



PROGRAMME

Thursday, March 19

10:30 12:30 Registration at Nový Zámek

12:30 13:30 Accommodation

14:00 15:40 Session I

chairperson: *Tomáš Obšil*

L1 3
Jiří Brynda

Carborane-Based Inhibitors of Carbonic Anhydrases and their Potential for Cancer Therapy

L2 4
Aleš Hnízda

Structural basis for hyperactivity of cN-II mutants

L3 4
Jana Škerlová

The unique mechanics of bacterial repressor DeoR: a structural study

L4 5
Adriana Baumlová

The crystal structure of the phosphatidylinositol 4-kinase IIa

L5 5
Vladena Bauerová-Hlinková

Insights into the structure OF THE human RyR2 N-terminal region and its mutations responsible for cardiac arrhythmias

15:40 16:00 *Coffee break*

16:00 17:40 Session II

chairperson: *Jan Dohnálek*

L6 6
Mariusz Jaskolski

Modulated protein crystal structure with 28 molecules in the asymmetric unit

L7 7
Kay Diederichs

CC* - Linking crystallographic model and data quality (30 min)

L8 7
Sergey Kalynych

Structural studies of human parechovirus 1 (30 min.)

L9 8
Edukondalu Mullapudi

Structure and genome release mechanism of Human Coronavirus Saffold virus-3 (SAFV-3)

17:40 17:55 *Coffee break*

17:55 18:55 Session III

chairperson: *Miroslav Klotz*

L10 8
Tereza Skálová

Structure of LLT1, a ligand for human NKR-P1, and its variability under various conditions

L11 9
Jost Ludwig

A refined atomic scale model of the yeast K⁺-translocation protein Trk1

L12 10
Janos Hajdu

The European XFEL and its potentials in structural biology

19:15 21:00 Dinner

Friday, March 20

7:30 8:45 Breakfast

9:00 10:20 Session IV

chairperson: *Jiří Vondrášek*

L13 10
Jaroslav Koča

Structural Bioinformatics - a Bridge between Structural Biology and Bioinformatics

L14
Hedi Hegyi

Enhancer-promoter interaction facilitated by transiently forming G-quadruplexes

L15 11
Lada Biedermannová

Hydration of amino acid residues in proteins: what can we learn from data mining

L16 12
David Jakubec

Large-scale quantitative assessment of binding preferences in protein – nucleic acid complexes

10:20 10:40 *Coffee break*

10:40 12:20 Session V

chairperson: *Jaroslav Koča*

L17 13
Alan Kádek

Structural dynamics of WrbA protein probed by mass spectrometry

L18 14
Petr Man

Hydrogen/deuterium exchange: moving from easy proteins to real life stories

L19 14
Tomáš Náhlík

Description of Algorithm for Analysis and 3D Reconstruction of Living Cell Inner Structures from Bright-Field Microscopy

L20 16
Lucie Bednářová

Spectroscopic studies of phosphoenolpyruvate carboxykinase from *Mycobacterium tuber*

