AN IN SILICO-BASED VIRTUAL SCREENING OF FINGERROOT-DERIVED PHYTOCHEMICALS ACTION ON EPSTEIN-BARR VIRUS LYTIC REPLICATION FOR EBV-ASSOCIATED MALIGNANCIES THERAPY

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In recent years, both pre-clinical and clinical studies of Epstein-Barr virus (EBV)-associated malignancies indicated the significant contribution of EBV lytic infection on viral carcinogenesis. There are currently no standard pharmaceutical products or specific vaccines, therefore, treatments focused on EBV lytic components have been elaborated as potential strategies for therapy of such diseases. Phytochemical compounds commonly found in fingerroot exhibited anti-viral activity and inhibited progression of several solid tumors. The effect of these compounds on EBV lytic replication is limited. Here, we integrate an *in silico* approach to investigate major bioactive compounds derived from *Kaempferia parviflora* Wall. ex Baker on the EBV lytic protein, an early late protein (BGLF4), as a target. The actions of these compounds were examined via flexible ligand docking, ADME property, and landscape of protein-ligand interaction. We also performed molecular dynamics (MD) simulations on such compounds to study the stability and the interactions of the protein-ligand complexes. Out of 20 bioactive compounds, pinocembrin and pinostrobin revealed the best binding affinity to BGLF4 with a high negative binding energy of -9.9 kcal/mol and -8.8 kcal/mol, respectively. Interestingly, the conformation of viral protein was altered with decreased surface area and higher stability when each ligand was applied as demonstrated by our MD simulation. Moreover, the calculation of the Root Mean Square Deviation (RMSD) of ligands and the viral protein also displayed the protein stability, indicating the applicable binding of both ligands in the viral protein target. Based on the ADME score, all of the pinocembrin and pinostrobin possess implying drug-likeness properties. Collectively, the present study accordingly evokes that pinocembrin and pinostrobin might be the potential inhibitors of BGLF4 protein and effective drug candidates for inhibition of EBV lytic infection. Nevertheless, these *in silico* findings still necessitate being supported by both *in vitro* and *in vivo* experiments to corroborate the exact mode of action (MoA) of these two phytochemical compounds.