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Binding studies of complexes of anticancer drugs with DNA and enzymes involved in DNA replication using molecular docking and cell culture techniques

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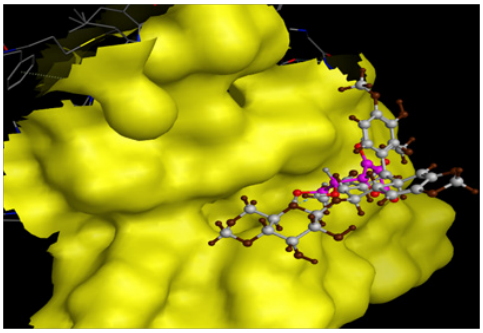
The presently studied twelve anticancer drugs are the cytotoxic agents which inhibit the replication of DNA and activities of enzymes involved in DNA replication namely topoisomerase-II, polymerase and helicase and have shown remarkable anticancer activity in clinical trials. In the studied work, we performed molecular docking studies of twelve antitumor drugs against DNA and DNA enzymes in the presence and absence of ascorbic acid (AA) and developed the quantitative structure activity relationship (QSAR) model for anticancer activity screening. A number of electronic and steric descriptors were calculated using MOE software package. QSAR was established showing a correlation of binding strength with various physicochemical descriptors.



Out of these twelve, eight cytotoxic drugs were tested on non small cell lung cancer cell lines (H-157 and H-1299) in the absence and presence of ascorbic acid and experimental IC_{50} values were calculated. From the docking studies binding constants were calculated indicating the strength of drug-DNA and drug-enzyme complex formation and it was correlated to the IC_{50} values (both experimental and theoretical). These results can offer useful references for directing the molecular design of DNA enzyme inhibitor with improved anticancer activity.

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