Supporting Information

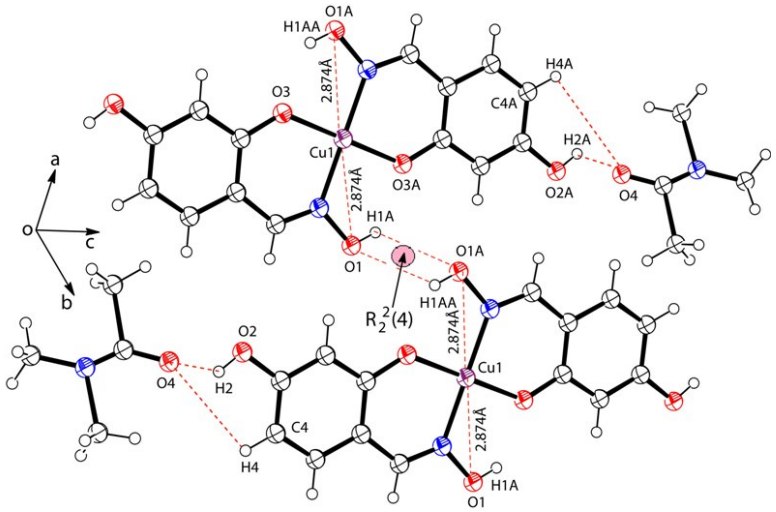


Figure S1: Structure of the complex **2**

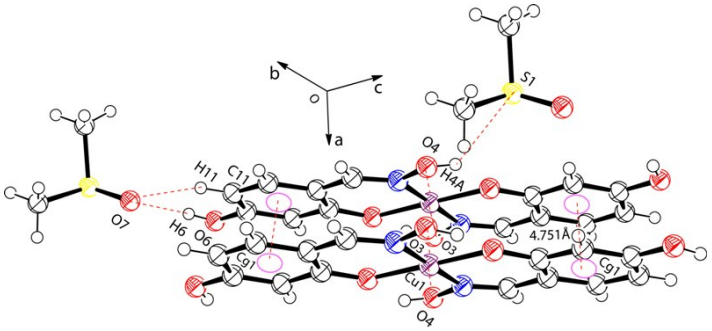


Figure S2: Structure of the complex **3**

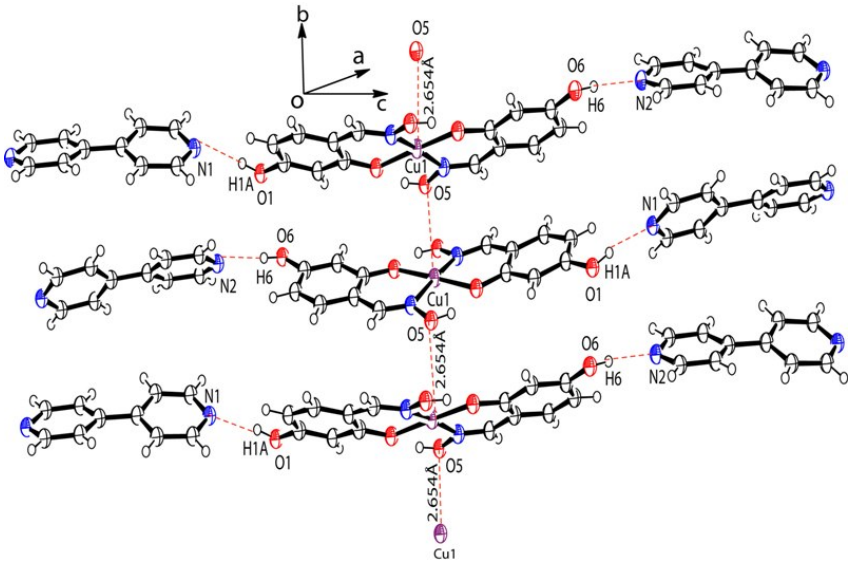


Figure S3: Structure of the complex **4**

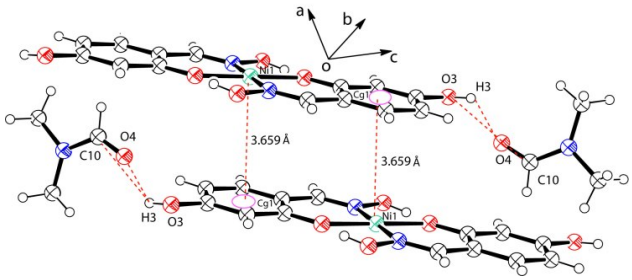


Figure S4: Structure of the complex **5**

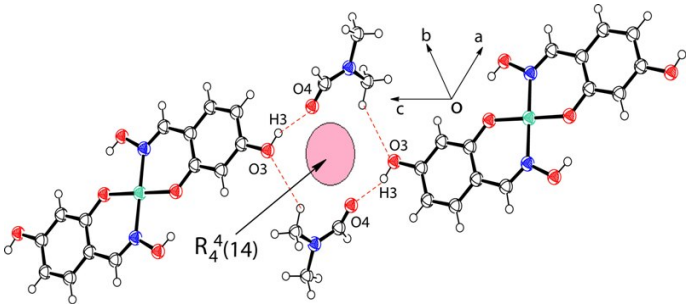


Figure S5: Solvent holding assemblies of the complex **5**

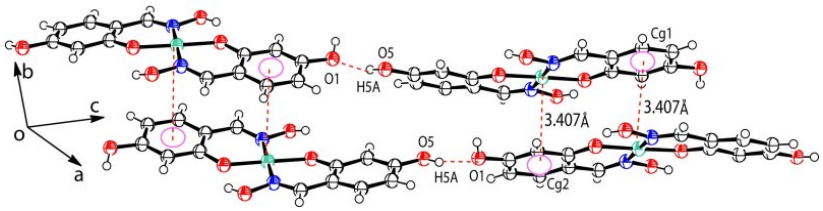


Figure S6: Structure of the complex **6**

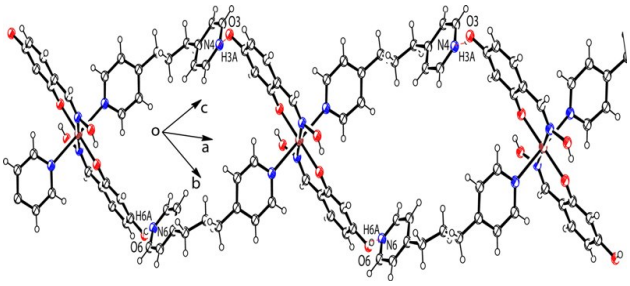
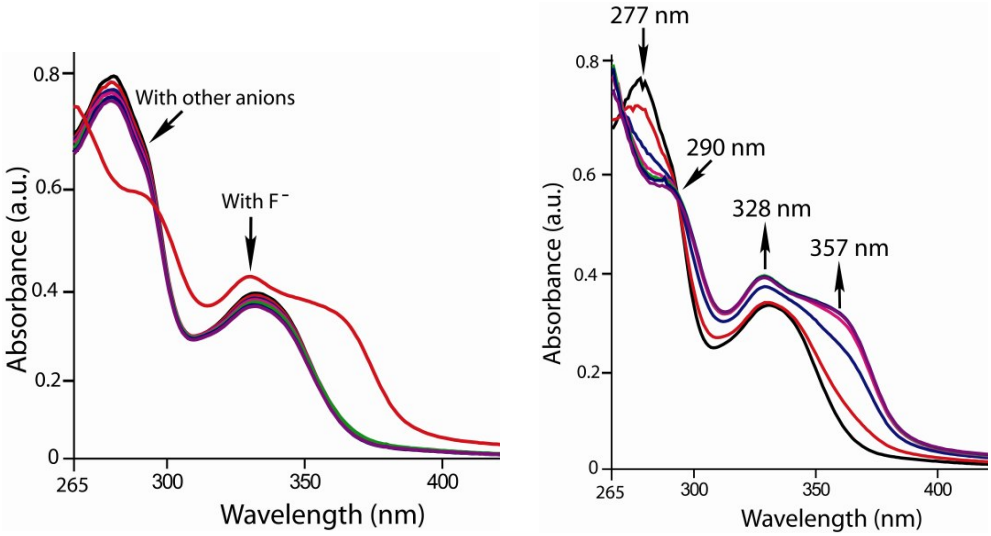
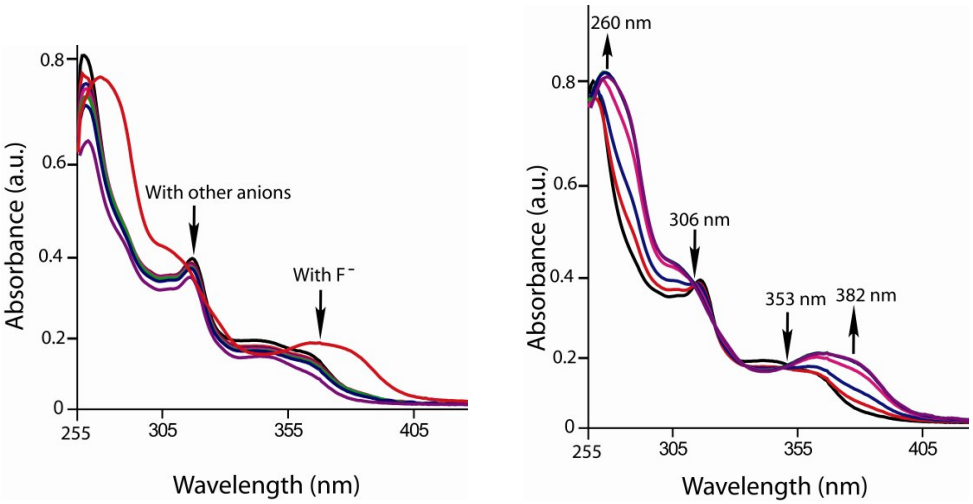


Figure S7: Self-assembly of the complex **7**



