CONFERENCE ABSTRACT

ISSN (O): 2349-5332
CODEN: IRJPHY

COMPUTER AIDED DRUG DESIGN- A REVIEW

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ABSTRACT

Drug discovery and developing a new medicine is a long, complex, costly and highly risky process that has few peers in the commercial world. This is why computer-aided drug design (CADD) approaches are being widely used in the pharmaceutical industry to accelerate the process. The cost benefit of using computational tools in the lead optimization phase of drug development is substantial. On an average, it takes 10-15 years and US $500-800 million to introduce a drug into the market, with synthesis and testing of lead analogs being a large contributor to that sum. Therefore, it is beneficial to apply computational tools in hit-to-lead optimization to cover a wider chemical space while reducing the number of compounds that must be synthesized and tested in vitro. The computational optimization of a hit compound involves a structure-based analysis of docking poses and energy profiles for hit analogs, ligand-based screening for compounds with similar chemical structure or improved predicted biological activity

KEYWORDS:lead analogs, ligand, computer-aided, docking poses.

Indian Research Journal of Pharmacy and Science; 24(2020)2150;
Journal Home Page: https://www.irjps.in