Supporting Information

Studies on the one-photon and two-photon properties of two water-soluble terpyridines and their zinc complexes

Pengfei Shi, *[a, b] Qin Jiang,[a] Xuesong Zhao,[b] Qiong Zhang[b] and Yupeng Tian*[b]

[a]School of Chemistry, Huaihai Institute of Technology, , Lianyungang, PR China, 222005;

[b]School of Chemistry, Anhui Universtiy, Hefei, PR China, 230601;

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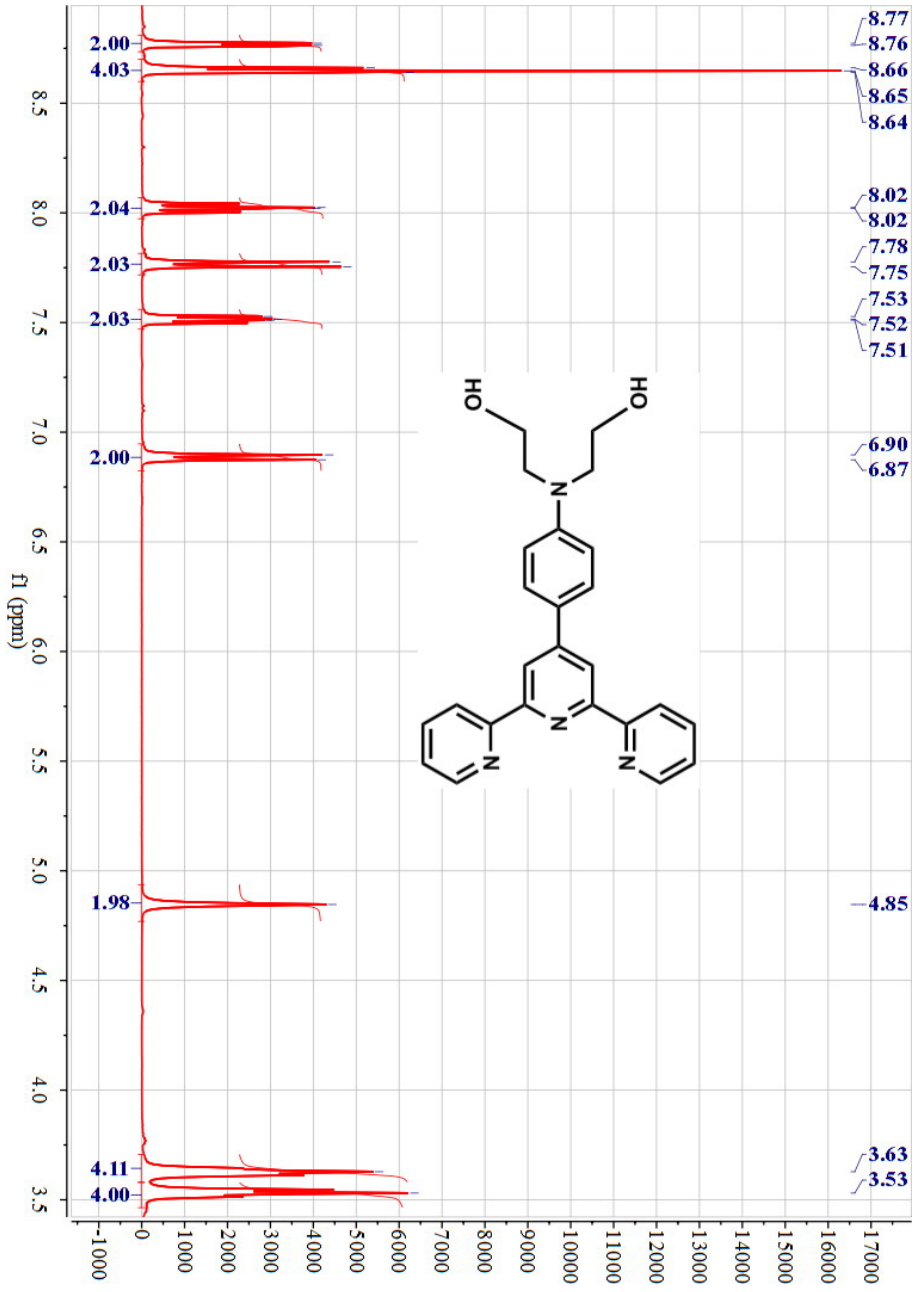

