



PROGRAMME

Thursday, March 17

- 10:30 12:30 Registration at Nový Zámek
 12:30 13:30 Accommodation
 13:59 14:00 Opening of XIV Discussions
- 14:00 15:40 **Session I** chairperson: *Imrich Barák*
- L1 3
Lenka Rezabkova
 Structural basis of katanin function at microtubule minus end (30 min.)
- L2 3
David Kopečný
 Structure-function study on plant aldehyde dehydrogenase from moss *Physcomitrella patens*
- L3 4
Josef Houser
 Lectins with beta-propeller fold in opportunistic pathogens (30 min.)
- L4 5
Rostislav Škrabaňa
 Structural and binding properties of a quadruple epitope regulating tau protein oligomerization
- 15:40 16:00 *Coffee break*
- 16:00 18:00 **Session II** chairperson: *Lenka Rezabkova*
- L5 5
Imrich Barák
 Asymmetric cell division during sporulation in *Bacillus subtilis* (30 min.)
- L6 6
Tomáš Kroupa
 Interaction of the Mason-Pfizer monkey virus matrix protein and its budding deficient mutants with the plasma membrane
- L7 7
Ladislav Bumba
 Calcium-driven folding of RTX domain β -rolls ratchets translocation of RTX proteins through Type I secretion ducts (30 min.)
- L8 7
Lukáš Chrást
 Structure-function relationship of paradoxically thermostable haloalkane dehalogenase of psychrophilic origin
- L9 8
Phuong Pham Ngoc
 Development of new protein scaffolds for directed evolution
- 18:30 20:30 Dinner

Friday, March 18

- 7:30 8:45 Breakfast
- 9:00 10:40 **Session III** chairperson: *Jan Dohnálek*
- L10 9
Jiří Brynda
 Second generation of Carborane-Based Inhibitors of Carbonic Anhydrases
- L11 10
Leona Švecová
 X-ray structure of bilirubin oxidase from *Myrothecium verrucaria* with ligand in oxidation center
- L12 10
Ondřej Cehlár
 The conformation of proline rich segment of neuronal protein tau studied by the X-ray crystallography, molecular dynamics simulations and biophysical methods
- L13 11
Tomáš Koval'
 Active site promiscuity in the S1-P1 nuclease family
- L14 11
Martin Kubala
 Identification of the RH421-binding site on Na⁺/K⁺-ATPase
- 10:40 11:00 *Coffee break*
- 11:00 12:30 **Session IV** chairperson: *Frederic Vellieux*
- L15 12
Piotr Wardega
 Affinity. Stability. Conformation (30 min.)
- L16 13
Stanislav Kukla
 Ultrafiltration master class
- L17 14
Raul Gomez
 Microcalorimetry: A versatile tool for the characterization of biomolecular interactions
- L18 14
Vernon Smith
 State-of-the-Art Pixel array detectors for crystallography
- 12:30 14:00 Lunch
- 14:15 15:55 **Session V** chairperson: *Filip Lankaš*
- L19 15
Zuzana Dunajová
 Molecular dynamics simulations of the transport of ligands through pathways of haloalkane dehalogenases DhaAwt and DhaA31
- L20 16
Tomáš Dršata
 Computer simulations of nucleosome positioning and allosteric effects in DNA (30 min.)



