Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

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

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Electronic supplementary information

*h*AChE & Donepezil Crystal

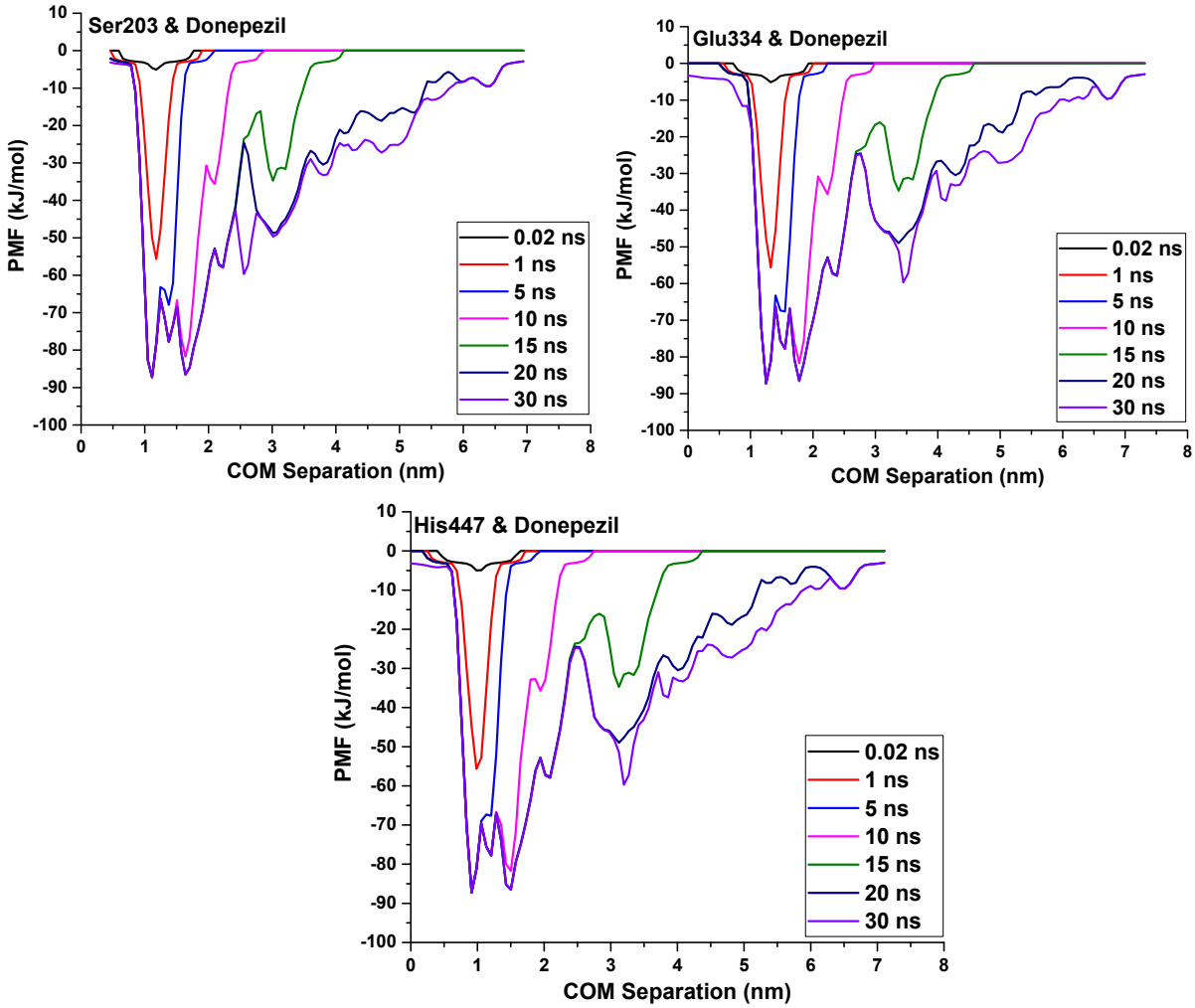

Fig. S1 The free energy profiles as a function of a CV namely Ser203, Glu334 and His447 with donepezil crystal were plotted at different time and compared with other to access the convergence of a well-tempered metadynamics simulation.