Figure S1. ^{1}H NMR spectrum of TPYOH in d_6-DMSO

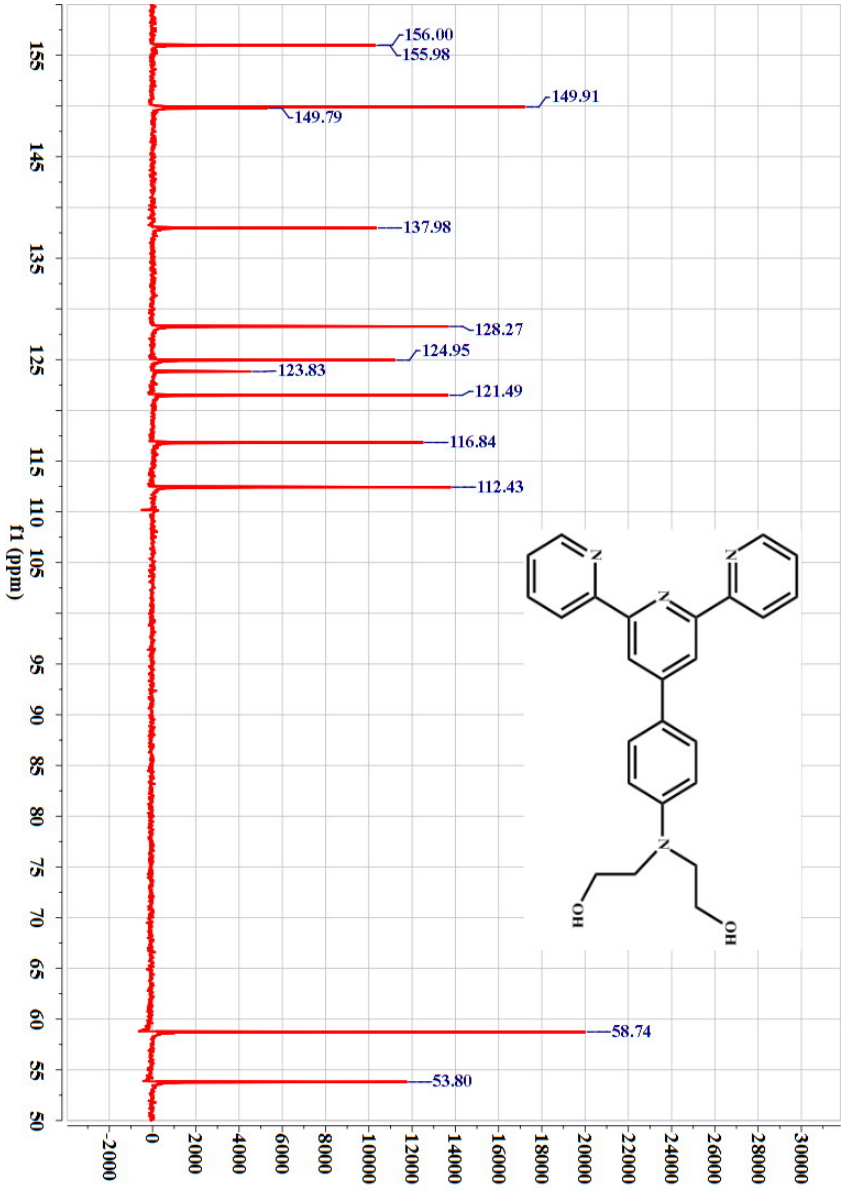

Figure S2. ^{13}C NMR spectrum of TPYOH in d_6-DMSO

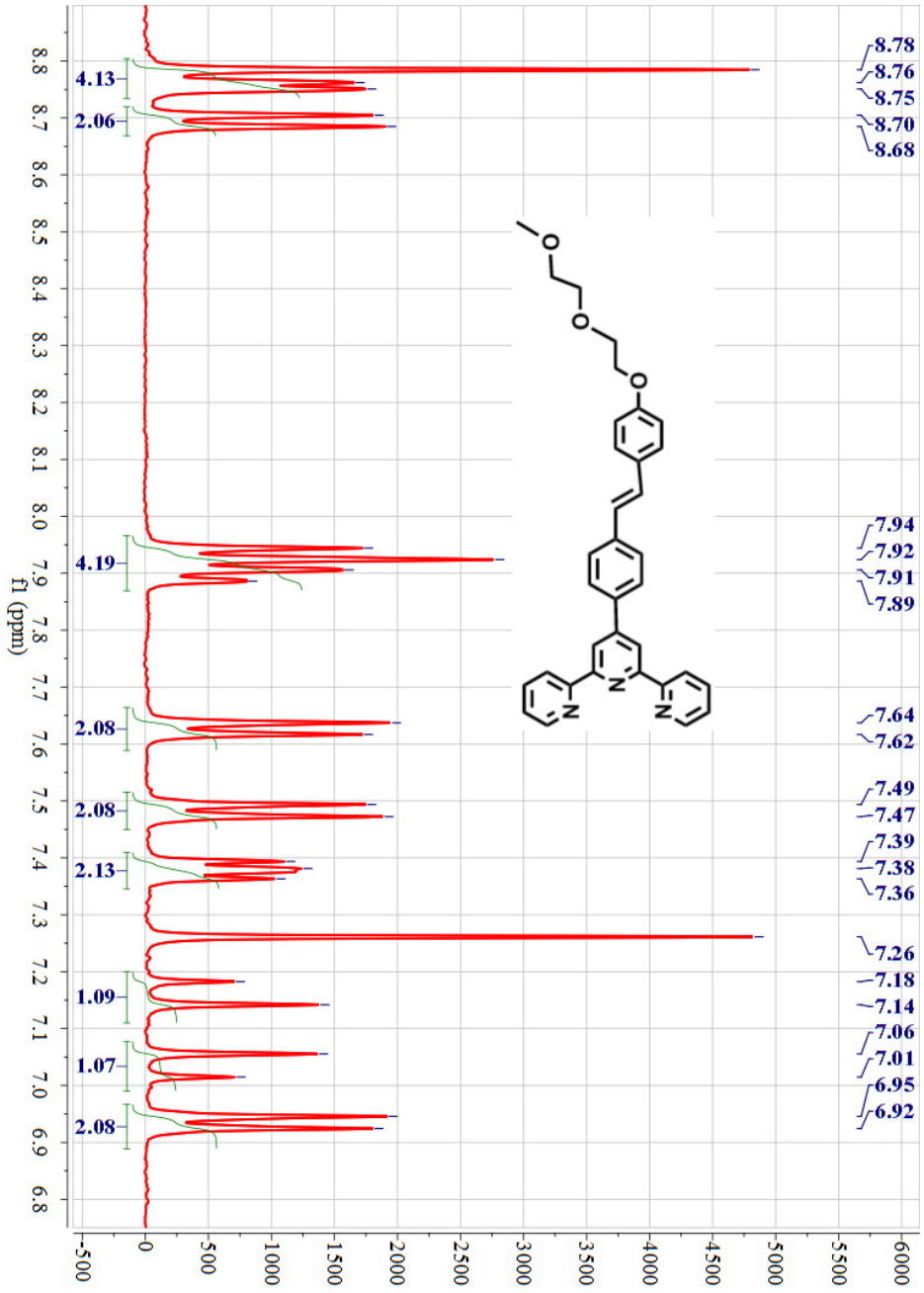

Figure S3. ^{1}H NMR spectrum of O3TPY in CDCl3

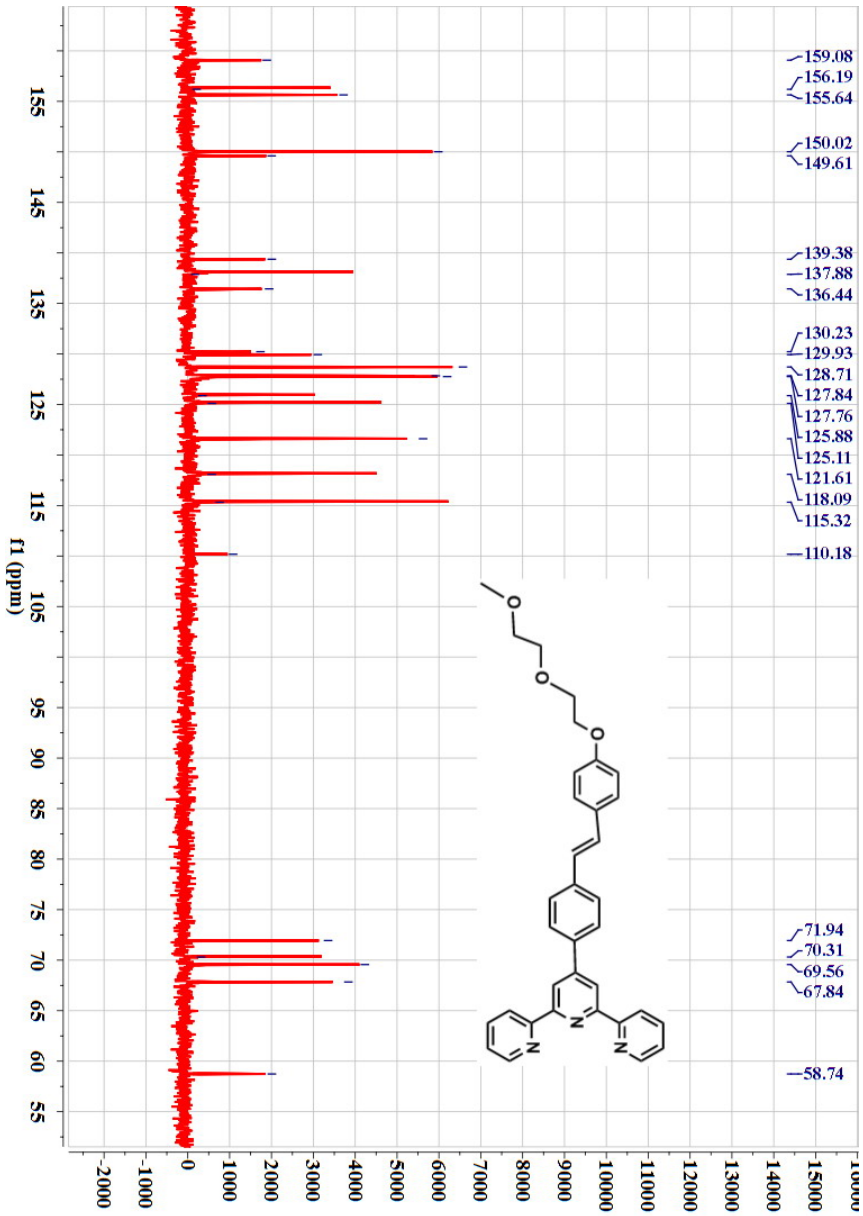

