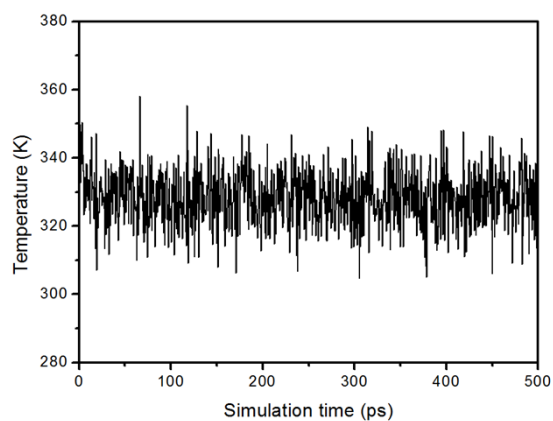
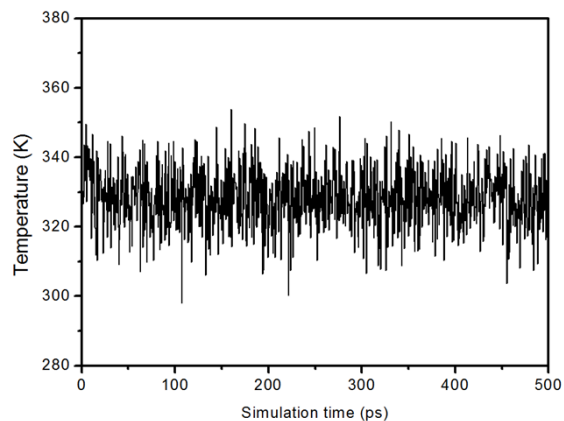


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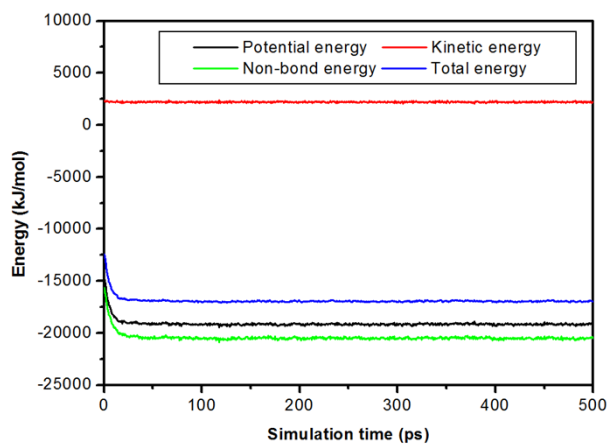


(a)

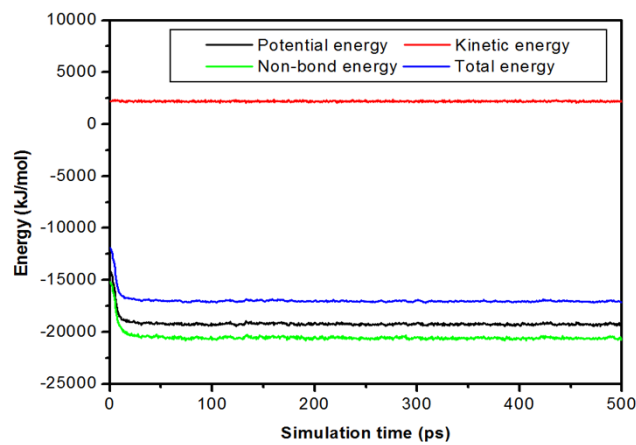


(b)

Fig. S1 Temperature equilibrium curve obtained from MD simulation for (a) 2-AB and (b) 3-AB at 328 K.



(a)



(b)

Fig. S2 Energy fluctuation curves obtained from MD simulation for (a) 2-AB and (b) 3-AB at 328 K.

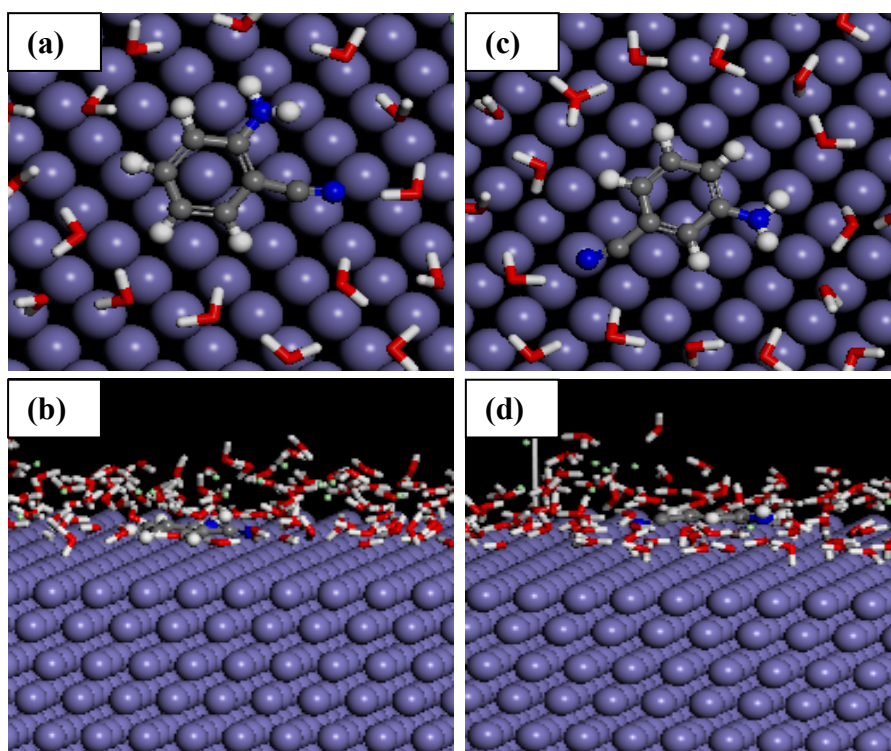


Fig. S3 Equilibrium adsorption configurations of inhibitors 2-AB (a and b) and 3-AB (c and d) on Fe (1 1 0) surface at 328 K obtained from MD simulations. Top: top view, Bottom: side view.