Electronic Supplementary Information for

Electrostatics-mediated α-chymotrypsin inhibition by functionalized single-walled carbon nanotubes

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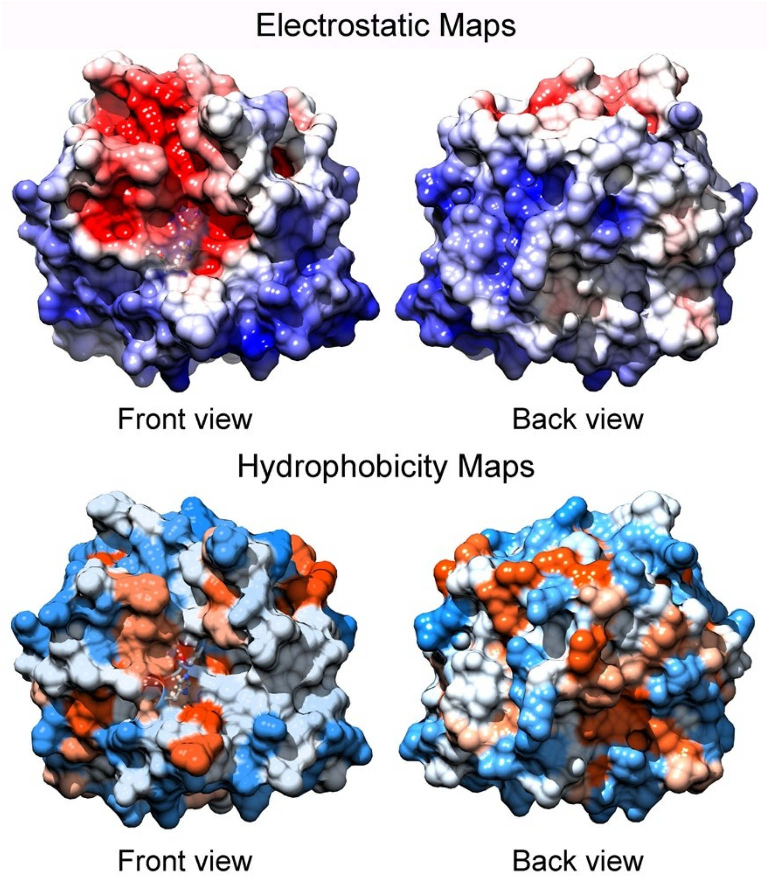

Figure S1. The electrostatic and hydrophobicity maps of α-ChT are shown in front and back views and the active sites are represented in stick mode. For electrostatic maps, the region in blue is for the part with positive potential, while that in red is for the part with negative potential. The white region has neutral potential. For hydrophobicity maps, it colors the surface ranging from dodger blue for the most polar residues to orange red for the most hydrophobic residues, with white in between.

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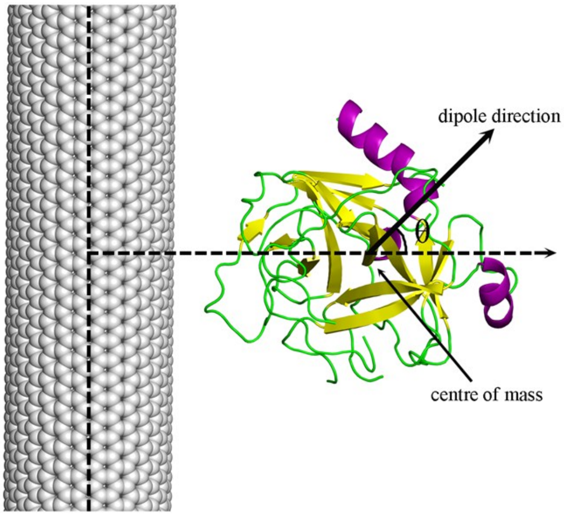


Figure S2. The definitions of protein orientation at CNTs. *θ* is the angle between the unit vector along the dipole of a protein and a vector connecting the CNT axis and the centre of mass of a protein (this vector is perpendicular to CNT axis).

