*Available online at* www.pelagiaresearchlibrary.com

Pelagia Research Library

European Journal of Experimental Biology, 2012, 2 (3):641-645

ISSN: 2248 –9215
CODEN (USA): EJEBAU

# Theoretical study on physicochemical and geometrical properties of Doxorubicin and Daunorubicin conjugated to PEO-b-PCL nanoparticles

**S. Bagheri[1*], S. M. Hassani[2] and Gh. Naderi[3]**

*[1]Department of Chemistry, Quchan Branch, Islamic Azad University, Quchan, Iran*
*[2]Department of Chemical Engineering, Shahrood Branch, Islamic Azad University, Shahrood, Iran*
*[3]Department of Biochemistry, Shahed University, Tehran, Iran*

---

**ABSTRACT**

*Daunorubicin (or daunomycin) and Doxorubicin (or adriamycin or 14-hydroxydaunomycin) are well-known anti-cancer agents used in cancer chemotherapy. They are anthracycline antibiotics and are commonly used in the treatment of a wide range of cancers. Doxorubicin and Daunorubicin were chemically conjugated to PEO-b-PCL (poly(ethylene oxide)-block-poly(□-caprolactone)) nanoparticles. In this research, the molecular structure, Binding Energy(BE), Dipole Moment (DM), Gibbs free energy of solvation ($\Delta G_{(solvation)}$) and some physicochemical properties of the Doxorubicin- PEO-b-PCL and Daunorubicin- PEO-b-PCL were investigated. Our results indicate that these complexes mentioned above can be used to improve the anti-cancer activity.*

**Keywords**: Anti-cancer drugs, Molecular geometry, Doxorubicin, Daunorubicin, PEO-b-PCL nanoparticles.

---

## INTRODUCTION

Daunorubicin (or daunomycin) and Doxorubicin (or adriamycin or 14-hydroxydaunomycin) are well-known drugs used in cancer chemotherapy. Biochemical data confirms that these drugs make complexes with DNA thereby blocking the any replication or transcription [1-4]. Doxorubicin has a wide range of anti-cancer activity and has been used to treat severe lymphoblastic and myeloblastic leukaemias, malignant lymphomas of both Hodgkins and non-Hodgkins types, carcinoma of different parts of the human body, e.g. breast, lung, bladder, thyroid and ovary cancer, etc. [5-13]. Daunorubicin is specifically useful in the cure of leukemia in man. Although the structures of Doxorubicin and Daunorubicin are only slightly different, their activities differ significantly (Fig. 1).

During the past few decades, a lot of research in the field of pharmaceuticals has been focused upon the development of new dosage vehicles that can change the normal outcome of drugs in a biological system and direct them toward their cellular or sub-cellular targets. Nano-delivery systems having suitable stability, size, and surface properties have been designed in such a way that they are able to avoid permeation through continuous capillary in normal tissue, evade glomerular filtration in kidneys and avert reception by the reticuloendothelial system (RES), thereby, circulating for longer periods in the blood and finally accumulating in solid tumors through the enhanced permeability and retention (EPR) phenomenon. However, the accumulation in the tumor by the carrier does not guarantee a preferential access of the incorporated drug to its targets. Further to the aforementioned qualities for