



PROGRAMME

Thursday, March 24

12:00 13:15 Registration

13:30 13:45 Opening

13:45 15:45 **Session I** chairperson: *Vladimír Sklenář*

L1 13
I. Barák

Lipid helices formation in *Bacillus subtilis* cell membrane * (30 min)

L2 13
P. Dvořák

Engineering of biochemical pathway for degradation of Anthropogenic environmental pollutant 1,2,3-trichloropropane

L3 14
J. Prchal

Expression and purification of myristoylated matrix protein of Mason-Pfizer monkey virus for Structural Studies

L4 15
J. Dohnálek

The molecular puzzle of C-type lectin like natural killer cell receptors

L5 15
P. Malý

Generation of artificial binders with affinity to human cytokines via computer-assisted mutagenesis of a stable protein scaffold and ribosome display selection *

15:45 16:00 *Coffee break*

16:00 18:00 **Session II** chairperson: *Petr Novák*

L6 16
D. Rozbeský

Chemical cross-linking and H/D exchange combined with mass spectrometry: A tool to validate and refine 3-D protein X-ray model

L7 17
P. Hanč

Structural details of NKR-P1D: Clrb interaction elucidated by protein cross-linking and mass spectrometry

L8 17
V. Andrushchenko

Supramolecular Assemblies Formed by Diolein and Stearyl Alcohol

L9 18
L. Řežábková

Structure of the 14-3-3/RGS3 complex: New details on architecture of complexes formed by 14-3-3 proteins

L10 19
M. Šebela

Structural and functional study on the glycosylation in maize cytokinin oxidase/dehydrogenase I

L11 20
P. Man

Accessibility changes within diphtheria toxin T domain upon membrane penetration probed by hydrogen exchange and mass spectrometry

18:30 20:00 Opening dinner at the Novy Zamek

20:00 22:00 **Poster Session I**, at the Novy Zamek

Friday, March 25

7:30 8:30 Breakfast

9:00 10:30 **Session III** chairperson: *Bohdan Schneider*

L12 21
Z. Chval

Mechanism of the Oxaliplatin Binding to the Double-Stranded 1,2-ds(pGpG) Dinucleotide in Aqueous Solution

L13 21
J. Přecechtělová

Torsion angle dependence of phosphorus chemical shifts in a nucleic acid backbone from combined molecular dynamics and density functional calculations*

L14 22
V. Sychrovský

Proposal of alternative pathway of the glycosidic bond cleavage mechanism of 8-oxoguanosine catalyzed by the human DNA repair protein hOGG1

L15 3
P. Kadeřávek

Complementation of 3D structure of delta subunit of RNA polymerase from *Bacillus subtilis* with description of internal motions in terms of reduced spectral density mapping

10:30 10:50 *Coffee break*

10:50 12:10 **Session IV** chairperson: *Vladimír Baumruk*

L16 23
V. Profant

Experimental and theoretical study of formation of polyproline II helix by means of Raman optical activity

L17 24
J. Hudecová

Conformational study of the cyclo(L-Trp-L-Trp)dipeptide

L18 24
Z. Futera

Application of New QM/MM Interface to Study of Ru Drugs Interacting with DNA

L19 25
I. Kishko

Kinetic analysis of *E. coli* WrbA redox activity



12:15 13:45 Lunch

14:00 16:00 **Session V** chairperson: *Petr Malý*

L20 26
J. Hašek

Reliability and Accuracy of Structure Determination in Diffraction Methods

L21 27
P. Řezáčová

Crystal structures of two protease inhibitors from tick saliva*

L22 28
A. Štěpánková

Three-dimensional structure of binunctional anhydrolase

L23 29
T. Koval

Structural analysis of a recombinant plant bifunctional nuclease TBN1

L24 30
L. Urbániková

Structural basis for substrate recognition by GH30 glucuronoxylanase from *Erwinia Chrysanthemi**

