



SUPPLEMENTARY MATERIAL TO
**Metal complexes with Schiff base and benzimidazolyphenol
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 (**H₂L¹**).
Decomposition point (Dec. p.): 138 °C. (+)ESI-MS (*m/z*): calculated for [C₁₈H₂₁NO₃]⁺ 299.4,
observed 297.3 (90.6 %) ([C₁₈H₂₁NO₃ - 2H]⁺ and 300.4 for ([C₁₈H₂₁NO₃ + H]⁺ (64.1 %).
Combustion analysis for C₁₈H₂₁NO₃: 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. ¹H NMR (500 MHz, DMSO-d₆, 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, OCH₃), 1.28 (s, 9H, –
C(CH₃)₃). ¹³C NMR (125 MHz, DMSO-d₆, δ / ppm): 161.6 (N=CH), 152.5 (C–OH(2')), 149.0
(C–OCH₃), 148.6 (C–OH(1')), 142.5 (C–C(CH₃)), 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 (OCH₃), 34.4 (–C(CH₃)₃). 31.8 (–
C(CH₃)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 (**HL²**): Dec.p.: 219 °C. (+)ESI-
MS (*m/z*): calculated for [C₁₈H₂₀N₂O₂]⁺ 296.4, observed 297.3 (100 %) ([C₁₈H₂₀N₂O₂ - H]⁺
and 298.3 for ([C₁₈H₂₀N₂O₂ + 2H]⁺ (20.7 %). Combustion analysis for C₁₈H₂₀N₂O₂: 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. ¹H NMR (500 MHz, DMSO-d₆, 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, OCH₃), 1.35 (*s*, 9H, -C(CH₃)₃). ¹³C NMR (125 MHz, DMSO-d₆, δ / ppm): 161.4 (C2), 152.7 (C-OCH₃), 149.6 (C-OH), 145.6 (C-C(CH₃)), 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 (OCH₃), 34.5 (-C(CH₃)₃), 31.7 (-C(CH₃)₃). UV-vis spectra (DMSO, λ_{max} / nm): 304m, 316m, 330m,br, 382m,br. Fluorescence spectra (EtOH, $c = 1 \times 10^{-4}$ mol L⁻¹, λ_{max} / nm): 463m.

[Co(L^I)(H₂O)₂] $\cdot$ H₂O (**1a**): Brown solid. Yield: 67 %. Dec. p.: 167 °C. Combustion analysis for C₁₈H₂₃NO₆Co (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} . A_{M} (DMF, 25 °C, S m² 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 H₂O); 150: 7.8; 200: 9.5 (1 mole of H₂O); 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^I)(H₂O)₂] (**1b**): Greenish brown solid. Yield: 70 %. Dec. p.: 186 °C. Combustion analysis for C₁₈H₂₃NO₅Ni (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} . A_{M} (DMF, 25 °C, S m² 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 H₂O); 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^I)(H₂O)] (**1c**): Brown solid. Yield: 73 %. Dec. p.: 295 °C. Combustion analysis for C₁₈H₂₁NO₄Cu (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} . A_{M} (DMF, 25 °C, S m² 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 H₂O); 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^I)(H₂O)] $\cdot$ H₂O (**1d**): Dark yellow solid. Yield: 65 %. Dec. p.: 173 °C. Combustion analysis for C₁₈H₂₃NO₅Zn (FW: 398.8): Calculated C 49.79, H 5.34, N 3.23; found C 49.90, H 5.20, N 3.11. A_{M} (DMF, 25 °C, S m² 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. ¹H NMR (500 MHz, DMSO-d₆, 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, OCH₃), 1.27 (*s*, 9H, -C(CH₃)₃). ¹³C NMR (125 MHz, DMSO-d₆, δ / ppm): 164.8 (N=CH), 161.3 (C-OH₂), 152.7 (C-OCH₃), 144.8 (C-OH1'), 142.4 (C-C(CH₃)), 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 (OCH₃), 32.2 (-C(CH₃)₃), 29.5 (-C(CH₃)₃). TGA (t / °C: weight loss, %): 50: 1.1; 75: 2.5; 100: 4.6 (1 mole of

H₂O); 150: 4.4; 200: 9.5 (1 mole of H₂O); 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(L¹)Cl]·H₂O (**1e**): Light brown solid. Yield: 77 %. Dec. p.: 265 °C. Combustion analysis for C₁₈H₂₁ClNO₄KPd (FW: 496.3): Calculated C 43.56, H 4.26, N 2.82; found C 43.70, H 4.11, 2.68. A_M (DMF, 25 °C, S m² mol⁻¹): 83.2. FT-IR (ATR, cm⁻¹): 3036m,br $\nu(\text{CH})_{\text{ar}}$, 2958m $\nu(\text{CH})_{\text{al}}$, 1646m $\nu(\text{C}=\text{N})$, 1611m $\nu(\text{C}=\text{C})$, 1506m, 1456m, 1351m, 1289m, 1257s $\nu(\text{C}-\text{O})$, 1204m $\nu(\text{C}-\text{O})$, 1097m, 1024m, 965m, 912m, 826m $\delta(\text{CH})_{\text{ar}}$, 730m, 673m $\nu(\text{N} \rightarrow \text{M})$, 564m, 540m $\nu(\text{O} \rightarrow \text{M})$, 500m, 462m. ¹H-NMR (500 MHz, DMSO-d₆, 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, J₁=8.7, J₂=8.5, H5'), 3.72 (s, 3H, OCH₃), 1.30 (s, 9H, -C(CH₃)₃). ¹³C NMR (125 MHz, DMSO-d₆, δ / ppm): 174.3 (N=CH), 161.5 (C-OH2), 148.4 (C-OCH₃), 146.9 (C-OH1'), 139.5 (C-C(CH₃)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 (OCH₃), 35.7 (-C(CH₃)₃), 32.1 (-C(CH₃)₃). TGA (t / °C: weight loss, %): 50: 0.7; 75: 2.0; 100: 3.7 (1 mole of H₂O); 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(L²)Cl(H₂O)] (**2a**): Dark brown solid. Yield: 72 %. Dec. p.: 201 °C. Combustion analysis for C₁₈H₂₁ClN₂O₃Co (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 . A_M (DMF, 25 °C, S m² mol⁻¹): 35.4. FT-IR (ATR, cm⁻¹): 3198m,br $\nu(\text{OH})$, 3088m,br $\nu(\text{CH})_{\text{ar}}$, 2960m $\nu(\text{CH})_{\text{al}}$, 1606m $\nu(\text{C}=\text{N})$, 1573m $\nu(\text{C}=\text{C})$, 1463m, 1435m, 1361m, 1244s $\nu(\text{C}-\text{O})$, 1195m, 1060m, 981m, 813m $\delta(\text{CH})_{\text{ar}}$, 786m, 732s, 66 m $\nu(\text{N} \rightarrow \text{M})$, 601m, 574m, 545m $\nu(\text{O} \rightarrow \text{M})$, 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 H₂O); 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, $c = 1 \times 10^{-4}$ mol L⁻¹, λ_{max} / nm): 425sh, 451m,br.

[Ni(L²)Cl(H₂O)]·H₂O (**2b**): Light brown solid. Yield: 70 %. Dec. p.: 198 °C. Combustion analysis for C₁₈H₂₃ClN₂O₄Ni (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 . A_M (DMF, 25 °C, S m² mol⁻¹): 38.8. FT-IR (ATR, cm⁻¹): 3373m,br $\nu(\text{OH})$, 3228m,br, 3070m,br $\nu(\text{CH})_{\text{ar}}$, 2962m $\nu(\text{CH})_{\text{al}}$, 2872m, 1611m $\nu(\text{C}=\text{N})$, 1598m $\nu(\text{C}=\text{C})$, 1545m, 1440m, 1362m, 1249m $\nu(\text{C}-\text{O})$, 1198m $\nu(\text{C}-\text{O})$, 1015m, 983m, 863m, 814m $\delta(\text{CH})_{\text{ar}}$, 731m, 671m $\nu(\text{N} \rightarrow \text{M})$, 581m, 540m $\nu(\text{O} \rightarrow \text{M})$, 457m, 420m. TGA (t / °C: weight loss, %): 50: 0.3; 75: 2.2; 100: 4.6 (1 mole of H₂O); 150: 7.8; 200: 9.0 (1 mole of H₂O); 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, $c = 1 \times 10^{-4}$ mol L⁻¹, λ_{max} / nm): 399w, 478m.

[Cu(L²)Cl] (**2c**): Brown solid. Yield: 76 %. Dec. p.: 235 °C. Combustion analysis for C₁₈H₁₉ClN₂O₂Cu (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 . A_M (DMF, 25 °C, S m² mol⁻¹): 48.8. FT-IR (ATR, cm⁻¹): 3215m,br $\nu(\text{OH})$, 3057w,br $\nu(\text{CH})_{\text{ar}}$, 2962m $\nu(\text{CH})_{\text{al}}$, 1608m $\nu(\text{C}=\text{N})$, 1589m $\nu(\text{C}=\text{C})$, 1543m, 1485m, 1384m, 1242s $\nu(\text{C}-\text{O})$, 1199m $\nu(\text{C}-\text{O})$, 1062m, 981m, 815m $\delta(\text{CH})_{\text{ar}}$, 786m, 732s, 667m $\nu(\text{N} \rightarrow \text{M})$, 576m, 543m $\nu(\text{O} \rightarrow \text{M})$, 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, $\lambda_{\max}$ / nm): 243w, 255m, 297sh, 307m, 321m, 335m,br, 371sh, 433m,br. Fluorescence spectra (EtOH, $c = 1 \times 10^{-4}$ mol L⁻¹, $\lambda_{\max}$ / nm): 404w,br, 461sh.

