

ABSTRACT

The present study explores the antiviral potential of the stem extract of *Nymphaea alba* against Human Metapneumovirus (HMPV) using a comprehensive in silico approach. Pharmacognostical and phytochemical investigations confirmed the presence of flavonoids, tannins, glycosides, and polyphenols—compounds known for their antiviral properties. FTIR analysis identified key functional groups such as hydroxyl, carbonyl, and aromatic rings, indicative of bioactive constituents. Twenty-four phytochemicals previously reported from *N. alba* were subjected to molecular docking against the HMPV fusion glycoprotein (PDB ID: 7LZE), an essential protein for viral entry. Among these, Naringin, Rutin, Corilagin, Orientin, and Ellagic acid-pentoside exhibited the highest binding affinities, with docking scores ranging from -7.2 to -7.8 kcal/mol, suggesting strong and specific interactions with the viral protein's active site. ADME and toxicity profiling of the top-ranked compounds was carried out using SwissADME and ProTox-III, respectively. Results indicated that Naringin, Orientin, and Rutin possessed favorable drug-likeness and solubility profiles, while Rutin showed the highest safety margin with a predicted LD₅₀ of 5000 mg/kg. Although some compounds showed predicted organ toxicities such as immunotoxicity and hepatotoxicity, most were non-carcinogenic, non-mutagenic, and non-cytotoxic. The combination of strong binding affinity, structural compatibility, and manageable toxicity profiles supports the therapeutic promise of *N. alba* phytoconstituents as potential antiviral agents. This study lays the groundwork for future in vitro and in vivo validation and highlights *N. alba* as a promising natural resource for the development of novel antiviral therapies targeting respiratory viruses like HMPV.

KEYWORDS: Antiviral study, N.Alba, Insilico study, HMPV