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12th WORLD NURSING FORUM

April 17, 2023 | Webinar

Received date: 07-03-2023 | Accepted date: 09-03-2023 | Published date: 27-04-2023

In Vitro and *In Silico* Potential Inhibitory Effects of New Biflavonoids from *Ochna rhizomatosa* on HIV-1 Integrase and *Plasmodium falciparum*

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The aim of this study was to identify bioactive secondary metabolites from *Ochna rhizomatosa* with potential inhibitory effects against HIV and *Plasmodium falciparum*. A phytochemical study of *O. rhizomatosa* root barks resulted in the identification of three new biflavonoids (1−3), along with four known ones (4−7). Compound 7 (Gerontoisoflavone A) was a single flavonoid present in the rootbark of the plant and was used as a reference. Compound 1 (IC50 = 0.047 µM) was the only one with a noteworthy inhibitory effect against HIV-1 integrase in vitro. Chicoric acid (IC50 = 0.006 µM), a pure competitive inhibitor of HIV-1 integrase, was used as control. Compound 2 exhibited the highest antiplasmodial activity (IC50 = 4.60 µM) against the chloroquine-sensitive strain of *Plasmodium falciparum* NF54. Computational molecular docking revealed that compounds 1 and 2 had the highest binding score (−121.8 and −131.88 Kcal/mol, respectively) in comparison to chicoric acid and Dolutegravir (−116 and −100 Kcal/mol, respectively), towards integrase receptor (PDB:3LPT). As far as Plasmodium-6 cysteine s48/45 domain inhibition is concerned, compounds 1 and 2 showed the highest binding scores in comparison to chloroquine, urging the analysis of these compounds in vivo for disease treatment. These results confirm the potential inhibitory effect of compounds 1 and 2 for HIV and malaria treatment. Therefore, our future investigation to find inhibitors of these receptors in vivo could be an effective strategy for developing new drugs.

Keywords: *Ochna rhizomatosa*; biflavonoids; HIV-1 replication; *Plasmodium falciparum* NF54; structure–activity relationships; molecular docking

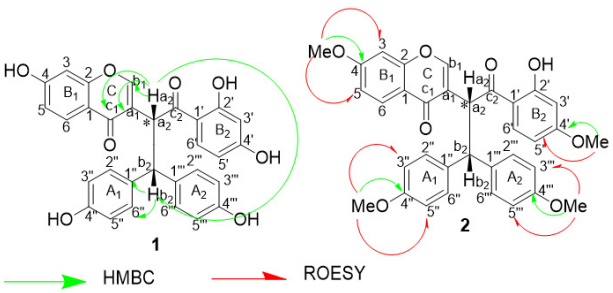

Figure 1. Key HMBC and ROESY correlations of (1–2).

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