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SUPPLEMENTARY MATERIAL TO

DFT calculation, biological activity, anion sensing studies and crystal structure of (*E*)-4-chloro-2-[(pyridin-2-ylimino)-methyl]phenol

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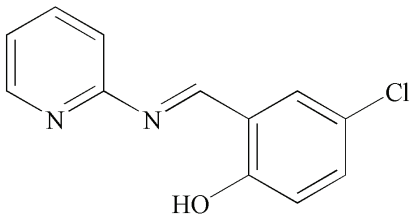

Fig. S-1. The molecular formula of (*E*)-4-chloro-2-[(pyridin-2-ylimino)methyl]phenol.

(E)-4-Chloro-2-[(pyridin-2-ylimino)methyl]phenol. Yield: 1.09 g, 90 %; Orange crystals; m.p.: 139–141 °C; Anal. Calcd. for $C_{12}H_9ClN_2O$: C, 62.07; H, 3.88; N, 12.06 %. Found: C, 61.85; H, 3.90; 12.06 %; IR (KBr, cm^{-1}, Fig. S-2) 3433 (O-H), 3107–3046 (Ar-H), 1616 (C=N), 1560 (C=C), 1478 (C-N), 1356 (C-O); ^{1}H-NMR (400.1 MHz, DMSO, δ / ppm, Fig. S-3): 12.49 (1H, *s*, Ar-OH), 8.94 (1H, *s*, Ar-CH=N-), 8.60–6.96 (7H, *m*, Ar-H); ^{13}C-NMR (100.6 MHz, DMSO, δ / ppm, Fig. S-4): 121.20 (C-1), 158.80 (C-2), 119.61 (C-3), 133.68 (C-4), 124.64 (C-5); 130.99 (C-6), 164.15 (C-7), 148.78 (C-8), 128.17 (C-9), 123.05 (C-10), 144.89 (C-11), 144.24 (C-12).

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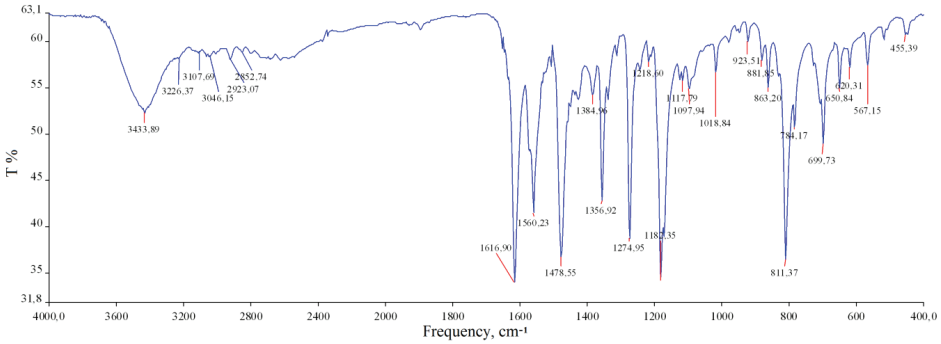

Fig, S-2. FT-IR spectrum of the title compound.

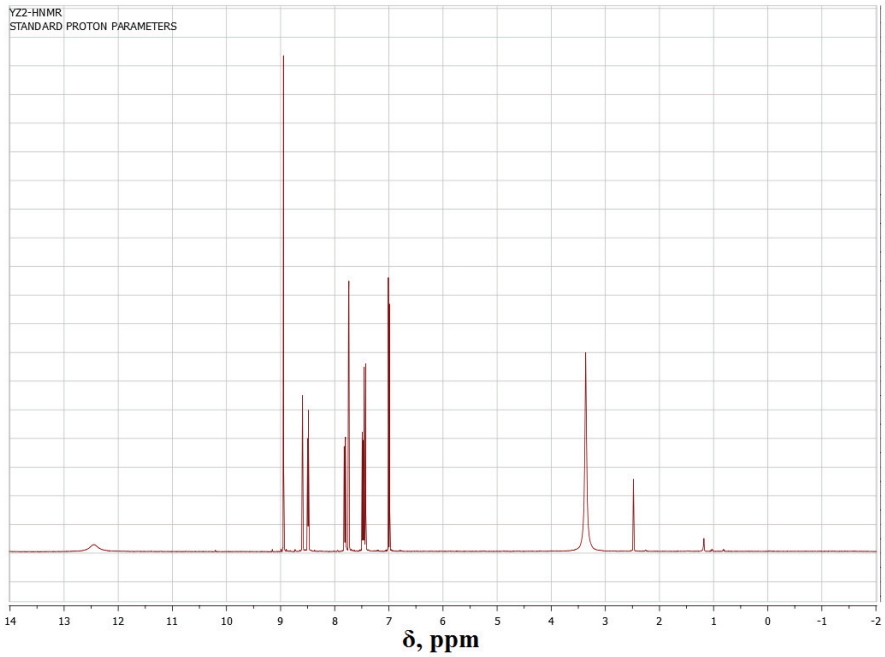

Fig. S-3. ^{1}H-NMR spectrum of the title compound.

