Supporting information

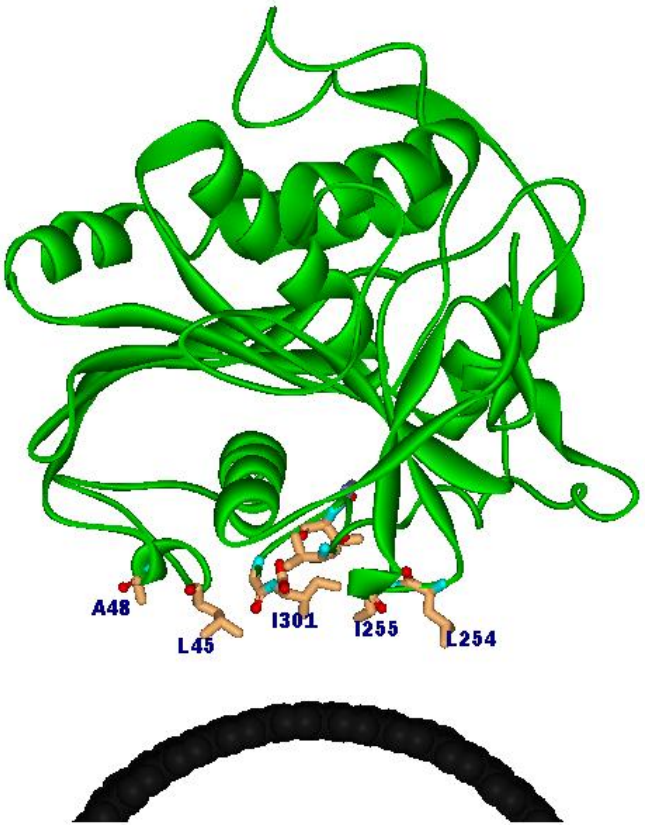
Table S1. Six orientations for the adsorption of the lipase on the CNT

Orientation	Residues initially above the CNT surface	Interaction energy between the lipase and CNT(kJ/mol)
I (Figure S4a)	Leu45, Ala48, Leu254, Ile255, Ile301	-417.6
II (Figure S4b)	Leu64, Ile100, Met101, Pro104	-381.3
III (Figure S4c)	Pro104, Leu105, Leu110, Leu124	-377.6
IV (Figure S4d)	Leu91, Ile95, ILe100, Met101, Val283, Val285, Ile286	-267.2
V (Figure S4e)	Val 1, Ala275, Leu279, Leu280, Val283	-246.9
VI (Figure S4f)	Gly34, Phe38, Pro40, Leu45, Ala48, Val298	-239.6

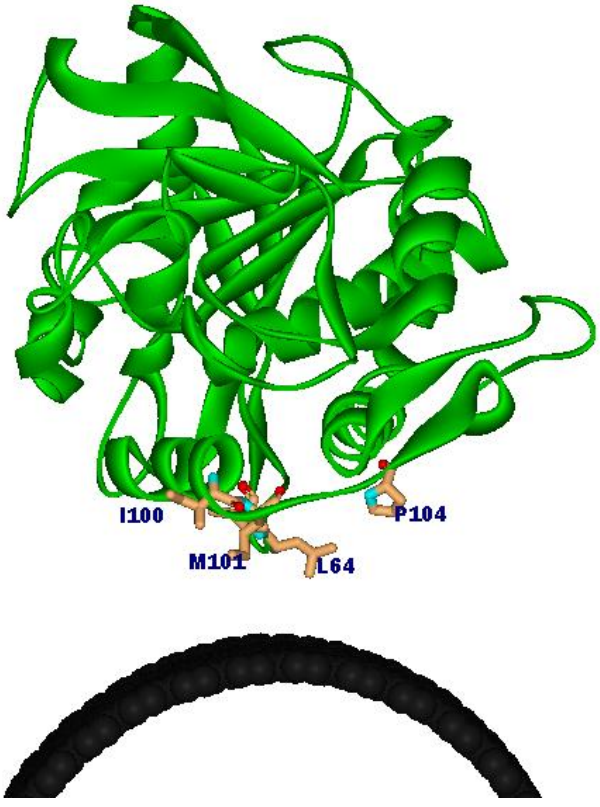
Table S2. Salt bridges for the immobilized lipases

