

Insilico analysis of biologically active plant products against cancer causing agents

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ABSTRACT

The deadliest disease in the world which is the reason behind 9.5 million people's death over the world. According to the WHO ovarian cancer is the most neglected cancer in women out of all cancers. The traditional medicine is having side effects as reoccurrence of the tumours in case of surgery, hair fall in chemotherapy and leading to other diseases. Thus, there is an extreme thrive for the alternate medicine other than traditional ones. To achieve this, we can seek from the mother nature which is a source of abundant medicinal plants whose potential is still unrevealed. Such plants are collected and the biologically active compounds are extracted from the plants which are capable of anti-cancer activity by literature review. These compounds are optimised under ligand preparation for further docking process. The proteins which are cancer causing potential exists are retrieved and pre-process of proteins is done. As the protein and ligand are prepared a grid formation is done where the specific coordinates of protein are fixed to form a grid where docking can take place. Now the prepared macromolecule and micro molecule are further proceeded to dock. The post docking analysis is done through manual visualization. The highly docked secondary metabolites are filtered according to the docking score and energy calculated. These potentially worth biologically active compounds of plant against ovarian cancer can further investigated for a promising drug for alternate treatment of ovarian cancer.

Keywords: Molecular Docking, Ovarian cancer, Plant secondary metabolites, biologically active compounds, Alternative medicine.

