

Electronic Supplementary Information for

**Simulated revelation for the adsorption behaviours of  
acetylcholinesterase on charged self-assembled monolayers**

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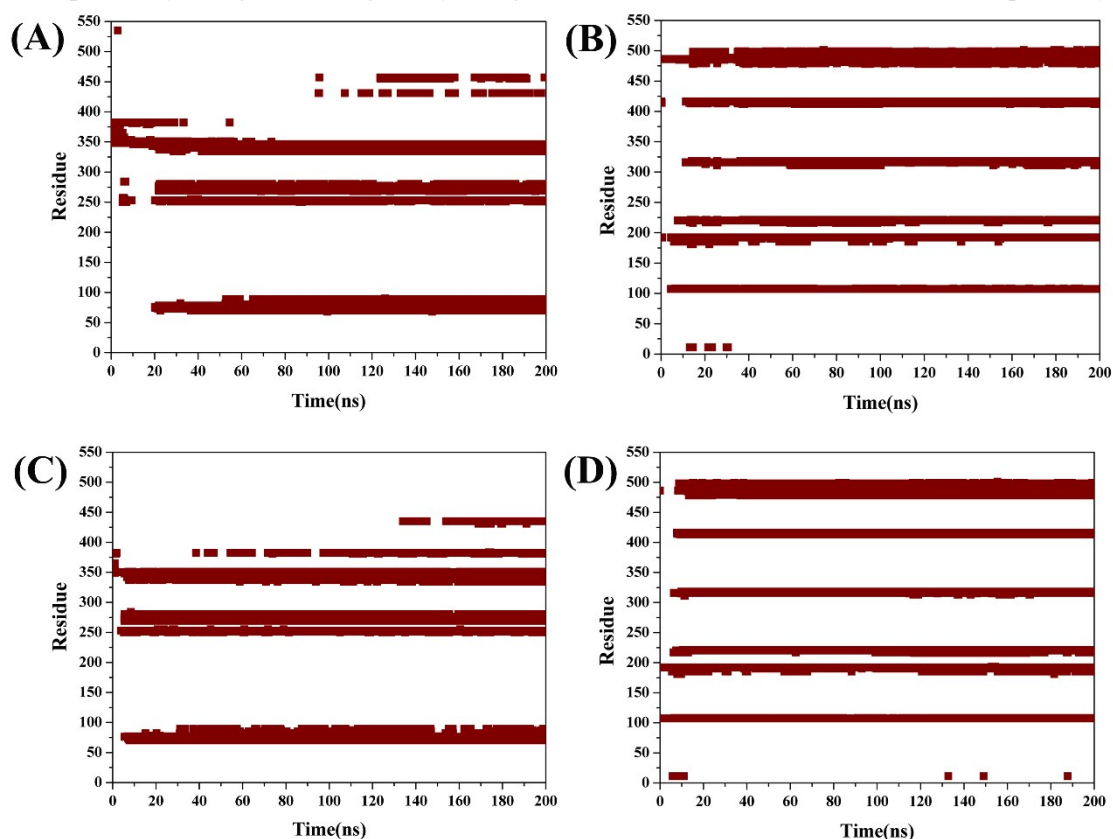
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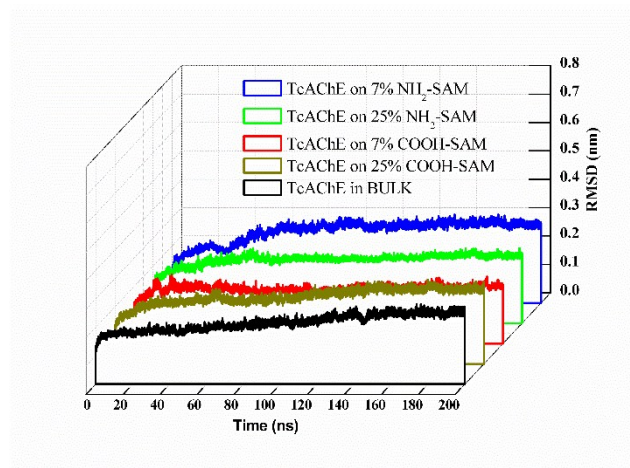
**Table S1.** The adsorption residues of TcAChE adsorbed on charged surfaces.

system	Contact residues (< 0.35 nm)
TcAChE on NH <sub>2</sub> -SAM (7%)	Tyr70, Asp72, Pro76, Gly77, Gly80, Glu82, Glu89, Asn253, Lys269, Lys270, Gln272, Glu273, Asp276, Val277, Tyr334, Ser340, Asp342, Ser343, Glu344, Lys346
TcAChE on NH <sub>2</sub> -SAM (25%)	Asp72, Glu73, Pro76, Gly77, Asn253, Gln272, Glu273, Asp276, Tyr334, Pro337, Gly338, Ser340, Asp342, Ser343, Glu344, Lys346, Ser348, Glu350, Asp351, Asn382
TcAChE on HOOC-SAM (7%)	Lys107, Lys192, Arg220, Lys316, Gln318, Lys413, Phe414, Asn416, Thr479, Asn481, Pro485, His486, Ser487, Gln488, Lys491, Leu494, Thr496, Lys498, Glu499
TcAChE on HOOC-SAM (25%)	Lys107, Ser108, Gln185, Asp190, Lys192, Asp217, Arg220, Arg221, Lys316, Gln318, Lys413, Phe414, Asn416, Thr479, Pro485, His486, Thr497, Lys498

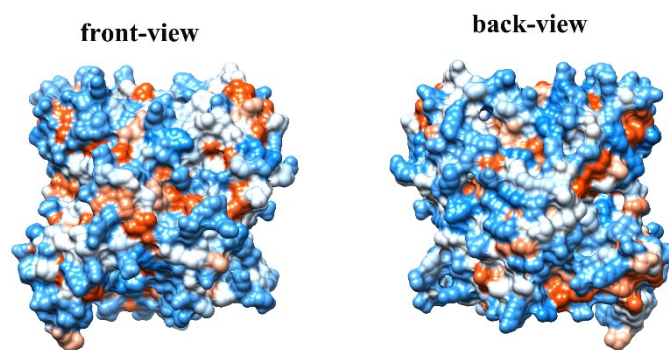
\*The positively charged, and negatively charged residues are colored in blue, and red, respectively



**Fig. S1.** Contact maps between TcAChE and charged SAMs during AAMD simulations: (A) 7% dissociated NH<sub>2</sub>-SAM; (B) 7% dissociated COOH-SAM; (C) 25% dissociated NH<sub>2</sub>-SAM; (D) 25% dissociated COOH-SAM.



**Fig. S2.** The time evolution of RMSD during overall processes of AAMD simulations.



**Fig. S3.** The hydrophobicity maps of TcAChE are shown in front and back views: the surface color changes from the blue for the strongest polar residue to orange-red for the most hydrophobic residue, with the intermediate residues in white.