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Abstract

Anthrarufin and Its Anionic Moieties as Potential Inhibitors of HIV-1 Reverse Transcriptase (RT) †

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Abstract: At the end of the last century, it was revealed that quinones with one, two, and three aromatic rings could inhibit HIV-1 protease, an enzyme crucial for HIV (Human Immunodeficiency Virus) replication. Since HIV-1 protease acts as key target for AIDS (Acquired Immunodeficiency Syndrome) medications, the development of efficient inhibitor of this protein would lead to an increase in medical treatment and a decrease in the drug resistance. Later research revealed that hydroxyquinones can block HIV-1 protease at the micromolar level, which enabled a direction for the creation of HIV medications. Anthrarufin (1,5-dihydroxy-9,10-anthraquinone) is an anthraquinone that possesses a moderate antioxidative capacity and antimalaric activity. In this study, molecular docking simulations were used to examine the molecular interactions between anthrarufin, its monoanion and dianion as ligands, and HIV-1 reverse transcriptase (HIV-1 RT) as a target protein. Using AGFR software, the binding site of the HIV-1 RT was identified. The three-dimensional crystal structure of HIV-1 RT was downloaded from the Protein Data Bank (PDB ID: 2ZD1). Dolutegravir, nevirapine, anthrarufin, anthrarufin-anion and anthrarufin-dianion are used as ligands in the molecular docking simulations together with rilpivirine (TMC278), a non-nucleoside inhibitor of estimated protein. The AutoDock 4.0 program is used for molecular docking simulations. Anthrarufin, its monoanion and dianion can be considered as a potential HIV-1 RT inhibitors because they have similar inhibitory potency to other ligands under consideration, according to the results of the free energy of binding (ΔG_{bind}) and inhibition constant (K_i) values.

Keywords: HIV-1 reverse transcriptase (RT); anthrarufin; anthrarufin-anion; anthrarufin-dianion; molecular docking

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