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34th NMR Valtice Program

SUNDAY MARCH 31, 2019

6:00-7:00 PM REGISTRATION – “VALTICKÉ PODZEMÍ“
entrance from Vinařská Street 47, Valtice (GPS 48.739789, 16.750063)

7:00-10:00 PM GET-TOGETHER PARTY IN “VALTICKÉ PODZEMÍ”

34th NMR Valtice Program

MONDAY APRIL 1, 2019

8:30-9:00 REGISTRATION

Sobotní Street 1029, Valtice (GPS 48.741502, 16.748558)

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

9:00 AM NMR, MS AND SCXRD STUDIES OF MOLECULAR CAPSULES
Kari Rissanen

9:45 AM ¹H DOSY NMR - POWERFULL TOOL IN
METALLOSUPRAMOLECULAR CHEMISTRY
Ondřej Jurček, Pia Jurček, Elina Kalenius, Kari Rissanen, Radek Marek

10:00 AM NMR STUDY OF COMPLEX OF CHOLESTEROL WITH HEPTAKIS(2,3,6-
TRI-O-METHYL)- β -CYCLODEXTRIN
Karolína Kučáková, Tereza Navrátilová, Bohumil Dolenský

10:15 AM BINDING OF ZWITTERIONIC RUTHENIUM(III) COMPLEXES WITH
CUCURBIT[7]URILS IN SOLUTION
Sanaz Malali, Jan Chyba, Michal Knor, Jan Novotný, Radek Marek

10:30 AM CONFERENCE PHOTO
Radovan Fiala

10:35 AM BREAK

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

11:00 AM POLYMORPHIC TRANSFORMATIONS OF DRUGS LOADED INTO
GLYCOPOLYMERIC MICELLES
Eliška Procházková, Cheng Cao, Aditya Rawal, Martin Dračínský, Saroj
Bhattacharyya, Ivana Císařová, James M. Hook, Martina H. Stenzel

11:15 AM VERSATILE RECEPTOR MOIETIES FOR ANION RECOGNITION AND
STRUCTURAL FEATURES THEREOF
Petra Cuřínová, Karolína Salvadori

11:30 AM UNPRECEDENTED ENANTIODISCRIMINATION OF INHERENTLY
CHIRAL CALIXARENE DERIVATIVES USING RDCS
Markéta Tichotová, Tomáš Landovský, Pavel Lhoták, Sharon Jeziorowski,
Christina M. Thiele, Hana Dvořáková

- 11:45 AM INTERMOLECULAR INTERACTIONS STUDIED BY NMR SPECTROSCOPY
Jakub R. Štoček, Lucie Čechová, Michal Šála, Martin Dračinský
- 12:00 LUNCH
- 2:00 PM SESSION 3 – R. HRABAL, Session Chair
- 2:00 PM MAGIC ANGLE SPINNING AND PROTON LINEWIDTH: HOW FAST IS FAST ENOUGH?
Zdeněk Tošner
- 2:15 PM HERMES – A SOFTWARE TOOL FOR PREDICTION AND ANALYSIS OF MAGNETIC FIELD-INDUCED RESIDUAL DIPOLAR COUPLINGS IN NUCLEIC ACIDS
Ilektra-Chara Giassa, Andrea Vavřinská, Jiří Zelinka, Jakub Sebera, Vladimír Sychrovský, Rolf Boelens, Radovan Fiala, Lukáš Trantírek
- 2:30 PM MULTI-FACES OF DISHEVELLED PROTEIN
Jitender Kumar, Jakub Harnoš, Marek Kravec, Vítězslav Bryja, Konstantinos Tripsianes
- 2:45 PM A GTP-DEPENDENT SWITCH THAT CONTROLS G-QUADRUPLEX MULTIMER FORMATION
Sofia Kolesnikova, Pavel Srb, Lukáš Vrzal, Michael S. Lawrence, Václav Veverka, Edward A. Curtis
- 3:00 PM HEDGEHOG IN THE CAGE II: DYNAMIC PARAMAGNETIC EFFECTS IN PROTEIN NMR SPECTRA
Pavel Srb, Michal Svoboda, Ladislav Benda, Martin Lepšík, Ján Tarábek, Václav Šícha, Bohumír Grüner, Klára Grantz-Šašková, Jiří Brynda, Pavlína Řezáčová, Jan Konvalinka, Václav Veverka
- 3:15 PM BREAK
- 3:45 PM SESSION 4 – V. SKLENÁŘ, Session Chair
- 3:45 PM WITH THE LITTLE HELP FROM MY FRIENDS: ON THE INTERACTIONS OF RECQ4 HELICASE WITH DNA AND DNA-BINDING PROTEINS
Anna C. Papageorgiou, Lumír Krejčí, Konstantinos Tripsianes
- 4:00 PM TARGETING CYTOSOLIC PURINE 5'-NUCLEOTIDASE II USING SMALL FRAGMENTS
Vítězslav Brinsa, Lukáš Vrzal, Pavel Srb, Michael Kugler, Milan Fabry, Václav Veverka

