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Supplementary Information

Iron Complexes Containing Electrochemically Active Diazocycle-bis(di-*tert*-butyl-phenol) Ligands

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Table S1. Select bond lengths (Å) and angles (degree) for complex **2**

Complex **2**			
Fe1–N1	2.177(3)	Fe1–O2	1.865(2)
Fe1–N2	2.186(3)	Fe1–Cl1	2.251(1)
Fe1–O1	1.868(2)		
N1–Fe1–O1	85.81 (9)	N2–Fe1–O1	145.00(1)
N2–Fe1–O2	87.80(1)	Cl1–Fe1–N1	100.25(7)
O1–Fe1–O2	97.99(9)	Cl1–Fe1–O1	112.26(7)
N1–Fe1–N2	72.60(1)	Cl1–Fe1–N2	98.18(7)
N1–Fe1–O2	148.80(1)		

Table S2. Select bond lengths (Å) and angles (degree) for complex **4**

Complex **4**			
Fe1–O1	1.900(7)	Fe2–O3	1.993(8)
Fe1–O2	1.867(8)	Fe2–O4	1.959(7)
Fe1–O3	2.055(7)	Fe2–O5	1.839(7)
Fe1–O4	2.022(8)	Fe2–N3	2.23(1)
Fe1–N1	2.25(1)	Fe2–Cl1	2.254(3)
Fe1–N2	2.295(7)		
Fe1–O3–Fe2	104.4(3)	Fe1–O4–Fe2	106.9 (4)
N1–Fe1–N2	60.0(3)	Cl1–Fe2–N3	101.5(3)
N1–Fe1–O1	84.9(3)	Cl1–Fe2–O3	102.3(2)
N1–Fe1–O2	110.3(3)	Cl1–Fe2–O4	127.0(2)
N1–Fe1–O3	76.7(3)	Cl1–Fe2–O5	106.2(3)
N1–Fe1–O4	149.4(3)	N3–Fe2–O3	151.4(3)
N2–Fe1–O1	142.3(3)	N3–Fe2–O4	77.7(3)
N2–Fe1–O2	82.2(3)	N3–Fe2–O5	88.2(3)
N2–Fe1–O3	76.8(3)	O3–Fe2–O4	75.5(3)
N2–Fe1–O4	114.6(3)	O3–Fe2–O5	100.0(3)
O1–Fe1–O2	99.0(3)	O4–Fe2–O5	126.6(3)
O1–Fe1–O4	102.7(3)		
O2–Fe1–O3	150.4(3)		
O2–Fe1–O4	98.0(3)		
O3–Fe1–O4	72.8(3)		

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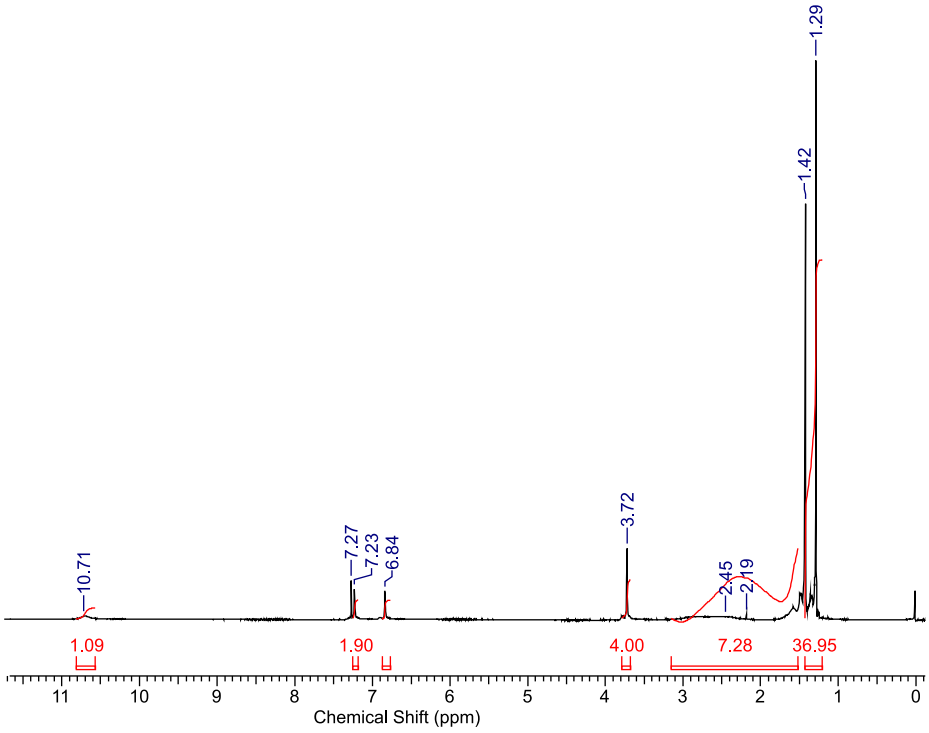

Figure S1. ^{1}H NMR spectrum ($CDCl_3$, 400 MHz) of the ligand H_2L1.

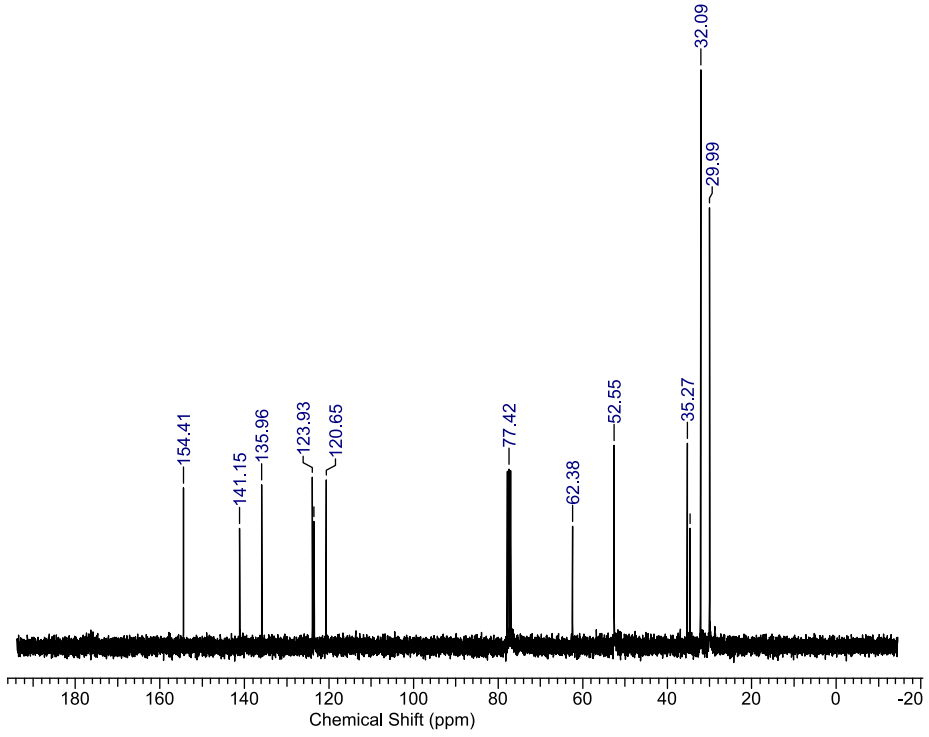

Figure S2. ^{13}C NMR spectrum ($CDCl_3$, 100 MHz) of the ligand H_2L1.

