N. Derevianko [1], A. Redaelli [2], A. Gautieri [2]

Flexible protein-ligand docking: preliminary results

[1] *Institute of Mathematics of NAS of Ukraine, Kyiv, Ukraine*
[2] *Department of Electronics, Information and Bioengineering, Politecnico di Milano, Milan, Italy*

We are working on development of new software for the protein-ligand docking. The scoring function is defined by using Lennard-Jones and Coulombic potentials. We consider two approaches: classical approach when protein is treated as rigit and ligand as flexible molecules and other approach when both protein and ligand are treated as flexible molecules. In addition, in both cases ligand has flexible torsion bonds. Preliminary results will be presented.