



INSTRUCT ULTRA

2nd Structural biology meeting

November 15 - 16, 2018

Hotel Tatra, Bratislava

Hall „GRAND“

Námestie 1. mája 5, 811 06 Bratislava

ISBN978-80-971156-6-1

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Programme

Thursday, November 15, 2018

12,30 -13,30

Lunch

13,30 – 13,40

INSTRUCT-ULTRA H2020

Miloš Hricovíni

Institute of Chemistry, Slovak Academy of Sciences, Bratislava

Chair:

Radovan Fiala

13,40 – 14,10

Long-range NMR restraints in integrated structural biology

Enrico Ravera¹, Giacomo Parigi¹ and Claudio Luchinat¹

Magnetic Resonance Center (CERM), and Department of Chemistry, University of Florence, and Interuniversity Consortium for Magnetic resonance of Metalloproteins, Via L. Sacconi 6, 50019 Sesto Fiorentino (FI), Italy

14,10 – 14,30

The function and structure of yeast phosphatidylinositol transfer protein Pdr17.

Zuzana Pevalová¹, Vladimír Pevala², Nicolas J. Blunsom³, Dana Tahotná¹, Roman Holič¹, Veronika Kotrasová², Barbora Keresztesová², Nina Kunová², Jacob A. Bauer², Július Košťan⁴, Eva Kutejová², Shamshad Cockcroft³, Peter Griač¹

¹*Centre of Biosciences, Institute of Animal Biochemistry and Genetics, Slovak Academy of Sciences, Dúbravská cesta 9, Bratislava, Slovakia*

²*Institute of Molecular Biology, Slovak Academy of Sciences, Dúbravská cesta 21, Bratislava, Slovakia*

³*Department of Neuroscience, Physiology and Pharmacology, Division of Biosciences, University College London, London, United Kingdom*

⁴*Max F. Perutz Laboratories, Vienna, Austria*

14,30 – 14,50

The structure of the cell wall binding domain of phage endolysin solved by program ARCIMBOLDO

Ľubica Urbániková¹, Martina Gerová¹, Jiří Brynda², Július Košťan³, Nora Halgašová¹ and Gabriela Bukovská¹

¹*Institute of Molecular Biology SAS, Dubravska cesta 21, Bratislava, Slovak Republic*

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³*Max F. Perutz Laboratories, University of Vienna, Vienna, Austria*

14,50 – 15,10	<p>Mitochondrial nucleoid proteins <u>Nina Kunová</u>¹, Gabriela Ondrovičová¹, Vladimír Pevala¹, Jacob Bauer¹, Veronika Kotrasová¹, Barbora Keresztesová¹, Peter Baráth², Jana Bellová² and Eva Kutejová¹ ¹<i>Department of Biochemistry and Structural Biology, Institute of Molecular Biology, Slovak Academy of Sciences, Bratislava, Slovakia</i> ²<i>Department of Glycobiology, Institute of Chemistry, Slovak Academy of Sciences, Bratislava, Slovakia</i></p>
15,10 – 15,30	<p>Coffee break</p> <p><i>Chair: Miloš Hricovíni</i></p>
15,30 – 16,00	<p>Hyperfine effects in paramagnetic NMR Spectroscopy Radek Marek <i>CEITEC – Central European Institute of Technology, Masaryk University Kamenice 5, CZ - 62500 Brno, Czechia</i></p>
16,00 – 16,20	<p>A mystery of a through-space indirect NMR spin-spin coupling between two hydrogen atoms Olga L. Malkina <i>Institute of Inorganic Chemistry, Slovak Academy of Sciences, Dúbravská cesta 9, SK-84536 Bratislava</i></p>
16,20 – 16,40	<p>Molecular modeling of an enzymatic mechanism of glycosyltransferases which used a manganese ion co-factor for catalytic activity <u>Juraj Kóňa</u>, Adela Bobovská, Vladimír Sládek <i>Department of Structure and Function of Saccharides, Institute of Chemistry, Slovak Academy of Sciences, Dúbravská cesta 9, SK-84538 Bratislava, Slovakia</i></p>
16,40 – 17,00	<p>Weak Te,Te interactions through the looking glass of NMR spin–spin coupling revisited Richard Szabó and <u>Irina Malkin Ondík</u> <i>Institute of Informatics, Information Systems and Software Engineering, Faculty of Informatics and Information Technologies STU in Bratislava, Ilkovičova 2, 842 16 Bratislava 4</i></p>
19,00	<p>Dinner</p>