	Simulation time	
	0 ns	50 ns
Case 1	Found 18 salt bridges. ASP153-LYS79 GLU54-LYS39 GLU54-HIS76 ASP251-ARG228 ASP230-HIS289 GLU58-LYS36 GLU296-ARG86 GLU19-ARG23 ASP61-ARG63 ASP93-HIS89 ASP212-LYS215 GLU209-LYS203 ASP219-LYS221 GLU19-HIS49 GLU247-ARG224 ASP181-LYS221 GLU57-LYS143 ASP181-LYS176	Found 20 salt bridges. ASP11-LYS215 ASP153-LYS79 GLU54-LYS39 GLU54-HIS76 ASP230-HIS289 GLU58-LYS36 GLU296-ARG86 ASP202-LYS203 GLU57-LYS143 ASP61-ARG63 ASP219-LYS218 GLU19-ARG23 ASP251-ARG228 ASP97-HIS126 GLU209-LYS203 ASP145-LYS143 GLU247-ARG224 ASP181-LYS221 GLU92-HIS89 ASP181-LYS176
Case 2	Found 14 salt bridges. ASP230-HIS289 GLU54-LYS39 ASP181-LYS221 ASP153-LYS79 GLU296-ARG86 GLU19-ARG23 ASP61-ARG63 ASP251-ARG228 ASP93-HIS89 GLU209-LYS203 ASP181-LYS176 GLU247-ARG224 GLU19-HIS49 GLU57-LYS143	Found 17 salt bridges. ASP230-HIS289 ASP251-ARG228 ASP181-LYS221 ASP219-LYS215 ASP153-LYS79 GLU296-ARG86 GLU54-LYS39 GLU19-ARG23 ASP61-ARG63 ASP97-ARG99 ASP93-HIS89 GLU209-LYS203 GLU54-HIS76 GLU247-ARG224 GLU13-LYS218 ASP67-ARG63 GLU57-LYS143

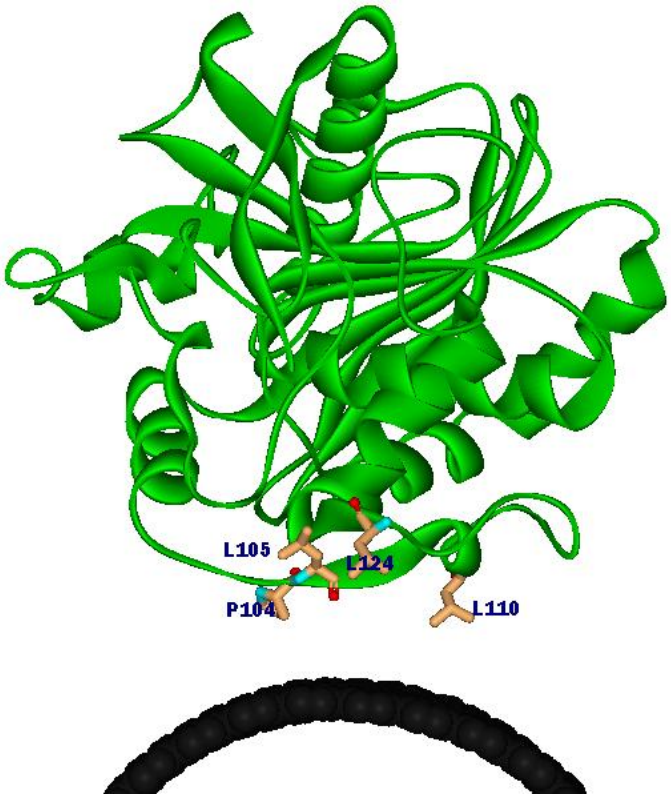
a)



