

**XX Discussions in Structural Molecular Biology
and
7th User Meeting of CIISB**

21-23 March 2024

Programme

Thursday, March 21

12:00 - 14:00 Registration and accommodation, coffee

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

14:30 **Opening of XX Discussions and 7th User Meeting of CIISB** (*Jan Dohnálek, Pavel Plevka*)

14:40 - 15:40 **Session I** *Chair person: Jan Dohnálek*

Lecture no. – page of abstract

Bohdan Schneider Institute of Biotechnology, Czech Academy of Sciences, Vestec	First twenty years of Discussions in Structural Molecular Biology (Invited lecture, 30 min)	<i>L1 – 7</i>
Kateřina Radilová Institute of Organic Chemistry and Biochemistry, Czech Academy of Sciences, Prague	Structural characterization of influenza A polymerase PA subunit domains in complex with novel inhibitors (PhD Thesis Award 2023 - winner's talk, 30 min)	<i>L2 – 8</i>

15:40 - 16:10 *Coffee break*

16:10 - 17:40 **Session II** *Chair person: Cyril Bařinka*

Karolína Šnajdarová Loschmidt Laboratories, Masaryk University, Brno	X-ray structures of (S)-enantioselective haloalkane dehalogenase DmmarA from <i>Mycobacterium marinum</i> reveal a new mode of homodimerization that is atypical for this enzyme family (Student talk)	<i>L3 – 9</i>
Tereza Skálová Institute of Biotechnology, Czech Academy of Sciences, Vestec	Solving X-ray structure at low resolution: Natural killer cell receptor NKp30 with its tumor ligand B7-H6	<i>L4 – 10</i>
Ondřej Vaněk Faculty of Science, Charles University, Prague	Structural immunology of (super)natural killer cell receptor-ligand recognition	<i>L5 – 11</i>
Evžen Bouřa Institute of Organic Chemistry and Biochemistry, Czech Academy of Sciences, Prague	Viral RNA-methyltransferases: function, structure and inhibition	<i>L6 – 12</i>
Martin Kopecký Specion, s.r.o., Prague	Modern Leica optic microscopy – product and application view (10 min)	<i>L7 – 12</i>

18:00 Dinner

20:00 **CIISB Executive committee**

Friday, March 22

7:30 - 9:00 *Breakfast*

9:00 - 10:30 **Session III** *Chair person: Veronika Obšilová*

Cyril Bařinka Institute of Biotechnology, Czech Academy of Sciences, Vestec	Structure-function studies of polyglutamylase TTL-11 <i>L8 – 13</i>
Tomáš Kouba Institute of Organic Chemistry and Biochemistry, Czech Academy of Sciences, Prague	RNA polymerase recycling by mycobacterial HeID: an alternative, HeID- protected pathway of transcription initiation <i>L9 – 13</i>
Zuzana Cieniková Masaryk University, CEITEC, Brno	The role of semi-disordered scaffold proteins in phage LUZ19 procapsid assembly <i>L10 – 14</i>
Alžbeta Dikunová Masaryk University, CEITEC, Brno	Assembly of torpedo termination complexes in thermophilic and mesophilic organisms (Student talk) <i>L11 – 14</i>
Josef Uskoba Bio Tech a.s., Prague	Assessment of sample quality with every measurement FIDA 1 fundamentals (10 min) <i>L12 – 15</i>

10:30 - 11:00 *Coffee break and group photo*

11:00 - 12:20 **Session IV** *Chair person: Gabriel Demo*

Josef Houser Masaryk University, CEITEC, Brno	Protein-protein interaction analysis in education – A model case of chymotrypsin inhibitor <i>L13 – 16</i>
Subhash Narasimhan Masaryk University, CEITEC, Brno	Structural characterization of novel binding partner of mycobacterial transcription initiation factor sigma-A (Student talk) <i>L14 – 17</i>
Petra Chrupková ELI Beamlines, Dolní Břežany	The Role of Carotenoid Excited State in Orange Carotenoid Protein Activation (Student talk) <i>L15 – 17</i>
Miroslav Kloz ELI Beamlines, Dolní Břežany	Multiple Retinal Isomerizations during the Early Phase of the Bestrodopsin Photoreaction <i>L16 – 19</i>

12:30 *Lunch*

15:00 – 16:10 **Session V** Chair person: **Josef Houser**

Ladislav Bumba Institute of Microbiology, Czech Academy of Sciences, Prague	A multifaceted role of filamentous hemagglutinin (FHA) in the virulence of pathogenic <i>Bordetella</i> species <i>L17 – 20</i>
Mohanraj Gopalswamy NanoTemper Technologies GmbH, Munich	Structural biology of Acute Myeloid Leukemia (AML) protein and small molecule inhibitor complex <i>L18 – 20</i>
Veronika Klápšřová Masaryk University, CEITEC, Brno	Structural characterization of the interaction between BRCA1-BARD1 and RNA polymerase II (Student talk) <i>L19 – 21</i>
Jacek Patryn Bio-Rad Laboratories, Warszawa	Bio-Rad: out of complexity, find the simplicity (10 min) <i>L20 – 21</i>