L21 16
Dalibor Štys

Measurement in biological systems



12:30	13:45	Lunch	
14:00	15:40	Session VI	chairperson: <i>Bohdan Schneider</i>
L22			17
<i>Piotr Wardega</i>			
Quantitative analysis of biomolecular interactions with Microscale Thermophoresis (MST)			
L23			18
<i>Dhiraj Sinha</i>			
Interdomain interaction in the motor subunit of the type I restriction-modification system EcoR124I and their functional relevance			
L24			18
<i>Miroslav Kloz</i>			
Coherent Raman spectroscopy - noninvasive structural tool for time resolved structures			
L25			19
<i>Salome Kylarová</i>			
Structural studies of ASK1-TBD:TRX1 complex by fluorescence spectroscopy and SAXS			
L26			20
<i>Tomáš Klumpler</i>			
Biological Small Angle X-ray Scattering at CEITEC-MU			
15:40	16:00	<i>Coffee break</i>	
16:00	18:00	Session VII	chairperson: <i>Jindřich Hašek</i>
L27			20
<i>Irena Kratochvílová</i>			
Theoretical and Experimental Study of Charge Transfer Through DNA: Impact of Mercury Mediated T-Hg-T Base Pair			
L28			21
<i>Babak Minofar</i>			
The interactions of soil natural organic matter (NOM) and polycyclic aromatic hydrocarbon (PAH) with biological interfaces studied by MD simulations			
L29			23
<i>Renáta Rychtáriková</i>			
Analysis of living cell 3D inner structures from high-resolution bright-field microscopy			
L30			23
<i>Vladimír Sychrovský</i>			
The activation of N-glycosidic bond cleavage operated by hOGG1 enzyme can be specifically controlled by electrophilicity/nucleophilicity			
L31			24
<i>Charles Sabin</i>			
Using Non-Crystallographic-Symmetry to solve the structure of a perfect merohedral twin crystal of Aichi virus (AiV)			
L32			25
<i>Daniel Němeček</i>			
Molecular Architecture of Encapsulin Nanocompartments			
18:15	19:30	Dinner	

19:30	20:45	General Assembly of the Czech Society for Structural Biology.	
Meeting will be held in the Czech and/or Slovak languages.			
21:00	23:00	Poster Session	

Saturday, March 21

7:30	8:45	Breakfast	
9:00	10:30	Session VIII	chairperson: <i>Michaela Wimmerová</i>
L33			26
<i>Radovan Dvorský</i>			
Miracle of multi-domain proteins: a case study of ROCK Kinase			
L34			26
<i>Petra Babková</i>			
Understanding structure-function relationships of haloalkane dehalogenaseS by ancestral sequence reconstruction			
L35			27
<i>Ladislav Bumba</i>			
Probing metal-ion-assisted - interaction in self-processing module of FrpC protein			
L36			27
<i>Tomasz Kabzinski</i>			
Structural basis for transcription termination coupled to RNA processing/degradation (30 min.)			
10:30	10:50	<i>Coffee break</i>	
10:50	12:40	Session IX	chairperson: <i>Lukáš Židek</i>
L37			28
<i>Klaudia Šarmírová</i>			
Functional analysis of a novel haloalkane dehalogenase DsvA isolated from thermophilic bacterium <i>Saccharomonospora viridis</i> DSM 4			
L38			29
<i>Magdalena Krejčíková</i>			
Combining NMR and Raman spectroscopy reveals structural and functional features of a new cisplatin derivative			
L39			29
<i>Vojtěch Kubáň</i>			
NMR Structural Study of Self-Processing Module			
L40			30
<i>Petr Těšina</i>			
LEDGF/p75 as a Target for Treatment of MLL-Dependent Leukemia and HIV Infection			
L41			30
<i>Josef Hritz</i>			
Complex binding scheme between 14-3-3zeta and phosphoproteins elucidated by NMR and computational studies (30 min.)			
12:45	14:00	Lunch	