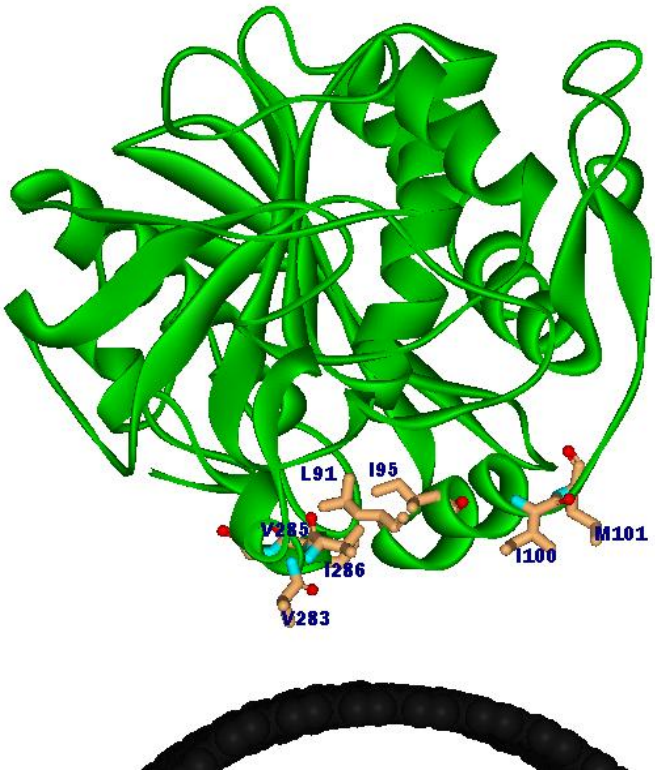
b)



c)



d)



