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22. Marta 2009. će održati workshop

"VEGA ZZ: A Versatile Toolkit for Drug Design"



10.30-12.30 – Uvodno predavanje, Sala za sednice Hemijskog fakulteta u Beogradu

(Visualization modes and atom selections, Measure of geometric properties, 2D and 3D molecular editors, Use of the solvent clusters, Counterion placement, File format conversion, Management of molecule databases, Analysis and visualization of the surface properties, Molecular similarity, Analysis of the protein structure, Molecular mechanics calculations (energy minimization, conformational search and molecular dynamics))

14.30-17.30 – Praktični deo, računarska učionica Hemijskog fakulteta u Beogradu

(Okvirno: Molecule editing, Structure optimisation, Conformational search, Molecular dynamics and result analysis, Surface analysis, Structure-based virtual screening)

Predavanje i praktični deo će biti izlagani na engleskom jeziku. Pored toga je potrebno elementarno poznavanje upotrebe programa za crtanje hemijskih formula. Ulaz slobodan.