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Hydrogen bond interaction with trypanosomal adenosine kinase; ornithine decarboxylase and triose phosphate isomerase could not be involved in the antitrypanosomal activity of stigmasterol: An *in silico* study

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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.

Biography

Aminu Mohammed, an academic staff from Ahmadu Bello University, Zaria-Nigeria obtained his PhD Biochemistry from the famous University of KwaZulu-Natal, South Africa in Biomedical Research Lab. His research interest focus on screening and isolation of potent ingredients/nutraceuticals with antidiabetic or antitrypanosomal potentials from vast wealth of plants located in African region using modern spectroscopic techniques. In addition, we are interested in elucidating the possible mode of actions of extracts, compounds or nutraceuticals derived from the plants using various *in vitro* and *in vivo* models. Presently, we focus on the *in silico* computer simulation and improving bioavailability of spice-derived nutraceuticals as possible antidiabetic or antitrypanosomal agents.

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