Figure S4. ^{13}C NMR spectrum of O3TPY in d_6-DMSO

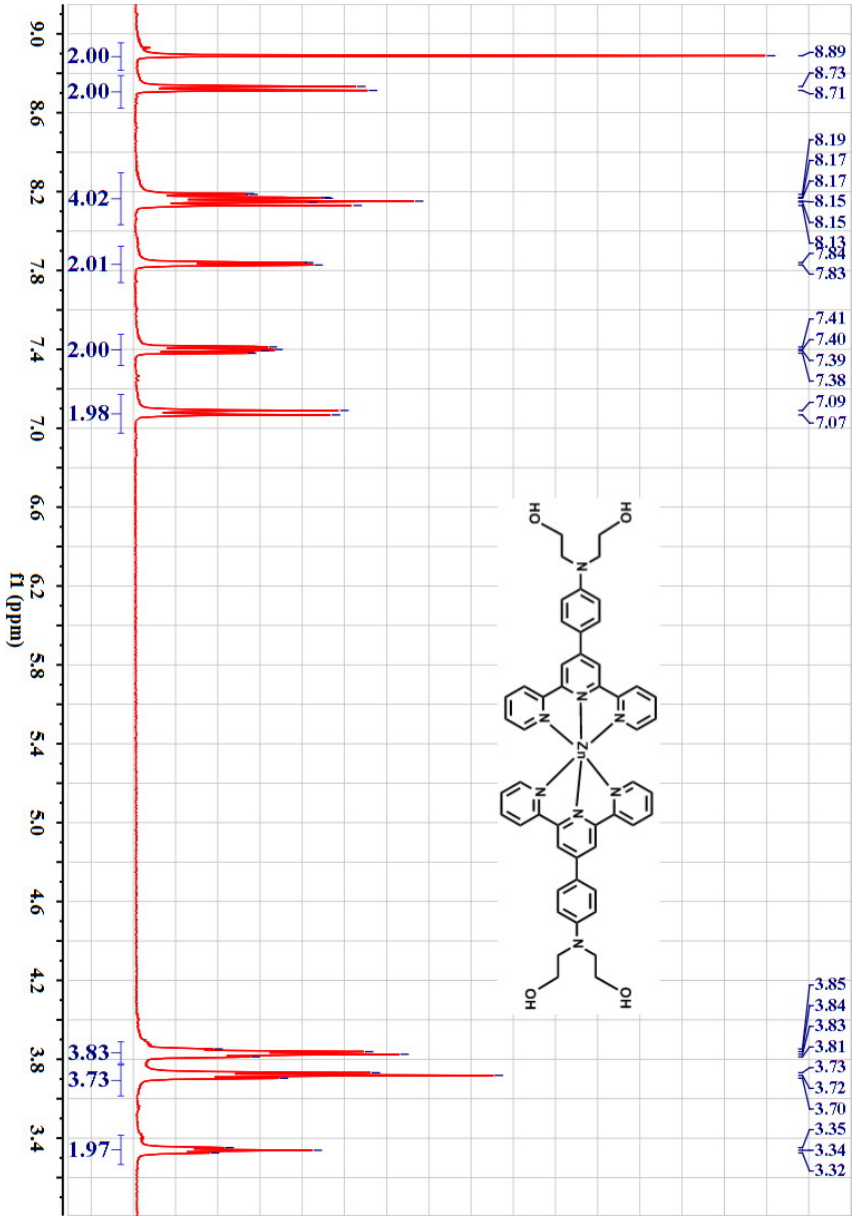

Figure S5. ^{1}H NMR spectrum of ZnTPYOH in d_3-CD_3CN

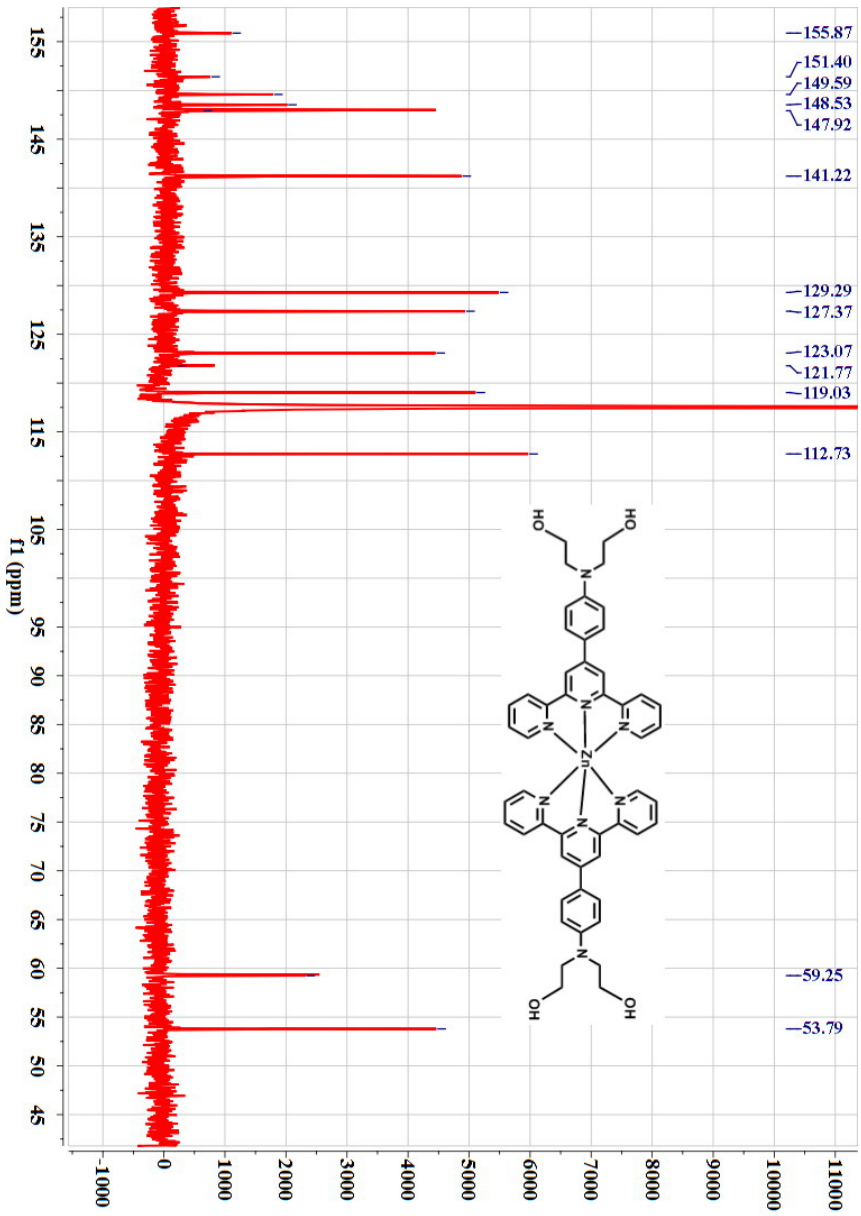

Figure S6. ^{13}C NMR spectrum of ZnTPYOH in d_3-CD_3CN

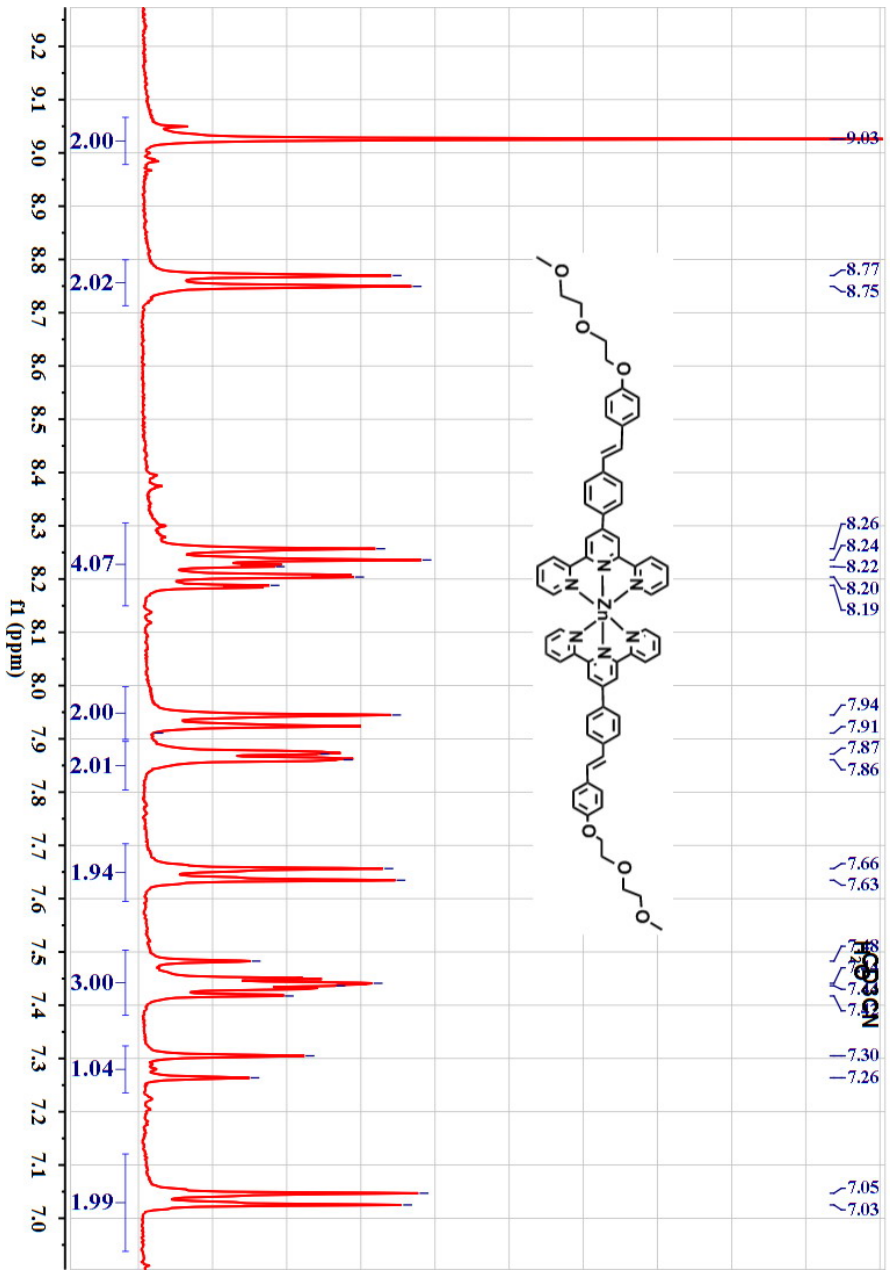