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|--|----------------------------------|---|
| L21 | 17 | Saturday, March 19 |
| <i>Rüdiger Ettrich</i> | | |
| Cation translocation in human ORAI channels: Modeling and simulations (30 min.) | | 7:30 8:45 Breakfast |
| L22 | 17 | 9:00 10:30 Session VII |
| <i>Jiří Kozelka</i> | | chairperson: <i>Karel Kubiček</i> |
| Lone-pair- interactions in nucleic acids and proteins: physical origin and significance (30 min.) | | L28 21 |
| | | <i>Frederic Vellieux</i> |
| | | The Centre of Molecular Structure (IBT, CAS) at Biocev (30 min.) |
| 15:55 16:15 <i>Coffee break</i> | | L29 22 |
| | | <i>Irena Kratochvilová</i> |
| 16:00 18:00 Session VI | chairperson: <i>Jiří Kozelka</i> | Freezing process in human cell nuclei: determination of cryoprotectant parameters strongly influencing the cell condition |
| L23 | 18 | L30 22 |
| <i>Evžen Bouřa</i> | | <i>Lucie Bednářová</i> |
| Structural insights and in vitro reconstitution of membrane targeting and activation of human PI4KB by the ACBD3 protein (30 min.) | | Chiroptical properties of the antimicrobial peptide lasiocepsin and of its analogs |
| L24 | 19 | L31 23 |
| <i>Kvido Strišovský</i> | | <i>Olivie Petřivalská</i> |
| The ins and outs of membrane-immersed catalysis: structure, mechanism and inhibition of rhomboid intramembrane proteases | | Structural insight into the 14-3-3 protein-dependent inhibition of protein kinase ASK1 |
| L25 | 19 | 10:30 10:50 <i>Coffee break</i> |
| <i>Sergey Kalynych</i> | | 10:50 11:50 Session VII |
| Large motions of the protruding domain in a native iflavirus | | chairperson: <i>Irena Kratochvilová</i> |
| L26 | 20 | L32 24 |
| <i>Jiří Nováček</i> | | <i>Milan Zachrdla</i> |
| Structure and genome delivery mechanism of <i>Staphylococcus aureus</i> phage therapy agent phi812-K1 determined by cryo-electron microscopy | | Structure and Dynamics of Sigma Subunit of RNA Polymerase from <i>Bacillus subtilis</i> |
| L27 | 20 | L33 25 |
| <i>Tibor Füzik</i> | | <i>Pavel Brázda</i> |
| Structural study of Tick-borne encephalitis virus using cryo-electron microscopy | | Recognition of pTyr1-CTD by the elongation factor Spt6 |
| 18:30 19:45 Dinner | | 12:00 13:30 Lunch |
| 19:30 20:45 | | |
| General Assembly of the Czech Society for Structural Biology. Meeting will be held in the Czech and/or Slovak languages. | | |
| 21:00 23:00 Poster Session | | |



POSTERS

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|--|----|--|----|
| P1 | 26 | P13 | 32 |
| <i>Valery Andrushchenko</i> | | <i>Marie Hlavničková</i> | |
| Eu ³⁺ -induced DNA condensation and chirality transfer | | Inhibitory binders derived from ABD-domain scaffold targeting human IL-17RA receptor as an alternative for modulation of Th17-mediated pro-inflammatory axis | |
| P2 | 27 | P14 | 33 |
