



## PROGRAMME

### Thursday, March 14

- 12:00 13:15 Registration at Nový Zámek
- 13:15 13:45 Accommodation in hotels
- 13:45 15:45 **Session I** chairperson: *Petr Novák*
- L1 3  
*John Engen*  
Hydrogen exchange mass spectrometry to probe the conformation of proteins both in solution and in membranes \* (45 min)
- L2 3  
*Alan Kádek*  
In-solution structure of cellobiose dehydrogenase probed by hydrogen / deuterium exchange mass spectrometry
- L3 4  
*Petr Novák*  
NKR-P1C Structural Model Revealed by Mass Spectrometry
- L4 5  
*Marek Šebela*  
Analysis of heterogeneous hinge-region O-glycosylation of human IgA1 using MALDI-TOF/TOF mass spectrometry \*
- 15:55 16:15 *Coffee break*
- 16:15 17:45 **Session II** chairperson: *Richard Štefl*
- L5 5  
*Jaroslav Nunvář*  
Evolution of genetic diversity of repetitive extragenic palindromic elements
- L6 6  
*Babak Minofar*  
Structure and dynamics of biomolecules in non-aqueous ionic solutions
- L7 6  
*Sinha Dhiraj*  
Interdomain communication and interaction in the motor subunit of restriction modification system EcoR1241 from *E.coli*
- L8 7  
*Bohdan Schneider*  
Analysis of protein/DNA interactions by novel bioinformatic tools \*
- 17:45 Dinner

### Friday, March 15

- 8:00 Breakfast
- 9:00 10:10 **Session III** chairperson: *Marek Šebela*
- L9 8  
*Mike Williams*  
Protein characterisation using DLS – measurement principle and technology typical applications, limitations and troubleshooting, the new Zetasizer Nano \*
- L10 8  
*Lucie Bednářová*  
Antimicrobial peptides interacting with model membranes. Spectroscopic study
- L11 9  
*Irena Kratochvilová*  
Charge transport through DNA/DNA duplexes and DNA/RNA hybrids: complex mechanism study
- 10:10 10:30 *Coffee break*
- 10:30 12:10 **Session IV** chairperson: *Jiří Brynda*
- L12 9  
*Jan Stránský*  
Plant nuclease TBN1 involved in apoptotic processes blocks its active site by a surface loop - sign of regulatory function?
- L13 10  
*Oksana Degtjarik*  
Preparation, Crystallization and Preliminary Structural Analysis of AHP2 Protein, the Signal Transmitter from *Arabidopsis thaliana*
- L14 11  
*Lubomír Borko*  
Human cardiac ryanodine receptor: structural study of the N-terminal region
- L15 12  
*Petr Těšina*  
Structural study of LEDGF/p75 binding partners
- L16 13  
*Josef Houser*  
Power is in detail - structural analysis of an *Aleuria aurantia* lectin mutant
- 12:15 13:30 Lunch
- 13:45 15:05 **Session V** chairperson: *Cyril Bařinka*
- L17 14  
*Vernon Smith*  
Bringing the Beamline Home: Increasing Productivity and Reducing Costs with the D8 VENTURE with METAJET X-Ray Source\*



L18	14
<i>Jan Dohnálek</i>	
Metals and ions in protein structures – from essential to marginal questions in identification of ions in enzymes and receptors*	
L19	15
<i>Ondrej Cehlár</i>	
Structural insight into the conformation of one of the microtubule binding motifs on the Alzheimer's disease-associated protein tau	
15:05 15:30 <i>Coffee break</i>	
15:30 17:30 <b>Session VI</b>	chairperson: <i>Tomáš Obšil</i>
L20	16
<i>Petr Kolenko</i>	
Inhibitors of glutaminyl cyclases against Alzheimer's disease *	
L21	17
<i>Jaroslav Burda</i>	
Reaction Mechanism of Ru(II) Piano-Stool Complexes; Umbrella Sampling QM/MM MD Study	
L22	17
<i>Radek Matuška</i>	
CH- $\pi$ Interaction between Carbohydrates and Aromatic Moieties: Electron Density Issue	
L23	18
<i>Žofie Sovová</i>	
Thylakoid membrane characterization and its interaction with PsbI protein from photosystem II	
L24	18
<i>Kvido Strišovský</i>	
Structural and mechanistic principles of intramembrane proteolysis - lessons from rhomboids*	
17:45 19:00 Dinner	
19:00	
<b>General Assembly of the Czech Society for Structural Biology</b> , at the Nový Zámek. Meeting will be held in the Czech and/or Slovak languages.	
20:15 22:45 <b>Poster Session at the Nový Zámek</b>	

**Saturday, March 26**

8:00 Breakfast	
9:00 10:40 <b>Session VII</b>	chairperson: <i>Rüdiger Ettrich</i>
L25	19
<i>Evžen Bouřa</i>	
The crystal structure of the Phi6 major capsid proteins*	
L26	19
<i>Daniel Němeček</i>	
Cryo-EM Reconstruction of the Bacteriophage phi6 Procapsid at Near-Atomic Resolution Shows Conformational Changes in dsRNA Virus Maturation	
L27	20
<i>Mikalai Lapkouski</i>	
Complexes of HIV-1 RT and DNA/RNA hybrid reveal structure compatible with RNA degradation*	
L28	20
<i>Lukáš Daniel</i>	
Role of the buried halide-binding site of haloalkane dehalogenase DbeA	
10:40 11:00 <i>Coffee break</i>	
11:00 12:10 <b>Session VIII</b>	chairperson: <i>Richard Hrabal</i>
L29	21
<i>Jan Frömmel</i>	
Aminoaldehyde dehydrogenase 1 from tomato – enzyme structure and possible use for the detection of aldehydes in beverages	
L30	22
<i>Tomáš Kroupa</i>	
Interaction of the myristoylated M-PMV matrix protein and his mutants with phospholipids	
L31	22
<i>Lukáš Židek</i>	
Molecular motions monitored by NMR relaxation – a conservative approach*	
12:10 12:12 <i>Closing remarks</i>	
12:15 <i>Lunch</i>	

Thirty minute talks are labeled by an asterisk, (\*), other talks have a limit of 20 minutes.

