Tarek M EL Gogary et al., Med chem 2016, 6:10(Suppl)
http://dx.doi.org/10.4172/2161-0444.C1.027

Synthesis of novel anthraquinone anti-cancer drugs: Molecular structure, molecular chemical reactivity descriptors and their interactions with DNA

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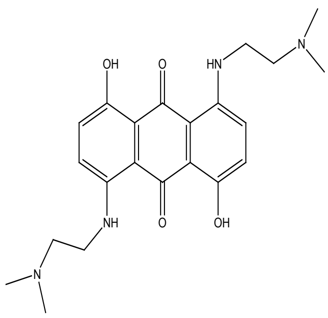
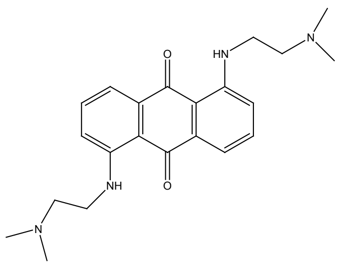
Background: Anthraquinones are well-known anticancer drugs. They carry out their cytotoxic activities through interaction with DNA and inhibition of topoisomerase II activity. Anthraquinones (AQ5 and AQ5H) were synthesized and studied with 5-DAAQ by computational and experimental tools.

Aim/Purpose: The purpose of this study is to shed more light on mechanism of interaction between anthraquinone DNA affinic agents and different types of DNA. This study will lead to gain of information useful for drug design and development.

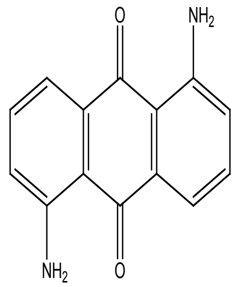
Methods: Molecular structures were optimized using DFT B3LYP/6-31+G(d). Depending on intra-molecular hydrogen bonding interactions four conformers of AQ5 were detected within the range of about 42kcal/mol. Molecular reactivity of the anthraquinone compounds was explored using global and condensed descriptors (electrophilicity and Fukui functions). NMR and UV-VIS electronic absorption spectra of anthraquinones/DNA were investigated at the physiological pH. The interaction of the anthraquinones (AQ5 and AQ5H) were studied with different DNA namely, calf thymus DNA, (Poly [dA]. Poly [dT]) and (Poly [dG].Poly [dC]). UV-VIS electronic absorption spectral data were employed to measure the affinity constants of drug/DNA binding using Scatchard analysis.

Results: NMR study confirms qualitatively the drug/DNA interaction in terms of band shift and broadening.





AQ5H



1,5-DAAQ

AQ5

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