Prophylactic and Therapeutic Roles of Glycyrrhiza glabra in the Prevention and Treatment of COVID19

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SARS-CoV-2 has struck as a major global pandemic causing COVID19, infecting over 109 million. Infection and pathogenesis of SARS-CoV-2 is mediated through the key proteins; Spike Protein and RNA-Dependent-RNA Polymerase (RdRp), aided by the nsp7/8/12 complex that are involved in the entry and replication of the virus. Screening tens/hundreds-of-thousands of known chemical-drug candidates through in silico methods to identify potential drug candidates are quickest ways to find treatments and also reduce costs and human exposures to dangerous pathogens like SARS-CoV-2. The purpose of our research is to screen, identify and predict the binding of natural compounds of the antiviral plant, Glycyrrhiza glabra, that can inhibit SARS-CoV-2 entry and replication through its interactions with the respective proteins. In this study, we have selected 20 known phytochemicals (GG1-GG20) from G.glabra to be tested for its binding efficacy with each protein based on Atomic Contact Energy (ACE) scores in molecular docking algorithm Patchdock. Chimera was used to visualize these interactions. GG3 and GG4 achieved lower ACE scores than -100.00 across all proteins, potentially inhibiting SARS-CoV-2 at multiple levels. GG4 binds to the Spike Protein near the Angiotensin-converting enzyme-2 receptor of the host cell, inhibiting the entry of the virus. However, GG3 binds close to the active site of the RdRp where the thumb, finger, and palm domains meet. GG3 and GG4 binds close to the active site of nsp7/8/12 complex, preventing viral replication. Overall, GG3 and GG4 from G.glabra have demonstrated the ability to prevent the spread of SARS-CoV-2 in silico.

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