Theoretical study on the interaction between candidate drugs and Coronavirus main protease (3CLPro) for inhibiting replication of SARS-CoV-2

조유미, 고은민, 신은혜, 곽상규†
UNIST
(skkwak@unist.ac.kr†)

We theoretically investigated the interactions of drug molecules with 3C-like protease (3CLPro), to inhibit the replication of SARS-CoV-2 using molecular dynamics (MD) simulation. Lopinavir, Ritonavir, CG376 and dipeptidyl series were used at different temperatures and concentrations. The adsorption behavior of drug candidates was compared by analyzing the root mean square fluctuation (RMSF), root mean square deviation (RMSD) of 3CLPro, minimum distances and interaction energies between 3CLPro and drug, and the number of aggregated drugs. The drugs were mainly adsorbed on the 3CLpro by the polar interactions. In specifically, dipeptidyl 7c was effective in inhibiting 3CLPro since it shows high binding energy, high number of attached active sites 3CLPro, and large dispersity of drugs in the adsorbed states compared to those of Lopinavir, Ritonavir, CG376. In specifically, alkyl groups within drugs mainly sticked to the active sites of 3CLPro. At high temperature, the interactions between drugs and the protein were increased, which was shown by larger adsorption area of drugs on the protein. Meanwhile, the number of adsorbed drugs was similar in different concentration of the drugs.