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Molecular Docking of Marrubiin in Candida Rugosa Lipase

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Abstract : Infections caused by Candida species manifest in a number of diseases, including candidemia, vulvovaginal candidiasis, endocarditis, and peritonitis. These Candida species have been reported to have lipolytic activity by secretion of lipolytic enzymes such as esterases, lipases and phospholipases. These Extracellular hydrolytic enzymes seem to play an important role in Candida overgrowth. Candidiasis is commonly treated with antimycotics such as clotrimazole and nystatin, which bind to a major component of the fungal cell membrane (ergosterol). This binding forms pores in the membrane that lead to death of the fungus. Due to their secondary effects, scientists have thought of another treatment basing on lipase inhibition but we haven't found any lipase inhibitors used as candidiasis treatment. In this work, we are interested to lipases inhibitors such as alkaloids as another candidiasis treatment. In the first part, we have proceeded to optimize the alkaloid structures and protein 3D structure using Hyperchem software. Secondly, we have docked inhibitors using Genetic algorithm with GOLD software. The results have shown ten possibilities of binding inhibitor to Candida rugosa lipase (CRL) but only one possibility has been accepted depending on the weakest binding energy.

Keywords : marrubiin, candida rugosa lipase, docking, gold
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