Supporting Information

Influence of a series of pyridine ligands on the structure and photophysical properties of Cd(II) complexes

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FTIR-ATR, ^{1}H, $^{13}C\{^{1}H\}$ and DEPT-135 NMR spectroscopies

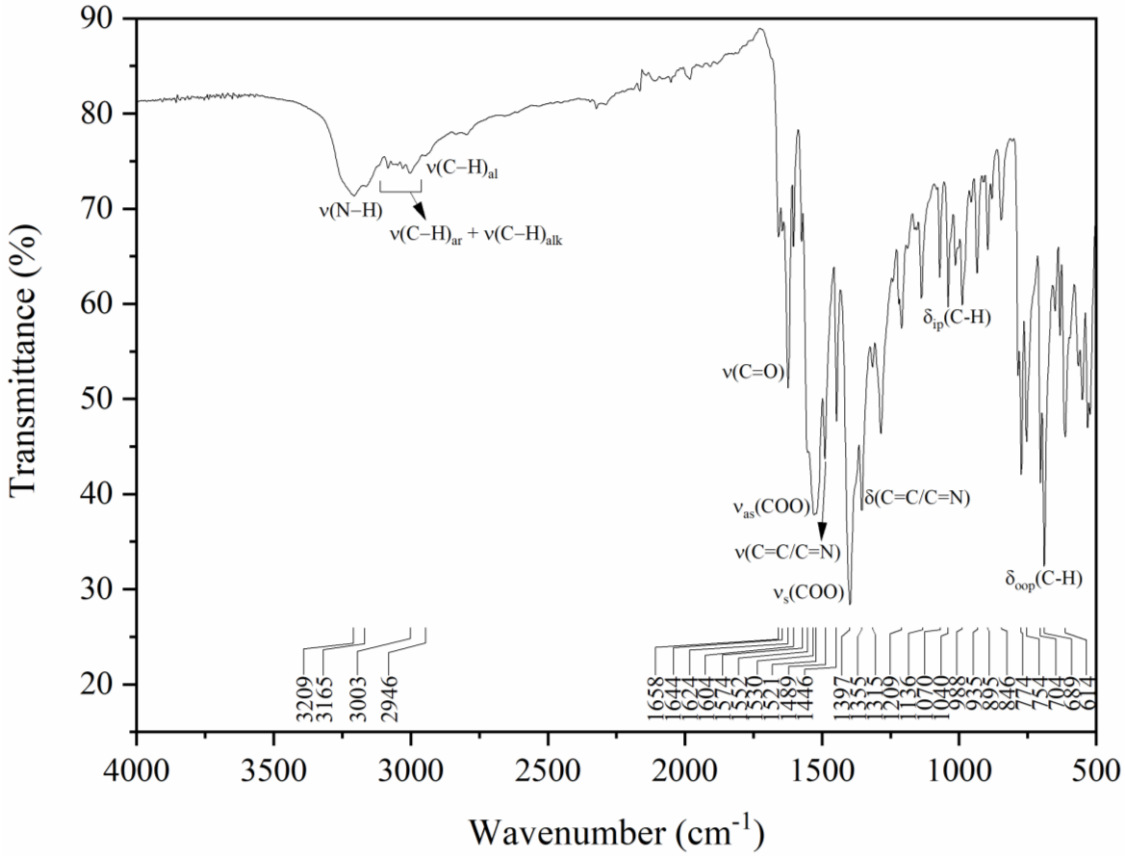

Figure S1. FTIR-ATR spectrum of compound $[Cd(\mu\text{-}O,O'\text{-}ACA)(ACA)(py)]_n$ (**1**).

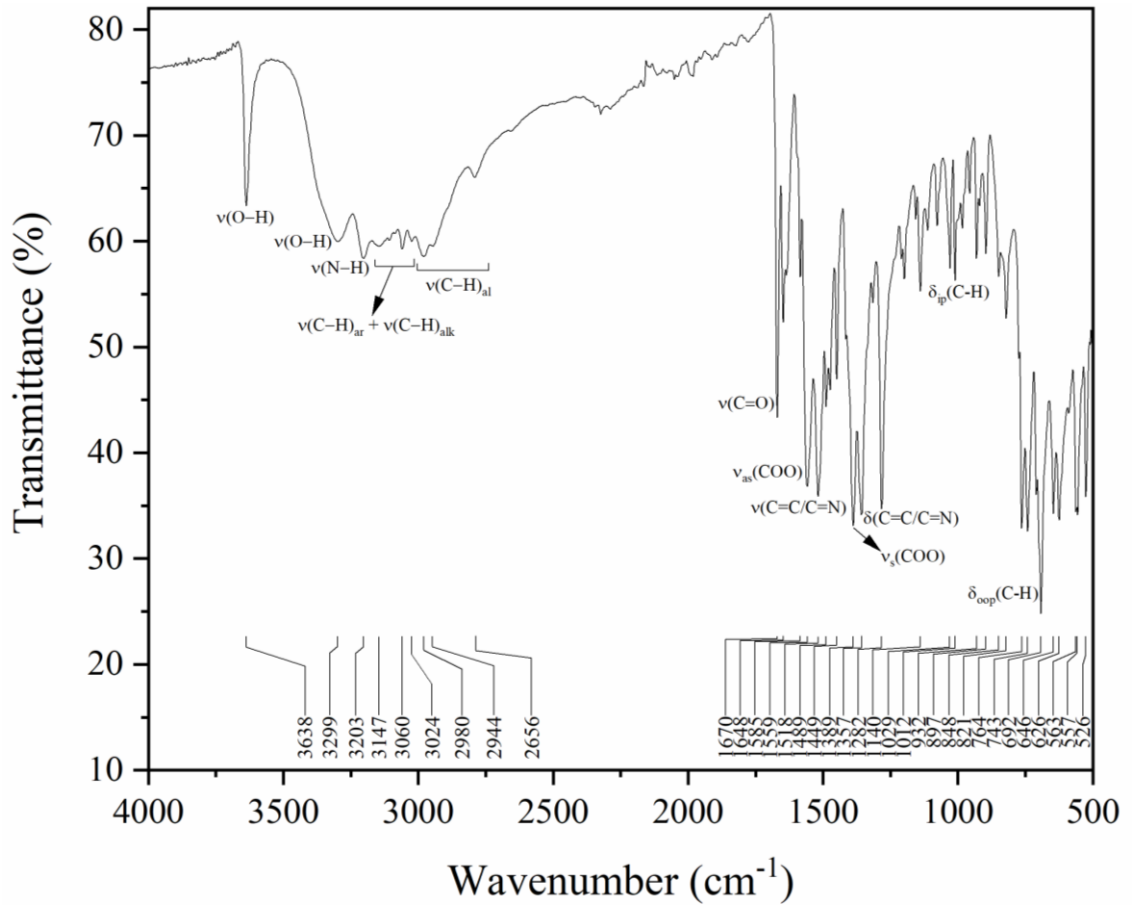

Figure S2. FTIR-ATR spectrum of compound $[Cd(ACA)_2(3\text{-phpy})_2(H_2O)_2]\cdot 2H_2O$ (**2**).

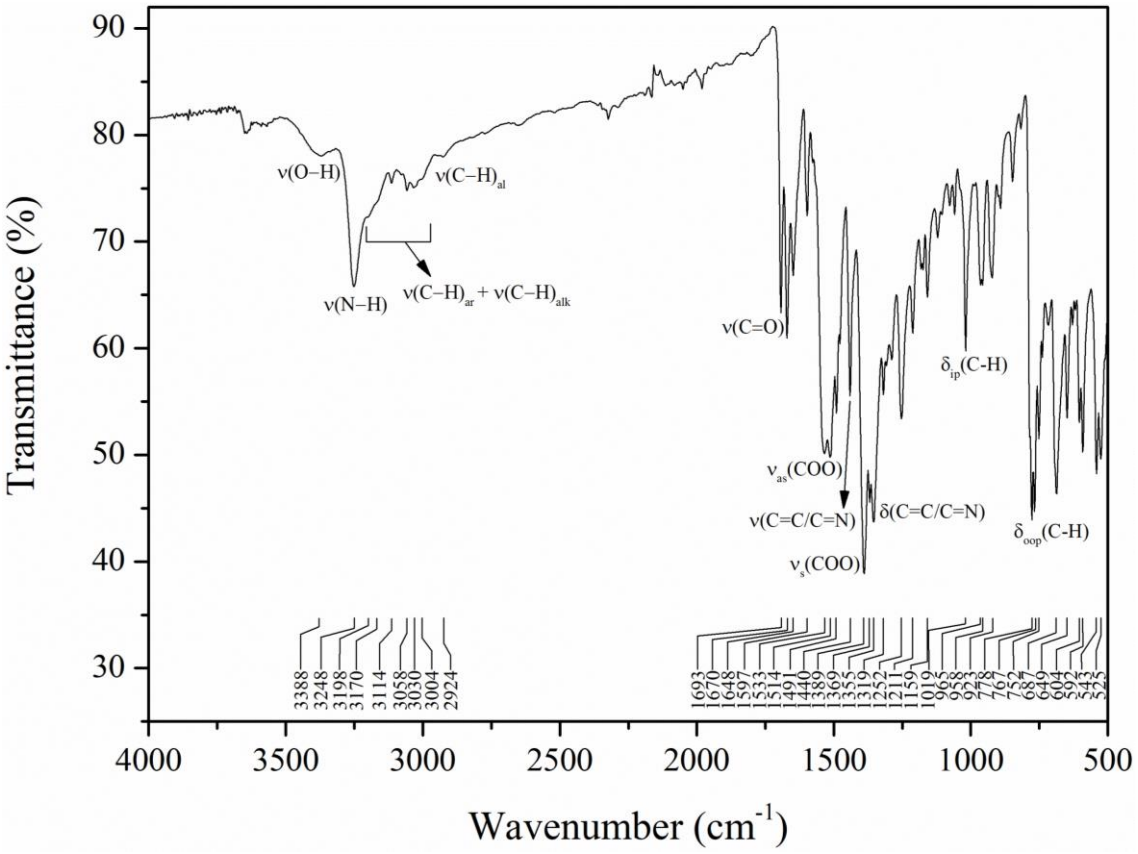

Figure S3. FTIR-ATR spectrum of compound $[Cd(ACA)_2(2,2'\text{-bipy})]_2\cdot 2MeOH$ (**3**).

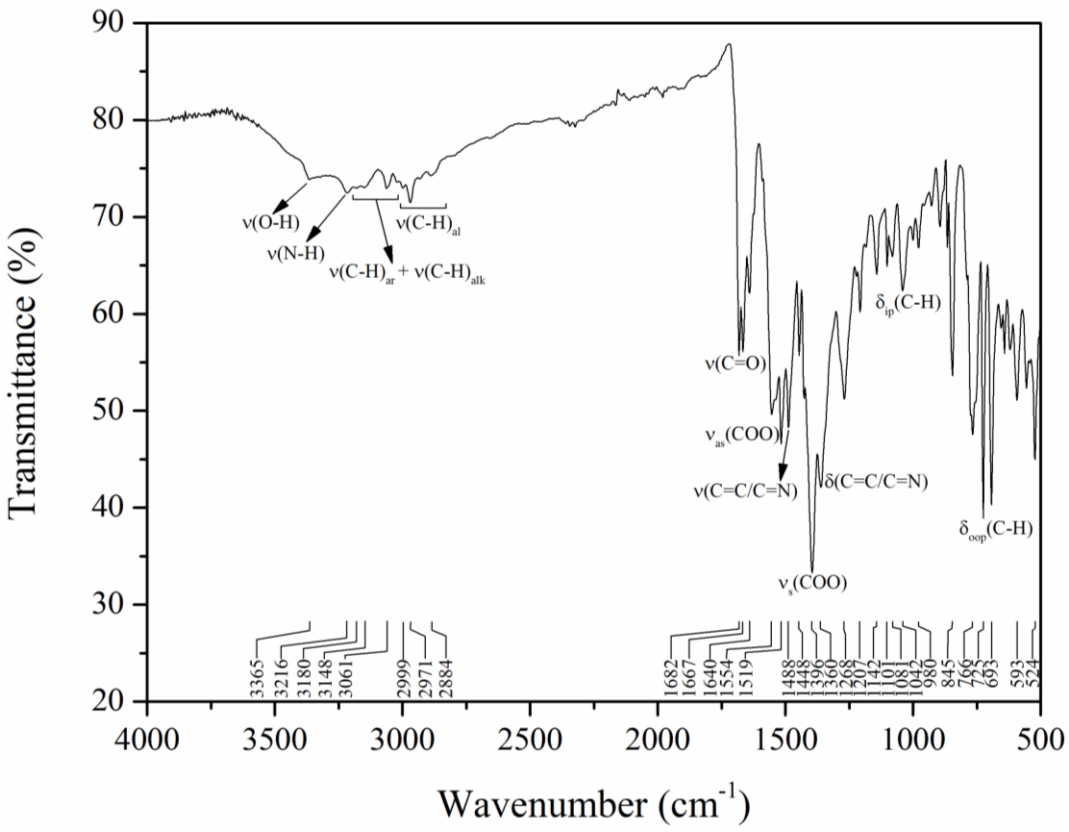

Figure S4. FTIR-ATR spectrum of compound [Cd(ACA)$_2$(1,10-phen)]·3EtOH (**4**).

