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

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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 (ERα) 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 β-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 ERα.

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

Results: Docking results indicated that curcumol, curcumenol, isocurcumenol, and β-sitosterol showed inhibitory activity againts estrogen receptor alpha (ERα). The order of potency is shown consecutively by isocurcumenol, curcumol, curcumenol, and β-sitosterol with values 0.584 M, 1.36 M, 1.61 M, and 7.35 M respectively. Curcumenol and estradiol interacts with ERα through hydrogen bonds and hydrophobic interactions, whereas curcumol, isocurcumenol, β-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.