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Computer aided screening of Mangrove ecosystem derived compound against Acetyl-cholinesterase

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Alzheimer's disease (AD) is considered as the most common type of dementia among older people. Almost 9 million people are suffering from AD in china and increasing with the course of time. Currently many different herbs are used for the treatment of AD including six Flavors Rehmannia Pills , Gastrodia and Uncaria Drink. It is been suggested that some Acetyl-cholinesterase inhibitors induced molecular and cellular change that directly influence AD pathogeneses. In our study literature search was perform to find Mangrove eco-system phytochemical structures by using Builder software implemented in Molecular operating environment (MOE 2009). Acetyl-cholinesterase (PDB ID 1EVE) structure with bound ligand was retrieved from protein data bank. Molecular docking was performed by triangular matcher placement method and rescore by London dG parameter. The crystal structure has bound ligand which was active against acetyl-cholinesterase. It can be concluded by docking analysis of different compounds that mangrove ecosystem compound may serve as good inhibitors against Acetyl-cholinesterase

Biography

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