***h*AChE & Docked Donepezil**

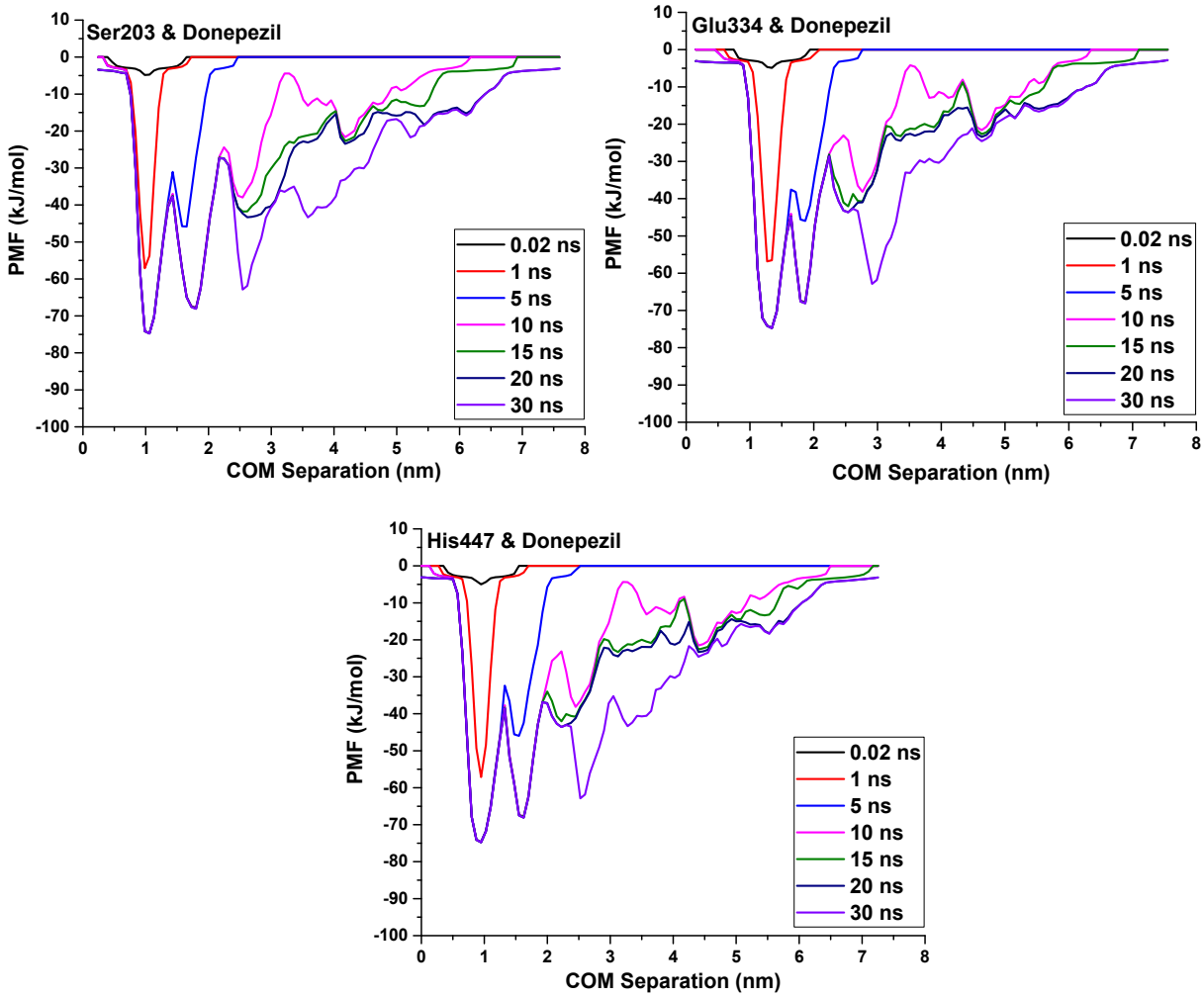

Fig. S2 The free energy profiles as a function of a CV namely Ser203, Glu334 and His447 with docked donepezil were plotted at different time and compared with other to access the convergence of a well-tempered metadynamics simulation.