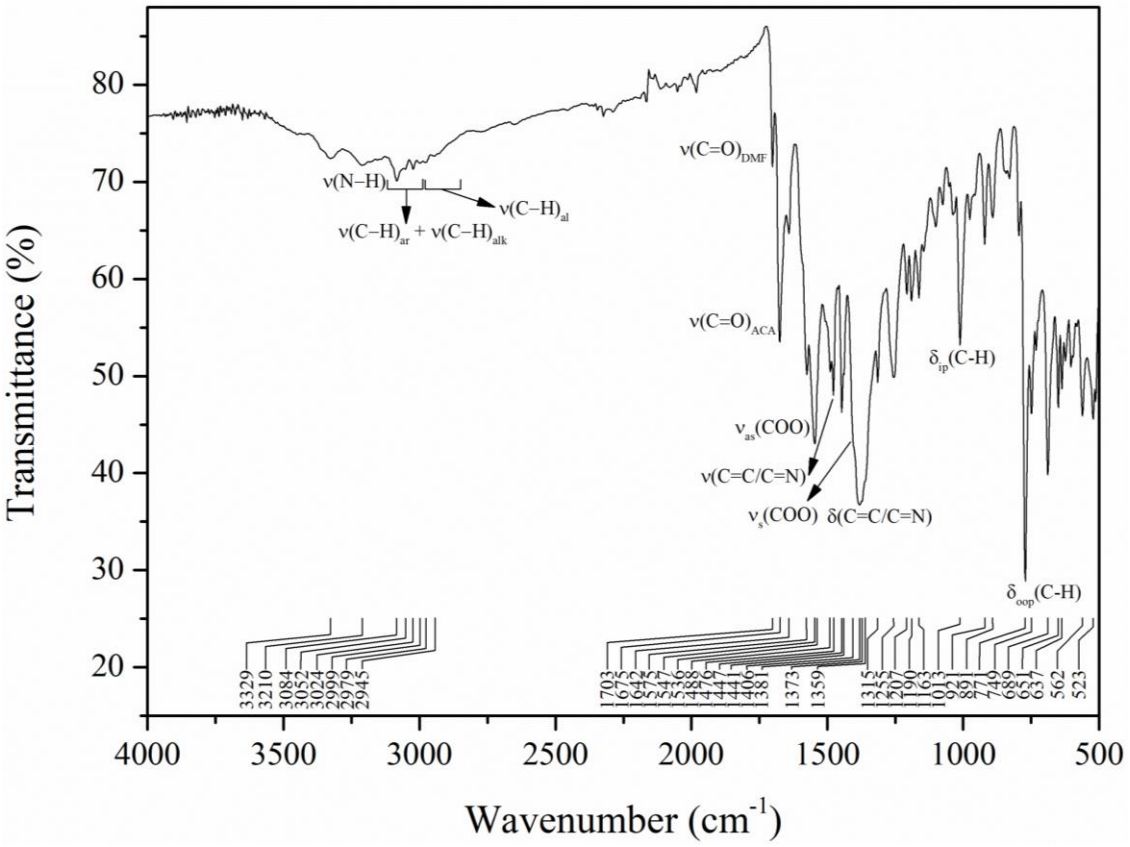

Figure S5. FTIR-ATR spectrum of compound [Cd(ACA)$_2$(terpy)]·2DMF (**5**).

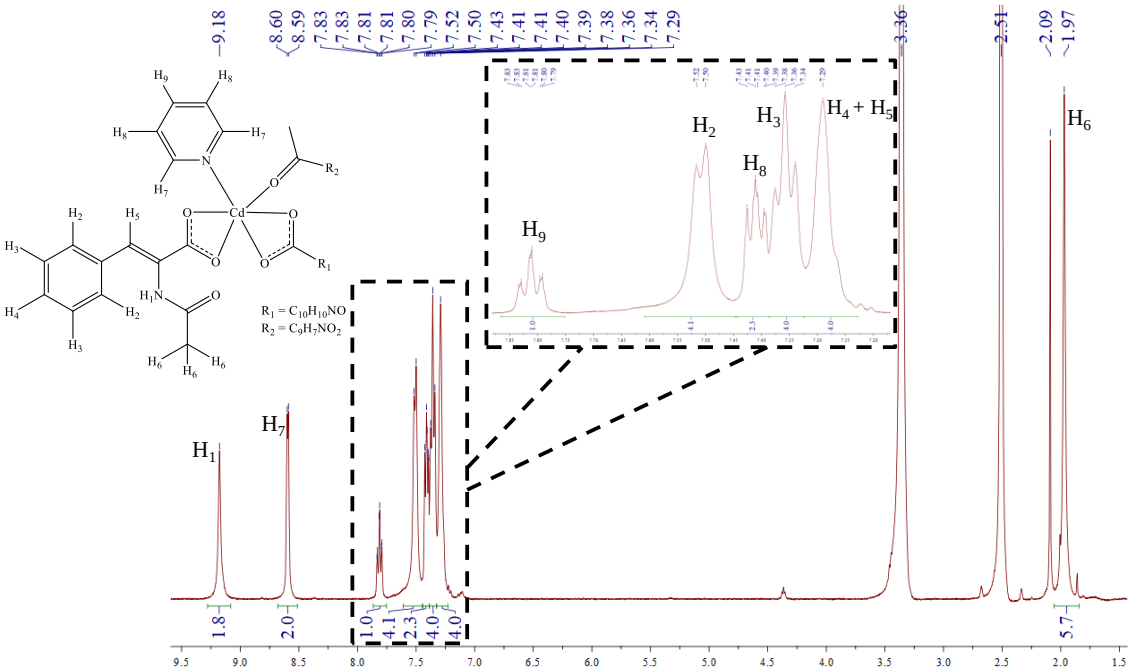

Figure S6. ^{1}H NMR spectrum of compound [Cd(μ-O,O'-ACA)(ACA)(py)]$_n$ (**1**) recorded at 298 K in DMSO-d_6.

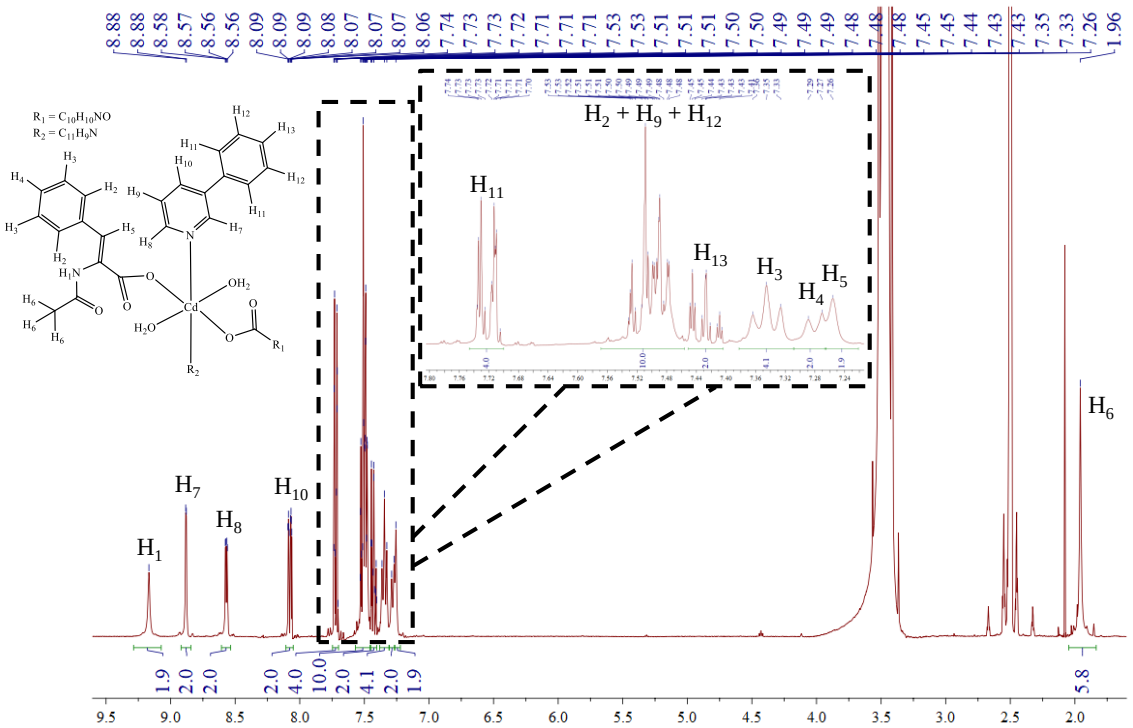

Figure S7. ^{1}H NMR spectrum of compound [Cd(ACA)$_2$(3-phpy)$_2$(H$_2$O)$_2$]·2H$_2$O (**2**) recorded at 298 K in DMSO-d_6.

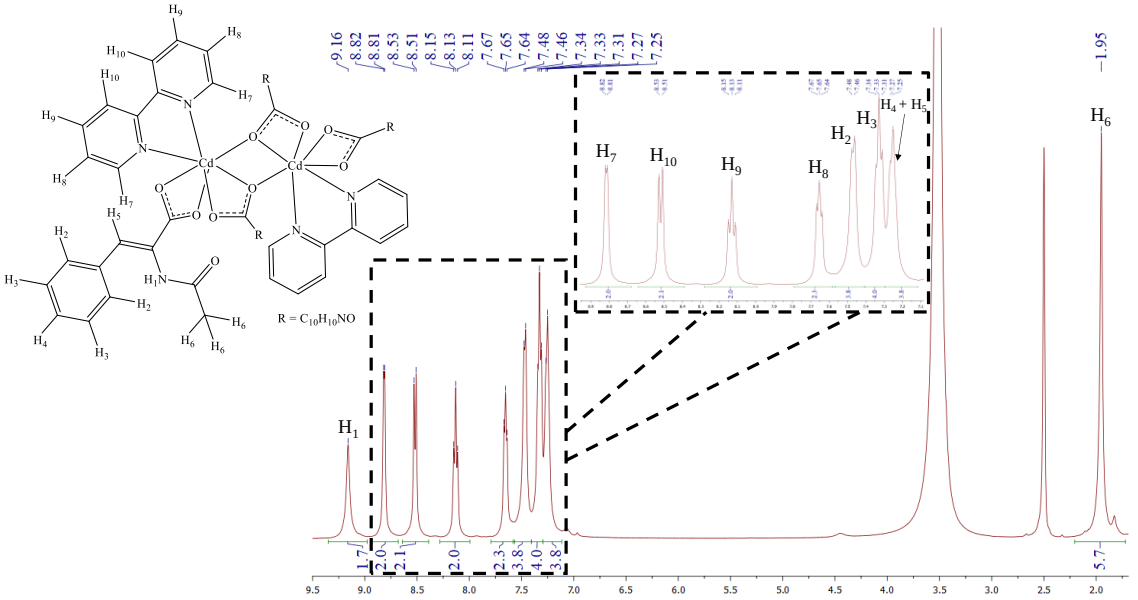

Figure S8. ^{1}H NMR spectrum of compound [Cd(ACA)$_2$(2,2'-bipy)]$_2$·2MeOH (**3**) recorded at 298 K in DMSO-d_6.

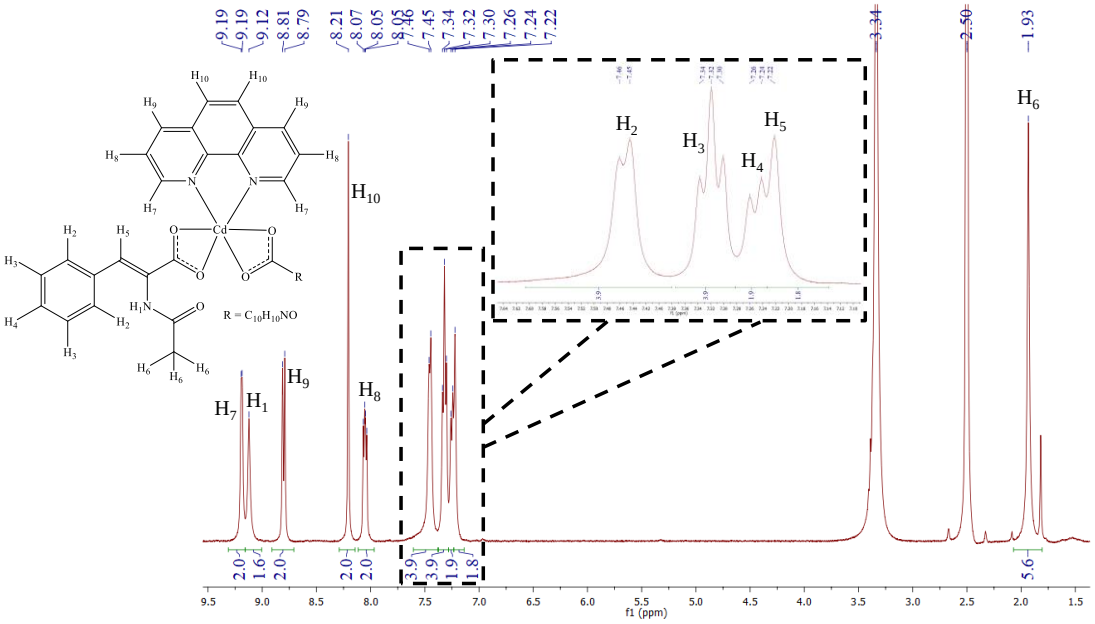

Figure S9. ^{1}H NMR spectrum of compound [Cd(ACA)$_2$(1,10-phen)]·3EtOH (**4**) recorded at 298 K in DMSO-d_6.

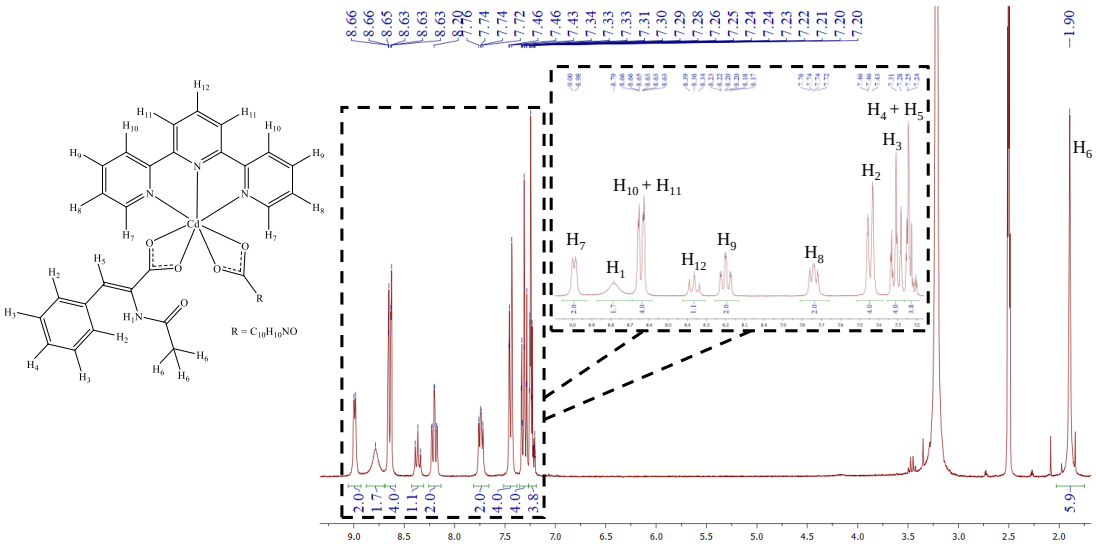

Figure S10. ^{1}H NMR spectrum of compound [Cd(ACA)$_2$(terpy)]·2DMF (**5**) recorded at 340 K in DMSO-d_6.

