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International Journal of Integrated Engineering
Volume 10, Issue 6, 2018, Pages 113-118

Molecular docking analysis of 6-paradol, zingerone and zerumbone against human estrogen receptor alpha (ERα) (Article)

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Abstract

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Molecular docking was done to assess the binding affinity of 6-paradol (6PRD), Zingerone (ZGR) and Zerumbone (ZRB) ligand-ERα 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-ERα, 6PRD-ERα and ZGR-ERα. 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-ERα was found to be drastically lower than HTMX-ERα, ZGR-ERα and ZRB-ERα. 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. © Penerbit UTHM.

Author keywords

6-paradol (6PRD) | Hydroxytamoxifen (HTMX) | Ligand-ERα complex | Molecular docking | Zerumbone (ZRB) | Zingerone (ZGR)

ISSN: 2229838X
Source Type: Journal
Original language: English
Document Type: Article
Publisher: Penerbit UTHM

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