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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 the most common type of dementia among older people. Almost 9 million people are suffering from an 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 the molecular and cellular change that directly influence AD pathogeneses. In our study literature search was performed to find Mangrove eco-system phytochemical structures by using Builder software implemented in the Molecular operating environment (MOE 2009). Acetyl-cholinesterase (PDB ID 1EVE) structure with bound ligand was retrieved from the protein data bank. Molecular docking was performed by triangular matcher placement method and rescore by London dG parameter. The crystal structure has bound the 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

Shahid Ullah, belong to Dir, a beautiful districts located in Khyber Pakhtunkhwa province of Pakistan. He has completed his doctorate of philosophy in Biochemistry and Molecular biology at School of Life Science and Technology, Huazhong University of Science and Technology (HUST), Wuhan, People Republic of China (2013-2016). During his doctoral period, he kept making effort to promote his capacity to scientific research in term of philosophy, methodology, knowledge and computational skill. He remained engaged in two government funded projects mainly focusing on PTM based computational studies. Through these projects, he have mastered a lot of computational skills, including collecting and sorting experimental data, extracting and analyzing pathway of data and developing database and tool by Perl and Java programing language. His main contribution to scientific community is developing a comprehensive phosphorylation site database (dbPAF) containing phosphorylated proteins with their modification sites in human, mouse, rat, fruit fly, nematode and yeast. dbPAF, is superior in both the number of p-sites and proteins in all the databases of the world. After the development of dbPAF database.He have further studied circadian related genes and their relationship with PTMs. Currently he is on postdoctoral position in Shenzhen University Shenzhen Guangdong, China.

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