In silico molecular screening of bioactive natural compounds of rosemary essential oil and extracts for pharmacological potentials against rhinoviruses	
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Abstract: Rhinoviruses (RVs) cause upper respiratory tract infections and pneumonia in children and adults. These non-enveloped viruses contain viral coats of four capsid proteins: VP1, VP2, VP3, and VP4. The canyon on VP1 used cell surface receptor ICAM-1 as the site of attachment and for the internalization of viruses. To date, there has been no drug or vaccine available against RVs. In this study, bioactive natural compounds of rosemary (Salvia rosmarinus L.), which are known for their pharmacological potential, were considered to target the VP1 protein. A total of 30 bioactive natural compounds of rosemary were taken as ligands to target viral proteins. The PkCSM tool was used to detect their adherence to Lipinski's rule of five and the ADMET properties of the selected ligands. Further, the CB-Dock tool was used for molecular docking studies between the VP1 protein and ligands. Based on the molecular docking and ADMET profiling results, phenethyl amine (4 methoxy benzyl) was selected as the lead compound. A comparative study was performed between the lead compound and two antiviral drugs, Placonaril and Nitazoxanide, to investigate the higher potential of natural compounds over synthetic drugs. Placonaril also targets VP1 but failed in clinical trials while Nitazoxanide was examined in clinical trials against rhinoviruses. It was discovered from this study that the (4 methoxy benzyl) phenethyl amine exhibited less toxicity in comparison to other tested drugs against RVs. More research is needed to determine its potential and make it a good medication against RVs.