Current Drug Targets

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Computer Aided Drug Design for Multi-Target Drug Design: SAR /QSAR, Molecular Docking and Pharmacophore Methods

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Graphical Abstract:
Abstract:
Multi-target drugs against particular multiple targets get better protection, resistance profiles and curative influence by cooperative rules of a key beneficial target with resistance behavior and compensatory elements. Computational techniques can assist us in the efforts to design novel drugs (ligands) with a preferred bioactivity outline and alternative bioactive molecules at an early stage. A number of in silico methods have been explored extensively in order to facilitate the investigation of individual target agents and to propose a selective drug. A different, progressively more significant field which is used to predict the bioactivity of chemical compounds is the data mining method. Some of the previously mentioned methods have been investigated for multi-target drug design (MTDD) to find drug leads interact simultaneously with multiple targets. Several cheminformatics methods and structure-based approaches try to extract information from units working cooperatively in a biomolecular system to fulfill their task. To dominate the difficulties of the experimental specification of ligand-target structures, rational methods, namely molecular docking, SAR and QSAR are vital substitutes to obtain knowledge for each structure in atomic insight. These procedures are logically successful for the prediction of binding affinity and have shown promising potential in facilitating MTDD. Here, we review some of the important features of the multi-target therapeutics discoveries using the computational approach, highlighting the SAR, QSAR, docking and pharmacophore methods to discover interactions between drug-target that could be leveraged for curative benefits. A summary of each, followed by examples of its applications in drug design has been provided. Computational efficiency of each method has been represented according to its main strengths and limitations.

Keywords: Multi-target, drug design, in silico, SAR, QSAR, molecular docking.
We recommend

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