

Fig. S1 Structure comparison of crystal structures of *Tr* cutinase and two lipases in closed form. The lid of *Tr* cutinase (PDB ID: 4PSD) and lipases (PDB ID: 1QGE and 3O0D) are colored red, cyan and purpleblue, respectively.

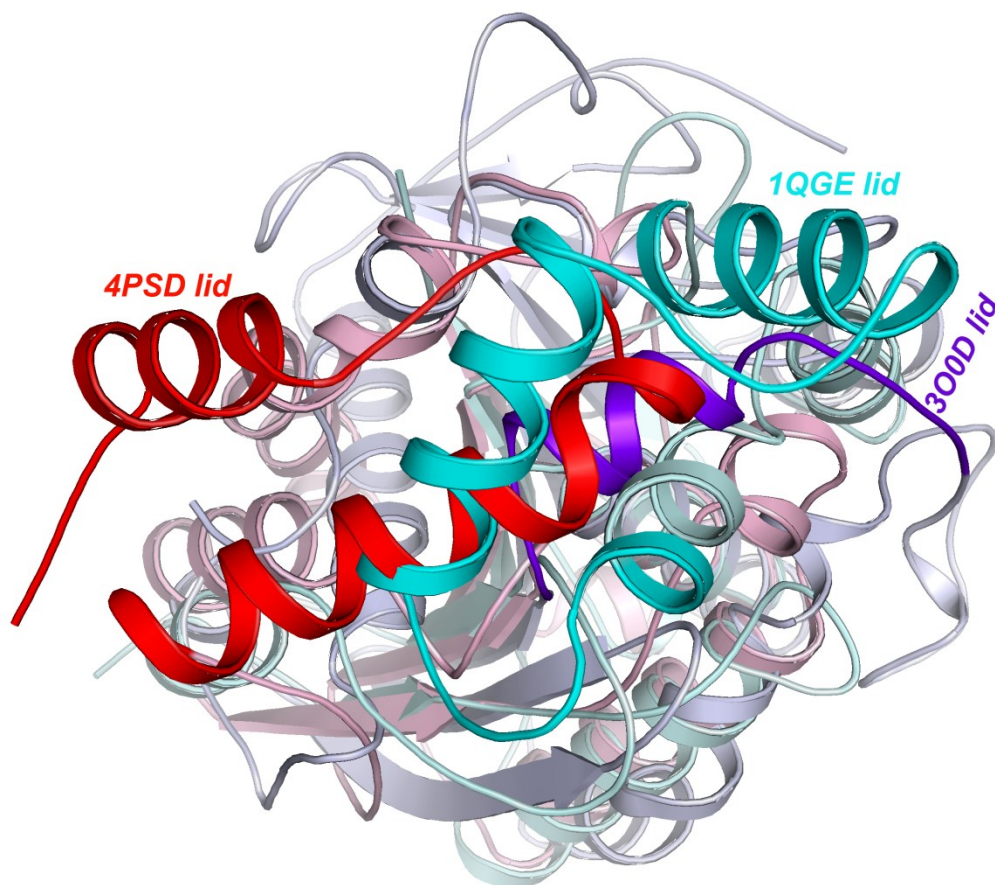


Fig. S2 RMSD and Rg plots of backbone atoms of protein for closed form. (A) RMSD plots at pH 6 (blue line) and pH8 (red line); (B) Rg plots at pH 6 (blue line) and pH8 (red line).

