5-(3,4-DICHLOROPHENYL)-3-{[4-(2-PYRIDYL)PIPERAZINE-1-YL]METHYL}-1,3,4-OXADIAZOLE-2(3H)-ONE: SYNTHESIS, CHARACTERIZATION, X-RAY AND DFT STRUCTURES

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5-(3,4-Dichlorophenyl)-3-{[4-(2-pyridyl)piperazine-1-yl)]methyl}-1,3,4-oxadiazole-2(3H)-one $C_{18}H_{17}Cl_2N_5O_2$ (**3**) is synthesized and characterized by IR, ^{1}H NMR, ^{13}C NMR, elemental analyses, single-crystal X-ray diffraction, and the molecular structure is also optimized at the B3LYP/6-31G(*d*,*p*) level using density functional theory (DFT). All data obtained from the spectral studies support the structural properties of **3**. The molecules are linked principally by C–H···O hydrogen bonds involving carbonyl atoms and carboxylate O atoms, forming $R_2^2(16)$ and $R_4^2(20)$ rings that link to give a one-dimensional network of molecules. An extensive two-dimensional network of C–H···O hydrogen bonds and π···π interactions are responsible for crystal stabilization.

Keywords: 1,3,4-oxadiazole, piperazine ring, synthesis, X-ray crystallography, DFT.