

# Pharmaceutical Science and Advanced Drug Delivery Systems

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## Computational and *In Vitro* experimental investigations reveal antiviral activity of Licorice and Glycyrrhizin against severe acute respiratory syndrome coronavirus 2

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**Introduction:** Without effective antivirals, the COVID-19 pandemic will likely continue to substantially affect public health. Medicinal plants and phytochemicals are attractive therapeutic options, particularly those targeting viral proteins essential for replication cycle.

**Methods:** A total of 179 phytochemicals of licorice (*Glycyrrhiza glabra*) were screened and scrutinized against the SARS-CoV-2 main protease (Mpro) with considerable binding affinities in the range of -9.831 to -2.710 kcal/mol. *In vitro* studies demonstrated robust anti-SARS-CoV-2 activity of licorice and glycyrrhizin under different treatment protocols (simulations treatment with viral infection, post-infection treatment, and pre-treatment), suggesting multiple mechanisms for action. Results: The top 10 compounds with the best docking scores, licuraside, glucoliquiritin apioside, 7,30-Dihydroxy-50 - methoxyisoflavone, licuroside, kanzonol R, neoisoliquiritin, licochalcone-A, formononetin, somucronulatol and licoricone, were redocked using AutoDock Vina, yielding -8.7 to -7.3 kcal/mol binding energy against Glycyrrhizin (-8.0 kcal/mol) as a reference ligand. Licorice and glycyrrhizin compounds

inhibited SARS-CoV-2 replication, the half-maximal inhibitory concentration (IC50) of glycyrrhizin was substantially lower than licorice.

**Conclusion:** Four compounds, licuraside, glucoliquiritin apioside, 7,30-Dihydroxy-50-methoxyisoflavone and licuroside, with glycyrrhizin (reference ligand) were considered for the 100 ns MD simulation and postsimulation analysis which support the stability of docked bioactive compounds with viral protein. This study supports proceeding with *in vivo* experimentation and clinical trials and highlights licorice and glycyrrhizin as potential therapeutics for COVID-19.

### Speaker Biography

Ahmed Majdi Tolah is currently an Assistant Professor at the King Abdulaziz University, Faculty of Applied Medical Science, Virology, Rabigh, Saudi Arabia and Researcher at Special Infectious Agents Unit, King Fahd Medical Research Center, Jeddah, Saudi Arabia. Science and Research Branch. He graduated Ph.D. Degree in Microbiology (Virology) in 2019. His research interests are diagnosis and treatment of viruses (SARS-CoV-2, MERS-CoV, Influenza virus and Dengue virus), drug and natural products discovery.

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