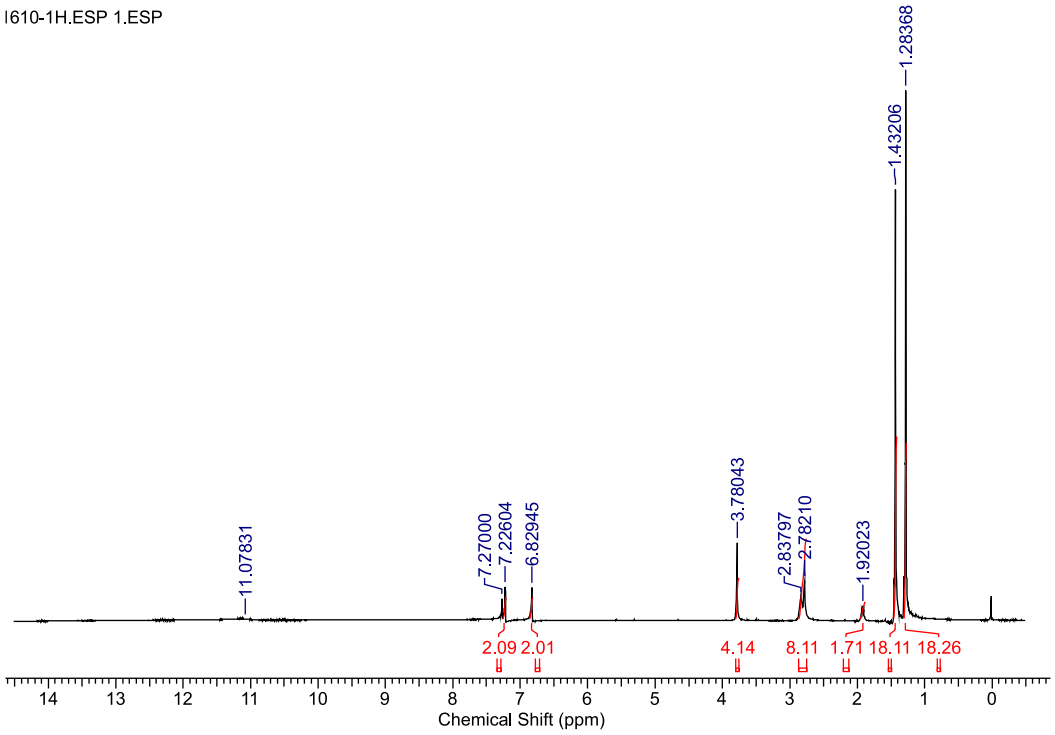

Figure S3. ^{1}H NMR spectrum ($CDCl_3$, 400 MHz) of the ligand H_2L2.

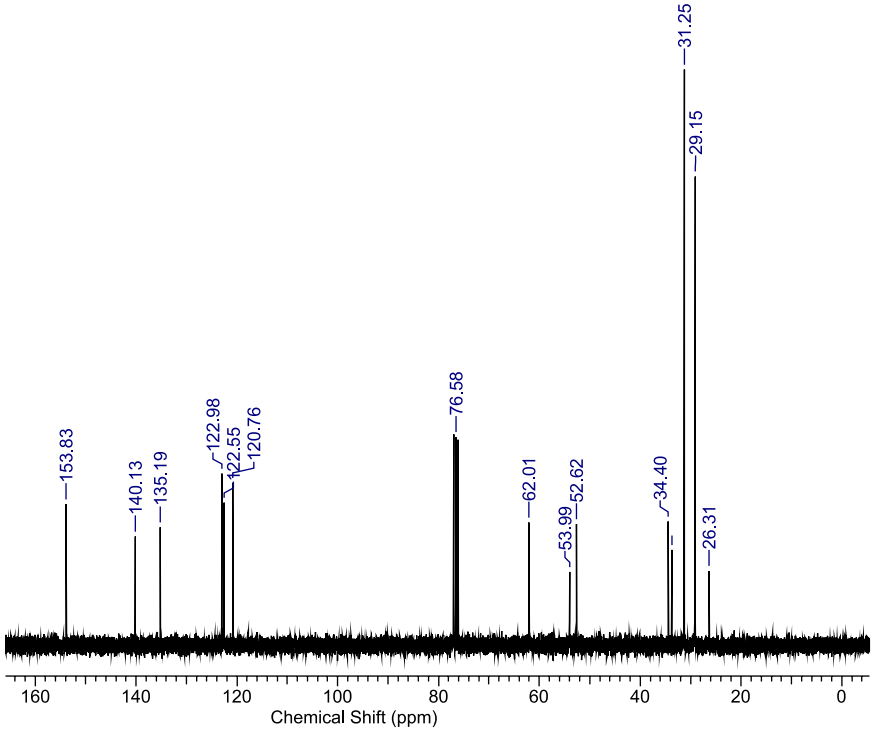

Figure S4. ^{13}C NMR spectrum ($CDCl_3$, 100 MHz) of the ligand H_2L2.

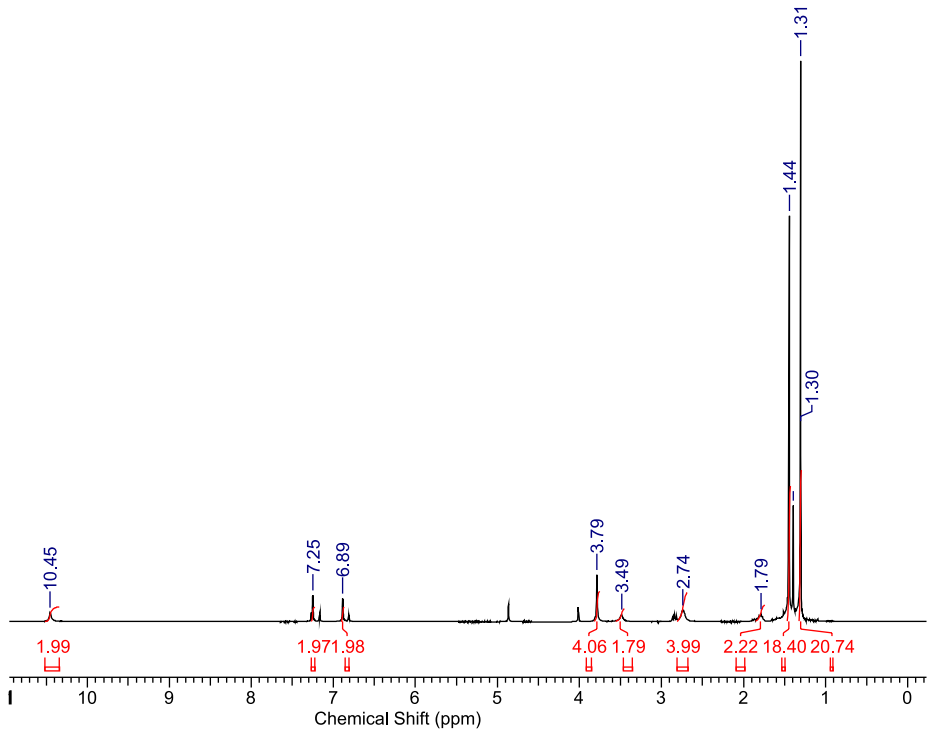

Figure S5. ^{1}H NMR spectrum ($CDCl_3$, 400 MHz) of the ligand H_2L3.

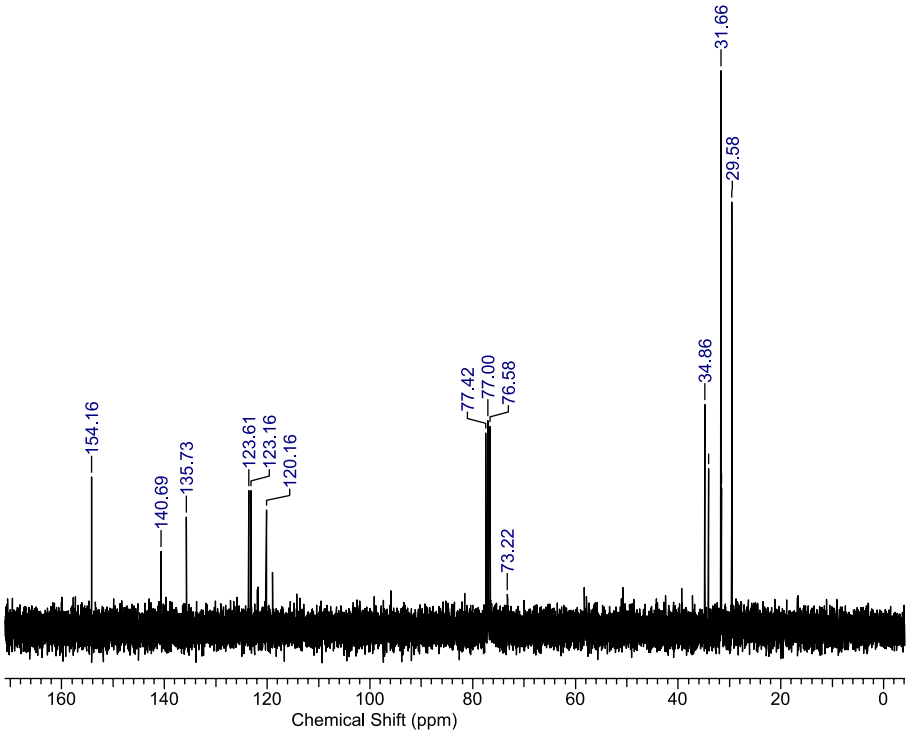

Figure S6. ^{13}C NMR spectrum ($CDCl_3$, 100 MHz) of the ligand H_2L3.

