

## عنوان مقاله:

In Silico Molecular Docking Studies of Natural Herbal Compounds as Aromatase Inhibitor in Breast Cancer Treatment

## محل انتشار:

یازدهمین کنگره بین المللی سرطان پستان (سال: 1394)

تعداد صفحات اصل مقاله: 2

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## خلاصه مقاله:

**INTRODUCTION:** Breast cancer is the second most common cancer worldwide and the most common malignancy in women. Aromatase, a cytochrome P450 enzyme is a key enzyme that plays a critical role in catalyzing the conversion of androgen substrates into estrogens and has a major effect in estrogen-dependent disease like breast cancer. Aromatase inhibitors (AIs) can stop the abnormal over expression of aromatase in postmenopausal women with estrogen receptor positive breast cancer. The purpose of this study is to analyze the potential inhibitory action of natural herbal AIs by computational docking studies. **MATERIALS AND METHODS:** In this study, molecular docking study of Exemestane (FDA approved drug) and six phytochemical compounds, including alkaloids (Berberine, Piperine), terpenoids (Spinasterol, Ursolic acid), flavonoids (Cyanidin, Amorphigenin) with aromatase (PDB ID: 3S79) has been done using Autodock 4.2.6. **RESULTS:** Molecular docking studies have indicated that among these six naturally AIs, Spinasterol showed higher binding affinity compared to others with the lowest binding energy (-10.14kcal/mol) and the high potential antibreast cancer activity. While, the lowest binding energy was observed in Cyanidin (-6.7kcal/mol). The binding energy of Exemestane to aromatase (- 9.75kcal/mol) was higher than Spinasterol. **Conclusion:** Natural herbal products that have been used traditionally as nutrition or medicine may also act as AIs. Current data show the potency of these herbal compounds to be effective in breast cancer chemoprevention or chemotherapy for postmenopausal women by less toxicity and more selectivity than chemical inhibitor and discovery of novel inhibitors in clinical

## کلمات کلیدی:

Molecular docking; Aromatase inhibitors; Herbal compounds; Breast cancer

## لینک ثابت مقاله در پایگاه سیویلیکا:

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