Tinospora cordifolia (Giloy) may curb COVID-19 contagion: Tinocordiside disrupts the electrostatic interactions between ACE2 and RBD

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Abstract

SARS-CoV-2 has been shown to bind the host cell ACE2 receptor through its spike protein receptor binding domain (RBD), required for its entry into the host cells. We have screened phytocompounds from a medicinal herb, Tinospora cordifolia, for their capacities to interrupt the viral RBD and host ACE2 interactions. We employed molecular docking to screen phytocompounds in T. cordifolia against the ACE2-RBD complex, performed molecular dynamics (MD) simulation, and estimated the electrostatic component of binding free energy. 'Tinocordiside' docked very well at the center of the interface of AEC2-RBD complex, and was found to be well stabilized during MD simulation. Tinocordiside incorporation significantly decreased electrostatic component of binding free energies of ACE2-RBD complex (23.5 and 17.10 kcal/mol in the trajectories without or with the ligand, respectively). It indicates that such an interruption of electrostatic interactions between the RBD and ACE2 would weaken or block COVID-19 entry and its subsequent infectivity. We postulate that natural phytochemicals like Tinocordiside could be the viable options for controlling COVID-19 contagion and its entry into host cells.

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