عنوان مقاله:

Comparative Study of binding affinity of Tamoxifen and Ridaifen-B drugs to the estrogen receptor in breast cancer cells in the In silico

محل انتشار:

یازدهمین کنگره بین المللی سرطان پستان (سال: 1394)

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خلاصه مقاله:

Background: One of the ways of enhancing the ability of cancer cells to multiply is by utilizing growth hormone receptors. Estrogen receptor(ER),is a hormone receptor and 80% of breast cancers are ER-positive. ER-α subtype is a transcription factor that induces the growth and differentiation of cancer cells through agonistic activity of estrogen hormone. Instead of the estrogen,Tamoxifen binds to ER-α,leading to inhibition of breast cancer cell proliferation and resulting in apoptosis. Ridaifen-B is a Tamoxifen derivative. Methods: First, the structure of ER and Tamoxifen from PDB and Ridaifen-B from Pubchem were received.The ER-α selection and determination of ligand binding site through Discovery Studio3.0 Client, docking and data analyzing by AutoDockTools4.2.6, the study of conformations and bindings through Pymol and the comparison and valuation of the data using SPSS, were accomplished. Results: The data from the calculations in 5 conformations for both ligands,for following values: Binding Energy, kI, Intermolecular Energy, Internal Energy, Torsional Energy, Unbounded Extended Energy, Cluster RMS and Ref RMS demonstrates more binding affinity of Ridaifen-B to ER-α compared with Tamoxifen. Conclusion: Due to the increasing resistance to Tamoxifen in cell lines of breast cancer MCF-7 and considering the results of the calculation of the interaction of receptor-ligand, it seems that Ridaifen-B can be a good alternative to Tamoxifen in the treatment .of breast cancer

کلمات کلیدی:

Breast Cancer,Tamoxifen,Ridaifen-B,AutoDockTools