Molecular docking to test for efficacy of porphyrin compounds in Alzheimer disease

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The cure for Alzheimer’s disease suggested by the Cholinergic Hypothesis involves searching for candidate compounds that can act as inhibitors for Acetylcholinesterase (AChE) enzyme. Regional cerebral blood flow can be increased in patients with Alzheimer’s disease by Acetylcholinesterase inhibitors. In this regard, Tetraphenylporphinesulphonate (TPPS), 5,10,15,20-Tetrakis (4-sulfonatophenyl) porphyrinato Iron(III) Chloride (FeTPPS) and 5,10,15,20-Tetrakis (4-sulfonatophenyl) porphyrinatoIron(III) nitrosyl Chloride (FeNOTPPS) were investigated as candidate compounds for inhibition of Acteylcholinesterase of Drosophila melanogaster (DmAChE) by use of Molecular Docking. The results show that FeNOTPPS forms the most stable complex with DmAChE.

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