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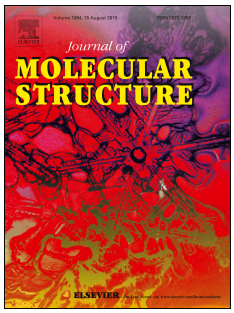

Crystal structure, non-covalent interaction and molecular docking studies of 2-{[2-phenylsulfonyl)hydrazinylidene]methyl}benzoic acid and its dysprosium catalysed cyclized product: 2-(phenyl-sulfonyl)phthalazin-1(2H)-one

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Crystal structure, non-covalent interaction and molecular docking studies of 2-{[2-phenylsulfonyl)hydrazinylidene]methyl}benzoic acid and its dysprosium catalysed cyclized product : 2-(phenyl-sulfonyl)phthalazin-1(2H)-one

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Abstract

The condensation reaction of equimolar benzenesulphonohydrazide and 2-carboxybenzaldehyde gave the Schiff base 2-{[2-(phenylsulfonyl)hydrazinylidene]methyl}benzoic acid(BSHOPA). The reaction of 2-{[2-(phenylsulfonyl)hydrazinylidene]methyl}benzoic acid with dysprosium(III)acetatetetrahydrate gave the cyclized product 2-(phenylsulfonyl)phthalazin-1(2H)-one (PSP). The compounds were characterized by elemental analysis, UV-VIS, IR, ^{1}H NMR, mass spectroscopy and single crystal X-ray determination. The asymmetric BSHOPA molecule crystallized in the triclinic, $P\bar{1}$ crystal system and space group respectively, while PSP crystallized in the monoclinic, $P2_1/n$ crystal system and space group respectively. In the crystal structure of the Schiff base (BSHOPA),the molecules are linked by intermolecular hydrogen bonds involving carboxylic oxygens, nitrogen atoms and sulphonyl oxygens. The chair structures of PSP are stacked through pi-pi interactions between benzene rings. Non-covalent interactions (NCI) analysis of the compounds revealed a number of intermolecular/intramolecular non-covalent interactions stabilizing the crystal structures. Antibiotic potency of the two compounds were investigated by docking against DNA gyrase. Results showed that they demonstrated affinity for the target antibiotic protein with free binding energies of -3.33 Kcal/mol (BSHOPA) and -5.67 Kcal/mol (PSP).