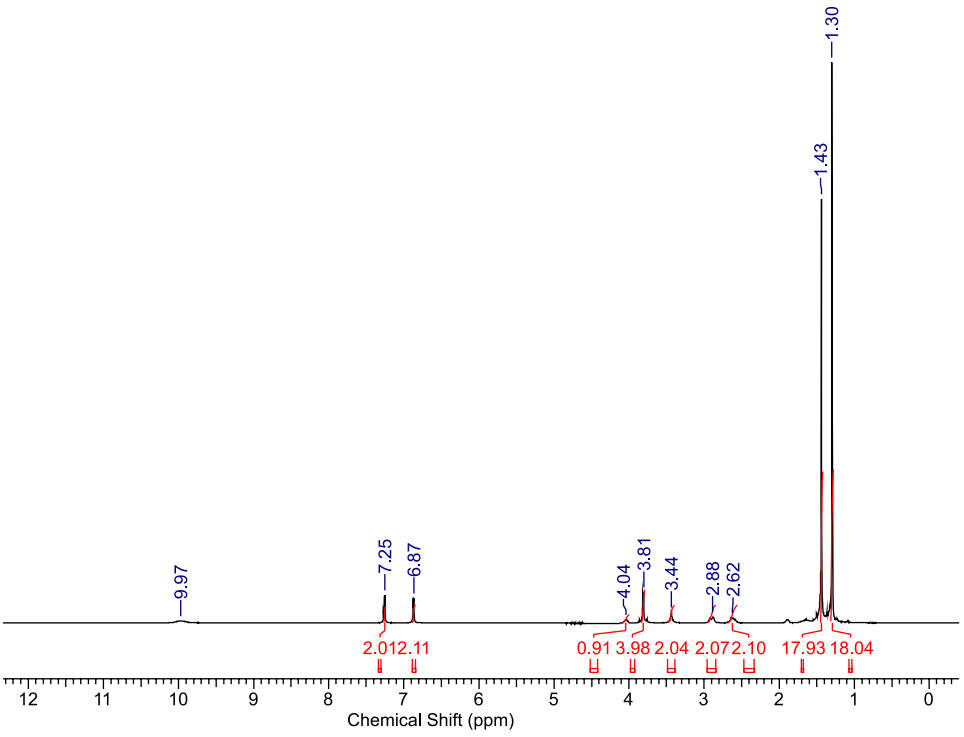

Figure S7. ^{1}H NMR spectrum ($CDCl_3$, 400 MHz) of the ligand H_3L4.

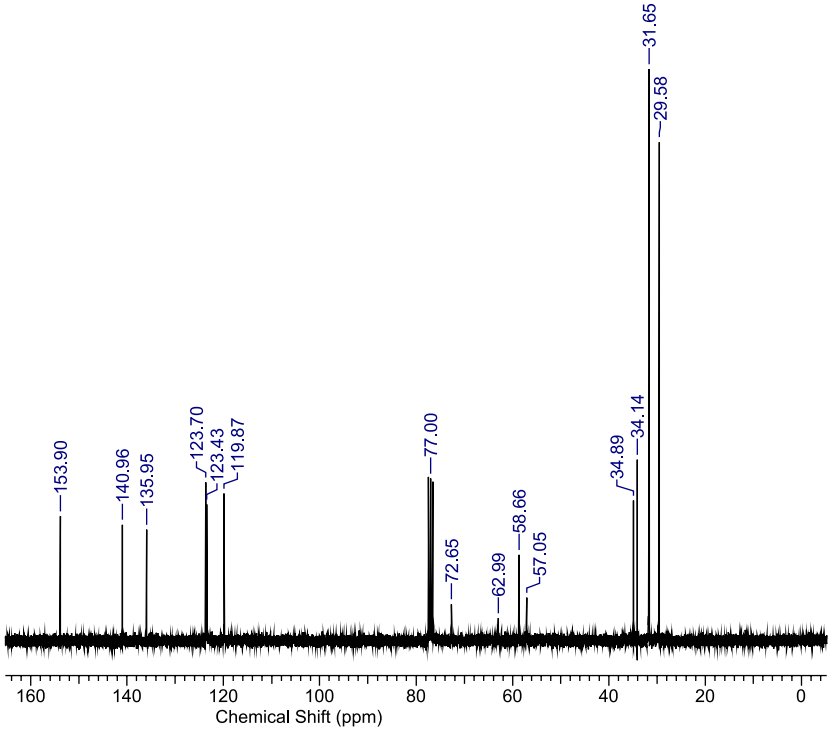

Figure S8. ^{13}C NMR spectrum ($CDCl_3$, 100 MHz) of the ligand H_3L4.

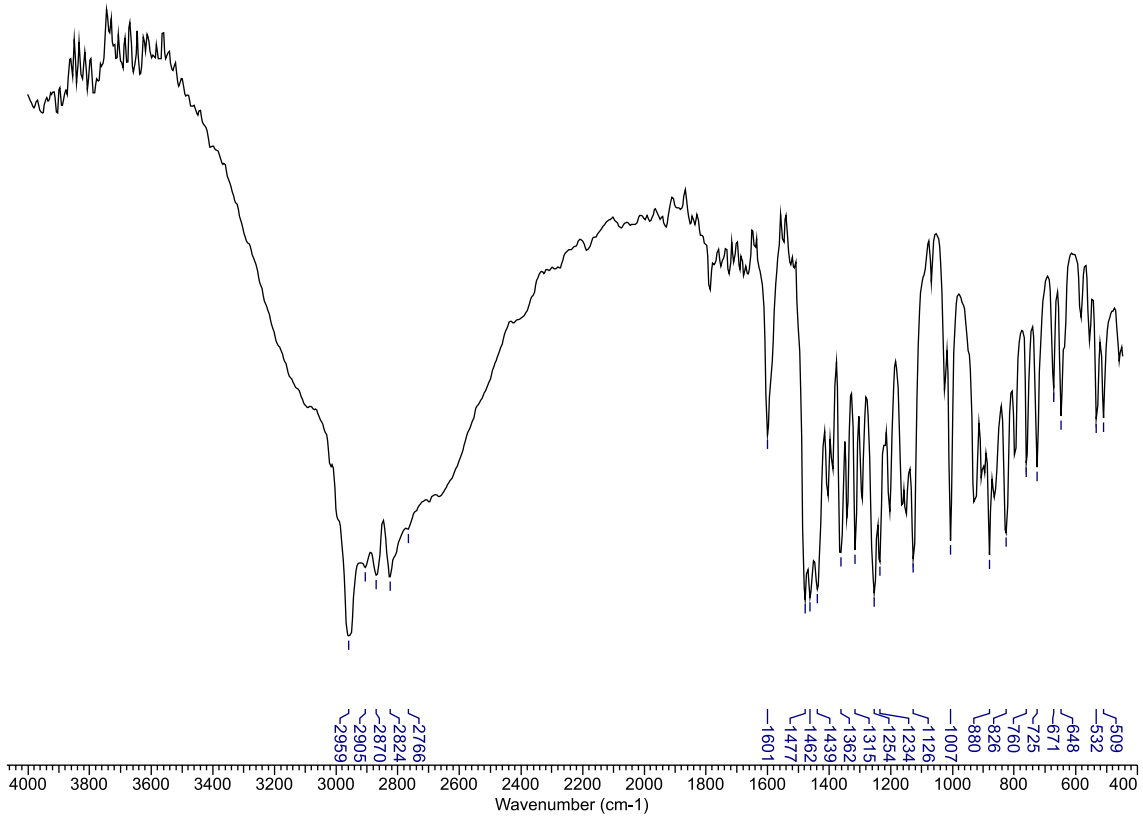

Figure S9. IR spectrum (KBr) of the ligand H_2L1.

