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SUPPLEMENTARY MATERIAL TO

Synthesis, characterization and antibacterial activities of Zn(II) and Cd(II) complexes of a 3-amino-2-phenylquinazolin-4(3*H*)--one Schiff base

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PHYSICAL, ANALYTICAL AND SPECTRAL DATA FOR THE LIGAND AND ITS Zn AND Cd COMPLEXES

*2-{2-[((4-oxo-2-phenyl-3(4*H*)-quinazolinyl)imino)methyl]phenoxy}acetic acid*. Yield: 74 %; white solid; m.p.: 174–178 °C, Anal. Calcd. for $C_{23}H_{17}N_3O_4$: C, 69.17; H, 4.29; N, 10.52 %. Found: C, 69.03; H, 4.33; N, 9.88 %; IR (KBr, cm^{-1}): 3230–3294 (–N–H stretching), 3084 (–O–H stretching, hydrogen bonded), 1734.6 (–C=O stretching –COOH group), 1653.8–1654.8 (–C=O stretching of $–CONH_2$ group) 1667 (–C=O, free), 1623 (–C=O, hydrogen bonded), 1602.7 (–C=N), 1215.1 ((>C–O–C< stretching), 930 (–N–N, stretching); ^{1}H-NMR (400 MHz, DMSO-d_6, δ / ppm): 4.79 (2H, *s*, O–CH_2), 6.99–8.56 (11H, *m*, Ar-H), 8.87 (1H, *s*, HC=N), 11.99–12.24 (1H, *s*, OH, hydrogen bonded with –N= group); ^{13}C-NMR (100 MHz, DMSO-d_6, δ / ppm): 169.94, 164.95, 164.51, 156.38, 144.61, 139.22, 134.26 132.56, 132.1, 131.68, 128.89, 128.59, 126.96, 125.82, 123.07, 122.29, 121.25, 120.88, 120.21, 112.61, 64.76; MS (*m*/*z*, (relative abundance, %)): 400.8 (M+1, 25).

[ZnL(AcO)]·H_2O. Yield 70 %; white solid; m.p.: >300 °C, Anal. Calcd. for $C_{25}H_{19}N_3O_6Zn$: C, 55.52; H, 3.91; N, 7.77. Found: C, 55.52; H, 3.43; N, 8.41; IR (KBr, cm^{-1}): 3435 (H_2O of crystallization), 3165 (–N–H stretching), 1684––1690 (–C=O stretching of –COOH group), 1653.8–1654.8 (–C=O stretching of $–CONH_2$ group), 1667 (–C=O, free), 1630 (–C=O stretching), 1590–1597.9 (–C=N stretching), 1232–1256 (>C–O–C< stretching), 963–960 (–N–N, stretching), 592.1 (M–N stretching frequency); Λ_M (DMF, S cm^2 mol^{-1}): 4.07.

[CdL(AcO)]·H_2O: Yield: 68 %, white solid, m.p.: >300 °C, Anal. Calcd. for $C_{25}H_{19}N_3O_6Cd$: C, 51.08; H, 3.60; N, 7.15 %. Found: C, 50.55; H, 3.03; N, 7.69 %; IR (KBr, cm^{-1}) 3420 (H_2O of crystallization), 3165 (–N–H stretching), 1684–

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–1690 (–C=O stretching of –COOH group), 1653.8–1654.8 (C=O stretching of $–CONH_2$ group), 1667 (–C=O, free), 1630 (–C=O stretching), 1590–1595.9 (–C=N stretching), 1232–1256 (>C–O–C< stretching), 963–960 (N–N, stretching), 594.1 (M–N stretching frequency); ^{1}H-NMR (400 MHz, DMSO-d_6, δ / ppm): 4.53 (2H, *s*, $O–CH_2$), 6.20–8.71 (11H, *m*, Ar-H), 8.73 (1H, *s*, HC=N); ^{13}C-NMR (100 MHz, DMSO-d_6, δ / ppm): 170.72, 169.79, 164.95, 155.33, 151.65, 139.26, 135.69, 133.11, 131.84, 131.30, 130.39, 129.93, 128.77, 127.33, 123.78, 122.41, 121.73, 121.41, 119.16, 113.11, 67.24; Λ_M (DMF, S cm^2 mol^{-1}): 5.64.