[Zn(L²)Cl(H₂O)]·H₂O (**2d**): Dark yellow solid. Yield: 65 %, Dec. p.: 229 °C. Combustion analysis for C₁₈H₂₃ClN₂O₄Zn (FW: 432.3): Calculated C 50.02, H 5.36, N 6.48; found C 50.30, H 5.44, N 6.34. A_M (DMF, 25 °C, S m² 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. ¹H NMR (500 MHz, DMSO-d₆, 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, OCH₃), 1.36 (*s*, 9H, –C(CH₃)₃). ¹³C NMR (125 MHz, DMSO-d₆, δ / ppm): 167.9 (C2), 159.0 (C–OCH₃), 131.9, 104.7, 54.2 (OCH₃), 32.8 (–C(CH₃)₃). TGA (t / °C: weight loss, %): 50: 1.9; 75: 4.1; 100: 4.3 (1 mole of H₂O); 150: 8.4; 200: 9.0 (1 mole of H₂O); 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, $\lambda_{\max}$ / nm): 237w, 254w, 296sh, 304m, 332sh, 354sh. Fluorescence spectra (EtOH, $c = 1 \times 10^{-4}$ mol L⁻¹, $\lambda_{\max}$ / nm): 424m,br.

[Pd(L²)Cl(H₂O)] (**2e**): Light brown solid. Yield: 77%, Dec. p.: 265. Combustion analysis for C₁₈H₂₁ClN₂O₃Pd (FW: 455.2): Calculated C 47.49, H 4.65, N 6.15; found C 47.12, H 4.63, N 5.90. A_M (DMF, 25 °C, S m² 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. ¹H NMR (500 MHz, DMSO-d₆, 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, OCH₃), 1.39 (*s*, 9H, –C(CH₃)₃). ¹³C NMR (125 MHz, DMSO-d₆, δ / ppm): 170.8 (C2), 166.2 (C–OCH₃), 159.8 (C–OH), 158.0 (C–C(CH₃)₃), 140.4, 139.3, 132.5, 119.0, 116.1, 56.2 (OCH₃), 33.2 (–C(CH₃)₃). TGA (t / °C: weight loss, %): 50: 0.2; 75: 0.5; 100: 0.6; 150: 3.3; 200: 5.1 (1 mole of H₂O); 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, $\lambda_{\max}$ / nm): 233m, 255m, 308m,br, 321m,br, 335m,br, 458m,br. Fluorescence spectra (EtOH, $c = 1 \times 10^{-4}$ mol L⁻¹, $\lambda_{\max}$ / nm): 393w, 472m,br.

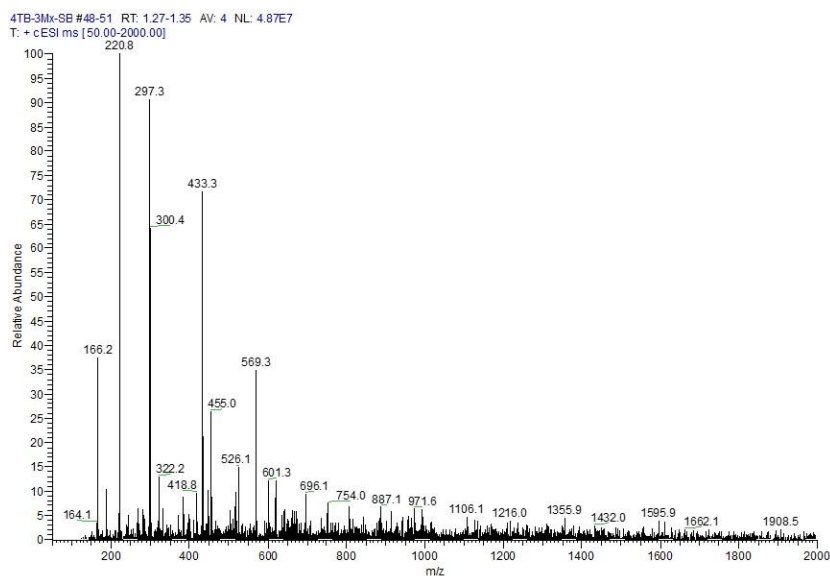
TABLE S-I. Crystal data and structure refinement parameters for **H₂L¹**

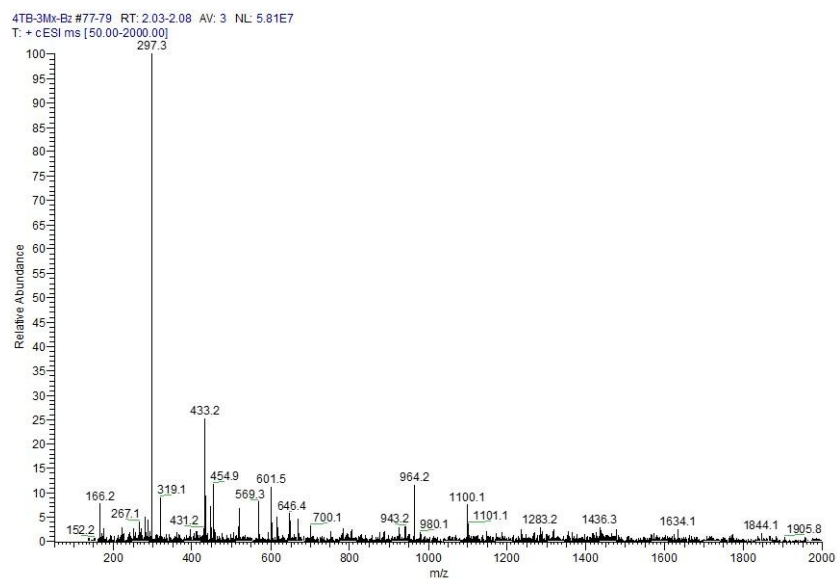
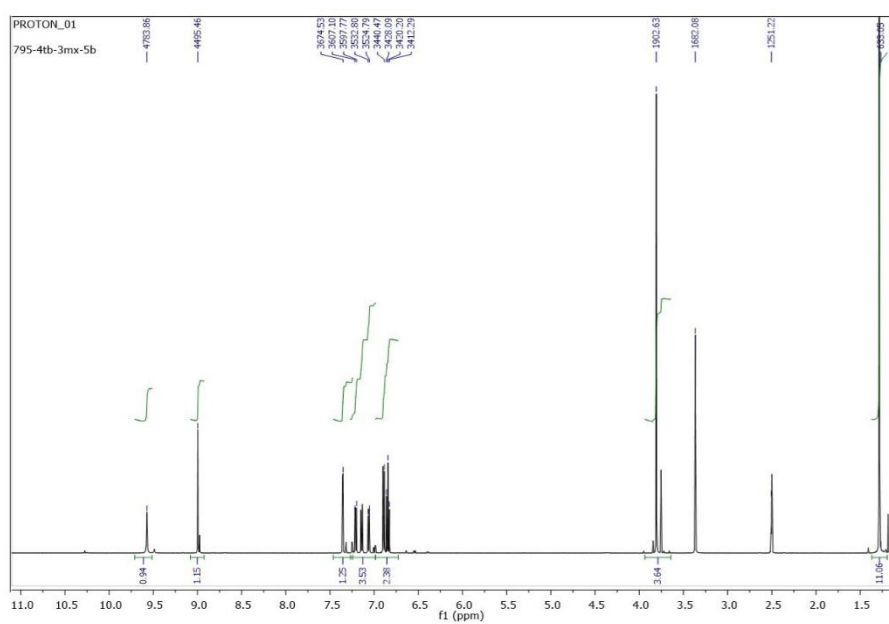
Empirical formula	C ₁₈ H ₂₁ NO ₃
Formula weight	299.36
Crystal system	Orthorhombic
Space group	<i>Pbca</i>
<i>a</i> (Å)	14.2349 (10)
<i>b</i> (Å)	9.5415 (5)
<i>c</i> (Å)	24.1061 (16)
α , β , γ (°)	90
<i>V</i> (Å ³)	3274.1(4)
<i>Z</i>	8
<i>D_c</i> (g cm ⁻³)	1.215
μ (mm ⁻¹)	0.082
θ range (°)	2.5–25.2

