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Synthesis, characterization and crystal structure of new tetrahydro-β-carboline as acetylcholinesterase inhibitor

Ahmad SaifuddinMohamad Arshada

Nelson Jeng YeouChearaMohammed OdayEzzatbNur AziahHanapiaRamuMeesalacSuhanaArshaddSharif MahsufiMansoraMohd NizamMordia

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Abstract

In this study, a new tetrahydro-β-carboline derivative, 2-benzoyl-6-methoxy-9-methyl-1-phenyl-1,2,3,4-tetrahydro-β-carboline has been synthesized through a three-steps reaction in good yield (76%). The structure of this compound was characterized by different spectroscopic methods including NMR (1D and 2D), UV, IR and MS. Molecular structure of the synthesized compound was also confirmed by single crystal X-ray diffraction technique. Further, evaluation of *in vitro* acetylcholinesterase (AChE) inhibitory activity showcased the potential of this compound as AChE inhibitor with an IC_{50} value of 26.52 ± 0.79 µM. In addition, this compound showed minimal toxicological profile at cellular level. Docking simulation illustrated a highly selective binding at peripheral side of AChE via hydrophobic

interactions. *In silico* prediction of blood-brain barrier (BBB) permeation and ADMET properties of the compound was also reported.

Keywords

Tetrahydro-β-carboline, Single crystal, Acetylcholinesterase, Molecular docking, Cytotoxicity, ADMET