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SUPPLEMENTARY MATERIAL TO

Metal complexes with Schiff base and benzimidazolylphenol ligands with *tert*-butyl and methoxy groups: Structural characterization and biological evaluation

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4-tert-*Butyl-2-{[(*E*)-(2-hydroxy-3-methoxyphenyl)methylidene]amino}phenol* (***H_2L^1***). Decomposition point (Dec. p.): 138 °C. (+)ESI-MS (*m/z*): calculated for $[C_{18}H_{21}NO_3]^+$ 299.4, observed 297.3 (90.6 %) ($[C_{18}H_{21}NO_3$ - 2H$]^+$ and 300.4 for ($[C_{18}H_{21}NO_3$ + H$]^+$ (64.1 %). Combustion analysis for $C_{18}H_{21}NO_3$: Calculated C 72.22, H 7.07, N 4.68; found C 72.41, H 7.11, N 4.60. FT-IR (ATR, cm^{-1}): 3509m,br ν(NH), 3054w ν$(CH)_{ar.}$, 2958m ν$(CH)_{al.}$, 1630m ν(C=N), 1619m ν(C=C), 1498m, 1455m, 1351m, 1289m, 1225m ν(C–O), 1204m ν(C–O), 1070s, 831m δ$(CH)_{ar.}$, 740m, 623m, 572m, 465m, 425m. ^{1}H NMR (500 MHz, DMSO-d_6, δ / ppm): 9.57 (*s*, 1H, OH1), 9.00 (*s*, 1H, N=CH), 7.36 (*d*, 1H, *J* = 2.4, H3), 7.21 (*dd*, 1H, J_1 = 7.9, J_2 = 1.4, H6'), 7.14 (*dd*, 1H, J_1 = 8.5, J_2 = 2.4, H5), 7.06 (*dd*, 1H, J_1 = 8.0, J_2 = 1.4, H4'), 6.89 (*d*, 1H, *J* = 8.5, H6), 6.84 (*t*, 1H, J_1 = 7.9, J_2 = 7.9, H5'), 3.81 (*s*, 3H, OCH_3), 1.28 (*s*, 9H, –$C(CH_3)_3$). ^{13}C NMR (125 MHz, DMSO-d_6, δ / ppm): 161.6 (N=CH), 152.5 (C–OH(2')), 149.0 (C–OCH_3), 148.6 (C–OH(1')), 142.5 (C–$C(CH_3)$), 134.0 (C2), 125.2 (C5), 124.3 (C6'), 119.7 (C3), 118.2 (C6), 116.7 (C1'), 116.5 (C5'), 115.5 (C4'), 56.3 (OCH_3), 34.4 (–$C(CH_3)_3$). 31.8 (–$C(CH_3)_3$). UV-vis spectra (DMSO, λ_{max} / nm): 315m,br, 348m,br, 456w,br.

2-(5-*tert*-Butyl-1*H*-benzimidazol-2-yl)-6-methoxyphenol (**HL^2**): Dec.p.: 219 °C. (+)ESI-MS (*m/z*): calculated for $[C_{18}H_{20}N_2O_2]^+$ 296.4, observed 297.3 (100 %) ($[C_{18}H_{20}N_2O_2$ - H$]^+$ and 298.3 for ($[C_{18}H_{20}N_2O_2$ + 2H$]^+$ (20.7 %). Combustion analysis for $C_{18}H_{20}N_2O_2$: Calculated C 72.95, H 6.80, N 9.45; found C 73.07, H 6.91, N 9.30. FT-IR (ATR, cm^{-1}): 3351m ν(NH+OH), 3072w ν$(CH)_{ar}$, 2960m ν$(CH)_{al}$, 1619m ν(C=N), 1604m ν(C=C), 1576m, 1462m, 1364m, 1254s ν(C–O), 1202m ν(C–O), 1059m, 972m, 808m δ$(CH)_{ar}$,, 785m, 732m, 655m, 557m, 511m, 457m, 425m. ^{1}H NMR (500 MHz, DMSO-d_6, δ / ppm): 13.12 (*s,br*, 2H, NH+OH),

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7.59 (*dd*, 1H, J_1 = 8.0, J_2 = 1.3, H6), 7.55 (*s,br*, 2H, H4+H6'), 7.36 (*dd*, 1H, J_1 = 8.5, J_2 = 1.5 Hz, H4'), 7.06 (*dd*, 1H, J_1 = 8.0, J_2 = 1.2, H7), 6.93 (*t*, 1H, J_1 = 8.0, J_2 = 8.0, H5'), 3.81 (*s*, 3H, OCH_3), 1.35 (*s*, 9H, $–C(CH_3)_3$). ^{13}C NMR (125 MHz, DMSO-d_6, δ / ppm): 161.4 (C2), 152.7 ($\underline{C}–OCH_3$), 149.6 ($\underline{C}–OH$), 145.6 ($\underline{C}–C(CH_3)$), 132.2 (C9), 131.3 (C8), 122.0 (C3'), 121.1 (C4'), 120.7 (C6), 120.1 (C2'), 117.1 (C7), 113.9 (C4), 109.3 (C5'), 56.2 (OCH_3), 34.5 ($–\underline{C}(CH_3)_3$), 31.7 ($–C(\underline{C}H_3)_3$). UV-vis spectra (DMSO, λ_{max} / nm): 304m, 316m, 330m,br, 382m,br. Fluorescence spectra (EtOH, $c = 1\times10^{-4}$ mol L^{-1}, λ_{max} / nm): 463m.

[Co(**L**^{1})$(H_2O)_2$]·H_2O (**1a**): Brown solid. Yield: 67 %. Dec. p.: 167 °C. Combustion analysis for $C_{18}H_{25}NO_6Co$ (FW: 410.33): Calculated C 52.69, H 6.14, N 3.41; found C 52.40, H 5.84, N 3.28. Magnetic moment, μ_{eff}: 4.06 μ_B. Λ_M (DMF, 25 °C, S m^2 mol^{-1}): 21.4. FT-IR (ATR, cm^{-1}): 3223m,br ν(OH), 3062w,br ν$(CH)_{ar}$, 2957m ν$(CH)_{al}$, 1646m ν(C=N), 1611m ν(C=C), 1565m, 1490m, 1440m, 1362m, 1257s ν(C–O), 1225m, 1096m, 1050m, 957m, 822m δ$(CH)_{ar}$, 723m, 684m ν(N→M), 541m ν(O→M), 495m, 452m. TGA (t / °C: weight loss, %): 50: 0.3; 75: 1.5; 100: 4.6 (1 mole of H_2O); 150: 7.8; 200: 9.5 (1 mole of H_2O); 250: 12.3; 300: 18.3; 350: 36.5; 400: 47.8; 450: 58.0; 500: 67.5; 550: 80.1; 600: 80.1; 650: 80.1; 700: 80.2 (Theoretical value of CoO: 18.3 %). UV-vis spectra (DMSO, λ_{max} / nm): 227w, 253m, 278m,br, 354m, 464m,br.

[Ni(**L**^{1})$(H_2O)_2$] (**1b**): Greenish brown solid. Yield: 70 %. Dec. p.: 186 °C. Combustion analysis for $C_{18}H_{23}NO_5Ni$ (FW: 392.07): Calculated C 55.14, H 5.91, N 3.57; found C 55.33, H 6.06, N 3.51. Magnetic moment, μ_{eff}: 2.04 μ_B. Λ_M (DMF, 25 °C, S m^2 mol^{-1}): 21.4. FT-IR (ATR, cm^{-1}): 3065w,br ν$(CH)_{ar}$, 2957m ν$(CH)_{al}$, 1633sh ν(C=N), 1615m ν(C=C), 1506m, 1440m, 1362m, 1245m ν(C–O), 1222s, 1129m, 1078m, 975m, 820m δ$(CH)_{ar}$, 732s, 682m ν(N→M), 587m, 536m ν(O→M), 496m, 454m, 425m. TGA (t / °C: weight loss, %): 50: 0.2; 75: 0.3; 100: 0.4; 150: 3.1; 200: 12.3 (2 mole of H_2O); 250: 15.5; 300: 22.1; 350: 27.2; 400: 60.1; 450: 78.9; 500: 80.0; 550: 80.0; 600: 80.0; 650: 80.0; 700: 80.0 (Theoretical value of NiO: 19.1 %). UV-vis spectra (DMSO, λ_{max} / nm): 232w, 255m, 300m,br, 343m,br, 356sh, 440m,br.

[Cu(**L**^{1})(H_2O)] (**1c**): Brown solid. Yield: 73 %. Dec. p.: 295 °C. Combustion analysis for $C_{18}H_{21}NO_4Cu$ (FW: 378.9): Calculated C 57.69, H 4.36, N 2.64; found C 57.43, H 4.21, N 2.49. Magnetic moment, μ_{eff}: 1.72 μ_B. Λ_M (DMF, 25 °C, S m^2 mol^{-1}): 32.0. FT-IR (ATR, cm^{-1}): 3346m,br ν(OH), 3080w,br ν$(CH)_{ar}$, 2962m ν$(CH)_{al}$, 1647m ν(C=N), 1612m ν(C=C), 1588m, 1506m, 1463m, 1351m, 1258m ν(C–O), 1093m, 1027m, 821m δ$(CH)_{ar}$, 781m, 731m, 688m ν(N→M), 584m, 537m ν(O→M), 477m, 422m. TGA (t / °C: weight loss, %): 50: 0.1; 75: 0.4; 100: 0.6; 150: 4.4; 200: 5.0 (1 mole of H_2O); 250: 10.5; 300: 29.8; 350: 45.1; 400: 47.0; 450: 59.7; 500: 68.0; 550: 79.2; 600: 79.4; 650: 79.9; 700: 79.9 (Theoretical value of CuO: 21.0 %). UV-vis spectra (DMSO, λ_{max} / nm): 242w, 254m, 272m,br, 307sh, 363m,br, 478w,br.

[Zn(**L**^{1})(H_2O)]·H_2O (**1d**): Dark yellow solid. Yield: 65 %. Dec. p.: 173 °C. Combustion analysis for $C_{18}H_{23}NO_5Zn$ (FW: 398.8): Calculated C 49.79, H 5.34, N 3.23; found C 49.90, H 5.20, N 3.11. Λ_M (DMF, 25 °C, S m^2 mol^{-1}): 23.4. FT-IR (ATR, cm^{-1}): 3336m,br ν(OH), 3211m,br, 3061w,br ν$(CH)_{ar}$, 2957m ν$(CH)_{al}$, 1637m ν(C=N), 1615m ν(C=C), 1506m, 1435m, 1363m, 1285m, 1234m ν(C–O), 1195m ν(C–O), 1022m, 875m, 819m δ$(CH)_{ar}$, 734m, 684m ν(N→M), 586m, 537m ν(O→M), 497m, 415m. ^{1}H NMR (500 MHz, DMSO-d_6, δ / ppm): 8.86 (*s*, 1H, N=CH), 7.50 (*s,br*, 1H, *J* = 2.4, H3), 7.19 (*d*, 1H, *J* = 7.1, H6'), 7.03 (*s,br*, 1H, H5), 6.88 (*s,br*, 1H, H4'), 6.78 (*d,br*, 1H, *J* = 6.8, H6), 6.38 (*t*, 1H, J_1 =7.7, J_2 = 7.8, H5'), 3.75 (s, 3H, OCH_3), 1.27 (*s*, 9H, $–C(CH_3)_3$). ^{13}C NMR (125 MHz, DMSO-d_6, δ / ppm): 164.8 (N=CH), 161.3 (C–OH2), 152.7 ($\underline{C}–OCH_3$), 144.8 (C–OH1'), 142.4 ($\underline{C}–C(CH_3)$), 130.1 (C2), 127.3 (C5), 123.8 (C6'), 119.4 (C3), 117.1 (C6), 114.3 (C1'), 111.5 (C5'), 107.6 (C4'), 55.0 (OCH_3), 32.2 ($–\underline{C}(CH_3)_3$), 29.5 ($–C(\underline{C}H_3)_3$). TGA (t / °C: weight loss, %): 50: 1.1; 75: 2.5; 100: 4.6 (1 mole of

H_2O); 150: 4.4; 200: 9.5 (1 mole of H_2O); 250: 12.2; 300: 23.1; 350: 29.5; 400: 33.0; 450: 63.0; 500: 78.6; 550: 78.8; 600: 78.9; 650: 79.0; 700: 79.0 (Theoretical value of ZnO: 20.4%). UV-vis spectra (DMSO, λ_{max} / nm): 228 w, 253 w, 279 m, 354 m,br, 464 m,br.