***h*AChE & Donepezil Crystal**

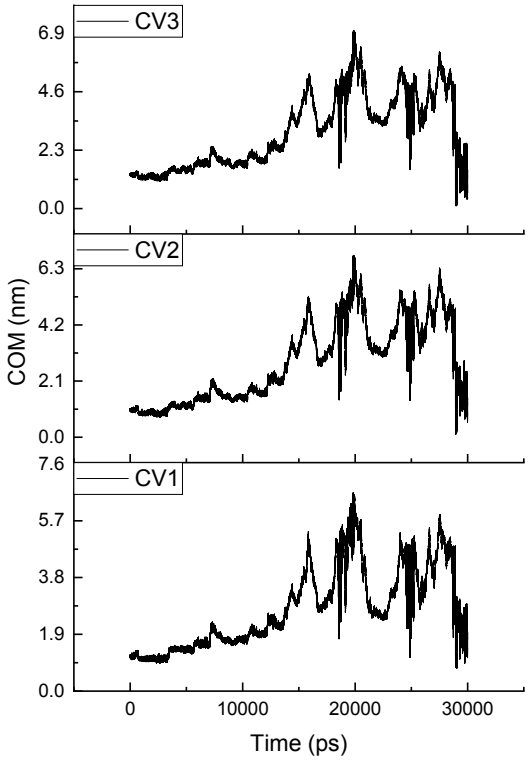

Fig. S3 Time evaluation plot of the examined CVs (CV1 = Ser203 & Donepezil; CV2 = His447 & Donepezil; CV3 = Glu334 & Donepezil) of the well-tempered metadynamics simulation for Donepezil crystal.

***h*AChE & Docked Donepezil**

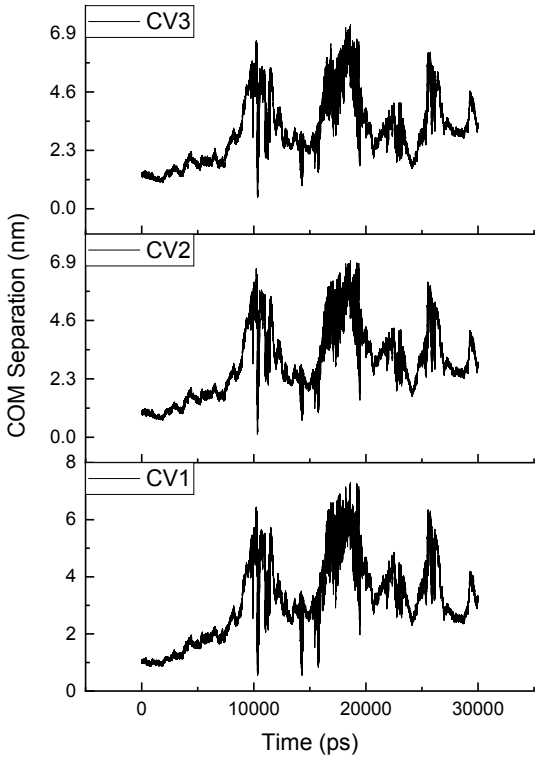

Fig. S4 Time evaluation plot of the examined CVs (CV1 = Ser203 & donepezil; CV2 = His447 & Donepezil; CV3 = Glu334 & Donepezil) of the well-tempered metadynamics simulation for docked donepezil.