

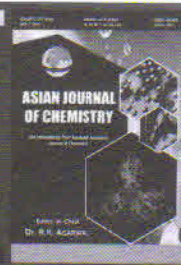


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## Electronic and Molecular Insights into Vericiguat: A Combined DFT, SAR and Molecular Docking Approach

D. JEBIXSON IMMANUEL<sup>✉</sup> and J. WINFRED JEBARAJ<sup>\*,✉</sup>

Department of Chemistry, St. John's College (Affiliated to Manonmaniam Sundaranar University, Abishekapatti), Palayamkottai, Tirunelveli-627002, India

\*Corresponding author: E-mail: winfred.chem@stjohnscollege.edu.in

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A medication called vericiguat is employed to treat symptomatic chronic heart failure. This work utilised Gaussian 16W in the gaseous phase to perform density functional theory (DFT) algorithms at the B3LYP/6-311++G(d,p) level. The electronic structure, Mulliken charge distribution and electrostatic potential (ESP) map were analyzed to explain the fundamental properties of molecule. The hole-electron interaction studies revealed the nature of charge transfer. Theoretical vibrational and UV-Vis spectral analyses were performed to support structural characterisation. Fukui function analysis was employed to predict reactive sites toward electrophilic, nucleophilic and radical attacks. Aromaticity indices, non-covalent interaction (NCI) analysis, shaded surface mapping and localised orbital locator (LOL) projections were generated using Multiwfn 3.8. Furthermore, molecular docking and structure-activity relationship (SAR) studies were performed with Maestro (Schrödinger) against target protein 6JT2, providing insights into binding interactions and the potential therapeutic significance of vericiguat.

**Keywords:** Vericiguat, DFT, Electrostatic potential, Wavefunction, Hole-electron interaction, Molecular docking.