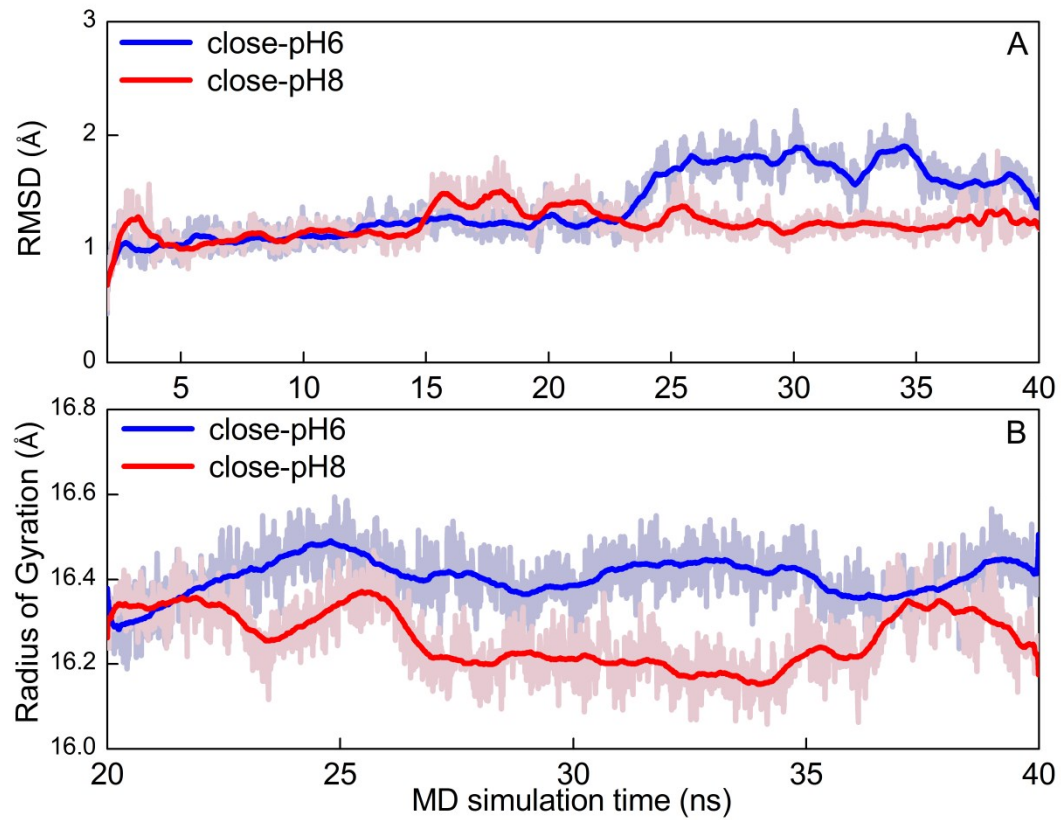


Fig. S3 RMSD plots of backbone atoms of protein and Rg plots of backbone atoms of the core structure of protein in open form. RMSD plots for *apo* state (A) and *holo* state (B), at pH 6 (blue line) and pH 8 (red line); Rg plots for *apo* state (C) and *holo* state (D), at pH 6 (blue line) and pH 8 (red line), respectively.

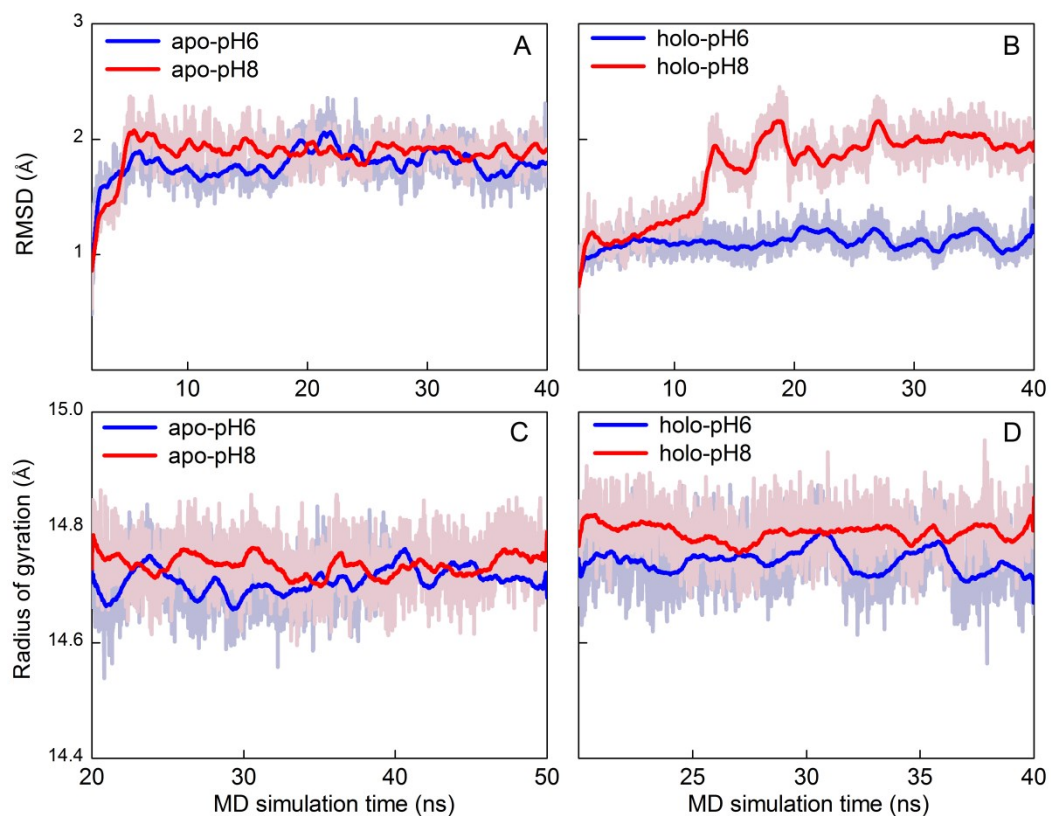


Fig. S4 Structure comparison of crystal structures of *Tr* and *Fs* cutinases in dark and light grey, respectively. The catalytic Ser164 is shown in stick representation. Region Cys212-Tyr232 and helix  $\alpha 2$  in *Tr* cutinase are colored hotpink and magenta. Region Cys178-Ala186 and Leu81-Ala85 in *Fs* cutinase are colored greencyan and green, respectively.

