

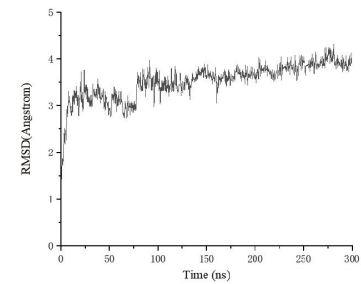
A



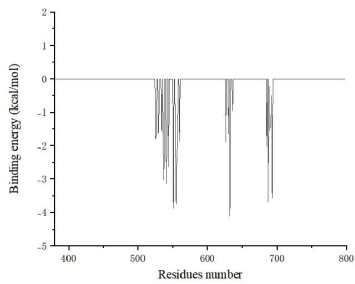
B

	Docking 1 (Kcal/mol)	Docking 2 (Kcal/mol)	Docking 3 (Kcal/mol)	Mean (Kcal/mol)
Docking score	-9.412	-9.254	-9.178	-9.281
predicted binding values (pKi, μ M)	6.920	6.800	6.750	6.820

C



D



Combine the free energy contribution items	NNK2 Energy value (kcal/mol)
ΔE_{vdw}	-58.08
ΔE_{elec}	-12.80
ΔG_{GB}	30.04
ΔG_{surf}	-18.31
ΔG_{bind}	-59.19

