



## **SILICOMOLECULAR DOCKING IN ANTICANCER POTENTIAL OF ISOLATED PHYTOCHEMICALS FROM HOPEA ODORATA AGAINST BREAST CANCER**

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**Abstract:**

**Objective:** Breast cancer could be a variety of cancer that develops from breast cells.

Carcinomas ordinarily originate the inner lining of milk ducts or the lobules that provide them with milk. a malignancy will unfold to different components of the body. . Cancer will unfold throughout one or each breast. Typically carcinoma spreads to different components of the body just like the bones the liver or elsewhere Moya et al. 2004 carcinoma in ladies could be a foremost unhealthiness each in developed and developing countries. The most issue of carcinoma is steroid hormone receptor alpha the current analysis was to screen the effective bioactive compounds from hopea-odorata.

**Methods:** The molecular docking approach can be used to model the collaboration between a small molecule and a protein at the nuclear level, which allow us to characterize the conduct of small molecules in the binding site of target proteins as well as to elucidate essential biochemical processes The docking process contains two basic steps: prediction of the ligand conformation as well as its position and orientation within these sites (usually referred to as pose) and assessment of the binding affinity

**Result:** specifically 4-hydroxyacetophenone bisnorstriatol grasshopper organic compound pcoumaric acid which can be very important inhibitors of steroid hormone receptor alpha  $\text{er-}\alpha$

for looking a drug against the carcinoma A large vary of docking score found throughout molecular docking by Schrodinger. ampelopsin h balanocarpol betulinic acid betulonic acid caryophyllene oxide friedelin showed the docking score -6.141 -1.823 -4.420 -3.976 -7.324 -4.510 respectively. Among all the compounds caryophyllene oxide showed the best docking score towards estrogen receptor alpha.

**Conclusion:** so caryophyllene oxide is the best compounds for focusing inhibitors of estrogen receptor alpha because it possessed the best value in molecular docking.

**Key Words**

Breast cancer ,Hopea odorata, Estrogen receptor alpha, Ampelopsin H, Balanocarpol, Betulinic acid, Betulonic acid, Caryophyllene oxide, Friedelin

## Introduction

The breast cancer rate is rising worldwide with a rise in violent neoplasia's in young women.[1]and a significant public health problem. The incidence is growing in most countries and is projected to increase any over future twenty years in spite of current efforts to avoid the illness.[2-5]The boosted incidence is not shocking since there has been, in most countries, growth in numbers of women with key breast cancer risk factors, as well as lower age of start, late age of first maternity, fewer pregnancies, shorter or no periods of breastfeeding, and later menopause. Alternative risk issues which boost the burden of carcinoma are the rise in fatness, alcohol intake, laziness, and hormone replacement therapy (HRT).[5] Breast cancer most typically Mature in cells from the inside layer of milk ducts and therefore the lobules that give the ducts with milk. Cancers developing from the ducts area unit referred to as ductal carcinomas, whereas those developing from lobules area unit referred to as lobe carcinomas.[6] The report of carcinoma is Designated by taking a biopsy of the about lump. Once the title is made, any experiments are done to see if cancer has unfolded on the far side the breast and that treatments it should reply to.[6] The molecular docking approach can be used to model the collaboration between a little molecule and a protein at the nuclear level, which permit us to characterize the conduct of small molecules in the binding position of mark proteins as well as to explain necessary biochemical processes The docking process include two fundamental steps: prediction of the ligand conformation as well as its position and orientation within these sites (usually referred to as pose) and assessment of the attraction affinity. Hopea odorata is a species of plant in the Dipterocarpaceae family which originates in Bangladesh, Cambodia, India, Malaysia, Myanmar, Thailand and Vietnam.[8] It is a large tree growing up to 45 m in height with the base of the trunk increasing a diameter of 4.5 m. It grows in woodlands, preferably near canals. In places such as West Bengal and the Andaman Islands, it is often planted as a shade tree.[9] Valued for its wood, it is a threatened species in its natural environment.[10] The dammar of this tree is stated to have medicinal assets utilized in treating sores and wounds.[11]Phytochemical studies informed that the heartwood of H. Odorata has certain kinds of phenolic compounds. These polyphenols are said to be beneficial as antioxidants, anticarcinogens, scavengers of free radicals and therefore have implications for the inhibition of pathologies such as cancer and cardiovascular

disease,[13,14] The goal of this Research was to monitor out the actual bioactive compounds from Hopeadorata, which can be potential inhibitors of estrogen receptor alpha (ER- $\alpha$ ) in future and may act as a drug which may be effective in preventing the breast cancer