K[Pd(**L**^{1})Cl]·H_2O (**1e**): Light brown solid. Yield: 77 %, Dec. p.: 265 °C. Combustion analysis for $C_{18}H_{21}ClNO_4KPd$ (FW: 496.3): Calculated C 43.56, H 4.26, N 2.82; found C 43.70, H 4.11, 2.68. Λ_M (DMF, 25 °C, S m^2 mol^{-1}): 83.2. FT-IR (ATR, cm^{-1}): 3036m,br ν(CH)$_{ar}$, 2958m ν(CH)$_{al}$, 1646m ν(C=N), 1611m ν(C=C), 1506m, 1456m, 1351m, 1289m, 1257s ν(C–O), 1204m ν(C–O), 1097m, 1024m, 965m, 912m, 826m δ(CH)$_{ar}$, 730m, 673m ν(N→M), 564m, 540m ν(O→M), 500m, 462m. ^{1}H-NMR (500 MHz, DMSO-d$_6$, δ / ppm): 8.64 (*s*, 1H, N=CH), 7.94 (*d*, 1H, J=3.0, H3), 7.43 (*d*, 1H, J=8.1 H6'), 7.30 (*d*, 1H, J=8.5, H5), 7.09 (*d*, 1H, *J* = 8.2, H4'), 7.02 (*d*, 1H, *J* = 8.6, H6), 6.72 (*t*, 1H, J_1 = 8.7, J_2 = 8.5, H5'), 3.72 (*s*, 3H, OCH_3), 1.30 (*s*, 9H, –C(CH_3)$_3$). ^{13}C NMR (125 MHz, DMSO-d$_6$, δ / ppm): 174.3 (N=CH), 161.5 (C–OH2), 148.4 (C–OCH_3), 146.9 (C–OH1'), 139.5 (C–C(CH_3)), 134.3 (C2), 126.3 (C5), 125.3 (C6'), 118.4 (C3), 118.3 (C6), 115.2 (C1'), 113.6 (C5'), 112.5 (C4'), 55.9 (OCH_3), 35.7 (–C(CH_3)$_3$), 32.1 (–C(CH_3)$_3$). TGA (t / °C: weight loss, %): 50: 0.7; 75: 2.0; 100: 3.7 (1 mole of H_2O); 150: 3.9; 200: 4.1; 250: 4.3; 300: 6.0; 350: 7.5; 400: 20.0; 450: 67.0; 500: 74.7; 550: 75.3; 600: 75.6; 650: 75.9; 700: 76.0 (Theoretical value of PdO: 24.6 %). UV-vis spectra (DMSO, λ_{max} / nm): 233w, 255m, 309sh, 318m,br, 337sh, 430m,br, 451sh.

[Co(**L**^{2})Cl(H_2O)] (**2a**): Dark brown solid. Yield: 72 %. Dec. p.: 201 °C. Combustion analysis for $C_{18}H_{21}ClN_2O_3Co$ (FW: 407.8): Calculated C 53.02, H 5.19, N 6.87; found C 54.10, H 5.00, N 6.72. Magnetic moment, μ_{eff}: 2.17 μ_B. Λ_M (DMF, 25 °C, S m^2 mol^{-1}): 35.4. FT-IR (ATR, cm^{-1}): 3198m,br ν(OH), 3088m,br ν(CH)$_{ar}$, 2960m ν(CH)$_{al}$, 1606m ν(C=N), 1573m ν(C=C), 1463m, 1435m, 1361m, 1244s ν(C–O), 1195m, 1060m, 981m, 813m δ(CH)$_{ar}$, 786m, 732s, 66 m ν(N→M), 601m, 574m, 545m ν(O→M), 501m, 470m, 420m. TGA (t / °C: weight loss, %): 50: 0.1; 75: 0.2; 100: 0.4; 150: 3.1; 200: 5.2 (1 mole of H_2O); 250: 9.9; 300: 29.0; 350: 66.0; 400: 67.1; 450: 68.2; 500: 69.4; 550: 82.4; 600: 82.5; 650: 82.6; 700: 82.6 (Theoretical value of CoO: 18.4 %). UV-vis spectra (DMSO, λ_{max} / nm): 240w, 253w, 307m,br, 320m,br, 334sh, 473w,br. Fluorescence spectra (EtOH, $c = 1\times10^{-4}$ mol L^{-1}, λ_{max} / nm): 425sh, 451m,br.

[Ni(**L**^{2})Cl(H_2O)]·H_2O (**2b**): Light brown solid. Yield: 70 %. Dec. p.: 198 °C. Combustion analysis for $C_{18}H_{23}ClN_2O_4Ni$ (FW: 425.5): Calculated C 50.81, H 5.45, N 6.58; found C 50.90, H 5.51, N 6.43. Magnetic moment, μ_{eff}: 2.05 μ_B. Λ_M (DMF, 25 °C, S m^2 mol^{-1}): 38.8. FT-IR (ATR, cm^{-1}): 3373m,br ν(OH), 3228m,br, 3070m,br ν(CH)$_{ar}$, 2962m ν(CH)$_{al}$, 2872m, 1611m ν(C=N), 1598m ν(C=C), 1545m, 1440m, 1362m, 1249m ν(C–O), 1198m ν(C–O), 1015m, 983m, 863m, 814m δ(CH)$_{ar}$, 731m, 671m ν(N→M), 581m, 540m ν(O→M), 457m, 420m. TGA (t / °C: weight loss, %): 50: 0.3; 75: 2.2; 100: 4.6 (1 mole of H_2O); 150: 7.8; 200: 9.0 (1 mole of H_2O); 250: 19.3; 300: 22.8; 350: 24.4; 400: 36.9; 450: 53.0; 500: 65.1; 550: 72.1; 600: 75.3; 650: 82.6; 700: 83.0 (Theoretical value of NiO: 17.5 %). UV-vis spectra (DMSO, λ_{max} / nm): 241w, 253w, 309m,br, 357m,br, 373m,br, 461m,br. Fluorescence spectra (EtOH, $c = 1\times10^{-4}$ mol L^{-1}, λ_{max} / nm): 399w, 478m.

[Cu(**L**^{2})Cl] (**2c**): Brown solid. Yield: 76 %. Dec. p.: 235 °C. Combustion analysis for $C_{18}H_{19}ClN_2O_2Cu$ (FW: 394.4): Calculated C 54.82, H 4.86, N 7.10; found C 55.90, H 5.05, N 6.92. Magnetic moment, μ_{eff}: 1.01 μ_B. Λ_M (DMF, 25 °C, S m^2 mol^{-1}): 48.8. FT-IR (ATR, cm^{-1}): 3215m,br ν(OH), 3057w,br ν(CH)$_{ar}$, 2962m ν(CH)$_{al}$, 1608m ν(C=N), 1589m ν(C=C), 1543m, 1485m, 1384m, 1242s ν(C–O), 1199m ν(C–O), 1062m, 981m, 815m δ(CH)$_{ar}$, 786m, 732s, 667m ν(N→M), 576m, 543m ν(O→M), 470m, 418m. TGA (t / °C: weight loss, %): 50: 0.2; 75: 0.3; 100: 0.4; 150: 0.5; 200: 1.6; 250: 4.2; 300: 6.4; 350: 13.4; 400: 26.5; 450: 43.0; 500: 65.0; 550: 76.0; 600: 78.1; 650: 80.0; 700: 81.0 (Theoretical value of CuO: 20.2 %). UV-

vis spectra (DMSO, λ_{max} / nm): 243w, 255m, 297sh, 307m, 321m, 335m,br, 371sh, 433m,br. Fluorescence spectra (EtOH, $c = 1\times10^{-4}$ mol L^{-1}, λ_{max} / nm): 404w,br, 461sh.

[Zn(**L**^{2})Cl(H_2O)]·H_2O (**2d**): Dark yellow solid. Yield: 65 %, Dec. p.: 229 °C. Combustion analysis for $C_{18}H_{23}ClN_2O_4Zn$ (FW: 432.3): Calculated C 50.02, H 5.36, N 6.48; found C 50.30, H 5.44, N 6.34. Λ_M (DMF, 25 °C, S m^2 mol^{-1}): 38.6. FT-IR (ATR, cm^{-1}): 3406m,br ν(OH), 3215m,br ν(NH), 3059w,br ν$(CH)_{ar}$, 2962m ν$(CH)_{al}$, 1614m ν(C=N), 1591m ν(C=C), 1554m, 1467m, 1386m, 1249s ν(C–O), 1199m ν(C–O), 1109m, 1078m, 975m, 852m, 825m δ$(CH)_{ar}$, 732s, 669m ν(N→M), 601m, 543m ν(O→M), 439m, 410m. ^{1}H NMR (500 MHz, DMSO-d_6, δ / ppm): 13.64 (*s,br*, 1H, NH), 7.65 (*dd,br*, 1H, $J_1 = 8.6$, $J_2 = 1.7$, H6), 7.37 (*d,br*, 2H, $J = 8.9$, H4+H6'), 7.05 (*s,br*, 1H, H4'), 6.95 (*d,br*, 1H, $J = 7.9$, H7), 6.89 (*t,br*, 1H, $J_1 = 8.0$, $J_2 = 8.1$, H5'), 3.82 (*s*, 3H, OCH_3), 1.36 (*s*, 9H, –$C(CH_3)_3$). ^{13}C NMR (125 MHz, DMSO-d_6, δ / ppm): 167.9 (C2), 159.0 (C–OCH_3), 131.9, 104.7, 54.2 (OCH_3), 32.8 (–$C(CH_3)_3$). TGA (t / °C: weight loss, %): 50: 1.9; 75: 4.1; 100: 4.3 (1 mole of H_2O); 150: 8.4; 200: 9.0 (1 mole of H_2O); 250: 21.7; 300: 34.3; 350: 75.6; 400: 80.9; 450: 81.1; 500: 81.5; 550: 81.6; 600: 81.8; 650: 82.0; 700: 82.1 (Theoretical value of ZnO: 18.8 %). UV-vis spectra (DMSO, λ_{max} / nm): 237w, 254w, 296sh, 304m, 332sh, 354sh. Fluorescence spectra (EtOH, $c = 1\times10^{-4}$ mol L^{-1}, λ_{max} / nm): 424m,br.