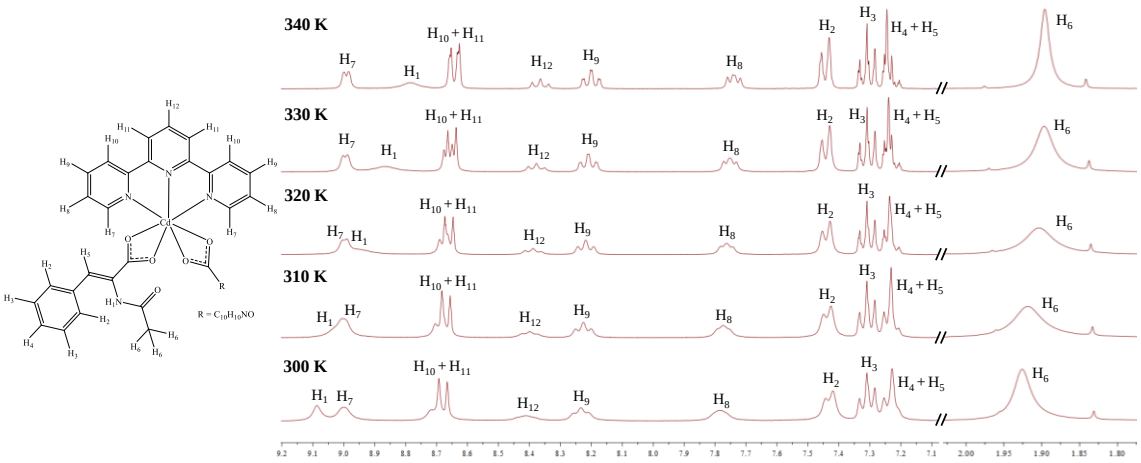

Figure S11. Temperature-Dependent ^{1}H NMR spectrum of compound [Cd(ACA)$_2$(terpy)]·2DMF (**5**) in DMSO-d_6.

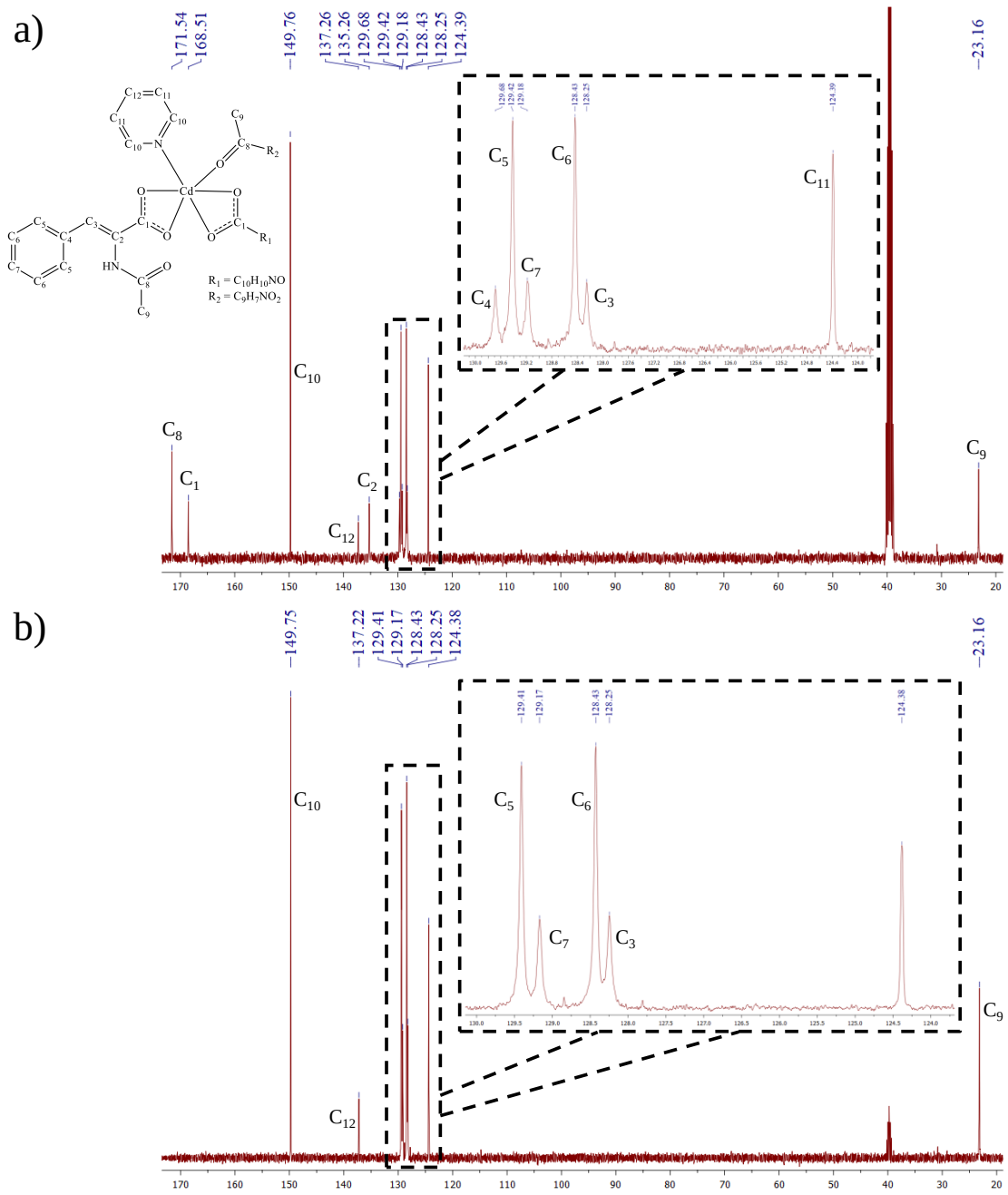

Figure S12. (a) $^{13}C\{^{1}H\}$ and (b) DEPT-135 NMR spectra of compound $[Cd(\mu\text{-}O,O'\text{-}ACA)(ACA)(py)]_n$ (**1**) recorded at 298 K in DMSO-d_6.

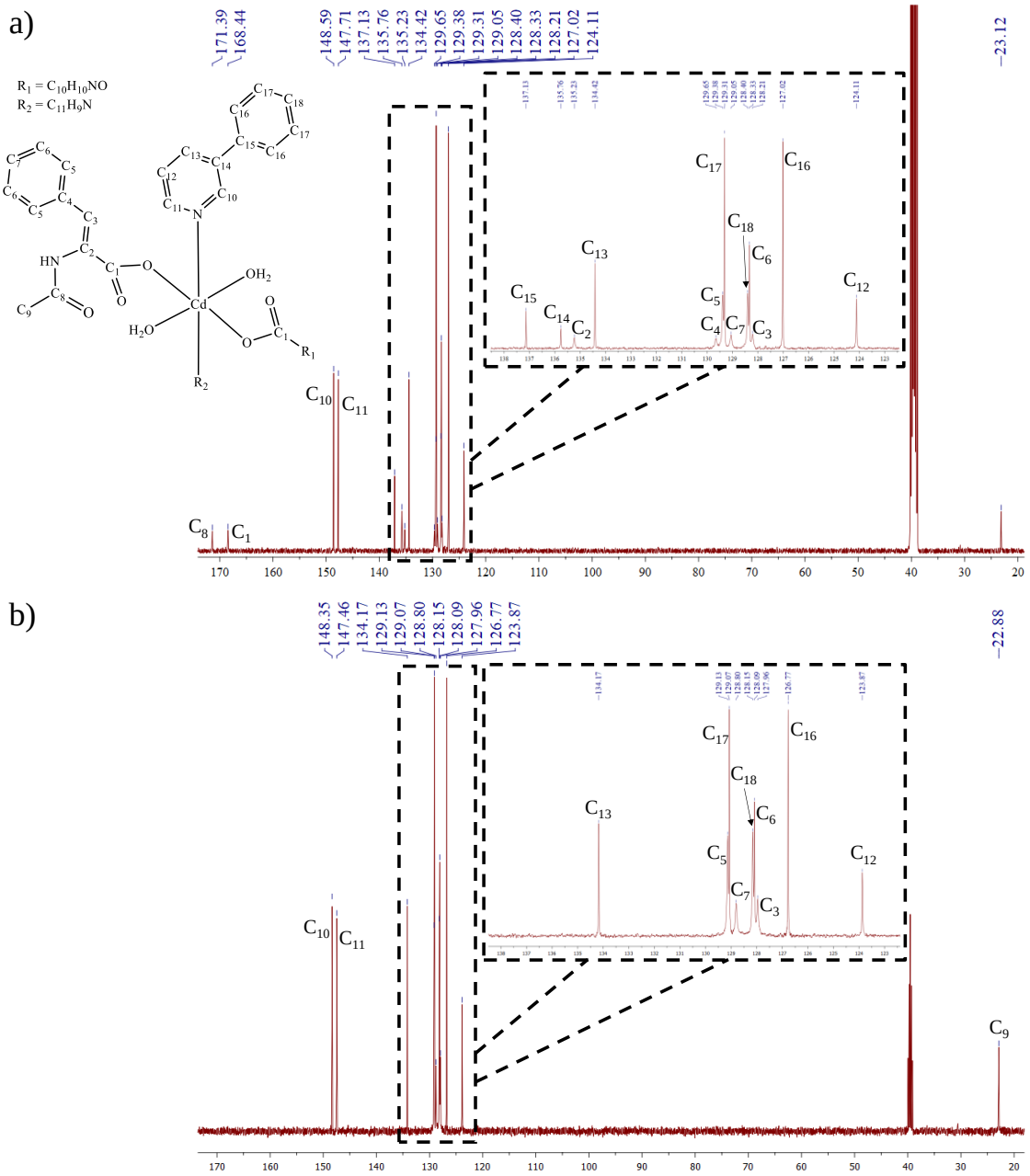

Figure S13. (a) $^{13}C\{^{1}H\}$ and (b) DEPT-135 NMR spectra of compound $[Cd(ACA)_2(3\text{-phpy})_2(H_2O)_2]\cdot 2\ H_2O$ (**2**) recorded at 298 K in DMSO-d_6.

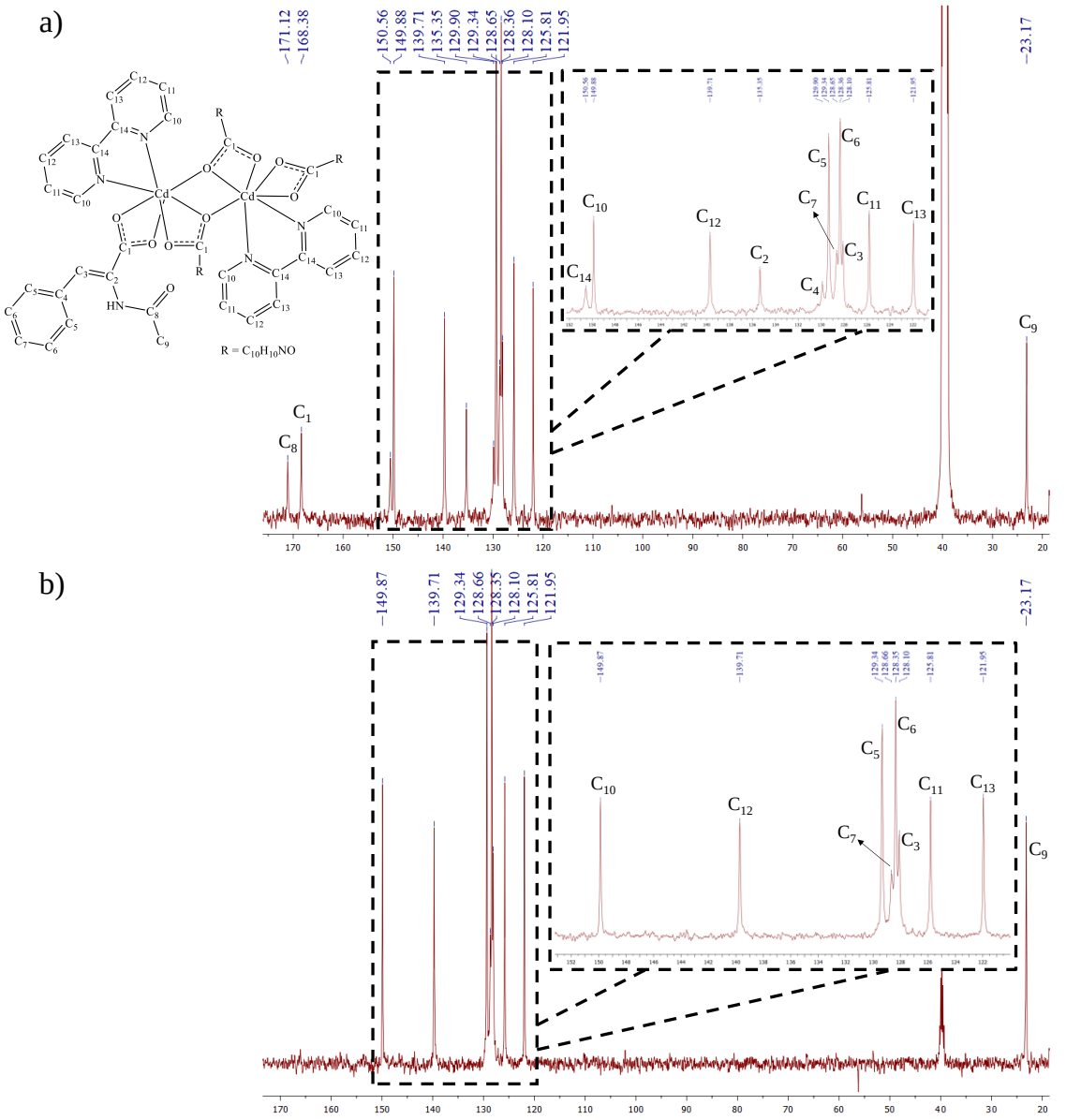

Figure S14. (a) $^{13}C\{^{1}H\}$ and (b) DEPT-135 NMR spectra of compound $[Cd(ACA)_2(2,2'\text{-bipy})]_2 \cdot 2MeOH$ (**3**) recorded at 298 K in DMSO-d_6.

