

Figure S1. RMSD complexes docked with compound 52/ Des4/ Des5/ Des6 for 100 ns simulations((A): The first time (B) : The second time(C) : The third time).

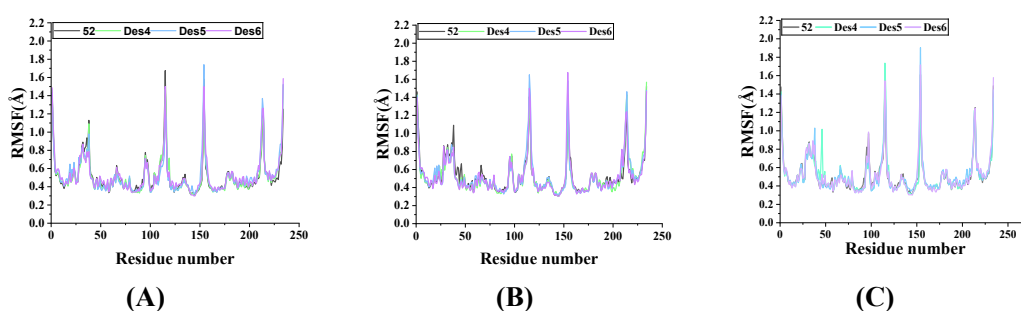


Figure S2. RMSF complexes docked with compound 52/ Des4/ Des5/ Des6 for 100 ns simulations((A): The first time (B) : The second time(C) : The third time).