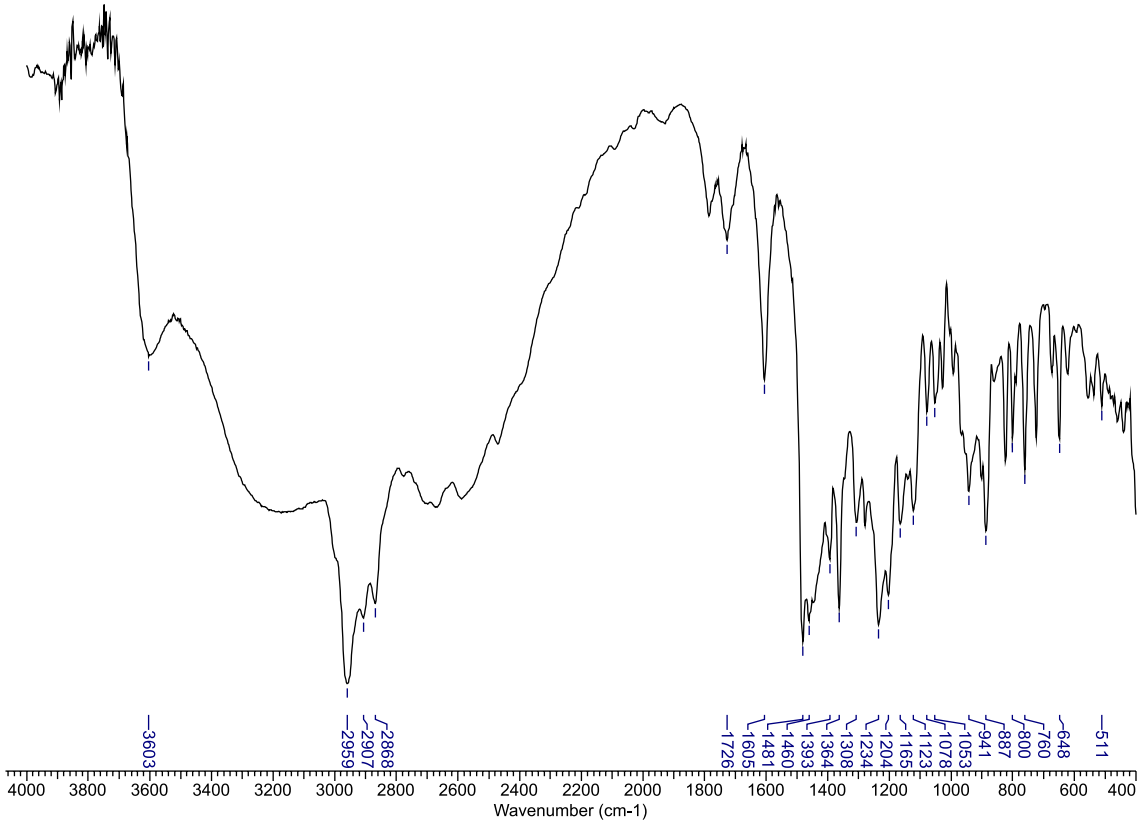

Figure S10. IR spectrum (KBr) of the compound **1**.

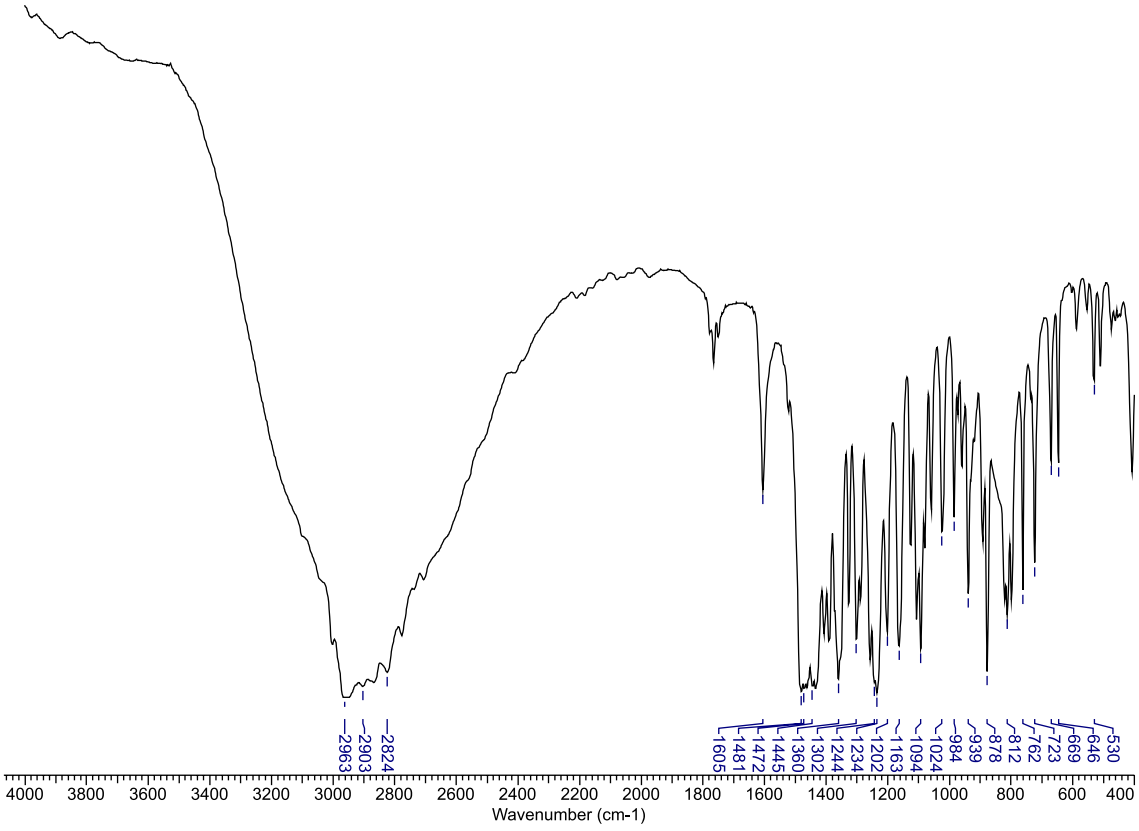

Figure S11. IR spectrum (KBr) of the ligand H_2L2.