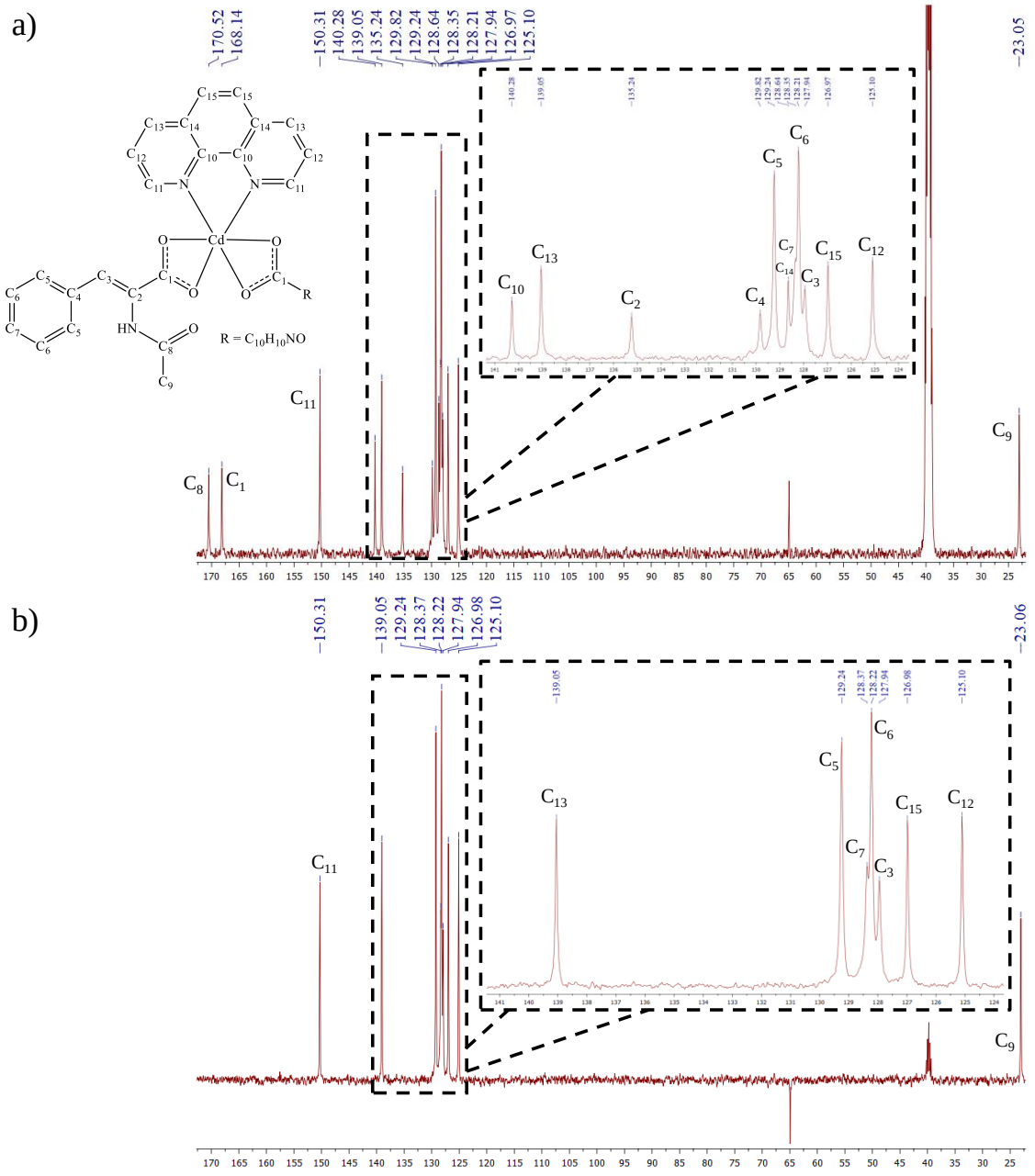

Figure S15. (a) $^{13}C\{^{1}H\}$ and (b) DEPT-135 NMR spectra of compound $[Cd(ACA)_2(1,10\text{-phen})]\cdot 3EtOH$ (**4**) recorded at 298 K in DMSO-d_6.

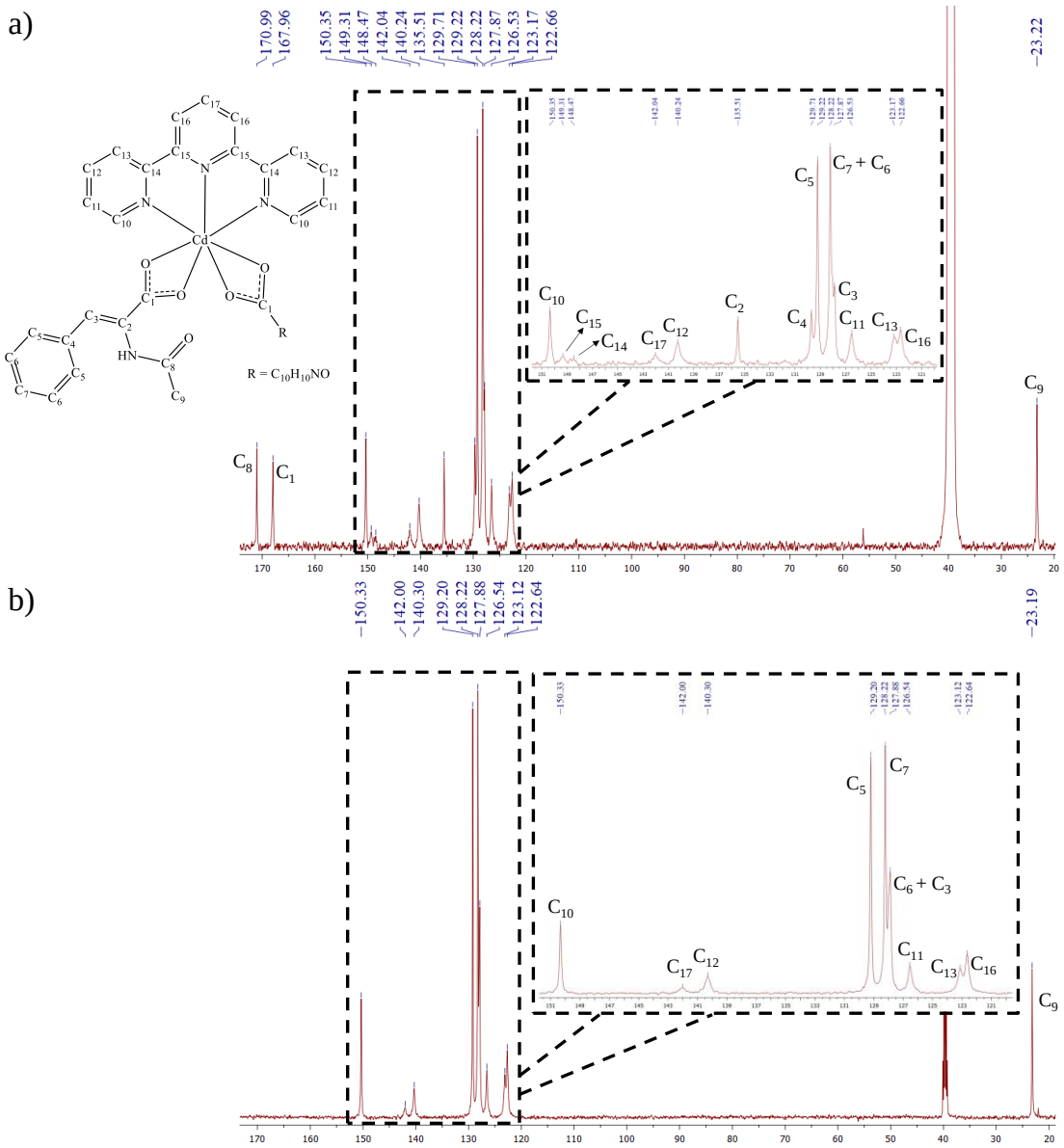

Figure S16. (a) $^{13}C\{^{1}H\}$ and (b) DEPT-135 NMR spectra of compound $[Cd(ACA)_2(terpy)]\cdot 2DMF$ (**5**) recorded at 298 K in DMSO-d_6.

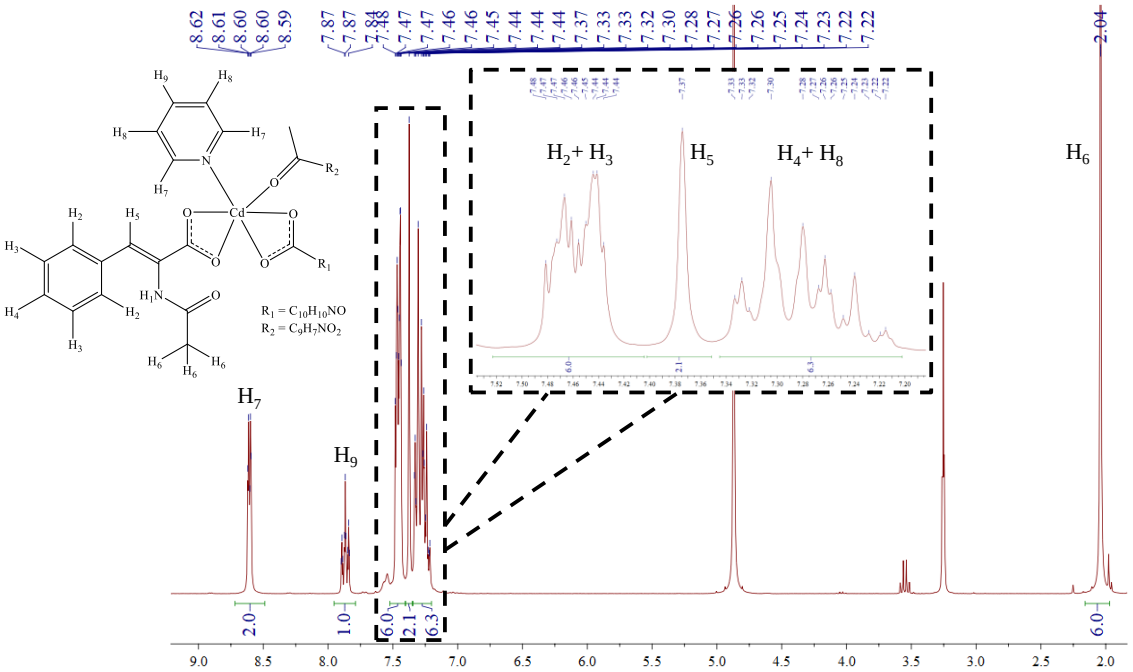

Figure S17. ^{1}H NMR spectrum of compound [Cd(μ-O,O'-ACA)(ACA)(py)]$_n$ (**1**) recorded at 298 K in MeOH-d_4.

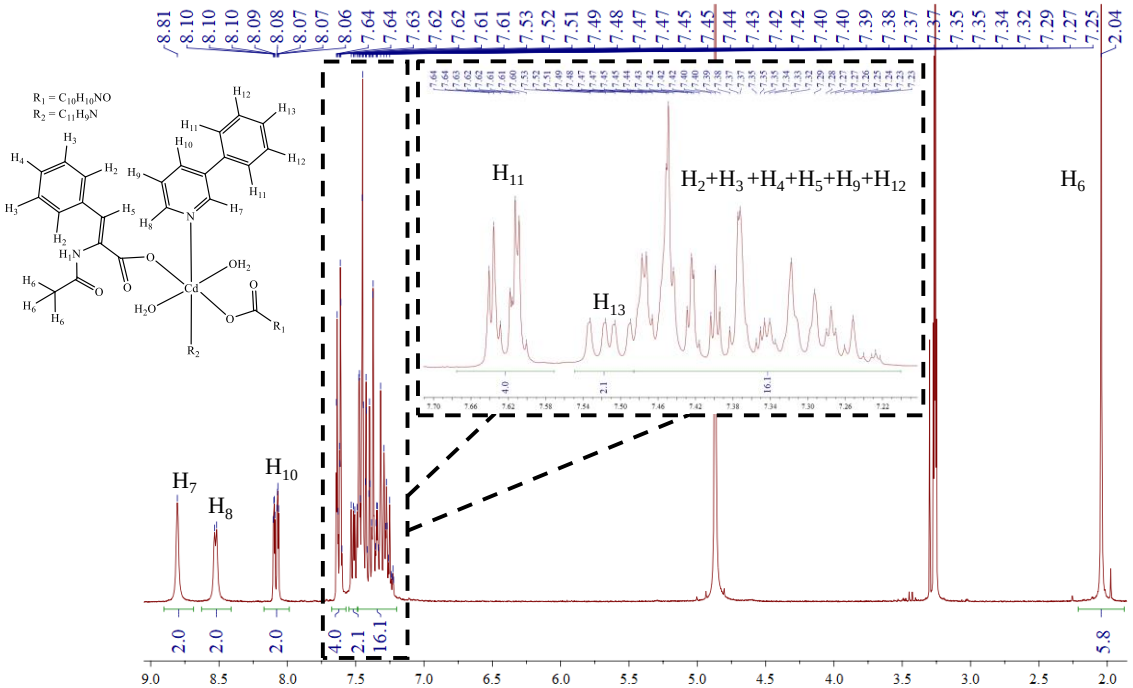

Figure S18. ^{1}H NMR spectrum of compound [Cd(ACA)$_2$(3-phpy)$_2$(H$_2$O)$_2$]$_2$·2H$_2$O (**2**) recorded at 298 K in MeOH-d_4.