Figure S7. ^{1}H NMR spectrum of ZnO3TPY in d_3-CD_3CN

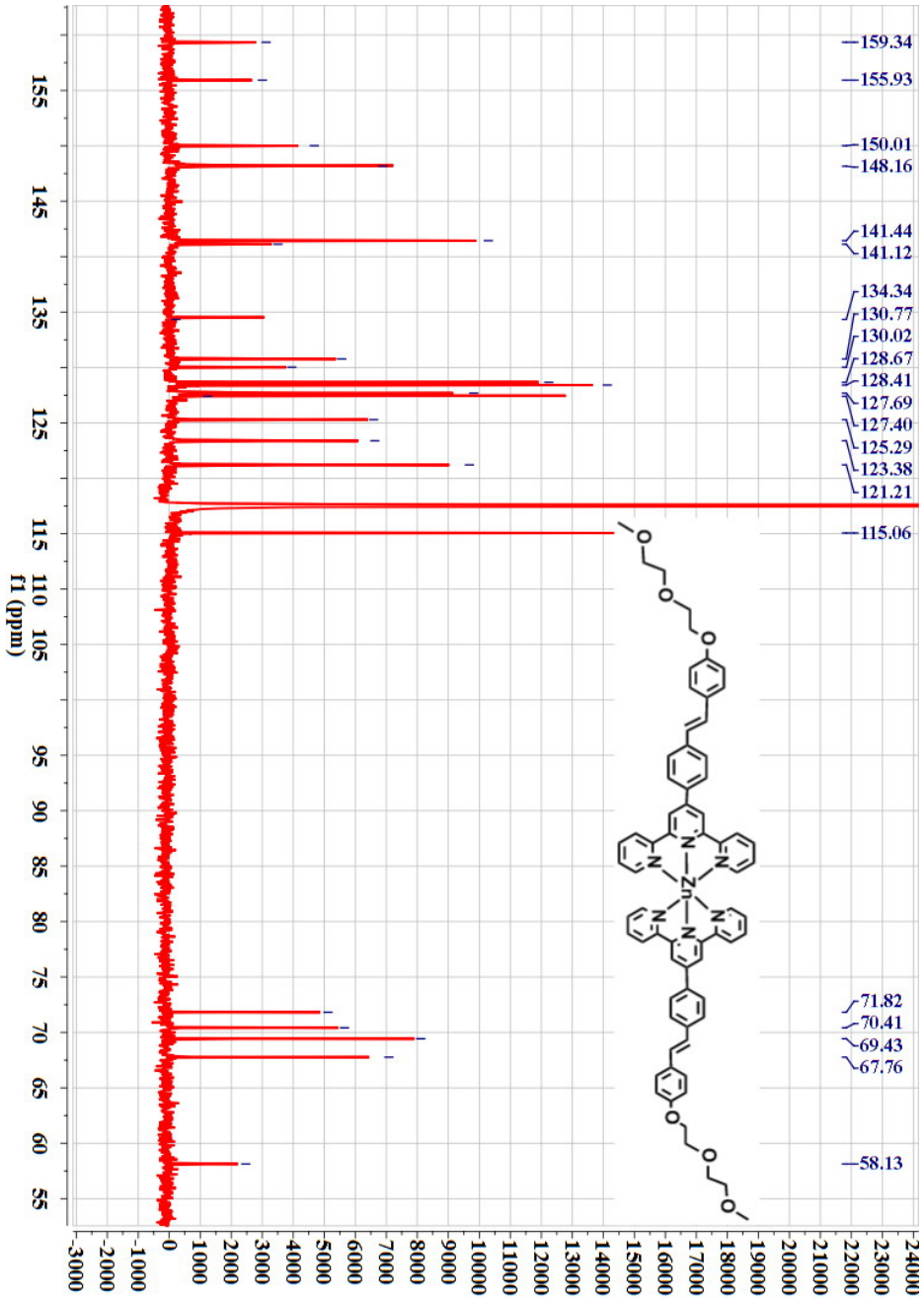

Figure S8. ^{13}C NMR spectrum of ZnO3TPY in d_3-CD_3CN

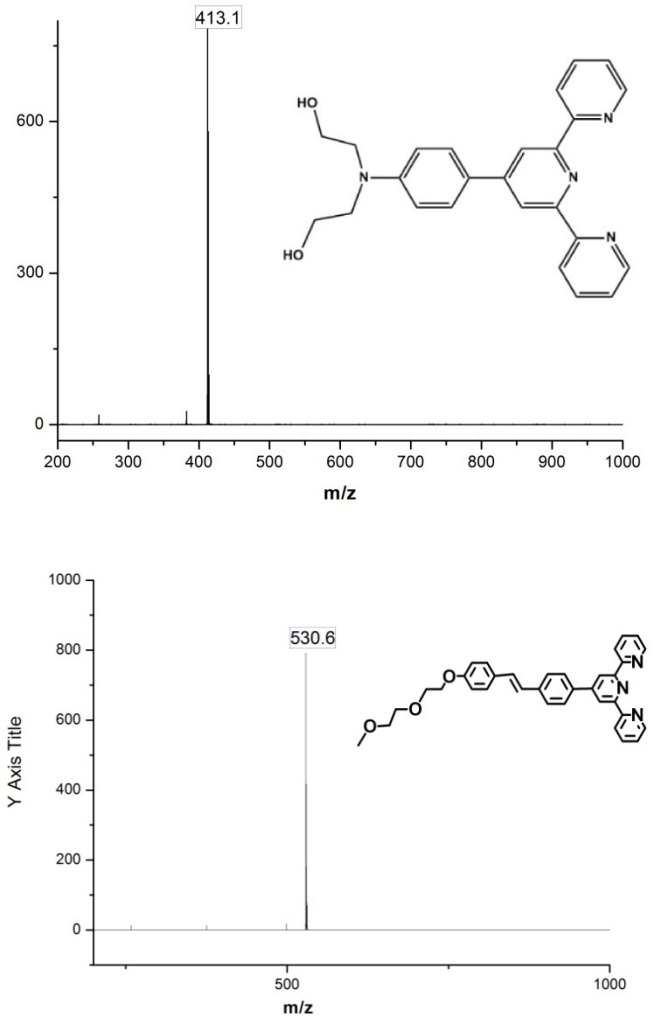

Figure S9. ESI-MS spectra for TPYOH (top) and O3TPY (bottom)

