Postgraduate student: **Fytros Marios**

Thesis Title:

Computational evaluation of potential binding molecules to protein targets with geometric criteria

Abstract:

The docking study of small molecules, mainly in organic compounds, to cavities or to binding sites of macromolecules (proteins), with computational methods (in silico) is a fundamental question of drug design and one of the main problems in contemporary structural bioinformatics. The docking of small molecule compounds (potential drug) is determined by the geometrical complementarity with the binding site (e.g. the catalytic site of the enzyme). Docking is distinguished in the following stages: (1) Identifying the binding sites (enzyme active site or other cavities of interest) of the macromolecule. The receptor is composed of amino acids that make up the binding site. (2) Searching for ligands that match with geometric criteria with the binding sites. (3) Evaluating (scoring) the energy of formation for each complex to succeed in minimization. Our work focused on (3), developing a Protein-Ligand docking algorithm with graphical methods in order to calculate the geometrical complementarity of the two molecules. In addition, we compared our algorithm to existing docking software which tries to solve the same problem.

SUBJECT AREA: Protein Docking

KEYWORDS: Protein Docking, Graphics, Enhanced Simulated Annealing, Geometry, Shape Complementarity, Binding Sites, PDB

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