

PROGRAMME

Thursday, March 13	Friday, March 14
10:30 12:00 Registration 12:00 12:45 Accommodation	8:00 Breakfast
12.00 12.43 Accommodation	9:00 10:00 Session II chairperson: <i>Tomáš Obšil</i>
13:00 14:15 Special Session celebrating IYCr	L9 11
chairperson: <i>Jan Dohnálek</i> Plenary lecture to celebrate	L9 11 Vernon. Smith
the International Year of Crystallography 3	Improvements to Data Quality with the PHOTON 100 de-
David Stuart	tector in Shutterless Mode
Challenges of virus crystallography	L10 Jiří Maršík
14:15 14:45 Coffee break	Latest Developments for Life Science from Rigaku
14:15 14:45 Coffee break	L11 11
14:45 16:05 Special Session celebrating IYCr	Jiří Brynda
chairperson: Bohdan Schneider	X-ray Structural Analysis of Carbonic Anhydrase and Carborane-Based Inhibitors Complexes
L1 3	10.00.10.20.6.6.1.1
Radomír Kužel	10:00 10:20 Coffee break
2014 - International Year of Crystallography L2 4	10:20 12:00 Session III chairperson: <i>Evžen Bouřa</i>
L2 4 Jindřich Hašek	10.20 12.00 Session III Champerson. Dv2ch Boura
International appreciation of crystallography	L12 12
L3 7	Kvido Stříšovký
Imre Barák	Crystal structures of rhomboid intramembrane protease
User consortium of serial femtosecond crystallography -	bound to substrate peptides elucidate the basis of substrate specificity and mechanism (30')
Slovak involvement L4 8	L13 12
J. Dohnálek	David Kopečný
Methods of structural biology of Instruct available to	Family of plant nucleoside N-ribohydrolases
Czech researchers	L14 13
	Veronika Lišková
16:05 16:30 Coffee break	Engineering enzyme access tunnels for protein stabilization
1620 10000	L15 14
16:30 18:00 Session I chairperson: <i>Petr Novák</i>	Sergio Maques
L5 8	Investigation of gating mechanisms in the access tunnel of
Daniel Němeček	haloakane dehalogenases (30')
Application of Difference 3D Electron Microscopy to Identify DSS1 Subunits and Induced Conformational	12:10 13:30 Lunch
Changes in the Complex with Rad52	13:45 15:35 Session IV chairperson: <i>Daniel Němeček</i>
L6 9 Tanvir Shaikh	13.43 13.33 Session IV Champerson. Damet Ivemecek
Initial bridges between the two ribosomal subunits are	L16 15
formed within 9.4 milliseconds: A time-resolved cryo-EM	Moran Jerabek
study	MicroScale Thermophoresis: Interaction analysis and be-
L7 10	yond (30') L17 15
Z. Kukačka	Lucie Bednárová
Chemical Cross-linking and Hydrogen-Deuterium Exchange –Tools for Precise Definition of Human	Raman microspectroscopy of Candida albicans vacuoles
Haptoglobin Structure	L18 16
L8 10	Irena Kratochvílová
E. Bouřa	Theoretical and experimental study of charge transfer
Combination of Xtal, SAXS, DEER and FRET data – the	through DNA: impact of mercury attached to mismatched base pairs
structure of ESCRT-I/II supercomplex and implications for membrane budding (30')	vase pairs

18:00 21:00 Dinner



L19

Tatsiana Charnavets

Structure, stability and thermodynamic characteristics of single stranded DNA in repetitive extragenic palindromic elements

L20 17

Josef Houser

RSL lectin - a complex approach to study carbohy-drate-protein interaction

15:35 16:00 Coffee break

16:00 17:40 **Session V** chairperson: *Richard Hrabal*

L21 18

Matej Zábrady

Recombinant antibodies for in vivo applications

L22 18

Jakub Ptáček

Selection and characterization of Anticalins specific for human glutamate carboxypeptidase II

