







OP21. *IN VITRO* AND *IN SILICO* EVALUATION OF THE ANTIVIRAL POTENTIAL OF EUCALYPTUS ESSENTIAL OILS

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The members of the genus *Eucalyptus* L. belonging to the Myrtaceae are well-known and have been utilized for millennia as aromatic and medicinal plants. Due to their antibacterial and antioxidant properties, eucalyptus essential oils are frequently used in flavorings, culinary preparations, as well as in medicinal and cosmetic applications. In the present study, *in vitro* enzyme inhibition assays were conducted for neuraminidase (NA), transmembrane serine protease 2 (TMPRSS2) and angiotensin-converting enzyme 2 (ACE2) to explore the antiviral potential of two different essential oils from *Eucalyptus* species. European-Pharmacopoeia-quality essential oils from *E. globulus* and *E. citriodora* were employed in the enzyme assays. The inhibitory activities of essential oils at 20 µg/mL against ACE2, TMPRSS2 and NA were measured using commercial kits. *E. globulus* essential oil inhibited ACE2, TMPRSS2 and NA by 94.3%, 74.82% and 67.59%, respectively. *E. citriodora* essential oil inhibited ACE2, TMPRSS2 and NA by 83.4%, 60.55% and 43.64%, respectively. Although both essential oils from the *Eucalyptus* species demonstrated good enzyme inhibitory activity, our *in vitro* results indicated that *E. globulus* essential oil possesses greater antiviral activity potential than *E. citriodora*. Furthermore, protein-ligand docking and interaction profiling studies were utilized to gain structural and mechanistic insights into the *in silico* ACE2, TMPRSS2 and NA inhibitory potentials of the major constituents of *Eucalyptus* essential oil, 1,8-cineole and citronellal. The results corroborated the *in vitro* findings. In conclusion, based on the results obtained in this study, both eucalyptus essential oils exhibit antiviral potential, making them viable candidates against cold, flu, and coronavirus. Further *in vivo* studies are required to confirm their activity.

Keywords: Eucalyptus; essential oil; antiviral; *in vitro* enzyme assay; molecular docking.

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