



PROGRAMME

Thursday, March 19

- 12:00 14:00 Registration and accommodation, coffee
- 14:00 14:15 Opening of XVI Discussions and 4th Users meeting of CIISB (*Jan Dohnálek, Vladimír Sklenář*)
- 14:15 16:45 **Session I**
chair person: *Jiří Pavlíček*
- L1 3
Pavčina Řezáčová (Institute of Organic Chemistry and Biochemistry, Czech Academy of Science - ASCR)
Structural studies of SorC family of transcriptional regulators (30 min)
- L2 4
Jan Dohnálek (Institute of Biotechnology, ASCR)
Unusual covalent bond between Trp and His in Bilirubin oxidase (CIISB User meeting)
- L3 5
Martin Malý (Institute of Biotechnology, ASCR)
Advantages of complete cross-validation in paired refinement (Student talk)
- L4 5
Jan Stránský (Institute of Biotechnology, ASCR)
Updates to instrumentation in the Centre of Molecular Structure in BIOCEV (CIISB User meeting)
- 15:45 16:15 *Coffee break*
- 16:15 18:20 **Session II**
chair person: *Lukáš Žlodek*
- L5 6
Bohdan Schneider (Institute of Biotechnology, ASCR)
Structural alphabet for structural analysis of nucleic acids
- L6 7
Martin Gajarský (CEITEC, Masaryk University)
Phylogenetically diverged structural motifs in telomeric DNA (Student talk, CIISB User meeting)
- L7 8
Kateřina Beková (CEITEC, Masaryk University)
Formation propensity of pseudo-circular G-hairpins (Student talk)
- L8 8
Aliaksei Chershneu (CEITEC, Masaryk University)
NACHRDB: solving the puzzle of structure-function relationships in nicotinic acetylcholine receptors (nAChRs) (Student talk)
- L9 10
Michal H. Kolář (University of Chemistry and Technology)
Large-scale atomistic simulations of the ribosome and its exit tunnel

- CL1 10
Piotr Wardega (NanoTemper Technologies Sp. z o.o.)
When protein stability matters (15 min)
- Invitation
Radomír Kužel (Faculty of Mathematics and Physics, Charles University, Prague)
25th General Assembly and Congress of the International Union of Crystallography (10 min)
- 18:30 Dinner, sponsored by Bruker AXS

Friday, March 20

- 7:30 9:00 Breakfast
- 9:00 10:20 **Session III**
chair person: *Vladimír Sklenář*
- L10 11
Klára Kohoutová (Faculty of Science, Charles University)
Modulating FOXO3 Transcriptional Activity by Small, DBD-binding Molecules (Student talk)
- L11 12
Daniel Krafcík (CEITEC, Masaryk University)
Investigation into G4-Ligand Complex in Living Human Cells Using In-cell NMR Spectroscopy (Student talk, CIISB User meeting)
- L12 13
Vanda Lux (Institute of Organic Chemistry and Biochemistry, ASCR)
Molecular mechanism of LEDGF/p75 dimerization
- L13 14
Pavčina Višková (CEITEC, Masaryk University)
Study of the i-motif stability during the cell cycle progression by in cell NMR spectroscopy (Student talk, CIISB User meeting)
- 10:20 10:50 *Coffee break*
- 10:50 12:25 **Session IV**
chair person: *Tomáš Obšil*
- L14 15
Pavol Bárdu (CEITEC, Masaryk University)
The story of *Rhodobacter capsulatus* gene transfer agent: Virus, organelle or both? (Student talk, CIISB User meeting)
- L15 16
Marta Šiborová (CEITEC, Masaryk University)
Structure of bacteriophage SU10 (Student talk, CIISB User meeting)



