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Supplementary material

SUPPLEMENTARY MATERIAL TO

Spectral, NLO and antimicrobial studies of Co(II), Ni(II) and Cu(II) complexes of Schiff base ligands of 2-amino-6-nitrobenzothiazole

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CHARACTERIZATION DATA FOR **L[1]**–**L[4]**

N-***(4-Methylbenzylidene)-6-nitrobenzothiazol-2-amine (HL[1])***. Anal. Calcd. for $C_{15}H_{11}N_3O_2S$ (FW: 297.33): C, 60.59; H, 3.73; N, 14.13; S, 10.78 %. Found: C, 59.19; H, 3.03; N, 13.05; S, 9.68 %; ^{1}H-NMR (300 MHz, DMSO-d_6, δ / ppm): 8.35 (1H, *s*, azomethine H), 7.46–6.93 (7H, *m*, Ar-H), 1.63 (3H, *s*, CH_3); ^{13}C-NMR (75 MHz, DMSO-d_6, δ / ppm): 22.3 (CH_3), 163 (N=CH), 129–142.3 (-C_6: A1–A6), 175.0 (S–C=N), 145–155 (-C6: A1–A6); ESI-MS (*m*/*z* (relative abundance, %)): 296.5 [M^+] (20), 281 (13), 250 (85), 206 (100).

N-*(4-Ethylbenzylidene)-6-nitrobenzothiazol-2-amine (**HL[2]**)*. Anal. Calcd. for $C_{16}H_{13}N_3O_2S$ (FW: 311.36): C, 60.59; H, 3.73; N, 14.13. S, 10.78 %. Found: C, 59.19; H, 3.03; N, 13.05, S, 9.68 %; ^{1}H-NMR (300 MHz, DMSO-d_6, δ / ppm): 8.41 (1H, *s*, azomethine H), 7.40–6.94 (7H, *m*, Ar-H), 1.89 (2H, *q*, CH_2), 1.63 (3H, *t*, CH_3); ^{13}C-NMR (75 MHz, DMSO-d_6, δ / ppm): 14.3 (CH_3), 28.0 (**C**$H_2$$CH_3$) 160.0 (N=CH), 129.1–146.6 (-C_6: A1–A6), 174.3 (S–C=N), 147–154 (-C_6: A1–A6); ESI-MS (*m*/*z* (relative abundance, %)): 310.5 [M^+] (20), 281 (14), 249 (83), 206 (100).

*4-[[(6-nitro-2-benzothiazolyl)imino]-methyl]phenol (**HL[3]**)*. Anal. Calcd. for $C_{14}H_9N_3O_3S$: C, 56.18; H, 3.05; N, 14.04; S, 10.71 %. Found: C, 55.22; H, 2.25; N, 13.26; S, 9.30 %; ^{1}H-NMR (300 MHz, DMSO-d_6, δ / ppm): 8.45 (1H, *s*, azomethine H), 7.26–6.95 (7H, *m*, Ar-H), 11.23 (*s*, phenolic H); ^{13}C-NMR (75 MHz, DMSO-d_6, δ / ppm): 160.0 (N=CH), 135.1–150.6 (-C_6: A1–A6), 174.6

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(S–C=N), 154–157.8 (-C_6: A1–A6). ESI-MS (*m*/*z* (relative abundance, %)): 298.90 [M^+] (16), 281 (24), 168(72), 205 (100).

*2-[[(6-nitro-2-benzothiazolyl)imino]-methyl]-phenol (**HL^4**)*. Anal. Calcd. for $C_{14}H_9N_3O_3S$ (FW: 299.36): C, 56.18; H, 3.05; N, 14.04; S, 10.71 %. Found: C, 55.22; H, 2.25; N, 13.26 S, 9.30 %; ^{1}H-NMR (300 MHz, DMSO-d_6, δ / ppm): 8.40 (1H, *s*, azomethine H), 7.36–6.94 (7H, *m*, Ar-H), 11.34 (*s*, phenolic H); ^{13}C-NMR (75 MHz, DMSO-d_6, δ / ppm): 175.5 160.5 (N=CH), 130–160.6 138––144.6 (-C_6: A1–A6), 175.5 (S–C=N), 150.3–158.0 (-C_6: A1–A6); ESI-MS (*m*/*z* (relative abundance, %)): 298.90 [M^+] (16), 281 (24), 168 (72), 205 (100).

