



## PROGRAMME

### Thursday, March 22

10:30 12:30 Registration at Nový Zámek

12:30 13:30 Accommodation

13:59 14:00 Opening of XV Discussions

#### 14:00 16:00 Session I

chairperson: *Jan Dohnálek*

L1 3

*Miroslav Kloz (ELI Beamlines)*

Spectral watermarking approach to stimulated Raman spectroscopy: background-free femtosecond vibration spectra

L2 5

*Irena Kratochvílová (Institute of Biotechnology)*

Critical defects in cryopreserved cell nuclei: DNA structure changes

L3 5

*Bohdan Schneider (Institute of Biotechnology)*

A DNA structural alphabet distinguishes the structural features of DNA bound to transcription factors and histone proteins

L4 6

*Edward A. Curtis (Institute of Organic Chemistry and Biochemistry)*

Mechanisms of G-quadruplex biochemical specificity

L5 6

*Giovanna Fragneto (Institut Laue-Langevin, Grenoble)*

The structure of model and natural lipid bilayers:

Moving towards complexity

16:00 16:20 Coffee break

#### 16:00 18:00 Session II

chairperson: *Edward Curtis*

L6 7

*Eva Hájková (Palacký University)*

Study on active site of nucleoside N-ribohydrolases from *Zea mays*

L7 8

*Emanuel K. Peter (Institute of Biotechnology)*

A method for accelerated free energy calculations of proteins in an extended experimental ensemble derived from the Protein Data Bank

L8 8

*David Jakubec (Inst. of Org. Chemistry and Biochemistry)*

3DPatch: fast sequence and structure residue-level information content annotation in a web browser

L9 9

*Klára Hlouchová (Charles University)*

Search into unevolved protein space

L10 9

*Jozef Hritz (Masaryk University)*

Protein homodimerization from perspective of structural biology and biophysics (30 min)

18:00 21:30 Dinner

Folows Meeting of the CIISB Exec. Com.

### Friday, March 23

7:30 8:45 Breakfast

#### 9:00 10:40 Session III

chairperson: *Klára Hlouchová*

L11 10

*Konstantinos Tripsianes (Masaryk University)*

Transforming biomolecular NMR to stay at the forefront of Structural Biology (30 min)

L12 10

*Pavel Srb (Inst. of Org. Chemistry and Biochemistry)*

Capturing dynamically interacting inhibitor by paramagnetic NMR spectroscopy

L13 11

*Martin Klíma (Inst. of Org. Chemistry and Biochemistry)*

Structural basis for hijacking of the host ACBD3 protein by picornaviruses

L14 11

*Václav Veverka (Institute of Organic Chemistry and Biochemistry)*

Targeting the LEDGF/p75 associated pathologies (30 min)

10:40 11:00 Coffee break

#### 11:00 12:20 Session IV

chairperson: *Bohdan Schneider*

L15 12

*Daniel Němeček (Thermo Fisher Scientific)*

Pipeline for protein structure determination by cryoEM (30 min.)

L16 56

*(PALL ForteBio)*

BLI technology as a tool for biomolecular interactions

L17 12

*Piotr Wardega (NanoTemper)*

NanoTemper Technologies – When protein quality matters. New arising star- Tycho NT.6 (30 min.)

12:20 13:15 Lunch

#### 13:30 15:45 Session V

chairperson: *Vladimír Sklenář*

##### 2nd Users Meeting of CIISB

L18 13

*Domink Hřebík (Masaryk University)*

Near-atomic structure of podovirus P68 provides insights into phage assembly and cell membrane penetration mechanism of bacteriophages infecting gram-positive bacteria

L19 13

*Liya Mukhamedova (Masaryk University)*

Cryo-EM structure of Kashmir bee virus

L20 14

*Kateřina Melková (Masaryk University)*

Microtubule Associated Protein 2c and Tau: insight into molecular basis of functional diversity of homologous regulatory intrinsically disordered proteins