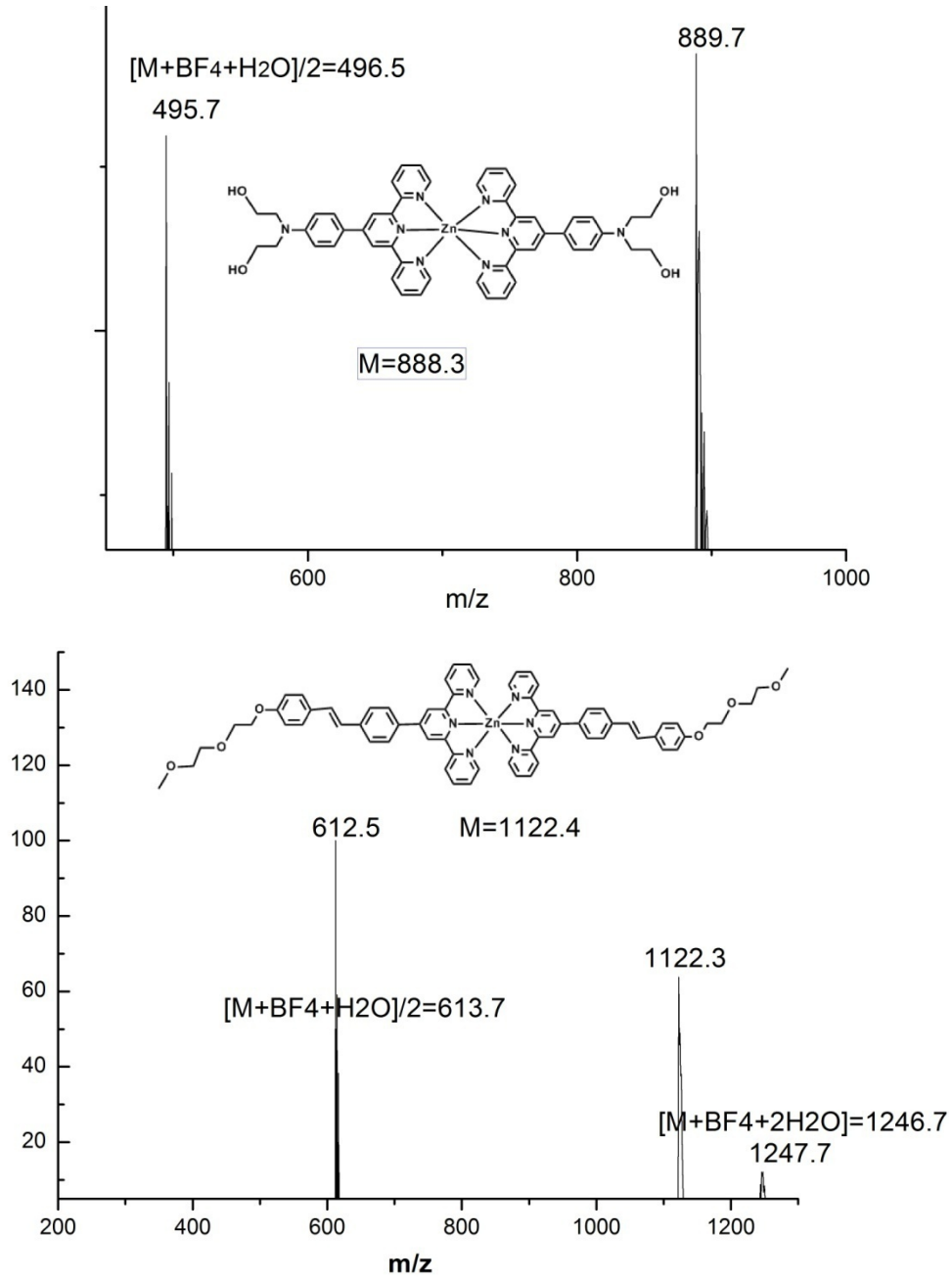

Figure S10. MALDI-TOF spectra for ZnTPYOH (top) and ZnO3TPY (bottom)

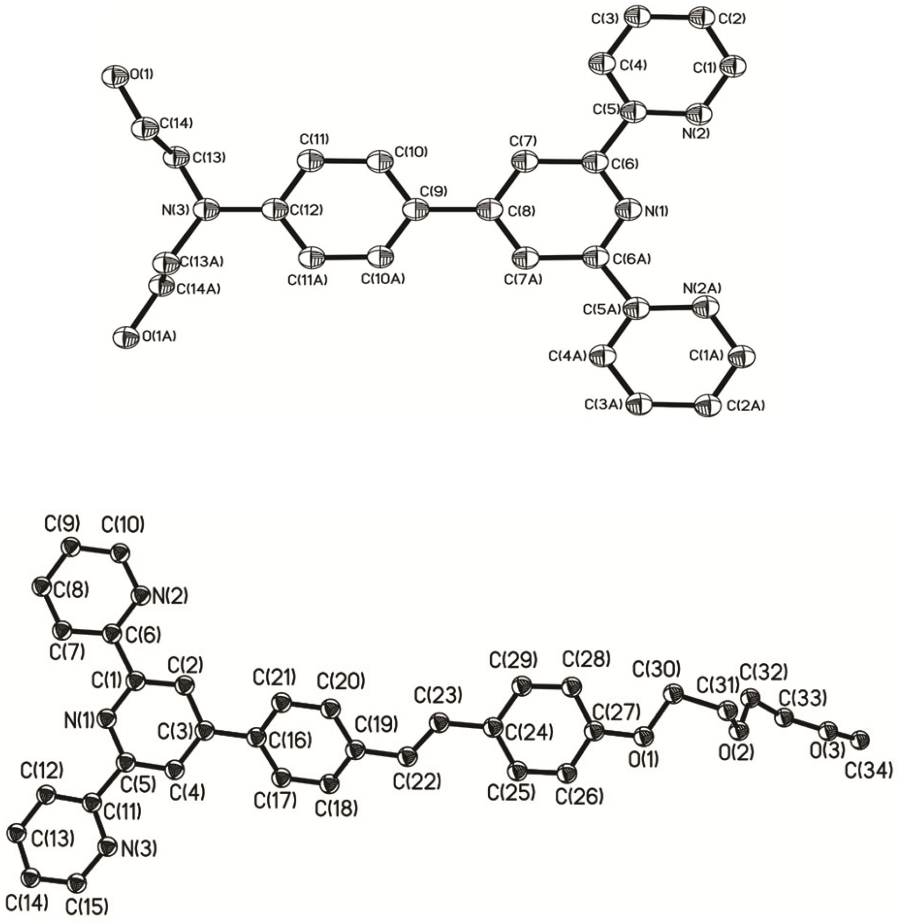

Figure S11. ORTEP drawing for TPYOH (top) and O3TPY(bottom). H atoms were omitted for clarity.

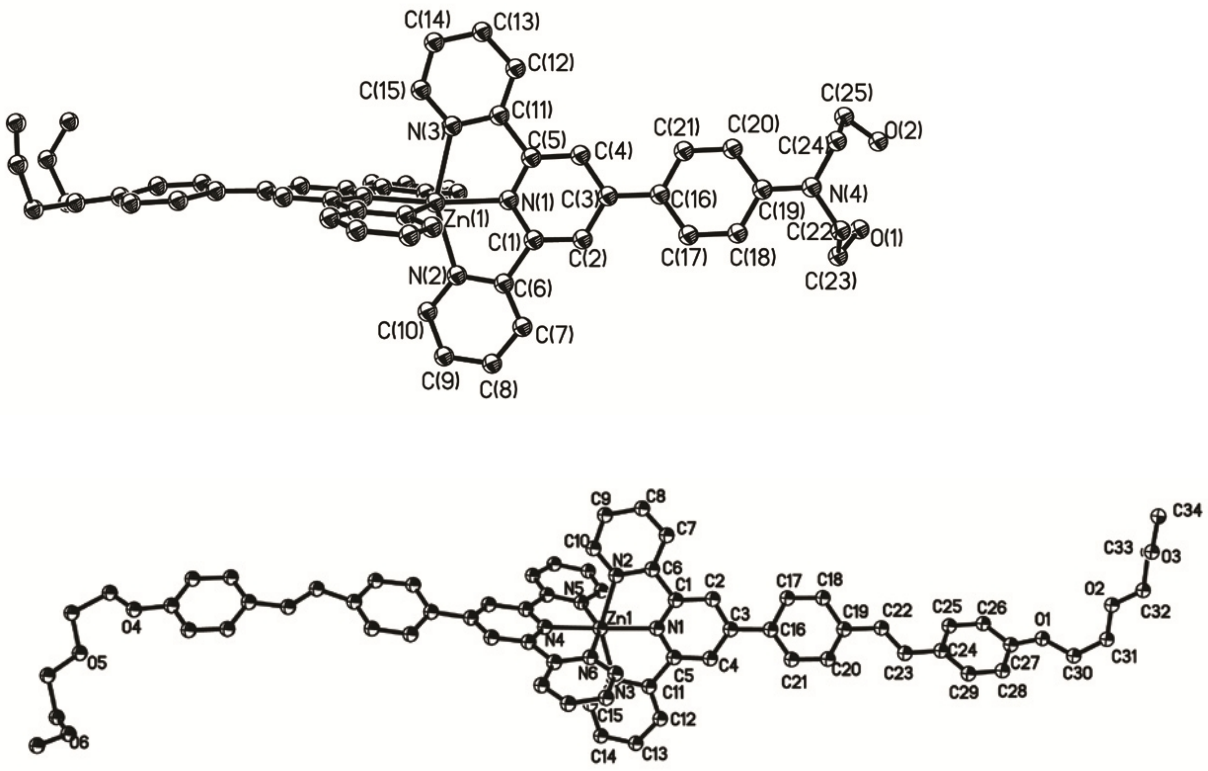

Figure S12. ORTEP drawing for ZnTPYOH (top) and ZnO3TPY (bottom). H atoms, BF_4^- and solvent molecules were omitted for clarity.

