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Abdulmujeeb T. Onawole, Saheed A. Popoola, Tawfik A. Saleh, Abdulaziz A. Al-Saadi



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Silver-loaded graphene as an effective SERS substrate for clotrimazole detection: DFT and spectroscopic studies

Abdulmujeeb T. Onawole^a, Saheed A. Popoola^b, Tawfik A. Saleh^a, Abdulaziz A. Al-Saadi^{a,*}

^aDepartment of Chemistry, King Fahd University of Petroleum and Minerals, Dhahran, Saudi Arabia

^bDepartment of Chemistry, Islamic University of Madinah, Saudi Arabia

*The corresponding Author; (asaadi@kfupm.edu.sa)

Abstract

Vibrational infrared, Raman and surface-enhanced Raman scattering (SERS) spectra of clotrimazole (CTZ) were documented and evaluated. Density-functional theory, B3LYP/6-311++G(d,p), approach was implemented to identify the possible conformations, develop the electrostatic potential map, evaluate frontier molecular orbitals and calculate the vibrational spectra of the target compound. The silver-loaded graphene was shown to be an effective SERS substrate for CTZ trace detection. The SERS spectrum showed two enhanced bands at 670 cm⁻¹ and 700 cm⁻¹ which confirmed the absorption of the silver substrate through chlorine and nitrogen atoms. A detection limit as low as 5 nM could be reached with a determination coefficient of 0.9988 using the band at 670 cm⁻¹. The protein-ligand interaction with Secreted Aspartic Proteinase 2 (SAP2) of *C. albicans* showed that the four stable forms of CTZ maintain a free energy of binding of 6-7 kcal/mol, which could give insights into the mode of action in treating Candidiasis.

Keywords: Clotrimazole, Surface-enhanced Raman scattering spectroscopy, DFT, Candidiasis, Molecular docking.

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