L23 19

Miroslava Kopecká

Role of EF-hand motif in the activation of neutral trehalase L24

Dalibor Kosek

Characterization of interactions between protein kinase ASK1 and its binding partners

L25 20

Ivana Nemčovičová

Cytomegalovirus gpUL141 exhibits unique receptor-binding domain to inhibit cell surface expression of CD155 and TRAIL death receptors

17:45 19:00 Dinner

20:00 21:00

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

20:15 22:45 **Poster Session**

Saturday, March 15

8:00 Breakfast

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9:15 10:45 **Session VI** chairperson: *Rüdiger Ettrich*

L26 21

Katsiaryna Tratsiak

Haloalkane dehalogenases: DmxA from *Marinobacter sp.* ELB 17 and DpcA from *Psychrobacter cryohalolentis* K5, from the crystallization to the structure analysis

L27 21

Radka Chaloupková

Comparison of catalytic performance of haloalkane dehalogenases in deep eutectic and organic co-solvents L28 22

Petra Szelcsányiová

Modification of substrate specificity and catalytic activity of haloalkane dehalogenase linb by opening de novo access tunnels

10:00 10:20 Coffee break

10:20 12:00 **SessionVII** chairperson: *Jiří Černý*

L29 23

Rüdiger Ettrich

Charybdotoxin unbinding from the mKv1.3 potassium channel: A Combined computational and experimental study (30')

L30 23

Saurabh Kumar Pandey

Binding competent states for L-arginine in E. coli arginine repressor apoprotein

L31 24

Hedi Hegyi

Domain Integrity Verification of Alternative Splicing - the DIVAS server

L32 24

Bohdan Schneider

Dynamics of biomolecules estimated by crystallographic B-factors (30')

12:00 12:05 Closing remarks

12:15 Lunch



POSTERS

P1	25	P12 32
Adriana Baumlová		Karla Fejfarová
Structural characterization of phosphatidylinositol 4-pl	10S-	Crystallization and preliminary X-ray diffraction analysis
phate IIalpha		of nepenthesin-1
phate Halpha		or neperioresia 1
P2	25	P13 32
Lada Biedermannová	23	Jan Frömmel
Hydration of amino acid residues in proteins: what car	1110	Aminoaldehyde dehydrogenase isoenzymes from <i>Pisum</i>
	ı wc	
learn from data mining?		sativum oxidize N-acylated aminoaldehydes
P3	26	P14 33
	26	
Kristýna Boušová	41	Pavel Grinkevich
Calmodulin and S100A1 protein interact with	tne	Structure and function of the C-terminal helical domain of
intracellular termini of the TRPM4 channel		the motor subunit HsdR from the type I restriction-modifi-
7.		cation system EcoR124I
P4	27	
Jiří Bufka		P15 33
Synthesis and Spectroscopy of Derivatives of the Fluo	res-	Dipanjan Guha
cent Protein Chromophore		Assembly and molecular architecture of the TSC1-TSC2
		complex
P5	27	
Zuzana Chromíková		P16 34
Crucial role of SpoIIE during Bacillus subtilis cell dif	fer-	Jiří Heller
entiation		Photosystem II PsbO protein from higher plants
P6	28	P17 34
Zdeněk Chval		Petr Hošek
Molecular dynamics calculations of Cy3 and Cy5 cyar	nine	Moving hills - new parallelizable metadynamic method
dyes terminally attached to DNA		with fixed amount of bias potential
ayes terminary accepted to DIVI		with fixed difficult of olds potential
P7	29	P18 35
Ladislav Csefalvay	2)	Dominik Hrebík
Purification and Initial Imaging of the type I DNA Res	tric	Interactions between receiver domain of cytokinin receptor
tion-Modification Enzyme EcoR124I by Elec		CKI1RD and AHP protein from <i>Arabidopsis thaliana</i>
Microscopy	uon	CKTIKD and ATTI protein from Arabidopsis indiana
Microscopy		P19 35
D0	20	
P8	30	Iulia Iermak
Oksana Degtjarik	D 0.6	Crystallization of glyceraldehyde dehydrogenase from
Crystallization and structural characterization of Lin	B86	Thermoplasma acidophilum
haloalkane dehalogenase mutant		700
70	• •	P20 36
P9	30	Michaela Jirků
Radka Dopitová		Characterization of the calmodulin and S100A1 binding
Crystal Structure of Phosphotransmitter AHP2 and Mo		domains on the N-terminus of TRPM1 receptor
ing of its Interaction with Sensor Histidine Kinase CK		
Towards Elucidating Molecular Recognition in	the	P21 36
Multistep Phosphorelay Signaling in Plants		Miroslava Kacířová
		Structural studies on Pdc/14-3-3 protein complex
P10	31	
David Dufour		P22 37
RNA structure prediction by knowledge-based statist	tical	Radka Končitíková
potentials and fragment assembly		Structure-function study on enzymes linked to cytokinin