POSTERS

P1	32	P12	38
<i>Kristýna Boušová</i>		<i>Kristýna Hudcová</i>	
PIP2 and PIP3 interact with N-terminus region of TRPM4 channel		Spectral and electrochemical analysis of miR-34a-5p	
P2	32	P13	39
<i>Petr Čech</i>		<i>Adéla Jilková</i>	
Automatic workflow for the classification of local DNA conformations		Activation route of the Schistosoma mansoni cathepsin B1 drug target	
P3	33	P14	39
<i>Jiří Černý</i>		<i>Michaela Jirků</i>	
Modeling of blocking of NMDA receptor channel by endogenous neurosteroids		PIP2 interact with cytosolic N-terminal region of the melastatin channel TRPM1	
P4	33	P15	40
<i>Dominika Chalupská</i>		<i>Miroslava Kacířová</i>	
Mechanism of phosphatidylinositol 4-kinase III β inhibition		Structural characterization of phosphoprotein phosphatidylinositol 4-kinase III β and its interaction with 14-3-3	
P5	34	P16	41
<i>Tatsiana Charnavets</i>		<i>Radka Končítiková</i>	
Repetitive extragenic Palindroms from Haemophilus Parasuis and their associated transposase RAYT		Structure-function study on plant aldehyde dehydrogenases from family 2 and family 7	
P6	34	P17	41
<i>Jindřich Fanfrlík</i>		<i>Miroslava Kopecká</i>	
The Semiempirical Quantum Mechanical Scoring Function for In-Silico Drug Design		Structural study of the yeast enzyme neutral trehalase and its complex with the 14-3-3 protein	
P7	35	P18	42
<i>Karla Fejfarová</i>		<i>David Kopečný</i>	
PDBCOP: PDB Comparison Program		Site-directed mutagenesis of two nucleoside N-ribonucleases from maize	
P8	35	P19	42
<i>Jindřich Hašek</i>		<i>Dalibor Kosek</i>	
Receptors expressed on the natural killer cells; Review of the molecular structure data		Sedimentation analysis of the interaction between ASK1 and its binding partners	
P9	37	P20	43
<i>Katarína Hlat-Glembová</i>		<i>Terézia Koval'ová</i>	
Identification of the Catalytic residues of glycosidases from Paenibacillus thiaminolyticus as a way to engineering of new glyco		Crystallographic and catalytic study of α -L-fucosidase from Paenibacillus thiaminolyticus	
P10	37	P21	43
<i>Josef Houser</i>		<i>Zuzana Kovářová</i>	
Possibilities for biomacromolecular crystallization at BIC Core Facility at CEITEC, Brno		Proteolytic system of blood-feeding ticks: an update on protein structures	
P11	38	P22	44
<i>Domink Hrebík</i>		<i>Tomáš Kroupa</i>	
NMR relaxation studies of receiver domain of cytokinin receptor CK1IRD mutants from Arabidopsis thaliana		Retroviral matrix proteins interaction with membranes	
		P23	44
		<i>Monika Krupová</i>	
		Studies of Lanthanide Complexes by a Combination of Spectroscopic Methods	



P24 <i>Petr Louša</i> Monitoring of phosphorylation progress of tyrosine hydroxylase and interaction with 14-3-3zeta elucidated by NMR	45	P36 <i>David Řeha</i> Structural characterization of NAD(P)H:quinone oxidoreductase WrbA from <i>E. coli</i> in complex with benzoquinone	51
P25 <i>Václav Mareška</i> Role of CH/ interactions in stabilizing the protein-carbohydrate complex	45	P37 <i>Mohammadmehdi Saberioon</i> Application of Multispectral Cameras for estimating Nitrogen and Grain Yield in Paddy fields	52
P26 <i>Katarína Muchová</i> Link between cytoskeleton and spore formation in <i>Bacillus subtilis</i>	46	P38 <i>Tanvir Shaikh</i> Integration of SPIDER workflows into Scipion for user-friendly analysis of electron microscopy data Type I restriction-modification enzyme EcoR124I	52
P27 <i>Gábor Nagy</i> Molecular Interactions of the 14-3-3-zeta protein	46	P39 <i>Marta Siborová</i> Mechanism of <i>Staphylococcus aureus</i> cell wall penetration by phage phi812/K1	53
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P29 <i>Vít Novák</i> Spectra Modelling Combining Molecular Dynamics and Quantum Mechanics	48	P41 <i>Michal Škultéty</i> Theoretical study of carbonic anhydrase IX	54
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<i>Mária Trundová</i>		<i>Anna Zhyrova</i>	
Expression of toxic recombinant proteins for structural studies in the <i>E. coli</i> Lemo21(DE3) expression system		Phase transition approach on the interpretation of the chemical oscillation in the Belousov-Zhabotinsky reaction	
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