Molecular Docking and Dynamics (MD) Simulation of 6-gingerol and 6-shogaol Against Human Estrogen Receptor Alpha (ER alpha)

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Abstract

Simulation and computational analysis of 6-gingerol and 6-shogaol is done to evaluate their binding affinity against ER alpha. Active site prediction was done using Computed Atlas of Surface Topography of Proteins (CASTp) to determine the binding pocket of ER alpha. Molecular docking and molecular dynamics (MD) simulation were done to assess the binding affinity and stability of the ligand-ER alpha complexes formed. Results showed that Tamoxifen have lowest binding energy (-9.61 +/- 0.39 kcal/mol) followed by 6-gingerol (-6.59 +/- 0.29 kcal/mol) and 6-shogaol (-5.70 +/- 0.36 kcal/mol). Inhibition constant (Ki) range of TMX-ER alpha was found to be drastically lower than both 6GN-ER alpha and 6SG-ER alpha. Based on the difference in the binding energy range and inhibition constant, 6-gingerol and 6-shogaol showed less potential in substituting tamoxifen for the inhibition of ER.. Docking complexes formed was supported with stability in root mean square deviation (RMSD) and total binding energy of the complexes. The study is concluded that 6-gingerol have high level of interactions with the ER alpha active site in terms of hydrogen bonding whereas hydrophobic interactions are observed with both 6-gingerol and 6-shogaol. However, both ginger bioactive compounds poses low potential as substitute in comparison with tamoxifen against ER alpha.

Keywords

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