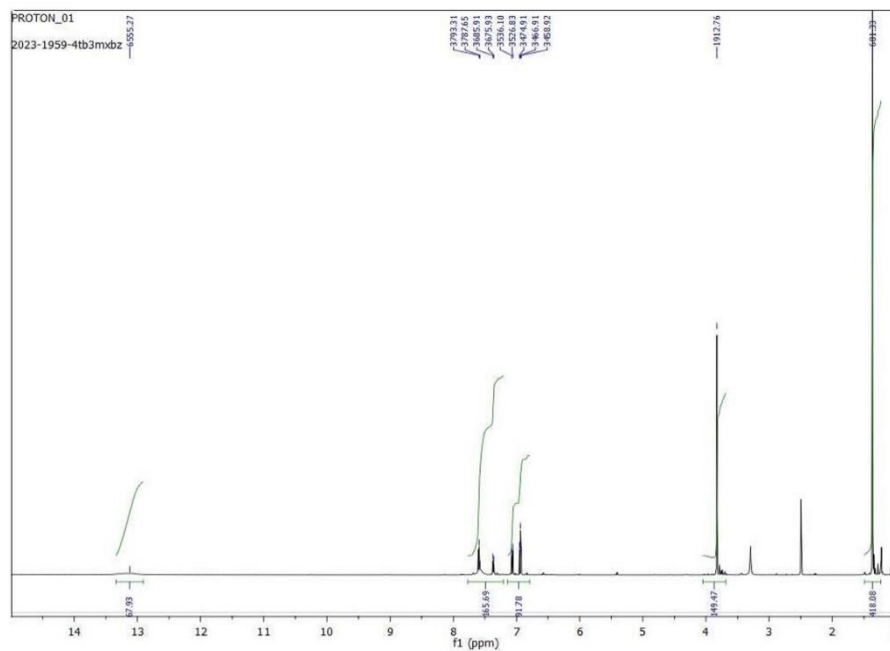
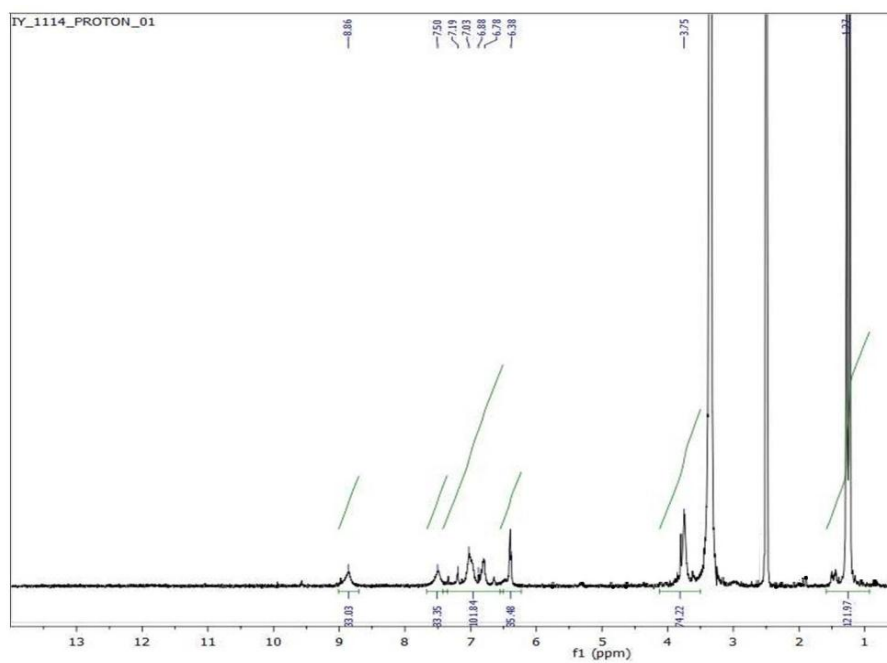
Measured refls.	46454
Independent refls.	3898
R_{int}	0.062
S	1.04
R1/wR2	0.059/0.154
$\Delta\rho_{\text{max}}/\Delta\rho_{\text{min}}$ (eÅ ⁻³)	0.19/-0.21
CCDC	2298000

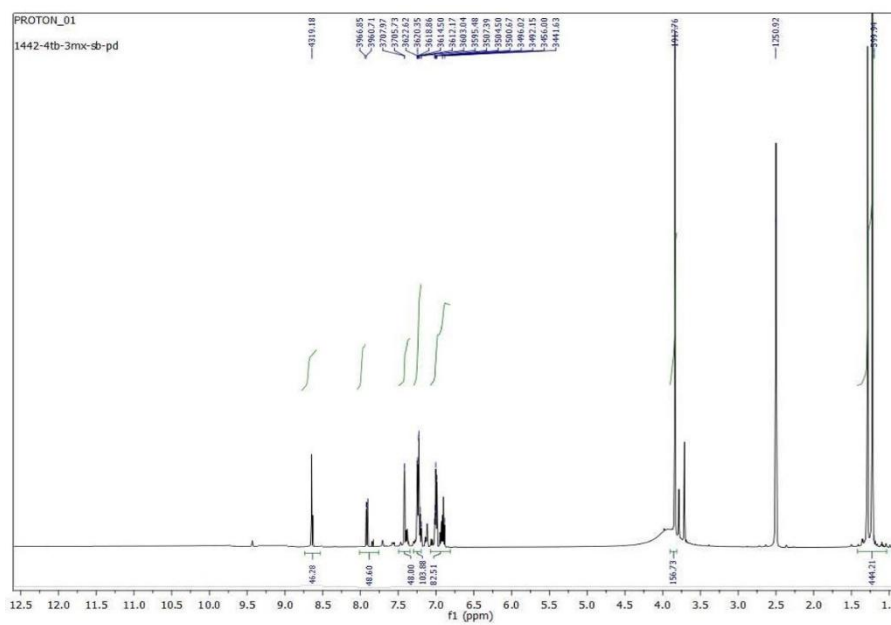
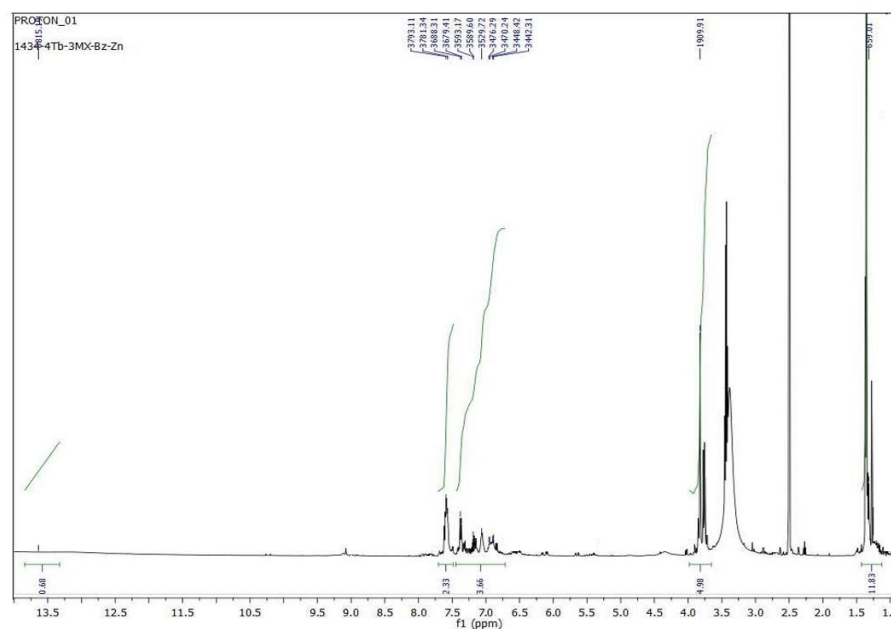
TABLE S-II. Selected bond distances and angles for **H₂L¹** (Å, °)

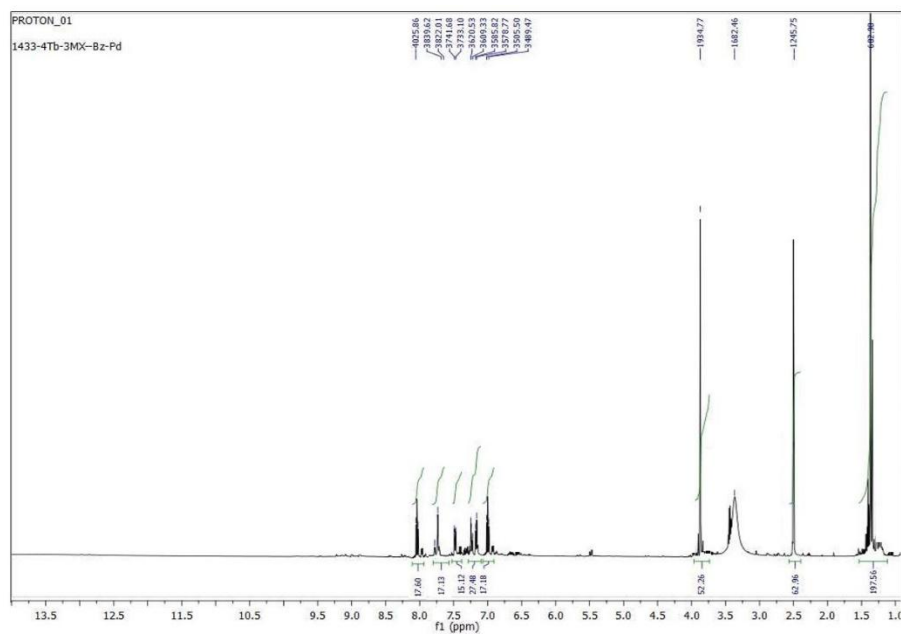
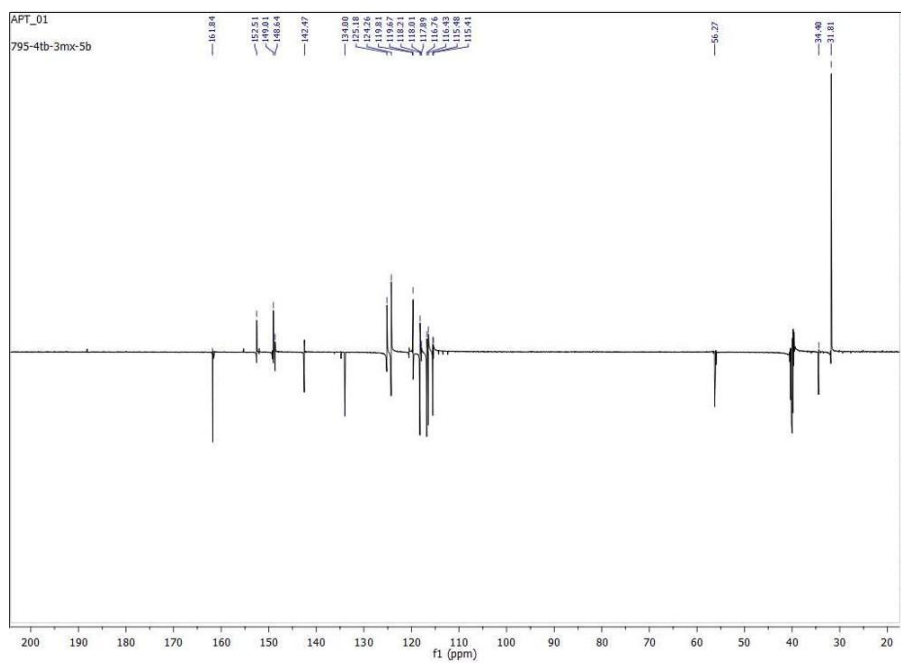
C8—N1	1.305(3)	C3—C2—O2	125.58(19)
C1—O1	1.289(2)	C13—C15—C18	110.40(19)
C2—O2	1.364(2)	C13—C15—C17	111.9(2)
C6—C8	1.407(3)	C16—C15—C13	108.3(2)
C7—O2	1.420(3)	O3—C10—C11	125.82(19)
C9—C14	1.384(3)	O3—C10—C9	116.1(2)
C9—C10	1.396(3)	C14—C9—N1	123.33(18)
C9—N1	1.414(3)	C10—C9—N1	115.90(18)
C10—O3	1.353(3)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