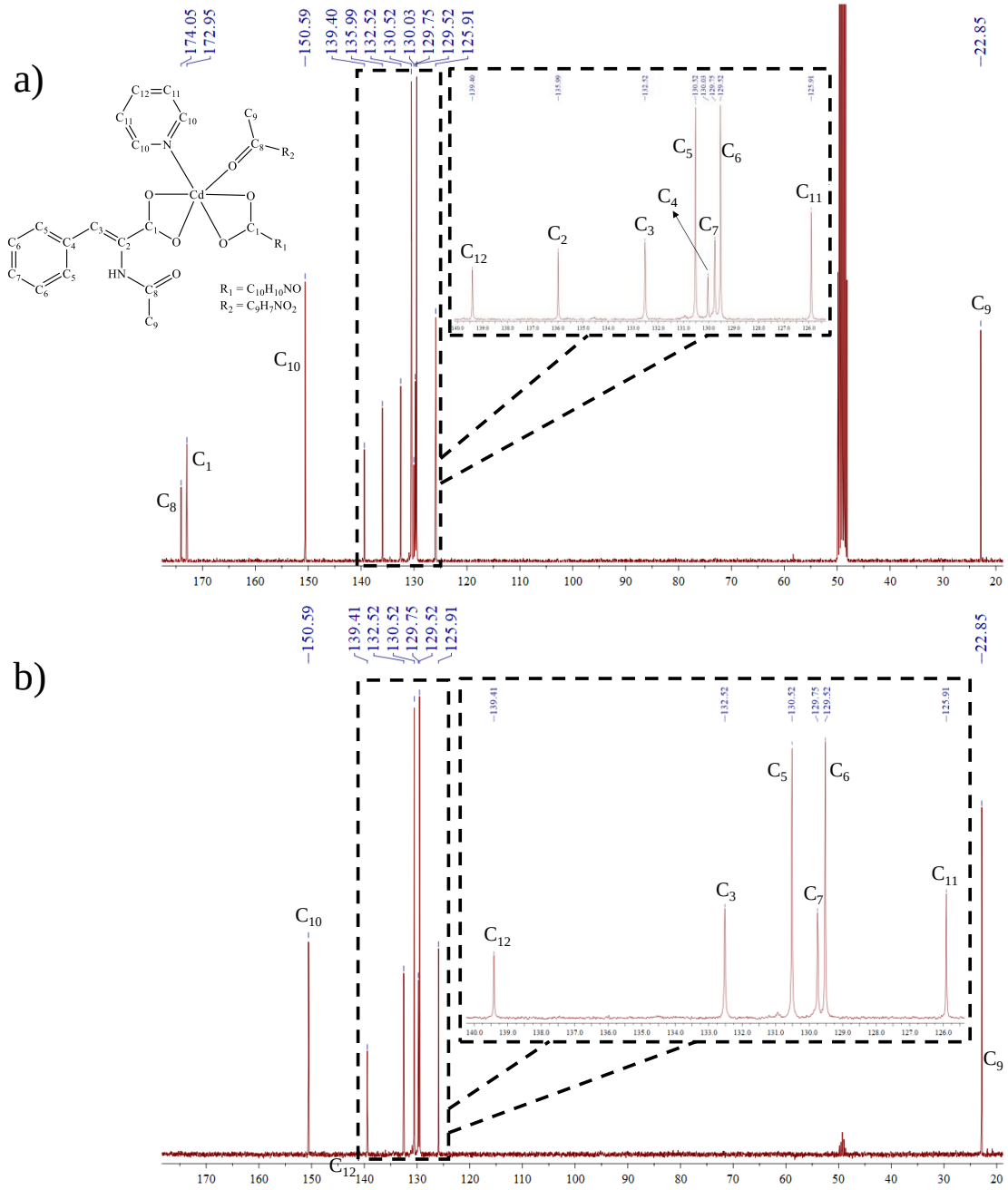

Figure S19. (a) $^{13}C\{^{1}H\}$ and (b) DEPT-135 NMR spectra of compound $[Cd(\mu\text{-}O,O'\text{-}ACA)(ACA)(py)]_n$ (**1**) recorded at 298 K in MeOH-d_4.

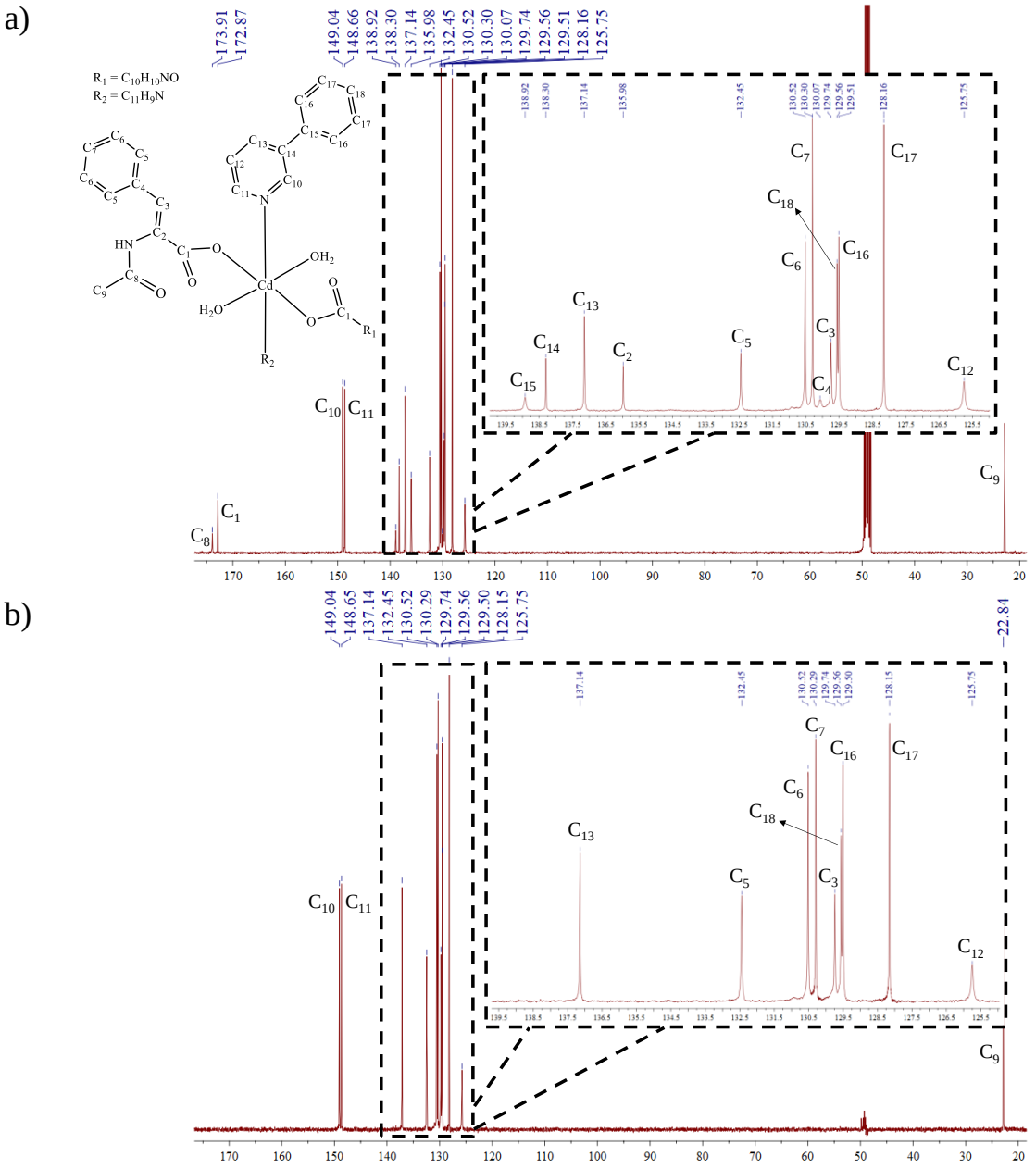

Figure S20. (a) $^{13}C\{^{1}H\}$ and (b) DEPT-135 NMR spectra of compound $[Cd(ACA)_2(3\text{-phpy})_2(H_2O)_2]\cdot 2H_2O$ (**2**) recorded at 298 K in MeOH-*d*4.

Crystal structure analysis

Table S1. Selected bond lengths (Å), bond angles (°), intra- and intermolecular interactions (Å) for **1**.

Bond lengths (Å)					
Cd(1)-O(1)		2.2502(14)	Cd(1)-O(5)#1	2.3239(14)	
Cd(1)-O(2)		2.4639(13)	Cd(1)-O(6)	2.2788(12)	
Cd(1)-O(4)#1		2.3457(13)	Cd(1)-N(3)	2.2669(16)	
Bond angles (°)					
O(1)-Cd(1)-O(2)		55.98(4)	O(6)-Cd(1)-O(2)	146.23(5)	
O(1)-Cd(1)-O(4)#1		90.91(5)	O(6)-Cd(1)-O(4)#1	98.81(4)	
O(1)-Cd(1)-O(5)#1		136.39(5)	O(6)-Cd(1)-O(5)#1	118.53(5)	
O(1)-Cd(1)-O(6)		92.48(5)	N(3)-Cd(1)-O(2)	96.43(5)	
O(1)-Cd(1)-N(3)		120.09(5)	N(3)-Cd(1)-O(4)#1	147.71(5)	
O(4)#1-Cd(1)-O(2)		93.88(5)	N(3)-Cd(1)-O(5)#1	91.96(5)	
O(5)#1-Cd(1)-O(2)		94.58(5)	N(3)-Cd(1)-O(6)	89.33(5)	
O(5)#1-Cd(1)-O(4)#1		56.69(5)			
Intramolecular interactions (Å)					
D-H···A	D-H (Å)	H···A (Å)	D···A (Å)	>D-H···A (°)	
N(2)-H(2N)···O(3)	0.88	2.05	2.917(2)	169	
C(16)-H(16)···O(3)	0.95	2.46	3.341(2)	154	
C(22)-H(22B)···O(3)	0.98	2.52	3.389(3)	148	
C(27)-H(27)···O(4)	0.95	2.44	3.238(2)	142	
Cg(I)···Cg(J)	d_{Cg-Cg}[a] (Å)	α[b] (°)	β, γ[c] (°)	$d_{plane-plane}$[d] (Å)	d_{offset}[e] (Å)
Cg(1)···Cg(2)	3.6304(12)	11.26(10)	20.6, 30.4	3.1297(8), 3.3987(8)	1.27 1.84
Intermolecular interactions (Å)					
D-H···A	D-H (Å)	H···A (Å)	D···A (Å)	>D-H···A (°)	
N(1)-H(1N)···O(2)	0.84(3)	2.10(3)	2.936(2)	174(3)	
C(18)-H(18)···Cg(3)	0.95	2.58	3.445(2)	151	

[a]Centroid-centroid distance. [b]Dihedral angle between the ring planes. [c]Offset angles: angle between Cg(I)-Cg(J) vector and normal to plane I, angle between Cg(I)-Cg(J) vector and normal to plane J (β = γ, when α = 0). [d]Perpendicular distance of Cg(I) on plane J and perpendicular distance of Cg(J) on plane I (equal when α = 0). [e]Horizontal displacement or slippage between Cg(I) and Cg(J) (equal for both centroids when α = 0). #1:-x+1/2,y-1/2,-z+1/2; Cg(1) = C(15) C(16) C(17) C(18) C(19) C(20); Cg(2) = N(3) C(23) C(24) C(25) C(26) C(27); Cg(3) = C(4) C(5) C(6) C(7) C(8) C(9)

Table S2. Selected bond lengths (Å), bond and torsion angles (°), intra- and intermolecular interactions (Å) for **2**.

Bond lengths (Å)				
Cd(1)-O(1)		2.2804(9)	Cd(1)-N(2)	2.3311(10)
Cd(1)-O(4)		2.3134(9)		
Bond angles (°)				
O(1)-Cd(1)-O(1)#1		180	O(4)-Cd(1)-O(4)#1	180
O(1)-Cd(1)-O(4)		91.26(3)	O(4)-Cd(1)-N(2)	88.86(4)
O(1)-Cd(1)-O(4)#1		88.74(3)	O(4)-Cd(1)-N(2)#1	91.14(4)
O(1)-Cd(1)-N(2)		87.54(3)	N(2)-Cd(1)-N(2)#1	180
O(1)-Cd(1)-N(2)#1		92.46(4)		
Torsion angle 3-phpy (º)			41.02	
Intramolecular interactions (Å)				
D-H···A	D-H (Å)	H···A (Å)	D···A (Å)	>D-H···A (°)
O(4)-H(4OB)···O(2)	0.87(2)	1.81(2)	2.661(1)	165(2)
Intermolecular interactions (Å)				
D-H···A	D-H (Å)	H···A (Å)	D···A (Å)	>D-H···A (º)
O(4)-H(4OA)···O(1W)	0.81(2)	1.90(2)	2.713(2)	174(2)
O(1W)-H(1WB)···O(3)	0.76(2)	1.95(2)	2.710(2)	170(2)
C(15)-H(15)···O(1)	0.95	2.52	3.453(2)	167
N(1)-H(1)···O(2)	0.88	2.02	2.855(1)	158
C(8)-H(8)···O(4)	0.95	2.44	3.382(2)	172
C(21)-H(21)···Cg(1)	0.95	2.97	3.7146(16)	136

#1: -x+1, -y+1, -z+1. Cg(1) = N(2) C(12) C(13) C(14) C(15) C(16)

Table S3. Selected bond lengths (Å); bond and torsion angles (°); intra- and intermolecular interactions (Å) for **3**.

Bond lengths (Å)				
Cd(1)-O(1)		2.4423(14)	Cd(1)-O(5)	2.3720(14)
Cd(1)-O(2)		2.3512(13)	Cd(1)-N(3)	2.3162(16)
Cd(1)-O(2)#1		2.4355(13)	Cd(1)-N(4)	2.3370(16)
Cd(1)-O(4)		2.3550(13)		
Bond angles (°)				
O(1)-Cd(1)-O(2)		54.58(4)	O(2)#1-Cd(1)-O(4)	101.77(5)
O(1)-Cd(1)-O(2)#1		125.75(4)	O(2)#1-Cd(1)-O(5)	80.96(5)
O(1)-Cd(1)-O(4)		84.00(5)	O(2)#1-Cd(1)-N(3)	83.24(5)
O(1)-Cd(1)-O(5)		137.18(5)	O(2)#1-Cd(1)-N(4)	142.45(5)
O(1)-Cd(1)-N(3)		102.49(5)	O(4)-Cd(1)-O(5)	55.84(5)
O(1)-Cd(1)-N(4)		87.25(5)	O(4)-Cd(1)-N(3)	167.51(5)
O(2)-Cd(1)-O(2)#1		71.17(5)	O(4)-Cd(1)-N(4)	98.81(5)
O(2)-Cd(1)-O(4)		94.04(5)	O(5)-Cd(1)-N(3)	114.55(5)
O(2)-Cd(1)-O(5)		133.63(5)	O(5)-Cd(1)-N(4)	85.18(5)
O(2)-Cd(1)-N(3)		98.42(5)	N(3)-Cd(1)-N(4)	71.16(6)
O(2)-Cd(1)-N(4)		138.10(5)		
Torsion angle 2,2'-bipy (º)			16.95	
Intramolecular interactions (Å)				
D-H···A	D-H (Å)	H···A (Å)	D···A (Å)	>D-H···A (°)
N(1)-H(1N)···O(5)	0.88	2.10	2.859(2)	144
C(23)-H(23)···O(4)	0.95	2.41	3.311(2)	158
Intermolecular interactions (Å)				
D-H···A	D-H (Å)	H···A (Å)	D···A (Å)	>D-H···A (°)
N(2)-H(2N)···O(1)	0.88	2.04	2.890(2)	161
C(31)-H(31)···O(3)	0.95	2.55	3.349(3)	142
O(1W)-H(1WO)···O(6)	0.84	1.94	2.696(10)	149
C(25)-H(25)···O(1W)	0.95	2.40	3.302(9)	159
C(29)-H(29)···Cg(1)	0.95	2.84	3.612(2)	139

#1: -x, -y+1, -z+1. Cg(1) = C(4) C(5) C(6) C(7) C(8) C(9)

Table S4. Selected bond lengths (Å), bond and torsion angles (°), and intermolecular interactions (Å) for **4**.

