

HP-SEE User Forum 2012, Belgrade

Friday 19 October 2012

Computational Chemistry Session 2 (12:00-14:30)

-Conveners: Nenad Vukmirovic

time	[id] title	presenter
12:00	[1] Design of novel nano-photonics materials	Dr PAPAPOPOULOS, Manthos
12:30	[31] Efficient Parallel Simulations of Large-Ring Cyclodextrins on HPC cluster	Dr ATANASSOV, Emanouil
13:00	[17] Free-energy surfaces of 2-[(carboxymethyl)sulfanyl]-4-oxo-4-arylbutanoic acids. Molecular dynamics study in explicit solvents.	DRAKULIC, Branko
13:30	[27] Investigations of biomolecular systems within the ISyMAB simulation framework	Mr VASILE, Ionut
14:00	[24] In the search of the HDAC-1 inhibitors. The preliminary results of ligand based virtual screening.	Mr ILIJA N., Cvijetić