Computational methods for drug discovery and personalized medication

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Abstract: Advanced computational methods have received wide attention in recent years due to its several applications relating to healthcare for opening new directions in the area of diagnostics and drug discovery including vaccine for unforeseen viruses. The drug discovery involves identifying a ligand that can optimally fit to a definite cavity on a target protein. The drug discovery has speeded up its process with advanced computational methods effectively. An enhanced quality of software and computational tools enables to reduce the drug discovery cycle. The bioinformatics research made available a noteworthy volume of data sources. This paper gives an overview of computational methods and databases that helps in acceleration of drug discovery and personalized medication.

Keywords: *Drug discovery, personalized medication, computational methods, Bioinformatics, molecular docking, deep learning.*

1. Introduction

The complexity in drug discovery needs combined effort to design effective drugs. In drug design it is required to detect a ligand that can fit effectively to a specific cavity on a targeted protein [1]. The traditional drug discovery methods take long process cycle with considerable cost. Current methods that utilize computational methods in structure-based drug design has improved the speed in the process of drug discovery effectively. An enhanced quality of software and computational tools enables to reduce the drug discovery cycle thus making more cost-effective.

The bioinformatics research made available a noteworthy volume of data sources that required in various phases of drug discovery and development pipeline. Some of the public databases that provide the biomolecular information are GenBank, PDB, SWISS-PROT, PIR, SCOP and CATH etc. The informatics practice tools like BLAST, FASTA and CLUSTALW perform sequence analysis using these databases. Further the molecular structures are visualized using software like Rasmol. PyMOL, UCSF Chimera etc.

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