

Design of Indole Based Acetylcholinesterase Inhibitors through Molecular Modeling, Docking, and ADMET Studies

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Alzheimer's disease (AD) the most common form of neurodegenerative senile dementia is associated with selective loss of cholinergic neurons and reduced levels of acetylcholine neurotransmitter, and it is characterized by loss of memory and progressive impairment in cognitive functions. Enhancement of cholinergic transmission is the basis of some drugs used in the treatment of AD. It is achieved by inhibiting acetylcholinesterase the

enzyme responsible for acetylcholine hydrolysis. In this work new indole- based acetylcholinesterase inhibitors were designed by investigating topology of the active site gorge of the enzyme. Molecular modeling studies was carried out using SANJEEVINI (a complete drug design software suite,SCFBIO,IITD). Designed inhibitors were found to be more effective than the currently used acetylcholinesterase inhibitors.