L16	16	L24	24
<i>David Buchta (CEITEC, Masaryk University)</i>		<i>Zdeněk Futera (Faculty of Science, University of South Bohemia)</i>	
Binding of neoFc receptor traps intermediate of pocket factor expulsion from echovirus 18 (Student talk, CIISB User meeting)		Electron Transfer Kinetics in Cytochrome C	
L17	17	18:00 19:00	
<i>Sebastian Zoll (Institute of Organic Chemistry and Biochemistry, ASCR)</i>		General Assembly of the Czech Society for Structural Biology. Meeting will be held in the Czech and/or Slovak languages.	
Invariant surface glycoproteins of trypanosomes as targets for structure-guided drug and vaccine design		19:00 20:00 <i>Dinner</i>	
CL2	17	(Meeting of the previous and new Council of CSSB)	
<i>Florence Husada (Thermo Fisher Scientific)</i>		20:00 22:00 Poster Session	
How Cryo-EM is revolutionizing structural biology complexes after the "resolution revolution" (15 min)			
12:30 14:00 <i>Lunch</i>			
14:00 15:00 <i>CIISB Executive Committee</i>			
15:00 16:00 Session V			
	chair person: <i>Pavlna Řezáčová</i>		
L18	18	L25	25
<i>Kateřina Slánská (Faculty of Science, Masaryk University)</i>		<i>Josef Lazar (Institute of Organic Chemistry and Biochemistry, ASCR)</i>	
Analysis and prediction of protein solubility (Student talk)		Fluorescent proteins as molecular antennas: structure and directionality	
L19	19	L26	26
<i>Petr Louša (CEITEC, Masaryk University)</i>		<i>Martin Marek (Loschmidt Laboratories, Masaryk University)</i>	
How phosphorylation impacts 14-3-3 dimerization (Student talk)		Structural Basis for Engineered Thermostability in Haloalkane Dehalogenases	
L20	20	L27	26
<i>Simona Lenhartová (Biomedical Research Center, Slovak Academy of Sciences)</i>		<i>Ladislav Bumba (Institute of Microbiology, ASCR)</i>	
Preliminary characterization of human CD160 and the influence of viral N-linked glycosylation related to this immune inhibitory pathway (Student talk)		Structure-function aspects of the TISS-mediated secretion of large RTX proteins	
16:00-16:20 <i>Coffee break</i>		L28	27
16:20 17:50 Session VI		<i>Tereza Skálová (Institute of Biotechnology, ASCR)</i>	
	chair person: <i>Jiří Vondrášek</i>	Crystal structure of heme-based oxygen sensor AfGcHK in complex with imidazole	
L21	22	L29	28
<i>Martin Lepšík (Centre de recherches sur les macromolécules végétales, CNRS)</i>		<i>Josef Houser (CEITEC, Masaryk University)</i>	
Calcium Bridging between Carbohydrates and Lectins: A Difficult Case for Classical Molecular Dynamics (30 min)		O-methylated saccharides as a neglected target for <i>Photobacterium</i> spp. Lectins	
L22	22	10:40 11:10 <i>Coffee break</i>	
<i>Francesco Luca Falginella (CEITEC, Masaryk University)</i>		11:10 12:30 Session VIII	
Elucidating Phospholipid Membrane Binding of DEP domain in the Wnt Signaling Pathway (Student talk)			chair person: <i>Imrich Barák</i>
L23	23	L30	29
<i>Dalibor Trapl (University of Chemistry and Technology)</i>		<i>Edward Curtis (Institute of Organic Chemistry and Biochemistry, ASCR)</i>	
Atomistic simulation of carbohydrate-protein complex formation: Hevein-32 domain (Student talk)		Making light with DNA	

Saturday, March 21

7:30 9:00 Breakfast

9:00 10:40 **Session VII**chair person: *Cyril Bařinka*



L31	29	L33	31
<i>Robert Vácha (CEITEC, Masaryk University)</i>		<i>Miroslav Kloz (ELI Beamlines, Institute of Physics, ASCR)</i>	
Effect of Helical Kink in Antimicrobial Peptides on Membrane Pore Formation		Comparative ultrafast spectroscopy and structural analysis of OCP1 and OCP2 protein from <i>Tolypothrix</i>	
L32	30	12:30-12:45	Evaluation of student presentations, prizes, concluding remarks
<i>David Kopečný (Faculty of Science, Palacký University)</i>		13:00	Lunch, departures
Urea-derived inhibitors of cytokinin oxidase/ dehydrogenase for agricultural applications			