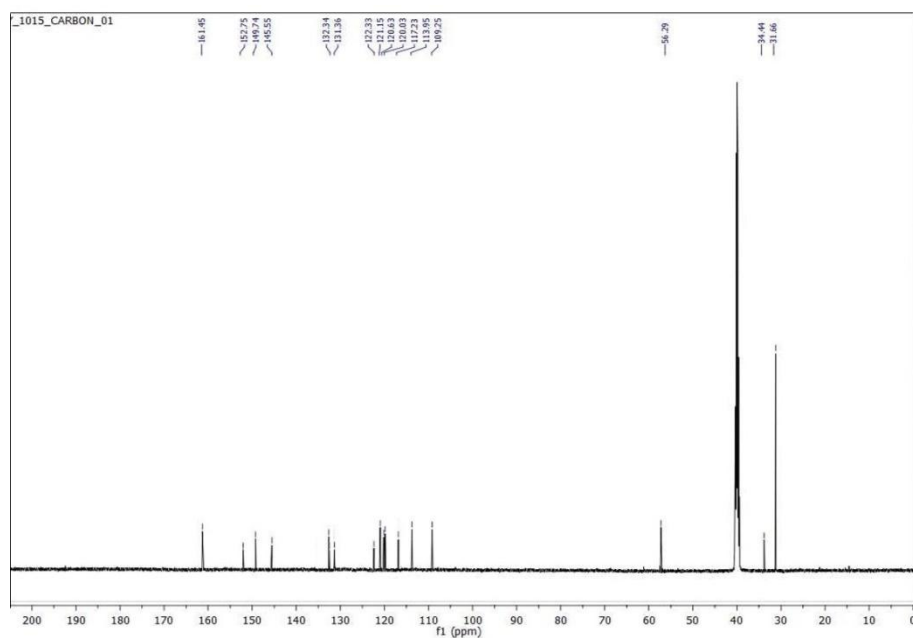
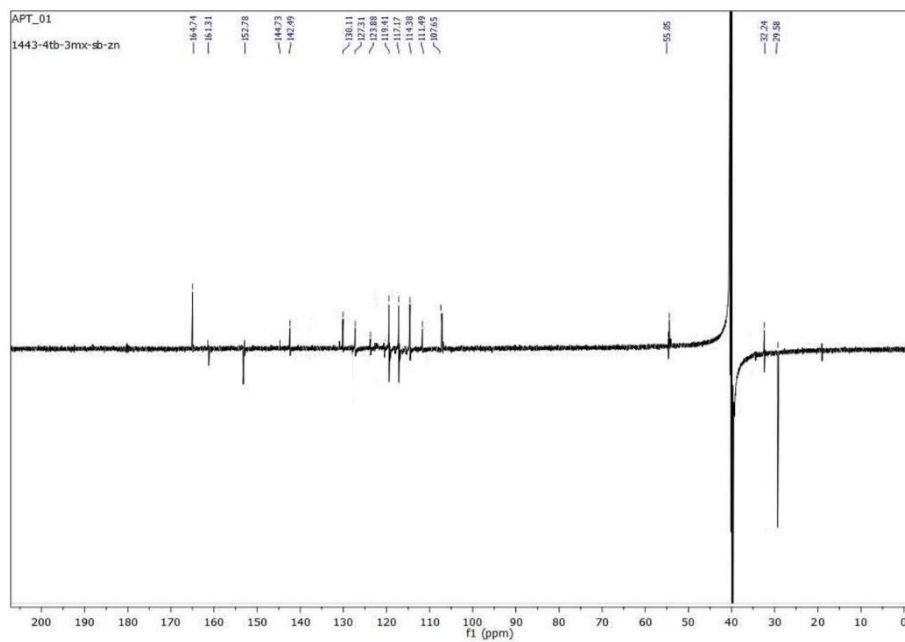
Fig. S1. ESI-MS spectrum of **H₂L¹**

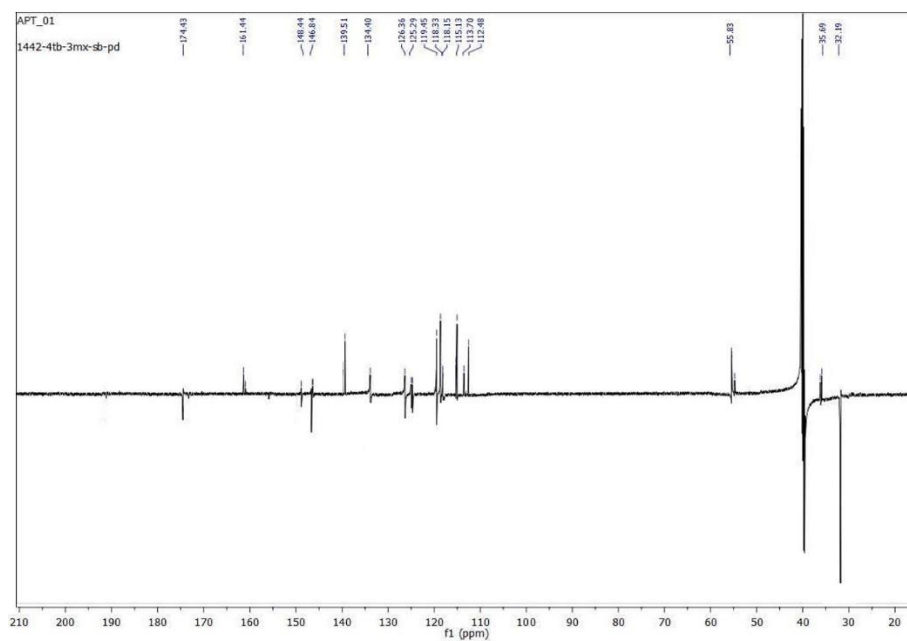
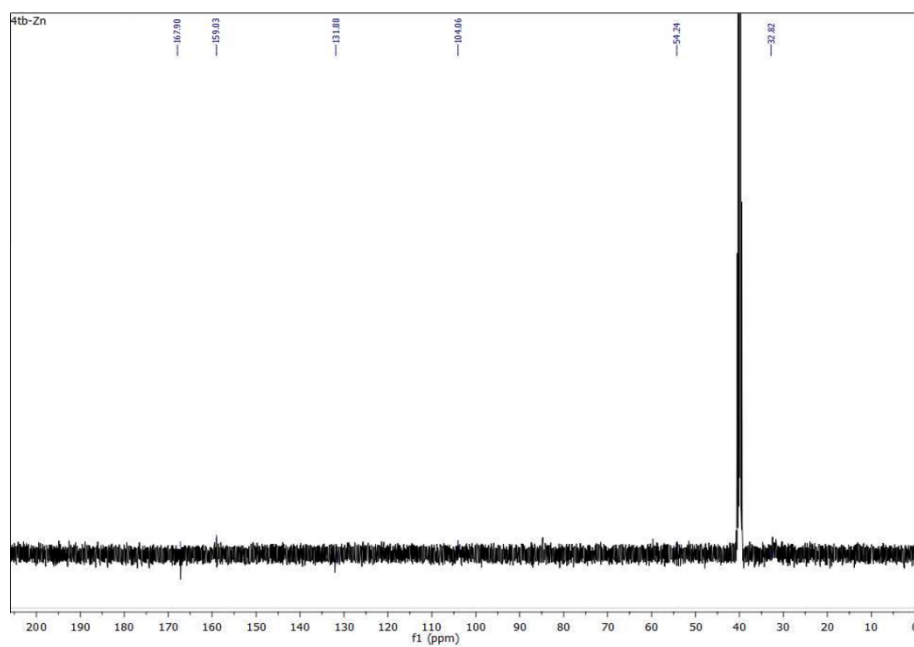
Fig. S2. ESI-MS spectrum of **HL²**Fig. S3. ¹H-NMR spectrum of **H₂L¹**

