Abstract

METHOD AND APPARATUS FOR COMPUTER AUTOMATED DETECTION OF PROTEIN AND NUCLEIC ACID TARGETS OF A CHEMICAL COMPOUND

A method and apparatus are disclosed for computer-automated detection of putative protein and nucleic acid targets of a chemical compound. The disclosed method and apparatus have potential applications in identification of unknown or secondary therapeutic targets and targets related to side-effect and toxicity of drugs, lead compounds or natural products. A ligand-biomolecule inverse-docking approach is disclosed as the method for finding putative targets, which searches a biomolecular cavity database to find protein and nucleic acid cavities that a chemical compound can be docked into. Docking is by shape-matching between a chemical compound (in single or multiple conformations) and a cavity model (a sphere cluster) using a disclosed vector-vector matching algorithm. Docked ligand-biomolecule structures are subject to conformation optimization. Putative targets are selected by evaluation of both ligand-biomolecule interaction energy and binding competitiveness against known binders. A method is also disclosed for computer-automated generation of a biomolecular cavity database from protein and nucleic acid 3D structure database.

(Figure 1 is to be published)

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