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(57) Abstract :
COMPUTATIONAL AND EXPERIMENTAL INSIGHTS INTO GLYCYRRHIZIN-LOADED NANOSTRUCTURED LIPID CARRIERS: DOCKING, DYNAMICS, DESIGN OPTIMIZATION, AND ANTICANCER EFFICACY IN LUNG CANCER CELLS Lung cancer (LC) remains a predominant global health concern, especially with escalating tobacco-smoking rates. Present study provides computational screening, molecular dynamics, DFT and simulation analysis of phytoconstituents on EGFR receptors (2ITY and W2O), followed by selection of highest docking score phytoconstituents among 45 for further analysis. Glycyrrhizin was found to possess maximum docking score -8.863 and -8.837 on both 2ITY and W2O respectively. The study unveils glycyrrhizin's interactions with EGFR pivotal in cancer progression and treatment. Molecular dynamics simulations highlighted the structural and dynamic interactions within a protein-ligand complex, indicating both stability and flexibility characteristics. DFT analysis of Glycyrrhizin revealed its molecular properties, suggesting stability and potential reactivity. Glycyrrhizin loaded nanostructured lipid carriers (GNLC) have been developed and analysed by various parameters like particle size and drug release zeta potential, SEM analysis, spectroscopic (UV, IR) and solubility analysis etc reveals critical insights into their optimization for effective drug delivery. The anticancer potential of GNLC have been further proved by experimental analysis through MTT assay. Both GNLC and Doxorubicin (0.78-50 µg/ml) were used for the activity. The anticancer potential at 12.50, 25 and 50µg/ml pf GNLC was found to be statistically significant and was comparable with that of standard group Doxorubicin. The observed structural transformations in Glycyrrhizin into a lipid matrix indicate potential enhancements in its bioavailability. The study concludes by emphasizing Glycyrrhizin's potential as a potent anticancer agent, acting through EGFR inhibition and influencing DNA replication processes will be more effective in GNLC formulation when compared with that conventional one.

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