



INSTRUCT ULTRA

3rd Structural biology meeting

November 14 - 15, 2019

Hotel Tatra, Bratislava

Hall „GRAND“

Námestie 1. mája 5, 811 06 Bratislava

INSTRUCT ULTRA

3rd Structural biology meeting

Programme

Thursday, November 14, 2019

- 12,30 -13,45** **Lunch**
- 13,45 – 14,00** **INSTRUCT-ULTRA H2020**
Miloš Hricovíni
Institute of Chemistry, Slovak Academy of Sciences, Bratislava
- Chair:* *Vladimír Pevala*
- 14,00 – 14,20** **Mechanics of single proteins**
Gabriel Žoldák
¹ *Center for Interdisciplinary Biosciences, Technology and Innovation Park, P.J. Šafárik University, Košice, Slovakia*
- 14,20 – 14,40** **Investigating the role of some key players of the human cytosolic iron-sulfur cluster assembly machinery**
Francesca Cantini^{1,2}, Vincenzo Maione¹, Lucia Banci^{1,2}
¹*Magnetic Resonance Center (CERM) – University of Florence, Italy,*
²*Department of Chemistry - University of Florence, Italy*
- 14,40 – 15,00** **Importance of Base-pair Probing for Mismatch Recognition**
Tomáš Bouchal^{1,2}, Ivo Durník^{1,2}, Petr Kulhánek^{1,2}
¹*CEITEC – Central European Institute of Technology, Masaryk University, 625 00 Brno, Czech Republic*
²*National Centre for Biomolecular Research, Faculty of Science, Masaryk University, 625 00 Brno, Czech Republic*
- 15,00 – 15,20** **Comparative structural analysis of lectin family from *Photorhabdus spp.***
Josef Houser^{1,2}, Eva Fujdiarová², Gita Jančaříková^{1,2}, Filip Melicher¹, Michaela Wimmerová^{1,2}
¹*CEITEC-Central European Institute of Technology, Masaryk University, Kamenice 5, 625 00 Brno, Czech Republic*
²*National Center for Biomolecular Research, Faculty of Science, Masaryk University, Kotlářská 2, 611 37 Brno, Czech Republic*
- 15,20 – 15,40** **Coffee break**

Chair:	<i>Miloš Hricovíni</i>
15,40 – 16,00	<p>Micro-Electron Diffraction: A Powerful Tool For Protein And Small Molecule Structure Determination</p> <p>Radovan Spurný¹ ¹<i>Thermo Fisher Scientific, Vlastimila Pecha 1282/12, Brno, Czech Republic</i></p>
16,00 – 16,20	<p>Local DNA structures and their importance in regulation of biological processes</p> <p>Václav Brázda <i>Institute of Biophysics, Academy of Sciences of the Czech Republic, Brno, Czech Republic</i></p>
16,20 – 16,40	<p>Weak Protein-Ligand Interactions: Advances in Saturation Transfer Difference (STD) NMR techniques</p> <p>Jesus Angulo¹ ¹<i>School of Pharmacy, University of East Anglia (UEA), Norwich Research Park, NR4 7LU, Norwich, U.K.</i></p>
16,40 – 17,00	<p>Human cardiac ryanodine receptor and its association with arrhythmias - milestones, achievements and perspectives</p> <p>Vladena Bauerová ¹<i>Institute of Molecular Biology SAS, Dubravská cesta 21, Bratislava, Slovak Republic</i></p>
17,00 – 17,20	<p>The exopolysaccharide produced by the cyanobacterium <i>Nostoc</i> sp. - a structural study</p> <p>Iveta Uhliariková¹, Mária Matulová¹, Vladislav Cepák², Jaromír Lukavský², Peter Capek¹ ¹<i>Institute of Chemistry, Center for Glycomics, Slovak Academy of Sciences, Dúbravská cesta 9, 84538 Bratislava, Slovakia</i> ²<i>Institute of Botany, Centre for Algology, Academy of Sciences of the Czech Republic, Dukelská 135, 37901 Třeboň, Czech Republic</i></p>
18,00	Dinner

Friday, November 15, 2019

Chair: Vladimír Frečer

8,45 – 9,05 Normal mode analysis as a routine part of a structural investigation

Jacob Bauer

*Institute of Molecular Biology, Slovak Academy of Sciences, Dúbravská cesta 21,
845 51 Bratislava*

9,05 – 9,25 Catalytic mechanisms of both inverting and retaining glycosyltransferases pass through oxocarbenium ion intermediates via S_Ni-like processes: Insights from DFT calculations.