| <i>Borislav Angelov</i> | | <i>Zuzana Jaseňáková</i> | |
| Time-resolved crystallography of proteins at the laser driven X-ray sources in ELI beamlines | | Structural study of the intracellular domains of the ethylene receptor ETR1 from <i>Arabidopsis thaliana</i> | |
| P3 | 27 | P15 | 33 |
| <i>Cyril Bařinka</i> | | <i>Petr Jeřábek</i> | |
| Human histone deacetylase 6: profiling of deacylase specificity | | Structure and dynamics of the membrane-anchored cytochrome P450 1A2–cytochrome b5 complex | |
| P4 | 28 | P16 | 34 |
| <i>Jakub Benýšek</i> | | <i>Barbora Kalousková</i> | |
| Novel inhibition scaffolds targeting human cysteine cathepsins | | Preparation of human NK cell activation receptor NKp80 and its ligand aicl | |
| P5 | 28 | P17 | 35 |
| <i>Lada Biedermannová</i> | | <i>Palani Kirubakaran</i> | |
| Atlas of protein hydration – connecting information from crystallography and ab initio calculations | | Artificial proteins modulate allostery of PDZ3 and SH3 in two domains constructs. A computational characterization of novel chimeric proteins | |
| P6 | 29 | P18 | 35 |
| <i>Michal Buša</i> | | <i>Eva Krascenitsova</i> | |
| Functional characterisation of novel cysteine protease inhibitor from <i>Fasciola hepatica</i> | | How Min systems from <i>Clostridia</i> species helps to find the mid-cell site during cell division? | |
| P7 | 29 | P19 | 36 |
| <i>Jan Dohnálek</i> | | <i>Magdalena Krejčíková</i> | |
| Towards structure of HelD – a partner protein of RNAP in gram positive bacteria | | Structural details of the interaction between pTyr1-CTD and the elongation factor Spt6 | |
| P8 | 30 | P20 | 36 |
| <i>Pavla Fajtová</i> | | <i>Monika Krupová</i> | |
| Prolyl oligopeptidase from the blood fluke <i>Schistosoma mansoni</i> : designing active-site inhibitors with anti-schistosomal activity | | Tracking of protein folding by chiral spectroscopic methods | |
| P9 | 30 | P21 | 37 |
| <i>Tereza Gerguri</i> | | <i>Sudhir Kumar Pal</i> | |
| Novel structure of membrane nanodisc | | Structure and dynamics of the methyl-transferase subunit of the <i>E.coli</i> restriction-modification system EcoR124I | |
| P10 | 31 | P22 | 37 |
| <i>Mária Gondová</i> | | <i>Adrian Leontovyč</i> | |
| Crystal structure of honey bee hexamerin 70b at 3.2 Å resolution | | Towards structural characterization of SmSP2 protease from parasitic blood fluke <i>Schistosoma mansoni</i> | |
| P11 | 31 | P23 | 38 |
| <i>Eva Hájková</i> | | <i>Petr Louša</i> | |
| Nucleoside N-ribohydrolases and adenosine kinases in maize (<i>Zea mays</i>) | | The kinetics of phosphorylation of tyrosine hydroxylase and its interaction with 14-3-3 zeta protein studied by NMR | |
| P12 | 32 | | |
| <i>Jiří Hausner</i> | | | |
| Dynamics of CIC-ec1 D417C mutant form studied by hydrogen/deuterium exchange | | | |



