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Physicochemical proprieties of Aspartic Proteinase-5 and natural compounds complex

The Secret Aspartic Proteinase enzyme plays an important role in promoting what can be established as a drug target for infections. As a result, inhibition of the enzyme's active center using phytochemicals would reduce the severity of the enzyme's virulence. Furthermore, it is one of 10 acid hydrolases that has a molecular weight of 37 KDa and is active at a potential of hydrogen of 3.0-7.0. The present work focuses on the *in silico* analysis of about 6 phytochemicals and the originally crystallized ligand, against the enzyme Secret Aspartic Proteinase 5 (code 2QZX) and phytochemicals from the database ZINC15, using Vina software. The docking results for the crystallized ligand, in kCal/mol, were -6.5 and the phytochemicals terpinyl valerate -6.2, azoxystrobin -6.6, timolol -6.7, terbutaline -6.8, terpecurcumin C -7.7 and higher binding of terpecurcumin A -7.9 and by amino acid interactions in relation to the crystallized ligand obtained Terpecurcumim A and Azoxystrobin with 18.75 and 25% respectively of interactions. Thus, these bioactive compounds can be used as clues to drugs that target secreted aspartic proteinase enzymes in the treatment of resistant Candida infections.

Keywords: Candida Albicans, Enzyme, Phytochemicals, Physicochemical proprieties, Interactions.