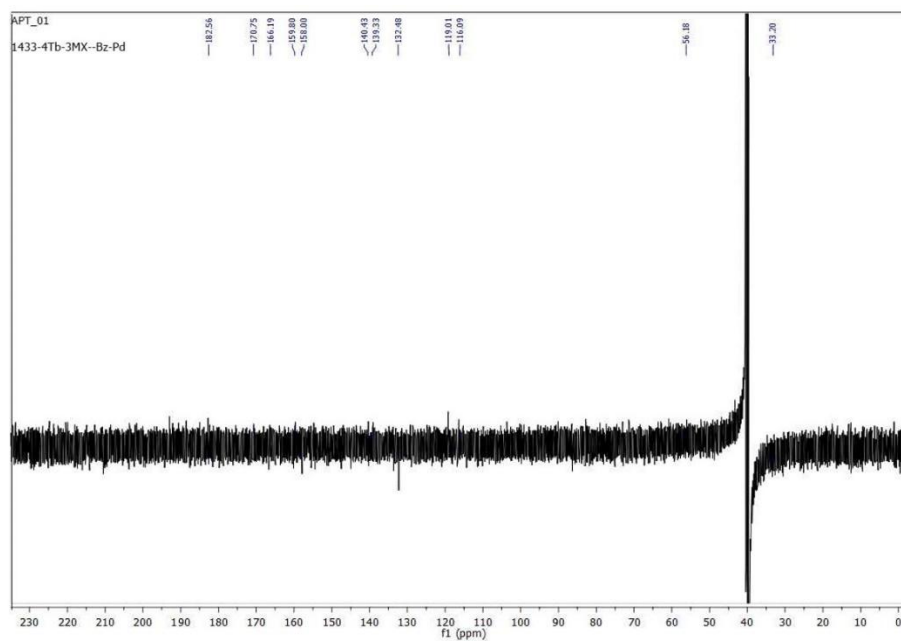
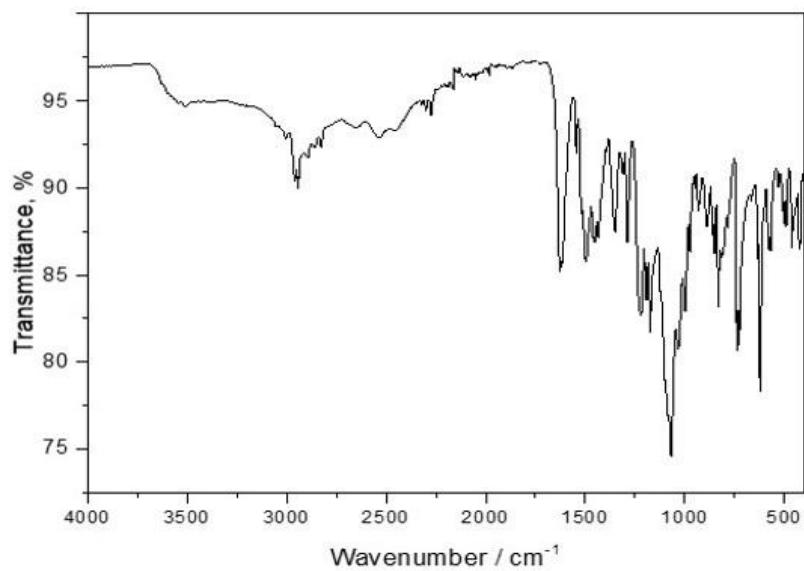
Fig. S4. ^1H -NMR spectrum of HL^2 

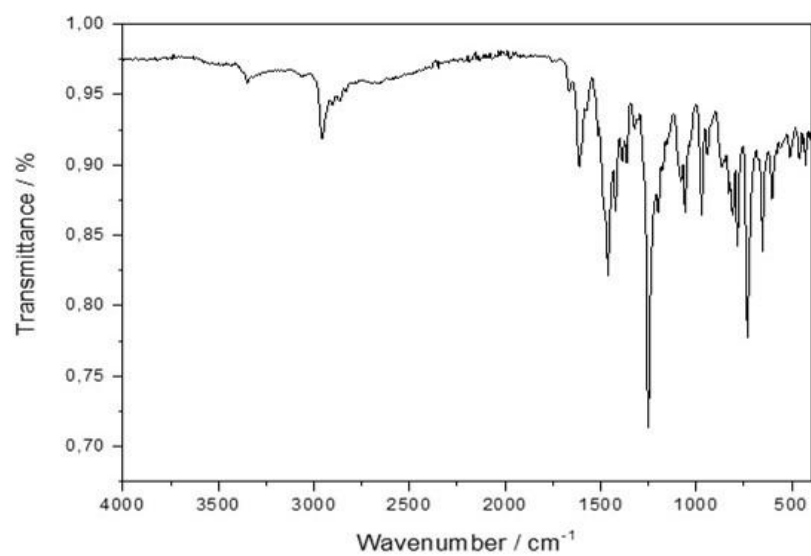
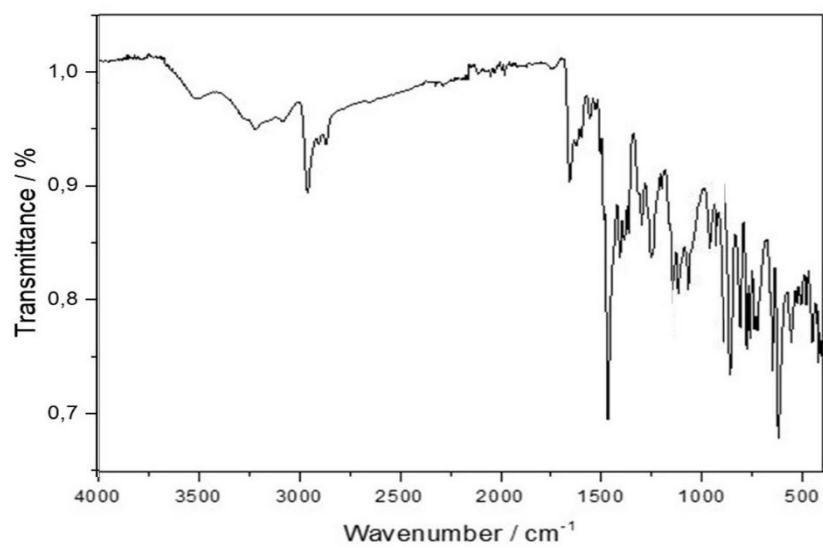
Fig. S6. ^1H -NMR spectrum of **1e** (Pd(II) complex of H_2L^1)Fig. S7. ^1H -NMR spectrum of **2d** (Zn(II) complex of HL^2)

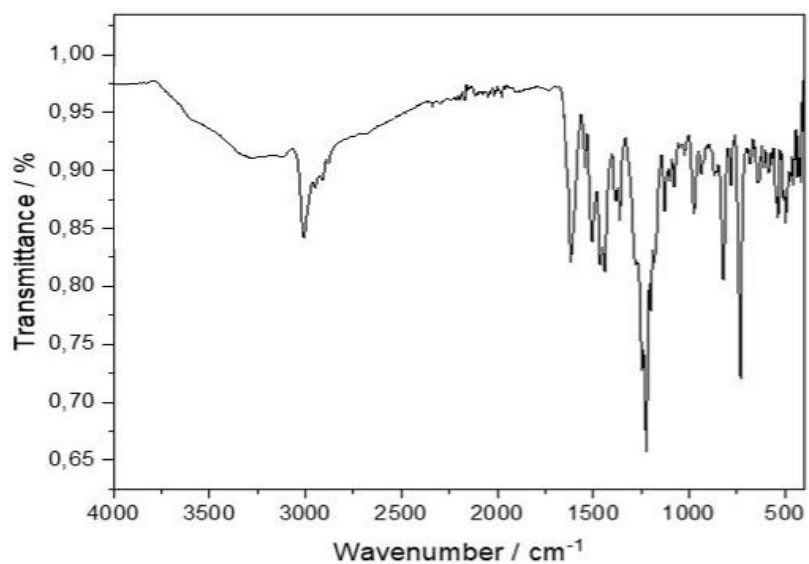
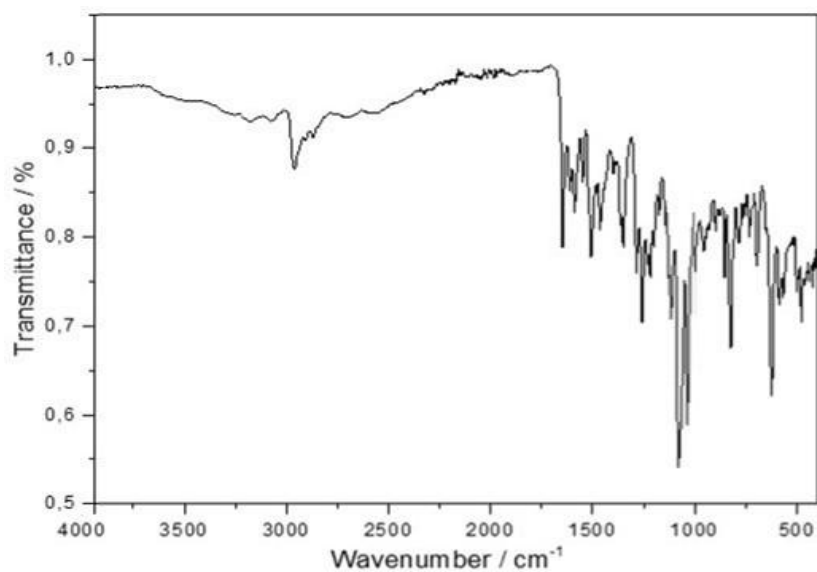
Fig. S8. ^1H -NMR spectrum of **2e** (Pd(II) complex of **HL**²)Fig. S9. ^{13}C -NMR spectrum of **H**₂**L**¹

