



PROGRAMME

Thursday, March 29

- 12:00 - 14:00 Registration
- 14:15 - 14:20 Introductory remarks
- 14:20 - 15:20 **Lecture session I**, chairperson: *P. Řezáčová*
 L1 p. 14
Pavel Plevka
 The Structure of Ryegrass Mottle Virus
- L2 p. 14
Petr Kolenko
 Crystallographic studies of intermolecular interactions of Fc-fragment of immunoglobulin
- L3 p. 15
Michal Kolář
 Protein as a Flexible Structure: Case Study of the HIV Pro-
 tease
- 15:20 - 15:30 Coffee break
- 15:30 - 16:20 **Lecture session II**, chairperson: *P. Řezáčová*
 L4 p. 15
Jiří Brynda
 TLS analysis of antibody structure shows stabilization by
 epitope binding
- L5 p. 16
Tomáš Obšil
 Interaction of DNA-binding domain of transcription factor
 FoxO4 with DNA
- 16:20 - 16:30 Coffee break
- 16:30 - 17:05 **Plenary lecture I**, chairperson: *B. Schneider*
 L6 p. 17
Filip Lankaš
 Structural mechanics of DNA: from atomic scale to
 bioinformatics
- 17:05 - 17:15 Coffee break
- 17:45 - 18:15 **Plenary lecture II**, chairperson: *J. Hašek*
 L7 p. 18
Tomáš Polívka
 Time-resolved structural dynamics - A challenge for future
- 18:00 - 19:00
 Concert of violin duo Lukáš Kuta & Václav Polívka
 J.M Leclair, J.S. Bach, S. Prokofjev and others
Detailed program will be available on registration desk
- 19:00 - 22:30 Banquet

Friday, March 30

- 7:00 - 8:45 Breakfast
- 9:00 - 10:50 **Lecture session III**, chairperson: *R. Hrabal*
 L8 p. 18
Lukáš Židek
 Orientational restraints in NMR structure determination
- L9 p. 19
Pavel Srb
 Is local flexibility of M-PMV matrix protein related to its
 binding affinity with a molecular motor?
- L10 p. 19
Richard Štefl
 RNA recognition by the ADAR2 dsRBMs: a 50 kDa pro-
 tein-RNA complex by NMRL8
- L11 p. 20
Vladimír Sychrovský
 Calculation of Scalar Couplings in the Backbone of Nu-
 cleic Acid
- 10:50 - 11:00 Coffee break
- 11:00 - 12:20 **Lecture session IV**, chairperson: *L. Židek*
 L12 p. 20
Zuzana Vokáčová
 Theoretical NMR Study of Watson-Crick/Sugar Edge
 RNA Base Pair Family
- L13 p. 21
Jaroslav Burda
 Computational study on spectral properties of the selected
 pigments from various photosystems; structure--transition
 energy relationship
- L14 p. 21
Jiří Mrázek
 Electronic structure of the non-heme iron center in
 photosynthetic apparatus of plants and bacteria. Computa-
 tional DFT study
- L15 p. 22
Tomáš Zimmerman
 Computational study of cysteine and methionine interac-
 tion with platinum(II) complexes in water
- 12:30 - 14:00 Lunch
- 14:00 - 15:20 **Lecture session V**, chairperson: *J. Pačes*
 L16 p. 22
Jan Adam
 Computational chemistry as a helpful tool for struc-
 ture-functional study and correlation, en route to protein
 engineering
- L17 p. 23
Rudiger Ettrich
 Structure and dynamics of the oxygen evolving complex of
 photosystem II: Role of the N-terminal loop
- L18 p. 23
Ondřej Šulák
 New approaches to structure and function studies of
 RS20L lectin from *Ralstonia solanacearum*



L19 <i>Navnit Mishra</i> Computational Studies on PA-IIL Lectin-Carbohydrate Interactions 15:20 - 15:30 Coffee break 15:30 - 17:25 Lecture session VI chairperson: <i>I. Kratochvilová</i> L20 <i>Bohdan Schneider</i> Conformational space of nucleic acids L21 <i>Dana Nachtigallová</i> Electronic coupling in the excited electronic state of stacked DNA bases L22 <i>Dalibor Štys</i> Mathematically-based studies of complex systems in physics, mathematics, chemistry, biology, economy and politics in Nove Hradý in the first half of 19th century and at the beginning of 21st century <i>Radomír Kužel</i> : Forthcoming meetings of the Czech and Slovak Crystallographic Association - short information. Correct typesetting of papers - general rules on correct typing and writing references. Future evaluation of publications. <i>Peter Šebo</i> Progress in building if the Biotechnology center in Vestec 17:30 - 18:30 Dinner 19:00 - 22:00 Poster session	p. 24	Saturday, March 31 7:00 - 9:10 Breakfast 9:15 - 10:15 Lecture session VII chairperson: <i>R. Zika</i> L23 <i>Irena Kratochvilová</i> New principle of the molecular photo-FET L24 <i>Jan Pačes</i> CHIPAS, Tool for ChIPonChip analysis L25 <i>Eva Brumovská</i> Structural and functional characterization of human protein kinase CKI epsilon 10:15 - 10:30 Coffee break 10:30 - 11:40 Lecture session VIII , chairperson: <i>T. Obšil</i> L2 <i>Jan Dohnálek</i> Subtilases and metal binding - the weak binding site of subtilisins revisited L27 <i>Jindřich Hašek</i> Ligand docking to biochemical targets - crystallography and modeling L28 <i>Pavčina Řezáčová</i> Structural studies of the repressor CggR from <i>Bacillus subtilis</i> 11:40 - 12:00 Concluding remarks 12:00 - 13:00 Lunch
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POSTERS

P1 <i>L. Benda</i> Calculation of the Effective Chemical Shielding Anisotropy in L-Alanyl-L-alanine, conformational and charge dependence study P2 <i>I. Beššeová</i> Computational simulations study of Helixes 90-92 P3 <i>E. Bouřa</i> Crystal structure of RGS3 RGS domain P4 <i>L. Bumba</i> Cryo-scanning electron microscopy of Bordetella pertussis adenylate cyclase toxin embedded in lipid vesicles	p. 31	P5 <i>J. Chmelík</i> Structure of <i>Bombyx mori</i> Chemosensory Protein 1 in Solution P6 <i>E. Fadrná</i> Computational study of restriction endonuclease hincii P7 <i>Z. Futera</i> Computational Study on Ruthenium(II) Complexes and their Interactions with NA bases P8 <i>L. Gorčík</i> NMR study of protein CD6	p. 33
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P9 <i>L. Gryčová</i> Lys735 participates on the ATP binding to the isolated C-terminus TRPV1	p. 34	P21 <i>J. Matulová</i> A cost-effective approach for amino-acid-type selective isotope labeling of proteins expressed in <i>Leishmania tarentolae</i>	p. 41
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