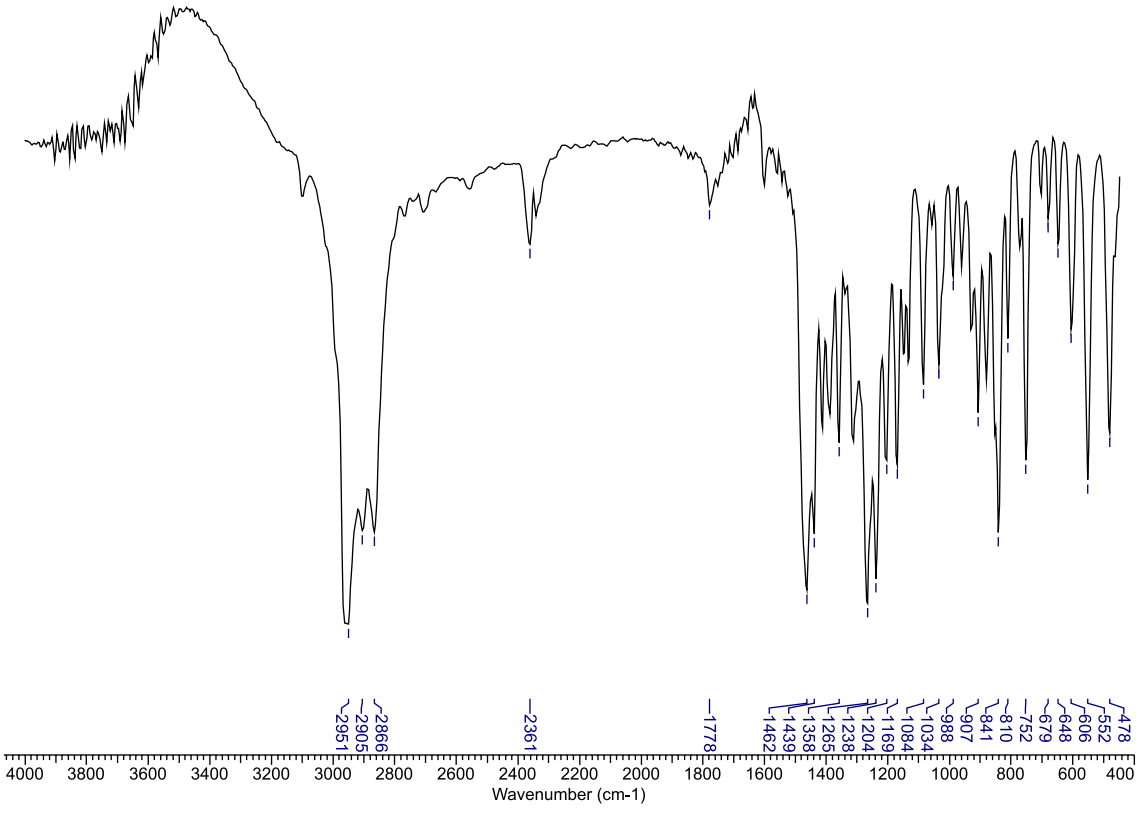

Figure S12. IR spectrum (KBr) of the compound **2.**

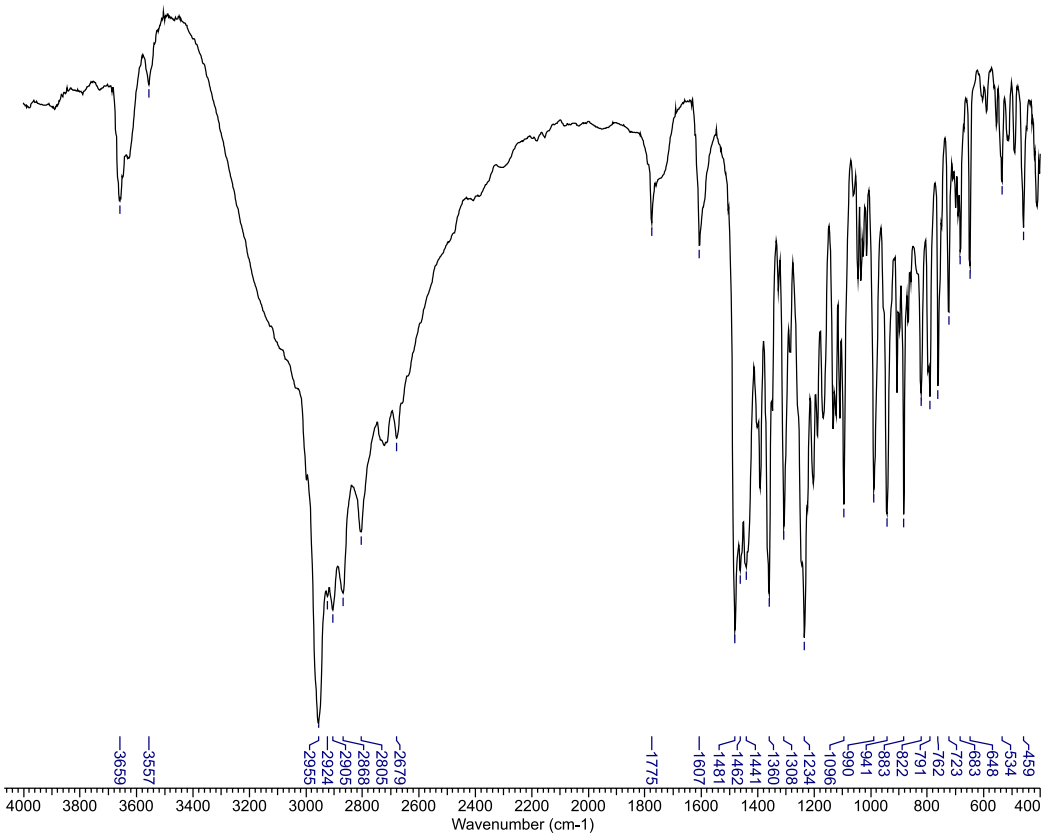

Figure S13. IR spectrum (KBr) of the ligand H_2L3.

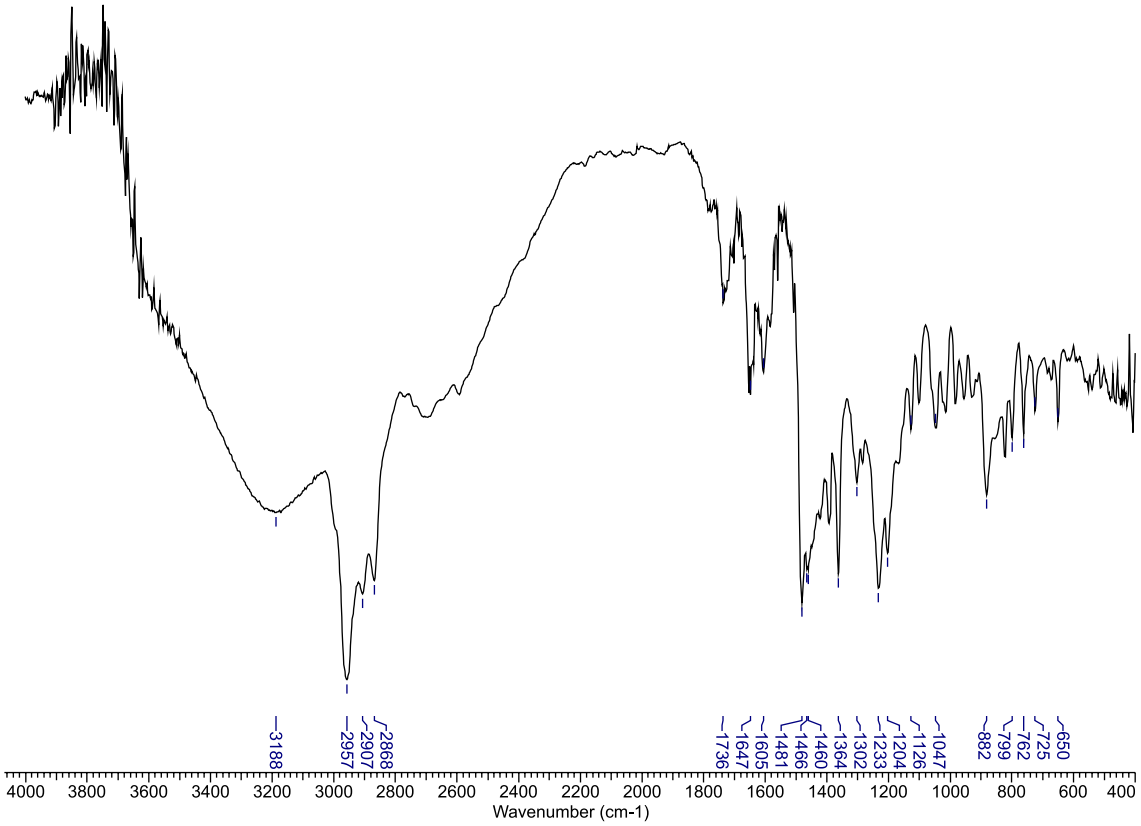

Figure S14. IR spectrum (KBr) of the compound **3**.

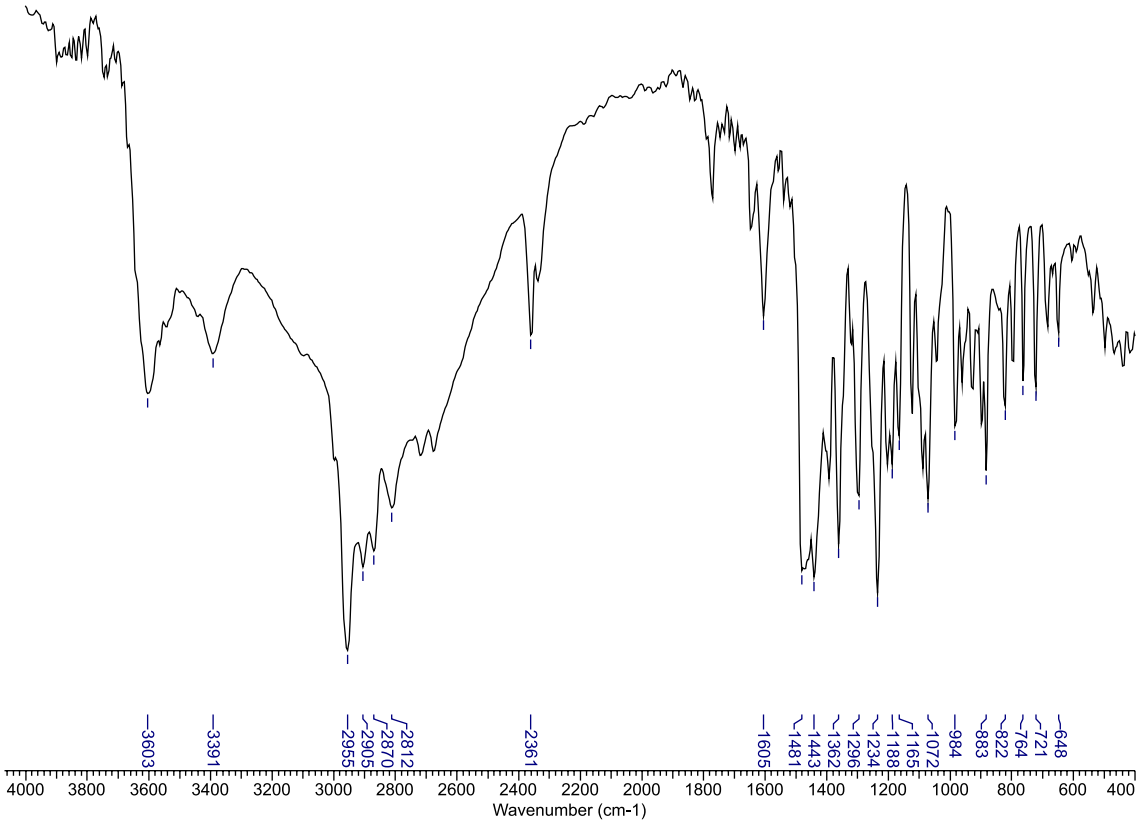

Figure S15. IR spectrum (KBr) of the ligand H_3L4.