16:00 16:15 *Coffee break*

16:15 17:45 **Session VI** chairperson: *Jiří Vondrášek*

L25 31
J. Brynda

Crystal structure of the mouse galectin-4 N-terminal carbohydrate recognition domain *

L26 31
D. Řeha

Biological Applications of QM/MM Calculations with Explicit MM Polarization

L27 32
O. Kroutil

Structure and Conformational Behavior of the DNA Oligonucleotide Attached to the Charged Surface: A Molecular Dynamics Study

L28 32
M. Krupička

Competing reactions of disulphides and hydroxyl anion - QM study

18:15 19:30 Dinner

20:00 21:00

First General Assembly of the Czech Society for Structural Biology, at the Nový Zámek. Meeting will be held in the Czech and/or Slovak languages.

21:00 23:00 **Poster Session II**, at the Nový Zámek

Saturday, March 26

7:00 9:00 Breakfast

9:15 10:45 **Session VII** chairperson: *Pavlna Řezáčová*

L29 33
R. Dvorský

Impact of Point Mutations on Protein Functions: Example Case of Ras GTPases*

L30 33
P. Páchl

Structure-based drug design of selective 5'-nucleotidases inhibitors

L31 34
M. Ruda

MetaCentrum in e-Infrastructure era

L32 35
A. Křenek

CERIT-SC Centre: Looking for Synergies in Scientific Computing

10:45 11:00 *Coffee break*

11:00 12:00 **Session VIII** chairperson: *Richard Hrabal*

L33 36
O. Skřehota

QSPR modeling - algorithms, challenges and IT solutions

L34 37
J. Houser

Aleuria aurantia lectin family - structural insight into differences of carbohydrate binding among related proteins

L35 38
R. Etrich

Functional coupling of DNA duplex translocation t

12:15 14:00 *Lunch*

Unless stated otherwise, all events are held at the Residence hotel.

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	39	P12	47
<i>T. Baikova</i>		<i>Jawid Ahmad</i>	
Crystallization and structure-functional analysis of coupling of translocation to DNA cleavage in type I restriction enzyme EcoR124I		Novel Ligands for IFN γ derived from <i>Streptococcal</i> Protein G scaffold	
P2	39	P13	47
<i>I. Beššeová</i>		<i>M. Kačířová</i>	
How could flexibility of RNA three way junction from the GTP-ase associated center of 50S assist to the accommodation of the tRNA into the ribosome?		Structural studies of 14-3-3/phosducin complex	
P3	41	P14	48
<i>V. Bičevich</i>		<i>J. Kohoutová</i>	
Helical-helicase 2 domains interactions in HsdR subunit of EcoR124I restriction-modification complex		Isolation of the extrinsic proteins from the oxygen-evolving complex of higher plants	
P4	42	P15	49
<i>L. Biedermannová</i>		<i>P. Kolenko</i>	
Investigation of ligand passage in proteins		Influence of RNA binding on the structure and functionality of Borna disease virus matrix protein	
P5	42	P16	50
<i>J. Bílý</i>		<i>M. Kopecká</i>	
Localization of calmodulin and PIP ₂ binding sites on the C-termini of the transient receptor potential cation channel TRPM5		Preparation of regulatory domain of tyrosine hydroxylase for NMR studies	
P6	43	P17	51
<i>J. Burda</i>		<i>D. Kopečný</i>	
Reduction mechanism of the Pt(IV) Satraplatin derivatives by guanosine monophosphate; quantum mechanical study		Biochemical characterization of a recombinant plant aldehyde dehydrogenase 7 from <i>Pisum sativum</i> (PsALDH7)	
P7	44	P18	51
<i>E. Dejmková</i>		<i>S. Kozmoň</i>	
Thermodynamical analysis of the mutant CV-IIL lectins from <i>Chromobacterium violaceum</i>		Carbohydrate CH/p interactions – Theoretical investigation of the favourable regions in the carbohydrate surroundings	
P8	45	P19	52
<i>R. Dopitová</i>		<i>Z. Kukačka</i>	
Preparation of AHP proteins for structural analysis		Structural assembly of β -N-acetylhexosaminidase complex	
P9	45	P20	52
<i>S. Geidl</i>		<i>P. Kulhánek</i>	
Predicting pK _a values of substituted phenols from atomic charges		PMFLib – a toolkit for free energy calculations	
P10	46	P21	53
<i>B. Holakovská</i>		<i>M. Kutý</i>	
Comparison of C-terminal segments of TRPV ion channel family members and their interactions with calmodulin		Thylakoid membrane and Photosystem II, structure and molecular dynamics simulations	
P11	46	P22	53
<i>J. Jamroškovič</i>		<i>M. Lahoda</i>	
The effect of <i>Escherichia coli</i> min proteins on <i>Bacillus subtilis</i>		Crystallization and structural analysis of DhaA31 protein from <i>Rhodococcus rhodochrous</i>	
		P23	54
		<i>E. Macáková</i>	
		Study of Structural Differences in H8-H9 Loop among 14-3-3 Protein Isoforms	