[Pd(**L**^{2})Cl(H_2O)] (**2e**): Light brown solid. Yield: 77%, Dec. p.: 265. Combustion analysis for $C_{18}H_{21}ClN_2O_3Pd$ (FW: 455.2): Calculated C 47.49, H 4.65, N 6.15; found C 47.12, H 4.63, N 5.90. Λ_M (DMF, 25 °C, S m^2 mol^{-1}): 49.6. FT-IR (ATR, cm^{-1}): 3293m,br ν(OH), 3197m ν(NH), 3058w,br ν$(CH)_{ar}$, 2958m ν$(CH)_{al}$, 2866m, 1602m ν(C=N), 1592m ν(C=C), 1561m, 1492m, 1436m, 1364m, 1242s ν(C–O), 1182m ν(C–O), 1075m, 981m, 812m δ$(CH)_{ar}$, 733m, 669m ν(N→M), 599m, 543m ν(O→M), 465m, 441m. ^{1}H NMR (500 MHz, DMSO-d_6, δ / ppm): 13.22 (*s,br*, 1H, NH), 8.02 (*d*, 1H, $J = 9.1$, H6), 7.61 (*d,br*, 1H, $J = 2.8$, H4), 7.39 (*d,br*, 1H, $J = 8.8$, H6'), 7.30 (*dd*, 1H, $J_1 = 8.4$, $J_2 = 1.8$, H4'), 7.23 (*dd*, 1H, $J_1 = 8.6$, $J_2 = 1.6$, H7), 6.96 (*t*, 1H, $J_1 = 8.3$, $J_2 = 7.9$, H5'), 3.84 (*s*, 3H, OCH_3), 1.39 (*s*, 9H, –$C(CH_3)_3$). ^{13}C NMR (125 MHz, DMSO-d_6, δ / ppm): 170.8 (C2), 166.2 (C–OCH_3), 159.8 (C–OH), 158.0 (C–$C(CH_3)$), 140.4, 139.3, 132.5, 119.0, 116.1, 56.2 (OCH_3), 33.2 (–$C(CH_3)_3$). TGA (t / °C: weight loss, %): 50: 0.2; 75: 0.5; 100: 0.6; 150: 3.3; 200: 5.1 (1 mole of H_2O); 250: 7.5; 300: 15.0; 350: 23.0; 400: 28.5; 450: 32.5; 500: 35.2; 550: 44.2; 600: 68.2; 650: 74.1; 700: 74.2 (Theoretical value of PdO: 26.8 %). UV-vis spectra (DMSO, λ_{max} / nm): 233m, 255m, 308m,br, 321m,br, 335m,br, 458m,br. Fluorescence spectra (EtOH, $c = 1\times10^{-4}$ mol L^{-1}, λ_{max} / nm): 393w, 472m,br.

TABLE S-I. Crystal data and structure refinement parameters for **H_2L^1**

Empirical formula	$C_{18}H_{21}NO_3$
Formula weight	299.36
Crystal system	Orthorhombic
Space group	*Pbca*
a (Å)	14.2349 (10)
b (Å)	9.5415 (5)
c (Å)	24.1061 (16)
α, β, γ (°)	90
V (Å^3)	3274.1(4)
Z	8
D_c (g cm^{-3})	1.215
μ (mm^{-1})	0.082
θ range (°)	2.5-25.2

Measured refls.	46454
Independent refls.	3898
R_{int}	0.062
S	1.04
R1/wR2	0.059/0.154
$\Delta\rho_{max}/\Delta\rho_{min}$ (eÅ^{-3})	0.19/-0.21
CCDC	2298000

TABLE S-II. Selected bond distances and angles for **H_2L^1** (Å, º)

C8—N1	1.305(3)	C3—C2—O2	125.58(19)
C1—O1	1.289(2)	C13—C15—C18	110.40(19)
C2—O2	1.364(2)	C13—C15—C17	111.9(2)
C6—C8	1.407(3)	C16—C15—C13	108.3(2)
C7—O2	1.420(3)	O3—C10—C11	125.82(19)
C9—C14	1.384(3)	O3—C10—C9	116.1(2)
C9—C10	1.396(3)	C14—C9—N1	123.33(18)
C9—N1	1.414(3)	C10—C9—N1	115.90(18)
C10—O3	1.353(3)	C8—N1—C9	127.13(19)
O1—C1—C6	122.17 (19)	N1—C8—C6	123.8(2)
O1—C1—C2	121.55 (18)	C2—O2—C7	117.37(17)
O2—C2—C1	113.32 (17)		

