

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)	L1 – 7
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)	L2 – 8

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)	L3 – 9
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	L4 – 10
Ondřej Vaněk Faculty of Science, Charles University, Prague	Structural immunology of (super)natural killer cell receptor-ligand recognition	L5 – 11
Evžen Bouřa Institute of Organic Chemistry and Biochemistry, Czech Academy of Sciences, Prague	Viral RNA-methyltransferases: function, structure and inhibition	L6 – 12
Martin Kopečný Specion, s.r.o., Prague	Leica optic microscopy – product and application view (10 min)	L7 – 12

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 HelD: an alternative, HelD-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>
Alřbeta Dikunová Masaryk University, CEITEC, Brno	Assembly of torpedo termination complexes in thermophilic and mesophilic organisms (Student talk) <i>L11 – 14</i>
Josef Uskoba Max Planck Institute of Biochemistry, Martinsried FIDA Biosystems?	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 Břeřany	The Role of Carotenoid Excited State in Orange Carotenoid Protein Activation (Student talk) <i>L15 – 17</i>
Miroslav Kloz ELI Beamlines, Dolní Břeřany	Multiple Retinal Isomerizations during the Early Phase of the Bestrhodopsin 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 Martinek** (University of South Bohemia, Faculty of Science, České Budějovice)
Characterization of *de novo* missense variants in individuals with neurodevelopment disorders and their impact on the structure and function of the protein SHP2
- Matyáš Suchý** (University of South Bohemia, Faculty of Science, České Budějovice)
Molecular dynamics simulations of single amino-acid substitution in BRAF:MEK1 complex
- Adam Polák** (Institute of Neuroimmunology, Slovak Academy of Sciences, Bratislava)
Production of monoclonal antibodies and their co-crystallization with intrinsically disordered protein tau
- Josef Cihhart** (University of Chemistry and Technology, Prague)
Computer simulations of the bacterial ribosome using coarse-grained models
- Radek Crha** (BOKU - University of Natural Resources and Life Sciences, Vienna)
Combining of hybrid QM/MM simulations with machine learned potentials
- Linda Kašiarová** (Loschmidt Laboratories, Masaryk University, Brno)
Towards unlocking the potential of staphylokinase for ischemic stroke treatment via a structure-based protein engineering
- Petr Škvára** (Institute of Organic Chemistry and Biochemistry, Czech Academy of Sciences, Prague)
Structural basis for RNA-cap recognition and methylation by the mpoX methyltransferase VP39
- 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 strukturální 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>Emiliana huxleyi</i> L30 – 30

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

12:30 *Lunch & departure*