Bond lengths (Å)					
Cd(1)-O(1)	2.3637(14)	Cd(1)-O(5)	2.3515(14)		
Cd(1)-O(2)	2.3123(15)	Cd(1)-N(3)	2.2979(16)		
Cd(1)-O(4)	2.3412(13)	Cd(1)-N(4)	2.2939(17)		
Bond angles (°)					
O(1)-Cd(1)-O(2)	56.32(5)	O(2)-Cd(1)-N(4)	154.07(6)		
O(1)-Cd(1)-O(4)	95.45(5)	O(4)-Cd(1)-O(5)	56.26(5)		
O(1)-Cd(1)-O(5)	130.74(5)	N(3)-Cd(1)-O(4)	148.34(5)		
O(1)-Cd(1)-N(3)	113.37(5)	N(3)-Cd(1)-O(5)	107.81(5)		
O(1)-Cd(1)-N(4)	105.33(5)	N(3)-Cd(1)-N(4)	73.19(6)		
O(2)-Cd(1)-O(4)	111.03(5)	N(4)-Cd(1)-O(4)	87.22(5)		
O(2)-Cd(1)-O(5)	94.09(5)	N(4)-Cd(1)-O(5)	111.62(5)		
O(2)-Cd(1)-N(3)	96.31(6)				
Torsion angles 1,10-phen (º)					
Cg(1)-Cg(2)	2.27	Cg(2)-Cg(3)	1.96		
Intermolecular interactions (Å)					
D-H···A	D-H (Å)	H···A (Å)	D···A (Å)	>D-H···A (º)	
N(2)-H(2N)···O(4)	0.88	1.94	2.789(2)	163	
O(1W)-H(1W)···O(2)	0.78(3)	1.99(3)	2.749(2)	164(3)	
C(18)-H(18)···O(6)	0.95	2.40	3.327(2)	165	
C(23)-H(23)···O(1W)	0.95	2.53	3.455(3)	163	
C(2W)-H(2WC)···O(3)	0.98	2.54	3.491(3)	165	
O(2W)-H(2OW)···O(3W)	0.84	1.95	2.788(3)	175	
N(1)-H(1N)···O(1W)	0.88	2.02	2.893(2)	170	
O(3W)-H(3OW)···O(6)	0.84	1.92	2.722(2)	159	
C(28)-H(28)···O(3)	0.95	2.32	3.037(3)	132	
Cg(I)···Cg(J)	d_{Cg-Cg}[a] (Å)	α[b] (º)	β, γ[c] (º)	$d_{plane-plane}$[d] (Å)	d_{offset}[e] (Å)
Cg(2)···Cg(2)	3.5193(12)	0	18.5	3.3367(8)	1.119
Cg(4)···Cg(2)	3.5862(11)	3.90(9)	21.7, 20.1	3.3676(8), 3.3311(8)	1.330, 1.232

[a]Centroid-centroid distance. [b]Dihedral angle between the ring planes. [c]Offset angles: angle between Cg(I)-Cg(J) vector and normal to plane I, angle between Cg(I)-Cg(J) vector and normal to plane J (β = γ, when α = 0). [d]Perpendicular distance of Cg(I) on plane J and perpendicular distance of Cg(J) on plane I (equal when α = 0). [e]Horizontal displacement or slippage between Cg(I) and Cg(J) (equal for both centroids when α = 0). Cg(1) = N(3) C(23) C(24) C(25) C(26) C(34); Cg(2) = C(26) C(27) C(28) C(29) C(33) C(34); Cg(3) = N(4) C(29) C(30) C(31) C(32) C(33); Cg(4) = C(15) C(16) C(17) C(18) C(19) C(20).

Table S5. Selected bond lengths (Å), bond and torsion angles (º), and intermolecular interactions (Å) for **5**.

Bond lengths (Å)			
Cd(1)-O(1)	2.522(2)	Cd(1)-N(3)	2.333(2)
Cd(1)-O(2)	2.322(2)	Cd(1)-N(4)	2.338(2)
Cd(1)-O(4)	2.237(2)	Cd(1)-N(5)	2.382(2)
Cd(1)-O(5)	2.670(2)		
Bond angles (º)			
O(1)-Cd(1)-O(2)	54.16(7)	O(4)-Cd(1)-O(5)	52.74(7)
O(1)-Cd(1)-O(4)	80.94(6)	O(4)-Cd(1)-N(3)	121.03(7)
O(1)-Cd(1)-O(5)	114.29(6)	O(4)-Cd(1)-N(4)	147.57(7)
O(1)-Cd(1)-N(3)	86.20(7)	O(4)-Cd(1)-N(5)	89.81(7)
O(1)-Cd(1)-N(4)	131.49(6)	O(5)-Cd(1)-N(3)	82.84(7))
O(1)-Cd(1)-N(5)	131.75(6)	O(5)-Cd(1)-N(4)	103.77(7)
O(2)-Cd(1)-O(4)	107.42(7)	O(5)-Cd(1)-N(5)	95.78(7)
O(2)-Cd(1)-O(5)	160.07(7)	N(3)-Cd(1)-N(4)	69.39(7)
O(2)-Cd(1)-N(3)	110.28(7)	N(3)-Cd(1)-N(5)	136.49(7)
O(2)-Cd(1)-N(4)	95.07(7)	N(4)-Cd(1)-N(5)	68.80(7)
O(2)-Cd(1)-N(5)	84.93(7)		
Torsion angles terpy (º)			
Cg(1)-Cg(2)	5.81	Cg(1)-Cg(3)	13.99

Intermolecular interactions (Å)				
D-H···A	D-H (Å)	H···A (Å)	D···A (Å)	>D-H···A (º)
N(1)-H(1N)···O(1)	0.88	2.07	2.906(3)	158
C(11)-H(11B)···O(4)	0.98	2.35	3.327(3)	177
C(34)-H(34)···O(5)	0.95	2.42	3.243(3)	144
C(26)-H(26)···O(3)	0.95	2.52	3.358(3)	147
C(16)-H(16)···O(8)	0.95	2.47	3.392(6)	165
C(24)-H(24)···O(8)	0.95	2.35	3.146(5)	142
N(2)-H(2)···O(7)	0.88	1.97	2.835(3)	166
C(22)-H(22C)···O(7)	0.98	2.52	3.382(4)	147
C(19)-H(19)···O(7)	0.95	2.56	3.424(7)	151

Cg(I)···Cg(J)	d_{Cg-Cg}[a] (Å)	α[b] (º)	β, γ[c] (º)	$d_{plane-plane}$[d] (Å)	d_{offset}[e] (Å)
Cg(1)···Cg(2)	3.5649(14)	5.81(12)	18.0, 23.0	3.2806(10), 3.3895(10)	1.101, 1.393
Cg(3)···Cg(1)	3.8055(15)	13.99(13)	20.9, 34.5	3.1367(12), 3.5544(10)	1.358, 2.155

[a]Centroid-centroid distance. [b]Dihedral angle between the ring planes. [c]Offset angles: angle between Cg(I)-Cg(J) vector and normal to plane I, angle between Cg(I)-Cg(J) vector and normal to plane J (β = γ, when α = 0). [d]Perpendicular distance of Cg(I) on plane J and perpendicular distance of Cg(J) on plane I (equal when α = 0). [e]Horizontal displacement or slippage between Cg(I) and Cg(J) (equal for both centroids when α = 0). Cg(1) = N(4) C(28) C(29) C(30) C(31) C(32); Cg(2) = N(5) C(33) C(34) C(35) C(36) C(37); Cg(3) = N(3) C(23) C(24) C(25) C(26) C(27).

Structural Comparison

Table S6. Structural parameters regarding the steric effects of the ligands in **1**-**5**[a].

Compound	Chelate angle ACA (º)	Bite angle dPy (º)	Outer atom angle[1] (º)
1	55.98(5), 56.69(5)	-	77.04
2	-	-	83.70
3	54.58(5), 55.84(5)	71.17(6)	144.05
4	56.26(5), 56.32(5)	73.19(6)	144.63
5	52.74(7), 54.16(7)	68.80(7), 69.39(7)	217.36

[a] The outer atom angles have been calculated using the two outer hydrogen atoms placed at the sides of the dPy ligands

UV-Vis and photoluminescence data

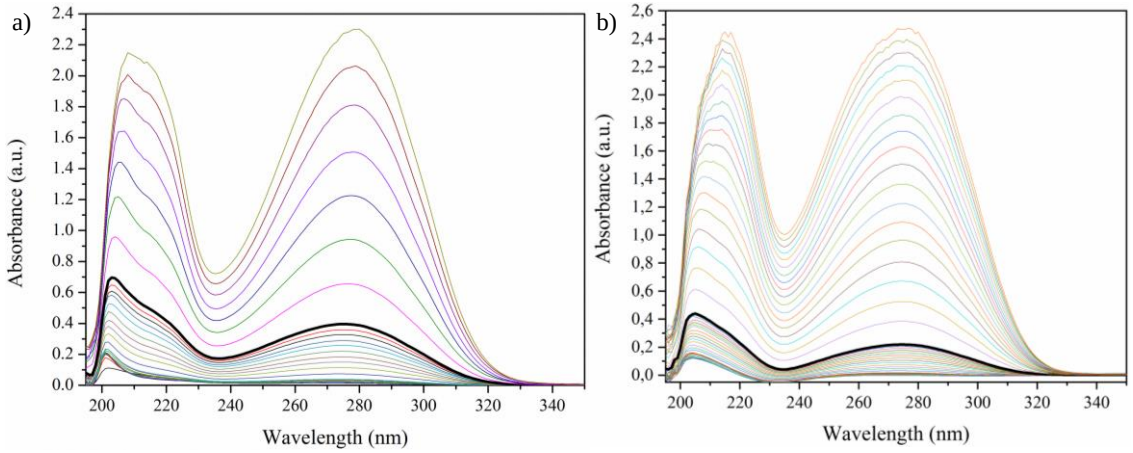

Figure S21. UV-Vis spectra of (a) HACA ligand and (b) ACA^- anion recorded at 298K, within a concentration range from ~$1 \cdot 10^{-9}$ to ~$1 \cdot 10^{-4}$ M.

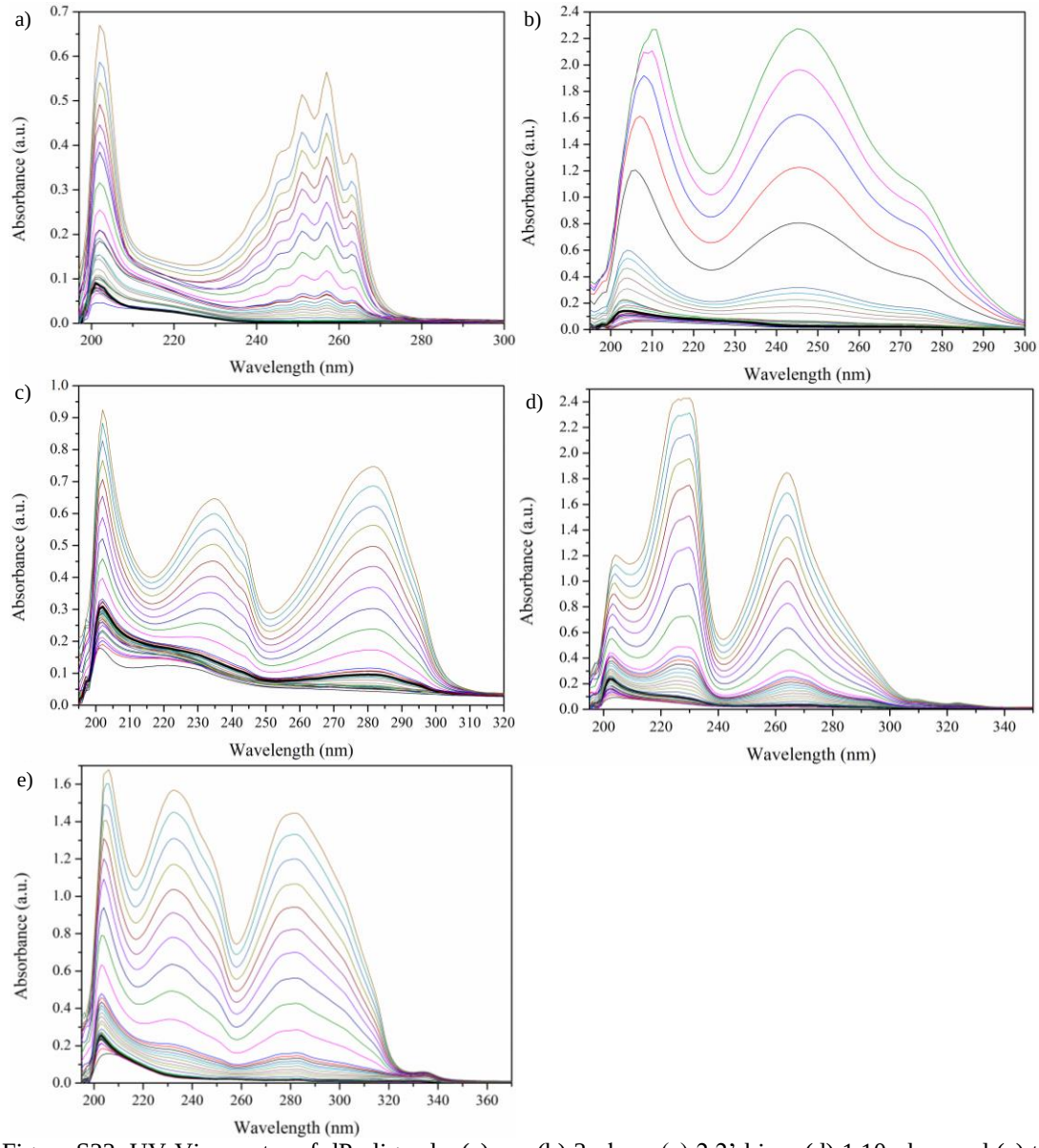

Figure S22. UV-Vis spectra of dPy ligands: (a) py; (b) 3-phpy; (c) 2,2'-bipy; (d) 1,10-phen and (e) terpy recorded at 298K, within a concentration range from ~$1 \cdot 10^{-9}$ to ~$1 \cdot 10^{-4}$ M.