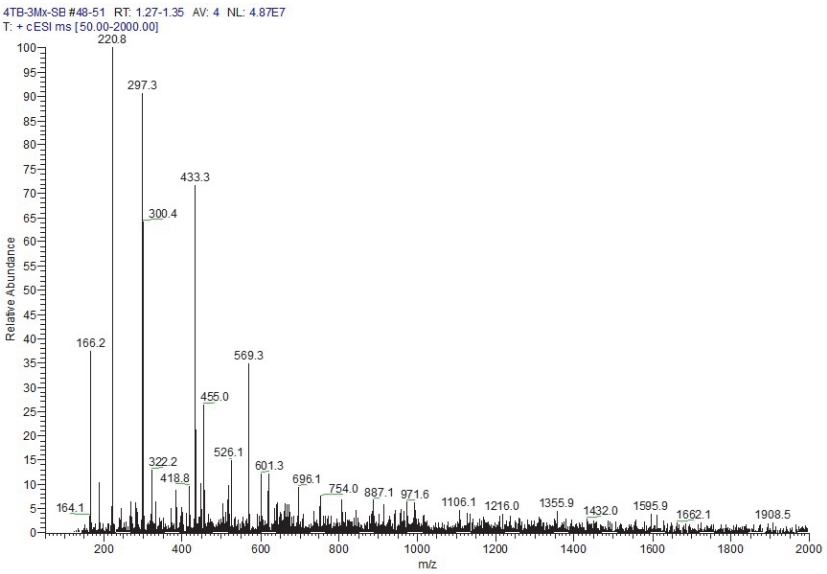

Fig. S1. ESI-MS spectrum of **H_2L^1**

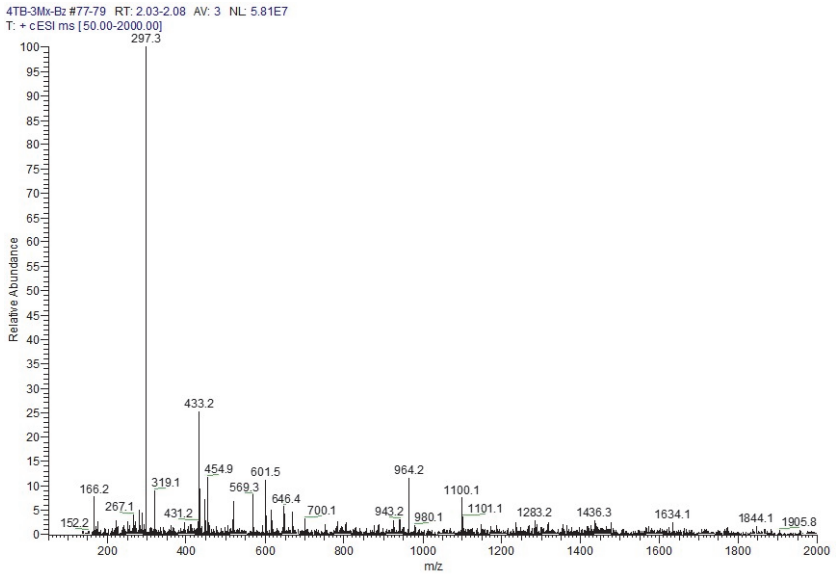

Fig. S2. ESI-MS spectrum of **HL²**

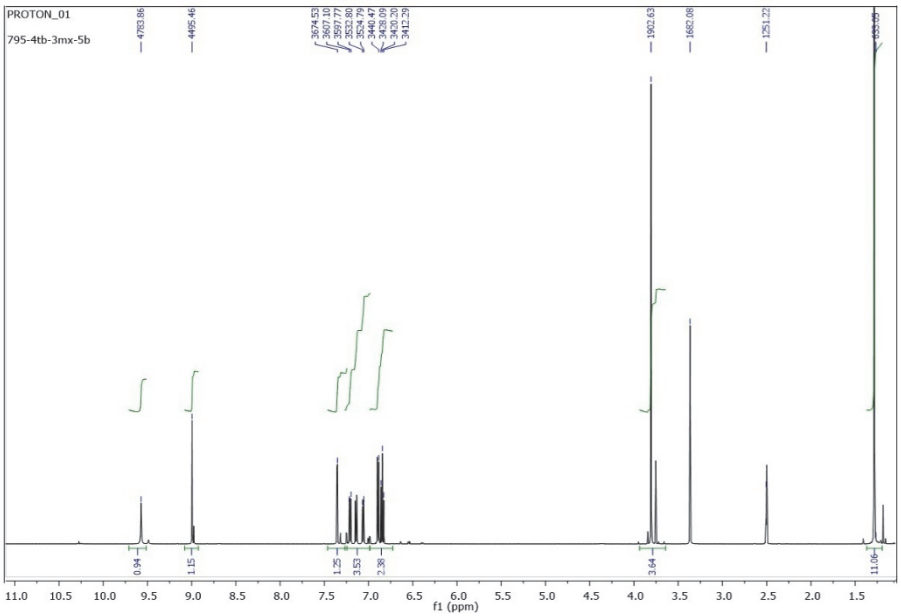

Fig. S3. ^{1}H-NMR spectrum of $\mathbf{H_2L^1}$

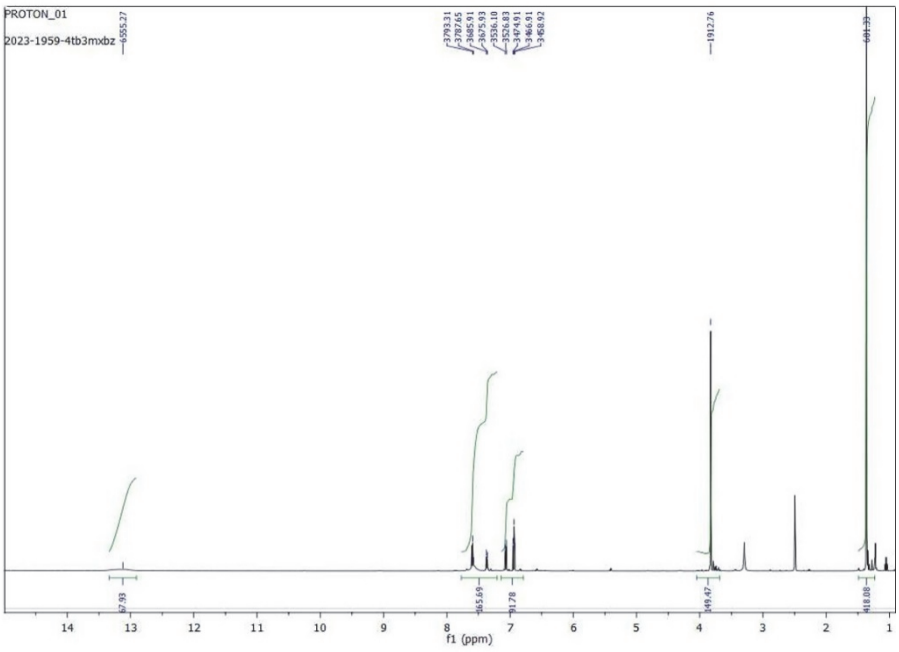

Fig. S4. ^{1}H-NMR spectrum of **HL^{2}**

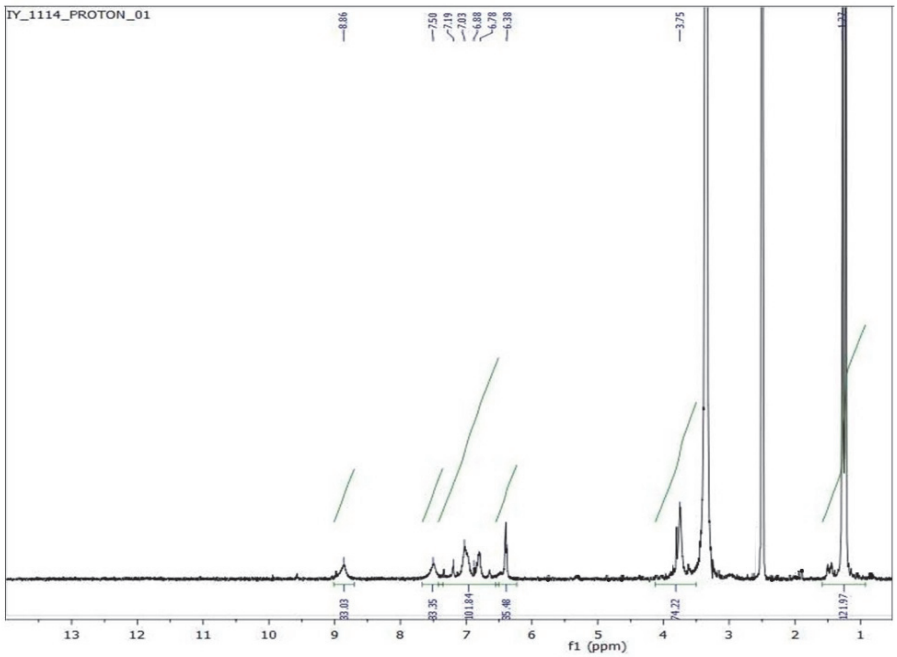

Fig. S5. ^{1}H-NMR spectrum of **1d** (Zn(II) complex of **H_2L^{1}**)

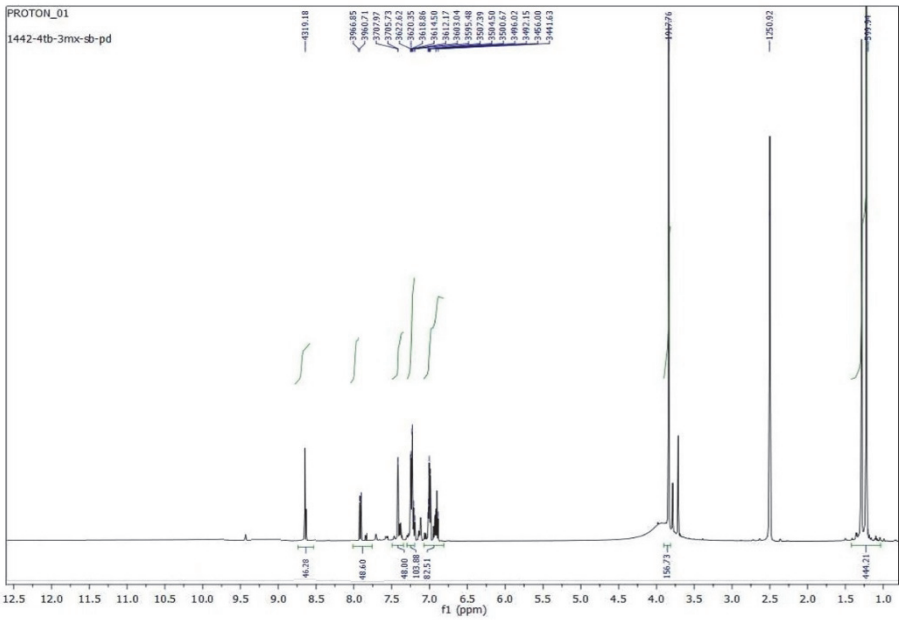

Fig. S6. ^{1}H-NMR spectrum of **1e** (Pd(II) complex of $\mathbf{H_2L^1}$)

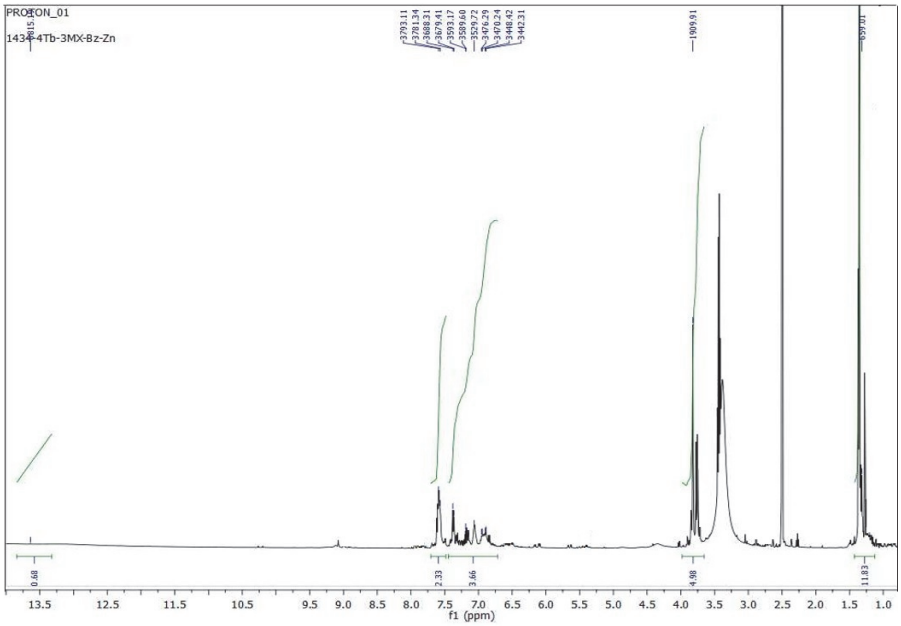

Fig. S7. ^{1}H-NMR spectrum of **2d** (Zn(II) complex of $\mathbf{HL^2}$)

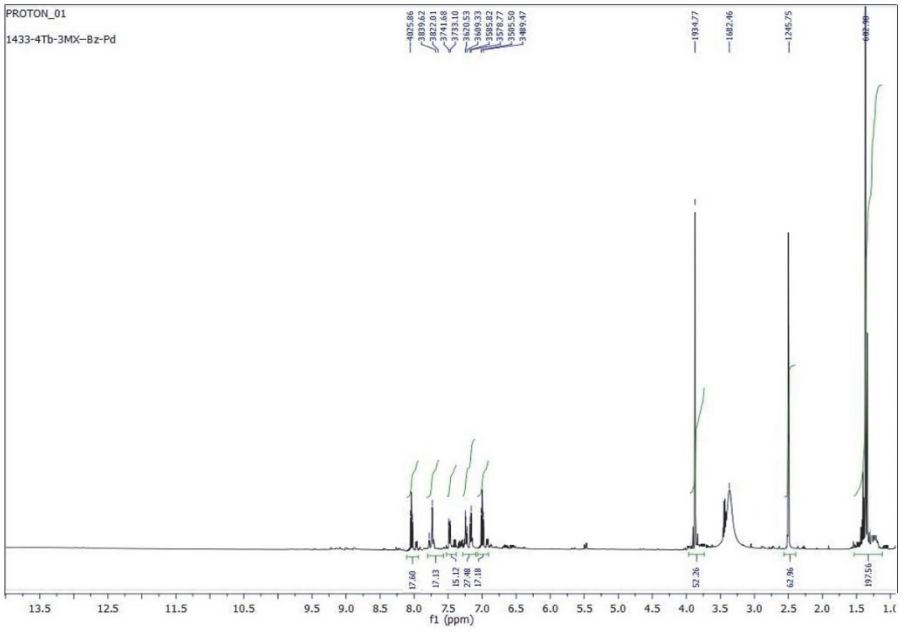

Fig. S8. ^{1}H-NMR spectrum of **2e** (Pd(II) complex of **HL^{2}**)