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|---|----|--|----|
| P24 | 38 | P36 | 46 |
| <i>Václav Mareška</i> | | <i>Marek Šebela</i> | |
| Electronic sculpting of AT2R ligands by metadynamics | | Oligonucleotide analysis and sequencing using MALDI-TOF mass spectrometry | |
| P25 | 39 | P37 | 46 |
| <i>Sara Matič</i> | | <i>Jan Šilhan</i> | |
| Computational study of specific ion effect on the graphene oxide surface | | Structural study of the reaction mechanism of 3' DNA phosphatase from <i>Neisseria meningitidis</i> | |
| P26 | 39 | P38 | 47 |
| <i>Kateřina Mudroňová</i> | | <i>Ondřej Škořepa</i> | |
| Effect of the ribose versus 2'-deoxyribose residue in guanosine-5'-monophosphates on the formation of G-quartets stabilized by K ⁺ and Na ⁺ | | Recombinant expression of rat natural killer cell inhibitory receptors NKRP1B-Clrb | |
| P27 | 41 | P39 | 47 |
| <i>Ivana Nemčovičová</i> | | <i>Vojtěch Spiwok</i> | |
| Characterization of a novel bidirectional NK activating ligand CD160 | | Moving Hills method | |
| P28 | 41 | P40 | 48 |
| <i>Joanna Oniskiewicz</i> | | <i>Jaroslav Srp</i> | |
| Recognition of different methylation states on histone H3 lysine 4 by Set3 protein | | Crystal structure of plant defense protein in complex with serine protease | |
| P29 | 42 | P41 | 48 |
| <i>Markéta Pazderková</i> | | <i>Jan Stránský</i> | |
| Spectroscopic study of protein fibrils | | A parameter of diffraction experiment with low attention: exposure | |
| P30 | 42 | P42 | 49 |
| <i>Samuel Pažický</i> | | <i>Ekaterina Sviridova</i> | |
| Relation of NKp30 glycosylation and C-terminal chain length to its structure | | Integrated structural biology study of the FrpD protein from <i>Neisseria meningitidis</i> | |
| P31 | 43 | P43 | 49 |
| <i>Václav Profant</i> | | <i>Katsiaryna Tratsiak</i> | |
| ROA study of chondroitin sulphate | | Structure-functional analysis of the α/β -hydrolase fold superfamily member | |
| P32 | 44 | P44 | 50 |
| <i>Tatyana Prudnikova</i> | | <i>Zuzana Trošanová</i> | |
| Structure-functional characterization of haloalkane dehalogenases | | Solvation of engrailed homeodomain mutant K52E | |
| P33 | 44 | P45 | 51 |
| <i>Katarína Pšenáková</i> | | <i>Ondřej Vaněk</i> | |
| Role of Cys residues on the stability of the complex between protein kinase ASK1 and thioredoxin | | Production of readily crystallizable glycoproteins in HEK293S GnTI cell line: A case study of human natural killer receptors | |
| P34 | 45 | P46 | 53 |
| <i>Jakub Ptáček</i> | | <i>Jiří Zahradník</i> | |
| Calcium ion is required for proper folding, dimerization and enzymatic activity of human glutamate carboxypeptidase II | | Structural study of the intracellular domains of the ethylene receptor ETR1 from <i>Arabidopsis thaliana</i> | |
| P35 | 45 | P47 | 52 |
| <i>David Řeha</i> | | <i>Vojtěch Zapletal</i> | |
| Theoretical study of crystal structure of WrbA from <i>E. coli</i> in complex with benzoquinone using QM calculations of charge transfer rates | | Comparison of computational and experimental results for intrinsically disordered proteins (IDPs) | |