Juraj Kóňa

Department of Structure and Function of Saccharides, Institute of Chemistry, Slovak Academy of Sciences, Dúbravská cesta 9, SK-84538 Bratislava, Slovakia

9,25 – 9,45 Analysis of Protein Dynamics and Structure by nt-PaCS-MD and ProGA

Vladimir Sladek^{1,2,*}, Ryuhei Harada³, Yasuteru Shigeta³

¹*Institute of Chemistry - Centre for Glycomics, Dubravská cesta 9, 84538 Bratislava, Slovakia.*

²*Agency for Medical Research and Development (AMED), Chiyoda-ku, Japan.*

³*Center for Computational Sciences, University of Tsukuba, Tennodai 1-1-1, Tsukuba, Ibaraki 305-8577, Japan*

9,45 – 10,05 Study of the N-acetylglucosaminyltransferase-V (GnT-V) interactions with substrates using computational chemistry tools

Barbora Stratilová^{1,2}, Stanislav Kozmon¹

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*

10,05 – 10,25 Photochemical properties of potential anticancer agents: Anti-syn isomerization of 2,3-di-substituted quinazolinones

Michal Hricovíni,¹ James Asher,² Miloš Hricovíni¹

¹*Institute of Chemistry, Slovak Academy of Sciences, Dúbravská cesta 9, 845 36 Bratislava, Slovak Republic*

²*Institute of Inorganic Chemistry, Slovak Academy of Sciences, Dúbravská cesta 9, 845 38 Bratislava, Slovak Republic*

10,25 – 10,45 Coffee break

Chair: Jesus Angulo

10,45 – 11,05 Building a center for research and teaching activities in structural biology for biomedicine and biotechnology – Interreg V-A Slovakia – Austria project StruBioMol

Vladimír Pevala¹, Gabriela Ondrovičová¹, Veronika Kotrasová¹, Barbora Keresztesová¹, Nina Kunová¹, Lucia Martináková¹, Jelena Pavlović¹, Vladena Bauerová¹, Jacob A. Bauer¹, Július Košťan², Kristina Djinović-Carugo², Eva Kutejová¹
¹*Institute of Molecular Biology, Slovak Academy of Sciences, Dúbravská cesta 21, Bratislava, Slovakia*

²*Department of Structural and Computational Biology, Max Perutz Labs, University of Vienna, Campus Vienna Biocenter 5, A-1030 Vienna, Austria*

11,05– 11,25

Amylolytic family GH126 - in silico analysis and preliminary experimental identification of potentially novel members

Lenka Kerényiová*, Zuzana Šramková, Domenico Pangallo & Štefan Janeček
Institute of Molecular Biology, Slovak Academy of Sciences, Dúbravská cesta 21, Bratislava, Slovakia

11,25 – 11,45

Bioinformatics analysis of acylesterases from family CE16

Ľubica Urbániková¹, Štefan Janeček^{1,2}

¹*Laboratory of Protein Evolution, Institute of Molecular Biology, Slovak Academy of Sciences, Dúbravská cesta 21, 845 51 Bratislava, Slovakia;*

lubica.urbanikova@savba.sk

²*Department of Biology, Faculty of Natural Sciences, University of SS. Cyril and Methodius in Trnava, Nám. J. Herdu 2, 917 01 Trnava, Slovakia*

11,45 – 12,05

Fragmentation analysis of O-specific bonded saccharides from bacterial samples using LC-MS and MALDI-MS

Filip Pancik¹, Jana Valarikova¹, Alzbeta Cizova¹, Slavomir Bystricky¹, Peter Barath¹

¹*Institute of Chemistry, Slovak Academy of Sciences, Dúbravská cesta 9, 845 38 Bratislava, Slovakia*

12,05 – 12,25

Pathogenicity of new *BEST1* variants identified in Italian patients with best vitelliform macular dystrophy assessed by computational structural biology

Vladimír Frečer¹, Giancarlo Iarossi², Anna Paola Salvetti³, Paolo Enrico Maltese⁴, Giulia Delledonne³, Marta Oldani³, Giovanni Staurenghi³, Benedetto Falsini⁵, Angelo Maria Minnella⁵, Lucia Ziccardi⁶, Adriano Magli⁷, Leonardo Colombo⁸, Fabiana D'Esposito^{9,10,11}, Jan Miertus¹², Francesco Viola¹³, Marcella Attanasio¹⁴, Emilia Maggio¹⁴ and Matteo Bertelli^{4,11}

¹*Faculty of Pharmacy, Comenius University in Bratislava, Bratislava, Slovakia.*

²*Bambino Gesù IRCCS Children's Hospital, Rome, Italy.*

³*Sacco Hospital, University of Milan, Milan, Italy.*

⁴*MAGI'S Lab S.R.L., Rovereto, TN, Italy.*

⁵*Institute of Ophthalmology, Fondazione Policlinico Gemelli/Università Cattolica del S. Cuore, Rome, Italy.*

⁶*GB Bietti Foundation IRCCS, Rome, Italy.*

⁷*University of Salerno, Salerno, Italy.*

⁸*San Paolo Hospital, University of Milan, Milan, Italy.*

⁹*Western Eye Hospital, Imperial College Healthcare NHS Trust, London, UK.*

¹⁰*University of Naples Federico II, Naples, Italy.*

¹¹*MAGI Euregio, Bolzano, Italy.*

¹²*Genius n.o., Trnava, Slovakia.*

¹³ *Fondazione IRCCS Cà Granda, Clinica Regina Elena, Milan, Italy.*

¹⁴ *IRCCS-Ospedale Sacro Cuore Don Calabria, Negrar, VR, Italy.*

12,30 – 12,35

Conclusions

12,35

Lunch