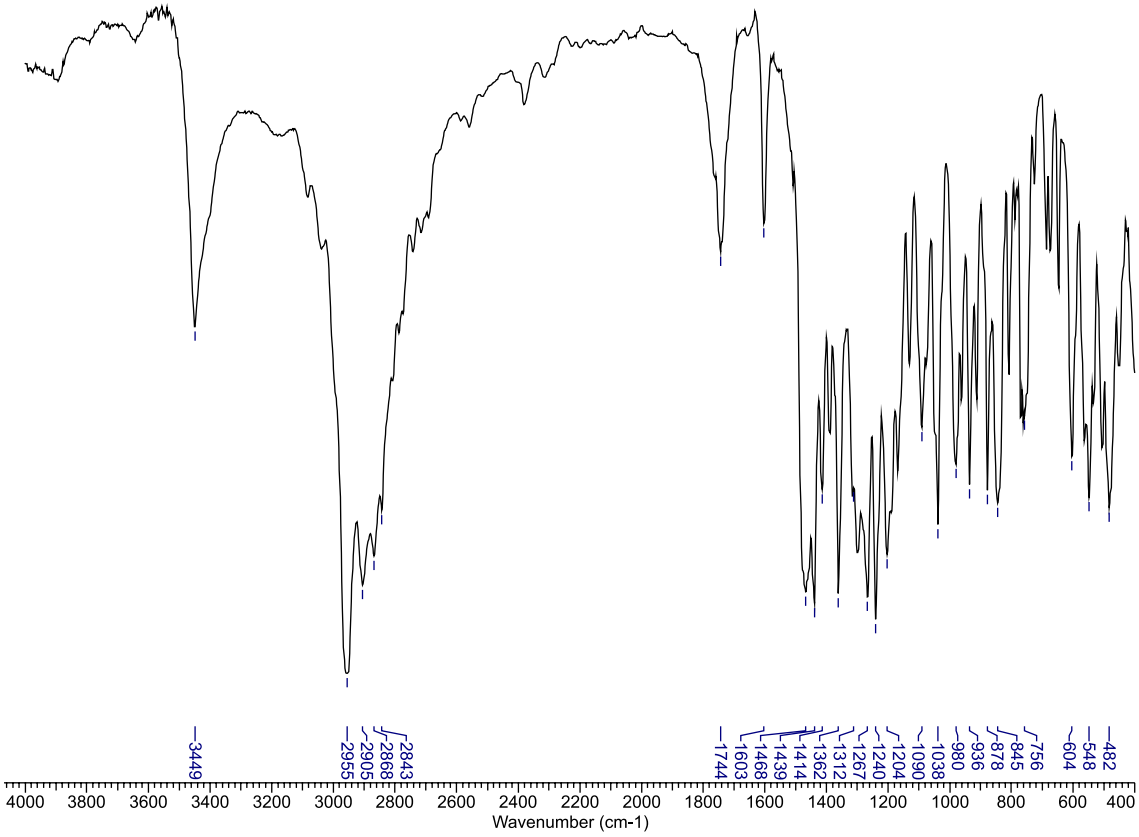

Figure S16. IR spectrum (KBr) of the compound **4**.

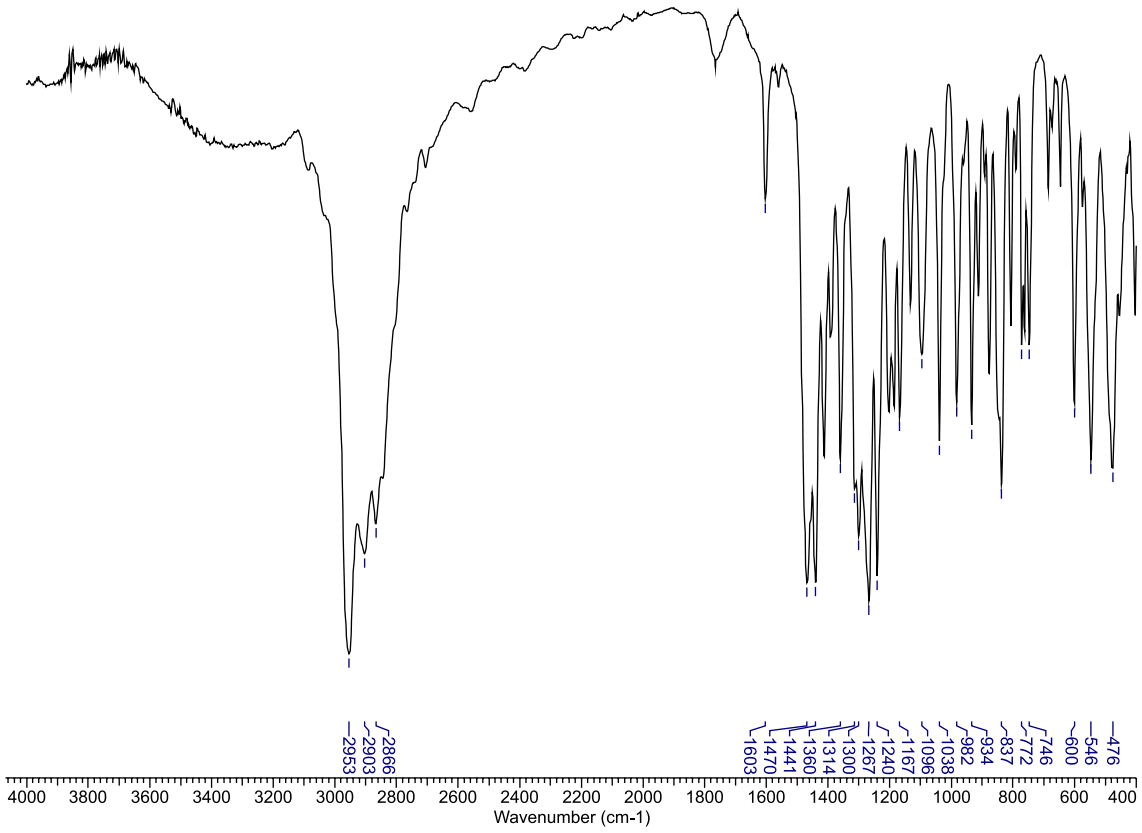

Figure S17. IR spectrum (KBr) of the compound **5**.

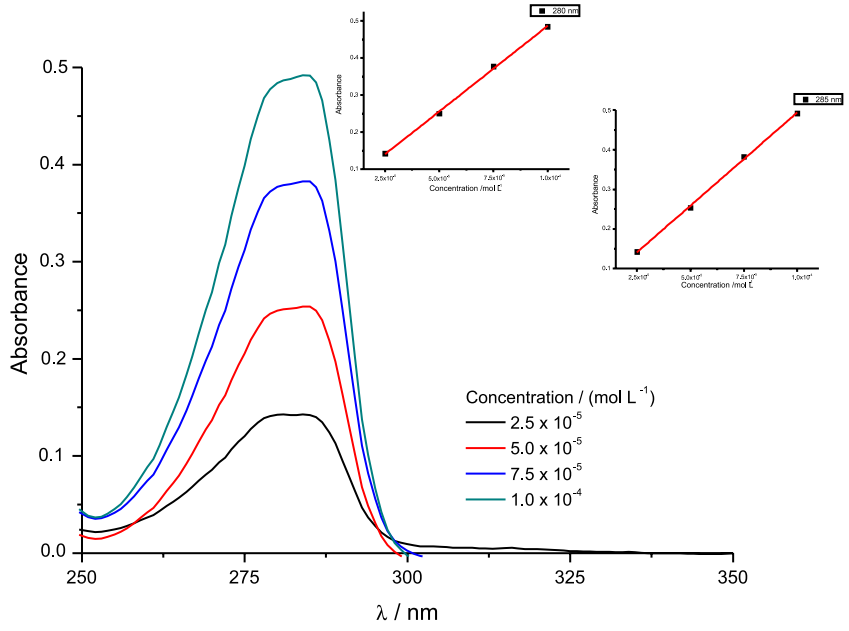

Figure S18. UV-Vis spectra of the ligand H_2L1 at different concentrations; solvent: CH_2Cl_2; λ = 280 nm (ε = 4.61 × 10^3 L mol^{-1} cm^{-1}); λ = 285 nm (ε = 4.71 × 10^3 L mol^{-1} cm^{-1}).

