



PROGRAMME

Thursday, March 12

- 12:00 - 14:00 Registration
- 14:10 - 14:15 Introductory remarks
- 15:15 - 16:30 **Lecture session I**, chairperson: *P. Řezáčová*
- L1 p. 3
Rudiger Ettrich
Structure of the motor subunit and translocation model for EcoR124I restriction-modification complex
- L2 p. 4
Patrik Florek
Structure of SpoIIISA-SpoIIISB toxin-antitoxin complex from *Bacillus subtilis*
- L3 p. 4
Jan Dohnálek
The Small Laccase from *Streptomyces coelicolor*
- L4 p. 5
Jindřich Hašek
Function analysis of cystathionine gamma-lyase mutants
- L5 p. 6
Andrea Štěpánková
Structure changes evoked by binding of ligands into the active site of enzyme beta-galactosidase from *Arthrobacter* sp. C2-2
- 16:15 - 16:30 Coffee break
- 16:30 - 17:50 **Lecture session II**, chairperson: *J. Damborský*
- L6 p. 7
Táňa Koudeláková
Directed evolution of haloalkane dehalogenase towards higher activity in buffer containing dimethyl sulfoxide
- L7 p. 8
Jiří Vondrášek
Structural interpretation of the sequential preferences
- L8 p. 8
Martin Krupička
QM/MM study of beta-1,4-galactosyltransferase-1
- L9 p. 8
Andrea Fořtová
Study of water molecule dynamics at the tunnel openings of haloalkane dehalogenase QM/MM study of beta-1,4-galactosyltransferase-1
- 17:50 - 18:15 Physiological break
- 18:15 - 18:45 Concert
- 19:00 - 22:30 Banquet

Friday, March 13

- 7:00 - 8:45 Breakfast
- 9:00 - 10:50 **Lecture session III**, chairperson: *J. Burda*
- L10 p. 9
Zuzana Jiroušková
Electronegativity Equalization Method - Fast Method For Charge Calculation
- L11 p. 10
Zdeněk Futera
Interaction of 'Piano-stool' Ruthenium Complexes with DNA; QM/MM Study
- L12 p. 10
Jan Kmuniček. Martin Kuba
Metacentrum: e-infrastructure for solving structural biology research challenges
- L13 p. 11
Václav Štumbauer
Random walk model of dispersion in bioreactors and its application to modelling of microbial growth
- 10:50 - 11:05 Coffee break
- 11:05 - 12:15 **Lecture session IV**, chairperson: *V. Sychrovský*
- L14 p. 11
Jaroslav Burda
Quantum chemical description of the properties and reaction mechanisms of selected anticancer metallodrugs with biomolecules
- L15 p. 12
Ladislav Benda
Solvation of nucleic acid backbone: A DFT study
- L16 p. 12
Jana Přecechtělová
The influence of backbone and solvent dynamics on 31P chemical shift tensors in Dickerson dodecamer: A combined MD/DFT study
- 12:30 - 13:45 Lunch
- 14:00 - 15:50 **Lecture session V**, chairperson: *V. Sklenář*
- L17 p. 13
Bohdan Schneider
DNA local conformations and their sequence preferences
- L18 p. 13
Ivana Beššeová
Molecular dynamics study: Intrinsic dynamics of RNA three-way junction
- L19 p. 14
Jiří Černý
Double-helical - ladder structural transition in the B-DNA is induced by a loss of dispersion energy



L20	p. 15	Saturday, March 18
<i>Petr Pacht</i>		
Structure-based drug design of selective 5-nucleotidases inhibitors		7:00 - 9:00 Breakfast
L21	p. 15	9:15 - 10:45 Lecture session VII , chairman: <i>I. Barák</i>
<i>Filip Lankaš</i>		
Simulating A-tract DNA: The influence of substates and the measure of bending		L27 p. 20
		<i>Vladimír Sklenář</i>
15:50 - 16:10 Coffee break		Quo vadis? NMR as an eminent tool for structural and systems biology
15:15 - 16:55 Lecture session VI , chairman: <i>P. Šebo</i>		L28 p. 20
		<i>Jiří Vlach</i>
L22	p. 16	Oligomerization of Non-Myristoylated M-PMV Matrix Protein
<i>Irena Kratochvílová</i>		L29 p. 21
Conductivity of natural and modified DNA measured by Scanning Tunneling Microscopy. The effect of sequence, charge and stacking		<i>Pavel Plevka</i>
L23	p. 17	Octahedral particles of bacteriophage MS2 coat protein mutant
<i>R. Chaloupková</i>		L30 p. 21
Thermodynamic analysis of the enantioselectivity of haloalkane dehalogenase DbjA and its variants DbjA and DbjA +H139A towards brominated esters and β -substituted bromoalkanes		<i>Dalibor Štys</i>
L24	p. 18	Buquoy's 'Fundamental laws of phenomenon of heat' and their meaning
<i>Vladena Bauerová</i>		10:45 - 11:00 Coffee break
Human Ryanodine receptor 2		11:00 - 12:00 Lecture session VIII , chairperson: <i>B. Schneider</i>
L25	p. 18	
<i>Zbyněk Halbhuber</i>		L31 p. 23
Direction of immune system in T1D pathogenesis: Analysis by using gene microarray and pathway analysis (GeneGo, MetaCore)		<i>Richard Štefl</i>
L26	p. 19	Transcription termination of nonpolyadenylated transcripts
<i>Tomáš Obšil</i>		L32 p. 23
Role of 14-3-3 proteins in the regulation of G-protein signaling		<i>Jiří Jonák</i>
		Proteosynthetic elongation factor EF-Tu domains: thermal adaptation and functions
18:30 - 19:30 Dinner		12:00 - 12:03 Concluding remarks
19:15 - 22:00 Poster session		12:15 - 14:00 Lunch