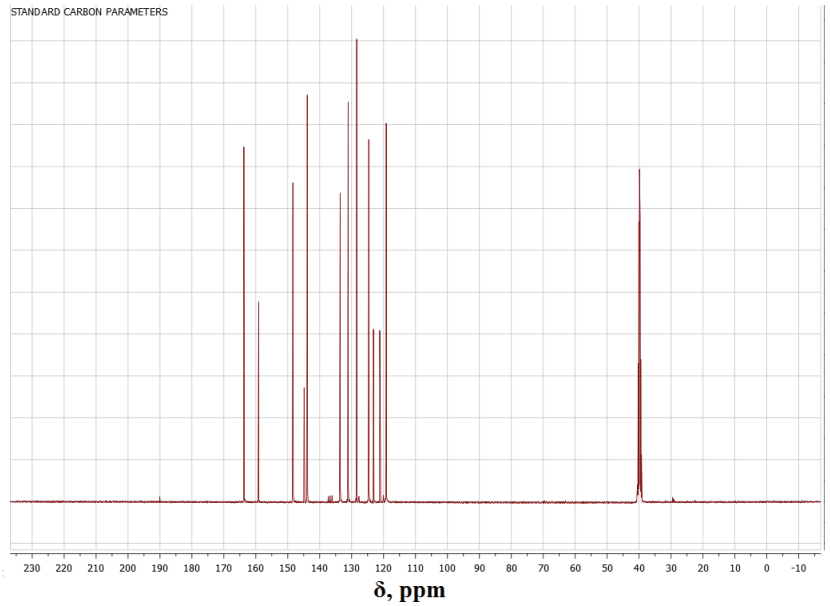

Fig. S-4. ^{13}C-NMR spectrum of the title compound.

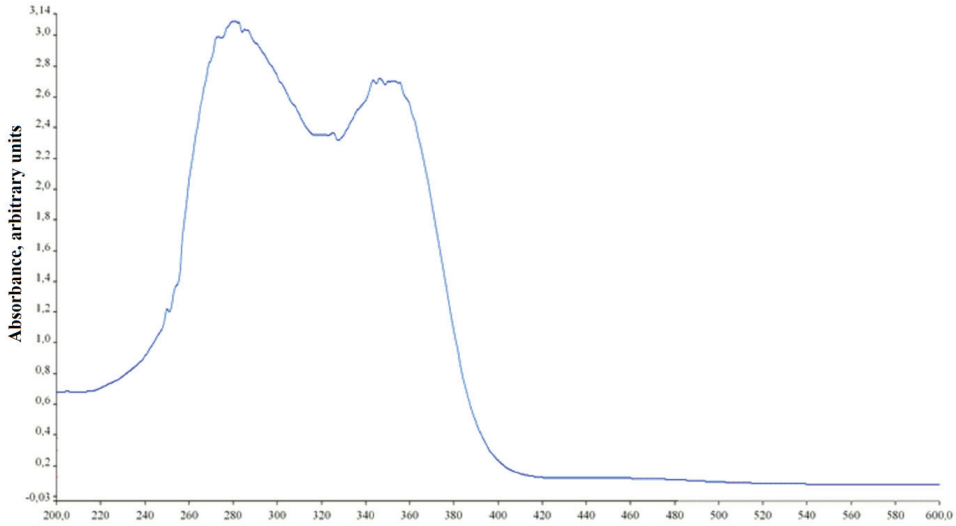

Fig. S-5. UV–Vis spectrum of the title compound.

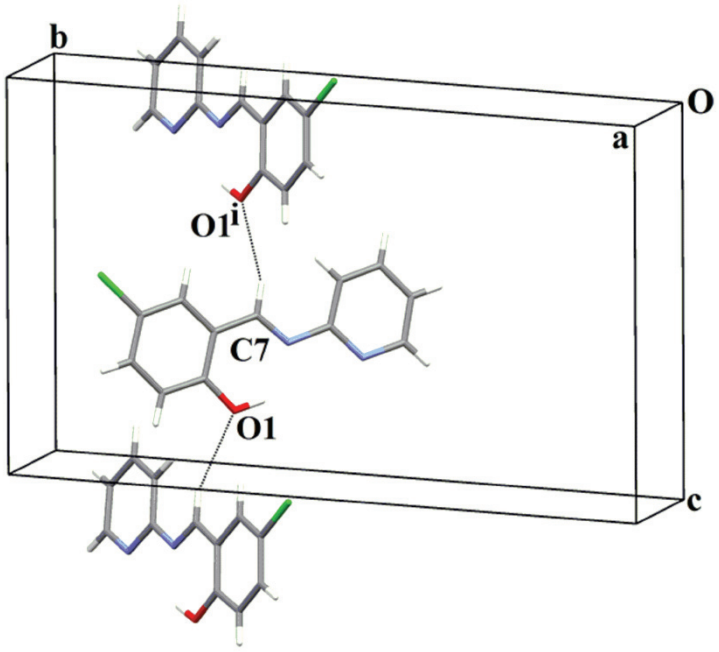

Fig. S-6. The C–H···O hydrogen bonds of the title compound.

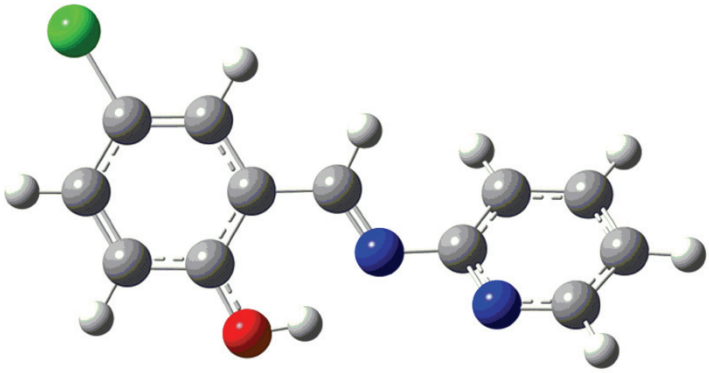

Fig. S-7. The theoretical geometric structure of the title compound (at the B3LYP/6-311++G(d,p) level).