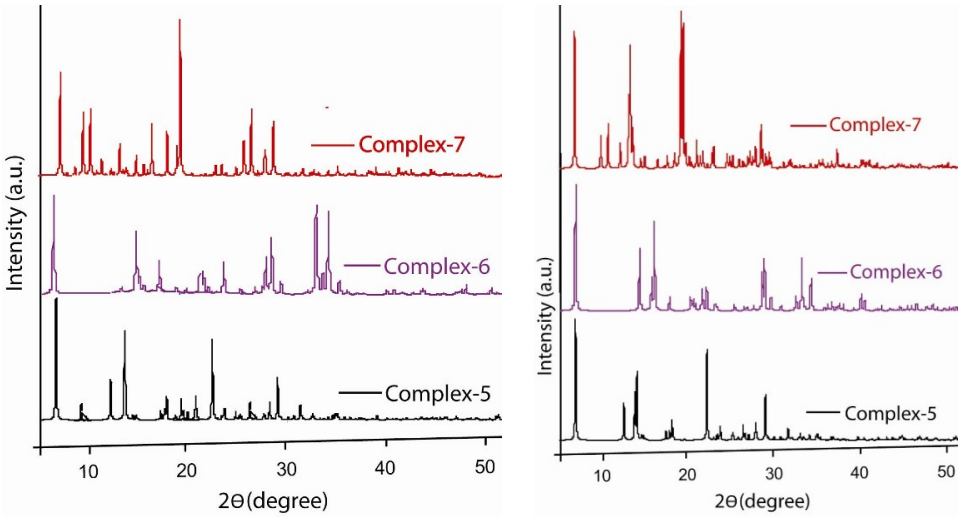
(a) (b)

Figure S8: UV-Vis spectra of the complex **1** (10^{-5} M solution in DMSO) on addition of different amounts of the (a) Tetrabutylammonium salts (fluoride, chloride, bromide, phosphate, carbonate) solution (50µl of 10^{-3}M) and (b) Tetrabutylammonium fluoride (10µl aliquot of 10^{-3} M in DMSO).



(a) (b)

Figure S9: UV-Vis spectra of the complex **5** (10^{-5} M solution in DMSO) on addition of different amounts of the (a) Tetrabutylammonium salts (fluoride, chloride, bromide, phosphate, carbonate) solution (50µl of 10^{-3}M) and (b) Tetrabutylammonium fluoride (10µl aliquot of 10^{-3} M in DMSO).



(a) **(b)**

Figure S10: (a) Experimental and (b) Simulated PXRD patterns of the complexes **5-7**:

