Revealing the Mechanistic Pathway of Cholinergic inhibition of Alzheimer’s disease by Donepezil: A Metadynamics Simulation Study

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Electronic supplementary information

hAChE & Donepezil Crystal

Fig. S1 The free energy profiles as a function of a CV namely Ser203, Glu334 and His447 with donepezil crystal were plotted at different time and compared with other to access the convergence of a well-tempered metadynamics simulation.
**$h$AChE & Docked Donepezil**

![Graphs](image)

**Fig. S2** The free energy profiles as a function of a CV namely Ser203, Glu334 and His447 with docked donepezil were plotted at different time and compared with other to access the convergence of a well-tempered metadynamics simulation.
**hAChE & Donepezil Crystal**

**Fig. S3** Time evaluation plot of the examined CVs (CV1 = Ser203 & Donepezil; CV2 = His447 & Donepezil; CV3 = Glu334 & Donepezil) of the well-tempered metadynamics simulation for Donepezil crystal.

**hAChE & Docked Donepezil**

**Fig. S4** Time evaluation plot of the examined CVs (CV1 = Ser203 & donepezil; CV2 = His447 & Donepezil; CV3 = Glu334 & Donepezil) of the well-tempered metadynamics simulation for docked donepezil.