L20	14	<b>Saturday, March 24</b>
<i>Karel Škubník (Masaryk University)</i>		
Virion structures and genome release mechanism of honeybee viruses from the family <i>Iflaviridae</i>		
L21	15	7:30 9:15 Breakfast
<i>Michaela Procházková (Masaryk University)</i>		
Structure of sacbrood honeybee virus reveals evolution of capsid protein features important for <i>Iflavirus</i> cell entry		
L22	16	9:30 10:20 <b>Session VII</b>
chairperson: <i>Veronika Obšilová</i>		
L28 20		
<i>Rüdiger Ettrich (Institute of Microbiology)</i>		
Computational Modeling of 3'-Phosphoadenosine 5'-Phosphosulfate Synthase PAPSS (30 min.)		
L29	21	L29 21
<i>Jan Mičan (Masaryk University)</i>		
Computational Enzyme Design of Haloalkane Dehalogenases for Yperite Degradation		
15:45 16:15 <i>Coffee break</i>		
16:00 18:00 <b>Session VI</b> chairperson: <i>Pavel Plevka</i>		
<b>2nd Users Meeting of CIISB</b>		
L23	16	10:20 10:40 <i>Coffee break</i>
<i>Tibor Füzik (Masaryk University)</i>		
Structure of tick-borne encephalitis virus and its neutralization by a monoclonal antibody (30 min.)		
L24	17	10:40 11:50 <b>Session VII</b>
chairperson: <i>Rüdiger Ettrich</i>		
L30 22		
<i>Veronika Obšilová (Institute of Physiology)</i>		
Molecular basis of the 14-3-3 protein-dependent activation of yeast neutral trehalase Nth1 (30 min)		
L25	18	L31 22
<i>Josef Houser (Masaryk University)</i>		
Looking for inhibitor: structural and functional analysis of novel bangle lectin PHL from <i>Photorhabdus asymbioticas</i>		
L32 23		
<i>Tereza Skálová (Institute of Biotechnology)</i>		
Crystal structure of globin domain of AfGcHK histidine kinase		
L26	18	L32 23
<i>Leona Švecová (Institute of Biotechnology)</i>		
Crystal structure of novel aryl-alcohol oxidase from thermophilic fungus		
L27	19	11:50-12:15 Student prizes & concluding remarks
<i>Kseniya Ustinova (Institute of Biotechnology)</i>		
Identification and characterization of microtubule-binding domain of HDAC6		
12:30 13:30 Lunch		
<i>Libor Grubhofer</i>		
Greetings by the president of the Czech Society for Biochemistry and Molecular Biology		
18:30 19:30 Dinner		
19:30 20:45		
<b>General Assembly of the Czech Society for Structural Biology.</b> Meeting will be held in the Czech and/or Slovak languages.		
20:30 22:30 <b>Poster Session</b>		



