Analysis of Quantitative Structure-Activity Relationship, Pharmacophore, and Molecular Docking of Tetracyclic Indenoquinoline Derivatives as Anticancer Agents

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Abstract: Topoisomerases have been the focus in the treatment of some diseases, such as bacterial gyrase (topoisomerase II) and topoisomerase IV which are the target of two classes of antibiotic drug: quinolones and coumarins; likewise Topoisomerase I and topoisomerase II are in cancer treatment. QSAR analysis has been performed on *tetracyclic indenoquinoline* derivatives as anticancer agents in three cell lines (HeLa, A-549, and MCF-7 cells). Ligand interaction analysis was performed by docking the derivatives against topoisomerase I receptor. Furthermore, the design of new derivatives and their prediction activities were based on the result of QSAR analysis and their interaction using MOE software. Design of new derivatives resulted 10 compounds that have been predicted better in biological activity than that of analogous compounds (camphtetocine) and the test compounds.

Keywords: QSAR, tetracyclic indenoquinoline, HeLa, A-549, MCF-7, pharmacophore, docking molecule.

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