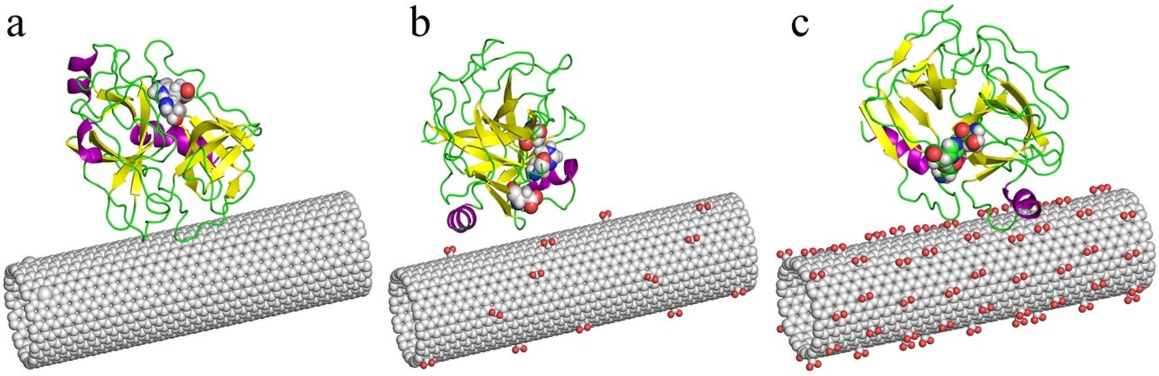
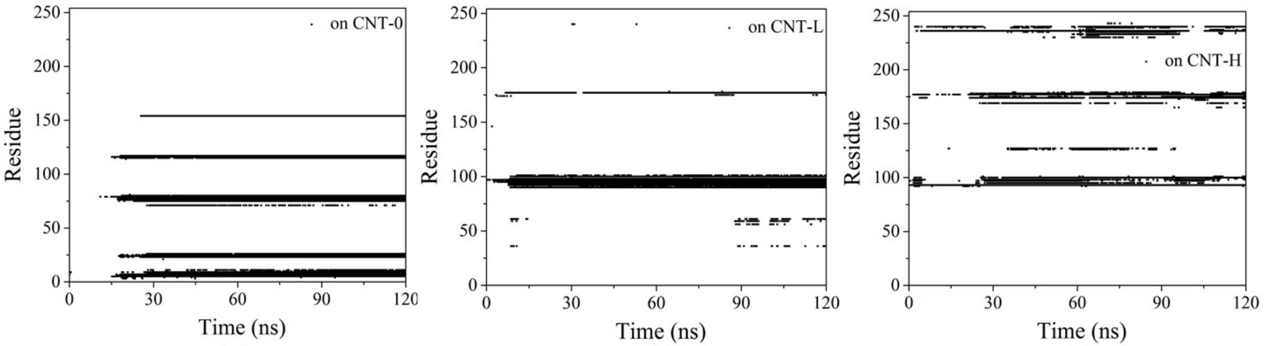


Figure S3. Typical structures of α-ChT adsorbed on (a) CNT-0, (b) CNT-L, and (c) CNT-H, respectively.



(a) (b) (c)

Figure S4. Residue contact maps of α-ChT adsorbed on (a) CNT-0, (b) CNT-L, and (c) CNT-H, respectively.