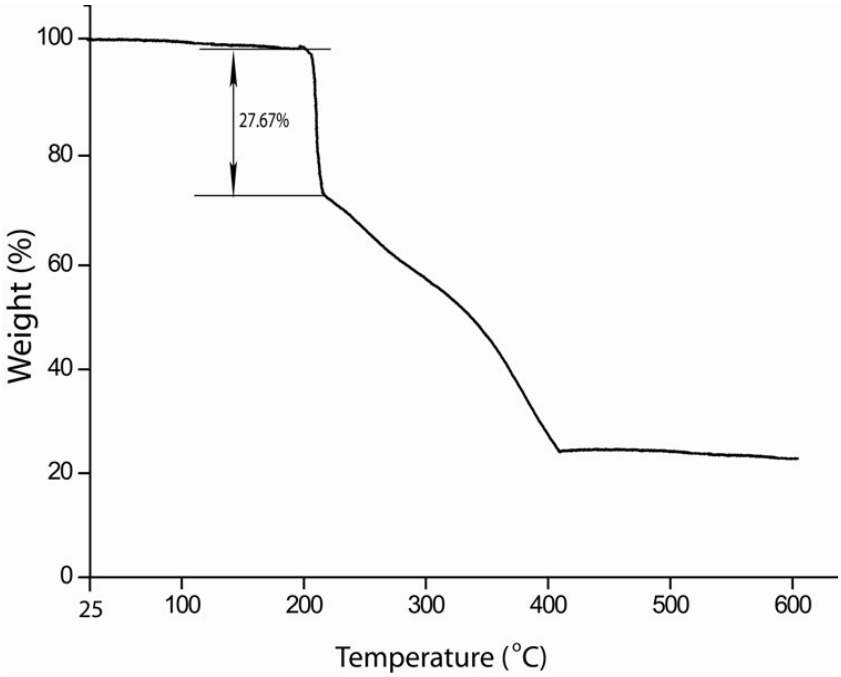


Figure S11: Thermogravimetry of the complex **1**

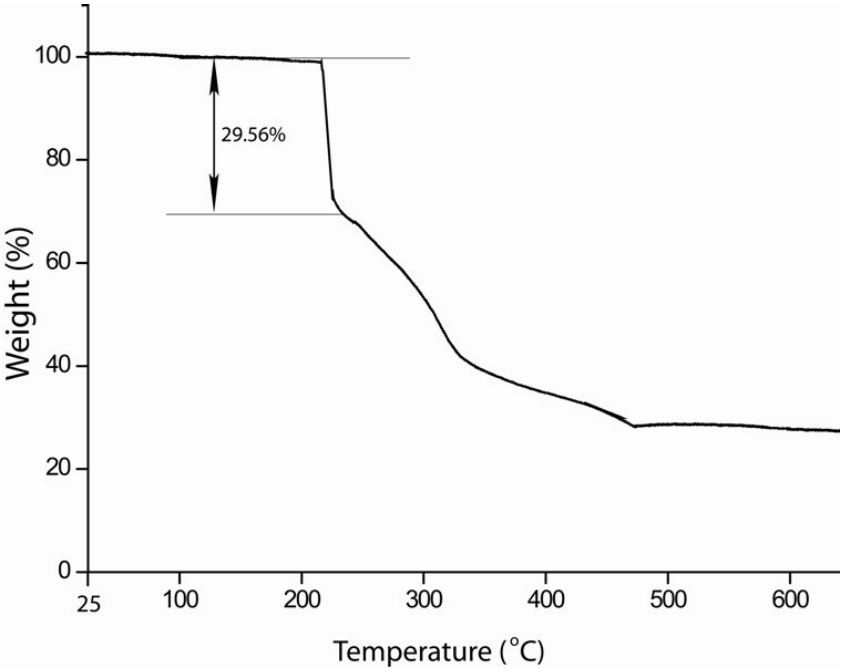


Figure S12: Thermogravimetry of the complex **2**

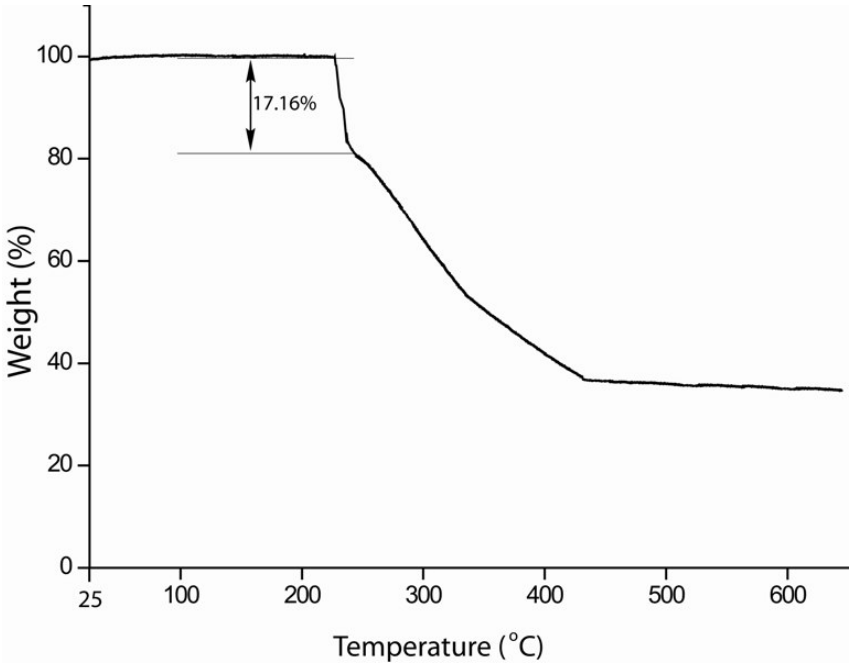


Figure S13: Thermogravimetry of the complex **3**

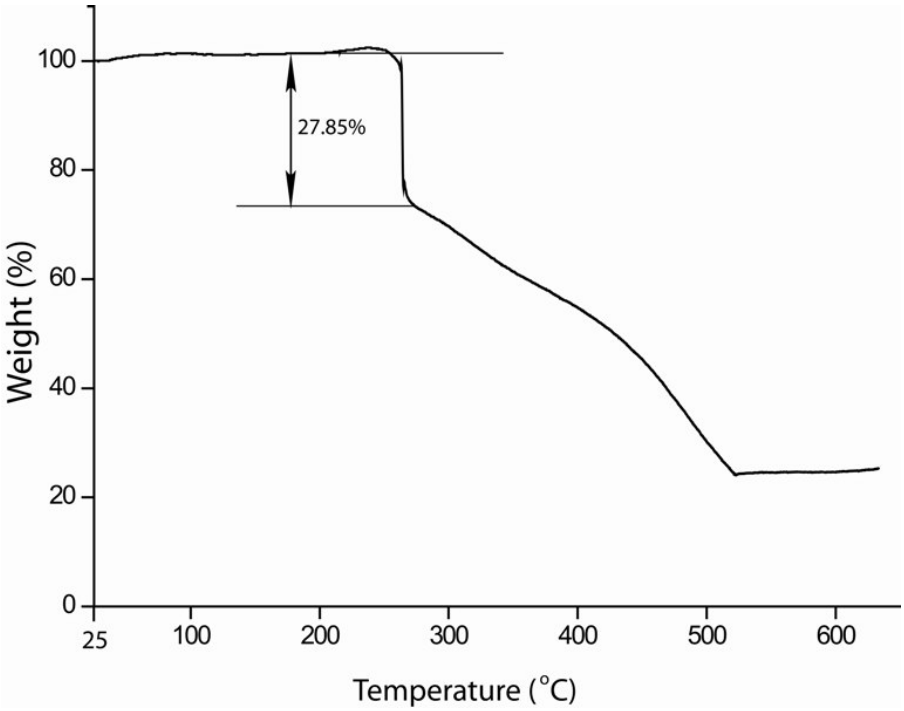


Figure S14: Thermogravimetry of the complex **5**

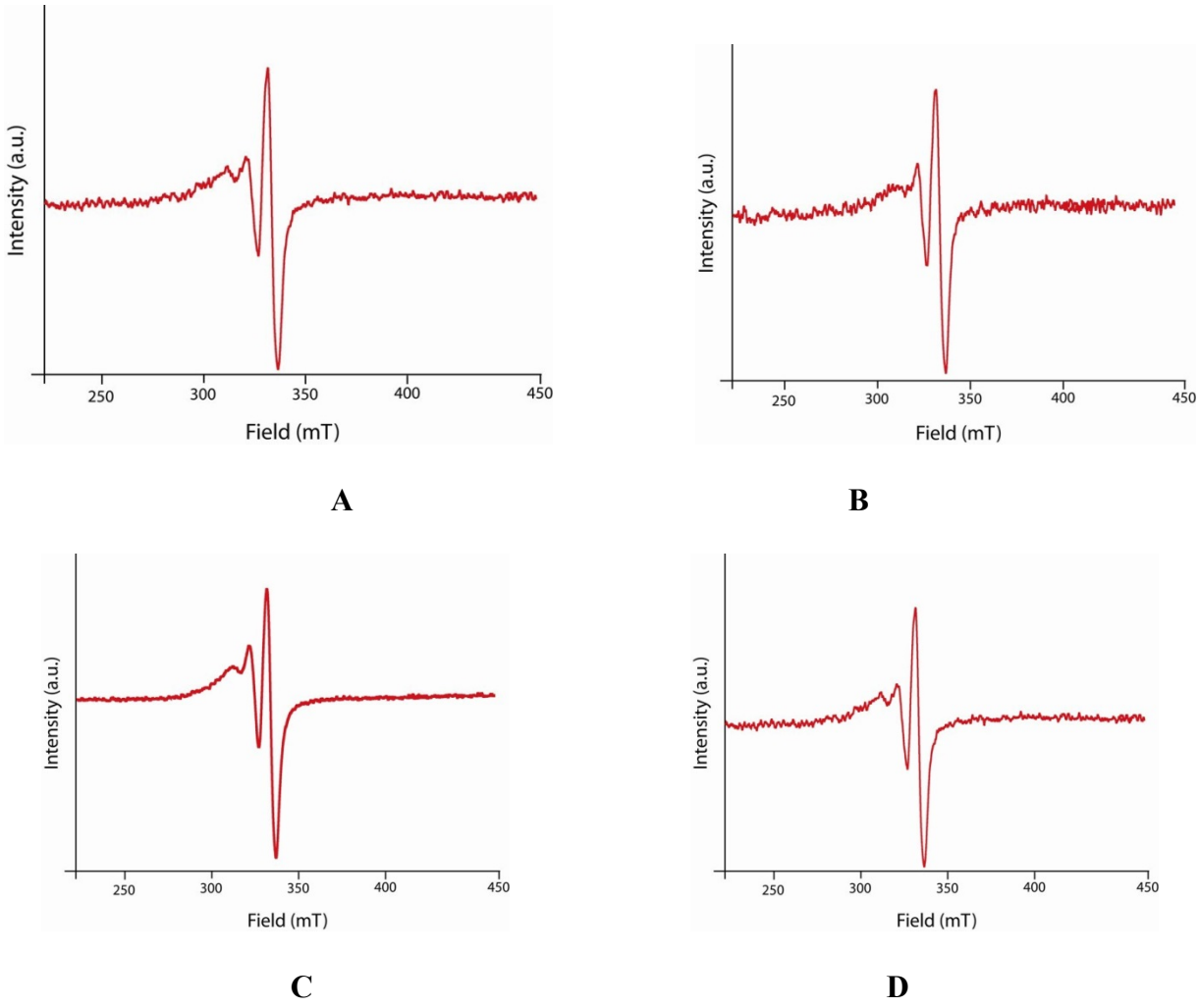


Figure S15: X-band ESR spectra of complex **1-4**: (A) **1**, (B) **2**, (C) **3**, and (D) **4.** Calculated g average (g_{av}) values are 2.031, 2.033, 2.032, and 2.031 respectively in DMSO solvent.

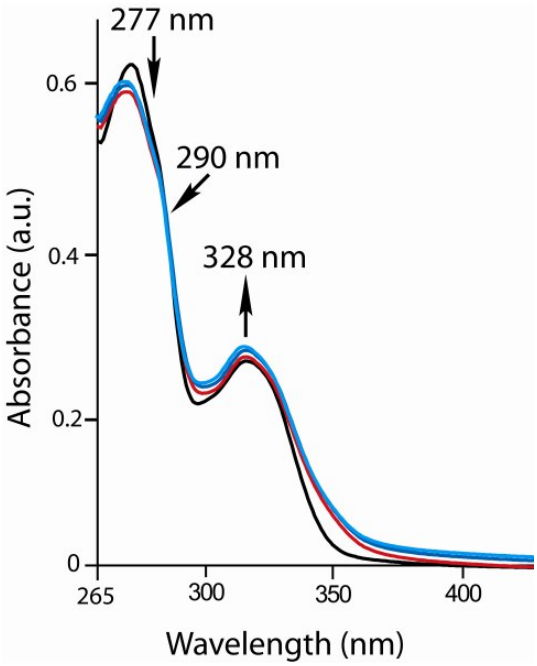
Table S1: Crystallographic parameters of the complexes **1-7**

	Complex **1**	Complex **2**	Complex **3**	Complex **4**
Formula	$C_{20}H_{26}CuN_4O_8$	$C_{22}H_{30}CuN_4O_8$	$C_{16}H_{18}CuN_2O_7S$	$C_{24}H_{20}CuN_4O_6$
CCDC no.	1402351	1402356	1402352	1402350
Mol. wt.	514.00	542.05	445.93	523.99
Space group	P -1	P 21/n	P -1	P 21
a/Å	6.1974(7)	9.3108(3)	8.3981(7)	10.6759(6)
b/Å	7.3044(9)	7.1558(2)	9.6705(9)	7.0765(4)
