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SUPPLEMENTARY MATERIAL TO

Computational, antimicrobial, DNA binding and anticancer activities of pyrimidine incorporated ligand and its copper(II) and zinc(II) complexes

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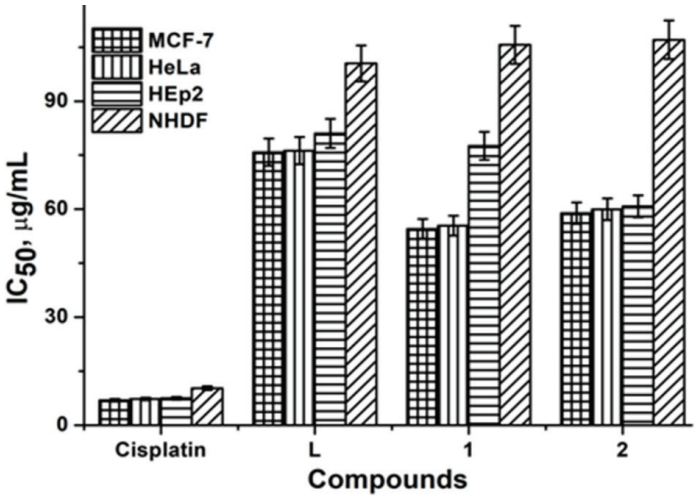

Fig. S-1. *In vitro* anticancer activities of ligand **L**, and complexes **1** and **2** on normal (NHDF) and cancer (MCF-7, HeLa and HEp2) cell lines.

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CHARACTERIZATION DATA FOR THE LIGAND AND ITS COMPLEXES

Ligand ***L***. Yield: 75 %; colour: lemon yellow solid; m.p.: 128 °C; Anal. Calcd. for $C_{16}H_{16}F_3N_5O$: C, 54.68; H, 4.56; N, 19.93 %. Found: C, 54.62; H, 4.49; N, 19.89 %; IR (KBr, cm^{-1}): 1544 (CH=N), 1591 (bend, NH), 3518 (stretch, NH), 1465 & 1402 (aromatic & C=N), 1317 (aromatic & C–N), 3053 & 3035 (aromatic sym & asym, C–H), 1151 (CF_3), 2939 & 2883 (aliphatic sym & asym, C–H), 1093 & 1232 (sym & asym, C–O–C), 1186 (morpholino-C–N); ^{1}H-NMR (400 MHz, DMSO-d_6, δ / ppm): 8.10 (1H, *s*), 9.90 (1H, *s*), 7.19 (1H, *d*), 8.77 (1H, *d*), 6.99 (2H, *d*), 7.55 (2H, *d*), 3.20 (4H, *t*), 3.75 (4H, *t*); ^{13}C-NMR (125 MHz, DMSO-d_6, δ / ppm): 119.91 (CF_3), 138.60 (azomethine (CH=N)), 160.61 (C_2 pyrimidine ring), 152.6 & 153.5 (pyrimidine ring C_4 & C_6), 108.10 (pyrimidine ring C_5), 152.25, 128.49, 114.93 & 125.49 (aromatic ring), 53.31 (–C–N–C–), 66.33 (–C–O–C– morpholine ring); UV–Vis (λ_{max} / nm): 266, 336; ESI mass (*m*/*z*): 351.

Complex ***1***. Yield: 85 %; colour: brown; m.p.: 220 °C; Anal. Calcd for $C_{32}H_{32}Cl_2CuF_6N_{10}O_{10}$: C, 39.82; H, 3.34; N, 14.51; Cu, 6.57 %. Found: C, 39.78; H, 3.39; N, 14.60; Cu, 6.52 %; IR (KBr, cm^{-1}): 1522 (CH=N), 1591 (bend, –NH), 3517 (stretch, –NH), 1463 & 1388 (aromatic & C=N), 1316 (aromatic, C–N), 3048 & 3033 (aromatic sym & asym, C–H), 1150 (CF_3), 2937 & 2881 (aliphatic sym & asym, C–H), 1091 & 1230 (sym and asym, C–O–C), 1184 (morpholine C–N); UV–Vis (λ_{max} / nm): 770; ESI Mass (*m*/*z*): 765.

Complex ***2***. Yield: 86 %; colour: dark brown; m.p.: 227 °C; Anal. Calcd. for $C_{32}H_{32}Cl_2F_6N_{10}O_{10}Zn$: C, 39.74; H, 3.33; N, 14.48; Zn, 6.76 %. Found: C, 39.69; H, 3.29; N, 14.51; Zn, 6.74 %; IR (KBr, cm^{-1}): 1535 (CH=N), 1589 (bend, –NH), 3515 (stretch, –NH), 1464 and 1384 (aromatic, CF_3–CH=N– and =CH–N=), 1315 (aromatic, C–N), 3049 & 3032 (aromatic sym & asym, C–H), 1151 (CF_3), 2936 & 2880 (aliphatic sym & asym, C–H), 1090 & 1231 (sym & asym, C–O–C), 1185 (morpholine –C–N); ^{1}H-NMR (400 MHz, DMSO-d_6, δ / ppm): 8.64 (1H, *s*) 9.94 (1H, *s*), 7.18 (1H, *d*), 9.51 (1H, *d*), 7.10 (2H, *d*), 7.77 (2H, *d*), 3.21 (4H, *t*), 3.76 (4H, *t*); ^{13}C-NMR: 119.91 (CF_3), 139.45 (azomethine CH=N), 161.10 (pyrimidine ring C_2), 152.6 & 154.16 (pyrimidine ring C_4 & C_6), 108.10 (pyrimidine ring C_5), 152.25, 128.49, 114.93 & 125.49 (aromatic ring C–H), 53.31 (morpholino ring –C–N–C–), 66.33 (morpholino ring –C–O–C–); UV–Vis (λ_{max}, nm): 270, 338; ESI Mass (*m*/*z*): 767.