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Anticancer and Molecular Docking Studies of Chalcone Derivatives

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Abstract: Chalcone derivatives namely (2E)-3-(4-hydroxy-3-ethoxyphenyl)-1-(4- hydroxyl phenyl) prop-2-en-1-one – (HEHP) and (2E)-3-(3,4dimethoxy phenyl)-1-(1-hydroxy-2 napthyl)prop-2-en-1-one – (DHNP) were synthesized by acid/ base catalyzedClaisen-Schmidt reaction. The cytotoxic activities of the compounds against normal Vero cell and breast cancer MCF7 cell lines were assessed by MTT assay method. Since cytotoxicity is inversely proportional to the cell viability, higher IC_{50} values with the Vero cell line suggests that the compounds are greatly non- toxic to normal Vero cell line. The IC_{50} values of 7.8 and 62.5µg/ml, exhibited against the MCF7 cells by the derivatives, HEHP and DHNP suggest the significant anticancer activity of the compound HEHP. Induced fit docking analysis was also carried out for the compounds and is compared with the same co-crystal ligand. The exemestane (co-crystal) has docked well at the active site of target protein O-H...N and O-H...O hydrogen bonds involving oxygen atom of the co-crystal with the nitrogen atom of the amino acid residue MET 374 and Oxygen atom of the residue Thr310, at a distance of 2.86 and 2.90Å, respectively, with the glide score of -9.473 and glide energy of -48.055Kcal/mol. The compounds HEHP and DHNP have been observed to be at the active site of target protein with the glide score of –8.505, -8.330 and glide energy of - 41.503, -50.661 Kcal/mol, respectively, which are comparable with the corresponding values of the co-crystal.
Keywords: Chalcone, Anticancer activity, cytotoxicity, Docking study, IC_{50} value, glide score, glide energy.

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