c/Å	13.1416(16)	19.0122(6)	12.5186(9)	14.7557(9)
α/°	91.394(5)	90.00	73.944(7)	90.00
β/°	102.247(5)	94.749(2)	86.252(6)	96.369(4)
γ/°	101.071(5)	90.00	67.507(9)	90.00
V/Å3	569.23(12)	1262.36(7)	901.77(13)	1107.88(11)
Density/g cm^{-3}	1.499	1.426	1.642	1.571
Abs. coeff./mm^{-1}	1.013	0.917	1.369	1.037
F(000)	267	566	458	538
Total no. of reflections	2040	2261	3252	3830
Reflections, $I > 2\sigma(I)$	1279	1830	2383	3231
Max. θ/°	25.24	25.24	25.25	25.24
Ranges (h, k, l)	$-7 \le h \le 7$ $-8 \le k \le 6$ $-10 \le l \le 14$	$-11 \le h \le 11$ $-8 \le k \le 8$ $-22 \le l \le 22$	$-10 \le h \le 9$ $-11 \le k \le 11$ $-15 \le l \le 13$	$-12 \le h \le 12$ $-8 \le k \le 8$ $-17 \le l \le 17$
Complete to 2θ (%)	98.70	98.90	99.80	99.50
Data/restraints/parameters	2040/0/155	2261/0/165	3252/0/250	3830/1/321
GooF (F^2)	1.034	1.086	1.027	1.086
R indices [$I > 2\sigma(I)$]	0.0387	0.0526	0.0430	0.0367
wR^2 [$I > 2\sigma(I)$]	0.1184	0.1438	0.0734	0.0684
R indices (all data)	0.0407	0.0602	0.0651	0.0473
wR^2 (all data)	0.1222	0.1537	0.0852	0.0713

