KEMIJSKI INŠTITUT

Vabilo na Forum40 / Invitation to the Forum40

dr. Janez Konc

D17, Department of Molecular Modeling

Četrtek / Thursday, 16.11.2017 ob / at 13:00

Velika predavalnica Kemijskega inštituta/ Great Lecture Hall, National Institute of Chemistry; Hajdrihova 19, Ljubljana

Protein-ligand binding sites comparison in drug discovery

We have developed new computational tools for protein-ligand binding prediction in drug discovery, based on graph theoretical approaches, combined with molecular simulations. We extended these approaches with genomic sequence variants information mapped to protein binding sites and with detection of conserved water sites in the novel GenProBiS and ProBiS H2O web servers. GenProBiS allows suggestion of functional effects of mutations on ligand binding and represents a key tool in drug discovery and personalized medicine. ProBiS H2O web server detects conserved water molecules that are important in ligand binding applied in drug development.

Vljudno vabljeni / Kindly invited