

XVIII Discussions in Structural Molecular Biology and 5th User Meeting of CIISB

24-26 March 2022

Programme

Thursday, March 24

11:30 - 13:30 Registration and accommodation, coffee

All talks are 20 minutes long unless indicated otherwise. All times are INCLUDING discussion.

14:00 **Opening of XVIII Discussions and 5th User Meeting of CIISB** (*Jan Dohnálek, Vladimír Sklenář*)

14:15 - 16:05 **Session I** *Chair person: Jan Dohnálek*

Lecture no. – page of abstract

Zdeněk Lánský Institute of Biotechnology, Czech Academy of Sciences	Tau generates protective envelopes on microtubules <i>L1 – 3</i>
Miroslav Kloz Institute of Physics, Czech Academy of Sciences	Structural changes of carotenoid echinenone in Orange Carotenoid Protein studied by femtosecond Raman spectroscopy <i>L2 – 4</i>
Rohit Joshi Institute of Physiology, Czech Academy of Sciences	Nedd4-2 binding to 14-3-3 modulates the accessibility of its catalytic site and WW domains (Student talk) <i>L3 – 4</i>
Aneta Kozeleková CEITEC, Masaryk University	Phosphomimicking Mutations ≠ Phosphorylation – a case study of 14-3-3 protein (Student talk, CIISB user meeting) <i>L4 – 5</i>
Mark Johnson / Lukáš Gajdoš Institut Laue-Langevin, Grenoble	Neutrons for Structural Biology at the Institut Laue Langevin / Neutron diffraction for deciphering lectin-carbohydrate interactions in bacterial infection (30 min) <i>L5 – 6</i>

16:05 - 16:35 *Coffee break*

16:35 - 18:25 **Session II** *Chair person: Pavlína Maloy Řezáčová*

Ján Biňovský CEITEC, Masaryk University	Baseplate structure of bacteriophage phi812 and mechanism of cell wall binding and penetration (Student talk, CIISB user meeting) <i>L6 – 7</i>
Zuzana Trebichalská CEITEC, Masaryk University	<i>In situ</i> cryo-electron tomography of enterovirus cell entry (Student talk, CIISB user meeting) <i>L7 – 7</i>
Miroslav Homola CEITEC, Masaryk University	Mechanism of virion formation of the <i>Emiliana huxleyi</i> virus 201 enveloped by two membranes (Student talk, CIISB user meeting) <i>L8 – 8</i>
Tomáš Koval' Institute of Biotechnology, Czech Academy of Sciences	Bacterial helicase-like transcription-associated factor HeID (CIISB user meeting) <i>L9 – 8</i>
Sebastian Zoll Institute of Organic Chemistry and Biochemistry, Czech Academy of Sciences	The structural basis of complement inhibition by the human parasite <i>Trypanosoma brucei gambiense</i> <i>L10 – 9</i>
Piotr Wardega NanoTemper Technologies	Characterize your most challenging interactions. The New Monolith (10 min) <i>L11 – 9</i>

18:30 Dinner

20:00 **CIISB Executive committee**

Friday, March 25

7:30 - 9:00 *Breakfast*

9:00 - 10:50 **Session III** *Chair person: Lukáš Židek*

Edward Curtis Institute of Organic Chemistry and Biochemistry, Czech Academy of Sciences	Supernova: a deoxyribozyme that catalyzes a chemiluminescent reaction L12 – 11
Maroš Huličiak Institute of Biotechnology, Czech Academy of Sciences	New Class of Structurally Robust Non-Antibody Protein Scaffolds for Directed Evolution (Student talk) L13 – 11
Jan Příbyl CEITEC, Masaryk University	Atomic force microscopy in structural biology (CIISB user meeting) L14 – 12
Petr Pompach Institute of Biotechnology, Czech Academy of Sciences	Structural Mass Spectrometry – An Advanced Tool in Protein Structure Analysis (CIISB user meeting) L15 – 13
Vilhelmiina Kontkanen Faculty of Science, University of South Bohemia	Structural Changes and Their Consequences for Azurin Oxidation in Vacuum and on Gold Interfaces L16 – 13
Patrick King SPECION, s.r.o.	Microfluidic Modulation Spectroscopy (MMS): A Novel IR-Based Technique Providing Automated, Highly-Sensitive Protein Secondary Structure Characterisation in <i>in situ</i> Conditions (10 min) L17 – 14