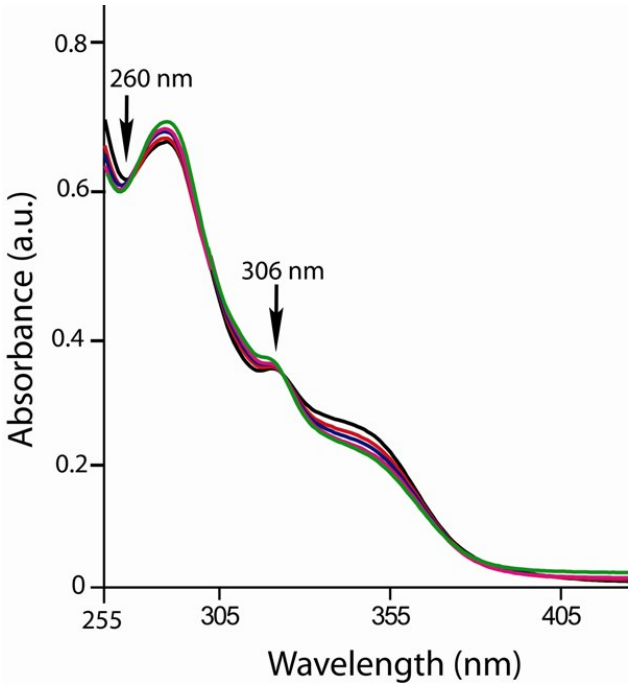
	Complex **5**	Complex **6**	Complex **7**
Formula	$C_{20}H_{26}NiN_4O_8$	$C_{14}H_{12}N_2NiO_6$	$C_{40}H_{40}N_6O_6Zn$
CCDC no.	1402354	1402353	1402355
Mol.wt.	509.14	362.95	766.17
Space group	P -1	$P2_1/c$	P -1
a/Å	6.2331(6)	6.8784(8)	7.7539(6)
b/Å	7.2148(6)	7.0931(8)	9.7058(8)
c/Å	13.1150(12)	27.221(3)	13.6203(10)
α/°	90.288(5)	90.00	75.256(5)
β/°	101.143(5)	90.610(3)	79.970(5)
γ/°	100.988(5)	90.00	72.318(5)
V/Å3	567.52(9)	1328.0(3)	939.22(13)
Density/g cm^{-3}	1.490	1.815	1.355
Abs. coeff./mm^{-1}	0.908	1.498	0.709
F(000)	266	744	400
Total no. of reflections	2044	2390	3398
Reflections, I > 2σ(I)	1883	1239	2704
Max. θ/°	25.00	25.24	25.25
Ranges (h, k, l)	$-7 \le h \le 7$ $-8 \le k \le 8$ $-15 \le l \le 15$	$-7 \le h \le 5$ $-4 \le k \le 7$ $-31 \le l \le 22$	$-9 \le h \le 9$ $-11 \le k \le 10$ $-16 \le l \le 15$
Complete to 2θ (%)	99.90	99.30	99.40
Data/restraints/parameters	2044/3/141	2390/0/209	3398/0/241
GooF (F^2)	1.015	1.077	1.008
R indices [I > 2σ(I)]	0.0738	0.0658	0.0358
wR^2 [I > 2σ(I)]	0.1888	0.1902	0.0818
R indices (all data)	0.0754	0.0887	0.0491
wR^2 (all data)	0.1880	0.2031	0.0882

Table S2: Selected bond parameters of complexes **5-7**

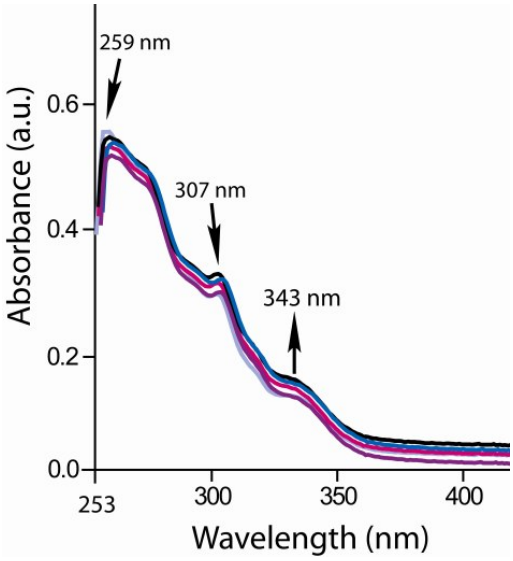
Complex **5**	Ni-O1 Ni-N1	1.843(8) 1.877(10)	O1-Ni-O1' O1-Ni-N1	179.99(2) 90.8(3)	O1'-Ni-N1 N1-Ni-N1'	89.2(3) 179.99(1)
Complex **6**	Ni1-O1 Ni1-O2 Ni1-N1 Ni1-N2	1.832(5) 1.829(5) 1.865(7) 1.865(7)	O2-Ni-O1 O2-Ni-N2 O1-Ni-N2	179.1(3) 92.6(3) 87.2(3)	O2-Ni-N1 O1-Ni-N1 N2-Ni-N1	87.3(3) 93.0(3) 178.0(3)
Complex **7**	Zn1-O2 Zn1-N1 Zn1-N2	2.010(13) 2.034 (16) 2.381 (18)	O2-Zn-O2' O2-Zn-N1 O2-Zn-N1' N1-Zn-N1' N1'-Zn-N3	180.0 90.02(6) 89.98(6) 180.0 85.85(6)	N1-Zn-N1' O2-Zn-N2 O2-Zn-N2' N1-Zn-N2 N1-Zn-N2	180.0 88.42(6) 91.57(6) 94.16(6) 85.84(6)



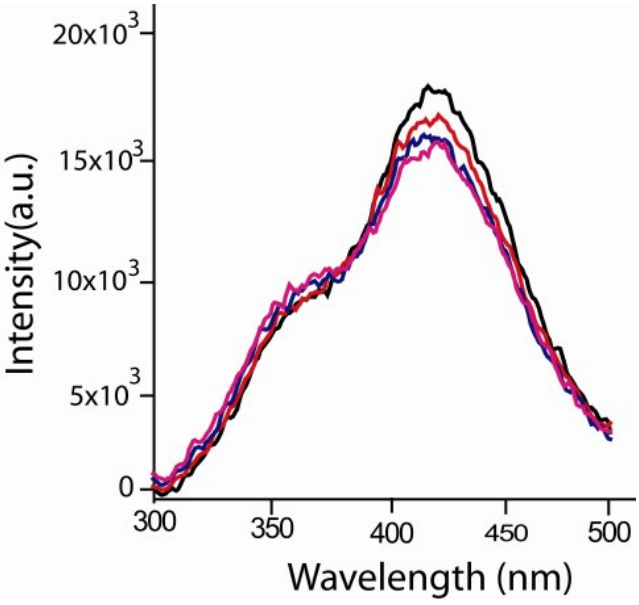
(a)



(b)