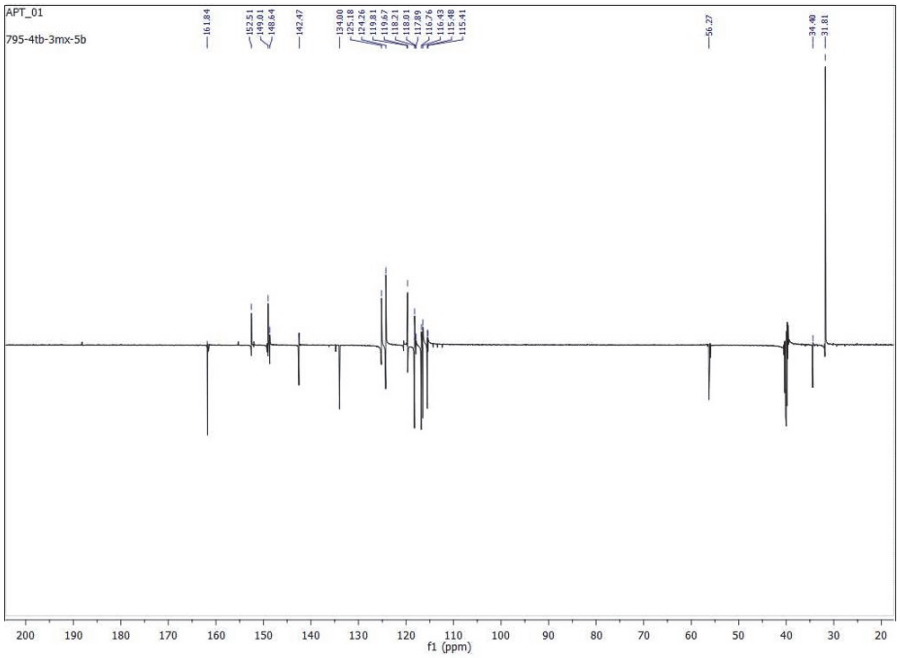

Fig. S9. ^{13}C-NMR spectrum of **H_2L^1**

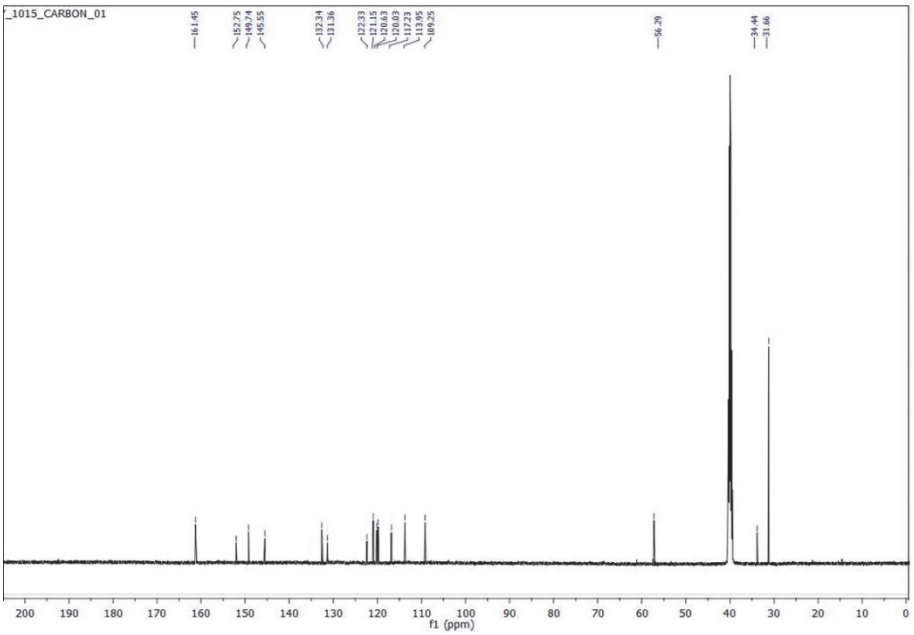

Fig. S10. ^{13}C-NMR spectrum of **HL^2**

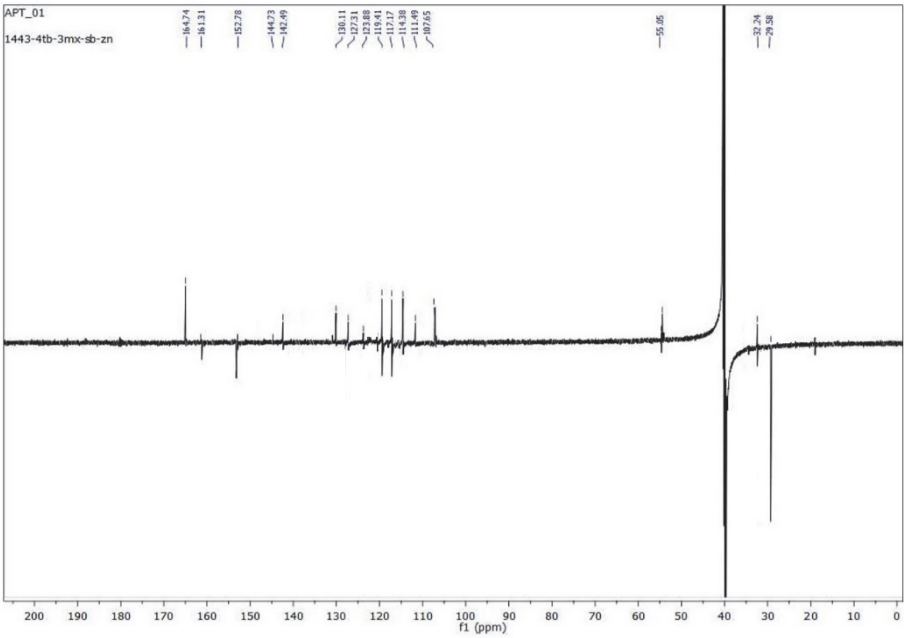

Fig. S11. ^{13}C-NMR spectrum of **1d** (Zn(II) complex of **H_2L^1**)

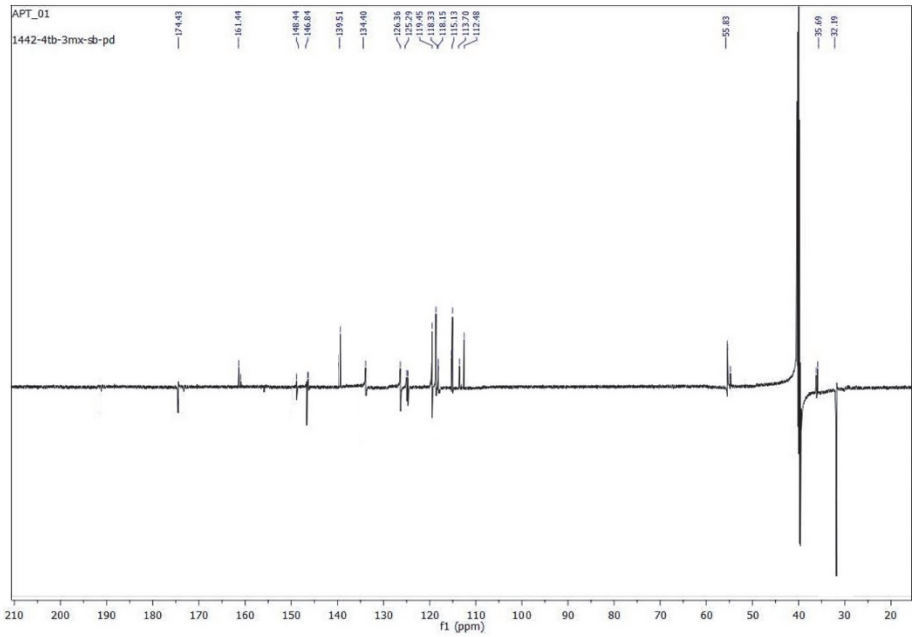

Fig. S12. ^{13}C-NMR spectrum of **1e** (Pd(II) complex of $\mathbf{H_2L^1}$)

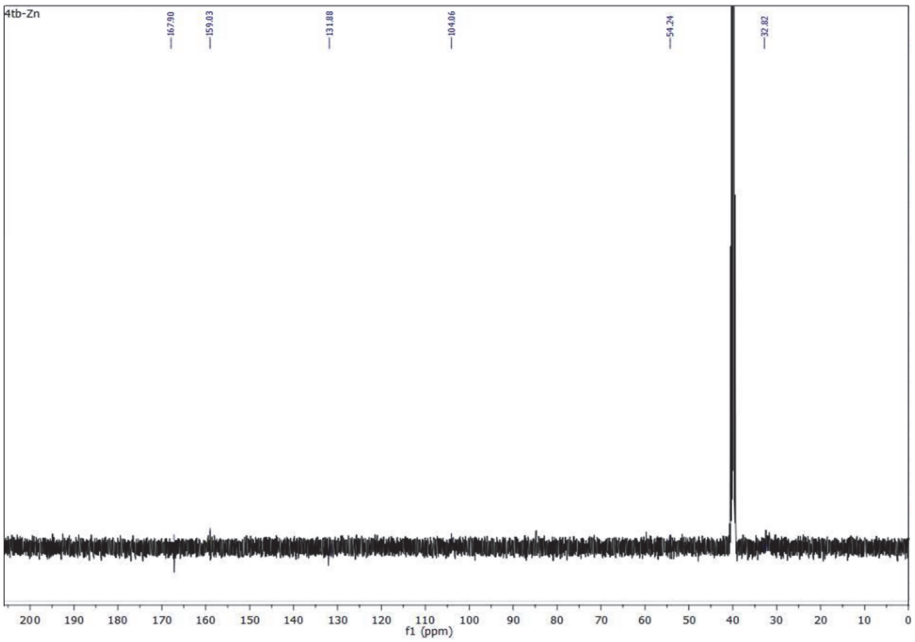

Fig. S13. ^{13}C-NMR spectrum of **2d** (Zn(II) complex of $\mathbf{HL^2}$)

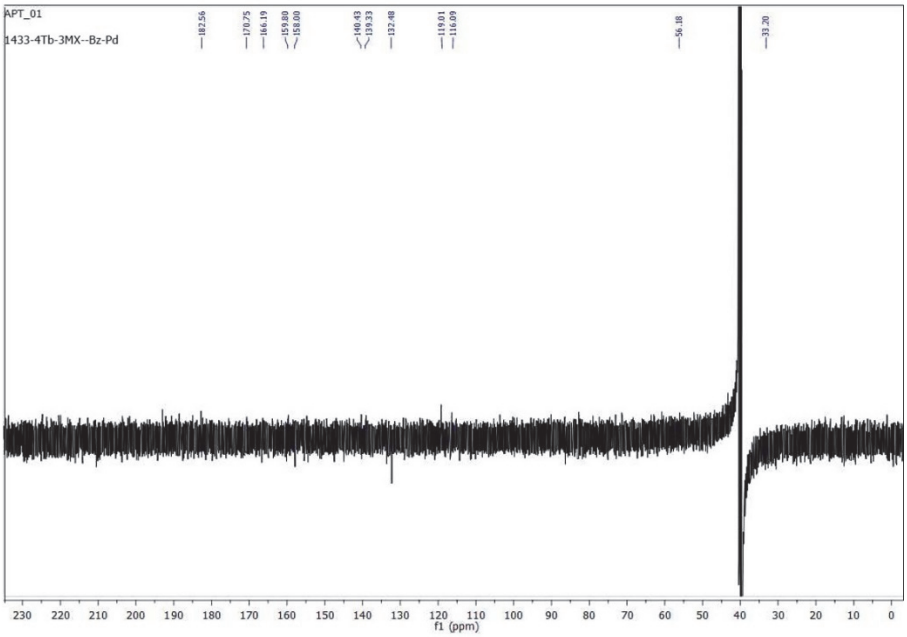

Fig. S14. ^{13}C-NMR spectrum of **2e** (Pd(II) complex of **HL^2**)

