Structural consequences in differently substituted haloarylcarboxylates and non-covalent interactions on crystal packing and biological efficacy of copper(II) complexes with N,N,N′,N′-tetramethylethylenediamine N-donor ligand

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Artykuł

In this work, we reported four new copper(II) halo-benzoate complexes (2-chloro-4-nitrobenzoate (2-Cl-4-NO2-BZ), 3,5-DICBZ, 2-chloro-5-nitrobenzoate (2-Cl-5-NO2-BZ), 3,5-difluoro benzoate (3,5-DIFBZ), and 3,5-dichlorobenzene (3,5-DICBZ) respectively in complexes **1–4**) with N,N,N',N'-tetramethylethylene diamine (*temed*) N-donor ligand in order to study the interesting coordination features and biological evaluation of such complexes under ambient reaction conditions. All the complexes **1–4** were characterized by elemental analyses, and spectroscopic techniques, including FT-IR, UV–vis, and EPR *etc.* Single crystal X-ray structure determination (SCXRD) of complexes revealed the distorted octahedral geometry in all complexes. Notably, the halobenzoate ligands exhibited a bidentate chelation mode in complexes **1** and **2**, while they showed a monodentate mode in complex **3**. In complex **4**, the carboxylate ligand exhibited both monodentate as well as bidentate coordination. Furthermore, detailed packing analyses of complexes **1–4** highlighted the significance of halogen bonding in lattice stabilization besides hydrogen bonding and π···π interactions as evidenced by Hirshfeld surface analyses and crystal analysis. Moreover, packing analyses displayed that complex **1** exhibited a layered or wave-like arrangement, while complex **2** featured a helical arrangement supported by a supramolecular halogen-bonded network guided by Cl···O interactions. Complex **3** displayed a zig-zag layered arrangement with a stacking topology, and Complex **4** showcased a ribbon-like arrangement stabilized by F···F and Cl···Cl halogen bonding interactions. Furthermore, sigma hole on halogen atoms has also been examined (which play an important role in halogen bonding) by electrostatic-potential isosurfaces. In order to exploit the biological efficacy of complexes **1–4** owing to the inherent biological activity of copper metal, molecular docking analyses against gram +ve bacteria *i.e. S. epidermidis* (PDB ID; 8DO6), *B. subtilis* (1QD9), as well as two gram -ve bacteria, namely, *P. aeruginosa* (5WZE) and *S. dysenteriae* (1DM0), have also been carried out. Interestingly, values of docking scores and inhibition constant of all complexes **1–4** (with a maximum binding score (inhibition constant) of -9.8 kcal/mol (0.063 µMol) i n **1** against 8DO6 and 1DM0) revealed higher biological efficacy than that of standard drugs.

Słowa kluczowe

Supramolecular, Copper(II), Single crystal, Halogen bonding, And sigma hole, Molecular docking

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