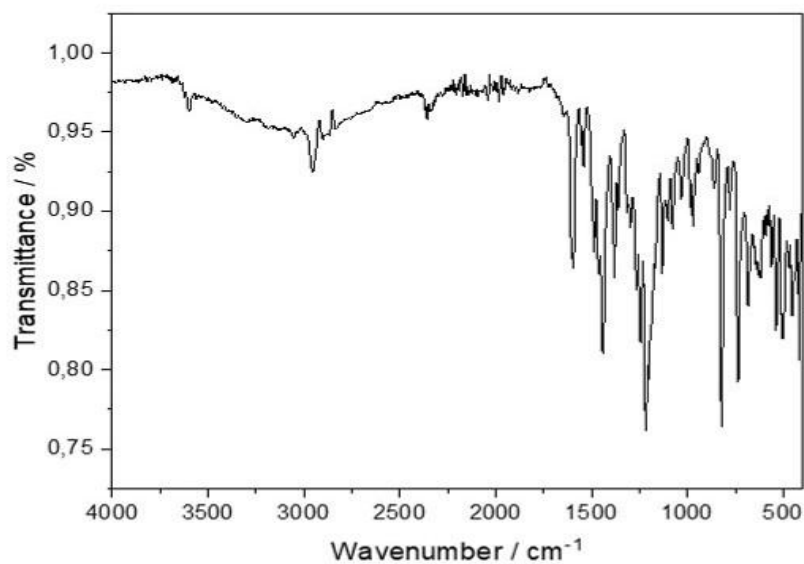
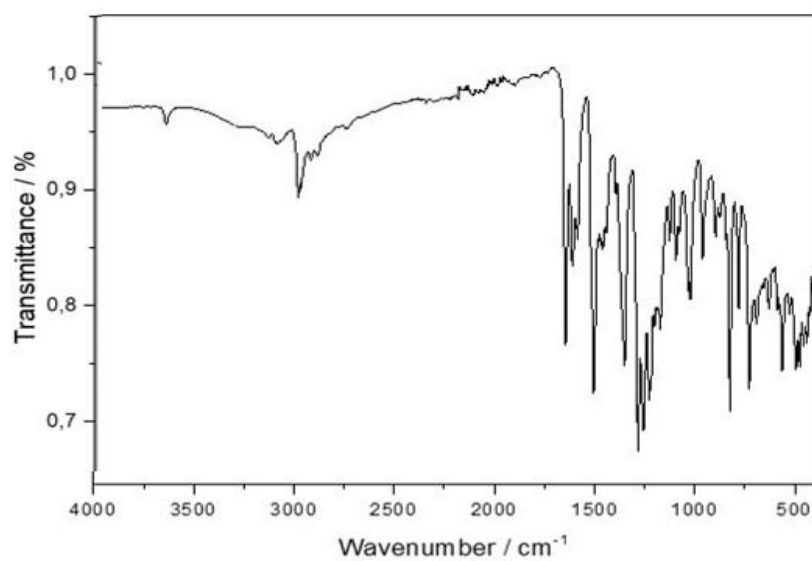
Fig. S10. ¹³C-NMR spectrum of **HL**²Fig. S11. ¹³C-NMR spectrum of **1d** (Zn(II) complex of **H**₂**L**¹)

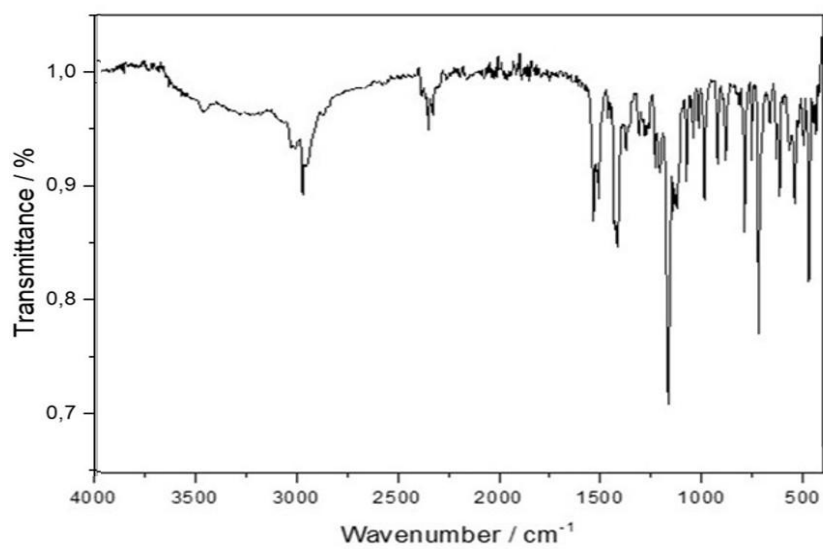
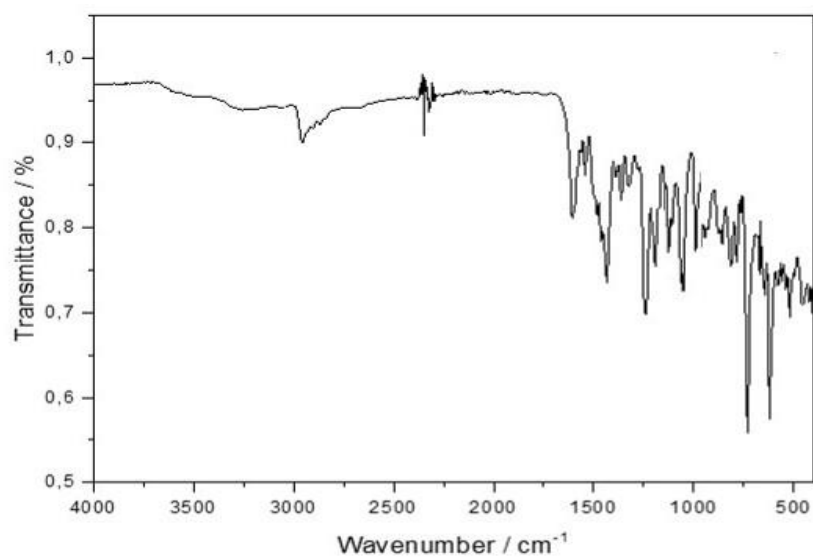
Fig. S12. ^{13}C -NMR spectrum of **1e** (Pd(II) complex of H_2L^1)Fig. S13. ^{13}C -NMR spectrum of **2d** (Zn(II) complex of HL^2)

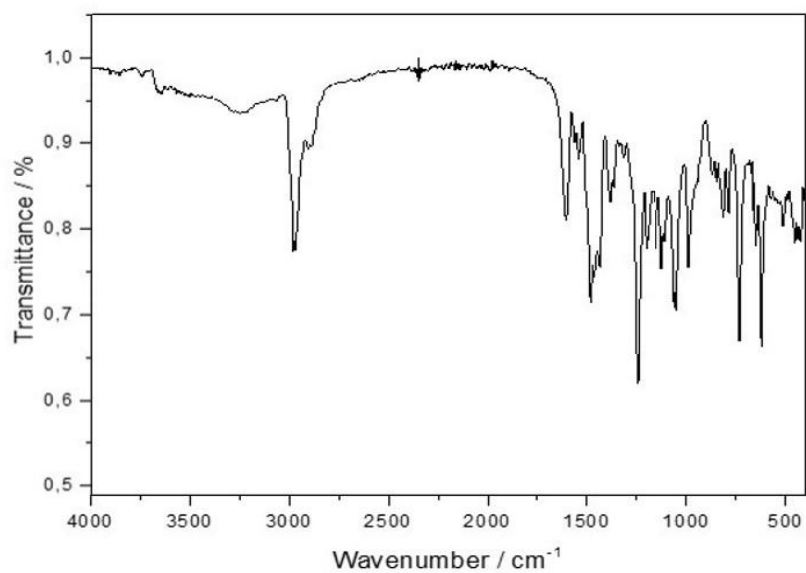
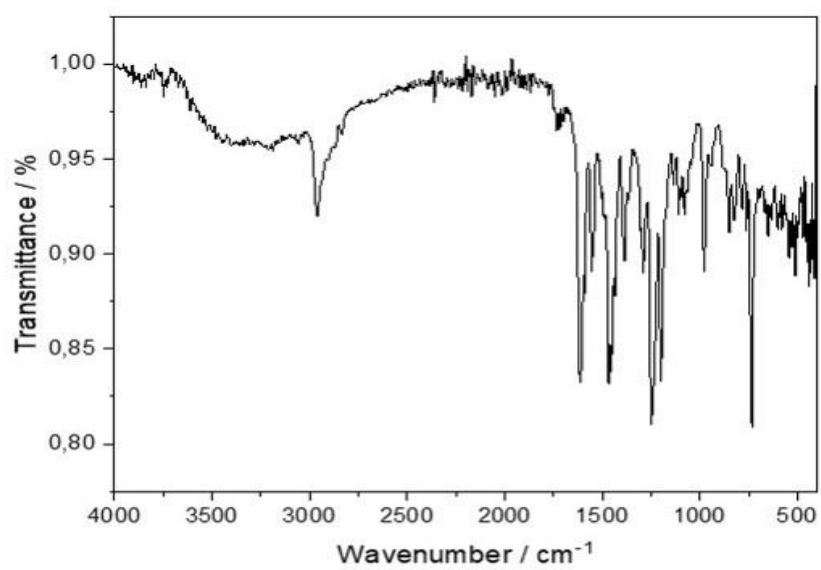
Fig. S14. ^{13}C -NMR spectrum of **2e** (Pd(II) complex of **HL**²)Fig. S15. FTIR spectrum of **H₂L**¹

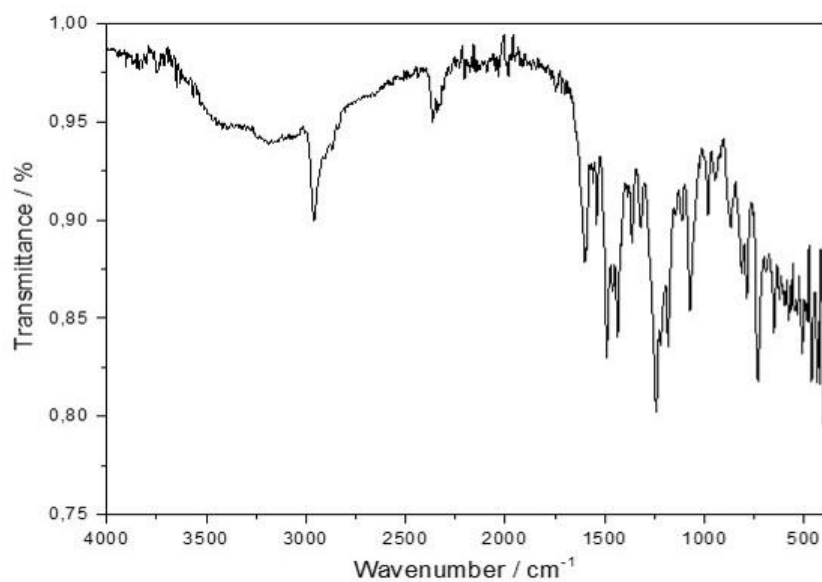
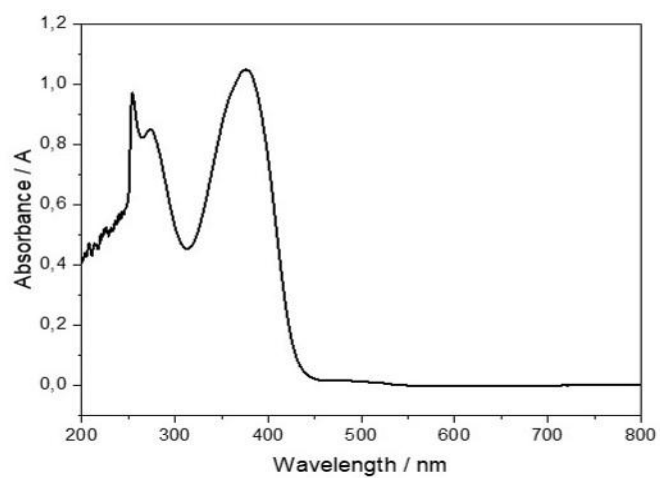
Fig. S16. FTIR spectrum of **HL**²Fig. S17. FTIR spectrum of **1a**