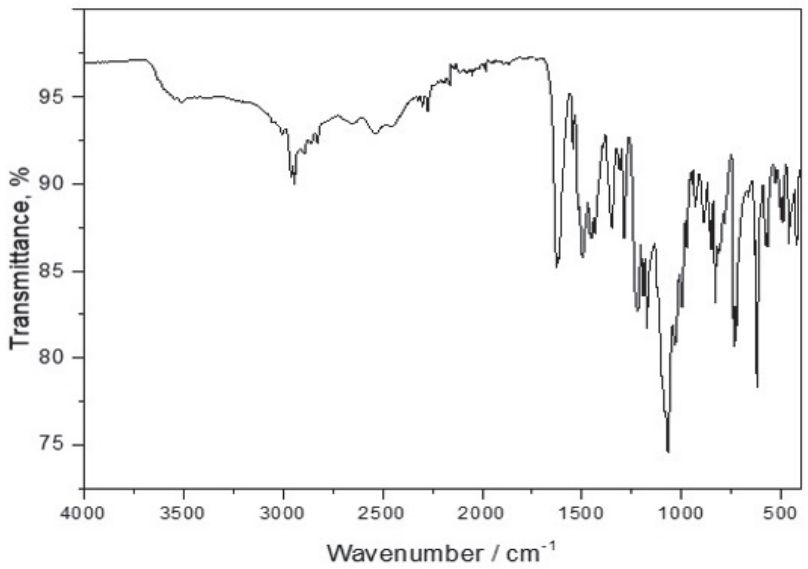

Fig. S15. FTIR spectrum of **H_2L^1**

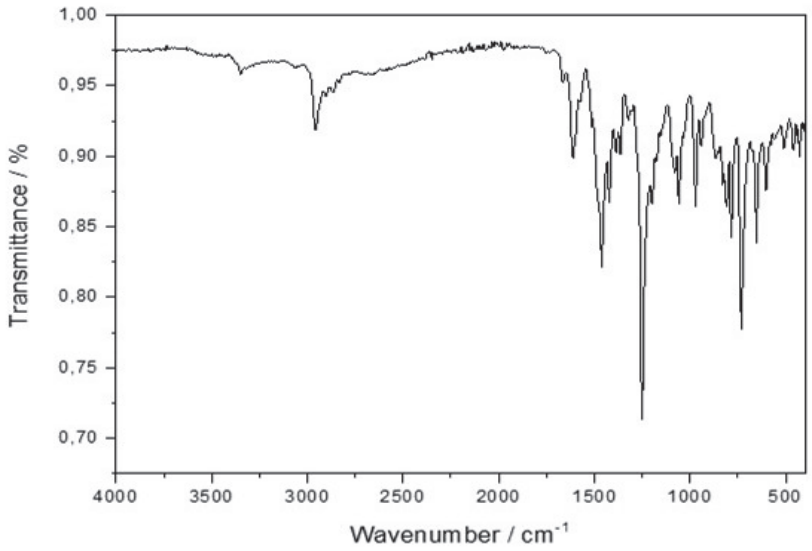

Fig. S16. FTIR spectrum of **HL^2**

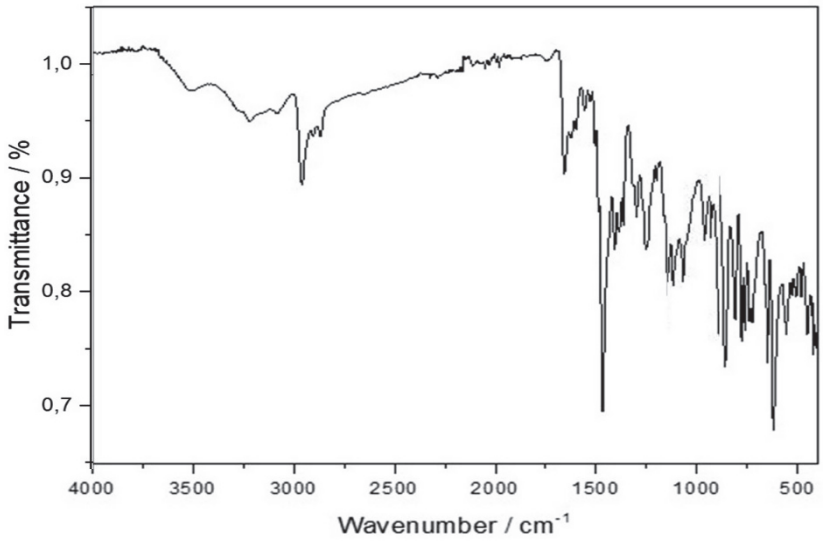

Fig. S17. FTIR spectrum of **1a**

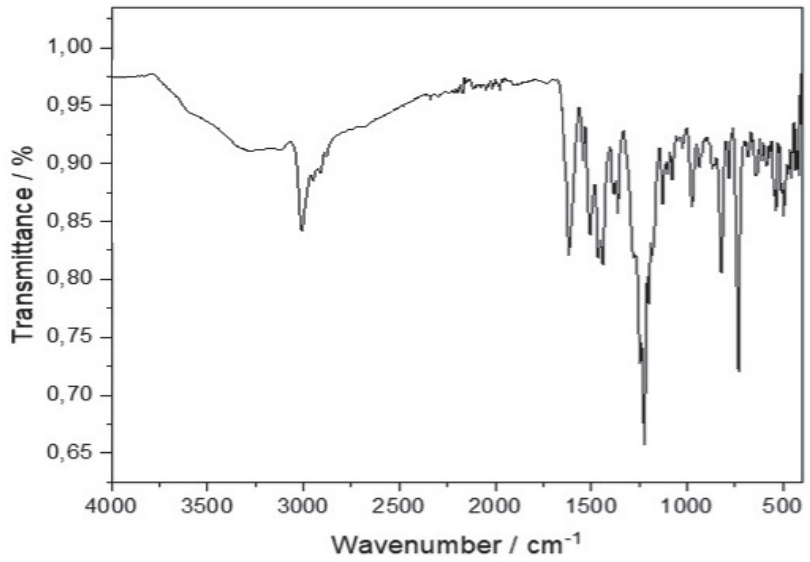

Fig. S18. FTIR spectrum of **1b**

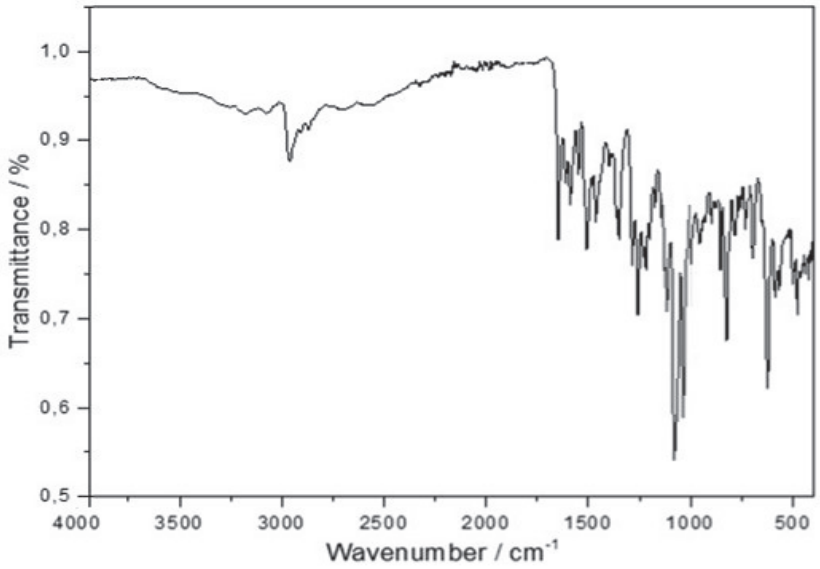

Fig. S19. FTIR spectrum of **1c**

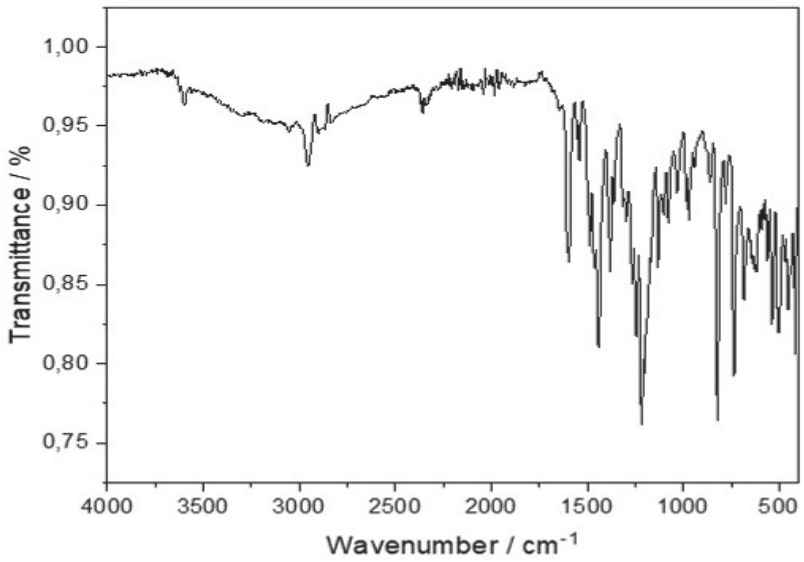

Fig. S20. FTIR spectrum of **1d**

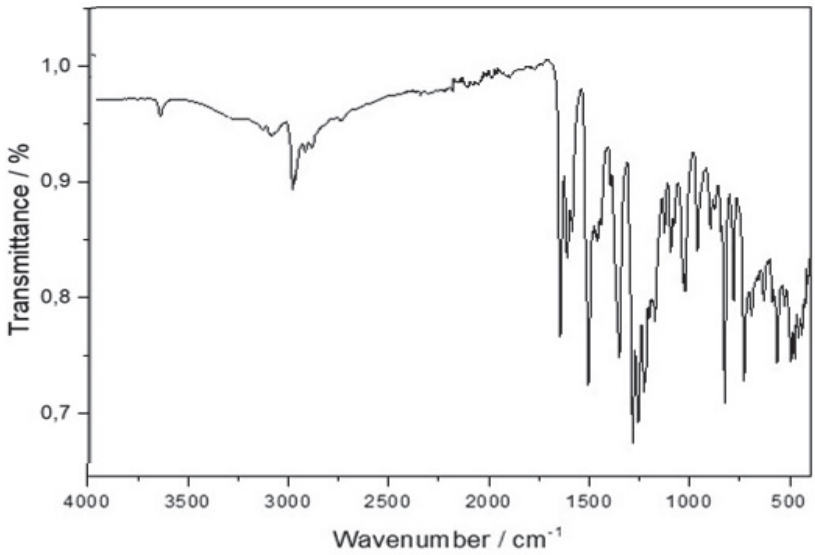

Fig. S21. FTIR spectrum of **1e**

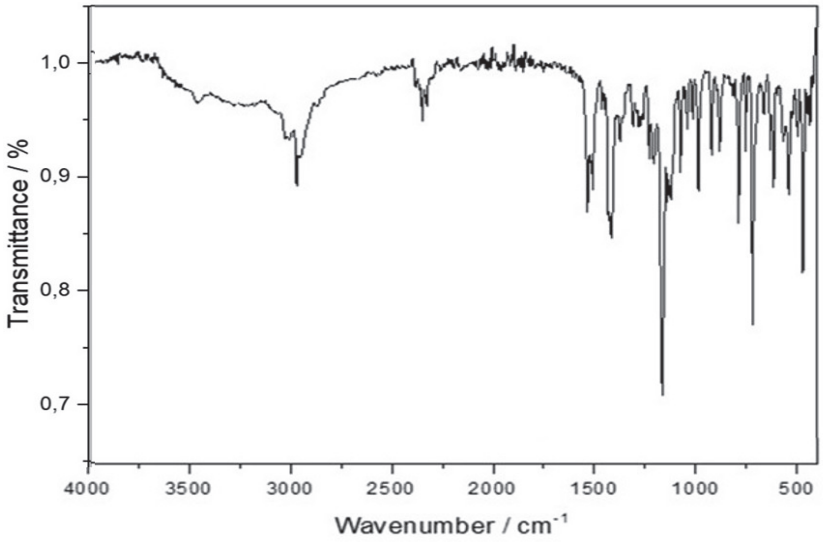

Fig. S22. FTIR spectrum of **2a**

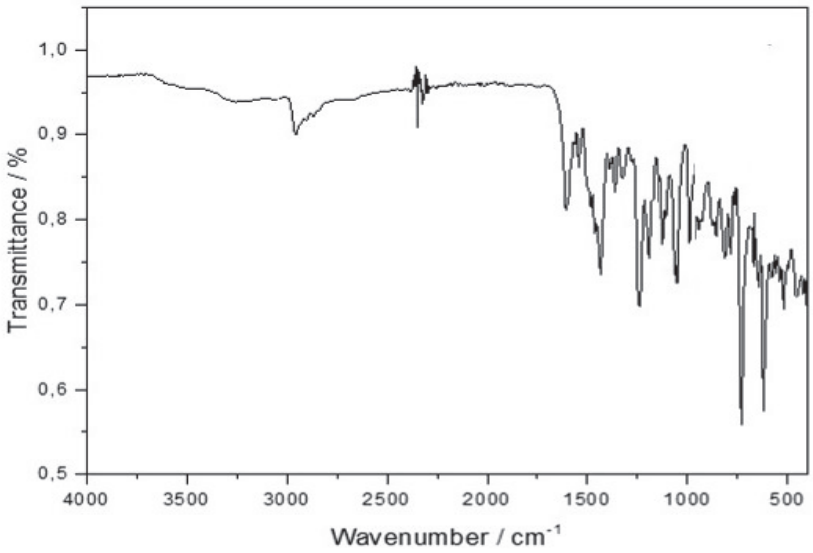

Fig. S23. FTIR spectrum of **2b**

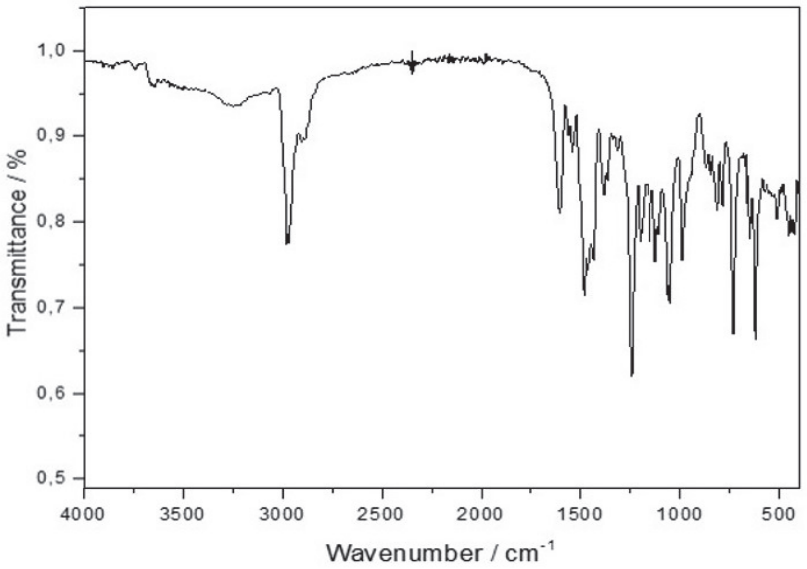

Fig. S24. FTIR spectrum of **2c**

