Title	**Structural investigations of new tridentate-phenylacetohydrazide Schiff base metal chelates: X-ray diffraction, Hirshfeld surface analyses, DFT, antibacterial and molecular docking studies**

Abstract

The coordination complexes of a tridentate-phenylacetohydrazide Schiff base (2-hydroxybenzylidene-2-phenylacetohydrazide, **HL**) with metal ions, namely, iron(II), zinc(II), palladium (II), silver(I) and cadmium(II), were synthesized and investigated using various analytical and spectroscopic techniques. A single-crystal X-ray diffraction analysis was performed on the silver derivative. The **HL** ligand and Ag complex were also analyzed via Hirshfeld surface analyses. Both X-ray and Hirshfeld surface analysis revealed intriguing structure and geometric characteristics, as well as remarkably intramolecular and intermolecular hydrogen bonding. All the metal ions, except palladium one, bonded to two molecules of ligand without deprotonation of the hydroxyl moieties. In addition, ^{1}H NMR studies of the diamagnetic complexes and X-ray analysis of the silver complex revealed the presence of the unprotonated OH. The spectroscopic analyses demonstrated that the ligand binds to metal ions through three binding sites. All metal ions, except for palladium, are bound to two ligand molecules to give the octahedral geometry, while the palladium ion is bound to one ligand molecule in addition to a water molecule to give a square planar structure. DFT-B3LYP calculations were used to determine the energy-minimized molecular geometric arrangements of the Pd(II), Ag(I), and Cd(II) derivatives. Quantum global reactivities of the complexes were also computed. Antibacterial and molecular docking studies of complexes were carried out to examine the potential applications of the derivatives as therapeutic reagents. The Ag(I) complex showed the highest antibacterial inhibition towards the tested bacteria with inhibition zone diameter = 21.7, 21.0, 19.3, and 15.7 mm. Molecular docking analysis revealed that the complexes have high binding affinities against the selected receptors (PDB: 1BNA, 1BQB and 5AEP) and demonstrated different DNA binding potencies. Among the compounds, the silver compound has proven its effectiveness as an antimicrobial agent, which is close to the antibiotic used and hopes to be used as a new drug after further research and clinical development.