Přichystal, Jan Novotný, Martin Sojka, Marek Nečas, Radek Marek

**11:00 AM      BREAK**

- 11:30 AM      SESSION 6 – P. CUŘÍNOVÁ, Session Chair**
- 11:30 AM      CONFORMATION OF MANNOBIOSE REVISITED BY NMR  
Radek Pohl, Jakub Kaminský
- 11:45 AM      STRUCTURAL INSIGHTS INTO ENANTIOSELECTIVE PEPTIDE-  
CATALYZED ACYLATION UTILIZING ADVANCED NMR METHODS  
Eliška Procházková, Julian Ilgen, Lukas Kaltschnee, Volker Schmidts, Maic  
Fredersdorf, Andreas Kolmer, Mira Schwab, Raffael C. Wende, Peter R.  
Schreiner, Christina M. Thiele
- 12:00          SLICE-SELECTIVE NMR APPROACHES FOR INVESTIGATION OF  
NONCOVALENT INTERACTIONS IN WATER  
Yavor Mitrev, Svetlana Simova
- 12:15          FLUXIONAL BEHAVIOUR OF UNSYMMETRICAL N-HETEROCYCLIC  
CARBENE Pd(II) COMPLEXES  
Miroslav Dangalov, Nikolay G. Vassilev, Rumen Lyapchev, Petar Petrov
- 12:30          PHOTOCHEMISTRY OF QUINAZOLINONE-DERIVED SCHIFF'S  
BASES: EPR, NMR AND DFT STUDY  
Michal Hricovíni, Miloš Hricovíni
- 12:45          RESONANCE-ASSISTED STABILISATION OF HYDROGEN BONDS  
PROBED BY NMR SPECTROSCOPY AND PATH INTEGRAL  
MOLECULAR DYNAMICS  
Martin Dračínský, Lucie Čechová, Zlatko Janeba, Eliška Procházková, Paul  
Hodgkinson
- 1:05 PM      LUNCH**
- 1:50 PM      FREE AFTERNOON – DISCUSSIONS**
- 7:00 PM      DINNER**

# 32<sup>nd</sup> NMR Valtice Program

**WEDNESDAY APRIL 26, 2017**

**9:00 AM      SESSION 7 – E. KLEINPETER, Session Chair**

9:00 AM      INVESTIGATION OF STRUCTURE AND STABILITY OF ALDEHYDE  
CELLULOSE

Jan Vicha, Lukáš Münster, Jiří Klofáč, Milan Masař, Ivo Kuřitka

9:15 AM      THERMORESPONSIVE POLYOXAZOLINE HOMOPOLYMERS AND  
COPOLYMERS IN AQUEOUS SOLUTIONS STUDIED BY NMR  
SPECTROSCOPY

Rafał Konefał, Jiří Spěváček, Peter Černoch, Eliezer Jäger

9:30 AM      THE WEAK INTERACTIONS RESPONSIBLE FOR THE FORMATION OF  
BILE ACID ALKYLAMIDE-BASED SUPRAMOLECULAR GELS

Riikka Kuosmanen, Rakesh Puttreddy, Karri Björklund, Sasu Jaakkola, Aleksii  
Tiusanen, Sonja Into, Hannu Salo, Kari Rissanen, Elina Sievänen

9:45 AM      BENZO-1,3-OXAZIN-4-ONE DERIVATIVES AS UV ABSORBERS: NMR  
AND UV-VIS DFT STUDY

Barbora Hanulíková, Ivo Kuřitka, Pavel Urbánek, Stanislav Kafka, Karel Proisl

10:00 AM      CALCULATION OF <sup>195</sup>Pt CHEMICAL SHIFTS IN Pt(II) COMPLEXES

Karolina Wawrocka, Matúš Durec, Radek Marek

10:15 AM      NON LINEAR EFFECTS IN SPIN NOISE NMR

Norbert Müller, Maria Theresia Pöschko, Stephan Ginthör, Matthias  
Bechmann, Victor V. Rodin, Judith Schlagnitweit, Hervé Desvaux

**10:30 AM      BREAK – SPONSORED BY EURISO-TOP**

**11:00 AM      SESSION 8 – N. MÜLLER, Session Chair**

11:00 AM      UNDERGRADUATE COURSE IN NATURAL PRODUCTS CHEMISTRY  
AND NMR METHODS FOR DETERMINATION OF MOLECULAR  
STRUCTURE

Nina Djapic

11:15 AM      ‘MXNMR’: AN ADVANCED DATA PROCESSING TOOL FOR  
SPIN-NOISE AND MULTIPLEX NMR

Stephan J. Ginthör, Kousik Chandra, Victor Rodin, Matthias Bechmann, Judith  
Schlagnitweit, Norbert Müller

- 11:30 AM CHARACTERIZATION OF NOVEL COMPOSITE MATERIALS  
CONSISTING OF MESOPOROUS METAL-ORGANIC FRAMEWORK  
AND POLY(*N*-ISOPROPYLACRYLAMIDE)  
Mária Šoltésová, Martin Hrubovský, Lenka Hanyková, Petr Kovář, Jan Demel,  
Jan Lang
- 11:45 AM OPTIMAL CONTROL OF CROSS POLARIZATION EXPERIMENT  
Zdeněk Tošner, Steffen Glaser, Bernd Reif
- 12:00 TOWARD THE NMR CRYSTALLOGRAPHY OF PARA-MAGNETIC  
COMPOUNDS. <sup>2</sup>H MAS NMR OF BIS(AMINO ACIDATO-*D<sub>N</sub>*)COPPER(II)  
COMPLEXES  
Gábor Szalontai, Róbert Csonka, József Kaizer, Petra Bombicz,  
Jasmina Sabolović
- 12:15 JOSEF DADOK PRIZE**
- 12:25 CLOSING REMARKS**
- 12:30 LUNCH**