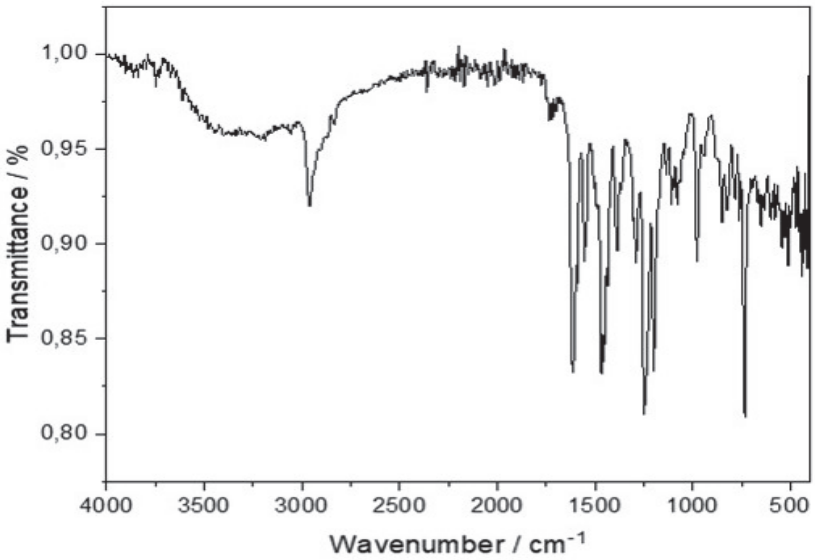

Fig. S25. FTIR spectrum of **2d**

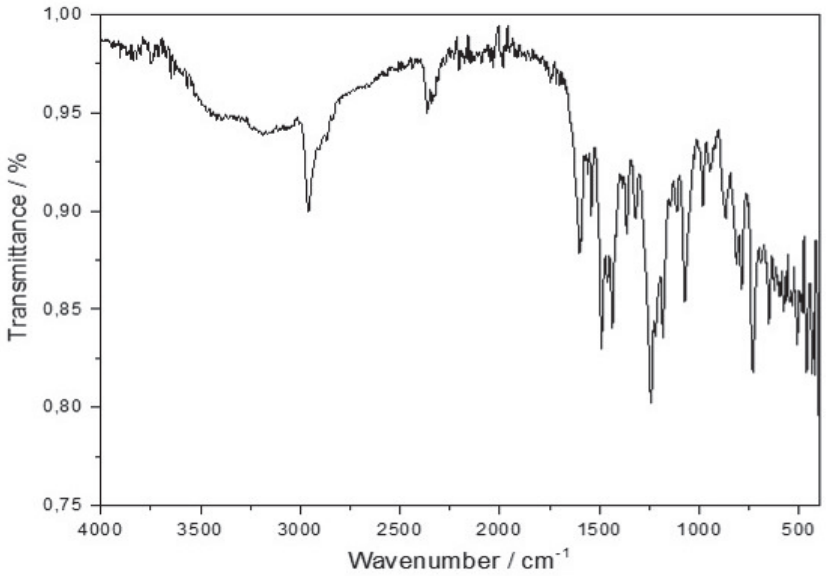

Fig. S26. FTIR spectrum of **2e**

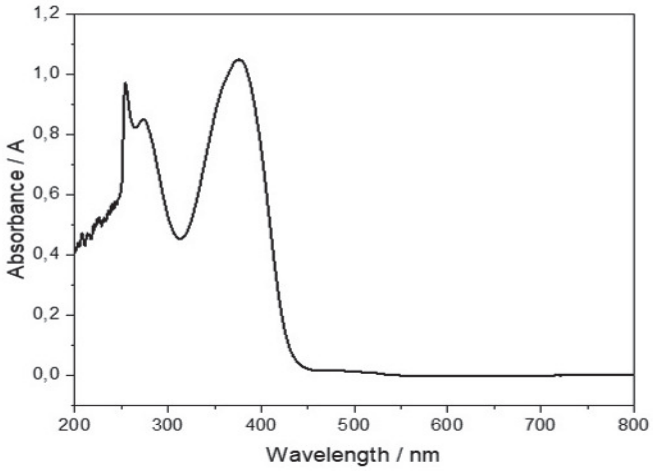

Fig. S27. UV-visible spectrum of $\mathbf{H_2L^1}$

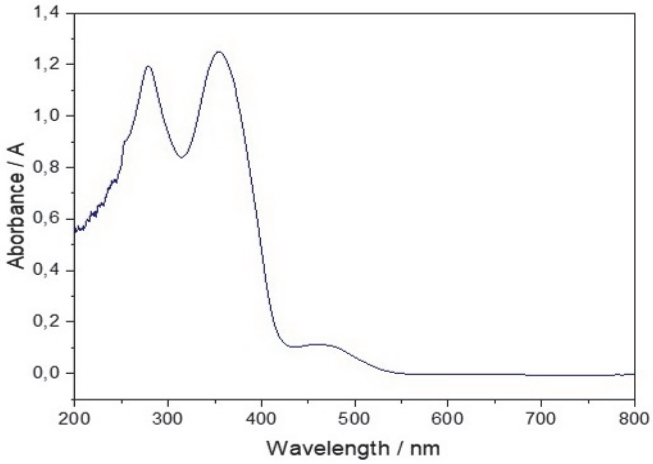

Fig. S28. UV-visible spectrum of **1a**

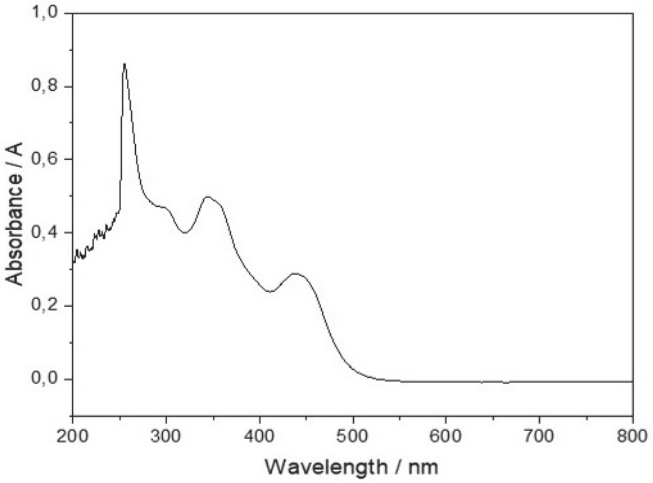

Fig. S29. UV-visible spectrum of **1b**

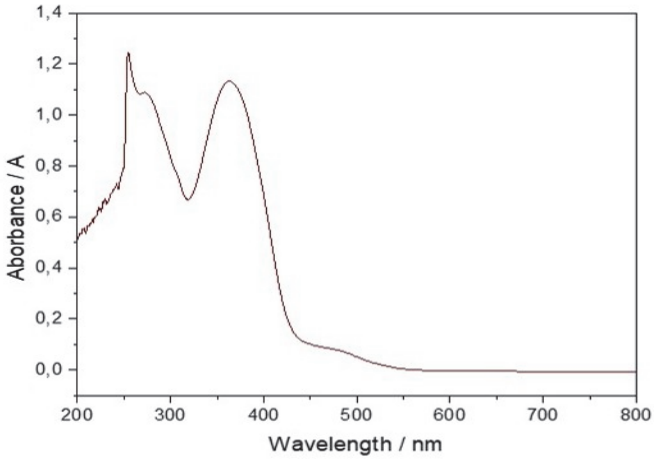

Fig. S30. UV-visible spectrum of **1c**

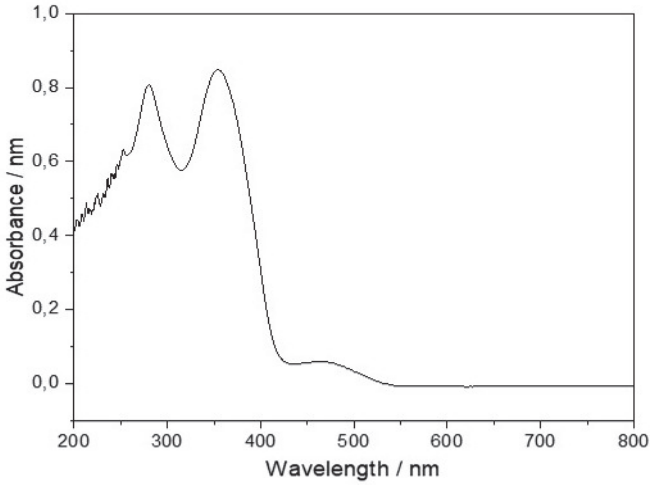

Fig. S31. UV-visible spectrum of **1d**

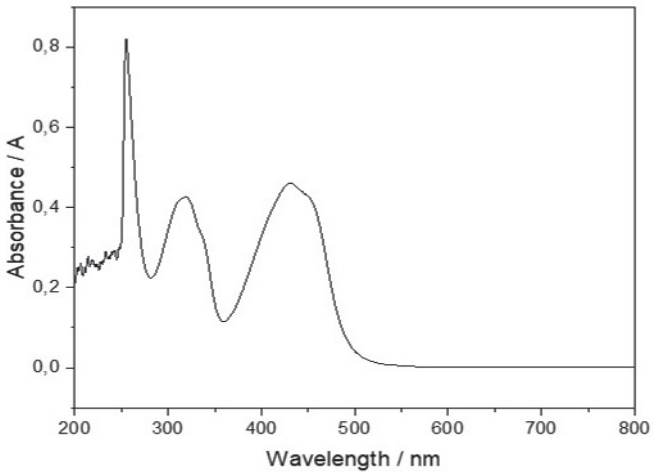

Fig. S32. UV-visible spectrum of **1e**

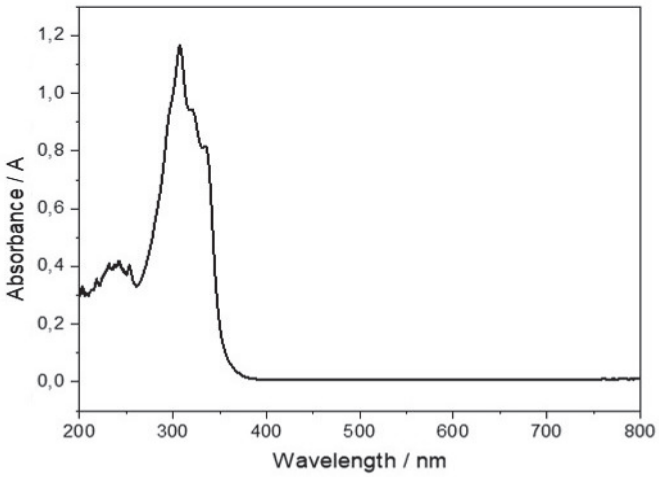

Fig. S33. UV-visible spectrum of **HL^2**

