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An ensemble docking-based virtual screening and molecular dynamics simulation of phytochemical compounds from Malaysian Kelulut Honey (KH) against SARS-CoV-2 target enzyme, human angiotensin-converting enzyme 2 (ACE-2)

Ismail, Che Muhammad Khairul Hisyam^{a, b}; Abdul Hamid, Azzmer Azzar^{a, b} ; Abdul Rashid, Nur Nadiah^c; Lestari, Widyad^d;Mokhtar, Khairani Idah^d; Mustafa Alahmad, Basma Ezzat^d; Abd Razak, Mohd Ridzuan Mohd^e; Ismail, Azlini^d

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Abstract

The human angiotensin-converting enzyme 2 (ACE-2) receptor is a metalloenzyme that plays an important role in regulating blood pressure by modulating angiotensin II. This receptor facilitates SARS-CoV-2 entry into human cells via receptor-mediated endocytosis, causing the global COVID-19 pandemic and a major health crisis. Kelulut honey (KH), one of Malaysian honey recently gained attention for its distinct flavour and taste while having many nutritional and medicinal properties. Recent study demonstrates the antiviral potential of KH against SARS-CoV-2 by inhibiting ACE-2 invitro, but the bioactive compound pertaining to the ACE-2 inhibition is yet unknown. An ensemble docking-based virtual screening was employed to screen the phytochemical compounds from KH with high binding affinity against the 10 best representative structures of ACE-2 that mostly formed from MD simulation. From 110 phytochemicals previously identified in KH, 27 compounds passed the ADMET analysis and proceeded to docking. Among the docked compound, SDC and FMN consistently exhibited strong binding to ACE-2's active site (-9.719 and -9.473 kcal/mol) and allosteric site (-7.305 and -7.464 kcal/mol) as compared to potent ACE-2 inhibitor, MLN 4760. Detailed trajectory analysis of MD simulation showed stable binding interaction towards active and allosteric sites of ACE-2. KH's compounds show promise in inhibiting SARS-CoV-2 binding to ACE-2 receptors, indicating potential for preventive use or as a supplement to other COVID-19 treatments. Additional research is needed to confirm KH's antiviral effects and its role in SARS-CoV-2 therapy, including prophylaxis and adjuvant treatment with vaccination. Communicated by Ramaswamy H. Sarma. © 2024 Informa UK Limited, trading as Taylor & Francis Group.

Author keywords

Ensemble-based virtual screening; Kelulut honey; molecular docking; molecular dynamic simulation; stingless bee

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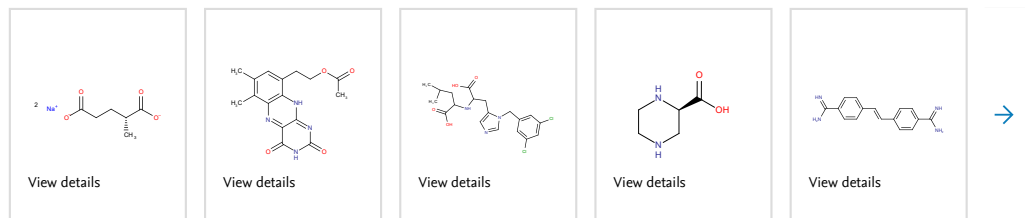
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Five chemical structures are displayed in a row, each within a rectangular box. Below each structure is a "View details" link. To the right of the fifth structure is a blue arrow pointing to the right.

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

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