POSTERS

P1	32	P10	36
<i>Kristýna Adámková (Institute of Biotechnology, ASCR)</i>		<i>Alžběta Dikunová (CEITEC, Masaryk university)</i>	
Zinc-dependent S1-P1-like nucleases from opportunistic human pathogens		Molecular mechanism of phase separation of RNA polymerase II	
P2	32	P11	37
<i>Jiří Bejček (University of Chemistry and Technology)</i>		<i>Stefan Djukic (Institute of Organic Chemistry and Biochemistry, ASCR)</i>	
Design of cardiac glycoside conjugates for improved cancer cell selectivity		Structural studies of purine nucleoside phosphorylase inhibitors	
P3	33	P12	37
<i>Lada Biedermannová (Institute of Biotechnology, ASCR)</i>		<i>Christos Feidakis (Faculty of Science, Charles University)</i>	
The first hydration level around biomolecules is site-specific		Predicting ion binding sites in proteins	
P4	33	P13	38
<i>Aleksandra Brzóstowicz (Faculty of Science, Masaryk University)</i>		<i>Eva Fujdiarová (CEITEC, Masaryk University)</i>	
Examination of interaction between regulatory domain of tyrosine hydroxylase and 14-3-3 protein		PLL3, a novel monomeric member of the seven-bladed beta-propeller lectin family	
P5	34	P14	39
<i>Michal Buša (Institute of Organic Chemistry and Biochemistry, ASCR)</i>		<i>Norbert Gašparik (CEITEC, Masaryk University)</i>	
Evolutionary upgrade of stefins for secretion in parasites		19F labelling of 14-3-3 recombinant protein for 19F NMR spectroscopy	
P6	34	P15	39
<i>Tatsiana Charnavets (Institute of Biotechnology, ASCR)</i>		<i>Ilektra - Chara Giassa (CEITEC, Masaryk University)</i>	
Biophysical research facilities at Centre of molecular structure of BIOCEV		HERMES – A software tool for prediction and analysis of magnetic field-induced residual dipolar couplings in nucleic acids	
P7	35	P16	40
<i>Aditya Chaudhari (Institute of Biotechnology, ASCR)</i>		<i>Mária Gondová (CEITEC, Masaryk university)</i>	
Photoinduced dynamics of EL222 monitored by multi-site-specific infrared spectroscopy		Role of hexamerin in regulation of pupa development	
P8	35	P17	40
<i>Nikola Chmúrčiaková (Institute of Organic Chemistry and Biochemistry, ASCR)</i>		<i>Petra Havlíčková (Institute of Chemistry, University of South Bohemia)</i>	
Cathepsin D protease of parasitic blood fluke <i>Schistosoma mansoni</i> as a target for inhibitory drugs		Crystallographic studies of TBEV NS5 RdRp domain	
P9	36	P18	41
<i>Zuzana Chromíková (Institute of Molecular Biology, Slovak Academy of Sciences)</i>		<i>Katarina Hesková (Institute of Neuroimmunology, Slovak Academy of Sciences)</i>	
Interaction of dynamic sporulation protein SpoIIE with novel cell cycle regulator protein GpsB		Preparation of a set of anti-tau monoclonal antibodies in CHO cell line using a robust system for eukaryotic expression	



