STUDY OF DOXORUBICIN IN GLUCOSAMINE(ETHYLENE GLYCOL) OLIGOMERS BY MOLECULAR MODELING

INTRODUCTION

In the recent year, people suffer from tumor sick expressing by surrounding environment and nutrition. This situation induces the DNA transcription to generate wrong amino acid translation. This wrong amino acid can become bad protein and causes cancer cell. This cancer cell can occur in many organelles in body such as skin, lung, breast, intestine, and thyroid.

The cancer cell treatment can be done by several methods such as operation, irradiation, and drug dosing to tumor cell. Currently, the drug treatment is a method of interest because this method decreases pain from operation and risk to other cells from irradiation. The drug treatment is normally used in the drug delivery form. This drug delivery consists of drug and carrier molecule. This carrier contains the functional group to carry drug to cancer cell. The design drug blocks the wrong DNA code transcription. Doxorubicin is an interesting drug because it treats the cancer cell in other organelles such as breast cancer, ovarian cancer, transitional cell bladder cancer, bronchogenic lung cancer, thyroid cancer, gastric cancer, soft tissue and estrogenic sarcomas, neuroblastoma, Wilms' tumor, malignant lymphoma (Hodgkin's and non-Hodgkin's), acute myeloblastic leukemia, acute lymphoblastic leukemia and Kaposi's sarcoma related to acquired immunodeficiency syndrome (AIDS) (U.S. National library of medicine, 2007).

Steinfeld *et al*. (2006) studied doxorubicin to treat the T lymphocytes cancer cell by mobilizing immune cells as therapeutic drug carrier systems. The doxorubicin treatment needs drug carrier to bring to cancer cell target because this molecule has side effect such as heart damage, nausea and vomit. This effect may last up to 24-48 hours after treatment. The carrier molecule can be used in many forms such as encapsulation, nanoaggregation, hydrogel, and micelle formation. The encapsulation is very interesting in drug delivery because this molecule protects the drug and normal cell. There are several research studies in drug delivery.

This research studies the probability of drug release from capsule and micelle formation by molecular simulation. The capsule carrier is glycol chitosan, because this molecule can protect the drug and form micelle structure with drug. The drug molecule studied is doxorubicin. The glycol chitosan capsule has ethylene glycol as a carrying group. The drug release is studied by polymer bond breaking in solution effect. The micelle formation can be examined by charge structure between drug and glycol chitosan molecule. This work also studies the length effect of ethylene glycol chitosan chain to polymer bond breaking of glycolchitosan capsule. According to the molecule of glycolchitosan is very big structure, the glycolchitosan molecule is insisted of glucosamine(ethylene glycol) oligomers for decreasing computational time in study by simulation. This simulation used the monomer of glycolchitosan is in range of 1 to 8 monomers which the polyglycolchitosan is called glucosamine(ethylene glycol) oligomers.

Objectives

To study and simulate structural and energetic properties of drug released from drug delivery system by molecular modeling.

Scopes of work

1. To study a breaking bond of glucosamine(ethylene glycol) oligomers, this is polymer capsule.
2. To study drug structure after released from glucosamine(ethylene glycol) capsule.
3. To study mechanism of drug delivery to cell in micelle formation.
4. To use GaussViewW and GAUSSIAN 03W as simulation softwares.

Expected results

1. Use of molecular simulation to determine drug release from capsule and delivery formation to the cancer cell.
2. Improvement of capsule to protect and carrier drug to cancer cell.