31

P11 Olga Dvořáčková

Influence of the substitution effects in the pyridine ring on the reactivity of the trans-[Pt(NH3)2(pyr)Cl]+ complex

N-ribohydrolases

metabolism - aldehyde dehydrogenases and nucleoside

46

47

48

48



P23 38 P34 43 Daniel Pokorný

Tereza Kovaľová

Structural and catalytic properties of a-L-fucosidase from Paenibacillus thiaminolyticus

P24 38 P35 44

Daniela Krajčíková

Studies of Self-assembly Properties of Bacillus Spore Coat **Proteins**

P25 39 P36 45

Tomáš Kroupa

Interaction of M-PMV matrix protein mutants with membranes

P26 P37 39 45

Monika Krupová

Detection of Molecular Chirality in Lanthanide Complexes by the Raman Optical Activity

P27 40 P38 46

Ivana Kutá Smatanová

Protein crystallization projects at the Faculty of Science of the USB CB

EcoR124I P28 40

P39

folding

P41

ence

P42

P43

Zoran Šućur

well-tempered metadynamics

Tereza Skálová

Salome Kylarová

Structural characterization of the thioredoxin-binding domain of protein kinase ASK1 and its interaction with thioredoxin

P29 41 Vojtěch Spiwok

Lucie Marečková

KLK2- and KLK11-binding proteins as novel class of recombinant capture ligands useful for improved Prostate Cancer diagnostics

Jan Stránský 41

P30 Zora Nováková

The role of the non-pharmacophore pocket of glutamate carboxypeptidase II in the design of small-molecule inhibi-

Exploring free energy surface of oxytocin by using

42

Jiří Pavlíček

P31

Crystal structures of complexes of GCPII with P1'-diversified urea-based inhibitors

Ekaterina Tutubalina Crystallization of FrpC protein Neisseria

P32 42

Miroslav Peterek

Assembly and molecular architecture of PI4K IIalpha complexes

P33 43

Maria Plevaka

Crystallization and preliminary diffraction analysis of Dha57, DhaA80 and DhaA106 mutants from Rhodococcus rhodochrous NCIMB 13064

P44 49

Structural and functional characterization of Ralstonia

Structural analysis of a novel haloalkane dehalogenase

Molecular dynamics comparison of E. coli WrbA

Pump-probe molecular dynamics (PPMD) simulations in

Interdomain communication in the endonuclease/motor

subunit of Type I restriction-modification enzyme

Structures of receptors and ligands of mammalian NK cells

Enhancement of linear vs. non-linear motions in protein

Critical parameters for S-SAD phasing – real case experi-

GROMACS and its testing on the PDZ domain

DbeA from Bradyrhizobium elkanii USDA94

solanacearum lectin mutant

apoprotein and holoprotein

Katsiaryna Shamayeva

Tatyna Prudnikova

David Řeha

Leona Šerá

Petra Zadravec

meningitidis

Development of lactic acid bacterium capable of binding Shiga toxin on the surface

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Vojtěch Zapletal

NMR study of haloalkane dehalogenase DhaA: resonance assignment and relaxation