All times include discussion and will be strictly observed.



## POSTERS

P1	23	P12	29
<i>Petr Ascheulov</i>		<i>M. Kacířová</i>	
Influence of specific boron defects on boron-doped diamond conductivity		Novel Ligands for IFNg derived from <i>Streptococcal</i> Protein G scaffold	
P2	23	P13	30
<i>Hana Barvíková</i>		<i>Alina Kevorková</i>	
Computational study of interactions of organic matter and biomolecules with mineral surfaces		Functional coupling of duplex translocation to DNA cleavage in a type I restriction enzyme	
P3	24	P14	30
<i>Vitali Bialevich</i>		<i>Petr Kolenko</i>	
Proposed translocation cycle of the restriction-modification system EcoR124I		Yfid from E.coli as a Pfl repair protein	
P4	25	P15	31
<i>Jarmila Dušková</i>		<i>Radka Končítíková</i>	
Extracellular chitinolytic enzymes of <i>Clostridium Paraputrificum</i> J4; separation and characterization		Structural characterization of two maize aldehyde dehydrogenases from family 2	
P5	25	P16	31
<i>Rüdiger Ettrich</i>		<i>Miroslava Kopecká</i>	
Biphasic kinetic behavior of FMN-dependent NAD(P)H:quinone oxidoreductase WrbA from E. coli: A molecular understanding		How calcium and Bmh1 activate yeast neutral trehalase Nth1?	
P6	26	P17	32
<i>Katarína Hlat-Glembová</i>		<i>Dalibor Kosek</i>	
Prediction and structural studies of active site of selected glycosyl hydrolases from <i>Paenibacillus thiaminolyticus</i>		Biophysical study of the complex between the 14-3-3 protein and the kinase domain of ASK1	
P7	26	P18	32
<i>Tatsiana Holubeva</i>		<i>Tomáš Koval'</i>	
Isolation and crystallization of the recombinant PsbR protein of higher-plant photosystem II		Structure of multifunctional plant nuclease TBN1	
P8	27	P19	33
<i>Petr Hošek</i>		<i>Natalia Kulik</i>	
Combination of alchemical free energy simulation and metadynamics in the simulation package GROMACS		Homology modeling of fungal hexosaminidase from <i>T. flavus</i> with high substrate promiscuity	
P9	27	P20	34
<i>Dominik Hřebík</i>		<i>Ivana Kutá Smatanová</i>	
Magnesium binding to the receiver domain of cytokinin receptor CK1IRD from <i>Arabidopsis thaliana</i>		Practical aspects of protein crystallography	
P10	28	P21	34
<i>Michaela Jirků</i>		<i>Michal Kutý</i>	
Ca <sup>2+</sup> binding proteins interact with the N-terminal region of TRPM1		Towards a structure of green plant Photosystem II	
P11	28	P22	35
<i>Ivo Kabelka</i>		<i>Lucie Marečková</i>	
Study of bsoBI endonuclease by molecular dynamics		Novel binders derived from an albumin-binding domain scaffold targeting Prostate Secretory Protein-94	
		P23	35
		<i>Petra Matunová</i>	
		Thermodynamic and kinetic parameters for interaction of selected Pt(II) complexes with guanine	



P24	36	P31	39
<i>Pavel Mikulecký</i>		<i>Tereza Skálová</i>	
Rational design of high-affinity variants of interferon-gamma receptor 1		Structural properties of NK receptors and ligands with C-type lectine-like fold	
P25	36	P32	40
<i>Pavel Oborský</i>		<i>Rostislav Škrabana</i>	
Digital metadynamics: New biased simulation concept and its testing on the conformational equilibrium of Ac-Ala-NHMe		Validation of a high-throughput setup for manual assembly of nanolitre vapour-diffusion protein crystallization screens	
P26	37	P33	41
<i>Saurabh Pandey</i>		<i>Katsiaryna Tratsiak</i>	
Computational simulation of trimer rotation in hexameric Arginine repressor from <i>E.coli</i>		Characterization of the selected haloalkane dehalogenases crystals specific activity towards to their substrates	
P27	37	P34	42
<i>Jiří Pavlíček</i>		<i>Lucie Vaňková</i>	
Gateway-based system for optimization of recombinant protein expression in <i>K. lactis</i>		Human IL-23 receptor antagonists derived from an albumin-binding domain scaffold inhibit IL-23-dependent ex vivo expansion of IL-17-producing T-cells	
P28	38	P35	42
<i>Jakub Ptáček</i>		<i>Milan Zachrdla</i>	
Selection and characterization of Anticalin-based binders targeting human glutamate carboxypeptidase II		NMR Investigation of Unstructured Malaria Surface Protein MSP2, Isoform 3D7	
P29	38	P36	43
<i>David Řeha</i>		<i>Vojtěch Zapletal</i>	
Biological Applications of QM/MM Calculations with Polarized Embedding		Motions of biomolecules monitored by spectral density mapping	
P30	39	P37	43
<i>Jakub Šebera</i>		<i>Jitka Židková</i>	
Theoretical Study of Metal Ion Binding in Modified and Natural Cytosine-Cytosine Base Pairs		Motions of biomolecules monitored by spectral density mapping	