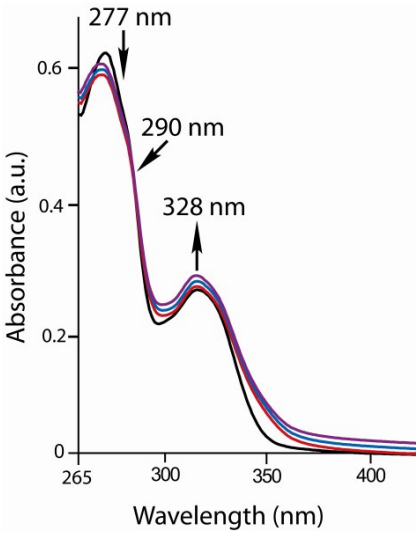


(c)

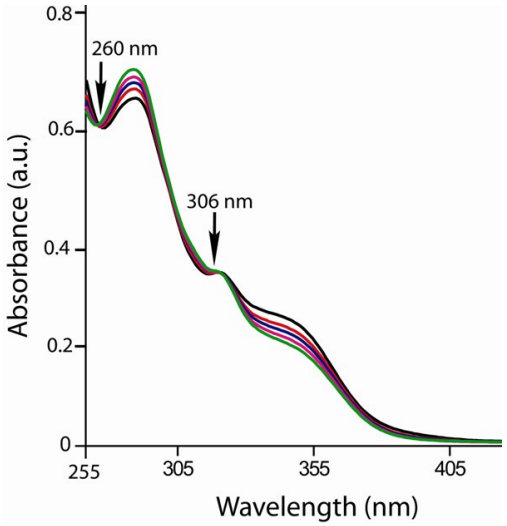


(d)

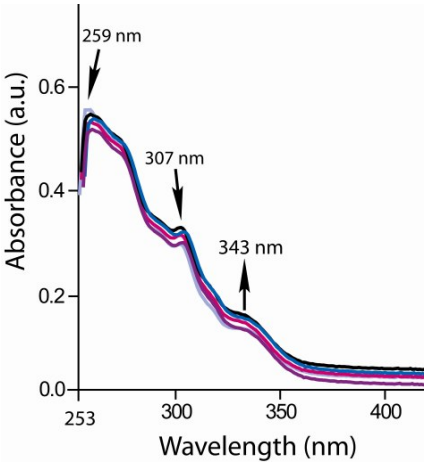
Figure S16: UV-Vis spectra (a) complex **1**, (b) complex **5** and (c) complex **7** in water on addition of different amounts of the tetrabutylammonium fluoride (100µl aliquot of 10^{-5} M in water). (d) Fluorescence spectra of complex **7** in water on addition of different amount of the tetrabutylammonium fluoride (100µl aliquot of 10^{-5} M in water).



(a)



(b)



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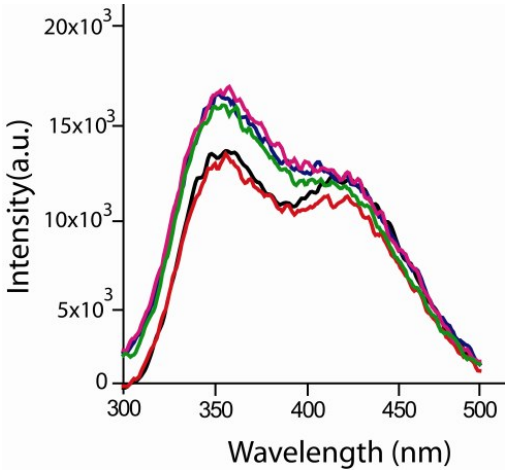


(d)

Figure S17: UV-Vis spectra (a) complex **1**, (b) complex **5** and (c) complex **7** in DMSO-Water mixture on addition of different amounts of the tetrabutylammonium fluoride (100µl aliquot of 10^{-3} M in DMSO-Water). (d) Fluorescence spectra of complex 7 in DMSO-Water on addition of different amount of the tetrabutylammonium fluoride (100µl aliquot of 10^{-3} M in DMSO-Water).

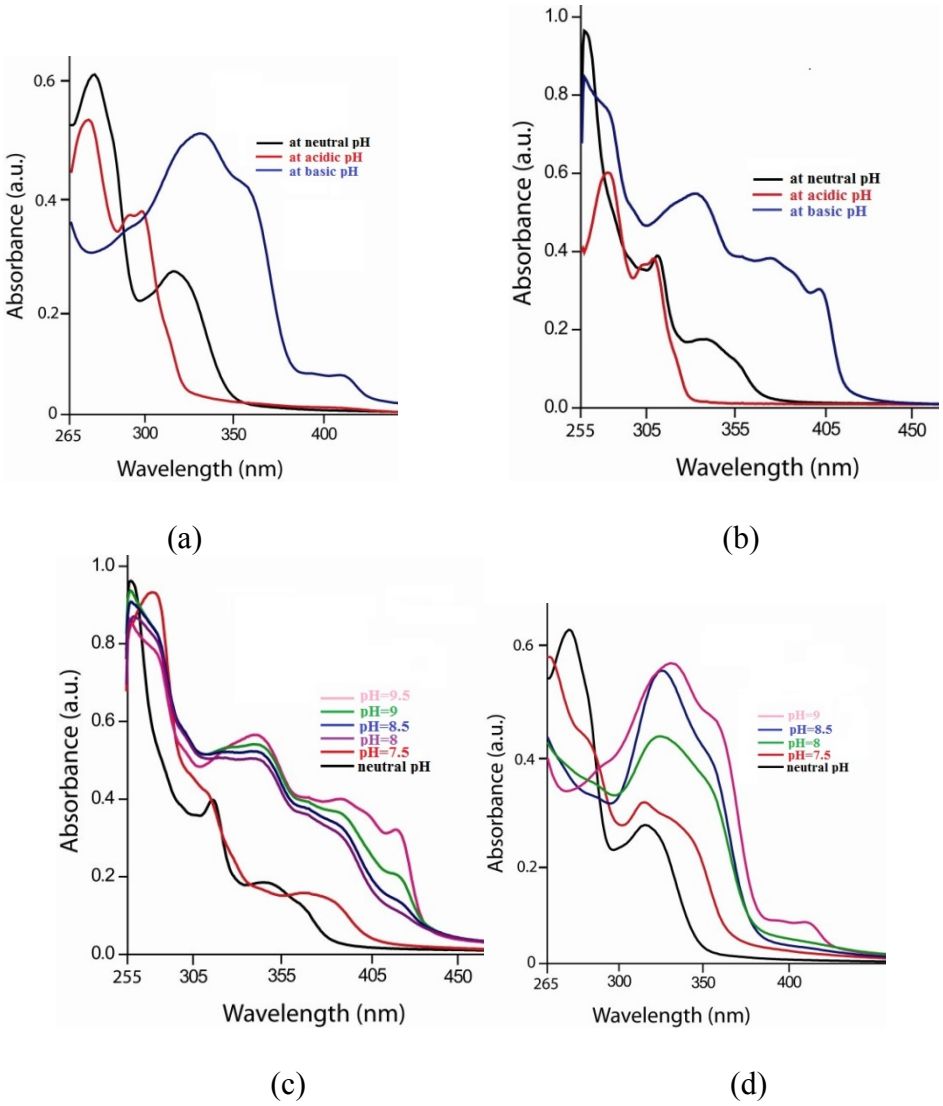
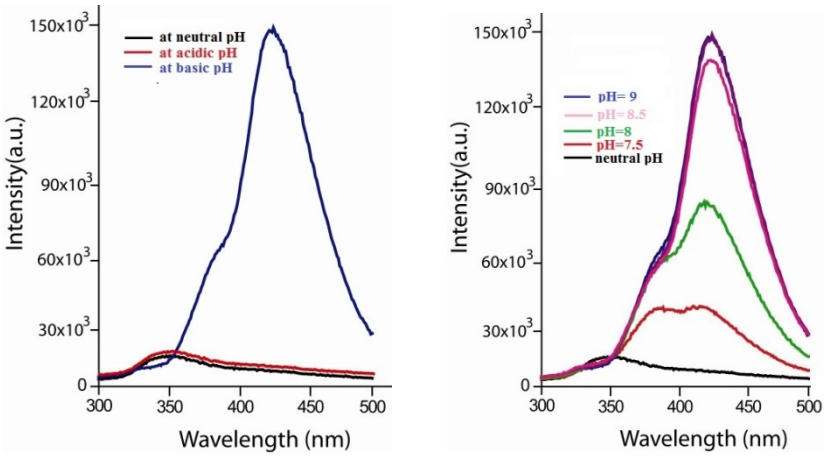
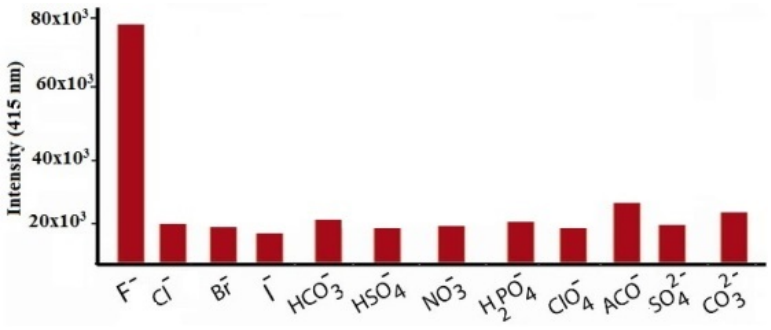