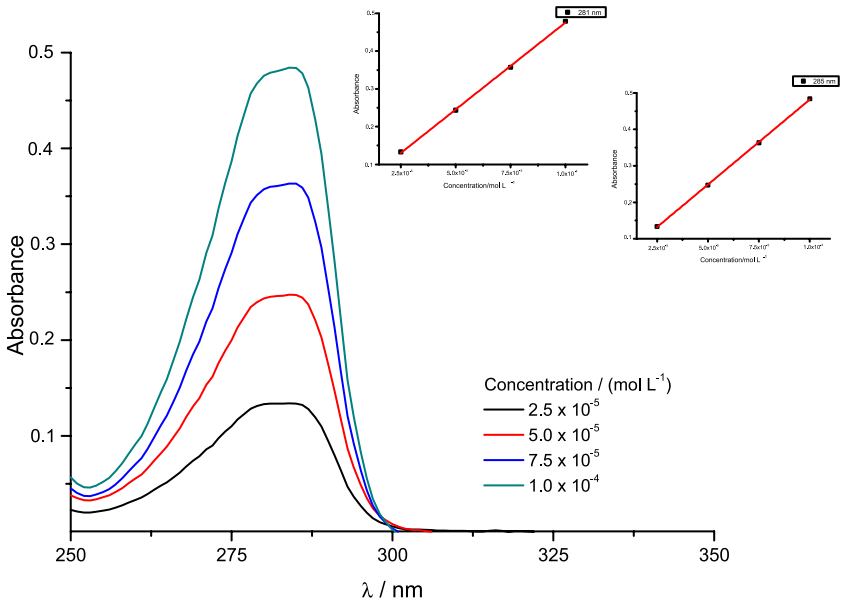

Figure S19. UV-Vis spectra of the ligand H_2L2 at different concentrations; solvent: CH_2Cl_2; λ = 281 nm (ε = 4.61 × 10^3 L mol^{-1} cm^{-1}); λ = 285 nm (ε = 4.67 × 10^3 L mol^{-1} cm^{-1}).

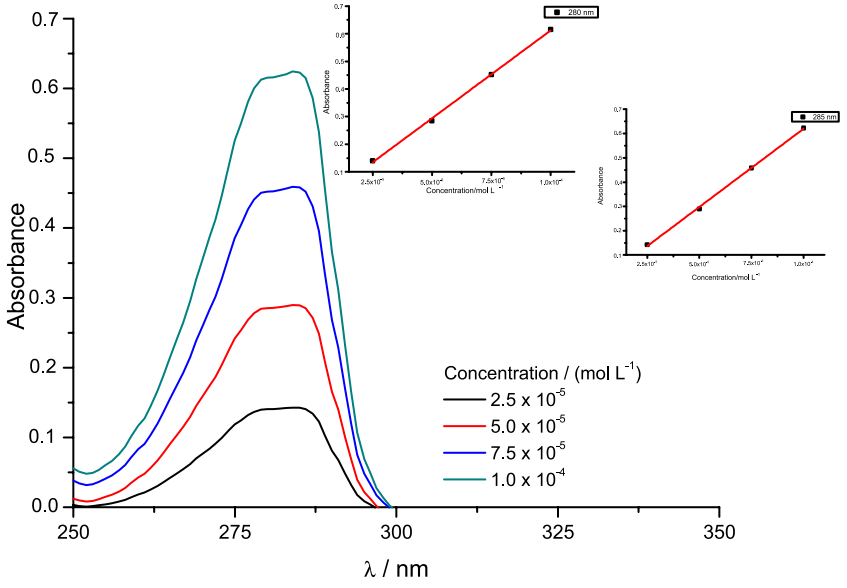

Figure S20. UV-Vis spectra of the ligand H_2L3 at different concentrations; solvent: CH_2Cl_2; λ = 280 nm (ε = 6.35 × 10^3 L mol^{-1} cm^{-1}); λ = 285 nm (ε = 6.46 × 10^3 L mol^{-1} cm^{-1}).

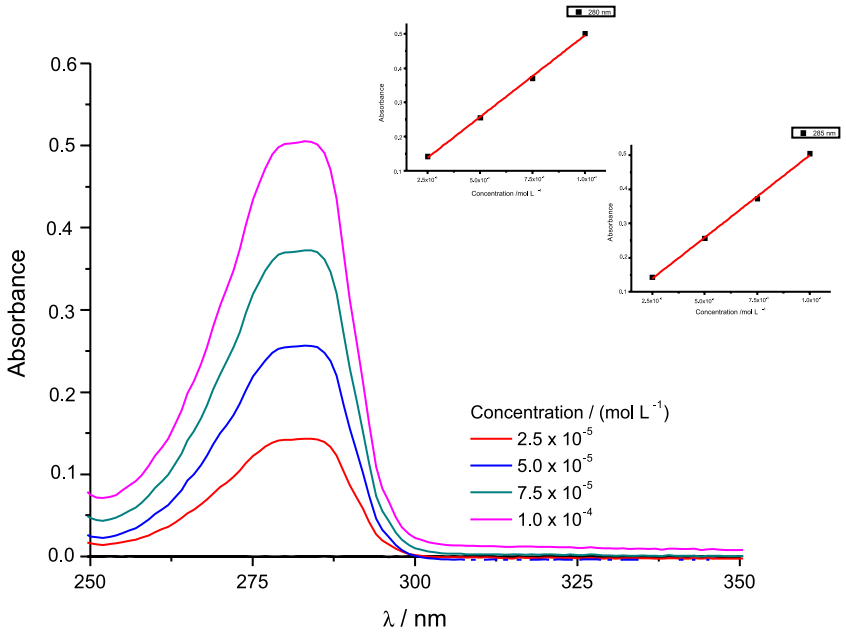

Figure S21. UV-Vis spectra of the ligand H_3L4 at different concentrations; solvent: CH_2Cl_2; λ = 280 nm (ε = 4.75 × 10^3 L mol^{-1} cm^{-1}); λ = 284 nm (ε = 4.77 × 10^3 L mol^{-1} cm^{-1}).

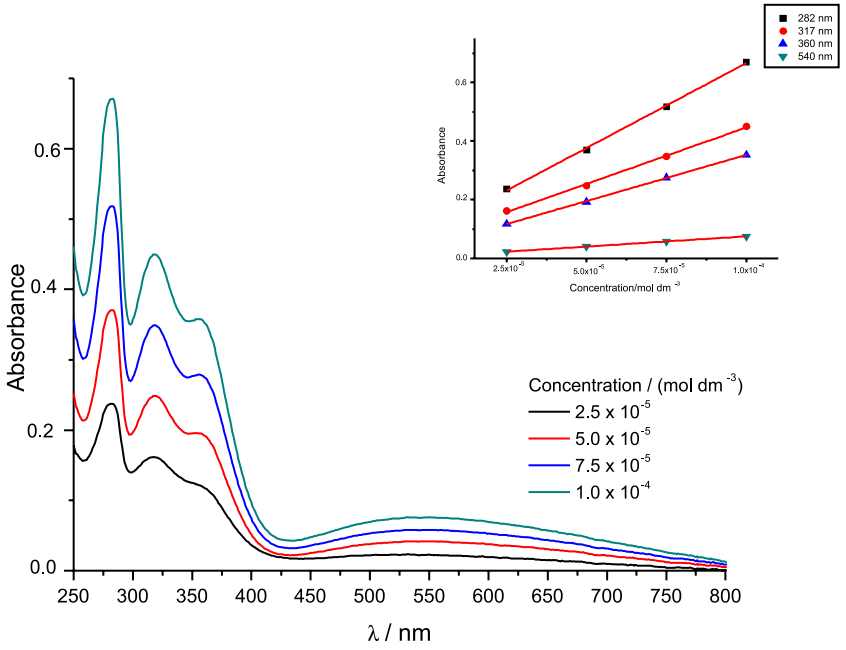

Figure S22. UV-Vis spectra of the compound **1** at different concentrations; solvent: CH_2Cl_2; λ = 282 nm (ε = 5.80 × 10^3 L mol^{-1} cm^{-1}); λ = 317 nm (ε = 3.86 × 10^3 L mol^{-1} cm^{-1}); λ = 360 nm (ε = 3.16 × 10^3 L mol^{-1} cm^{-1}); λ = 540 nm (ε = 7.00 × 10^2 L mol^{-1} cm^{-1}).

