

**CENTRAL EUROPEAN NMR MEETING**

**35<sup>th</sup> NMR VALTICE**

**Valtice, Czech Republic**

**April 24-27, 2022**

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

Printed by: Tribun EU s.r.o.

**ISBN**

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

**SUNDAY      APRIL 24, 2022**

**4:30-6:00 PM    REGISTRATION – “VALTICKÉ PODZEMÍ“  
(GPS: 48.7396914N, 16.7501669E)**

**6:00 PM          GET-TOGETHER PARTY IN “VALTICKÉ PODZEMÍ”**

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

**MONDAY APRIL 25, 2022**

**8:30-8:55 REGISTRATION “CENTRUM EXCELENCE“ (GPS: 48.7411942N, 16.7485308E)**

**8:55 OPENING – R. MAREK**

**9:00 AM SESSION 1 – V. SKLENÁŘ, Session Chair**

9:00 AM MAPPING STRUCTURAL EPITOPES ON SMALL PROTEINS INTERACTING WITH INTACT MABS USING HYDROGEN / DEUTERIUM EXCHANGE MEMORY NMR  
Martina Di Muzio, Sabrina Wildner, Sara Huber, Gabriele Gadermaier, Mario Schubert

9:15 AM MULTIFUNCTIONAL DISORDER IN RECQ4 HELICASE WITH THE INHERENT ABILITY TO UNFOLD AND TRAP G-QUADRUPLEXES  
Anna C. Papageorgiou, Raghbir Ashraf, Michaela Pospíšilová, Christopher A. Waudby, Pavel Kadeřávek, Jakub Cibulka, Lumir Krejčí, Konstantinos Tripsianes

9:30 AM A PHYSICAL INTERACTION BETWEEN RECQ4 HELICASE AND XERODERMA PIGMENTOSUM GROUP A PROTEIN  
Klára Odehnalová, Anna C. Papageorgiou, Konstantinos Tripsianes

9:45 AM NMR DIRECTED MUTATIONS OF COILED-COIL INTERACTION SITES RESTORE WILD TYPE BEHAVIOR OF A PATHOGENIC STIM1 PROTEIN MUTANT  
Agrim Gupta, Christian Manuel Kitzler, Adriana Rathner, Petr Rathner, Marc Fahrner, Christoph Romanin, Norbert Müller

10:00 AM THE POWER OF SELF-CONTROL IN PROTEIN KINASE: A ZOOM ON CK1  
Sara Bologna, Kristína Gômôryová, Vítězslav Bryja, Konstantinos Tripsianes

10:15 AM PYRENE-LABELLED G-QUADRUPLEXES DERIVED FROM THE KIT PROTO-ONCOGENE  
Kateřina Peterková, Ivo Durník, Radek Marek, Janez Plavec, Peter Podbevšek

10:30 AM CONFERENCE PHOTO  
Radovan Fiala

**10:40 AM BREAK**

- 11:00 AM      SESSION 2 – R. HRABAL, Session Chair**
- 11:00 AM      DECORIN BINDING PROTEINS A FROM EUROPEAN *BORRELIAE* AND THEIR VARIETY IN GAG BINDING  
Libor Hejduk, Petr Rathner, Martin Strnad, Libor Grubhoffer, Jan Štěrba, Ryan O. M. Rego, Norbert Müller, Adriana Rathner
- 11:15 AM      DUAL BINDING MODE OF DISHEVELLED PDZ DOMAIN  
Jitender Kumar, Jan Komárek, Cyril Bařinka, Vítězslav Bryja, Konstantinos Tripsianes
- 11:30 AM      PHOSPHORYLATION DYNAMICS OF DISHEVELLED  
Miroslav Micka, Vítězslav Bryja, Konstantinos Tripsianes
- 11:45 AM      HIGH-RESOLUTION RELAXOMETRY APPLIED TO STUDY DYNAMICS OF C-TERMINAL DOMAIN OF  $\delta$  SUBUNIT OF RNA POLYMERASE FROM *BACILLUS SUBTILIS*  
N. Salvi, Vojtěch Zapletal, Petr Padrta, Zuzana Jaseňáková, Milan Zachrdla, Nicolas Bolik-Coulon, Thorsten Marquardsen, Jean-Max Tyburn, Lukáš Žídek, Fabiene Ferrage, Martin Blackledge, Pavel Kadeřávek
- 12:00              LUNCH – HOTEL KLARET (48.7413239N, 16.7505050E)**
- 2:00 PM            SESSION 3 – P. KADEŘÁVEK, Session Chair**
- 2:00 PM            SPIN–LATTICE ( $T_1$ ) AND SPIN–SPIN ( $T_2$ ) NMR RELAXATION IN ELECTRICALLY STRESSED GLYCEROL  
Adam D. Wexler, Jakob Woisetschläger, Ursula Reiter, Gert Reiter, Michael Fuchsjäger, Elmar C. Fuchs, Lothar Brecker
- 2:15 PM             $Al^{3+}$  SOLVATION IN SOLUTIONS OF ALUMINUM NITRATE IN A PROTIC IONIC LIQUID: NUCLEAR MAGNETIC RESONANCE VERIFICATION OF THE SOLVATION SHELL COMPOSITION  
Vladimir V. Matveev, Alexandr Ievlev, Mária Šoltésová, Helena Štěpánková, Erkki Lähderanta, Luis M. Varela
- 2:30 PM            PARAMAGNETIC NMR OF LANTHANIDE(III) COMPLEXES  
David Rajský, Iaroslav Doroshenko, Jaromír Toušek, Jiří Pinkas, Radek Marek, Jan Novotný
- 2:45 PM            ISOMERS INTERCONVERT BY PHOSPHONATE ROTATION IN MACROCYCLIC LANTHANIDE(III) COMPLEXES  
Adam Svítok, Petr Hermann, Zdeněk Tošner
- 3:00 PM            PARAMAGNETIC NMR SHIFTS IN SUPRAMOLECULAR HOST-GUEST SYSTEMS OF RUTHENIUM(III) COMPLEXES  
Petra Pikulová, Jan Chyba, Pia Jurček, Jan Novotný, Radek Marek