10:50 - 11:10 *Coffee break*

11:10 - 12:50 **Session IV** *Chair person: Pavel Plevka*

Kristýna Adámková Institute of Biotechnology, Czech Academy of Sciences	Zinc-dependent nuclease from <i>Stenotrophomonas maltophilia</i> : Structural analysis of the active site (Student talk, CIISB user meeting) L18 – 15
Ondrej Cehlár Institute of Neuroimmunology, Slovak Academy of Sciences	Biophysical characterization of novel monoclonal antibodies targeting epitopes on the SARS-CoV-2 Spike protein (CIISB user meeting) L19 – 16
Martin Malý Faculty of Nuclear Sciences and Physical Engineering, Czech Technical University	Integrative structural analysis of antibiotic-inactivating enzyme from <i>Stenotrophomonas maltophilia</i> (Student talk, CIISB user meeting) L20 – 17
Michal Koblížek Institute of Microbiology, Centre Algatech, Czech Academy of Sciences	2.4 Å structure of the double concentric ringed light harvesting complex from phototrophic bacterium <i>Gemmatimonas phototrophica</i> L21 – 18
Zuzana Hlavenková Thermo Fisher Scientific	Thermo Scientific™ Tundra Cryo-TEM: 100kV Cryo-TEM dedicated for Single Particle Analysis (10 min) L22 – 18
Poster flash talks, 2 minutes each	
Alexandra Náplavová (Faculty of Science, Masaryk University) Multiple approaches for protein phosphorylation: a story of 14-3-3 (Student poster)	
Jan Šimek (Faculty of Science, Masaryk University) To homodimerize or to heterodimerize: story of 14-3-3 protein dimer formation (Student poster)	
Pavel Pohl (Institute of Physiology, Czech Academy of Sciences) 14-3-3-protein regulates Nedd4-2 by modulating interactions between HECT and WW domains (Student poster)	
Olívia Petrválská (Institute of Physiology, Czech Academy of Sciences) 14-3-3 directly interacts with the kinase domain of CaMKK1 and inhibits calmodulin binding	

12:50 - 14:00 *Lunch*

14:00 - 15:50 **Session V** *Chair person: Vojtěch Spiwok*

Martin Lepšík Institute of Organic Chemistry and Biochemistry, Czech Academy of Sciences	On the Importance of Physically Correct Models for Protein-Ligand Binding <i>L23 – 19</i>
Michal Malý Institute of Biotechnology, Czech Academy of Sciences	"ReDNATCO" - making DNATCO more useful for crystallographers <i>L24 – 20</i>
Ladislav Bartoš Faculty of Science, Masaryk University	Designing transmembrane proteins to enhance transport of peptides across cell membranes (Student talk) <i>L25 – 21</i>
Zdenek Futera Faculty of Science, University of South Bohemia	Mechanisms of Charge Transfer through Multiheme Protein Junctions, Their Distance and Band-Alignment Dependencies <i>L26 – 22</i>
Lubomír Rulišek Institute of Organic Chemistry and Biochemistry, Czech Academy of Sciences	Exploring Reaction Mechanisms of Metalloproteins by Correlating Theory and Experiment <i>L27 – 23</i>
Martin Máša Beckman Coulter, Life Sciences Sales Dpt	EMnetik 24 System - DNA Cleanup for Genetic Engineering (10 min) <i>L28 – 24</i>

15:50 - 16:10 *Coffee break*

16:10 - 18:00 **Session VI** *Chair person: Tomáš Koval'*

Martin Marek Faculty of Science, Masaryk University	Can misfolded enzymes be beneficial? Yes, they can <i>L29 – 25</i>
Jitka Plucarová Faculty of Science, Masaryk University	Interactions of adaptor protein Grb2 with microtubule associated protein 2c (Student talk, CIISB user meeting) <i>L30 – 25</i>
Radim Novotný Faculty of food and biochemical technology, University of Chemistry and Technology	Structure and biological functions of TBEV Capsid protein (Student talk) <i>L31 – 26</i>
Raju Mandal Faculty of Science, Charles University	Biophysical characterization of the FOXO4:p53 complex (Student talk) <i>L32 – 27</i>
Dávid Tužinčín CEITEC, Masaryk University	Seeing the invisible – Study of transiently formed protein conformation found in domain 1.1 of bacterial transcription factor (Student talk, CIISB user meeting) <i>L33 – 28</i>
Poster flash talks, 2 minutes each	
<p>Andreas Santamaria (Institut Laue-Langevin, Grenoble) Strikingly different roles of SARS-CoV-2 fusion peptides uncovered by neutron scattering (Student poster)</p> <p>Lucie Valentová (CEITEC, Masaryk University) A hunting strategy and virion structure of <i>P. aeruginosa</i> bacteriophage JBD30 revealed by cryo-electron microscopy (Student poster)</p> <p>Peter Pajtinka (CEITEC, Masaryk University) Synergistic antimicrobial activity of magainin 2 and PGLa revisited (Student poster)</p> <p>Patricia Hrašnová (Institute of Neuroimmunology of Slovak Academy of Sciences) Structural and Biophysical Aspects of Lactoferrin and Its Interaction with Plasminogen (Student poster)</p> <p>Andrej Bitala (Institute of Virology, Biomedical Research Center Slovak Academy of Sciences) Immunoprecipitation pull-down assay revealed binding between human CD160 and viral UL144 (Student poster)</p>	

