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In-Silico Investigation of Phytochemicals from Ocimum Sanctum as Plausible Antiviral Agent in COVID-19

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Abstract : COVID-19 has ravaged the globe, and it is spreading its Spectre day by day. In the absence of established drugs, this disease has created havoc. Some of the infected persons are symptomatic or asymptomatic. The respiratory system, cardiac system, digestive system, etc. in human beings are affected by this virus. In our present investigation, we have undertaken a study of the Indian Ayurvedic herb, Ocimum sanctum against SARS-CoV-2 using molecular docking and dynamics studies. The docking analysis was performed on the Glide module of Schrödinger suite on two different proteins from SARS-CoV-2 viz. NSP15 Endoribonuclease and spike receptor-binding domain. MM-GBSA based binding free energy calculations also suggest the most favorable binding affinities of carvacrol, β elemene, and β caryophyllene with binding energies of −61.61, 58.23, and −54.19 Kcal/mol respectively with spike receptor-binding domain and NSP15 Endoribonuclease. It rekindles our hope for the design and development of new drug candidates for the treatment of COVID19.

Keywords : molecular docking, COVID-19, ocimum sanctum, binding energy
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