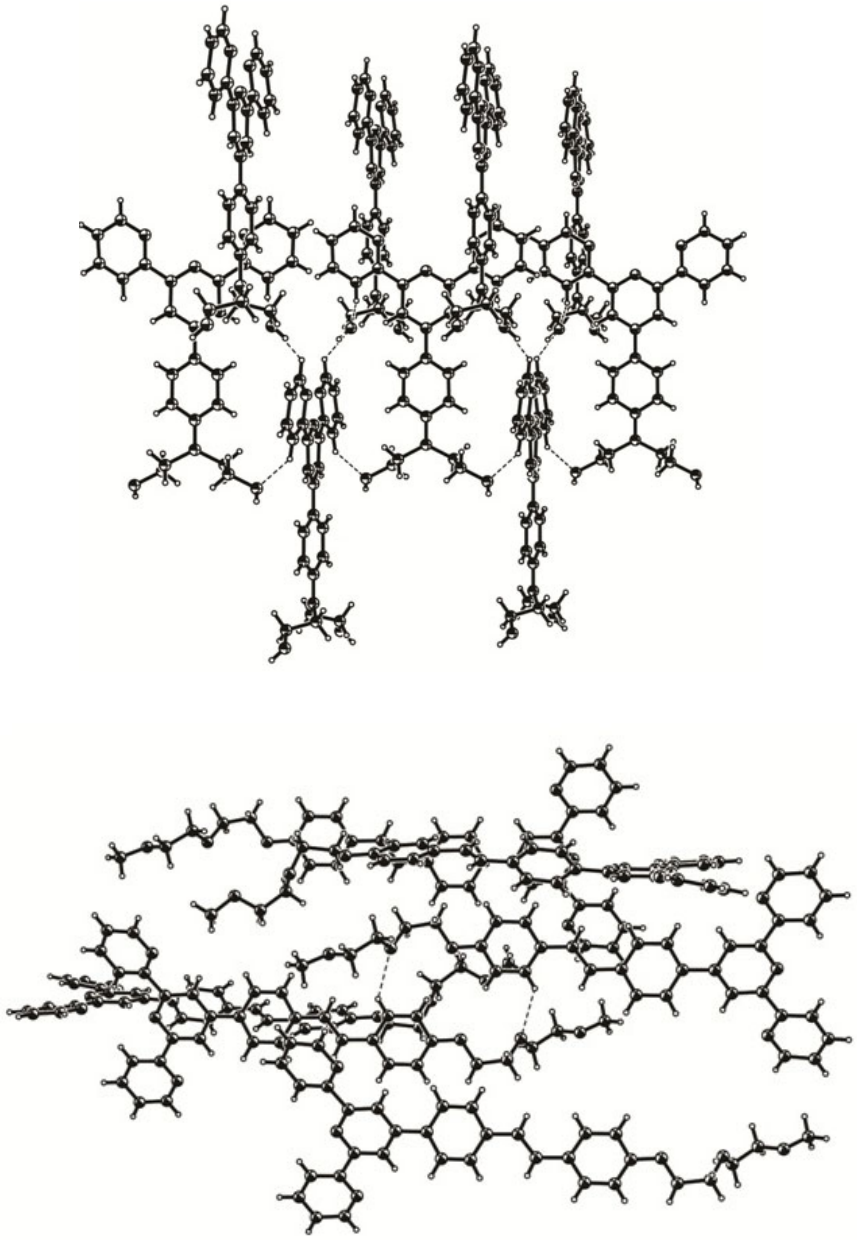

Figure S13. Diagrams of hydrogen bonds existed in TPYOH and O3TPY. TPYOH (top); O3TPY(bottom)