## POSTERS

P1	24	P13	30
<i>Kristýna Adámková (Institute of Biotechnology)</i>		<i>Ondrej Cehlár (Institute of Neuroimmunology)</i>	
Interaction of zinc-dependent nuclease from S1-P1 family with RNA		Conformational biases of tau protein's microtubule binding repeat regions r modulation of Th17-mediated pro-inflammatory axis	
P2	24	P14	31
<i>Miroslava Alblová (Institute of Physiology)</i>		<i>Dominika Chalupská (Institute of Organic Chemistry and Biochemistry)</i>	
Structural studies of the 14-3-3 protein and neutral trehalase (Nth1) complex		Structural and biophysical characterization of the PI4KB:14-3-3 protein complex	
P3	25	P15	32
<i>Petra Babková (Masaryk University)</i>		<i>Tatsiana Charnavets (Institute of Biotechnology)</i>	
Structural analysis of resurrected ancestral haloalkane dehalogenases		Facilities at the Centre of Molecular Structure of BIOCEV	
P4	26	P16	32
<i>Pavol Bárdy (Masaryk University)</i>		<i>Klaudia Chmelová (Masaryk University)</i>	
Grand theft among bacteria and phages: the structure of the gene transfer agent		Structure-function analysis of DhmeA, a haloalkane dehalogenase of subfamily III from <i>Haloferax mediterranei</i>	
P5	26	P17	33
<i>Roman Baška (Masaryk University)</i>		<i>Zuzana Cieniková (Masaryk University)</i>	
Structural study of staphylococcal phage phi812K1/420 proteins BmpA, BmpB and BmpC		Structural studies of the <i>Myoviridae</i> bacteriophage 812 portal complex	
P6	27	P18	33
<i>Ivana Berková (University of South Bohemia)</i>		<i>Alžběta Dikunová (Masaryk University)</i>	
Crystallization studies of novel haloalkane dehalogenase DgaA from <i>Glacieocola agarylitica</i> NO2		Expression, purification and structural analysis of recombinant chronic bee paralysis virus RNA-dependent-RNA-polymerase	
P7	27	P19	34
<i>Ján Biňovský (Masaryk University)</i>		<i>Anna Dubanková (Institute of Organic Chemistry and Biochemistry)</i>	
Phage adhesion to <i>S. aureus</i> : structure-functional studies of Receptor Binding Protein 1		Structural and functional characterisation of Aichi virus RNA dependent RNA polymerase	
P8	28	P20	34
<i>Pavlna Božíková (Institute of Biotechnology)</i>		<i>Pavla Fajtová (Inst. of Org. Chemistry and Biochemistry)</i>	
Structural alphabets for conformational analysis of nucleic acidssite inhibitors with anti-schistosomal activity		SmSP2: an anti-hemostatic serine protease secreted by the blood fluke pathogen, <i>Schistosoma mansoni</i>	
P9	28	P21	35
<i>Barbora Břenková (Masaryk University)</i>		<i>Jiří Fukal (Inst. of Org. Chemistry and Biochemistry)</i>	
Novel structure of membrane nanodisc		The benchmark of <sup>31</sup> P NMR parameters in phosphate: a case study on structurally constrained and flexible phosphate	
P10	29	P22	36
<i>David Buchta (Masaryk University)</i>		<i>Valerio Guido Giacobelli (Charles University)</i>	
Virion structure and inhibition of genome release of human echovirus 18		Test of genetic code evolution hypotheses: Reverse evolution of specific target proteins by mRNA-display technique	
P11	29		
<i>Michal Buša (Inst. of Org. Chemistry and Biochemistry)</i>			
Functional characterisation of novel cysteine protease inhibitor from <i>Fasciola hepatica</i>			
P12	30		
<i>Carina R. Büttner (Masaryk University)</i>			
Structures of three infection cycle intermediates of Cocksackievirus A6			