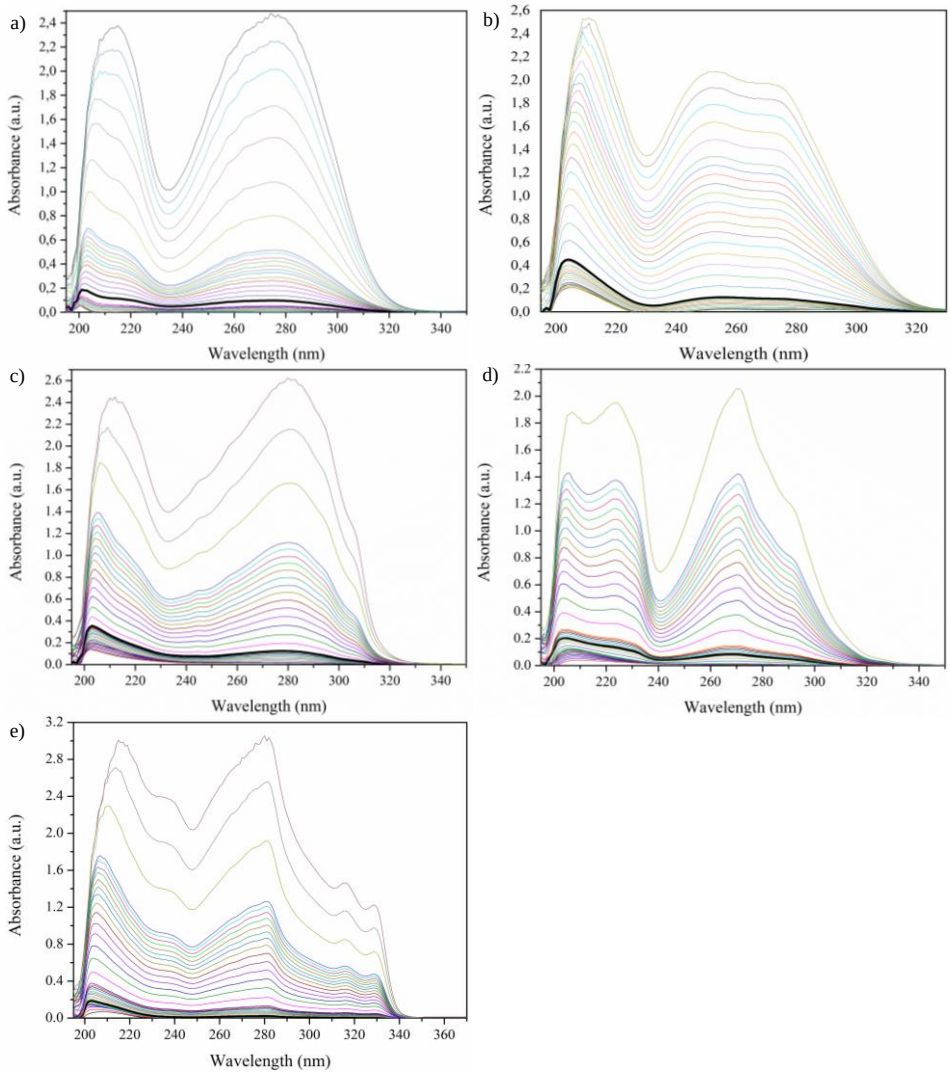

Figure S23. UV-Vis spectra of complexes **1**-**5** recorded at 298K, within a concentration range from ~$1 \cdot 10^{-9}$ to ~$1 \cdot 10^{-4}$ M. (a) **1**; (b) **2**; (c) **3**; (d) **4** and (e) **5**.

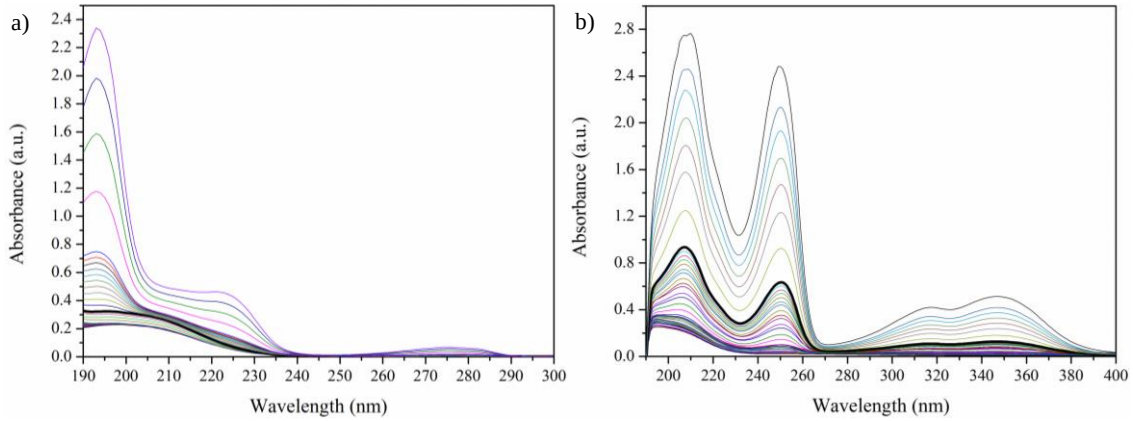

Figure S24. UV-Vis spectra of standards (a) L-tyrosine (L-tyr) and (b) quinine sulphate (QS) recorded at 298K, within a concentration range from ~$1 \cdot 10^{-9}$ to ~$1 \cdot 10^{-4}$ M.

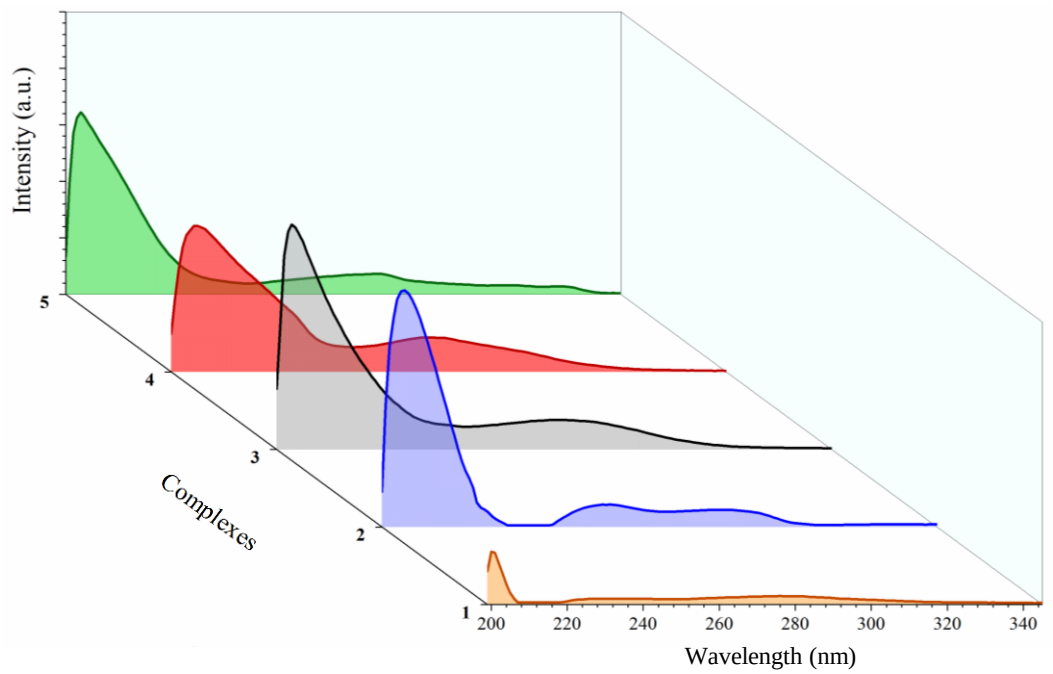

Figure S25. UV-Vis spectra of complexes **1**-**5** recorded at 298 K at a concentration of $1.00 \cdot 10^{-7}$ M.

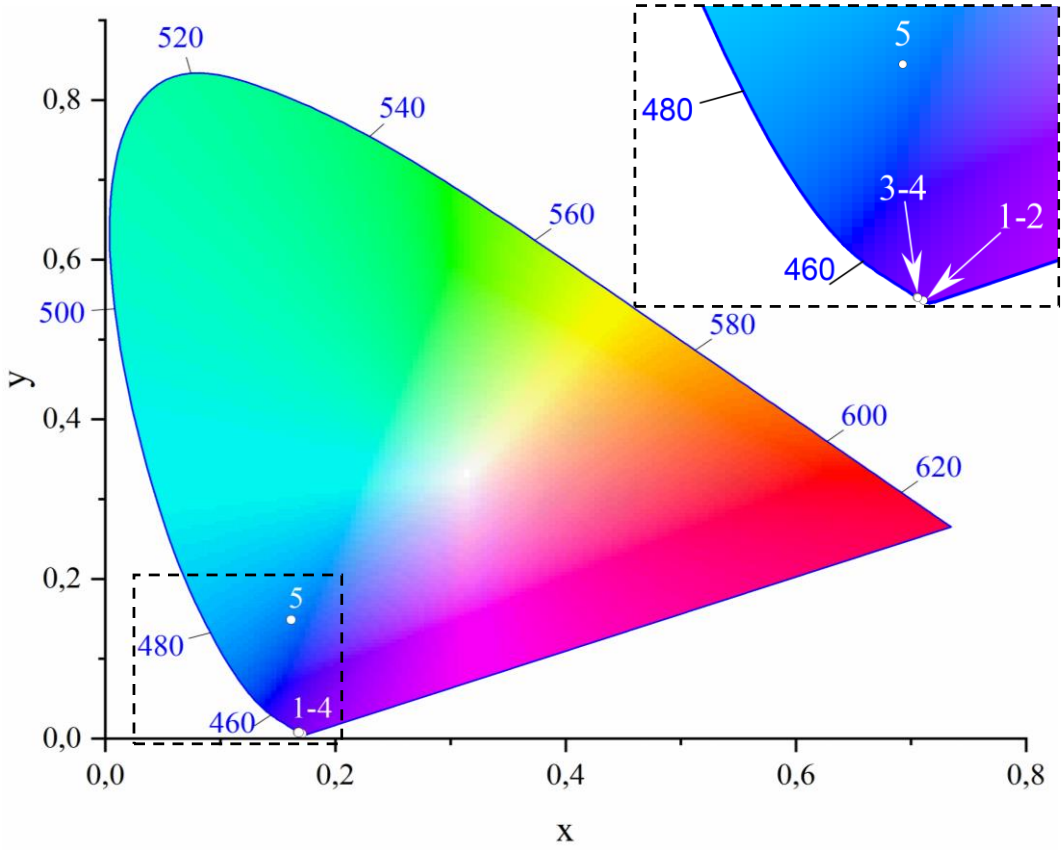

Figure S26. CIE 1931 chromaticity diagram of compounds **1**-**5**.

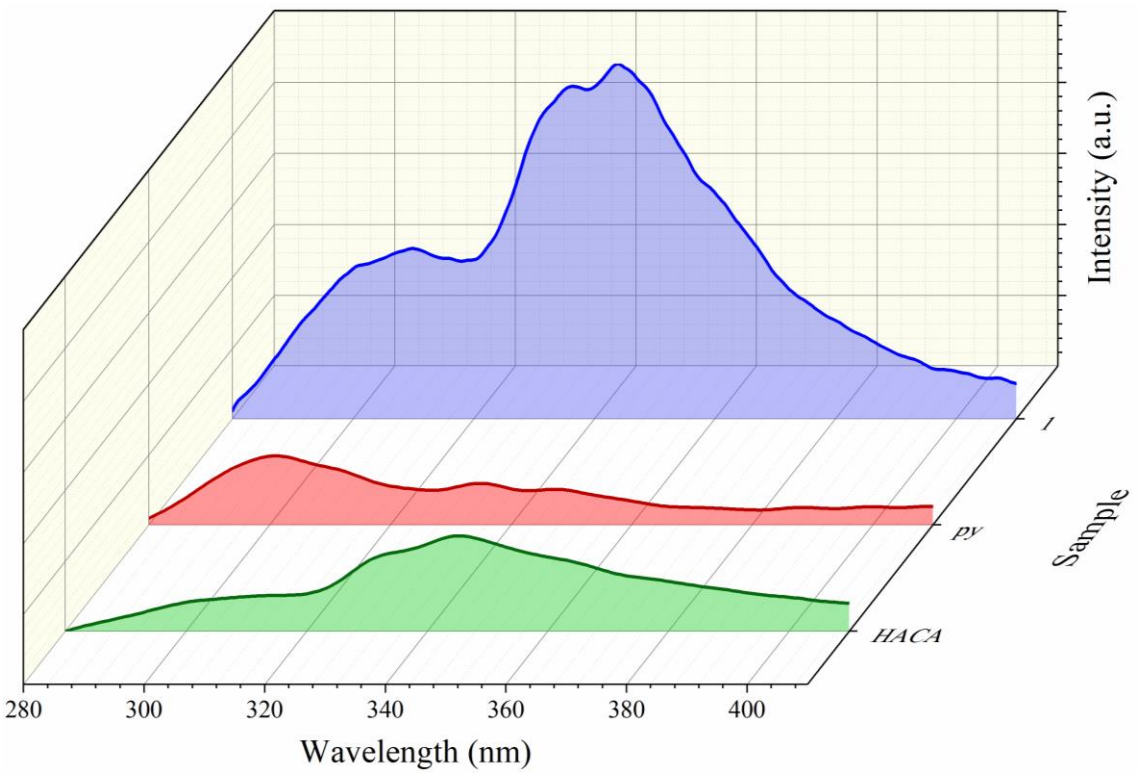

Figure S27. Emission spectra of **1** and their corresponding ligands (HACA and py) irradiated at the excitation maxima of **1** using $1.00 \cdot 10^{-7}$ M solutions.