Figure S18: UV-Vis spectra of the (a) complex **1**, (b) complex **5** at different pH and (c) and (d) at pH = 8.5 spectra of complex **1** and **5**.

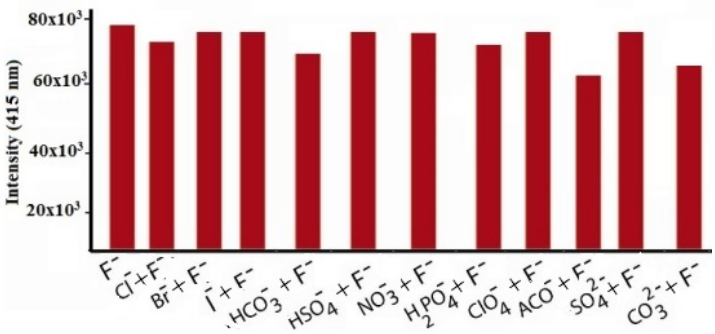


(a) (b)

Figure S19: Fluorescence spectra of complex **7** (a) at different pH and (b) at different basic pH.



(a)



(b)

Figure S20: (a) Fluorescence intensities at 415 nm for the complex **7** (10^{-5}M) in the presence of 10^{-3}M different anions. (b) Fluorescence intensities at 415 nm for complex 7 (10^{-5}M) in the presence of 10^{-3}M of F^- and with the addition of 10^{-3}M of different anions respectively.

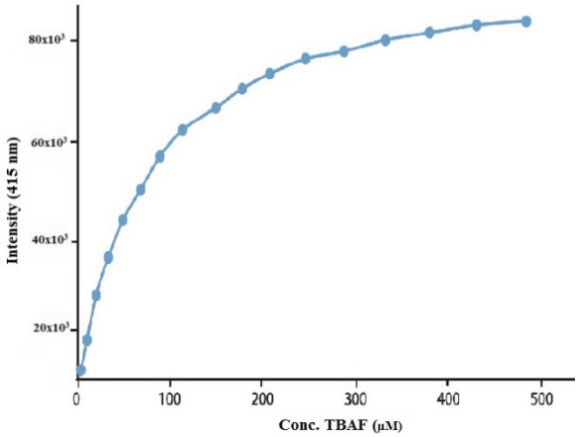


Figure S21: Fluorescence intensity versus tetrabutylammonium fluoride [TBAF] plot of zinc complex at 415nm.

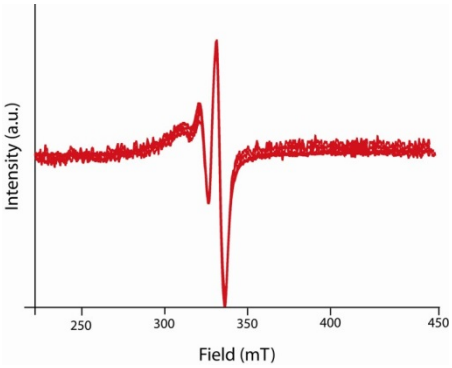


Figure S22: EPR spectrum of copper complex **1** with tetrabutyl ammonium fluoride.

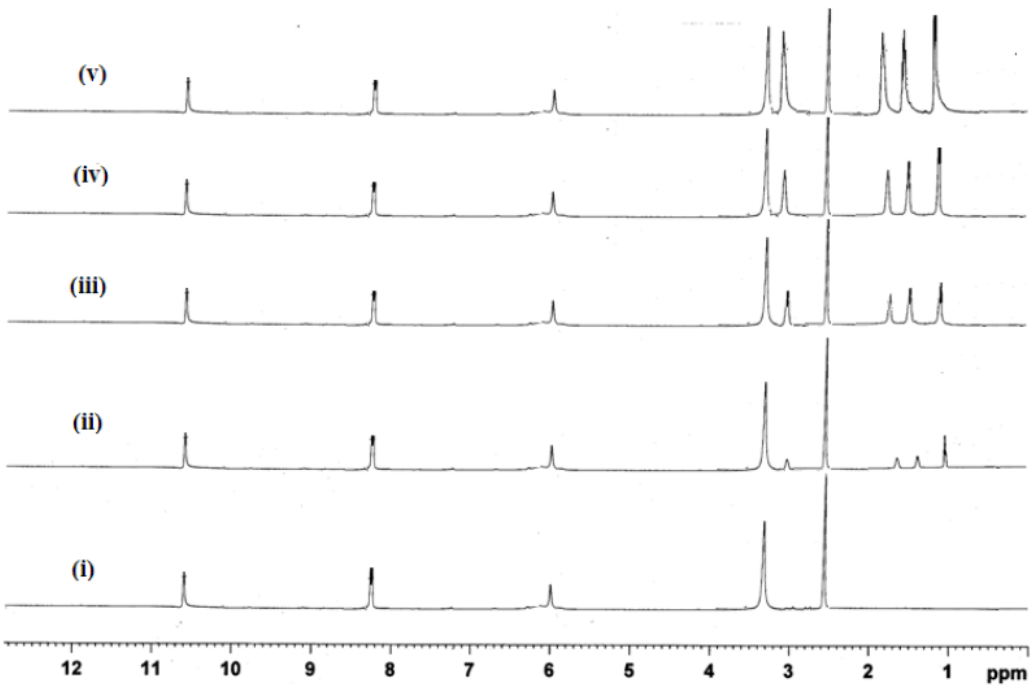


Figure S23: ^{1}H-NMR (DMSO-d^{6}) spectra during titration of complex **5**(i), with tetrabutyl ammonium fluoride 0.5(ii), 1(iii), 1.5(iv) and 2(v) equivalents.

