Construction of marine compound library.

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ABSTRACT

The Computer-aided drug design technologies appeared poised to deliver diverse lead compounds for any biological target. Specifically, the present study targeted the marine compound and their analogs through Computer-aided drug design method and led to the discovery of marine compound library.The marine pharmacy currently holds more than 35,054 marine-derived biological samples. The existing Marine Compounds were collected from Pubchem. To ensure a clean dataset for the Computer Aided Drug Design work, a combination of Schrodinger's LigPrep, QikProp, Premin and Macromodel packages are used to prepare the input file. LigPrep is used to generate accurate 3D molecular structures including tautomeric, stereochemical, and ionization variations, as well as energy minimization and flexible filters to generate fully customized ligand libraries that are optimized for further computational analysis.The generated structures were filtered using QikProp. QikProp is a quick, accurate and easy-to-use absorption, distribution, metabolism and excretion (ADME) prediction program designed by Professor William L. Jorgensen. Using QikProp the widest variety of pharmaceutically relevant properties namely octanol / water and water / gas log P, log S, log BB, overall CNS activity, CaCo2 and MDCK cell permeability's, human oral absorption, log Khsa for human serum albumin binding and log IC50 for HERG K+ Channel blockage were predicted for the above filtered molecules. In addition to predicting molecular properties, QikProp provides ranges for comparing a particular molecule's properties with those of 95% of known drugs. Virtual screening is increasingly gaining acceptance in the pharmaceutical industry as a cost effective and timely strategy for analyzing very large chemical datasets and Maestro Packages offers the full spectrum of speed and accuracy from high-throughput virtual screening of millions of compounds to extremely accurate binding mode predictions, providing consistently high enrichment at every level. In this study, we collected the Marine Compound from Pubchem database. A Marine Compound Library with optimized structure are generated by LigPrep, for the above collected Compounds. The ADME property also calculated for the generated compounds using QikProp.The success of these studies in identifying compounds with enhanced biological properties underscores the continuing importance of Marine Compounds as starting points for chemical biology and drug discovery efforts through rational molecular design and chemical synthesis.

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