

CENTRAL EUROPEAN NMR MEETING

33rd NMR VALTICE

Valtice, Czech Republic

April 23-25, 2018

33rd NMR Valtice Program

MONDAY APRIL 23, 2018

8:45-9:45 REGISTRATION

9:50 AM OPENING REMARKS
Radek Marek

10:00 AM SESSION 1 – L. TRANTÍREK, Session Chair

10:00 AM TWO-FIELD NMR SPECTROMETER AND ITS APPLICATIONS
Kadeřávek P., Cousin, S. F., Charlier, C., Marquardsen, T., Tyburn, J.M., Bovier, P.A., Ulzega, S., Speck T., Wilhelm D., Strouk, L., Engelke, F., Maas, W., Sakellariou D., Bodenhausen, G., Pelupessy, P., Ferrage F.

10:30 AM SHARPER NMR
Ariana B. Jones, Guy C. Lloyd-Jones, Elaine Adair, Dušan Uhrín

10:45 AM PROTON DETECTION OF CARBON-CARBON COUPLINGS BETWEEN CHEMICALLY EQUIVALENT NUCLEI
Vratislav Blechta, Jan Sýkora

11:00 AM DETERMINATION OF THE SIZE OF SMALL MOLECULES FROM THEIR DIFFUSION COEFFICIENT
Petr Dvořák, Mária Šoltésová, Jan Lang

11:15 AM RADICAL IONS OF A 2,3-DIAMINO-1,4-NAPHTHOQUINONE DERIVATIVE AS A CANDIDATE FOR SINGLET FISSION (STRUCTURAL VARIATIONS IN SOLUTION STUDIED BY EPR AND DFT)
Ján Tarábek, Jin Wen, Paul I. Dron, Lubomír Pospíšil, Radek Pohl, Josef Michl

11:30 AM PARAMAGNETIC NMR EFFECTS IN Ru(III) HOST-GUEST COMPLEXES
Jan Chyba, Martin Novák, Petra Munzarová, Jan Novotný, Radek Marek

11:45 AM CONFERENCE PHOTO
Radovan Fiala

12:00 LUNCH

2:00 PM SESSION 2 – M. DRAČÍNSKÝ, Session Chair

2:00 PM THE SOFTWARE POSEL: POLYMORPH SELECTOR BASED ON SSNMR AND COMPUTATIONAL DATA
Jiří Czernek, Jiří Brus

- 2:15 PM EXPLORING SYSTEMATIC DISCREPANCIES IN DFT CALCULATIONS OF CHLORINE NUCLEAR QUADRUPOLE COUPLINGS
Ondřej Socha, Paul Hodgkinson, Cory M. Widdifield, Jonathan R. Yates, Martin Dračínský
- 2:30 PM LINKING THE CHARACTER OF THE METAL-LIGAND WITH SPIN-ORBIT EFFECTS ON THE LIGAND NMR CHEMICAL SHIFTS
Jan Novotný, Jan Vícha, Pankaj L. Bora, Michal Straka, Stanislav Komorovsky, Michal Repisky, Radek Marek
- 2:45 PM RELATIVISTIC SPIN-ORBIT HEAVY ATOM ON THE LIGHT ATOM NMR CHEMICAL SHIFTS ACROSS THE PERIODIC TABLE
Jan Vícha, Stanislav Komorovsky, Michal Repisky, Radek Marek, Michal Straka
- 3:15 PM BREAK**
- 3:45 PM SESSION 3 – D. UHRÍN, Session Chair**
- 3:45 PM INVESTIGATION OF DIALDEHYDE CELLULOSE CROSSLINKED POLY(VINYL)ALCOHOL HYDROGELS
Lukáš Münster, Jan Vícha, Jiří Klofáč, Milan Masař, Anna Hurajová, Ivo Kuřitka
- 4:00 PM CHASING BIOCHEMICAL SPECIFICITY OF G-QUADRUPLEXES
Pavel Srb, Lukáš Vrzal, Sofia Kolesnikova, Edward A. Curtis and Václav Veverka
- 4:15 PM NMR STUDY OF GA REPETITIONS WITH I-MOTIF ANCHOR
Aleš Novotný, Jan Novotný, Iva Kejnovská, Radovan Fiala, Michaela Vorlíčková, Radek Marek
- 4:30 PM EVALUATION OF FORMATION OF DNA I-MOTIFS IN THE NUCLEI OF LIVING MAMMALIAN CELLS USING IN CELL NMR SPECTROSCOPY
Šimon Džatko, Michaela Krafcikova, Robert Hänsel-Hertsch, Tomas Fessel, Radovan Fiala, Tomas Loja, Daniel Krafcik, Jean-Louis Mergny, Silvie Foldynova-Trantírková, Lukas Trantírek
- 5:00 PM PETR SEDMERA PRIZE AWARDED BY THE CZECH J. M. MARCI SPECTROSCOPIC SOCIETY
Radovan Fiala
- 7:00-9:00 PM BUFET DINNER AND BRUKER EVENING:
VISIT OF “SALON VÍN ČESKÉ REPUBLIKY“**

