



PROGRAMME

Thursday, March 18

12:00 - 13:15 Registration

13:30 - 14:30 **Open forum about the future of structural biology in Europe**

chair person: *V. Sklenář*

Introduction

L1 p. 3

Jan Dohnálek

INSTRUCT – An Integrated Structural Biology Infrastructure for Europe. Do we need formal professional organization?

14:30 - 15:00 Coffee break

15:00 - 15:05 **Opening of the conference**

15:05 - 17:05 **Lecture session I**, chair person: *B. Schneider*

L2 p. 4

Zdeněk Tošner

Solid-state NMR of biological samples

L3 p. 4

Pavel Srb

Dynamical analysis of WT M-PMV matrix protein and its single point mutant R55F with respect to their different oligomerization properties

L4 p. 5

Jan Prchal

Interaction of the M-PMV matrix protein with phosphatidylinositol bisphosphate

L5 p. 6

Vladimír Kopecký

Structure differences between protein crystals and solution structures monitored by Raman spectroscopy – case study of PsbP protein

L6 p. 6

Valery Andrushchenko

Structure of guanine octamers d(G)₈ determined by combination of VCD spectroscopy and theoretical computations

L7 p. 7

Irena Kratochvílová

Charge transport in DNA oligonucleotides with various base-pairing patterns

17:05 - 17:20 Coffee break

17:20 - 19:20 **Lecture session II**, chair person:

J. Damborský

L8 p. 8

Pavel Jungwirth

The interface between oxidized phospholipid bilayers and aqueous solutions

L9 p. 8

Babak Minofar

Aqueous salt solution of organic solvents as a media for enzymatic reactions

L10 p. 9

Veronika Štěpánková

Effect of organic solvents on structure and function of haloalkane dehalogenases

L11 p. 10

Tomáš Mozga

Biochemical and structural characterization of novel haloalkane dehalogenase DbeA from *Bradyrhizobium elkani* USDA94 possessing two halide-binding sites

L12 p. 11

Rudiger Ettrich

Was binding of free amino acids an early innovation in the evolution of allostery?

19:30 - 22:30 Banquet

Friday, March 19

7:00 - 8:45 Breakfast

9:00 - 10:50 **Lecture session III**, chair person: *T. Obšil*

L13 p. 12

Jaroslav Koča

Computational methods as a component of modern structural biology

L14 p. 12

Vojtěch Spiwok

Free Energy Modelling of Substrate Distortion in the Enzyme Active Site: An Example of Influenza Neuraminidase

L15 p. 13

Radka Svobodová-Vařeková

SiteBinder – software tool for superimposing multiple structural motives

L16 p. 14

Jiří Černý

Improving protein binding, in silico approach

10:30 - 10:50 Coffee break

11:05 - 12:15 **Lecture session IV**, chair person: *J. Koča*

L17 p. 14

Ladislav Benda

Computational analysis of the stabilization effects in successive U-Hg-U base pairs

L18 p. 15

Crina Maria Ionescu

Fast methods of atomic charge calculation: parameterization of EEM for applicability to metal containing proteins

L19 p. 15

Jan Alán

Employment of free energy calculations to estimation of carbohydrates affinities towards PA-IIL superfamily lectins



L20 <i>Imre Barák</i> Molecular and structural mechanisms of cell division site recognition in <i>Bacillus subtilis</i>	p. 16	19:45 - 21:00 First plenary meeting of NFSB chair person: <i>B. Schneider</i> Organization of the NFSB National forum for structural biology Legal framework Membership Election of the NFSB committee
12:10 - 13:45 Lunch		
14:00 - 16:00 Lecture session V , chair person: <i>J. Dohnálek</i>		
L21 <i>Tomáš Obšil</i> Structure of the 14-3-3/FOXO4 complex derived from the fluorescence spectroscopy data	p. 17	21:00 - 23:00 Poster session
L22 <i>Kateřina Procházková</i> Structural and molecular mechanism for autoprocessing of MARTX toxin of <i>Vibrio cholerae</i> at multiple sites	p. 18	
L23 <i>Pavel Mader</i> Human carbonic anhydrase complexes with isoquinoline inhibitors	p. 18	
L24 <i>David Kopečný</i> Structural analysis of plant aminoaldehyde dehydrogenases	p. 19	
L25 <i>Julie Wolfová</i> Defining structural features of the family of tetrameric flavoproteins Wrba	p. 19	
L26 <i>Tomáš Klumpler</i> Solving phase problem using a Se-Met derivative of the flavoenzyme NAD(P)H:acceptor oxidoreductase (FerB)	p. 20	
16:00 - 16:30 Coffee break		
16:30 - 18:20 Lecture session VI , chair person: <i>R. Ettrich</i>		
L27 <i>Bohdan Schneider</i> Bioinformatic analyses of the first solvation shell of nucleic acids	p. 24	
L28 <i>Jindřich Hašek</i> Using the Cambridge Structure Database of Organic and Organometallic Compounds in Structure Biology	p. 24	
L29 <i>Martin Kuba</i> MetaCentrum - On the Way from Distributed Computing to Cyber Infrastructure for Research	p. 26	
L30 <i>Dalibor Štys</i> Three dimensional information structure of living cell fate	p. 27	
18:30 - 19:30 Dinner		
<hr/> Saturday, March 20		
7:00 - 8:45 Breakfast		
9:15 - 10:45 Lecture session VII , chair person: <i>R. Štefl</i>		
L31 <i>Veronika Motáčková</i> Structure and dynamics of RNA polymerase delta subunit from <i>Bacillus subtilis</i> determined by NMR spectroscopy	p. 28	
L32 <i>Fruzsina Hobór</i> The role of Nrd1-Nab3 complex in transcription termination	p. 28	
L33 <i>Karel Kubíček</i> Structural insights into recruitment and dissociation of RNA polymerase II termination factors	p. 29	
10:20 - 10:45 Coffee break		
10:45 - 12:05 Lecture session VIII , chair person: <i>J. Vondrášek</i>		
L34 <i>Václav Veverka</i> Structural insight into regulation of the Wnt/b-catenin signalling pathway by sclerostin: implications for osteoporosis treatments	p. 29	
L35 <i>Michaela Wimmerová</i> High-affinity lectins from pathogens: the potential targets for antiadhesive drug design	p. 30	
L36 <i>Richard Dvorský</i> From Structural Biology to the Drugs against Inflammatory Bowel Diseases	p. 30	
12:05 - 12:07 Concluding remarks		
12:15 - 14:00 Lunch		



POSTERS

P1 <i>D. Antoš</i> MetaCentrum -- e-Infrastructure for Computational and Data Challenges	p. 31	P13 <i>J. Hrudíková</i> Raman and Raman optical activity conformational study of a cyclic hexapeptide	p. 37
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