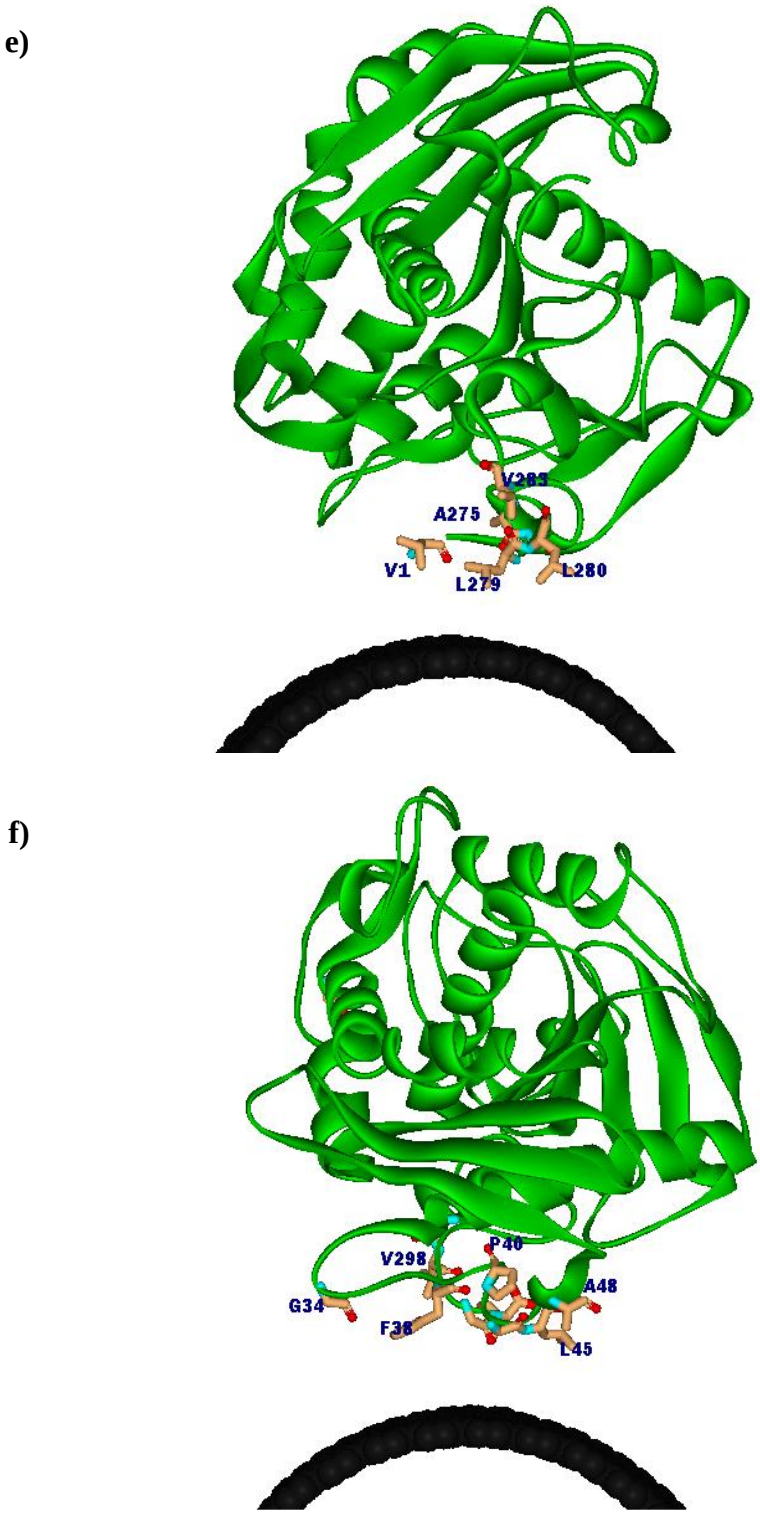


Figure S1. Six starting orientations with the residues in orange above the CNT surface.