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TUESDAY APRIL 24 2018

9:00 AM SESSION 4 – V. BLECHTA, Session Chair

9:00 AM OCEAN-DCP: DOUBLING SIGNAL INTENSITY IN BIOLOGICAL SOLID STATE NMR

Zdeněk Tošner, Riddhiman Sarkar, Johanna Becker-Baldus, Clemens Glaubitz, Sebastian Wegner, Frank Engelke, Steffen Glaser, Bernd Reif

9:15 AM OPTIMIZED CROP IRRIGATION USING A COST-EFFECTIVE *IN-SITU* NMR SOIL WATER PROBE

Cathy Clewett, Kevin Derby, Pablo Prado, Brice Ruthardt, Steven R. Evett

9:30 AM GAIN OF FUNCTION MUTATION IN STIM1 PROTEIN STUDIED BY SOLID AND SOLUTION STATE NMR

Petr Rathner, Michael Stadlbauer, Linda Cerofolini, Enico Ravera, Marc Fahrner, Claudio Luchinat, Giacomo Parigi, Christoph Romanin, Norbert Müller

9:45 AM DETECTION OF SUCCINIMIDE AS DEGRADATION PRODUCT IN PROTEIN

Luigi Grassi, Christof Regl, Arthur Hinterholzer, Sabrina Wildner, Gabriele Gadermaier, Christian G. Huber, Chiara Cabrele, Mario Schubert

10:00 AM STRUCTURAL CHARACTERIZATION OF β -CELL DIFFERENTIATION FACTOR NKX6.1

Vojtěch Duchoslav, Pavel Srb, Rozálie Hexnerová, Irena Siegllová, Milan Fábry, Václav Veverka

10:15 AM INVESTIGATION DNA LIGAND INTERACTIONS BY IN-CELL NMR SPECTROSCOPY

Michaela Krafčíková, Šimon Džatko, Radovan Fiala, Anthon Granzhan, Tomáš Loja, Marie-Paule Teulaude-Fichou, Coralie Caron, Tomáš Fessl, Robert Hänsel-Hertsch, Silvie Foldynová-Trantírková, Lukáš Trantírek

10:30 AM BREAK

11:00 AM SESSION 5 – A. LYČKA, Session Chair

11:00 AM BRUKER NEWS

Pavel Kessler

11:25 AM JEOL NEWS

Michal Maloň

- 11:45 AM OXFORD INSTRUMENT NEWS
Barry Jones
- 12:05 AM MAGRITEC NEWS
Ullrich Koch
- 12:25 AM SPIN-DOC NEWS
Bert Heise
- 12:45 LUNCH**
- 1:45 PM EPR WORKSHOP
Marta Kolesko
- 2:30 PM FREE DISCUSSIONS**
- 5:00 PM CONCERT IN BAROQUE THEATRE IN VALTICE CASTLE**
- 7:00 PM DINNER AND PARTY IN HUBERTUS HOTEL (Valtice castle area)**

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WEDNESDAY APRIL 25, 2018

9:00 AM SESSION 7 – H. PELANTOVÁ, Session Chair

9:00 AM MULTINUCLEAR NMR SPECTROSCOPY OF AZO DYES: PAST AND PRESENT
Antonín Lyčka

9:15 AM DETERMINATION OF OPTICAL PURITY OF ARYLPROPANOIC ACIDS
Petra Cuřínová, Roman Holakovský, Pavel Izák, Petr Hájek, Kristýna Janků

9:30 AM STRUCTURAL ELUCIDATION OF ISOLATED ALKALOIDS FROM *PAPAVER RHOEAS* EMPLOYING NMR SPECTROSCOPY
Jana Maříková, Jakub Radek Štoček, Jiří Kuneš, Jakub Chlebek

9:45 AM BREAK

10:30 AM SESSION 8 – M. SCHUBERT, Session Chair

10:30 AM APPLICATION OF E-LEARNING IN THE TEACHING OF NMR AT UCT PRAGUE
Hana Dvořáková, Jan Prchal, Tomáš Kroupa, Richard Hrabal

10:45 AM PLASMA BIOMARKERS IN ALZHEIMER'S DISEASE
Kristýna Dobšíková, Martina Bugáňová, Helena Pelantová, Jakub Zápal, Blanka Šedivá, Vladimír Setnička, Lucie Habartová, Marek Kuzma

11:00 AM INHIBITION OF FOXO3-DNA INTERACTION BY SMALL MOLECULE INHIBITORS
Katarína Pšenáková, Miroslava Alblová, Jan Veselý, Michael J. Ausserlechner, Veronika Obsilová, Tomáš Obsil

11:15 AM NMR-ASSISTED FRAGMENT-BASED DRUG DISCOVERY
Lukáš Vrzal, Hana Dvořáková, Pavel Srb, Václav Veverka

11:30 AM JOSEF DADOK PRIZE
Radovan Fiala

11:40 AM CLOSING REMARKS

11:45 AM LUNCH