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IN SILICO EVALUATION OF NATURAL MONOTERPENES AGAINST THE SARS-COV-**2 MAIN PROTEASES**

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Abstract

Severe acute respiratory syndrome coronavirus 2 (SARS-CoV-2) promotes challenging immune and inflammatory phenomena in the human body [1]. The main objective of the current study is to investigate the impact of the major components of propolis on the active sites of key SARS-CoV-2 main proteases (7N5Z, 6LU7, and 7E6L). Molecular simulations were employed to explore potential interactions between these viral active sites and major components, with the aim of contributing to the development of potential therapeutic strategies against SARS-CoV-2.

Keywords : SARS-CoV-2, α -Pinene, limonene, GC/MS, ADMET.

