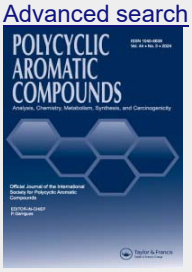

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Antibacterial Potential of Trihydroxycyclohexa-2,4-Diene-1-Carboxylic Acid: Insight from DFT, Molecular Docking, and Molecular Dynamic Simulation

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Abstract

In this study, (z)-5-((3-(2,3-dihydroxyphenyl) acryloyl) oxy)- 1,3,4-trihydroxycyclohexa-2,4-diene-1-carboxylic acid (chlorogenic acid) was isolated and characterized using UV-Visible, ^{1}H NMR and ^{13}C NMR, FT-IR, along with detailed investigation using density functional theory (DFT), *in-silico* molecular docking, and molecular dynamics (MD) simulation. Results from DFT calculation indicates that the titled compound is very stable with energy gap of 3.7–7.8 for variable functionals, and similarly, the structural parameters show very close agreement with X-ray data for bond lengths and angles.

The FT-IR spectrum results revealed stretching vibration O–H (3366 cm^{-1}), C=O (1689 cm^{-1}), C–H (1636, 1606, 1522, and 1442 cm^{-1}), C–O (1192 and 1122 cm^{-1}). The drug-likeness analyses and ADME studies showed drug-likeness ability and good oral behavior of the investigated compound as it obeys Lipinski, Ghose, Veber and Egan rules. Hepatotoxic and immunotoxic activities were indicated for the toxicity/toxicological endpoints of the studied compound. The molecular docking indicates a binding affinity of −8.30 and 9.5 kcal/mol for the titled compound, which is higher than the standard drug. From the molecular dynamic simulation results, chlorogenic-2H14 (complex B) revealed variations in RMSD values of less than 3Å, indicating that the protein structure underwent minor conformational changes throughout the simulation. Chlorogenic-protein complexes had average RGyr values of 3.704 − 4.907Å, which indicates compaction during the simulation. Therefore, it can be said that the titled compound has potential to be effective as an agent for cholera management, and the results obtained can be platform further in-vitro, vivo and clinical trials.

Keywords:

- DFT
- ADMET
- molecular docking
- molecular dynamic simulation

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Author contributions

Hitler Louis: Project administration, Conceptualization, design, supervision, writing, and editing. Chioma M. Chima and Aniekan E. Owen: Results analysis, writing, editing, and manuscript first draft. Ernest C. Agwamba: Analysis, writing and manuscript final draft. and editing. Iqrar Ahmad and Harun Patel: Analysis and Discussion of molecular dynamics. Eze Ahuekwe and Wilfred Emori: Resources, analysis, writing, and editing. Innocent Benjamin, Mmefone A. Ojong, and Chioma B. Ubah: Analysis, writing and editing. Chun-Ru Cheng and Amanda-Lee E. Manicum: Resources validation, writing and editing.

Disclosure statement

All authors assert zero financial and inter-personal incompatibility of interest that could have influenced the research work or results reported in this research paper. No potential conflict of interest was reported by the author(s).

Data availability statement

All data are contained within the manuscript and manuscript supporting information document (ESI).

Additional information

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