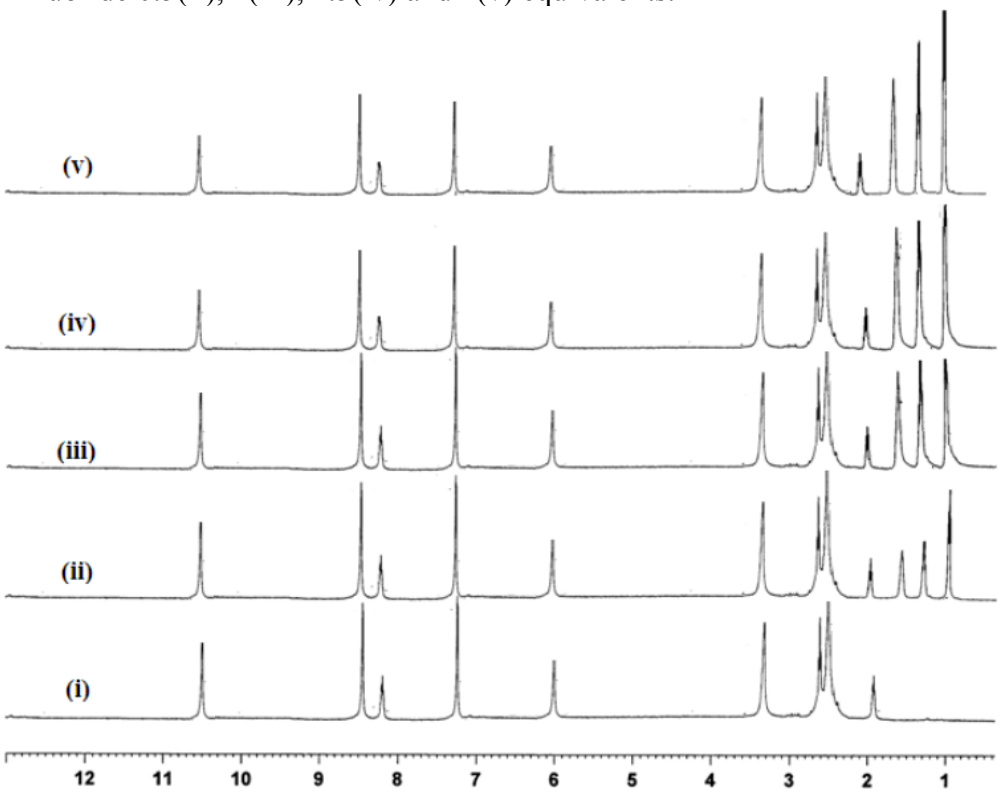


Figure S24: ^{1}H-NMR (DMSO-d^{6}) spectra during titration of complex 7(i) with tetrabutyl ammonium fluoride 0.5(ii), 1(iii), 1.5(iv) and 2(v) equivalents.

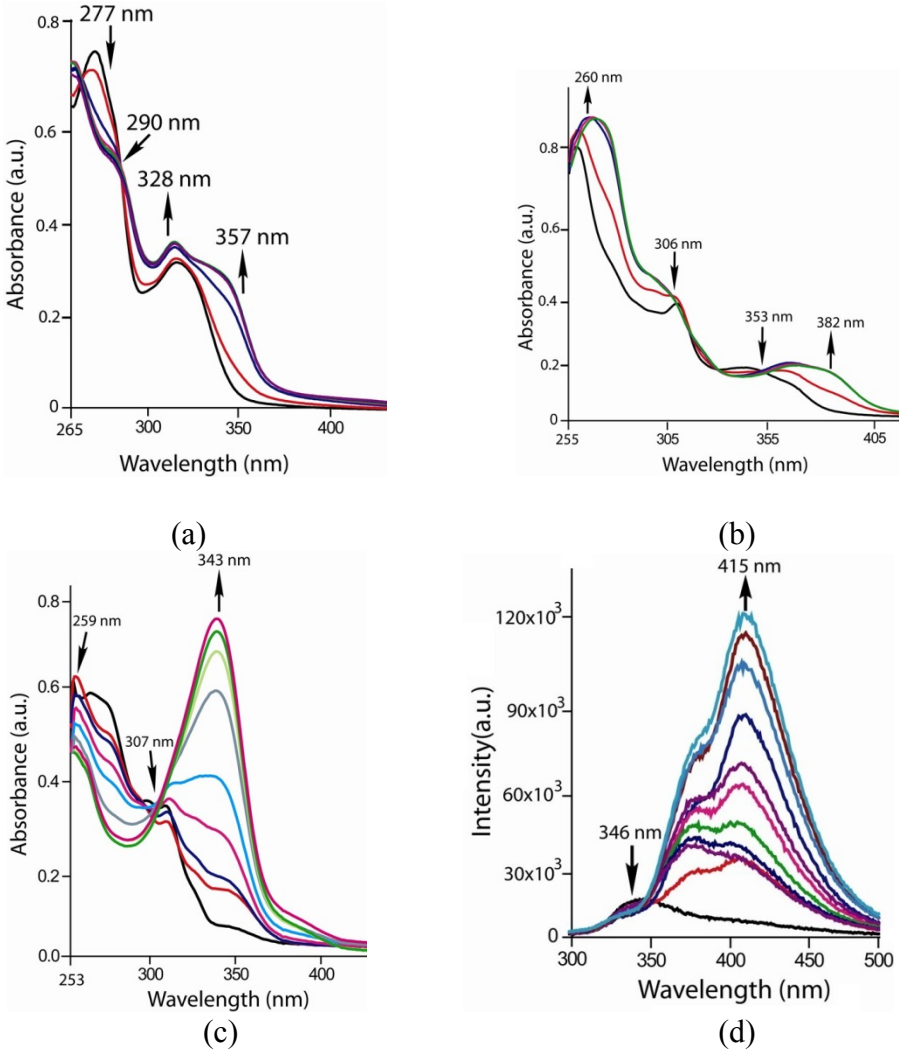


Figure S25: UV-Vis spectra (a) complex **1**, (b) complex **5** and (c) complex **7** on addition of different amount of tetrabutylammonium hydroxide. (d) Fluorescence spectra of complex 7 on addition of different amount of tetrabutylammonium hydroxide.