

Theoretical Study on Interaction between Cancer Cell Membrane and Targeting Agents for Oncolytic Virus

박세영, 고은민, 신은혜, 신선우, 곽상규[†]
울산과학기술원
(skkwak@unist.ac.kr[†])

An oncolytic virus is a genetically modified virus to target and destroy the tumor cells through replication mechanism and autoimmunity of the human body, which have less side effect and less toxicity. To commercialize the oncolytic virus, however, improvement of targeting efficiency is a key factor. In this study, the interaction between cancer/normal cell and virus membrane model with new targeting agents are compared via coarse-grained molecular dynamics (CGMD). Glycan and DOTAP are attached on virus model for targeting the cancer cell. First, glycan induced the adsorption of HA and sialic acid, which is the receptor of virus on cell membrane. Second, we checked the optimal chain length of poly(ethylene oxide) (PEO), which was linking ligand for POPE and DOTAP, and model with 27 constitutional monomers was adopted. Cancer cell membrane showed increased fluctuation by the interaction with DOTAP. We confirmed the preferred interaction between our oncolytic virus and cancer cell membrane than normal cell by analyzing the radial distribution function and the behavior of lipid in cell membrane.