



PROGRAMME

Thursday, March 16

13:00 - 15:00 Registration

15:10 - 15:15 Introductory remarks

15:15 - 16:30 **Lecture session I**, chairman: *V. Sychrovský*
L1 p. 3
Tomáš Obšil

Regulation by molecular interference: How 14-3-3 protein controls activity of forkhead transcription factor FOXO4
L2 p. 4
Karel Bezouška

Optical spectroscopy, mass spectrometry and NMR are essential tools in the production of soluble receptors of natural killer cells
L3 p. 5
Jiří Vlach

A single-point mutation of M-PMV matrix protein causes reorientation of protein domains and changes the phenotype of the virus
L4 p. 5
Zuzana Vokáčová

NMR parameters in RNA molecules and their correlation with molecular structure

16:30 - 17:00 Coffee break

17:00 - 18:00 **Plenary lecture I**, chairman: *V. Sychrovský*
PL1 p. 6
Vladimír Sklenář

BioNMR: Contemporary Trends, Challenges, and Future Prospects

18:30 - 22:30 Banquet

Friday, March 17

7:00 - 8:45 Breakfast

9:00 - 10:00 **Plenary lecture II**, chairman: *D. Štys*
PL2 p. 6
Vladimír Baumruk

Methods of optical spectroscopy for structural biology

10:00 - 10:20 Coffee break

10:20 - 12:00 **Lecture session II**, chairman: *D. Štys*
L5 p. 6
Jan Florian

DNA replication fidelity: Theory and experiment
L6 p. 7
Pavel Macek

Molecular dynamics study of major urinary protein-pheromone interactions: A structural model for ligand induced flexibility increase
L7 p. 7
Jiří Šebek

MD and Ab Initio Modeling of Electronic Spectra of

N-methylacetamide and Peptides in Water Solutions
L8 p. 8
Peter Flecker

Molecular Modelling studies with Bowman Birk inhibitors
L9 p. 8
Michal Hušák

The use of GPU based calculations in structural biology
L10 p. 9
Patrik Florek

Bacterial programmed cell death - genetical, biochemical, and structural insight

12:15 - 14:00 Lunch

14:15 - 15:00 **Plenary lecture III**, chairman: *B. Schneider*
PL3 p. 10
Rudiger Ettrich

Molecular systems biology: Molecular simulations of proteins and their complexes

15:00 - 15:15 Coffee break

15:15 - 16:55 **Lecture session III**, chairman: *B. Schneider*
L11 p. 10
Matěj Lexa

The accuracy of domain boundary detection in proteins based on segment co-occurrence compared to other methods
L12 p. 11
Peter Palenčár

Crystal structure of photosystem II from *Thermosynechococcus elongatus* refined and studied by molecular dynamics
L13 p. 12
Jiří Brynda

From non-peptide towards non-carbon protease inhibitors: metallocarboranes as specific and potent inhibitors of HIV protease
L14 p. 13
Veronika Krejčířková

Structural studies of galectin-4 N-terminal domain in complex with lactose
L15 p. 13
Daniel Svozil

DNA Conformational Families

16:55 - 17:15 Coffee break

17:15 - 18:00 **Plenary lecture IV**, chairman: *B. Schneider*
PL4 p. 14
Jiří Šponer

Structure and dynamics of RNA and DNA. Advanced computational studies

18:30 - 19:30 Dinner

19:45 - 22:00 **Poster session**

**Saturday, March 18**

7:00 - 9:10 Breakfast

9:15 - 10:15 **Plenary lecture V**, chairman: *J. Brynda*

PL5 p. 14

Jan Dohnálek

Structure elucidation by diffraction methods - contribution to structural biology

10:15 - 10:30 Coffee break

10:30 - 11:50 **Lecture session IV**, chairman: *J. Damborský*

L16 p. 15

Zbyněk Prokop

Discovery of Stereoselective Haloalkane Dehalogenase: New Tool for Asymmetric Synthesis

L17 p. 16

Tomáš Mozga

Structure-enantioselectivity relationships of haloalkane dehalogenases

L18 p. 17

Radka Chaloupková

Physical variables as a control of enzyme stereoselectivity

L19 p. 17

Táňa Chrobáková

Engineering of enantioselective haloalkane dehalogenase by cumulative mutagenesis

L20 p. 18

Martin Klvana

Modelling of Product Release and Identification of Export Routes in Haloalkane Dehalogenase DhaA

11:55 - 12:00 Concluding remarks

12:15 - 14:00 Lunch

POSTERS

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M. Haeubl

Expression and Purification of apo-Micro-Myoglobin and its Reconstitution to the Heme binding Micro-Myoglobin

P2 p. 20

K. Hofbauerová

Human protein CD69 studied by combination of vibrational spectroscopy and molecular

P3 p. 21

E. Chovancová

Evolution of haloalkane dehalogenase protein family

P4 p. 22

P. Jeřábek:

Computer-Assisted Design of Fluorescent Probes for Solvent Relaxation Experiments

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V. KopeckýBehavior of the human α_1 -acid glycoprotein in water-low aliphatic alcohol systems

P7 p. 24

I. Kutá SmatanováCrystals of photosystem II core complex from *Pisum sativum*

P8 p. 25

M. Kutý

Photosynthetic reaction centre and chlorosomal pigments, a computational study

P9 p. 26

M. LapkouskiOverexpression, purification and crystallization attempts of the recombinant R subunit *EcoAI*

P10 p. 26

P. Mader

Stabilization of antibody structure upon binding epitope peptide: x-ray, microcalorimetry and molecular dynamics study

P11 p. 27

L. MaršálkováTemperature dependence of human α_1 -acid glycoprotein behavior induced by mixed solvents and acid pH

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V. MartínekTheoretical investigation of the effects of mutations of the charged amino acids on the dissociation and rate constants for the DNA replication by human DNA polymerase β

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M. Monincová

High-throughput characterization of enzymes from genomic and proteomic projects: – Multivariate statistical approach

P14 p. 29

V. Mrázíková

Structural study on C-terminus of the vanilloid receptor TRPV1

P15 p. 30

M. Nálezková

NMR study of protein CD69



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