Interactions of terpenoid compounds with main protease and RNA-dependent RNA-polymerase protein targets of SARS-CoV-2

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ABSTRACT

Introduction: The novel Coronavirus, SARS-CoV-2 causing the COVID-19 pandemic has become a serious public health issue worldwide. This has created a huge demand for discovering antiviral drugs for treating COVID-19. Phytocompounds especially terpenoids have potential for effective antiviral activities against SARS-CoV-2. In this study, a library of terpenoid compounds was screened for their interactions with protein targets of SARS-CoV-2 using the computational docking approach. **Materials and methods:** Terpenoid compounds were retrieved from data bases such as PubChem (NCBI, USA), Naturally-occurring Plant-based Anti-cancer Compound-activity Target (NPACT) and Kyoto Encyclopaedia for Gene and Genome (KEGG). Docking of terpenoid compounds with the main protease (Mpro) and RNA-dependent RNA-polymerase (RdRP) was performed using Autodock Vina. Drug-likeness properties were predicted using SwissADME web tool. **Results and conclusion:** Out of 850 terpenoid compounds docked with SARS-CoV-2 protein targets, Agavoside A showed the highest interaction energy value of -9.1kcal/mol against Mpro and formed hydrogen bond (HB) interactions with Lys137, Asp197, Thr199 and Leu287. Labriformidin and Absinthin showed interaction energy values of -9 and -8.8kcal/mol, respectively, with Mpro. Against RdRp, Absinthin showed the highest interaction energy value of -9.9 kcal/mol and formed HB interactions with Asp760, Asp623 and Cys622. Agavoside A and Labriformidin showed interaction energy values of -9.6 and -9.4kcal/mol, respectively, with RdRp. ADMET analysis revealed that all three compounds possess non-toxic and non-carcinogenic properties. The lead terpenoid compounds Agavoside A, Labriformidin, and Absinthin could be potential antiviral agents for treating COVID-19. However, further *in-vitro* and *in-vivo* studies are required.