Research Article

Polypharmacology of some medicinal plant metabolites against SARS-CoV-2 and host targets: Molecular dynamics evaluation of NSP9 RNA binding protein

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Abstract

manually curated, procuring a library of 521 metabolites; this was virtually screened against NSP9, including some other viral and host targets and were evaluated for polypharmacological indications. Leads were identified via rigorous scoring thresholds and ADMET filtering. MM-GBSA calculation was deployed to select NSP9-Lead complexes and the complexes were evaluated for their stability and protein-ligand communication via MD simulation. We identified 5 phytochemical leads for NSP9, 23 for Furin, 18 for ORF3a, and 19 for IL-6. Ochnaflavone and Licoflavone B, obtained from *Lonicera japonica* (Japanese Honeysuckle) and *Glycyrrhiza glabra* (Licorice), respectively, were identified to have the highest potential polypharmacological properties for the aforementioned targets and may act on multiple pathways simultaneously to inhibit viral entry, replication, and disease progression. Additionally, MD simulation supports the robust stability of Ochnaflavone and Licoflavone B against NSP9 at the active sites via hydrophobic interactions, H-bonding, and H-bonding facilitated by water. This study promotes the initiation of further experimental analysis of natural product-based anti-COVID-19 therapeutics.

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Keywords: Virtual screening;s phytochemicals | NSP9 | Orf3a | furin | Interleukin-6 | molecular dynamics simulation | COVID-19 | SARS CoV-2

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