16:10 - 16:40 *Coffee break*

16:40 – 17:40 **Session VI** Chair person: **Pavel Srb**

Robert Vácha Masaryk University, CEITEC, Brno	New Scramblases with Moonlighting Functions Identified in Mitochondria <i>L21 – 22</i>
Michal H. Kolář University of Chemistry and Technology, Prague	Three epochs of nascent protein translocation through the ribosome exit tunnel <i>L22 – 23</i>
Poster flash talks, 2 minutes each	
Irena Kratochvílová (Institute of Physics, Czech Academy of Sciences, Prague) Study of the relationship between embryo quality, speed of development and clinical pregnancy in PGT cycles	
Lukáš Martínek (University of South Bohemia, Faculty of Science, České Budějovice) Characterization of <i>de novo</i> missense variants in individuals with neurodevelopment disorders and their impact on the structure and function of the protein SHP2 (Student poster)	
Matyáš Suchý (University of South Bohemia, Faculty of Science, České Budějovice) Molecular dynamics simulations of single amino-acid substitution in BRAF:MEK1 complex (Student poster)	
Adam Polák (Institute of Neuroimmunology, Slovak Academy of Sciences, Bratislava) Production of monoclonal antibodies and their co-crystallization with intrinsically disordered protein tau (Student poster)	
Josef Cikhart (University of Chemistry and Technology, Prague) Computer simulations of the bacterial ribosome using coarse-grained models (Student poster)	
Radek Crha (BOKU - University of Natural Resources and Life Sciences, Vienna) Combining of hybrid QM/MM simulations with machine learned potentials (Student poster)	
Linda Kašiarová (Loschmidt Laboratories, Masaryk University, Brno) Towards unlocking the potential of staphylokinase for ischemic stroke treatment via a structure-based protein engineering (Student poster)	
Yevgen Yurenko (Institute of Organic Chemistry and Biochemistry, Czech Academy of Sciences, Prague) Accurate Multi-Scale Computations of Binding Free Energies in Insulin/Insulin Receptor Complex	

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. Revize členské základny
7. Hlasování o změně sídla společnosti a o související změně stanov ČSSB
8. Schválení tříčlenné volební komise pro volby Rady ČSSB v roce 2025 na období 2025-2030
9. Infrastruktury se vztahem ke strukturní biologii, přístupy, financování, vývoj Instructu a jiných
10. Různé

19:00 - 20:00 *Dinner*

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

(20:00 - 22:00 CSSB Council meeting)

Saturday, March 23

7:30 - 9:00 *Breakfast*

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

Alastair Gardiner Institute of Microbiology, Czech Academy of Sciences, Prague	Cryo-EM structure of the large photosynthetic complex from two species of Gemmatimonadota L23 – 24
Michal Koblížek Institute of Microbiology, Czech Academy of Sciences, Třeboň	Cold-loving bacterium from a mountain lake harvests light energy using both bacteriochlorophyll-containing photosystems as well as proton-pumping rhodopsins L24 – 25
Edward Curtis Institute of Organic Chemistry and Biochemistry, Czech Academy of Sciences, Prague	A fluorescent deoxyribozyme for high-throughput screening L25 – 25
Jiří Zahradník First Faculty of Medicine, Charles University, Prague	Dual Perspectives on the Evolution of SARS-CoV-2 Receptor Binding Domain L26 – 26

10:20 - 10:50 *Coffee break*

10:50 - 12:10 **Session VIII** *Chair person: Vojtěch Spiwok*

Gabriel Demo Masaryk University, CEITEC, Brno	Distinct 30S subunit dimerization architecture facilitated by a novel ribosome dimerization factor in archaea L27 – 27
Tibor Füzik Masaryk University, CEITEC, Brno	Asymmetric reconstructions of immature Tick-borne encephalitis virus particles reveal assembly mechanism of flaviviruses L28 – 28
Dominik Hrebík Max Planck Institute of Biochemistry, Martinsried	High-resolution <i>in situ</i> structures of HIV-1 matrix protein by single particle analysis L29 – 28
Pavel Plevka Masaryk University, CEITEC, Brno	Structure and replication cycle of a virus infecting climate-modulating alga <i>Emiliania huxleyi</i> L30 – 29

12:10 - 12:30 **Evaluation of student presentations, prizes, concluding remarks**

12:30 *Lunch & departure*