- 3:15 PM      BREAK**
- 3:45 PM      SESSION 4 – M. ŠOLTÉSOVÁ, Session Chair**
- 3:45 PM      PARAMAGNETIC COMPLEXES FOR <sup>19</sup>F MRI  
Filip Koucký, Tereza Dobrovolná, Ivana Císařová, Jan Kotek
- 4:00 PM      STRUCTURAL TRANSFORMATIONS OF HOST-GUEST COMPLEXES  
BETWEEN PLATINUM(II) COMPOUNDS AND MACROCYCLES  
Shib S. Paul, Jan Novotný, Jan Chyba, Radek Marek
- 4:15 PM      AZOPYRIMIDINE PHOTOSWITCHES AND THEIR INTERACTIONS  
WITH BETA-CYCLODEXTRIN  
Anna Hružíková, Lucie Mužíková Čechová, Sille Štěpánová, Markéta  
Tichotová, Aleš Růžička, Václav Kašička, Eliška Procházková
- 4:30 PM      PHOSPHATE-BASED SELF-IMMOLATIVE SYSTEMS FOR DRUG  
DELIVERY  
Markéta Tichotová, Petr Šimon, María García Gallardo, Ondřej Baszczyński,  
Eliška Procházková
- 4:45 PM      BREAK – Sandwich & Refreshment**
- 5:15 PM      SESSION 5 – R. FIALA, Session Chair**
- 5:15 PM      PETR SEDMERA PRIZE AWARDED BY THE CZECH J. M. MARCI  
SPECTROSCOPIC SOCIETY  
Radovan Fiala & Viktor Kanický
- 6:00 PM      BREAK**
- 7:00-9:00 PM      BRUKER EVENING: “SALON VÍN ČESKÉ REPUBLIKY“  
(GPS: 48.7395550N, 16.7557533E)**

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

**TUESDAY APRIL 26, 2022**

**9:00 AM SESSION 6 – E. PROCHÁZKOVÁ, Session Chair**

9:00 AM NMR CRYSTALLOGRAPHY IN THE PURSUIT OF A CRYSTAL  
STRUCTURE OF N-FORMYL-MLF-OH TRIPEPTIDE  
Jiri Czernek, Martina Urbanová, Jiří Brus

9:15 AM KINETICS OF RESORCINOL-FORMALDEHYDE  
POLYCONDENSATION BY <sup>1</sup>H-NMR RELAXOMETRY  
Eva Kinertová, Václav Slovák

9:30 AM EFFECTS OF WORKERS EXPOSURE TO NANOPARTICLES STUDIED  
BY NMR METABOLOMICS  
Lenka Michálková, Štěpán Horník, Vladimír Ždímal, Jan Sýkora, Daniela  
Pelclová

9:45 AM NMR AEROSOLOMICS: AN OVERVIEW  
Štěpán Horník, Petr Vodička, Petra Pokorná, Jaroslav Schwarz, Vladimír  
Ždímal, Jan Sýkora

10:00 AM <sup>2</sup>H NMR STUDY OF ANOMALOUS REACTION MECHANISM IN SOME  
BENZAZABORoles  
Martin Hejda, Antonín Lyčka

10:15 AM OBSCURE NMR NUCLEI BACK TO THE SCENE; A CASE STUDY OF  
BORON-11  
Jan Vrána, Josef Holub, Aleš Růžička

10:30 AM NMR STUDY OF GLYCOSYL <sup>15</sup>N-ANILINES  
Nina Habanová, Radek Pohl