P24	54	P35	61
<i>J. Makroczyová</i>		<i>K. Shamayeva</i>	
Functional and biochemical analysis of truncated SpoIIISA toxin in <i>Bacillus subtilis</i>		Identification of amino acid residues important for coupling ATPase and restriction activity in EcoR124I endonuclease	
P25	55	P36	62
<i>P. Maloň</i>		<i>O. Schmidt</i>	
Vibrational and electronic optical activity of amide and disulfide groups in neurohypophyseal hormones and their models		Higher plant photosystem II	
P26	56	P37	63
<i>T. Náhlík</i>		<i>T. Skálová</i>	
The state trajectory of cell		Structure of mouse CLRG – a ligand of NK cell receptor	
P27	56	P38	63
<i>V. Papoušková</i>		<i>V. Spiwok</i>	
NMR study of RNA polymerase delta subunit unique for gram-positive bacteria		Molecular Simulation with Elastic Network Model Potential in Gromacs	
P28	57	P39	64
<i>A. Pautsina</i>		<i>P. Srb</i>	
Biological systems state variable identification using joint analysis of biological and technical hypothesis in the time-lapse tissue culture development experiment		Protein oligomerization and backbone flexibility	
P29	58	P40	64
<i>T. Pazderka</i>		<i>Z. Strělcová</i>	
Raman and infrared spectroscopy of amino acids and its implication for improvement of the protein secondary structure determination		Computational study of the dimethylphosphate hydrolysis as the reference system for the understanding of the restriction endonucleases mechanism	
P30	59	P41	65
<i>M. Pazderková</i>		<i>A. Stsiapanava</i>	
Antibacterial peptides in interaction with model membranes studied by various spectroscopic methods		Crystallization and preliminary crystallographic analysis of <i>Rhodococcus rhodochrous</i> wild-type DhaA protein and its variant DhaA13 complexed with different ligands	
P31	59	P42	66
<i>B. Pekárová</i>		<i>E. Sviridova</i>	
Structure and binding specificity of the receiver domain of sensor histidine kinase CKII from <i>Arabidopsis thaliana</i>		<i>Neisseria Meningitidis</i> iron-regulated protein FrpD: Crystallization and crystallographic characterization	
P32	60	P43	67
<i>J. Písačková</i>		<i>J. Urban</i>	
Preparation, characterization and crystallization of recombinant fragment of anti-CD3 antibody MEM-57		Decomposition of cellular system via causal relations	
P33	60	P44	67
<i>M. Raab</i>		<i>D. Veisová</i>	
The binding properties of the H5N1 neuraminidase - molecular dynamics studies		The activity of NTH1 enzyme is mediated by yeast 14-3-3 isoforms	
P34	61	P45	19
<i>J. Ryška</i>		<i>M. Šebela</i>	
Docking study of matrix metalloproteinase inhibitors		Structural and functional study on the glycosylation in maize cytokinin oxidase/dehydrogenase1	