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MMAChEI-Molecular modeling studies for exploring structural requirement of acetylcholinesterase inhibitors

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The enzyme acetylcholinesterase (AChE) plays an important role in the central and peripheral nervous system. Acetylcholine (ACh) acts through the regulation of the AChE activity which can play a key role in accelerating senile amyloid β-peptide (Aβ) plaque deposition. The inhibition of the enzyme prevents ACh depletion, one of the key principles for the treatment of alzheimer's disease. The present study has been emphasized to explore both ligand- and structure-based pharmacophore studies on a set of structurally diverse compounds to explore prime structural features responsible for selective binding to AChE, and vis-à-vis inhibiting enzyme activity. Both the studies showed the importance of aromatic ring and hydrophobic features of the molecule for effective binding. Systematic comparisons revealed that structure-based pharmacophore has advantages in efficiently identifying potent hits with structural diversity over simple ligand-based pharmacophore search. Structure-based pharmacophore mapping (Q^2=0.862, R^2_{pred}=0.694) study adjudged the significance of the features obtained from ligand-based energy optimized pharmacophore model (EF=20.326, GH=0.617, BEDROC=0.932). Presence of electronegative groups, and acyclic and aromatic rings in the molecular scaffold depict their importance in AChE inhibition.

Biography

Tabassum Hossain, MSc in Bio-informatics, is pursuing PhD in University of Calcutta as a Junior Research Fellow under the Moulana Azad National Fellowship of University Grant Commission, India. She has published 8 research papers and presented a research article in 5th FIP Pharmaceutical Sciences World Congress 2014 at Melbourne, Australia.

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