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Supporting information

for

Design, Synthesis and Biological Evaluation of Tacrine 1,2,3-Triazole Derivatives as Potent Cholinesterase Inhibitors

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Schematic representation of protein-ligand interaction of compound 8a2 and Tacrine in hAchE



Schematic representation of protein-ligand interaction of compound 8a2 and Tacrine in hBchE



The comparison of binding poses of 8a2 with Tacrine in hAchE and hBchE.



Reproduce the Tacrine binding mode with docking simulation.



<u>Tacrine</u> X-ray Docking RMSD = 0.05Å

Schematic representation of protein-ligand interaction of compound III, and IV in hAchE and hBchE, respectively.



Electric eel acetylcholinesterase (eeAChE) (Sigma-Aldrich, USA; Enzyme Information Download Website:

https://www.sigmaaldrich.com/content/dam/sigmaaldrich/docs/Sigma/Product_Information_Shee t/c3389pis.pdf)

Horse serum butyrylcholinesterase (hsBChE;) (Sigma-Aldrich, USA; Enzyme Information Download Website:

https://www.sigmaaldrich.com/content/dam/sigma-aldrich/docs/Sigma/Datasheet/c1057dat.pdf)