## **MATERIALS AND METHODS**

### **In silico analysis**

#### **Molecular docking analysis of isolated compounds**

##### **Protein Preparation**

Three-dimensional crystal Structure of estrogen receptor alpha (PDB id: 3ERT) was taken in pdb format from the protein data store. After that, the structure was organized and developed using the Protein Preparation Wizard of Schrödinger-Maestro v10.1. Charges and bond orders were allocated, hydrogens were added to the heavy atoms, selenomethionines were converted to methionines, and all waters were deleted. Using force field OPLS\_2005, minimization was carried out setting extreme heavy atom RMSD (root-mean-square deviation) to 0.30 Å.[15, 16]

##### **Ligand Preparation**

Compounds were retrieved from PubChem databases, i.e. Ampelopsin H, Balanocarpol, Betulinic acid, Betulonic acid, Caryophyllene oxide, Friedelin. [17-19]

##### **Glide Standard Precision (SP) ligand docking**

SP flexible ligand docking was carried out in Glide of Schrödinger-Maestro v 10.1 within which penalties were convenient to non-cis/trans amide bonds. Van der Waals scaling factor and partial charge cutoff were designated to be 0.80 and 0.15, respectively for ligand atoms. Final scoring was performed on energy-minimized poses and displayed as Glide score. The best -docked pose with lowest Glide score value was recorded for each ligand

