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Spectroscopic, single crystal X-ray, Hirshfeld, *in vitro* and *in silico* biological evaluation of a new series of potent thiazole nucleus integrated with pyrazoline scaffolds

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ABSTRACT

In the present study, the spectroscopic characterization of a new series of substituted thiazole linked pyrazoline scaffolds **4a-l** was performed. The formation of **4a-l** from the intermediate 3-(4-chlorophenyl)-5-[4-(propan-2-yl)phenyl]-4,5-dihydro-1*H*-pyrazole-1-carbothioamide **2** and substituted 2-bromo-1-phenylethanone **3a-l** was evidenced through the changes in FTIR, ^{1}H NMR, ^{13}C NMR, LCMS data. The X-ray diffraction studies revealed that compound **2** and **4g** crystallized in monoclinic crystal system with $P2_1/n$ space group. Compound **4j** crystallized in triclinic system, *P-1* space group with Z = 4. The percentage of intermolecular contacts and distribution of electrostatic potential of molecular crystal structures was resolved by Hirshfeld surface analysis with 2D finger plots and electrostatic potential map. The newly synthesized derivatives were screened for their *in vitro* antioxidant and antimicrobial activity. The single crystal studies revealed that, for compounds **2**, **4g** and **4j** the isopropyl