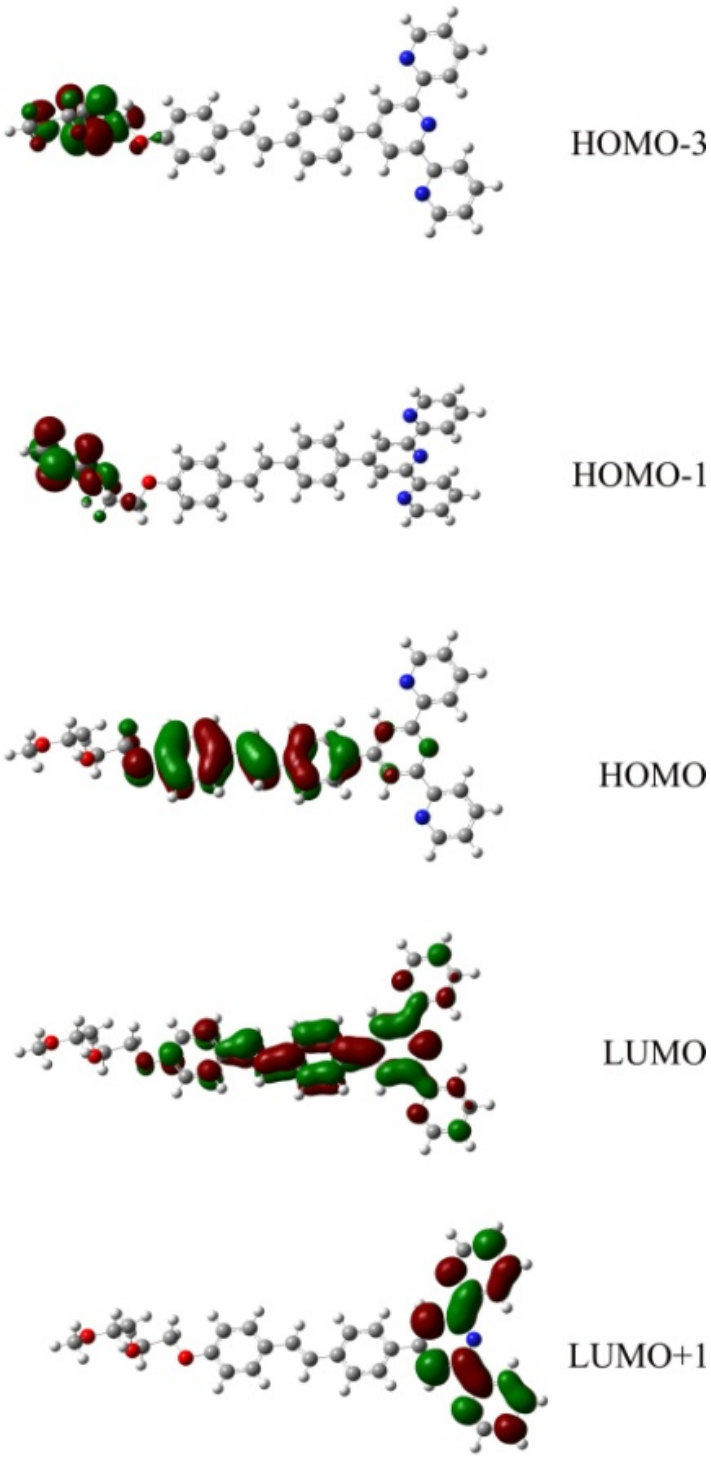

Figure S14. Molecular orbitals for O3TPY based on TD-DFT calculations

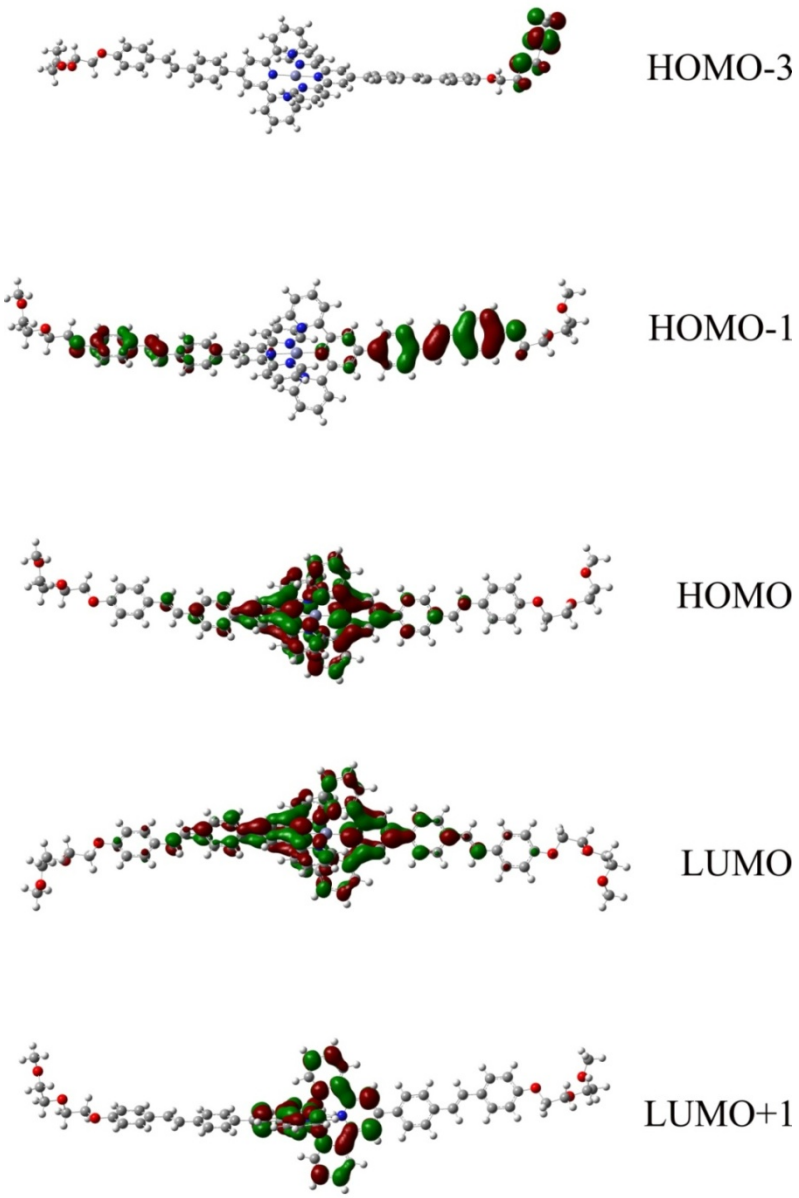

Figure S15. Molecular orbitals for ZnO3TPY based on TD-DFT calculations

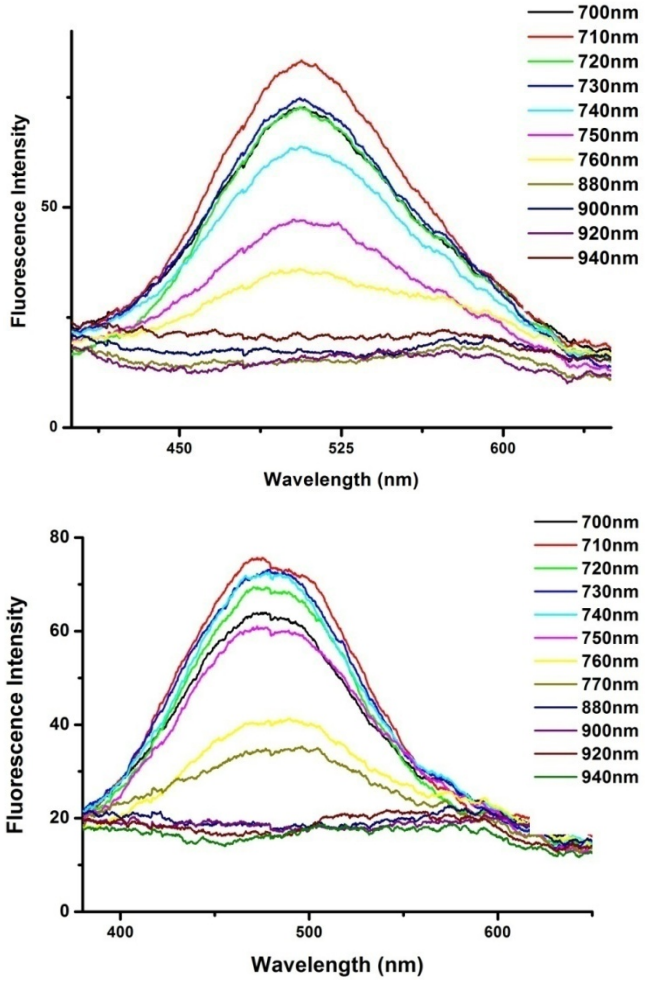

Figure S16. Two-photon excited fluorescence for TPYOH (top) and O3TPY (bottom) under different laser. The concentrations were 5×10^{-4} mol/L.

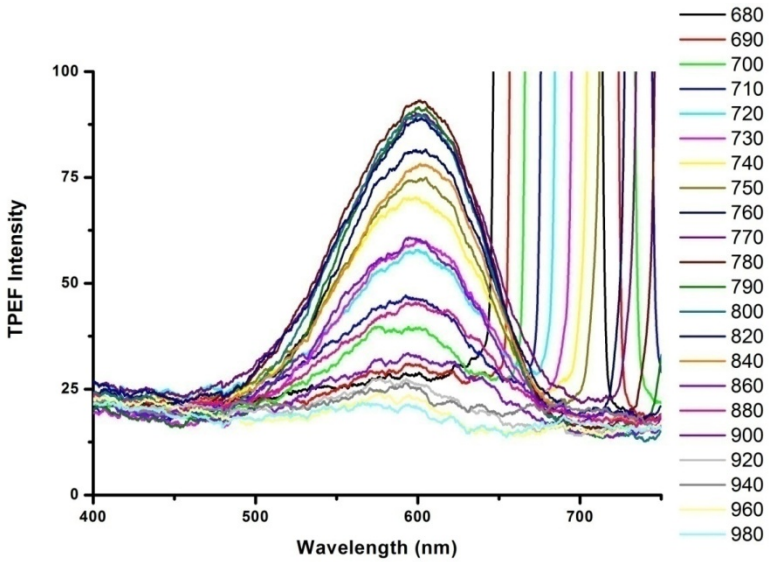

Figure S17. Two-photon excited fluorescence for ZnO3TPY in H_2O/DMSO. The concentration was 1×10^{-3} mol/L. (O3TPY was firstly dissolved in H_2O containing 1% DMSO with the concentration was 1mmol/L, then excess of $Zn(NO3)_2$ was added to completely convert the ligand into ZnO3TPY)

