CECAM Workshop
Free energy calculations: From theory to applications
Poster session

Arash Azari

Dynamical properties of the solution environment near the microtubule surface and their implication to the interaction with motor proteins.

◆◆◆◆◆◆◆

Luciana Capece

Molecular insights of heme proteins by means of free energy calculations

◆◆◆◆◆◆◆

Pragya Chohan

Exploring the energetic barriers to transport of hydrophobic solutes across the outer membranes of Gram-negative bacteria.

◆◆◆◆◆◆◆

Rob Horton

Towards an efficient method of calculating free energies of charged systems.

◆◆◆◆◆◆◆

Anela Ivanova

Aggregation Patterns of Dodecyl Oligo(ethylene glycol) Dimers in Aqueous Solution

◆◆◆◆◆◆◆

Gavin Melaugh

Liquids with Intrinsic Micro-Porosity

◆◆◆◆◆◆◆

Mauro Lorenzo Mugnai

Retaining the self-interactions in thermodynamic cycles using dual topology: a proof and a comprehensive test

◆◆◆◆◆◆◆

Wojtek Plazinski

The dynamics of calcium binding by alginates. Application of the transition path sampling method.

◆◆◆◆◆◆◆

Vasileios Tatsis

Classical Molecular Dynamics at constant pH. Applications to peptides immersed in explicit solvent.

⬩⬩⬩◆⬩⬩⬩

Kanin Wichapong

Binding Free Energy Calculation for Predicting Binding Affinities of Kinase Inhibitors

⬩⬩⬩◆⬩⬩⬩

Yoshiteru Yonetani

Free energy profiles for DNA-protein dissociation: Adaptive biasing force calculation

⬩⬩⬩◆⬩⬩⬩

Tsvetan Zahariev

Theoretical Assessment of C12E3 Propensity to Aggregation

⬩⬩⬩◆⬩⬩⬩