# Theoretical study on encapsulation and release of anti-cancer drug in PEG-PLA vesicle

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Drug encapsulation and release are directly related to the efficiency of biological therapy. In this work, dynamics of vesicle for encapsulating and releasing the anti-cancer drug were studied by coarse-grained molecular dynamics; amphiphilic block-copolymer (i.e. polyethylene glycol (PEG) and polylactic acid (PLA)) for vesicle and gemcitabine for anti-cancer drug. In particular, the self-assembly of vesicle covering drug and the shape control of the vesicle were investigated. First, we observed that the self-assembly occurred only if the volume ratio of PEG-PLA became 3:7, where the optimal area per the number of polymer chain was 0.3 nm2. Controlling the inner and outer surface areas of the membrane of vesicle induced anisotropic shape of vesicle with the aspect ratio of 1.1. Second, the effective mole ratio of block-copolymer and drug was found to be 100 to 1, which worked for loading drug into vesicle. Finally, the rupture of the vesicle in low pH environments (i.e. pH 3 ~ pH 7) mimicking the inside of cancer cell, was studied for the drug release. Hydrolysis of PEG and crystalline PLA were heavily involved in the drug release