Friday, November 16, 2018

Chair: *Ludovít Škultéty*

- 8,45 – 9,05** **Molecular determinants of juvenile hormone action as revealed by 3D QSAR analysis in *Drosophila*.**
Denisa Beňová-Liszeková, Milan Beňo and Robert Farkaš
Laboratory of Developmental Genetics, Institute of Experimental Endocrinology, Biomedical Research Center, Slovak Academy of Sciences, Dúbravská cesta 9, 845 05 Bratislava, Slovakia
- 9,05 – 9,25** **The structure, occurrence and biological role of G-quadruplexes**
Viktor Víglaský
¹*Department of Biochemistry, Institute of Chemistry, Faculty of Sciences, P. J. Šafárik University in Košice*
- 9,25 – 9,45** **New acridine cytostatics – structure and properties**
Ján Imrich¹, Mária Vilková¹, Danica Sabolová², Michal Bečka¹
¹*Department of Organic Chemistry and NMR laboratory,* ²*Department of Biochemistry, Institute of Chemistry, Faculty of Science, P. J. Šafárik University, Šrobárova 2, 040 01 Košice, Slovakia*
- 9,45 – 10,05** **The use of time-domain data for metabolite quantification**
Michal Kaliňák¹, and Martin Kopčík¹
¹*Central laboratories, Faculty of Chemical and Food Technology, Slovak University of Technology, Radlinského 9, 812 37 Bratislava, Slovakia*
- 10,05 – 10,25** **Study of the Xyloglucan endotransglycosylase (XET) interactions with substrates using computational chemistry tools**
Barbora Stratilová^{1,2}, Stanislav Kozmon¹, and Eva Stratilová¹
¹*Institute of Chemistry, Slovak Academy of Sciences, Dúbravská cesta 9, 845 38 Bratislava, Slovakia*
²*Department of Physical and Theoretical Chemistry, Faculty of Natural Sciences, Comenius University in Bratislava, Mlynská dolina, Ilkovičova 6, 842 15 Bratislava, Slovakia*
- 10,25 – 10,40** **Coffee break**
- Chair:* *Radek Marek*
- 10,40 – 11,10** **Structural studies of non-B DNA by NMR spectroscopy**
Radovan Fiala¹, Martin Gajarský¹, Martina Lenarčíč Živkovič², Janez Plavec², Šimon Džatko¹, Michaela Krafcíková¹, Lukáš Trantírek¹, Aleš Novotný¹, and Radek Marek¹
¹*Central European Institute of Technology, Masaryk University, Kamenice 5, 625 00 Brno, Czech Republic*
²*Slovenian NMR Centre, National Institute of Chemistry, Hajdrihova 19, SI-1000 Ljubljana, Slovenia*

- 11,10 – 11,30** **How Mutations to the N-Terminal Domain of the Human Cardiac Ryanodine Receptor Affect its Dynamics: A Molecular Dynamics Study**
Jacob Bauer^{1*}, Eva Kutejová¹, Vladena Bauerová¹
¹*Institute of Molecular Biology, Slovak Academy of Sciences, Bratislava Slovakia*
- 11,30 – 11,50** **Study of the substrate modification influence on the O-GlcNAc transferase reaction mechanism by QM/MM molecular dynamics.**
Stanislav Kozmon^{1,2}, Igor Tvaroška^{1,2}
¹*Institute of Chemistry, Slovak Academy of Sciences, Dúbravská cesta 9, 845 38 Bratislava, Slovakia*
² *Central European Institute of Technology (CEITEC), Masaryk University, Kamenice 5, 615 00 Brno, Czech Republic*
- 11,50 – 12,10** **Mass Spectrometry, a Tool for Discovery Proteomics Fishing for Specific Biomarkers, Virulence Factors, and Stress Related Proteins**
Gabriela Flores-Ramirez, Maksym Danchenko, Katarina Palkovicova, Nikola Babitsova, Ludovit Skultety
Department of rickettsiology, Institute of Virology, Biomedical Research Center, Dubravská c. 9, 845 05 Bratislava, Slovakia
- 12,10 – 12,15** **Conclusions**
- 12,30 -13,30** **Lunch**