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Molecular docking and dynamic simulation of phytochemical components from *Clitoria ternatea* against different hormone-dependent cancer cell lines

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Creating novel non-toxic drug candidates targeting breast cancer (BC) cells with no effects on normal cells is at the top of research objectives. Blue *Clitoria ternatea* (*C. ternatea*) flowers were macerated in ethanol and evaporated using a precision economy incubator at 40°C to isolate the major phytochemical compounds. The GC-MS technique was used to identify the chemical structure of isolated components. Molecular docking, molecular dynamic simulation, and pharmacokinetics analytical tools were used to measure the binding affinity, stability, and solubility degree of isolated compounds bound to caspase-3. Normal HSF and different BC cell lines were grown for 24 h and 48 h to evaluate antiproliferative and caspase-3 activity against the metastatic BC cell line (of interest) MDA-MB-231. Computational analysis of compound 4CT: CID-22212496 (Cholesta-8,24-dien-3-ol) showed poor solubility, stable binding affinity (–7.6 kcal/mol), and strong interactions across several amino acid residues. Antiproliferative experiments showed no toxic activities of isolated compounds on cell growth of the normal cell line HSF with a IC_{50} value of 869.6±5.04 µg/mL compared to cells treated with DOX following 24 h. In contrast, significant inhibition of cell viability was observed, particularly in the BC cell line MDA-MB-231, with IC_{50} values of 363.06±6.94 µg/mL and 209.4±4.06 µg/mL following 24 h and 48 h, respectively, with increased levels of caspase-3 enzyme (*p-value* < 0.001). We suggest that the Cholesta-8,24-dien-3-ol compound may have potential anticancer activity by blocking the estrogen receptor and consequently inhibiting estrogen biosynthesis through the activation of the intrinsic caspase-3 pathway.

Keywords: Blue tea flowers, Caspase-3, Cholesta-8,24-dien-3, Cytotoxicity, Pharmacokinetics, Metastatic TNBC cells