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|---|----|---|----|
| P48 | 53 | P50 | 54 |
| <i>Nina Zemanová</i> | | <i>Lucie Zimová</i> | |
| Structural and biophysical characterization of the projection domain of neuronal tau protein | | The role of the S1-S4 sensor domain in the activation and modulation of the TRPA1 ion channel | |
| P49 | 54 | | |
| <i>Hana Zigová</i> | | | |
| Improved interpretation of 14-3-3 fluorescence measurements by molecular dynamics simulations | | | |

Author Index

| | | | | | |
|-------------------|------------------------|------------------|----------------|--------------------|--------------------|
| Adam, M. | 14 | Dunajová, Z. | 15 | Klíma, M. | 18 |
| Akhmanova, A. | 3 | Durst, R. | 14 | Klímová, N. | 7 |
| Andreasson, J. | 27 | Dušková, J. | 11 | Kloz, M. | 27 |
| Andrushchenko, V. | 26, 36 | Dvorský, R. | 10 | Kolářová, L. | 8 |
| Angelov, B. | 27 | Dvořák, J. | 30, 37 | Kolenko, P. | 11, 48, 52 |
| Baldwin, G.S. | 46 | Ettrich, R. | 17, 37, 45 | Komárek, J. | 4 |
| Balla, T. | 18 | Fábry, M. | 9 | Končítíková, R. | 3, 31 |
| Barák, I. | 5, 35 | Fajtová, P. | 30 | Kontseková, E. | 5 |
| Barvík, I. | 54 | Falk, M. | 22 | Kopečná, M. | 3 |
| Bařinka, C. | 7, 27, 45 | Fejfarová, K. | 11 | Kopečný, D. | 3, 31 |
| Baumlová, A. | 18 | Filipčík, P. | 5 | Kosek, D. | 23, 44 |
| Baumruk, V. | 22, 42, 43 | Florián, J. | 33 | Kouřil, Š. | 46 |
| Bazgier, V. | 11 | Formanová, P. | 20 | Kovačech, B. | 5 |
| Bazzi, S. | 17 | Freemont, P.S. | 46 | Koval, T. | 10, 11, 29 |
| Bednářová, L. | 7, 22 | Frischauf, I. | 17 | Kovářová, Z. | 28 |
| Benešik, M. | 20 | Fűzik, T. | 20 | Kozelka, J. | 17, 50 |
| Benýšek, J. | 28 | Gerguri, T. | 30 | Kralovičová, J. | 5 |
| Berka, K. | 11 | Golan, M. | 22 | Krascsenitsová, E. | 35 |
| Biedermannová, L. | 8, 28 | Gondová, M. | 31 | Kratochvílová, I. | 22 |
| Bíbová, I. | 7 | Goméz, R.P. | 14 | Králová, B. | 38 |
| Bláha, J. | 34, 42, 47, 51 | Grűner, B. | 9 | Krásný, L. | 24, 29 |
| Bouř, P. | 26, 36, 43 | Hajková, E. | 31 | Krejčíková, M. | 36 |
| Bouřa, E. | 18 | Halada, P. | 29 | Kroupa, T. | 6 |
| Brázda, P. | 25, 36 | Harlos, K. | 51 | Krupová, M. | 36 |
| Brezovský, J. | 7, 15 | Hašek, J. | 11 | Kubala, M. | 11 |
| Briozzo, P. | 3 | Hausner, J. | 32 | Kubáň, V. | 52 |
| Brynda, J. | 9, 28 | Hejátko, J. | 33 | Kubiček, K. | 25, 36 |
| Bumba, L. | 7, 49 | Herman, P. | 23 | Kukačka, Z. | 23 |
| Buratowski, S. | 41 | Hexnerová, R. | 18 | Kukla, S. | 13 |
| Buša, M. | 28, 29 | Hlavničková, M. | 32 | Kuchař, M. | 32 |
| Caffrey, C.R. | 30 | Horn, M. | 28, 30, 37, 48 | Kumar, A. | 4 |
| Capitani, G. | 3 | Houser, J. | 4 | Kumar Pal, S. | 37 |
| Carrey, J. | 45 | Hrabal, R. | 6 | Kutá Smatanová, I. | 7, 44, 45, 49 |
| Cehlár, O. | 5, 10, 53 | Hradílek, M. | 30 | Kutil, Z. | 27 |
| Chaloupková, R. | 7, 49 | Hritz, J. | 38, 52, 53 | Kutý, M. | 44, 45, 49 |
| Chalupská, D. | 18 | Huličiak, M. | 11 | Kúdelová, M. | 41 |
| Charvanets, T. | 21 | Humpolíčková, J. | 18 | Kylarova, S. | 44 |
| Chrást, L. | 7, 49 | Hýlová, A. | 3 | Kyslík, P. | 52 |
| Chromíková, Z. | 5 | Hynková, A. | 54 | Kyslíková, E. | 52 |
| Cígler, P. | 9 | Iermak, I. | 44 | Labajová, N. | 35 |
| Cramer, P. | 25, 36 | Jančaříková, G. | 4 | Lankaš, F. | 16 |
| Černý, J. | 8, 28, 52 | Jamroškovíc, J. | 35 | Lednev, I.K. | 42 |
| Dalton, J. | 29 | Jansen, S. | 50 | Lehmbeck, J. | 11 |
| Damborský, J. | 7, 15, 49 | Janubová, M. | 10, 53 | Leontovyč, A. | 37 |
| Daniel, L. | 7 | Jaseňáková, Z. | 33 | Levdansky, Y. | 19 |
| Degtjarik, O. | 44, 45, 49 | Jeřábek, P. | 33 | Louša, P. | 38, 52 |
| Dejmková, E. | 41 | Jiang, K. | 3 | Macek, P. | 7 |
| De Miranda, J. | 19 | Jílková, A. | 30 | Magnani, F. | 38 |
| Demo, G. | 4 | Kachala, M. | 7 | Makroczyová, J. | 35 |
| Derler, I. | 17 | Kalousková, B. | 34, 42, 51 | Maloň, P. | 22 |
| Dohnálek, J. | 10, 11, 21, 29, 48, 51 | Kalynych, S. | 19 | Malý, P. | 32 |
| Doškař, J. | 20 | Kammerer, R.A. | 3 | Man, P. | 18, 32 |
| Dršata, T. | 16 | Kavan, D. | 32 | Marečková, L. | 32 |
| Dubánková, A. | 18 | Keredche, S. | 42 | Marek, R. | 17 |
| Dukor, R.K. | 42 | Kirubakaran, P. | 35 | Mareš, M. | 28, 29, 30, 37, 48 |