

**Quantum chemical studies of Doxorubicin loaded Acetylated cashew gum Nanoparticles as drug delivery system.**

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**Abstract**

In this investigation, the therapeutic potential of Doxorubicin, a well-established anti-cancer agent, is explored. Despite its proven efficacy, the drug faces challenges such as poor bioavailability, solubility issues, and toxicity, necessitating the development of a targeted delivery system to enhance effectiveness while minimizing adverse effects. A promising candidate for this purpose is acetylated cashew gum, a naturally synthesized polymer derived from the cashew tree (*Anacardium occidentale*). This study primarily focuses on the computational modeling of Doxorubicin-loaded acetylated cashew gum nanoparticles. Quantum chemical calculations, specifically Density Functional Theory (DFT) with a basis set of 6-31+ (d, p), were employed to investigate various properties of these nanoparticles. The analysis included essential bonding parameters, geometry, UV-Visible spectra, HOMO-LUMO (highest occupied molecular orbital - lowest unoccupied molecular orbital), and harmonic vibrational frequencies. The computational approach involved using the GAMESS-US software for DFT calculations and Avogadro for molecular modeling. Geometry optimization, an initial step in DFT calculations, was conducted without constraints, utilizing the optimized geometric parameters for subsequent vibrational frequency calculations to characterize stationary points as minima. The calculated wave numbers (B3LYP) demonstrated proper agreement with the determined wave numbers. The final Restricted Hartree-Fock (RHF) energy after 17 iterations was -2369.0373728027. Additionally, total Mulliken and Lowdin atomic populations, bond order, valence analysis, and electrostatic moments were determined through DFT calculations. It is noteworthy that the study acknowledges the importance of future research aiming to calculate solubility parameters, bioavailability, and pharmacokinetic properties based on the obtained data. This comprehensive approach holds potential for advancing our understanding of Doxorubicin-loaded acetylated cashew gum nanoparticles and their applicability in drug delivery systems for cancer treatment.

**Keywords:** Doxorubicin, Cashew gum, DFT, Quantum chemistry, Drug delivery systems