- 4:15 PM UNRAVELLING DIMERIZATION OF THE EPIGENETIC READER
LEDGF/P75
Vanda Lux, K. Čermáková, M. Fábry, M. Hořejší, M. Mádlíková, T. Brouns, F.
Christ, J. Demeulemeester, Z. Debyser, P. Řezáčová, V. Veverka
- 4:30 PM COUPLING TRANSCRIPTION TERMINATION TO mRNA
PROCESSING / DEGRADATION
Tomasz Kabzinski, Jana Laláková, Andrea Fořtová, Tomáš Klumpler,
Karel Kubíček, Štěpánka Vaňáčová, Richard Štefl
- 4:45 PM PETR SEDMERA PRIZE AWARDED BY THE CZECH J. M. MARCI
SPECTROSCOPIC SOCIETY
Radovan Fiala & Viktor Kanický
- 5:30 PM BREAK**
- 7:00-9:00 PM BUFET DINNER AND BRUKER EVENING:
VISIT OF “SALON VÍN ČESKÉ REPUBLIKY“
Zámek 1, Valtice (GPS 48.739709, 16.755265)**

34th NMR Valtice Program

TUESDAY APRIL 2, 2019

9:00 AM SESSION 4 – A. LYČKA, Session Chair

9:00 AM APPLICATION OF NMR-BASED METABOLOMICS FOR MICROBIAL
COMETABOLITES EVALUATION
Martina Čermáková, Helena Pelantová, Marek Kuzma

9:15 AM NMR METABOLOMICS STUDY OF THE ASSOCIATION BETWEEN
PANCREATIC CANCER AND DIABETES MELLITUS
Lenka Michálková, Štěpán Horník, Jan Sýkora, Lucie Habartová, Vladimír
Setnička

9:30 AM NMR AEROSOLOMICS AS A TOOL TO DISTINGUISH VARIOUS TYPES
OF AEROSOL SAMPLES
Štěpán Horník, Jaroslav Schwarz, Vladimír Ždímal, Jan Sýkora

9:45 AM PREDICTION OF WINE'S TASTE BIOMARKERS THROUGH NMR AND
CHEMOMETRICS
Alberto Juan Ruiz, Antonio Chorques, Jaroslav Havlik

10:00 AM BREAK

10:30 AM SESSION 5 – T. BARTL, Session Chair

10:30 AM JEOL NEWS 2019
Michal Maloň

10:50 AM BRUKER NEWS 2019
Matúš Durec and Pavel Kessler

11:20 AM WORKSHOP – ASK AN EXPERT
(Bruker representatives will answer your questions or try help to solve your problems in 1 to 1
discussions. If you wish, you may send your question in advance to pavel.kessler@bruker.com)

12:30 LUNCH

2:00 PM FREE DISCUSSIONS

34th NMR Valtice Program

WEDNESDAY APRIL 3, 2019

9:00 AM SESSION 7 – R. POHL, Session Chair

9:00 AM STRUCTURAL INTERPRETATION OF THE ³¹P NMR CHEMICAL SHIFT
IN PHOSPHOROTHIOLATE AND PHOSPHATE

Jiří Fukal, Ondřej Páv, Miloš Buděšínský, Ivan Rosenberg, Jakub Šebera,
Vladimír Sychrovský

9:15 AM DETERMINATION OF THE FULL ²⁰⁷Pb CHEMICAL SHIFT TENSOR OF
THE NATURAL MINERALS PHOSGENITE (Pb₂Cl₂CO₃) AND
WULFENITE (PbMoO₄) BY SINGLE-CRYSTAL NMR SPECTROSCOPY
ONLY

Otto E. O. Zeman, Jennifer Steinadler, Rupert Hochleitner, Thomas Bräuniger

9:30 AM ¹⁵N, ¹³C AND 1H NMR STUDY OF TAUTOMERISM IN 3-METHYL-1-
PHENYL-4-[(*E*)-4-SUBSTITUTED-PHENYLDIAZENYL]-1*H*-PYRAZOL-
5-AMINES

Antonín Lyčka

9:45 AM BREAK

10:15 AM SESSION 8 – Z. TOŠNER, Session Chair

10:15 AM SOLID- AND LIQUID-STATE NMR: A FRUITFUL SYMBIOSIS FOR
PARAMAGNETIC COMPLEXES

Jan Blahut, Kevin J. Sanders, Arthur L. Lejeune, Ladislav Benda, Guido
Pintacuda

10:30 AM PARAMAGNETIC ACETYLACETONATE RUTHENIUM(III)
COMPLEXES - ORBITAL AND HYPERFINE CONTRIBUTIONS TO THE
NMR CHEMICAL SHIFTS

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

10:45 AM PHOTOREDOX CATALYSIS OF AEROBIC BENZYLIC OXIDATION BY
ETHYLENE-BRIDGED FLAVINIUM. TOWARDS A DEVELOPMENT OF
AN ARTIFICIAL METAL-FREE “FLAVOENZYME”

Jan Zelenka, Eva Svobodová, Ján Tarábek, Irena Hoskovcová, Veronika
Boguschová, Sarah Bailly, Marek Sikorsky, Jana Roithová, Radek Cibulka

11:00 AM CONFORMATION OF TRIMANNOSIDE BOUND TO CYANOVIRIN-N
Radek Pohl

11:15 AM JOSEF DADOK PRIZE
Radovan Fiala

11:25 AM CLOSING REMARKS

11:30 LUNCH