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Identification of Natural Estrogenic and Anti-estrogenic Compounds for Treating Cancers in Humans Using Bioinformatics Approach

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Medicinal compounds play a vital role in healthcare system of world's population. They help to cure various diseases including cancer without causing toxicity. About 50% drugs in clinical use are obtained from natural products and they have the ability to control cancer cells. Over 1400 genera of herbs have a history for being used in cancer treatments. The base for drug discovery which includes isolation and characterization of pharmacologically active compounds from plant sources is a dynamic research field worldwide. There is an increasing demand to identify and analyze the target proteins with active sites and potential drug molecules that can bind to their sites specifically. Hormones such as estrogen and progesterone play a very important role in human growth and are responsible in regulating the complex cellular events associated with differentiation, function and growth of female reproductive tissues. Natural estrogens mostly used include estradiol (E2), estrone (E1) and estriol (E3) and genistein (from soy and red clover), which are reported to have no side effects. These phytoconstituents may act as natural alternatives for Hormone Replacement Therapy (HRT). Some phytochemicals have also been shown to possess antiestrogenic activity by suppressing estrogen mediated transcriprtion or proliferation. This study was aimed to identify phytoestrogens acting as estrogens or antiestrogens using Computer Aided Drug Designing (CADD) approach. The receptor site is known (ET-α) so we used receptor based molecular design or structure based drug design using docking through Database searching or Virtual screening. 11 different compounds were selected based upon Lipinski Rule of Five and toxicity, which served either as agonist or antagonist for ET-α receptor. These compounds were targeted to identify their effect on the receptor by docking and finally an effective anticancerous compound was chosen based upon its binding interactions and energy using scoring functions.