

## In silico study of curcumol, curcumenol, isocurcumenol and B-sitosterol as potential inhibitors of estrogen receptor alpha of breast cancer

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Deskripsi Lengkap: <https://lib.ui.ac.id/detail?id=20496674&lokasi=lokal>

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### Abstrak

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Based on data from the Hospital Information System (HIS) in 2007, breast cancer is the top ranked diagnosed cancer in Indonesia. Estrogen receptor alpha (ER $\alpha$ ) is associated with breast cancer because it is found in high levels in cancer tissues. Curcumol, curcumenol, isocurcumenol of white tumeric rhizomes (*Curcuma zedoaria* (Christm.) Roscoe), and  $\beta$ -sitosterol from seeds of pumpkin (*Cucurbita pepo* L.) have been reported to have inhibitory activity against cancer cells. This study presents the in silico study of these compounds as inhibitors of ER $\alpha$ .

**Methods:** Docking simulations are carried out in this paper to visualize molecular-level interactions between the four compounds with ER $\alpha$ . Docking simulations between estradiol and tamoxifen on ER $\alpha$  are carried out as well.

**Results:** Docking results indicated that curcumol, curcumenol, isocurcumenol, and  $\beta$ -sitosterol showed inhibitory activity againsts estrogen receptor alpha (ER $\alpha$ ). The order of potency is shown consecutively by isocurcumenol, curcumol, curcumenol, and  $\beta$ -sitosterol with values 0.584 M, 1.36 M, 1.61 M, and 7.35 M respectively. Curcumenol and estradiol interacts with ER $\alpha$  through hydrogen bonds and hydrophobic interactions, whereas curcumol, isocurcumenol,  $\beta$ -sitosterol and tamoxifen through hydrophobic interactions in succession.

**Conclusion:** Natural products containing all four compounds have the potential to be used as drugs or adjuvant drugs in breast cancer therapy.