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Ruiwen Zhang
Texas Tech University Health Sciences Center
1300 Coulter Drive
Amarillo, TX 79106
USA

The Structural Bioinformatics analysis of Biophenolic Lignan-Estrogen Receptor interaction
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Author(s): Farzaneh Mohamadyar-Toukanlou, Mina Esfandiari, Mahshid Sadat Kashef-Saberi, Mahboubeh Kabini Renani, Masoud Soleimani.

Abstract:
Background: Plant lignans have proven efficacious in blocking estrogen receptors of breast cancer cells. However, available studies have mostly dealt with anti-cancer effects of groups of lignans in certain foods or plants and the effects of specific lignans, especially from a molecular interaction viewpoint, has been rarely addressed in the literature. Objective: We aimed to computationally predict the binding ability and binding strength of pinosinol, matairesinol, lariyiresinol and secoisolariciresinol as potent ligands of estrogen receptor alpha (ER-α), in order to study these lignans as drugs. Methods: Blind Docking method was utilized to predict the binding orientation of lignans to their targets by AutoDock 4.2 software. Docking results of lignan-receptor complexes were compared to tamoxifen-receptor complex separately. Hydrophobic interactions and hydrogen bonds between lignans and ER were perfused and the binding energy was calculated. Results: The best binding affinity of tamoxifen, matairesinol, pinosinol, lariyiresinol and secoisolariciresinol were respectively -8.7, -7.5, -6.7, -6.7, -5.8 kcal/mol, and matairesinol showed the minimum binding energy than other studied lignans. Matairesinol showed the most similar interactions with tamoxifen with small molecule-receptor complex in the following residues: Leu 391, Ala 350, Ile 424 and Phe 404. Conclusion: Among the studied lignans, matairesinol showed the least binding energy as well as the most similar hydrophobic interactions to tamoxifen suggesting that matairesinol can display more efficacious biological activity to inhibit ER in comparison with pinosinol, lariyiresinol and secoisolariciresinol. Thus, our results introduce matairesinol as a potentially effective anti-ER drug.

Keywords: Biophenolic lignan, Structural bioinformatics, Matairesinol, Docking

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