Theoretical Study of Functionalized Oncolytic Virus on Cancer Cell Targeting via Coarse-grained Molecular Dynamics Simulation using Nurion-KNL System

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Oncolytic virus that is functionalized to target and destroy cancer cell is a developing method for cancer treatment. For effective treatment and accurate targeting on cancer cell, understanding the interaction between oncolytic virus and cancer cell membrane is of great importance. In this study, spherical oncolytic virus models (i.e., diameter of 30 and 80 nm) were constructed including DOTAP (N-[1-(2,3-dioleoyloxy)propyl]-N,N,N-trimethylammonium), which were attached to POPE (i.e., 25 % and 50 % of total number of POPE in the virus), and Hemagglutinin (HA) with and without glycan, where the virus-cell membrane model system was constructed in water condition. Note that total number of particles used for the system was about 4.5×10^9. To perform coarse-grained molecular dynamics (CGMD), huge computational resource, 2,500 nodes of Nurion-KNL system, have been employed. We found that oncolytic virus containing 25 % of DOTAP closely interacted with the cancer cell, which was more fluctuating and thinning than normal cell. Through this study, we demonstrated that the application of DOTAP could be an effective method for enhancing the anti-cancer nature of oncolytic virus.