

Monday May 23, 2016

8:30 – 9:00 Register at Mehmet Akif Ersoy Hall

Morning Session:

9:00 – 9:30 Alexander Schug (Invited Talk)

Protein and RNA structure prediction by integration of co-evolutionary information into molecular simulation

9:30 – 10:00 Sebastian Kmiecik (Invited Talk)

CABS-dock web server for protein-peptide docking with significant structural flexibility

10:00 – 10:30 Break

10:30 – 11:00 Turgut Baştuğ (Invited Talk)

Recent developments in calculation of free energies in biological systems

11:00 – 11:30 Maciej Blaszczyk (CBSB2016 Outstanding Young Researcher)

Modeling of protein-peptide interactions using the CABS-dock web server for binding site search and flexible docking

11:30 – 12:00 Panel Discussion

12:00 – 13:30 Lunch

Afternoon Session

13:30 – 14:00 Wolfhard Janke (Invited Talk)

Knots as Stable Order Parameter for Semiflexible Polymers

14:00 – 14:30 Giovanni La Penna (Invited Talk)

Probing copper catalysis in biology with multiple simulations

14:30 – 15:00	Break
15:00 – 15:30	Şahin Büyükdağlı (Invited Talk) Electrostatic interactions in polymer translocation through nanopores
15:30 – 16:00	Bogdan Lesyng (Invited Talk) Simulations and analysis of fret processes in (bio)molecular systems using a QM-MD approach
16:00 – 16:20	Murat Çavuş (Contributed Talk) Free energy calculation for navab channel with no equilibrium requirement
16:20 – 16:50	Panel Discussion
16:50 – 18:00	Poster Session

Tuesday May 24, 2016

Morning Session

9:00 – 9:30	Canan Atılgan (Invited Talk) Molecular level strategies for the assesment of drug resistance in bacteria
9:30 – 10:00	Adam Sieradzan (Invited Talk) What make tellomers unique?
10:00 – 10:30	Break
10:30 – 11:00	Haleh Abdizadeh (CBSB2016 Outstanding Young Researcher) Multiple computational approaches disclose principles underlying human serum transferrin functioning

11:00 – 11:30 Sofia Piepoli (CBSB2016 Outstanding Young Researcher)
Analysis on target specific transcription activator-like effectors by perturbation-response scanning and free energy calculations

11:30 – 12:00 Panel Discussion

12:00 – 13:30 Lunch

Afternoon Session

13:30 – 14:00 Franklin Hays (Invited Talk)

Imatinib binding to human c-Src is coupled to inter-domain allostery and suggests a novel kinase inhibition strategy

14:00 – 14:30 M. Wiśniewska (CBSB2016 Outstanding Young Researcher)

Hydration effects in protein kinases

14:30 – 15:00 Break

15:00 – 15:30 Caroline Ross (CBSB2016 Outstanding Young Researcher)

Structural-based prediction of novel linear b-cell epitopes in picornaviruses

15:30 – 15:50 Tandıç F. Güçlü (Contributed Talk)

Centrality of residues and redundancies in their communication explain the disruptive mutations in DHFR

15:50 – 16:10 Gökşin Liu (Contributed Talk)

Iron and synergistic anion binding specificity of haemophilus influenzae ferric binding protein

16:10 – 16:40 Panel Discussion

19:00 – 21:00 Conference dinner at Beyaz Ev

Wednesday May 25, 2016

Morning Session

- | | |
|---------------|--|
| 9:00 – 9:30 | Ulrich H.E. Hansmann (Invited Talk)

Generalized-Ensemble Sampling and Modeling of Protein Aggregation |
| 9:30 – 10:00 | Emre Taşcı (Invited Talk)

Going from bottom to top and relating the intermediates: Applications of computational group theory |
| 10:00 – 10:30 | Break |
| 10:30 – 10:50 | Emine Deniz Tekin (Contributed Talk)

Self-assembled peptide amphiphiles with molecular dynamics simulations |
| 10:50 – 11:10 | Meral Eryürek (Contributed Talk)

Microcanonical molecular dynamics study of melting of small Pt clusters |
| 11:10 – 11:30 | Parting Words |

Conference ends