P23	36	P35	43
<i>Mária Gondová (Masaryk University)</i> Crystal structure of honeybee hexamerin 70b provides insight into regulation of juvenile hormone levels in haemolymph of pupae		<i>Radka Končítiková (Palacký University)</i> Study on several plant aldehyde dehydrogenases from moss <i>Physcomitrella patens</i>	
P24	37	P36	44
<i>Petra Havlíčková (University of South Bohemia)</i> Crystallization studies and preliminary X-ray crystallographic analysis of a newly prepared histidinol-phosphate phosphatase Tt82 from <i>Thermococcus onnurineus</i>		<i>Salome Kylarová (Charles University)</i> Structural insights into the regulation of CaMKK2 by calmodulin and 14-3-3 protein	
P25	37	P37	44
<i>Rozálie Hexnerová (Institute of Organic Chemistry and Biochemistry)</i> Abbreviation paradise: The Taz2 (CBP) TAD (C/EBP $\beta$ ) interaction		<i>Barbora Landová (Institute of Organic Chemistry and Biochemistry)</i> Molecular mechanisms of DNA interstrand cross-link formation	
P26	38	P38	45
<i>Miroslav Homola (Masaryk University)</i> Structure and replication of <i>Emiliana huxleyi</i> virus 86		<i>Domenico Lentini Santo (Charles University)</i> Structural studies of 14-3-3 complexes with peptides containing 14-3-3 binding motifs of protein kinase CaMKK2	
P27	38	P39	46
<i>Martin Horn (Inst. of Org. Chemistry and Biochemistry)</i> Novel macrocyclic inhibitors of human cathepsin D		<i>Václav Mareška (University of Chemistry and Technology)</i> Electronic sculpting of AT2R ligands by well-tempered and Flying Gaussian metadynamics	
P28	38	P40	46
<i>Matej Horváth (Charles University)</i> Structural basis of ASK1 inhibition by DJ-1		<i>Kludia Mihalovičová (Institute of Neuroimmunology)</i> Construction of vectors enabling eukaryotic expression of antibody Fabs aimed at crystallography of tau filament core	
P29	39	P41	47
<i>A. Ishemgulova (Masaryk University)</i> Vaccinia virus as vector for human rhinovirus C3 expression		<i>Jana Moravcová (Masaryk University)</i> Cryo-electron microscopy of mammalian cells	
P30	40	P42	47
<i>Adéla Jílková (Masaryk University)</i> Exploring druggable hot spots in <i>Schistosoma mansoni</i> cathepsin B1 for structure-based design of vinyl sulfone inhibitors		<i>Erik Nomilner (Masaryk University)</i> Study of dynamics of intrinsically disordered protein MAP2c using NMR relaxation	
P31	40	P43	48
<i>Dana Kalábová (Institute of Physiology)</i> Human procaspase-2 phosphorylation at both S139 and S164 is required for 14-3-3 binding		<i>Jan Prchal (University of Chemistry and Technology)</i> Interaction of MoMLV and MMTV matrix proteins with membrane phospholipids	
P32	41	P44	49
<i>Barbora Kaščáková (University of South Bohemia)</i> Structure-functional studies of protein P4 from bacteriophage $\phi$ 8		<i>Jakub Ptáček (Institute of Biotechnology)</i> Engineered fragments of anti-PSMA antibodies and their use in immunotherapy of prostate cancer	
P33	42	P45	49
<i>Lucie Kolářová (Institute of Biotechnology)</i> Interferons type II and their receptors R1 and R2 in fish species: structure, function and evolution		<i>Michal Růžička (Masaryk University)</i> Structural and Elastic Properties of DNA Mutation Motifs	
P34	42	P46	50
<i>Petr Kolenko (Institute of Biotechnology)</i> Weak ligand binding: data processing and electron density calculation methods		<i>Bohdan Schneider (Institute of Biotechnology)</i> Dinucleotide hydration sites	

P47 Vladimír Sychrovský (Institute of Organic Chemistry and Biochemistry) The theoretical study of charge transfer efficiency through damaged DNA duplexes	50	P52 Jaroslav Srp (Institute of Organic Chemistry and Biochemistry) Biomolecular simulations by combination of flying Gaussian method and parallel tempering	53
P48 Marta Šiborová (Masaryk University) Structure of Virus like Particles of Merkel Cell Polyomavirus	51	P53 Zoran Šucur (Univ. of Chemistry and Technology) Flying Gaussian method: New applications	53
P49 Jan Šilhan (Inst. of Org. Chemistry and Biochemistry) The study of the role of FANCI phosphorylation in FANCD2 monoubiquitylation and DNA crosslink repair	51	P54 Vyacheslav Tretyachenko (Charles University) Into the wild: expression and characterization of random protein libraries	54
P50 Aneta Šmídová (Institute of Physiology) Structural characterization of the complex between the procaspase-2 and the 14-3-3 protein	52	P55 Zuzana Trošanová (Masaryk University) Thermodynamic and kinetic study of 14-3-3 protein	54
P51 Vojtěch Spiwok (Univ. of Chemistry and Technology) Biomolecular simulations by combination of flying Gaussian method and parallel tempering	53	P56 Lukáš Židek (Masaryk University) Intrinsically disordered Microtubule Associated Protein 2c (MAP2c) studied via computational methods and nuclear magnetic resonance	55



**Harrachov, hotel Svornost**

**18.-21.6. 2018**

[www.xray.cz/kolokvium](http://www.xray.cz/kolokvium)

Výpočetní metody, strukturní databáze, kursy, výuka.  
Novinky v přístrojovém vybavení.

Příspěvky z oblasti krystalografie a strukturní analýzy.