Pirawat Thongjun 2007: Study of Doxorubicin in Glucosamine(Ethylene Glycol) Oligomers by Molecular Modeling. Master of Engineering (Chemical Engineering), Major Field: Chemical Engineering, Department of Chemical Engineering.
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This research studied the release of doxorubicin from a capsule of glucosamine(ethylene glycol) oligomers by the molecular modeling method. This drug formed a micelle with glucosamine(ethylene glycol). The release mechanism can be studied through the polymer bond-breaking of glucosamine(ethylene glycol) oligomers in three conditions: acid, normal (water) and base solutions. This simulation calculated the relative energy by B3LYP/6-31G//AM1 and B3LYP/6-31G//PM3 methods. The activated energies were 176.58, 166.60 and 257.57 kcal/mol by B3LYP/6-31G//AM1, and 145.51, 135.78 and 287.60 kcal/mol by B3LYP/6-31G//PM3. Interpreting from these energies, the doxorubicin can be released in acid and water solutions, but not in base solution because of the higher activated energy. The amount of ethylene glycol chains in glucosamine(ethylene glycol) has an effect on drug release. As the length of ethylene glycol increased, the drug release increased in the acid condition, but decreased in the normal and base conditions. When the drug was released from glucosamine(ethylene glycol) oligomers, this drug molecule, together with the glucosamine(ethylene glycol) molecule formed a micelle. The possibility of micelle formation was studied by the B3LYP/6-31G//PM3 method and showed that the ethylene glycol promoted the glucosamine(ethylene glycol) to form the micelle structure. If the length of ethylene glycol chains increases, the micelle structure is easily formed. According to micelle simulation, the ethylene glycol chain helps glucosamine(ethylene glycol) for micelle formation with doxorubicin. The optimum form is glucosamine-di(ethylene glycol) oligomer. The ethylene glycol group can carry doxorubicin in micelle formation to cancer cells.

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