Table S1 Selected bond lengths and bond angels for the four compounds

Compound	Bond Length		Bond Angel	
TPYOH	N(1)-C(6)	1.333(5)	C(6)-N(1)-C(6)#1	117.8(5)
	N(1)-C(6)#1	1.333(5)	C(5)-N(2)-C(1)	117.1(5)
	N(2)-C(5)	1.328(6)	C(12)-N(3)-C(13')	117.2(6)
	N(2)-C(1)	1.356(6)	C(12)-N(3)-C(13')#1	117.2(6)
	N(3)-C(12)	1.394(10)	C(13')-N(3)-C(13')#1	125.6(12)
	N(3)-C(13')	1.51(3)	C(12)-N(3)-C(13)	115.7(6)
	N(3)-C(13')#1	1.51(3)	C(13')-N(3)-C(13)	51.8(7)
	N(3)-C(13)	1.55(2)	C(13')#1-N(3)-C(13)	102.8(9)
	N(3)-C(13)#1	1.55(2)	C(12)-N(3)-C(13)#1	115.7(6)
			C(13')-N(3)-C(13)#1	102.8(9)
			C(13')#1-N(3)-C(13)#1	51.8(7)
			C(13)-N(3)-C(13)#1	128.6(12)
			C(14)-O(1)-H(1)	109.5
			C(14')-O(1')-H(1')	109.5
			N(2)-C(1)-C(2)	122.7(6)
			N(2)-C(5)-C(4)	121.8(4)
			N(2)-C(5)-C(6)	116.8(4)
			C(4)-C(5)-C(6)	121.4(4)
			N(1)-C(6)-C(7)	122.5(4)
			N(1)-C(6)-C(5)	116.3(4)
ZnTPYOH	Zn(1)-N(5)	2.061(4)	N(5)-Zn(1)-N(1)	171.54(16)
	Zn(1)-N(1)	2.071(4)	N(5)-Zn(1)-N(2)	109.54(15)
	Zn(1)-N(2)	2.165(4)	N(1)-Zn(1)-N(2)	75.64(15)
	Zn(1)-N(6)	2.169(4)	N(5)-Zn(1)-N(6)	75.72(16)
	Zn(1)-N(3)	2.207(4)	N(1)-Zn(1)-N(6)	111.05(16)
	Zn(1)-N(7)	2.208(4)	N(2)-Zn(1)-N(6)	94.23(16)
	N(1)-C(1)	1.339(6)	N(5)-Zn(1)-N(3)	98.84(15)
	N(1)-C(5)	1.347(6)	N(1)-Zn(1)-N(3)	75.60(15)
	N(2)-C(10)	1.344(6)	N(2)-Zn(1)-N(3)	151.19(15)
	N(2)-C(6)	1.350(6)	N(6)-Zn(1)-N(3)	97.52(15)
	N(3)-C(15)	1.333(6)	N(5)-Zn(1)-N(7)	75.74(15)
	N(3)-C(11)	1.353(6)	N(1)-Zn(1)-N(7)	97.79(15)
	N(4)-C(19)	1.369(6)	N(2)-Zn(1)-N(7)	91.05(15)
	N(4)-C(22)	1.448(7)	N(6)-Zn(1)-N(7)	151.10(15)
	N(4)-C(24)	1.460(7)	N(3)-Zn(1)-N(7)	91.21(14)
	N(5)-C(26)	1.340(6)	C(1)-N(1)-C(5)	120.3(4)
	N(5)-C(30)	1.349(6)	C(1)-N(1)-Zn(1)	120.0(3)
	N(6)-C(35)	1.335(6)	C(5)-N(1)-Zn(1)	119.6(3)
	N(6)-C(31)	1.344(6)	C(10)-N(2)-C(6)	118.3(5)
	N(7)-C(40)	1.335(6)	C(10)-N(2)-Zn(1)	125.4(4)
	N(7)-C(36)	1.348(6)	C(6)-N(2)-Zn(1)	116.2(3)

	N(8)-C(44)	1.380(6)	C(15)-N(3)-C(11)	118.4(4)
	N(8)-C(47)	1.445(7)	C(15)-N(3)-Zn(1)	126.6(3)
	N(8)-C(49)	1.475(7)	C(11)-N(3)-Zn(1)	114.9(3)
			C(19)-N(4)-C(22)	120.4(4)
			C(19)-N(4)-C(24)	119.9(4)
			C(22)-N(4)-C(24)	118.5(4)
			C(26)-N(5)-C(30)	119.9(4)
			C(26)-N(5)-Zn(1)	120.2(3)
			C(30)-N(5)-Zn(1)	119.9(3)
			C(35)-N(6)-C(31)	118.3(5)
			C(35)-N(6)-Zn(1)	126.3(4)
			C(31)-N(6)-Zn(1)	115.4(3)
			C(40)-N(7)-C(36)	118.7(4)
			C(40)-N(7)-Zn(1)	127.0(3)
			C(36)-N(7)-Zn(1)	114.3(3)
			C(44)-N(8)-C(47)	122.8(5)
			C(44)-N(8)-C(49)	121.0(5)
			C(47)-N(8)-C(49)	116.2(5)
O3TPY	N(1)-C(5)	1.339(6)	C(5)-N(1)-C(1)	118.2(4)
	N(1)-C(1)	1.340(6)	C(10)-N(2)-C(6)	117.3(5)
	N(2)-C(10)	1.334(7)	C(11)-N(3)-C(15)	116.9(5)
	N(2)-C(6)	1.335(6)	N(1)-C(1)-C(2)	122.6(4)
	N(3)-C(11)	1.334(7)	N(1)-C(1)-C(6)	115.3(4)
	N(3)-C(15)	1.336(7)	N(1)-C(5)-C(4)	122.5(4)
			N(1)-C(5)-C(11)	115.9(4)
			N(2)-C(6)-C(7)	122.9(5)
			N(2)-C(6)-C(1)	116.8(4)
			N(2)-C(10)-C(9)	123.3(6)
			N(2)-C(10)-H(10)	118.3
			N(3)-C(11)-C(12)	122.7(5)
			N(3)-C(11)-C(5)	116.8(4)
			N(3)-C(15)-C(14)	124.0(6)
			N(3)-C(15)-H(15)	118.0
ZnO3TPY	Zn(1)-N(4)	2.055(4)	N(4)-Zn(1)-N(1)	175.28(16)
	Zn(1)-N(1)	2.087(4)	N(4)-Zn(1)-N(3)	107.42(15)
	Zn(1)-N(3)	2.165(4)	N(1)-Zn(1)-N(3)	75.62(16)
	Zn(1)-N(2)	2.185(4)	N(4)-Zn(1)-N(2)	101.92(15)
	Zn(1)-N(5)	2.186(4)	N(1)-Zn(1)-N(2)	75.06(16)
	Zn(1)-N(6)	2.203(4)	N(3)-Zn(1)-N(2)	150.65(16)
	N(1)-C(1)	1.336(7)	N(4)-Zn(1)-N(5)	75.71(15)
	N(1)-C(5)	1.344(6)	N(1)-Zn(1)-N(5)	107.71(16)
	N(2)-C(10)	1.337(7)	N(3)-Zn(1)-N(5)	97.49(15)
	N(2)-C(6)	1.345(6)	N(2)-Zn(1)-N(5)	90.29(16)
	N(3)-C(11)	1.339(6)	N(4)-Zn(1)-N(6)	75.97(15)

	N(3)-C(15)	1.345(6)	N(1)-Zn(1)-N(6)	100.67(16)
	N(4)-C(35)	1.337(6)	N(3)-Zn(1)-N(6)	89.02(15)
	N(4)-C(39)	1.346(6)	N(2)-Zn(1)-N(6)	97.47(16)
	N(5)-C(44)	1.325(7)	N(5)-Zn(1)-N(6)	151.61(16)
	N(5)-C(40)	1.345(6)	C(1)-N(1)-C(5)	120.3(4)
	N(6)-C(49)	1.324(7)	C(1)-N(1)-Zn(1)	120.3(3)
	N(6)-C(45)	1.347(6)	C(5)-N(1)-Zn(1)	119.4(3)
	N(7)-C(69)	1.14(3)	C(10)-N(2)-C(6)	118.4(5)
	N(8)-C(71)	1.087(8)	C(10)-N(2)-Zn(1)	125.8(3)
			C(6)-N(2)-Zn(1)	115.7(3)
			C(11)-N(3)-C(15)	119.3(4)
			C(11)-N(3)-Zn(1)	115.9(3)
			C(15)-N(3)-Zn(1)	124.6(3)
			C(35)-N(4)-C(39)	119.8(4)
			C(35)-N(4)-Zn(1)	120.0(3)
			C(39)-N(4)-Zn(1)	119.9(3)
			C(44)-N(5)-C(40)	119.0(4)
			C(44)-N(5)-Zn(1)	126.3(4)
			C(40)-N(5)-Zn(1)	114.3(3)
			C(49)-N(6)-C(45)	119.4(5)
			C(49)-N(6)-Zn(1)	126.4(4)
			C(45)-N(6)-Zn(1)	113.7(3)