Computer Applications

Theories and Applications

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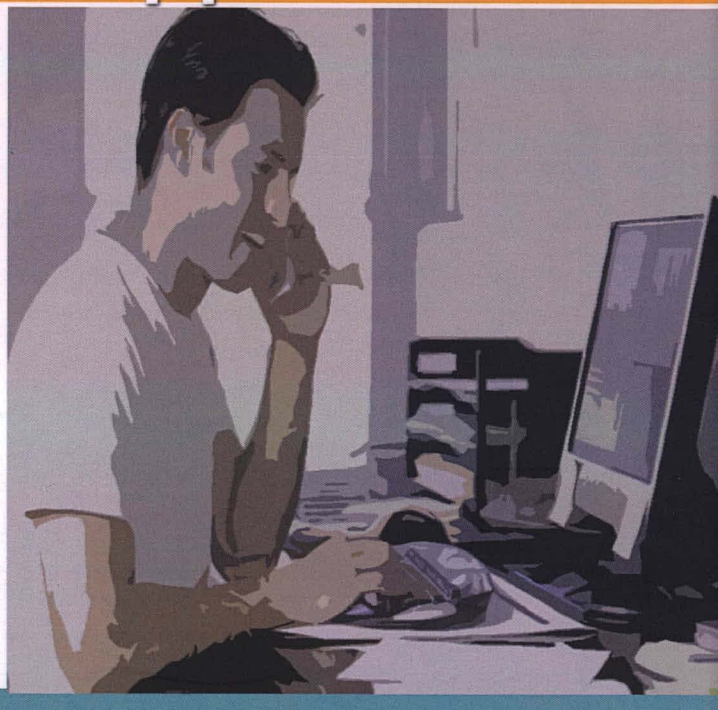

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2. In-Silico Drug Target Design & Its Approaches

Hassen Mohammed Abduallah Alsafi, Imad Fakhri Taha Al-Shaikhli, Asadullah Shah

ABSTRACT

Drug design and drug discovery are critical importance aspects in human life. Its successes rate depends on the depth understanding in the biological and chemical research employing computational approach. The main objective of studying rational drug design is to identify a key drug target based on a thorough understanding the structure of drugs. The pharmacophore expresses constraints on the 3D structure of the molecule by using certain techniques and software. In order to optimize the search, genetic algorithm has been implemented and used in some docking software's. It plays essential roles in the field of rational drug design. Moreover, it demonstrates their suitability in a variety of areas, including *quantitative structure-activity relationships* (QSARs) and variable selection, conformation searching, receptor docking, receptor and pharmacophore elucidation,