18:00 - 19:00 **General Assembly of the Czech Society for Structural Biology**

The meeting will be held in the Czech and/or Slovak languages

1. Volba zapisovatele
2. Schválení programu
3. Výroční zpráva Rady ČSSB o činnosti a hospodaření
4. Zpráva revizní komise
5. Schválení výroční zprávy Rady ČSSB o činnosti a hospodaření
6. Infrastruktury se vztahem ke strukturální biologii, přístupy, financování, vývoj Instructu a jiných
7. Různé

19:00 - 20:00 *Dinner*

20:00 - 22:00 **Poster session**

Saturday, March 26

7:30 - 9:00 *Breakfast*

9:00 - 10:20 **Session VII** *Chair person: Jiří Pavlíček*

Václav Veverka Institute of Organic Chemistry and Biochemistry, Czech Academy of Sciences	A ubiquitous disordered protein interaction module orchestrates transcription elongation <i>L34 – 28</i>
Zuzana Cieniková CEITEC, Masaryk University	Structures of phage 812 neck suggest a mechanism for genome retention and release in <i>Herelleviridae</i> (CIISB user meeting) <i>L35 – 29</i>
Markéta Šoltysová Institute of Organic Chemistry and Biochemistry, Czech Academy of Sciences	How do SorC proteins recognize their DNA operators? (Student talk) <i>L36 – 29</i>
Vladena Bauerová Institute of Molecular Biology, Slovak Academy of Sciences	Structure-functional insights into the dantrolene binding site of the human cardiac ryanodine receptor: towards a deeper understanding of heart arrhythmias <i>L37 – 30</i>

10:20 - 10:40 *Coffee break*

10:40 - 12:20 **Session VIII** *Chair person: Veronika Obšilová*

Dalibor Košek Institute of Physiology, Czech Academy of Sciences	Mechanism of replicative "rolling-circle" DNA transposition in eukaryotes <i>L38 – 31</i>
Robert Vácha CEITEC, Masaryk University	How Viruses and Virus-like Nanoparticles Can Release Their Cargo/Genome (CIISB user meeting) <i>L39 – 32</i>
Tibor Füzik CEITEC, Masaryk University	Structure of tick-borne encephalitis virus immature particle solved by cryo-electron microscopy and sub-tomogram averaging (CIISB user meeting) <i>L40 – 33</i>
Richard Štefl CEITEC, Masaryk University	Cryo-EM of mouse RNase III–RNA complexes (CIISB user meeting) <i>L41 – 34</i>
Gabriel Demo CEITEC, Masaryk University	Cryo-EM ensemble reveals the mechanism of +1 ribosomal frame shifting <i>L42 – 35</i>

12:20 - 12:40 **Evaluation of student presentations, prizes, concluding remarks**

