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Antiplasmodial Activity of Drimane Sesquiterpene Isolated from Warburgia salutaris

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Abstract : Background: Malaria remains a life-threatening disease in tropical regions despite the advances in the treatment of this disease, it still remains a significant burden as some parasites have become resistant to the currently available drugs. This has created a necessity for the development of alternative, more efficient antimalarial drugs. Warburgia salutaris is a traditional medicinal plant used in malaria treatment by Zulu traditional healers. Materials and methods: The W. salutaris stem-bark was extracted with dichloromethane and the compound was isolated through column chromatography. The compound was identified and characterized by spectroscopic analysis (1H NMR, 13C NMR, IR and MS) and the structure was also confirmed by x-ray crystallography. The anti-plasmodial activity (in vitro) was studied on NF54 Plasmodium falciparum strain (CQS). Cytotoxicity was measured using the MTT assay on HEK239 and HEPG2 cell lines. Docking of Mukaadial acetate was conducted in AutoDock Vina. Structural modifications were conducted in UCSF Chimera and molecular interactions examined in LigPlot. Results: The compound, Mukaadial Acetate showed appreciable inhibition (IC50 0.44±0.10 µg/ml) of the parasite growth and cytotoxicity activity of 0.124±0.109 and 0.199±0.083 (µg/ml) on HEK293 and HEPG2 cells respectively. Molecular docking revealed that Mukaadial Acetate binds to the purine, pyrophosphate and ribose binding sites of the PfHGXPRT with an optimum binding conformation and forms hydrogen bond, steric and hydrophobic interactions with the residues inhabiting the respective binding sites. Conclusion: It is apparent that W. salutaris contains components (including Mukaadial Acetate) that exhibit antimalarial activity. This study scientifically validates the use of this plant in folk medicine.

Keywords : plasmodium falciparum, molecular docking, antimalarial activity, PfHGXPRT, Warburgia salutaris, mukaadial acetate

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