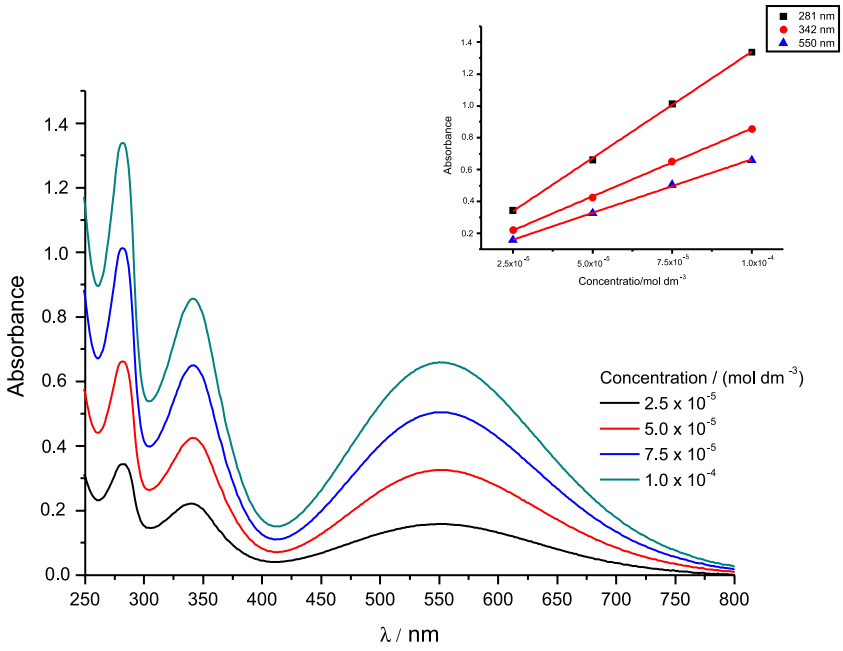

Figure S23. UV-Vis spectra of compound **2** at different concentrations; solvent: CH_2Cl_2; λ = 281 nm (ε = 1.33 × 10^4 L mol^{-1} cm^{-1}); λ = 342 nm (ε = 8.53 × 10^3 L mol^{-1} cm^{-1}); λ = 550 nm (ε = 6.72 × 10^3 L mol^{-1} cm^{-1}).

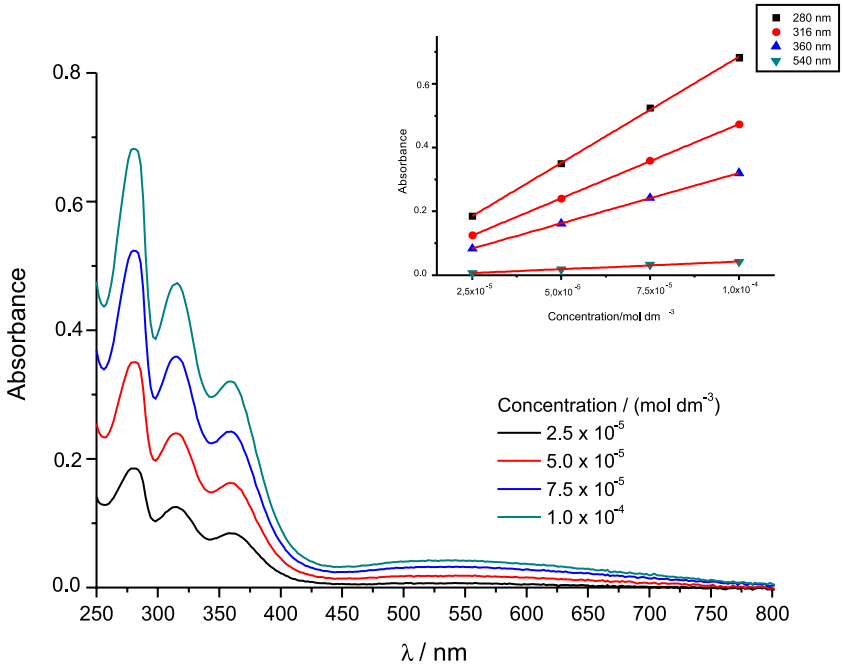

Figure S24. UV-Vis spectra of the compound **3** at different concentrations; solvent: CH_2Cl_2; λ = 280 nm (ε = 6.66 × 10^3 L mol^{-1} cm^{-1}); λ = 316 nm (ε = 4.65 × 10^3 L mol^{-1} cm^{-1}); λ = 360 nm (ε = 3.15 × 10^3 L mol^{-1} cm^{-1}; λ = 540 nm (ε = 4.78 × 10^2 L mol^{-1} cm^{-1}).

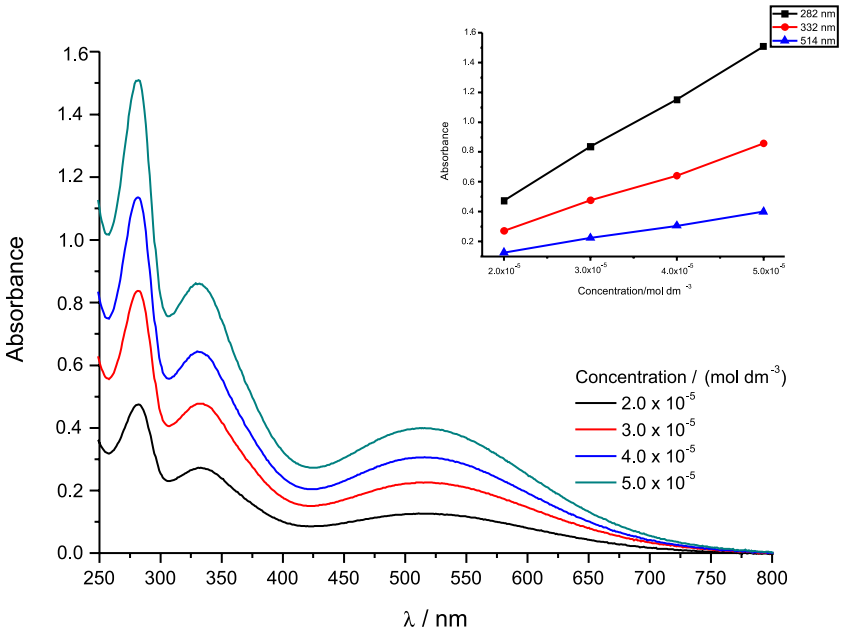

Figure S25. UV-Vis spectra of the compound **4** at different concentrations; solvent: CH_2Cl_2; λ = 282 nm (ε = 3.40 × 10^4 L mol^{-1} cm^{-1}), λ = 332 nm (ε = 1.93 × 10^4 L mol^{-1} cm^{-1}); λ = 514 nm (ε = 9.00 × 10^3 L mol^{-1} cm^{-1}).

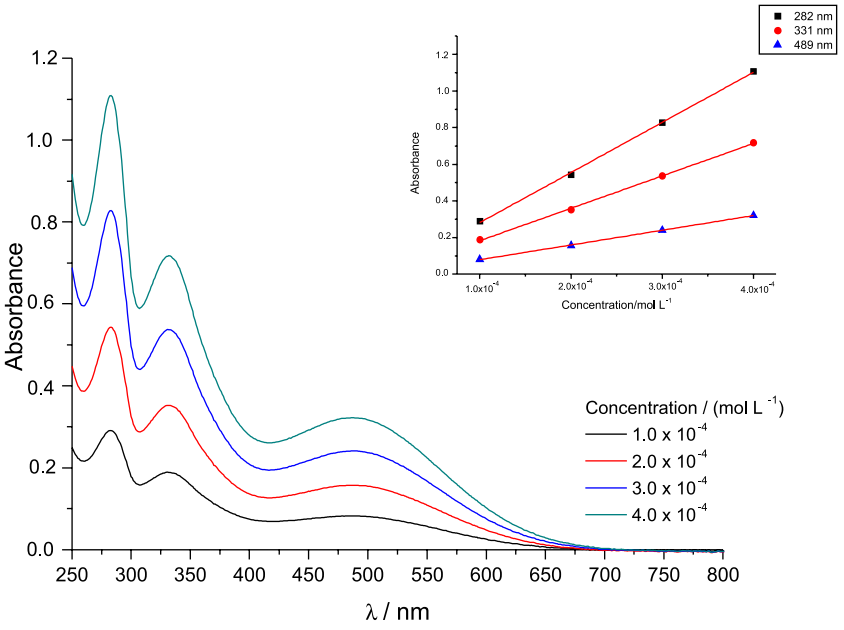

Figure S26. UV-Vis spectra of the compound **5** at different concentrations; solvent: CH_2Cl_2; λ = 282 nm (ε = 2.74 × 10^3 L mol^{-1} cm^{-1}); λ = 331 nm (ε = 1.77 × 10^3 L mol^{-1} cm^{-1}); λ = 489 nm (ε = 8.03 × 10^2 L mol^{-1} cm^{-1}).