12:40 *Lunch & departure*

Posters

P01	Jiří Bejček	Design and evaluation of RNA-dependent RNA polymerase inhibitors of Severe acute respiratory syndrome coronavirus-2	p.36
P02	Daniel Berdát	Structural variability of base pairs in DNA	p.36
P03	Andrej Bitala	Immunoprecipitation pull-down assay revealed binding between human CD160 and viral UL144	p.37
P04	Tomáš Brom	Critical interactions of neuronal transcription factor REST with stabilizer TRF2	p.38
P05	Tatsiana Charnavets	Biophysical research facilities at Centre of molecular structure	p.38
P06	Radek Crha	Changes of the transient secondary structure motifs within Tau protein induced by its phosphorylation	p.39
P07	Arun Dhillon	Understanding the structural basis of interaction between adenovirus 5 type C and host receptors in viral entry and immune defence	p.39
P08	Christos Feidakis	AHoJ: Rapid, tailored search and retrieval of apo and holo protein structures	p.40
P09	Eva Fujdiarová	Detailed analysis of binding sites in the PLL family	p.40
P10	Norbert Gašparik	¹⁹ F labelling of disordered and hybrid proteins for ¹⁹ F NMR spectroscopy	p.41
P11	Karolína Honzejková	Thioredoxin inhibits ASK1 by keeping it in reduced state	p.41
P12	Josef Houser	Methods for characterization of biomolecules at BIC Core Facility	p.42
P13	Patricia Hrašnová	Structural and biophysical aspects of lactoferrin and its interaction with plasminogen	p.43
P14	Jakub Hrubý	Ni-replacement in Zn-dependent S1 nuclease	p.44
P15	Blanka Husťáková	Biochemical characterization of S1-P1 nuclease from human opportunistic pathogen <i>Stenotrophomonas maltophilia</i>	p.44
P16	Andrea Hušková	Structural architecture of NEIL3 glycosylase in abasic site DNA repair	p.45
P17	Klára Kohoutová	Modulating FOXO3 transcriptional activity by small, DBD-binding molecules	p.45
P18	Eliška Koutná	Conservation of H3K36 di- and trimethylated nucleosome recognition by PWWP	p.46
P19	Kateřina Krejčová	Non-nucleotide RNA-dependent RNA polymerase inhibitors that block SARS-CoV-2 and flaviviral replication	p.47
P20	Gytis Kučinskas	Structure of recombinant Tau40 protein fibrils prepared without enhancers of fibrilization	p.47
P21	Barbora Landová	Structural studies of MutM and abasic site interstrand crosslink	p.48
P22	Kateřina Linhartová	Recognition of RNA polymerase II C-terminal domain by RPRD2	p.48
P23	Yingliang Liu	Effect of a LOV protein matrix on flavin photocycle probed by transient resonance Raman spectroscopy and theoretical calculations	p.49

P24	Olga Matsarskaia	SARS-CoV-2 and more: how neutron provide insights into biological questions	p.50
P25	Andrea Náplavová	Multiple approaches for protein phosphorylation: a story of 14-3-3	p.50
P26	Stefana Niemoga	Multiapproach docking study for binding of intrinsically disordered tau peptides to monoclonal antibodies	p.51
P27	Zora Nováková	Prostate cancer: development of PSMA-directed antibody-based molecules intended for immunotherapy	p.52
P28	Kateřina Orsághová	Immunomodulatory cathepsin B from the house dust mite dermatophagoides farinae: Functional and structural characterization	p.52
P29	Peter Pajtinka	Synergistic antimicrobial activity of magainin 2 and PGLa revisited	p.53
P30	J. Pavlíček	New instrumentation available in Centre of molecular structure. Institute of Biotechnology CAS (Biocev)	p.54
P31	Olivia Petrvalská	14-3-3 directly interacts with the kinase domain of CaMKK1 and inhibits calmodulin binding	p.54
P32	Pavel Pohl	14-3-3-protein regulates Nedd4-2 by modulating interactions between HECT and WW domains	p.55
P33	Andreas Santamaria	Strikingly different roles of SARS-CoV-2 fusion peptides uncovered by neutron scattering	p.56
P34	Věra Schrenková	Raman optical activity of nucleotides – theoretical and experimental study	p.57
P35	Tereza Skálová	Crystal structure of human natural killer cell receptor NKp30 in complex with its tumor ligand B7-H6	p.57
P36	Simona Slušná	Mechanism of aggregation of tau protein forms associated with Alzheimer's disease and influence of the local structural motif on tau functions	p.58
P37	Anna Sobotková	Visualization of phage propagation in a <i>staphylococcus aureus</i> biofilm	p.59
P38	Vojtěch Spiwok	Metadynamics driven by alphafold output	p.59
P39	Jan Stránský	CF diffraction techniques in Centre of Molecular Structure: Employing high-end X-ray technologies for laboratory structural biology	p.60
P40	Hagen Sülzen	To each their own: Overcoming challenges in structural characterisation of closely related protein-protein complexes using single particle cryo-EM	p.60
P41	Jan Šimek	To homodimerize or to heterodimerize: story of 14-3-3 protein dimer formation	p.61
P42	Petr Škvara	Viral capsids as tools for structural biology	p.62
P43	Karolína Špeldová	Searching for the specific inhibitor of S1-P1 nuclease using fragment screening	p.62
P44	Leona Švecová	Fragment-based characterization of substrate for novel FAD-dependent oxidoreductase from <i>Chaetomium thermophilum</i>	p.63
P45	Lucie Valentová	A hunting strategy and virion structure of P. aeruginosa bacteriophage JBD30 revealed by cryo-electron microscopy	p.64
P46	Martina Zánová	Cryo-EM refinement and model building of protein-RNA complexes	p.64