

Construction of Oncolytic Virus Model for Targeting Cancer Cell via Coarse-grained Molecular Dynamics

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An oncolytic virus is an effective alternative to anti-cancer drug, which can cause secondary damage, due to low side effect. However, oncolytic virus should have targeting ability for the cancer treatment. In this regard, the effective targeting materials were investigated by comparing the interaction between cancer/normal cell membrane and oncolytic virus via coarse-grained molecular dynamics (CGMD). Simulation was performed with 70 million of particles and the size of virus was ~80 nm. Glycan and DOTAP (N-[1-(2,3-dioleoyloxy)propyl]-N,N,N-trimethylammonium) were used for targeting materials by attaching to oncolytic virus. Six oncolytic virus models were constructed depending on the concentration of DOTAP, which were attached to 25 % and 50 % of POPE (i.e., DOTAP 25 % and DOTAP 50 %, respectively), and the existence of glycan. Targeting ability of oncolytic virus was simply tested by root mean square fluctuation of lipid of cancer cell and the distance between virus and cancer cell. Oncolytic virus, containing DOTAP 25 % or both DOTAP 25 % and glycan, showed strong attraction to cancer cell and induced large fluctuation on cancer.