**10:45 AM BREAK**

**11:15 AM SESSION 7 – A. RŮŽIČKA, Session Chair**

11:15 AM NMR STRUCTURE ELUCIDATION OF QUAMBALARINES  
Eliška Procházková, Oleksandr Kucherak, Eva Stodůlková, Zdeněk Tošner,  
Ivana Císařová, Miroslav Fliieger, Miroslav Kolařík, Ondřej Baszczyński

11:30 AM LONG-RANGE C–F COUPLINGS IN CONFORMATIONAL ANALYSIS OF  
DISACCHARIDES  
Ema Chaloupecká, Martin Kurfířt, Lucie Červenková Šťastná, Jindřich Karban,  
Martin Dračínský

- 11:45 AM HYDROGEN-BONDING INTERACTIONS OF 8-OXOPURINE  
NUCLEOBASES  
Zuzana Osifová, Michal Šála, Martin Dračínský
- 12:00 WHAT CAN JOSEF DADOK NATIONAL NMR CENTRE DO FOR YOU  
Radovan Fiala
- 12:15 JEOL UPDATES 2022: ECZ LUMINOUS  
Michal Maloň
- 12:35 BRUKER UPDATES  
Tangi Jezequel & Michael Hammer
- 1:00 PM LUNCH IN KLARET (48.7413239N, 16.7505050E)**
- 2:30 PM FREE DISCUSSIONS**
- 6:30 PM MĚŘICÍ TECHNIKA MORAVA EVENING: DINNER IN FELDSBERG  
(GPS: 48.7419097N, 16.7585175E)**

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

**WEDNESDAY APRIL 27, 2022**

**9:00 AM      SESSION 8 – M. DRAČÍNSKÝ, Session Chair**

9:00 AM      DIMERIZATION OF ACETIC ACID IN THE GAS PHASE – NMR  
EXPERIMENTS AND QUANTUM-CHEMICAL CALCULATIONS  
Ondřej Socha, Martin Dračínský

9:15 AM      AD-MD METHOD FOR CALCULATION OF NMR SHIFT AND INDIRECT  
SPIN-SPIN SCALAR COUPLING INCLUDING THE EFFECTS DUE TO  
MOLECULAR DYNAMICS  
Jiří Fukal, Jakub Šebera, Miloš Buděšínský, Ivan Rosenberg, Petr Jurečka,  
Vladimír Sychrovský

9:30 AM      CALCULATION OF NMR SPIN-SPIN COUPLINGS FOR  
INTRINSICALLY DISORDER PROTEINS: A PROSPECTIVE TOOL TO  
FACILITATE EXPERIMENTAL NMR STUDIES  
Amina Gaffour, Krishnendu Bera, Jana Pavlíková Přecechtělová

9:45 AM      SPIN-ORBIT HEAVY ATOM ON THE LIGHT ATOM <sup>1</sup>H NMR CHEMICAL  
SHIFTS INDUCED THROUGH H···F HYDROGEN BOND  
Jan Vícha, Petr Švec, Zdeňka Růžičková, Maksim A. Samsonov, Kateřina  
Bártová, Aleš Růžička, Michal Straka, Martin Dračínský

10:00 AM      TEMPERATURE INDUCED SALT TO COCRYSTAL  
TRANSFORMATION  
Jakub Štoček, Martin Dračínský, Ivana Císařová, Tomáš Slanina, Ondřej Socha

10:15 AM      NANOSTRUCTURED ALUMINOSILICATES AS REFERENCE  
MATERIALS FOR <sup>27</sup>Al SOLID-STATE NMR  
Martin Kejík, Lukáš Jeremias, Jiří Brus, Aleš Stýskalík, Zdeněk Moravec,  
Lucie Šimoníková, Craig Barnes, Jiří Pinkas

**10:30 AM      BREAK**

**11:00 AM      SESSION 9 – J. BRUS, Session Chair**

11:00 AM      DFT-BASED CALCULATIONS OF <sup>27</sup>Al QUADRUPOLAR NMR  
PROPERTIES IN ALUMINOSILICATE MATERIALS  
Lukáš Jeremias, Martin Kejík, Jiří Brus, Aleš Stýskalík

11:15 AM      SENSITIVITY-ENHANCED SEQUENCES IN SOLID-STATE NMR  
Jan Blahut, Matthias Brandl, Bernd Reif, Zdeněk Tošner



- 11:30 AM VISUALIZATION OF SPIN DYNAMICS DURING CROSS  
POLARIZATION EXPERIMENT  
Zdeněk Tošner
- 11:45 AM PROBING ELECTROSTATICS OF IDPS BY COMPUTATION AND  
EXPERIMENT  
Franz Mulder, Rupashree Dass, Enrico Corliano
- 12:00 JOSEF DADOK PRIZE**  
Radovan Fiala
- 12:10 CLOSING REMARKS**  
Radek Marek
- 12:15 LUNCH IN KLARET (48.7413239N, 16.7505050E)**