6th International Conference on
Obstetrics, Infertility and Mental health

Investigation of the interaction of tamoxifen drug with p70 S6 kinase protein using molecular docking analysis

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Abstract

To determine the consequence and activity of drugs, the evaluation of binding of drug with protein is a key process in cancer treatment. Molecular docking is a computational simulation method for analysis of the conformation of a drug molecule into the binding site of a protein macromolecule. In this research, molecular docking analysis was applied to investigate the interaction of tamoxifen (TAM) drug with p70 S6 kinase protein. The information of the mentioned drug and protein were obtained from pubchem.ncbi.nlm.nih.gov and www.uniprot.org sites, respectively. The simplification of p70 S6 kinase protein was performed using Chimera software. Then, the molecular docking process was started using PyRx software. According to the values of binding affinity and RMSD obtained from docking analysis, it was predicted that TAM drug possessed an appropriate interaction with P70 S6 kinase protein. Thus, TAM-P70 S6 kinase protein docking was a predominant binding mode. The TAM drug can be used as an inhibitor in the growth of cancer cells.

Keywords: Molecular docking, Tamoxifen, p70 S6 kinase, Protein, binding affinity

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