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(57) Abstract :
The Present Invention says that in the United States, lung cancer is the biggest cause of cancer-related mortality, ranking in second only to colon cancer. As of 2020, 247,270 persons had been diagnosed with lung cancer, with a total of 116,930 of those cases being women and 130,340 of those being males. EGFR is a type of tyrosine kinase receptor which promotes uncontrolled cell division. In some types of cancer cells, genetic mutation (EGFR) promotes the EGFR proteins at greater levels than normal. By inhibiting EGFR may be useful for preventing or reducing the growth of lung cancer against NSCLC. In this study 16 phyto-chemicals were selected from IMPPAT, a manually curated database. The crystal structure of EGFR kinase domain (2ITY and 3WTO) was downloaded from Protein Data Bank. These derivatives' binding affinities were predicted using Glide, which indicated that EGFR-kinase inhibitors had good binding energies, ranging from -10.49 to -3. 643 kcal/mol. Olmutinib and Osimertinib are used as standard. All the compounds were examined for their ADMET characteristics using SwissDock. The docking results were validated by molecular dynamics simulations to show the durability of hydrogen bonding interactions. Results reveals that Epigallocatechin Gallate (EGCG) had superior docking score when compared with both the standard drugs. The possible Mechanism of action of EGCG in treatment of cancer by modifying cell signalling pathways is also explored.

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