(البحث رقم 10 في القائمة)

عنوان البحث : (باللغة الأنجليزية)	**Structural investigations of new tridentate-phenylacetohydrazide Schiff base metal chelates: X-ray diffraction, Hirshfeld surface analyses, DFT, antibacterial and molecular docking studies**	
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ملخص موجز للبحث :

In this research, a ligand was prepared from phenylacetohydrazide derivatives (2-hydroxybenzylidene-2-phenylacetohydrazide, HL) and then new complexes with transition metal ions: iron, zinc, palladium, silver, and cadmium. The structures of the compounds were confirmed using infrared spectroscopy, proton nuclear magnetic resonance (1HNMR), elemental analysis, magnetic moment measurements, electrical .conductivity, mass spectrometry, and thermogravimetric analysis

The spatial structure of the silver complex was confirmed using single-crystal X-ray diffraction and surface Hirschfeld analysis. Both X-ray diffraction and surface Hirschfeld analysis revealed an interesting structure and unique geometric properties. They also demonstrated the presence of intramolecular and intermolecular hydrogen bonds and confirmed the octahedral structure of the silver complex. Spectroscopic analysis confirmed that the ligand binds to metal ions through three sites. All metal ions, except palladium, are bound to two ligand molecules to form an octahedral geometry, while the palladium ion is bound to one ligand and a water molecule to form a square-planar geometry. Computational simulations using LANL2DZ were used to study some of the properties of the prepared materials. Docking and antibacterial studies were performed to examine the potential applications of the complexes as therapeutic reagents. The Ag(I) complex showed superior antibacterial inhibition against the tested bacteria, including E. coli, K. pneumoniae, S. aureus, and S. mutans, with inhibition zone diameters of 21.7, 21.0, 19.3, and 15.7 mm, respectively. Computer simulations were performed using the MOE program to study the binding capacity of the complexes to several proteins (PDBs: 1BNA, 1BQB, and 5AEP). Molecular docking simulations indicated that the complexes exhibited high affinities to DNA. Iron and silver derivatives exhibited the highest affinities toward the examined receptors, with nearly equal binding affinities (S = -5.10 and S = -5.01 kcal/mol, respectively). Experimental and theoretical results indicated the remarkable activity of the complexes against various bacterial species. The silver

complex demonstrated remarkable antimicrobial activity, bringing it closer to the existing antibiotic, which is hoped to be used as a new drug after further clinical research and development.