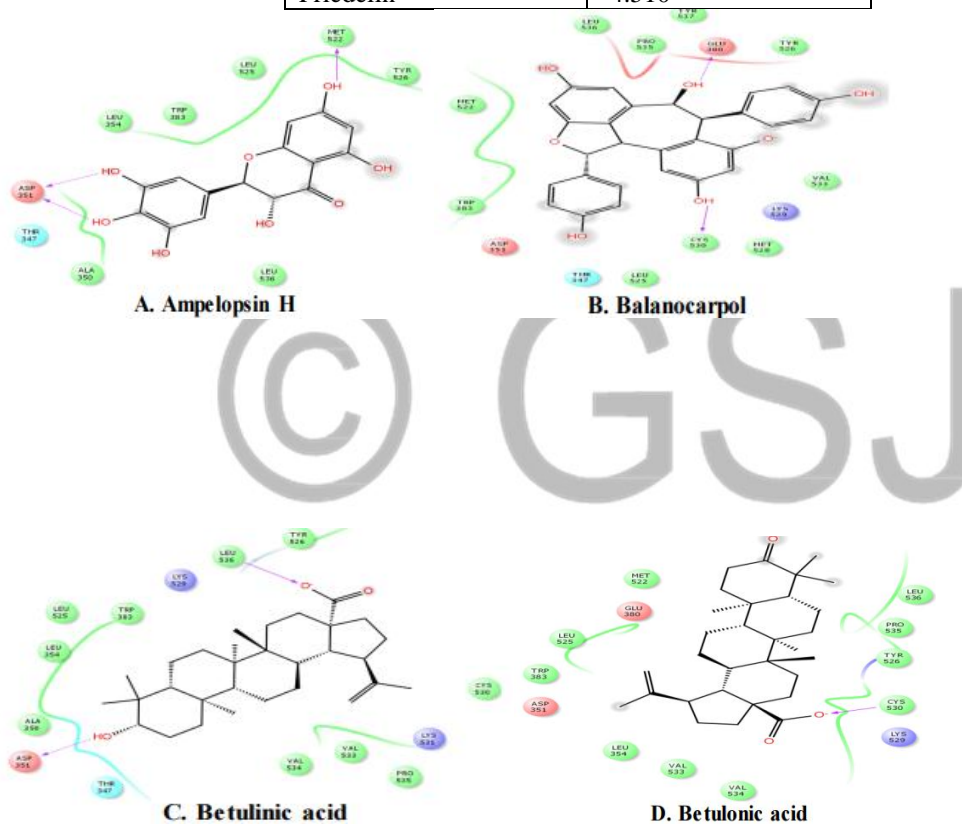
### **In silico analysis**

#### **Molecular docking analysis**

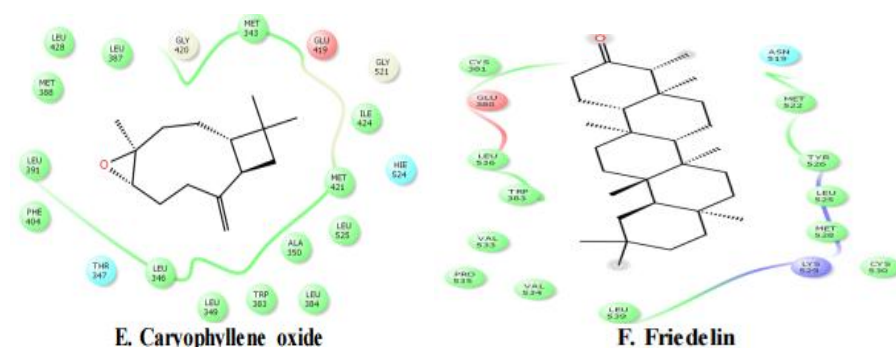
A number of scientific studies show that aberrance in redox balance with an elevated level of oxygen-free radicals, reactive oxygen species (ROS), and reactive nitrogen species (RNS) plays a significant role in the source and progression of most human diseases including cancer.[23, 24] Reactive oxygen species (ROS) act as a secondary messenger in intracellular signaling cascades and elevated level of ROS related to carcinogenesis by supporting the initiation, progression, and metastasis of cancer cells. It also induced DNA injury leading to genetic lesions that initiate tumorigenicity and subsequent tumor progression.[25] Extracts of medicinal plants have been used for the treatment of various diseases, as well as cancer all over the world, as they are easily prepared, standardized, and stored. Herbal extracts are also charged effective which development their accessibility to the patients of all financial status. [26, 27] Global health policies sponsor the therapeutic use of the herbal extract. World Health Organization (WHO) also encourages the use of medicinal plants in the treatment of disease.[28] Medicinal plants used for health benefit are not taken under the appropriate instruction and consultant of a physician. The current approach to discover a new drug molecule includes either isolation from a natural source or the synthesis of a particular compound responsible for a therapeutic effect.[29] And in the silico way of finding new potential compounds from the isolated compounds of the plant becoming more standard over the years. In this study, the binding mode of estrogen receptor was investigated by doing computational analysis, glide docking. In cooperation glide standard (SP) and extra precision (XP) mode had been presented, where extra precision mode used for cross-validation purpose. The results of docking analysis were described in Table 1 and the docking figure showed in Figure 1. Binding energy is the primary parameter which is generated as a result of molecular docking. It provides us the idea of strength and affinity of the collaboration between the ligand and the receptor. The larger the binding energy is, the weaker the contact is and vice versa. Thus, during any docking study, we put forward to look for the ligand which displays the least binding energy, thus the best affinity among the test molecules.[30] Among all the compounds, Caryophyllene oxide showed a good docking score.

**Table 1:** Docking results of Ampelopsin H, Balanocarpol, Betulinic acid, Betulonic acid, Caryophyllene oxide, Friedelin with estrogen receptor alpha (PDB: 3ERT). Compound Name Docking Score Glide emodel Glide energy

Compound Name	Docking Score
Ampelopsin H	-6.141
Balanocarpol	-1.823
Betulinic acid	-4.420
Betulonic	-3.976
Caryophyllene oxide	-7.324
Friedelin	-4.510



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**Figure 1:** Docking results of A. Ampelopsin H, B. Balanocarpol, C. Betulinic acid, D. Betulonic acid, E. Caryophyllene oxide, F. Friedelin with estrogen receptor alpha (PDB: 3ERT).

**Conclusion:**

Among all the compounds Caryophyllene oxide showed best docking score towards estrogen receptor alpha. So, Caryophyllene oxide is the best compounds for selective inhibitors of estrogen receptor alpha, as it possessed best worth in Molecular docking. Further in vitro and in vivo study need to recognize estrogen receptor alpha inhibitory activity of isolated compounds from. *Hopes odorata*

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**Consent for publication**

Not applicable

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