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Identification of potential inhibitors for Ebola virus: An *in silico* approach

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Ebola virus (EBOV) is a fatal virus that causes severe hemorrhagic fever in human and animals. However, there is currently no FDA-approved drug for treating Ebola virus infection. Identification of potential inhibitors for Ebola virus has gained much attention of medicinal chemists in the last few years. Although few lead compounds were identified, the drug discovery for Ebola virus is significantly more challenging. In this study, *in silico* approaches were applied to explore potential inhibitors for EBOV infection. Initally, four protein targets for EBOV were identified through their important roles in viral pathogenesis and disease, namely VP24 (PDB id: 4MOQ), VP30 (PDB id: 5DVW), VP35 (PDB id: 3FKE), và VP40 (PDB id: 1H2C), respectively. The ligands were taken from some drugs which are in clinical testings from other anti-viruses potential compounds. Through blind dockings and focused dockings, the potential inhibitors and binding sites were discovered for different protein targets of EBOV. The docking results of the trial drugs are consistent with the experiment data. In the group of other potential compounds, there were some ligands which had abilities to well-bind with Ebola proteins such as Silybin (-9.5 kJ.mol-1), Harringtonine (-8.0 kJ.mol-1), Homoharringtonine (-8.3 kJ.mol-1), Chat 5 (-8.2 kJ.mol-1). Among these ligands, after screening through Lipinski 5 rules, Silybin was the only suitable one which could be used as lead compounds for EBOV drug discovery. This study provided helpful information to considerably assist in drug discovery of antiviral agents for Ebola virus.

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