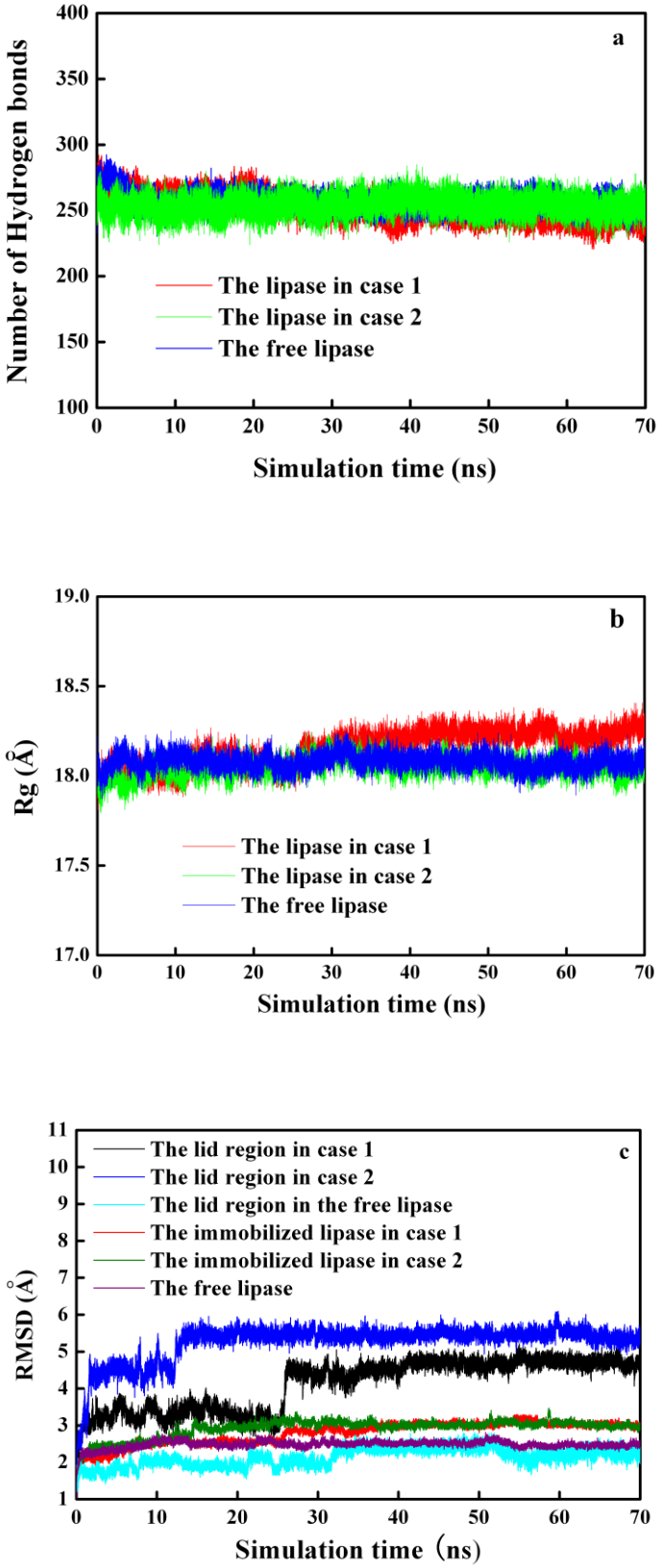


Figure S2. Number of hydrogen bonds (a), radius of gyration (b), and RMSD (c).