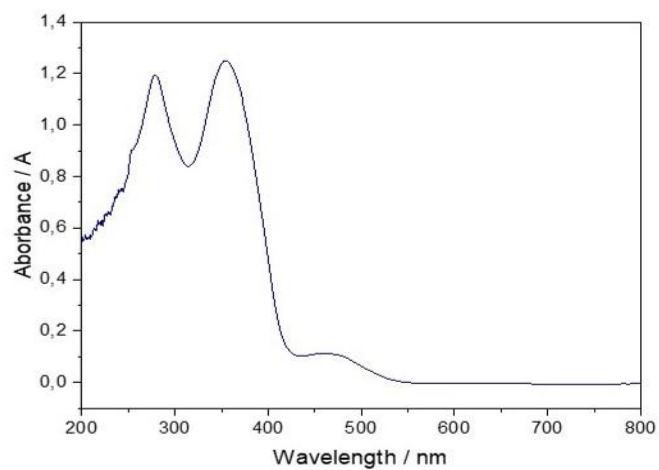
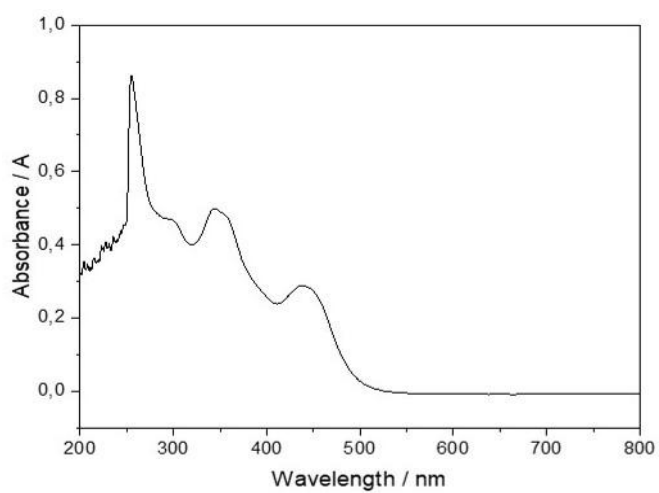
Fig. S18. FTIR spectrum of **1b**Fig. S19. FTIR spectrum of **1c**

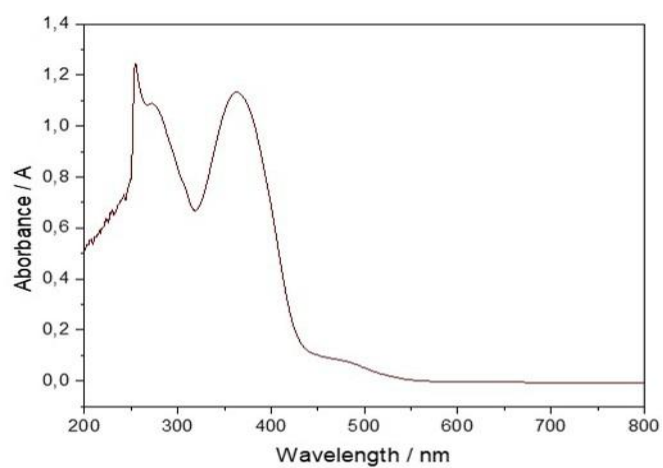
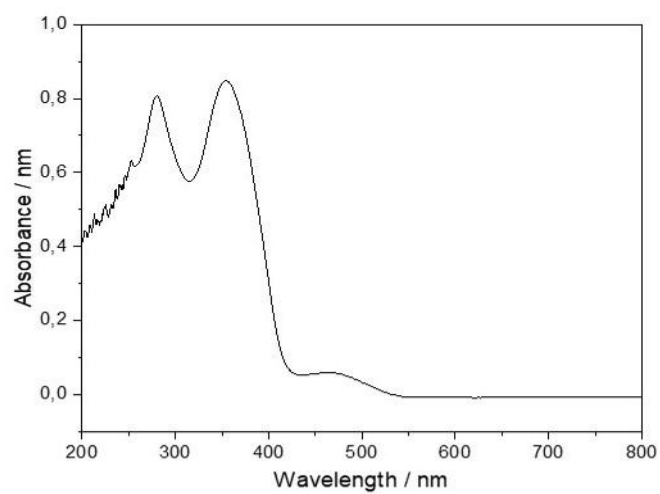
Fig. S20. FTIR spectrum of **1d**Fig. S21. FTIR spectrum of **1e**

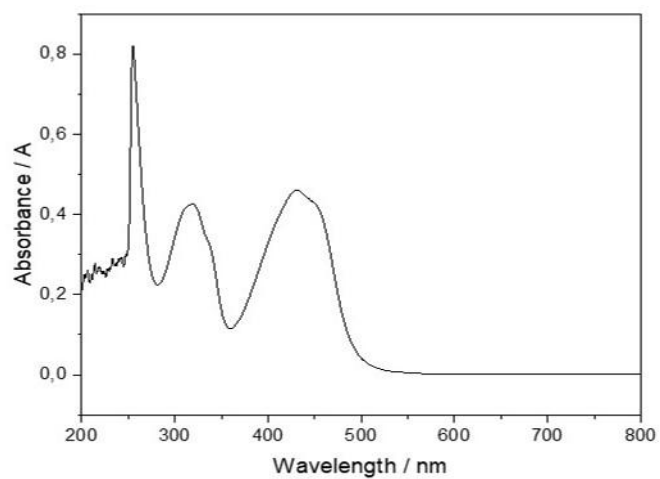
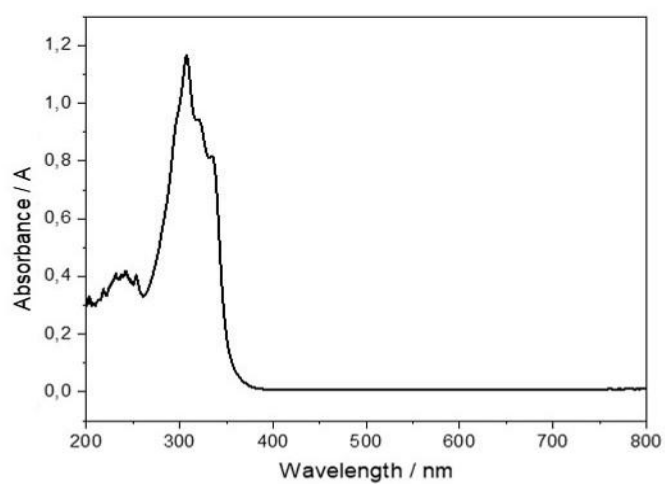
Fig. S22. FTIR spectrum of **2a**Fig. S23. FTIR spectrum of **2b**

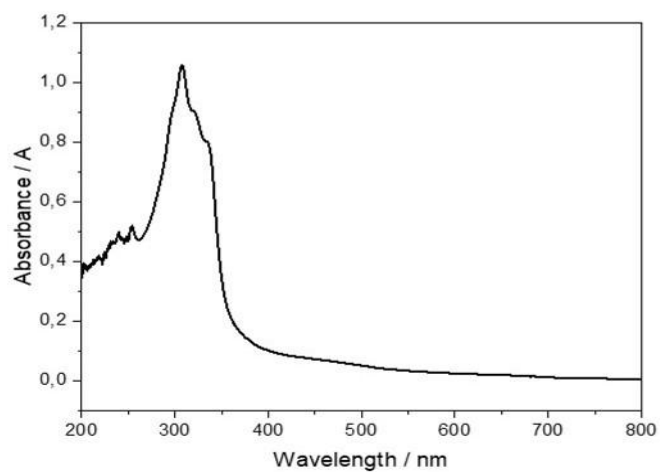
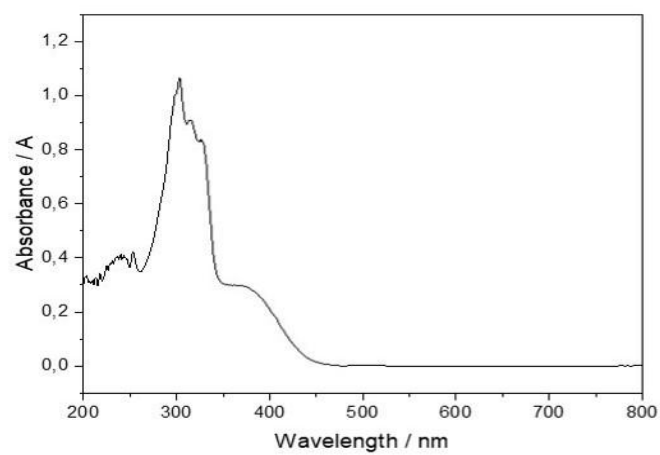
Fig. S24. FTIR spectrum of **2c**Fig. S25. FTIR spectrum of **2d**