P19	42	P30	49
<i>Alena Hofrová (CEITEC, Masaryk University)</i>		<i>Martina Kopečná (Faculty of Science, Palacký University)</i>	
Structural study of KIX domain by NMR		Study on aldehyde dehydrogenases from low and high plants using X-ray crystallography, microscale thermophoresis and site-directed mutagenesis	
P20	43	P31	50
<i>Karolína Honzejková (Faculty of Science, Charles University)</i>		<i>Eliška Koutná (Institute of Organic Chemistry and Biochemistry, ASCR)</i>	
Biophysical characterization of the N-terminal part of ASK1 and its interaction with TRX		LEDGF/p75 interaction network in the nucleosomal context	
P21	43	P32	50
<i>Lenka Horňáková (Institute of Neuroimmunology, Slovak Academy of Sciences)</i>		<i>Michaela Krafcíková (CEITEC, Masaryk University)</i>	
The reactivity of the C-terminal antibody shows differences possibly due to the changes in the global folds of tau isoforms		Study of DNA-Protein Interactions in Living Cells by in-cell NMR Spectroscopy	
P22	44	P33	51
<i>Matěj Horváth (Faculty of Science, Charles University)</i>		<i>Kateřina Linhartová (CEITEC, Masaryk University)</i>	
Role of 14-3-3 protein in the regulation of Death-associated protein kinase 2 (DAPK2)		Recognition of RNA Polymerase II C-terminal domain by RPRD2	
P23	45	P34	52
<i>Dominik Hřebík (CEITEC, Masaryk University)</i>		<i>Mikhail Makarov (Faculty of Science, Charles University)</i>	
Cryo-EM structure of human rhinovirus 14 in complex with its receptor ICAM-1		Life prior to aromatic residues: reverse engineering of a dephosphocoenzyme A kinase	
P24	45	P35	53
<i>Iveta Jahodová (Institute of Neuroimmunology, Slovak Academy of Sciences)</i>		<i>Raju Mandal (Faculty of Science, Charles University)</i>	
Structural and biophysical study of the first N-terminal insert of tau protein in the complex with monoclonal antibody		Molecular insight into the interaction between Forkhead box O4 (FOXO4) and p53 transcription factors	
P25	46	P36	53
<i>Nikola Jantová (Institute of Neuroimmunology, Slovak Academy of Sciences)</i>		<i>Eva Maturová (CEITEC, Masaryk University)</i>	
Structural and biophysical principles of natural protection of organism mediated by lactoferrin – a milk glycoprotein		In-cell NMR spectroscopy as a tool for studying the influence of changing intracellular environment on non-B DNA structures	
P26	47	P37	54
<i>Rohit Joshi (Institute of Physiology, ASCR)</i>		<i>Yuliia Mironová (CEITEC, Masaryk University)</i>	
Study of protein-protein interactions of human E3 ubiquitin ligase NEDD4L using fluorescence spectroscopy		Structural characterisation of phage infection in bacterial biofilm	
P27	48	P38	55
<i>Barbora Kaščáková (Institute of Chemistry, University of South Bohemia)</i>		<i>Veronika Obšilová (Institute of Physiology, ASCR)</i>	
Structure Comparison of Salivary Serpins from <i>Ixodes ricinus</i>		14-3-3 protein binding blocks both the nuclear localization sequence and the dimerization interface of caspase-2	
P28	48	P39	56
<i>Veronika Klápšová (CEITEC, Masaryk University)</i>		<i>Katarína Orsághová (Institute of Organic Chemistry and Biochemistry, ASCR)</i>	
Structural characterization of the interaction between BRCA1-BARD1 and RNA polymerase II		Immunomodulatory cathepsin B from the house dust mite <i>Dermatophagoides farinae</i> : functional and structural characterization	
P29	49	P40	56
<i>Jan Komárek (Institute of Biotechnology, ASCR)</i>		<i>Jiří Pavlíček (Institute of Biotechnology, ASCR)</i>	
X-ray structure of PDZ domain of Dishevelled-3 protein		Centre of Molecular Structure in BIOCEV – Current status and updates	



P41	57	P46	60
<i>Jitka Plucarová (CEITEC, Masaryk University)</i>		<i>Marek Šebesta (CEITEC, Masaryk University)</i>	
Microtubule Associated Protein 2c interacts with multiple partners at specific sites		Structural insights into the function of ZRANB3 in replication stress response	
P42	57	P47	61
<i>Pavel Pohl (Institute of Physiology, ASCR)</i>		<i>Leona Švecová (Institute of Biotechnology, ASCR)</i>	
Initial structural studies of regulation of ubiquitin ligase Nedd4-2 by 14-3-3 proteins		Structural data-based identification of substrate nature for novel FAD-dependent oxidoreductase from <i>Chaetomium thermophilum</i>	
P43	58	P48	61
<i>Michaela Procházková (CEITEC, Masaryk University)</i>		<i>Lucie Valentová (CEITEC, Masaryk University)</i>	
Excursion into the <i>Staphylococcus aureus</i> cell during bacteriophage infection		Structure of <i>T. castaneum</i> storage protein solved by cryo-electron microscopy	
P44	59	P49	62
<i>Riccardo Rigo (CEITEC, Masaryk University)</i>		<i>Lisa-Maria Weinhold (Institute of Organic Chemistry and Biochemistry, ASCR)</i>	
Structural characterization of a G-rich region within EGFR promoter		Structural relationship between subunits of the non-canonical BAF chromatin remodeling complex	
P45	60		
<i>Jaroslav Srp (Institute of Organic Chemistry and Biochemistry, ASCR)</i>			
A novel inhibitory motif against aspartic proteases identified in thyropins			