Molecular Docking Analysis of 6-paradol, Zingerone and Zerumbone Against Human Estrogen Receptor Alpha (ER alpha)

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INTERNATIONAL JOURNAL OF INTEGRATED ENGINEERING
Volume: 10 **Issue:** 6 **Pages:** 113-118 **Special Issue:** SI
DOI: 10.30880/ijie.2018.10.06.015
Published: 2018
Document Type: Article

Abstract

Molecular docking was done to assess the binding affinity of 6-paradol (6PRD), Zingerone (ZGR) and Zerumbone (ZRB) ligand-ER alpha complex in comparison to Hydroxytamoxifen (HTMX). Docking results showed that Glu353 and Arg394 active residues forms hydrogen bonding with 6PRD and ZGR. Glu353, Leu387 and Arg394 were the three identical residues found to formed hydrophobic interaction in HTMX-ER alpha, 6PRD-ER alpha and ZGR-ER alpha. HTMX showed lowest binding energy (-10.71 +/- 0.43 kcal/mol) followed by ZRB (-8.66 +/- 0.04 kcal/mol), 6PRD (-6.92 +/- 0.14 kcal/mol) and ZGR (-5.93 +/- 0.31 kcal/mol). Inhibition constant (Ki) range of 6PRD-ER alpha was found to be drastically lower than HTMX-ER alpha, ZGR-ER alpha and ZRB-ER alpha. Based on the docking analysis, the three bioactive compounds were showed to poses low potential as substitute towards tamoxifen. Future study is recommended for analysing 6PRD potential in substituting estradiol as Hormone Replacement Therapy (HRT) for breast cancer.

Keywords

Author Keywords: 6-paradol (6PRD); Zingerone (ZGR); Zerumbone (ZRB); Hydroxytamoxifen (HTMX); ligand-ER alpha complex; molecular docking
KeyWords Plus: HUMAN BREAST-CANCER; BETA

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Funding

Funding Agency	Grant Number
International Islamic University Malaysia	RIGS 15-120-0120

View funding text

Publisher

UNIV TUN HUSSEIN ONN MALAYSIA, 86400 PARIT RAJA, BATU PAHAT, JOHOR, 00000, MALAYSIA

Categories / Classification

Research Areas: Engineering
Web of Science Categories: Engineering, Multidisciplinary

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