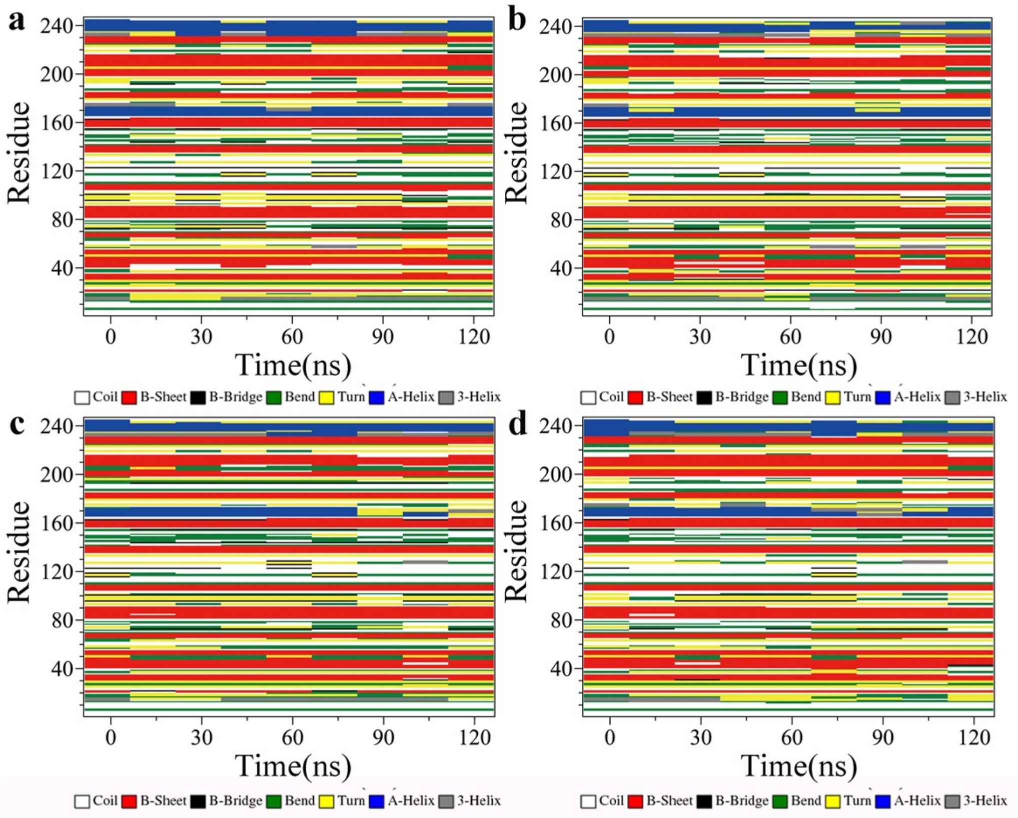


Figure S5. Time evolution of the secondary structures of α-ChT in water (a) and adsorbed on (b) CNT-0, (c) CNT-L, and (d) CNT-H, respectively.

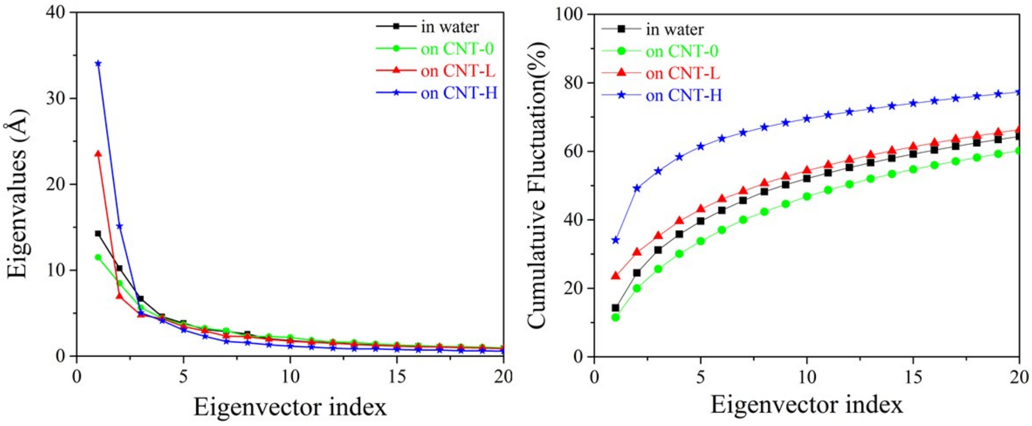


Figure S6. (a) The eigenvalues (Å^2) and (b) the percentages of cumulative eigenvalues (%) plotted against the first 20 eigenvector indices obtained from the C_α covariance matrix constructed from the last 20 ns of MD simulations.