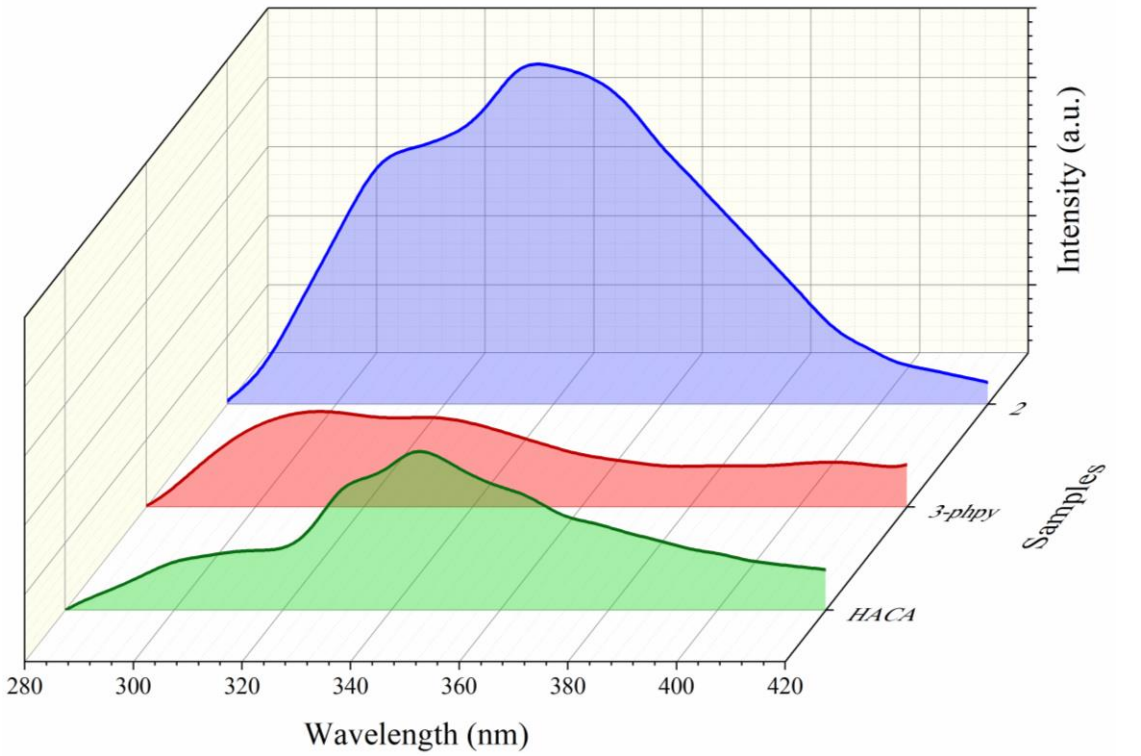

Figure S28. Emission spectra of **2** and their corresponding ligands (HACA and 3-phpy) irradiated at the excitation maxima of **2** using $1.00 \cdot 10^{-7}$ M solutions.

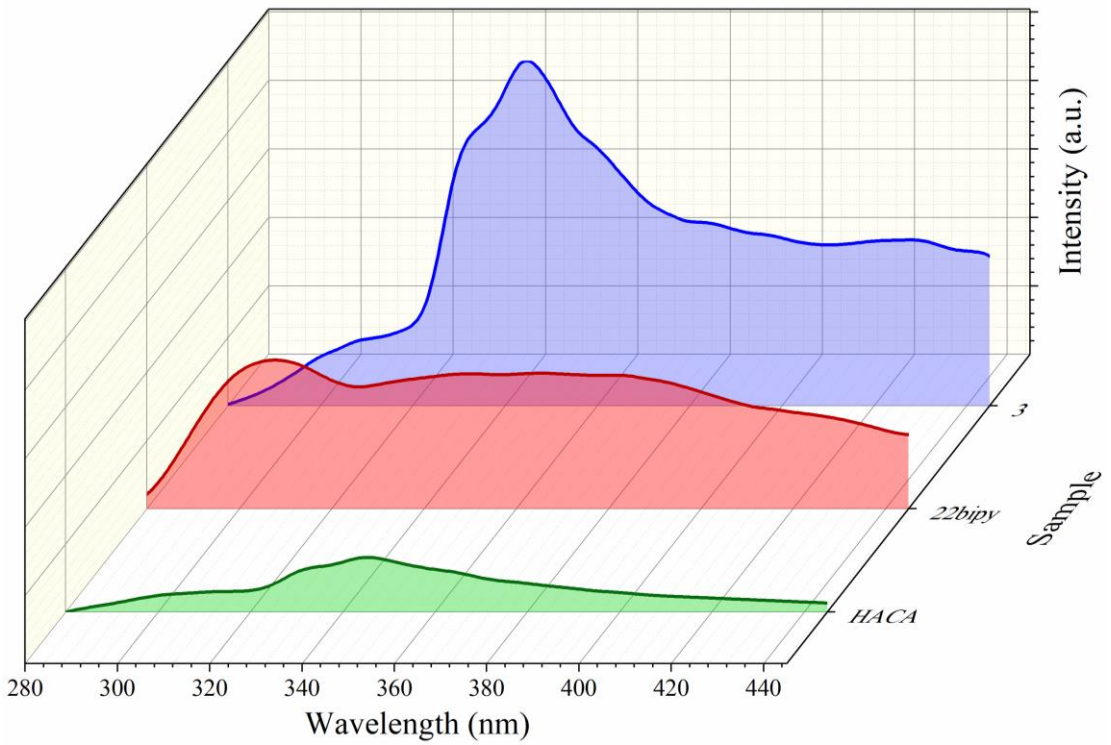

Figure S29. Emission spectra of **3** and their corresponding ligands (HACA and 2,2'-bipy) irradiated at the excitation maxima of **3** using $1.00 \cdot 10^{-7}$ M solutions.

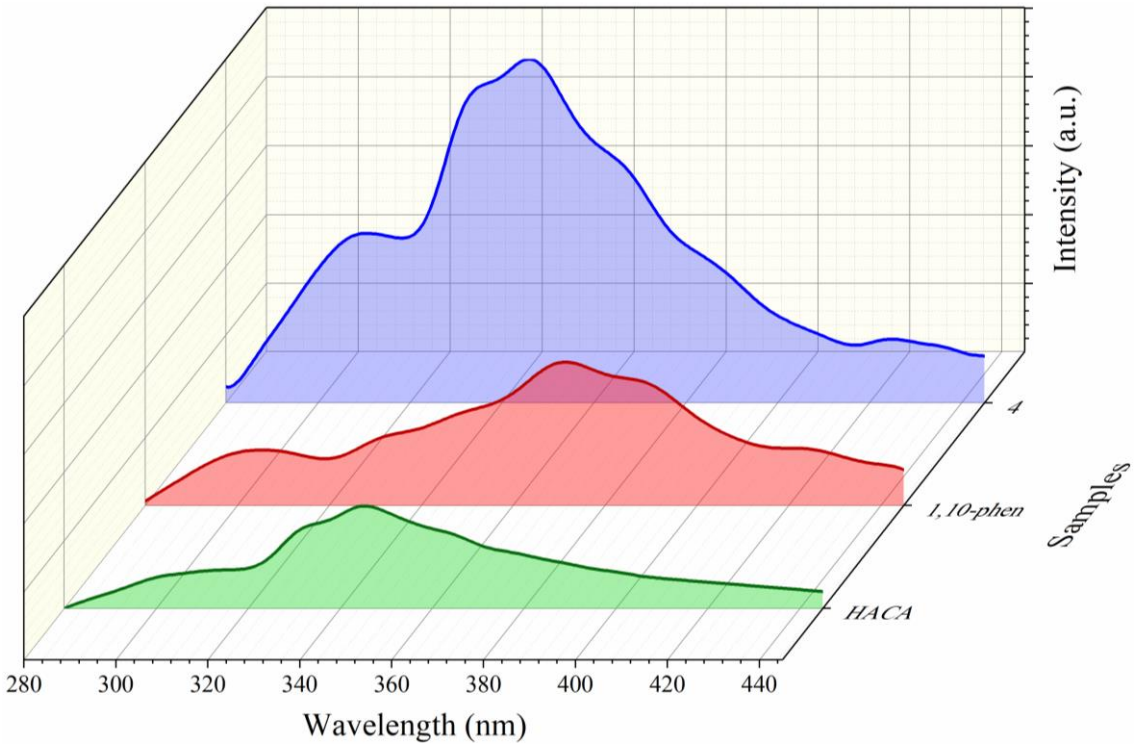

Figure S30. Emission spectra of **4** and their corresponding ligands (HACA and 1,10-phen) irradiated at the excitation maxima of **4** using $1.00 \cdot 10^{-7}$ M solutions.

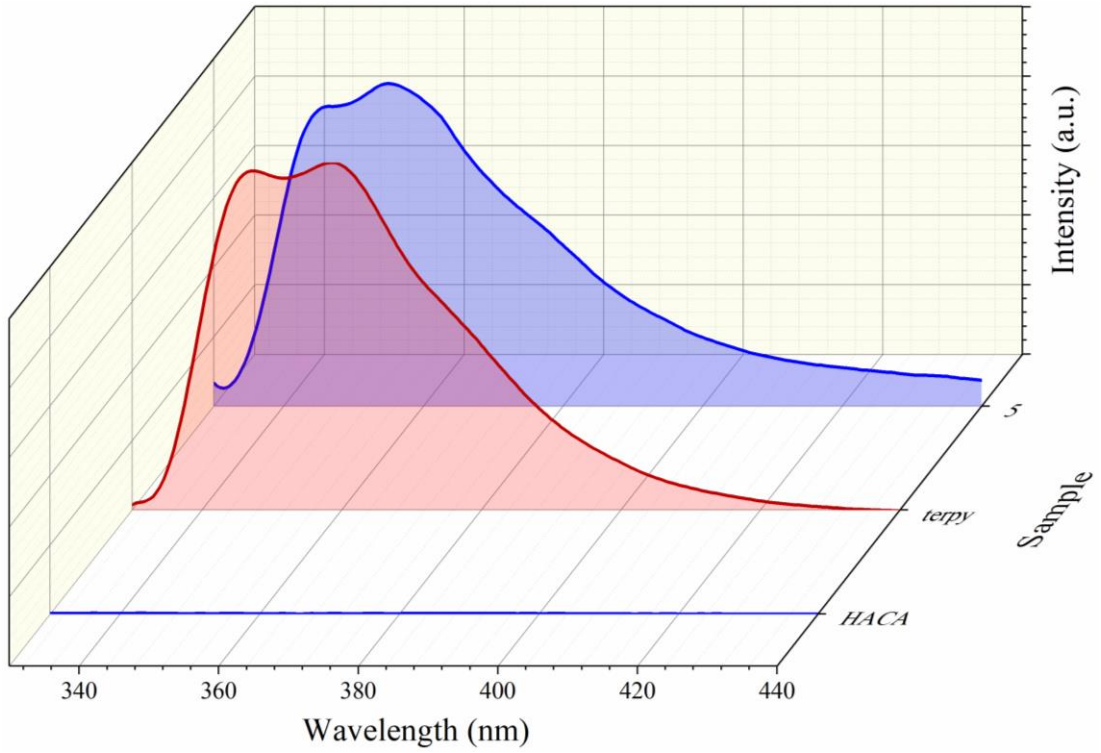

Figure S31. Emission spectra of **5** and their corresponding ligands (HACA and terpy) irradiated at the excitation maxima of **5** using $1.00 \cdot 10^{-7}$ M solutions.

Table S7. Detailed parameters extracted from the photophysical properties of L-tyr, QS, HACA and dPy ligands[a].

Sample	$\lambda_{max\text{-}abs}$ (log (ε))	λ_{ex} (nm)	$\lambda_{max\text{-}em}$ (nm)	Φ_s
L-tyr	197 (5.26), 228 (3.78), 278 (3.07)	275	315	0.14
QS	207(4.65), 250(4.60), 315(3.64), 347(3.74)	350	455	0.577
HACA	201 (4.58), 218 (4.61) 272 (4.44)	229	345	0.039[b]
		320	-	-[c]
py	201 (4.05), 249 (3.64), 252 (3.72), 255 (3.69), 263 (3.60)	229	301	0.046[b]
3-phpy	204(4.44), 245(4.23), 275(3.90)	229	312	0.013[b]
2,2'-bipy	202(4.00), 231(3.84), 243(3.79), 280(3.94)	229	308	0.039[b]
1,10-phen	202(4.38), 226(4.60), 264(4.44), 308(3.10)	229	371	0.023[b]
terpy	203(4.41), 231(4.30), 277(4.26), 283(4.25), 333(3.20)	320	359	0.11[d]

[a]All the wavelengths are given in nm. ε values are given in $M^{-1} \cdot cm^{-1}$. $\lambda_{max\text{-}abs}$ = maximum of absorption; λ_{ex} = excitation maximum; $\lambda_{max\text{-}em}$ = maximum of emission. [b]Relative quantum yield values using L-tyrosine as standard (Φ_s = 0.14).[2] [c]Non-fluorescent samples at the selected excitation wavelength. [d]Relative quantum yield values using quinine sulphate as standard (Φ_s = 0.577).[3]

References

1 F. Sánchez-Férez, J. M. Rius-Bartra, T. Calvet, M. Font-Bardia and J. Pons, *Inorg. Chem.*, 2021, **60**, 3851–3870.

2 R. F. Chen, *Anal. Lett.*, 1967, **1**, 35–42.

3 J. W. Eastman, *Photochem. Photobiol.*, 1967, **6**, 55–72.