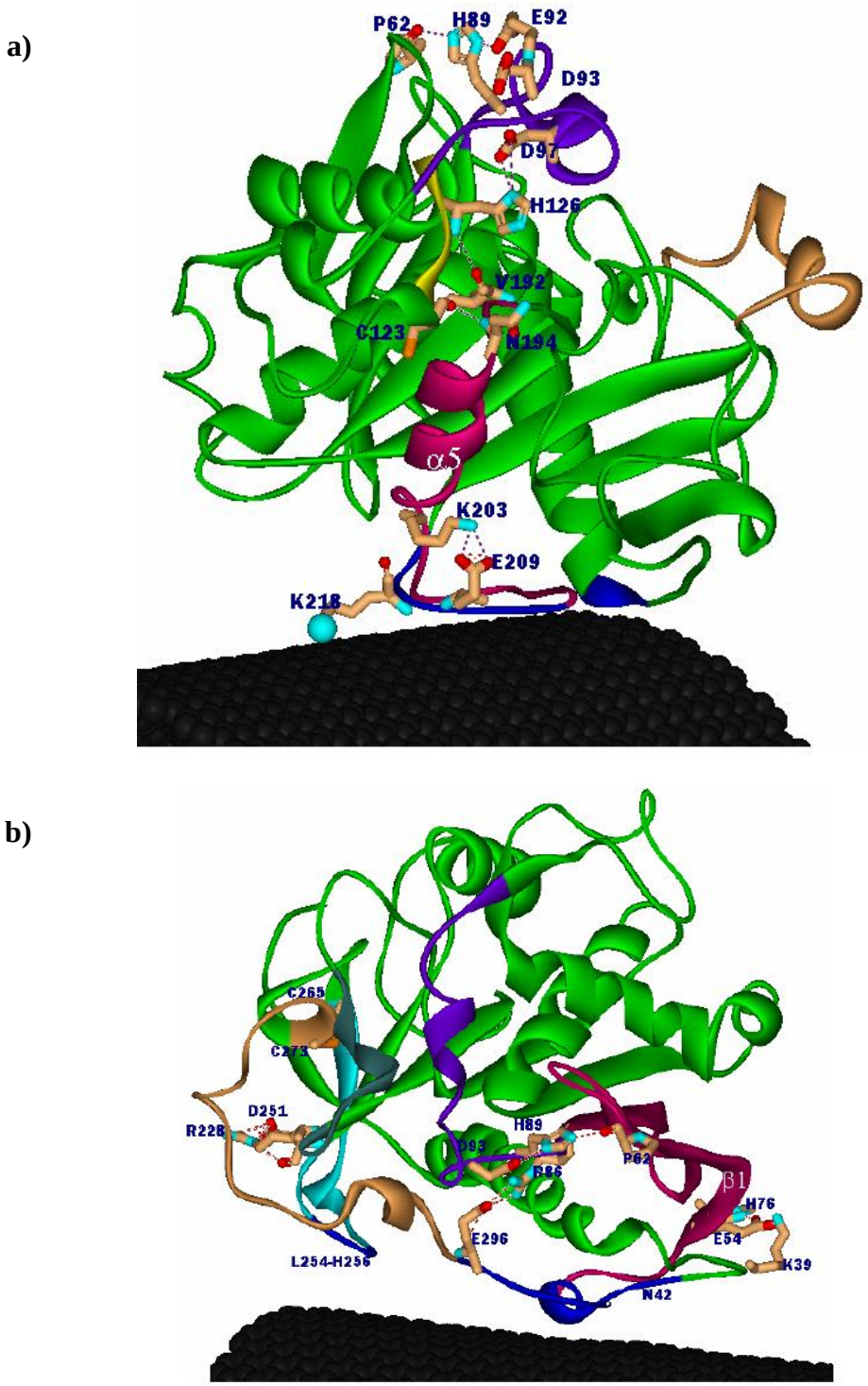


Figure S3. Simulation snapshots at 50 ns for case 1 (a) and case 2 (b).

In the snapshots, the segments in contact with the CNT are shown in blue. The lid is shown in violet, and the segment (Asn 277 – Leu 290) is shown in orange. The hydrogen bond and salt bridge interactions between the residues, which contribute to the propagation of the interactions, are indicated by the dashed lines.

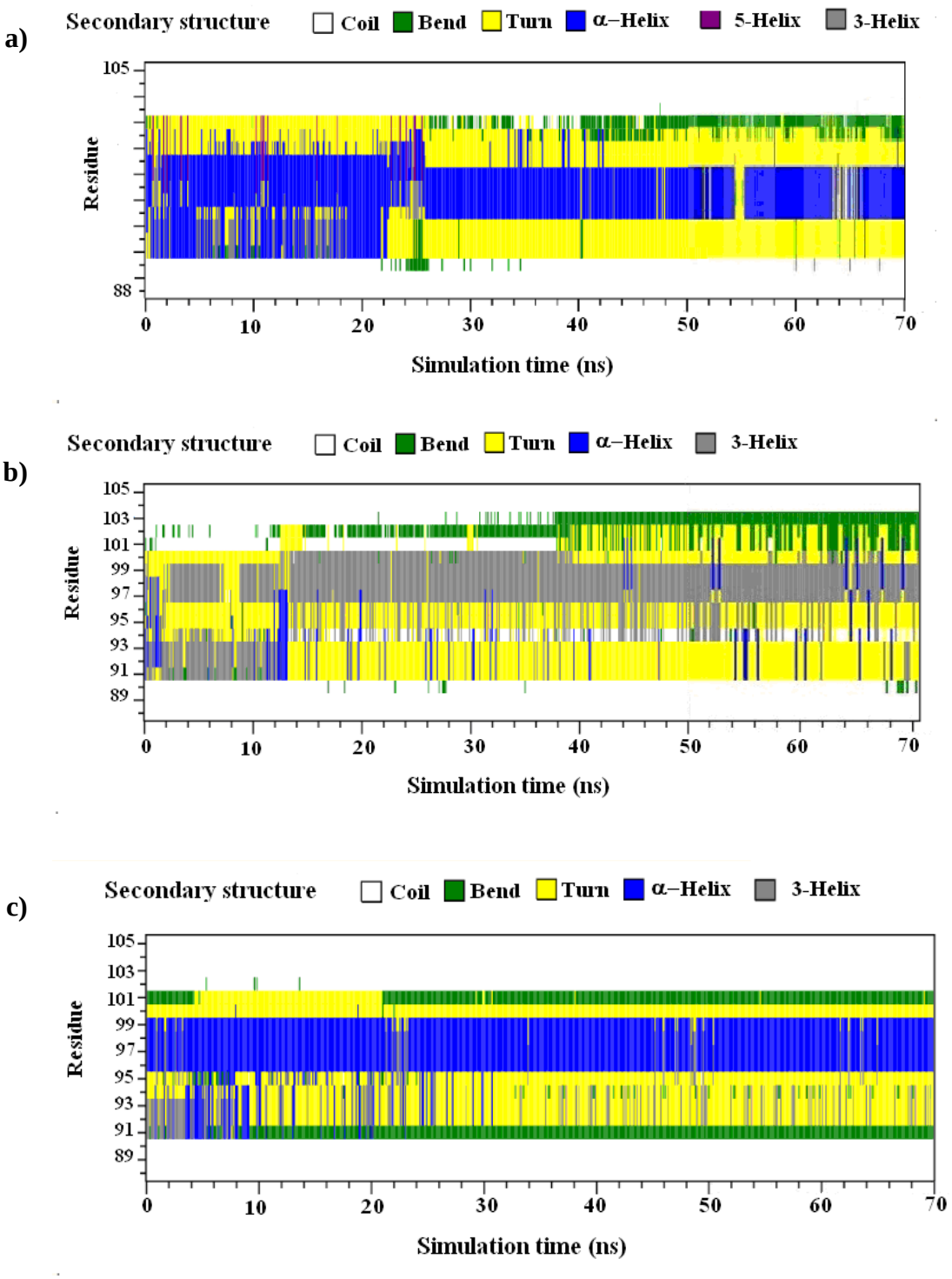
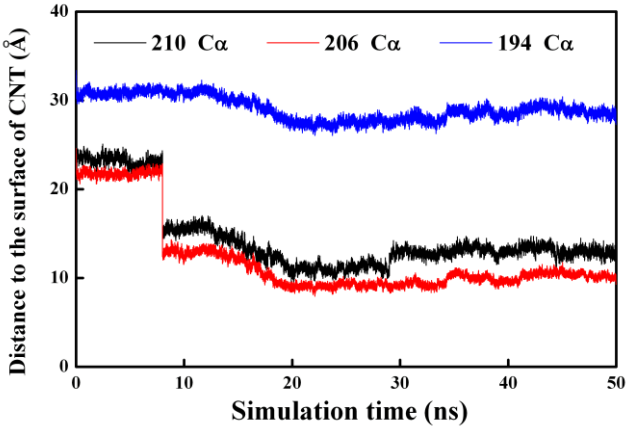
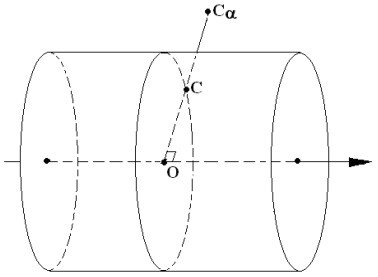


