An In Silico Approach for Identification of Novel Inhibitors as Potential Therapeutics Targeting HIV-1 Viral Infectivity Factor from Parijoto (*Medinilla speciosa*)

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Abstract

Human Immunodeficiency Virus (HIV) is a virus that attacks the human immune system and tends to develop into AIDS. The United Nations through a joint program called UNAIDS (Joint United Nations Program on HIV and AIDS) has a target of ending the HIV/AIDS epidemic by 2030 in line with SDGs 3. Protease inhibitors (PIs) are crucial drugs in highly active antiretroviral therapy for human immunodeficiency virus-1 (HIV-1) infections. Parijoto (*Medinilla Speciosa*) is one of the famous plants cultivated around the muria mountains Kudus and has many properties, especially to develop as an anti virus. This study aims to identify potential therapeutic inhibitors for HIV-1 PR derived from the parijoto plant using an in silico approach. Potential compounds were extracted using ethanol and determined using Gas Chromatography-Mass Spectrometer (GC-MS). Molecular docking was carried out using the Autodock Vina integrated in PyRx program with the HIV-1 protease receptor active site (PDB ID: 3S43) and the native ligand Amprenavir. The results showed that there were 3 peaks in gas chromatography with 6 compounds resulting from parijoto extraction. The compound with the best binding energy affinity for the HIV-1 protease receptor is 1-(4-Chlorophenyl)-2-phenyl-4-piperidino-5-hydroxy-4,5-dihydroimidazole with a value of -10.0 kcal/mol.

Keywords: Parijoto, HIV, HIV-1 Protease, In silico

Identifikasi Inhibitor Terapi Potensial Bagi Infeksi Virus HIV-1 Berbahan Parijoto (*Medinilla speciosa*) melalui Pendekatan in Silico

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Abstrak

HIV merupakan virus yang menyerang sistem kekebalan tubuh manusia dan cenderung berkembang menjadi AIDS. PBB melalui program gabungan bernama UNAIDS (*Joint United Nations Programme on HIV and AIDS*) memiliki target mengakhiri epidemi HIV/AIDS pada tahun 2030 yang selaras dengan SDGs 3. Inhibitor protease (PI) adalah obat penting dalam terapi antiretroviral yang sangat aktif untuk infeksi human immunodeficiency virus-1 (HIV-1). Parijoto *(Medinilla Speciosa L.)* merupakan salah satu tanaman khas yang dibudidayakan di sekitar pegunungan muria dan mempunyai banyak khasiat terutama untuk dikembangkan sebagai anti virus. Penelitian ini bertujuan untuk mengidentifikasi inhibitor terapi potensial bagi HIV-1 PR yang berasal dari tanaman parijoto melalui pendekatan in silico. Senyawa potensial diekstraksi menggunakan etanol dan ditentukan menggunakan *Gas Chromatography-Mass Spectrometer* (GC-MS). Penambatan molekul dilakukan menggunakan program Autodock Vina yang terintegrasi pada PyRx dengan situs aktif reseptor protease HIV-1 (PDB ID: 3S43) dan *native ligand* Amprenavir. Hasil penelitian menunjukkan terdapat 3 *peak* pada gas chromatography dengan 6 senyawa hasil ekstraksi parijoto. Senyawa dengan afinitas energi ikatan terbaik terhadap reseptor protease HIV-1 yaitu 1-(4-Chlorophenyl)-2-phenyl-4-piperidino-5-hydroxy-4,5-dihydroimidazole dengan nilai -10.0 kkal/mol.

Kata kunci : Parijoto, HIV, Protease HIV-1, *In silico*