ABSTRACT

A global challenge in many sectors including health and disease management, is posed by the rapidly spreading coronavirus disease 2019 (COVID-19). This research serves as a preliminary investigation by screening potential compounds from Nigella sativa essential oils that may perform as COVID-19 prophylaxis by a set of *in silico* studies, including chemical characterization, ADMET prediction, molecular docking, density functional theory, and gene enrichment analysis. Through molecular docking, 117 candidate compounds were collectively predicted for their inhibitory effects against crucial protein targets (Mpro, PLpro, Nucleocapsid, Spike, TMPRSS2 and ACE2). DFT analysis was performed to examine the degree of reactivity of the 10 best performing compounds. In addition, a gene enrichment analysis was conducted to gain insight on the modulation of relevant genes and pathways in relation to COVID-19 and the immune system.. Together, the study has revealed a number of promising compounds including cyclododecene, a-phellandrene, a-pinene, terpinolene limonene, eucalyptol and allo ocimene which are predicted to possess good inhibition activity towards target proteins and the ability to modulate relevant genes including, GAPDH, HMOX1, and NFE2L2. Overall, this study proposed that the prophylactic effect may be achieved by 2 mechanisms, by immune system enhancement and suppression of proinflammatory cytokines.

Keywords: *In silico* studies, *Nigella sativa,* SARS CoV-2, COVID-19

ABSTRAK

Tantangan global di banyak sektor termasuk kesehatan dan manajemen penyakit, ditimbulkan oleh coronavirus disease 2019 (COVID-19) *yang menyebar dengan begitu cepat. Penelitian ini ditujukan sebagai investigasi awal dengan menyaring senyawa potensial dari minyak atsiri Nigella sativa yang dapat berfungsi sebagai profilaksis* COVID-19 *melalui serangkaian studi in silico, termasuk karakterisasi kimia, prediksi ADMET, docking molekuler, teori fungsi densitas, dan analisis pengayaan gen. Melalui docking molekuler, 117 senyawa kandidat diprediksi secara kolektif untuk efek penghambatannya terhadap target protein penting (Mpro, PLpro, Nucleocapsid, Spike, TMPRSS2 dan ACE2). Analisis DFT dilakukan untuk menguji tingkat reaktivitas 10 senyawa berkinerja terbaik. Selain itu, analisis pengayaan gen dilakukan untuk mendapatkan wawasan tentang modulasi gen dan jalur yang relevan dalam kaitannya dengan* COVID-19 *dan sistem kekebalan. Bersama-sama, penelitian ini telah mengungkapkan sejumlah senyawa yang menjanjikan termasuk* cyclododecene, a-phellandrene, a-pinene, terpinolene limonene, eucalyptol *dan* allo ocimene *yang diperkirakan memiliki aktivitas penghambatan yang baik terhadap protein target dan kemampuan untuk memodulasi gen yang relevan termasuk, GAPDH, HMOX1, dan NFE2L2. Secara keseluruhan, penelitian ini mengusulkan bahwa efek profilaksis dapat dicapai dengan 2 mekanisme, dengan peningkatan sistem kekebalan tubuh dan penekanan sitokin proinflamasi.*

Kata kunci : Studi In-siliko, Nigella sativa, SARS-CoV 2, COVID-19