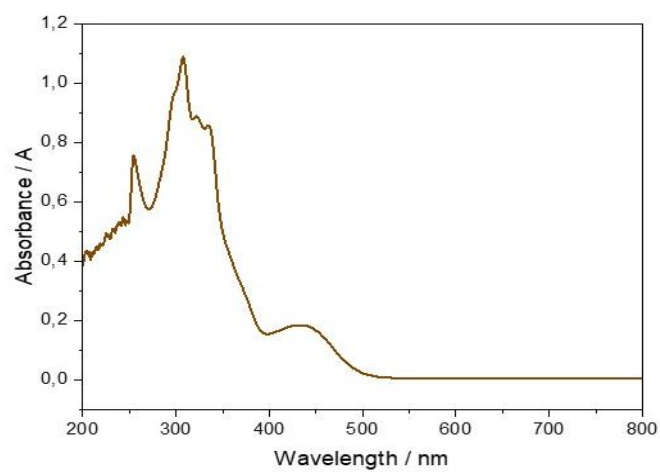
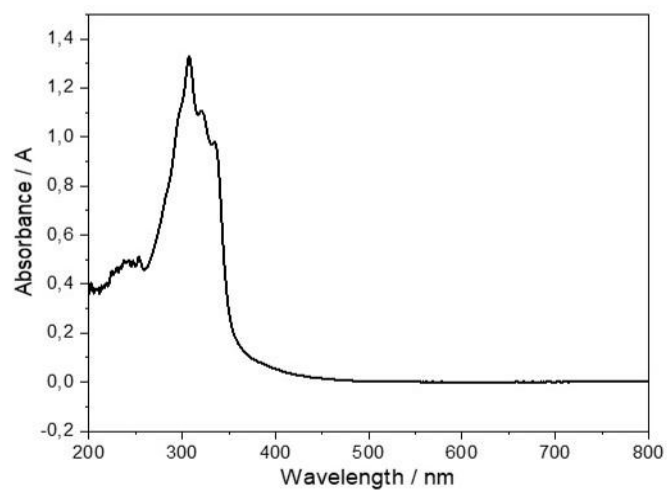
Fig. S26. FTIR spectrum of **2e**Fig. S27. UV-visible spectrum of **H₂L¹**

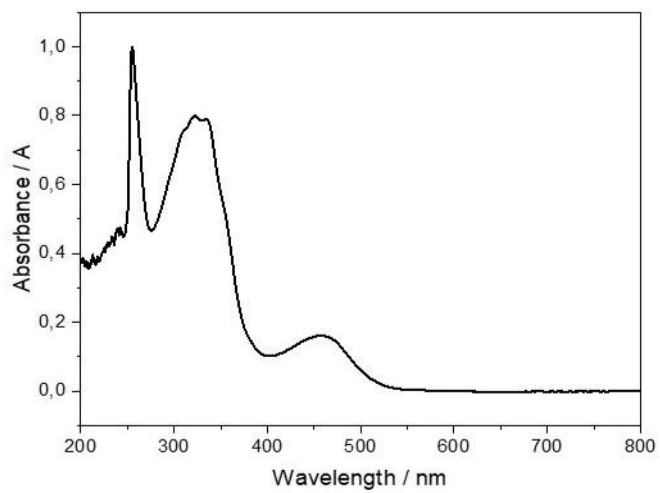
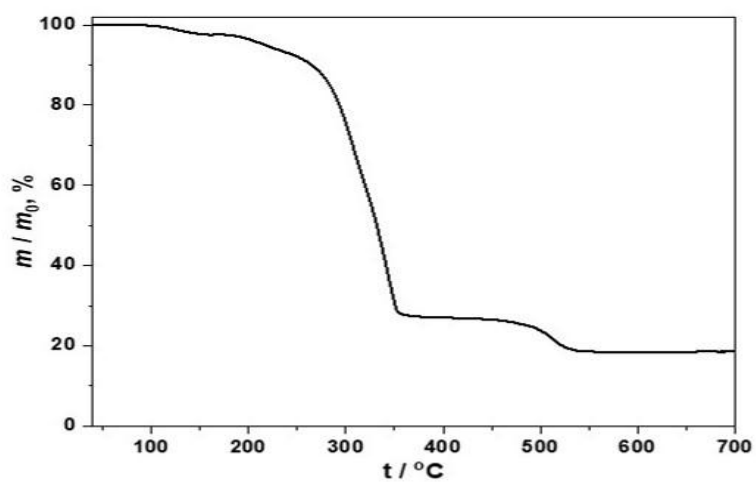
Fig. S28. UV-visible spectrum of **1a**Fig. S29. UV-visible spectrum of **1b**

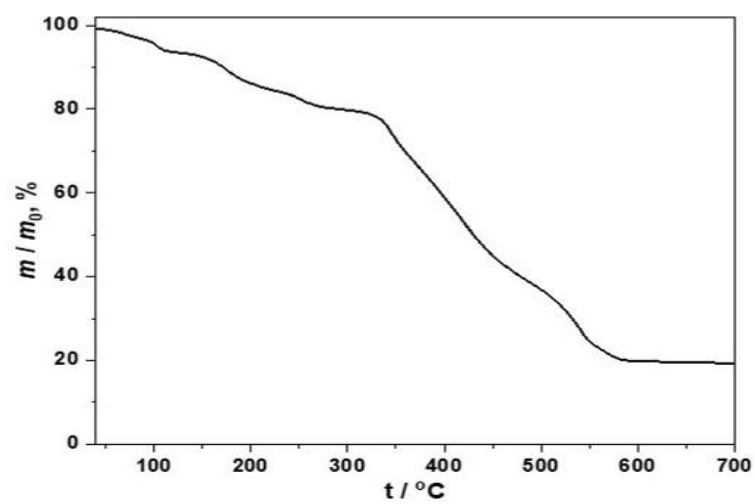
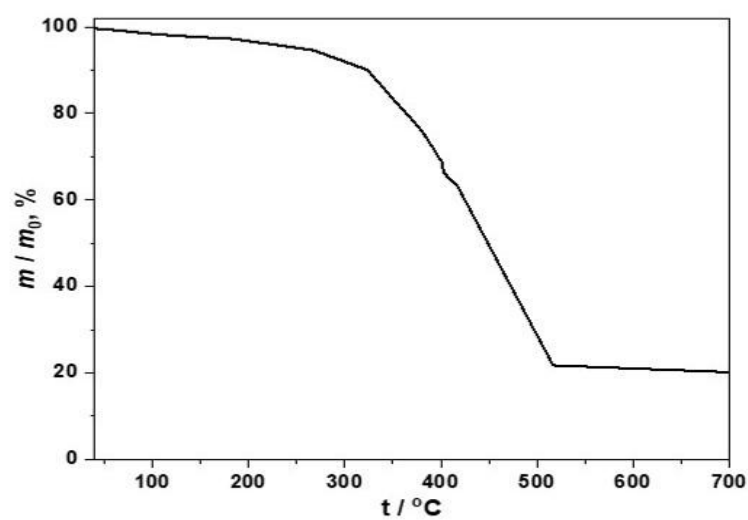
Fig. S30. UV-visible spectrum of **1c**Fig. S31. UV-visible spectrum of **1d**

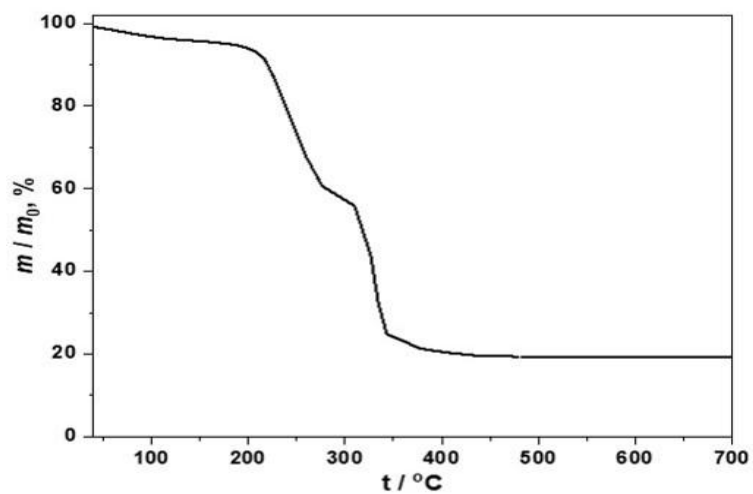
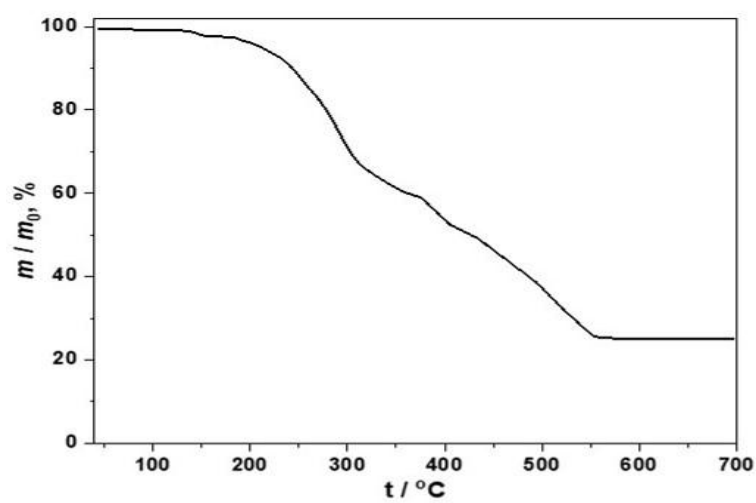
Fig. S32. UV-visible spectrum of **1e**Fig. S33. UV-visible spectrum of **HL²**

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**.