ANALYTICAL DATA FOR THE METAL(II) COMPLEXES OF **HL^1**–**HL^4**

HL^1–Co. Anal. calcd. for $C_{30}H_{22}Cl_2CoN_6O_4S_2$: C, 49.73; H, 3.06; N, 11.60; S, 8.85 %. Found: C, 48.20; H, 2.78; N, 10.33; S, 7.80 %.

HL^1–Ni. Anal. calcd. for $C_{30}H_{22}Cl_2N_6NiO_4S_2$: C, 49.75; H, 3.06; N, 11.60; S, 8.85 %. Found: C, 48.10; H, 2.88; N, 10.43; S, 7.85 %.

HL^1–Cu. Anal. calcd. for $C_{30}H_{22}Cl_2CuN_6O_4S_2$: C, 49.42; H, 3.04; N, 11.53; S, 8.80 %. Found: C, 48.12; H, 2.84; N, 10.33; S, 7.85 %.

HL^2–Co. Anal. calcd. for $C_{32}H_{26}Cl_2CoN_6O_4S_2$: C, 51.07; H, 3.48; N, 11.17; S, 8.52 %. Found: C, 50.70; H, 2.95; N, 10.05; S, 7.25.

HL^2–Ni. Anal. calcd. for $C_{32}H_{26}Cl_2N_6NiO_4S_2$: C, 51.09; H, 3.48; N, 11.17; S, 8.51 %. Found: C, 50.70; H, 2.95; N, 10.00; S, 7.35 %.

HL^2–Cu. Anal. calcd. for $C_{32}H_{26}Cl_2CuN_6O_4S_2$: C, 50.76; H, 3.46; N, 11.10; S, 8.45 %. Found: C, 49.85; H, 2.75; N, 10.15; S, 7.65 %.

HL^3–Co. Anal. calcd. for $C_{28}H_{18}Cl_2CoN_6O_6S_2$: C, 46.17; H, 2.49; N, 11.54; S, 8.80 %. Found: C, 45.20; H, 1.55; N, 10.50; S, 7.85 %.

HL^3–Ni. Anal. calcd. for $C_{28}H_{18}Cl_2N_6NiO_6S_2$: C, 46.18; H, 2.49; N, 11.54; S, 8.81 %. Found: C, 45.25; H, 1.50; N, 10.50; S, 7.75 %.

HL^3–Cu. Anal. calcd. for $C_{28}H_{18}Cl_2CuN_6O_6S_2$: C, 45.88; H, 2.47; N, 11.46; S, 8.75 %. Found: C, 45.00; H, 2.05; N, 10.35; S, 7.65 %.

HL^4–Co. Anal. calcd. for $C_{28}H_{16}CoN_6O_6S_2$: C, 51.30; H, 2.46; N, 12.82; S, 9.78 %. Found: C, 50.70; H, 1.75; N, 11.75; S, 8.85 %.

HL^4–Ni. Anal. calcd. for $C_{28}H_{16}N_6NiO_6S_2$: C, 51.32; H, 2.46; N,12.82; S, 9.79 %. Found: C, 50.65; H, 1.80; N, 11.78; S, 8.80 %.

HL^4–Cu. Anal. calcd. for $C_{28}H_{16}CuN_6O_6S_2$: C, 50.94; H, 2.44; N, 12.73; S, 9.71 %. Found: C, 50.15; H, 1.92; N, 11.95; S, 8.70 %.