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Antitrypanosomal Activity of Stigmasterol: An in silico Approach

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Abstract : Stigmasterol has previously been reported to possess antitrypanosomal activity using in vitro and in vivo models. However, the mechanism of antitrypanosomal activity is yet to be elucidated. In the present study, molecular docking was used to decipher the mode of interaction and binding affinity of stigmasterol to three known antitrypanosomal drug targets viz; adenosine kinase, ornithine decarboxylase and triose phosphate isomerase. Stigmasterol was found to bind to the selected trypanosomal enzymes with minimum binding energy of -4.2, -6.5 and -6.6 kcal/mol for adenosine kinase, ornithine decarboxylase, and triose phosphate isomerase respectively. However, hydrogen bond was not involved in the interaction of stigmasterol with all the three enzymes, but hydrophobic interaction seemed to play a vital role in the binding phenomenon which was predicted to be non-competitive like type of inhibition. It was concluded that binding to the three selected enzymes, especially triose phosphate isomerase, might be involved in the antitrypanosomal activity of stigmasterol but not mediated via a hydrogen bond interaction.

Keywords : antitrypanosomal, in silico, molecular docking, stigmasterol
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