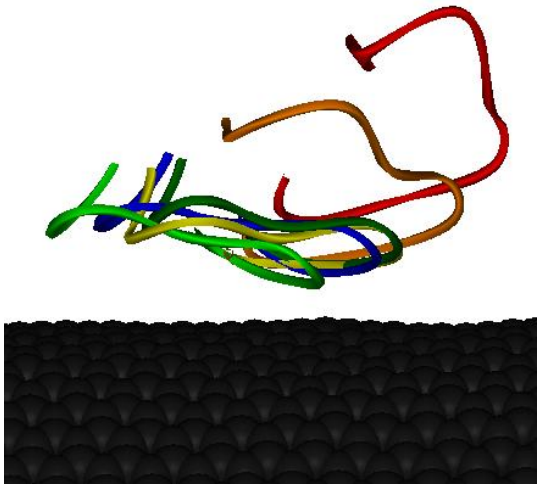
Figure S4. The conformational change of the lid with simulation time. (a) The lipase in case 1; (b) The lipase in case 2; (c) The free lipase.



a



b



c

Figure S5. (a) The distance between the Cα atoms and the surface of the CNT. (b) Illustrating the distance between the Cα and the carbon atom of the CNT, which equals to the distance OCα minus the radius OC of the CNT. (c) The movement of the loop (Phe 206–Arg 220) toward the CNT surface with simulation time for case 1, in which red (0 ns), orange (10 ns), yellow (20 ns), green (30 ns), olive (40 ns), and blue (50 ns)