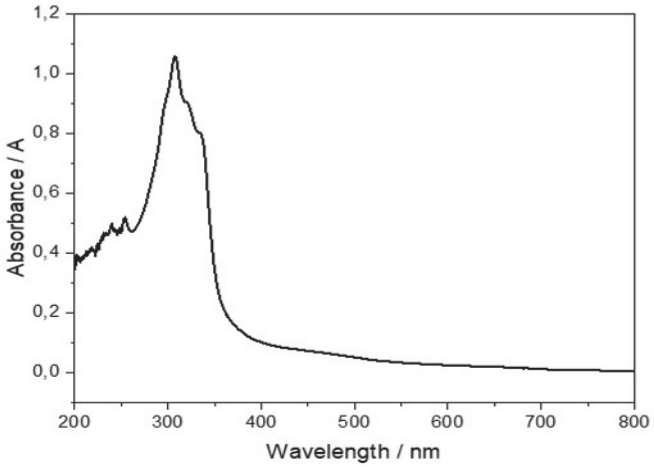

Fig. S34. UV-visible spectrum of **2a**

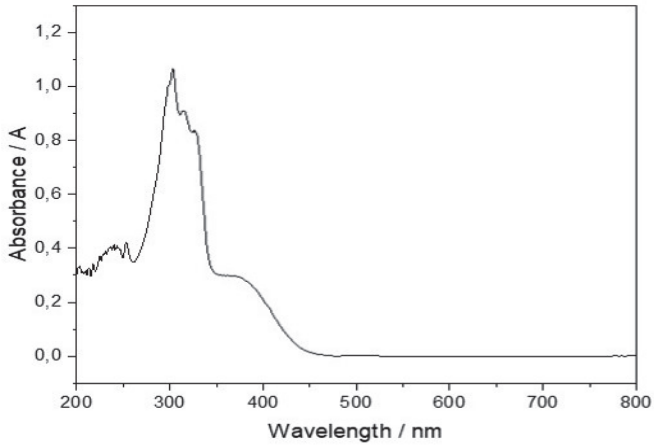

Fig. S35. UV-visible spectrum of **2b**

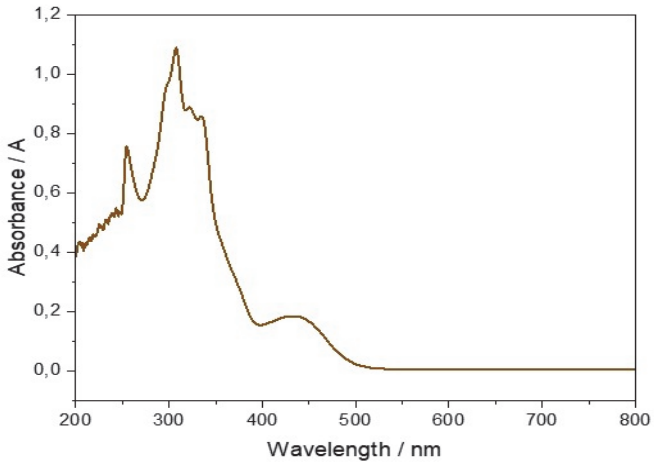

Fig. S36. UV-visible spectrum of **2c**

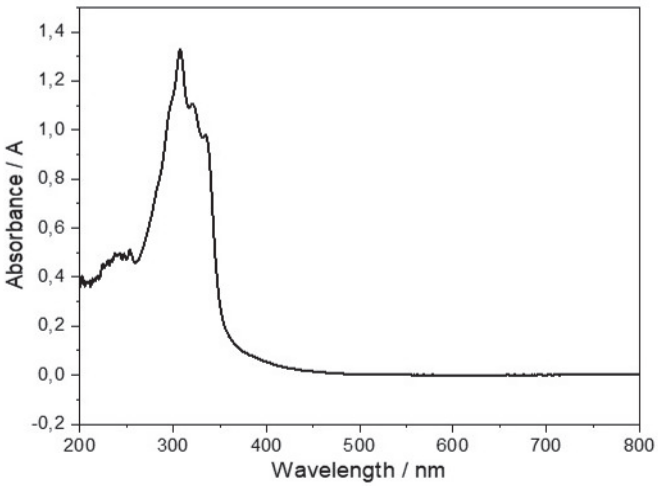

Fig. S37. UV-visible spectrum of **2d**

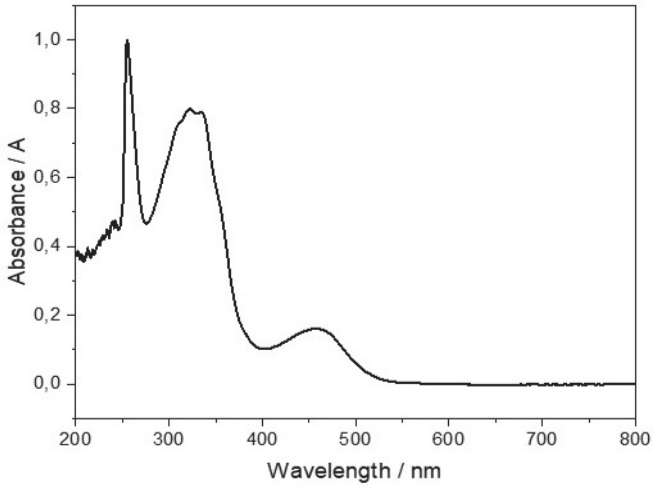

Fig. S38. UV-visible spectrum of **2e**

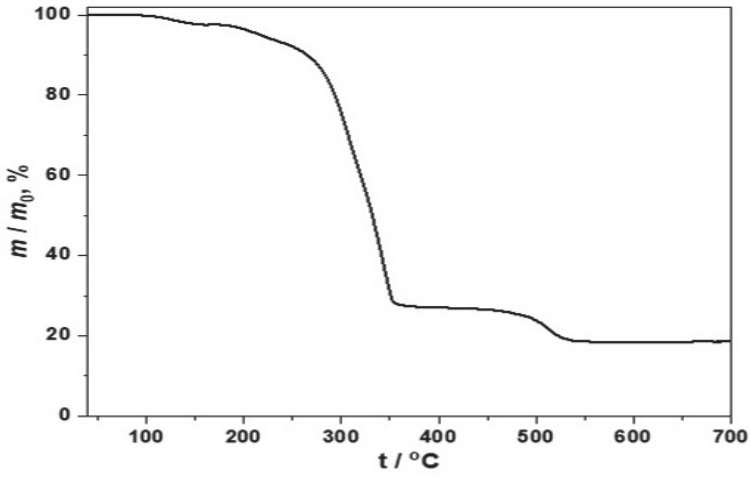

Fig. S39. TGA curve of **2a**

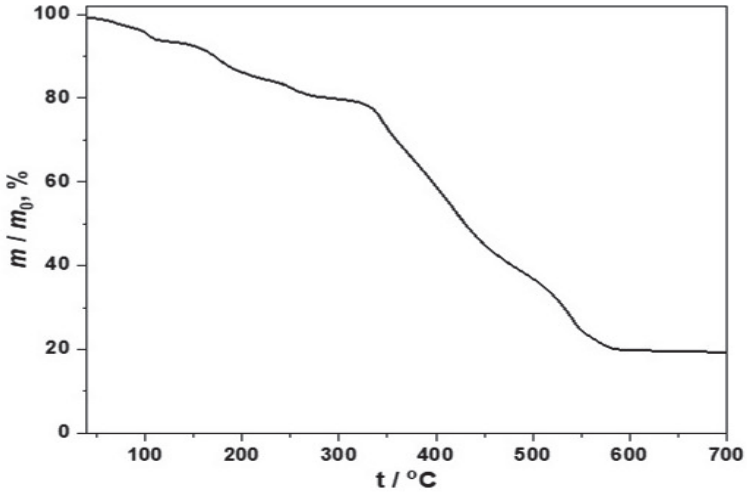

Fig. S40. TGA curve of **2b**

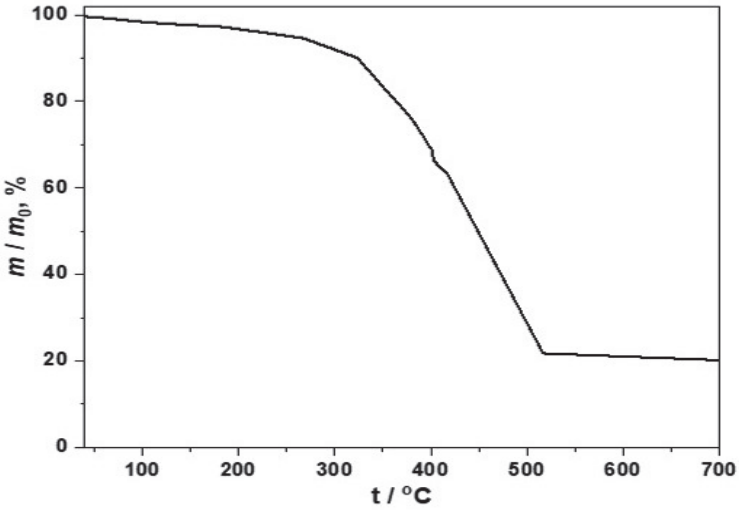

Fig. S41. TGA curve of **2c**

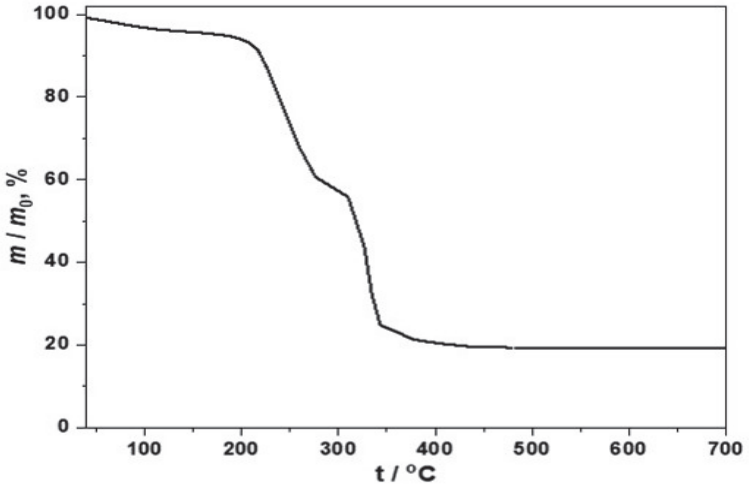

Fig. S42. TGA curve of **2d**

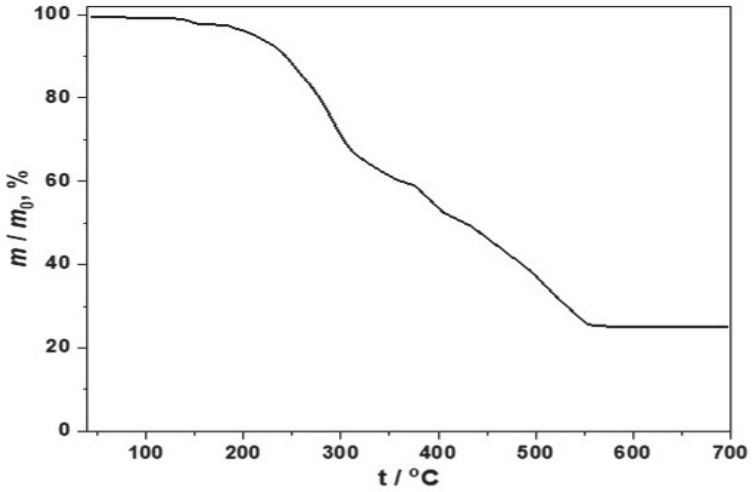

Fig. S43. TGA curve of **2e**.