Supporting information

An AIE fluorescent switch with multi-stimuli responsive property and application for quantitatively detecting pH value, sulfite anion and hydrostatic pressure

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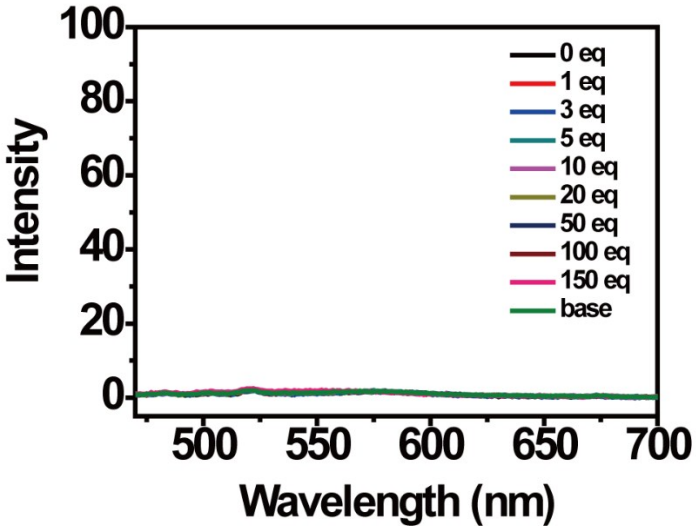

Fig. S1 PL spectra of TPE-Sp-CN in acetonitrile solution (1×10^{-5} M) before and after different equivalent of acid addition then sufficient base treatment.

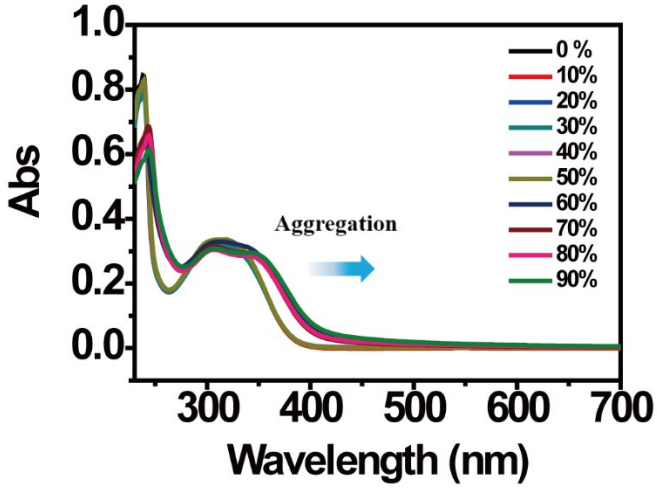

Fig. S2 Absorption spectra of TPE-Sp-CN (1×10^{-5} M) in different volume fraction of MeCN/H_2O mixture.

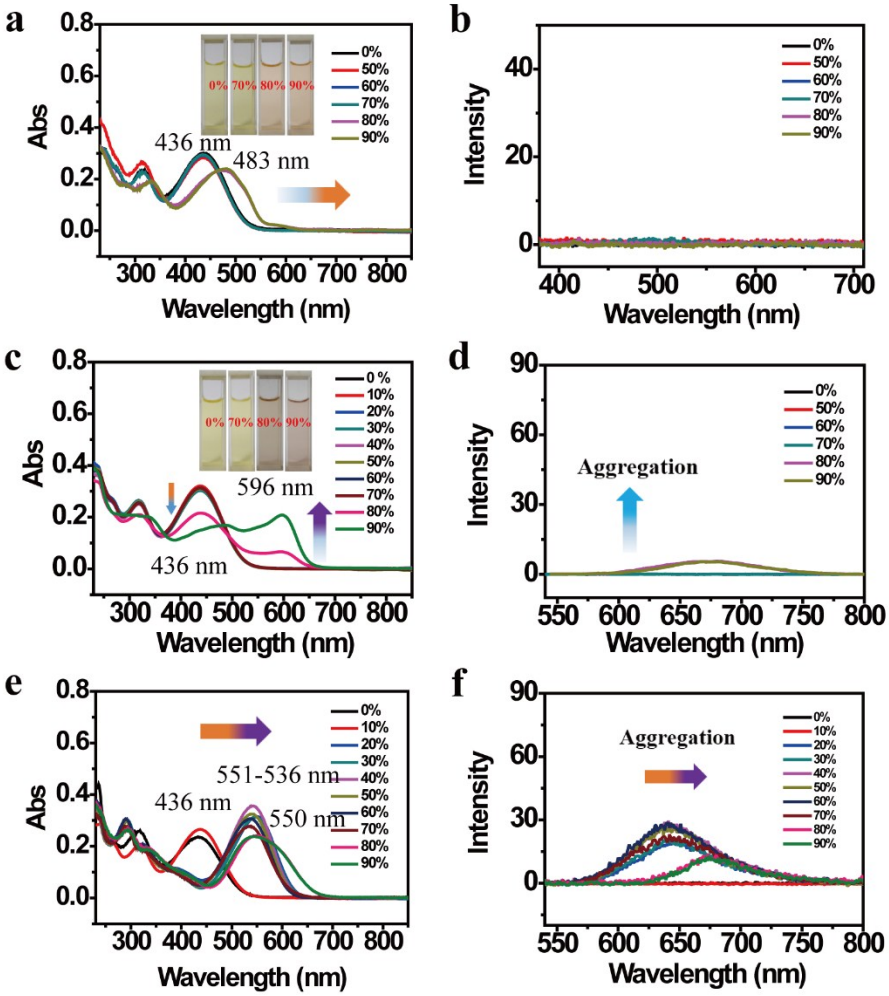

Fig. S3 (a), (c), (e) Absorption spectra and (b), (d), (f) PL spectra of TPE-Sp-CN (1×10^{-5}M) with 500 eq., 80 eq., 20 eq. HCl in different volume fraction of MeCN/H_2O mixture, respectively.

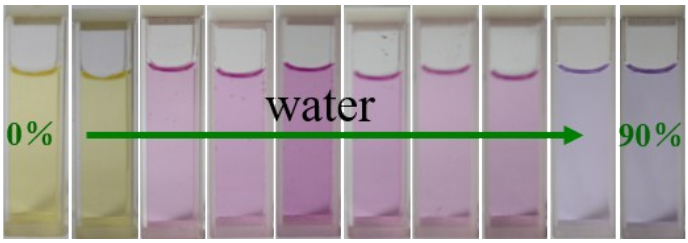

Fig. S4 The pictures of TPE-Sp-CN with 20 eq. HCl addition in different volume fraction of water/acetonitrile mixture. The pictures were taken under ambient light and the concentration of TPE-Sp-CN is 1×10^{-5} M.

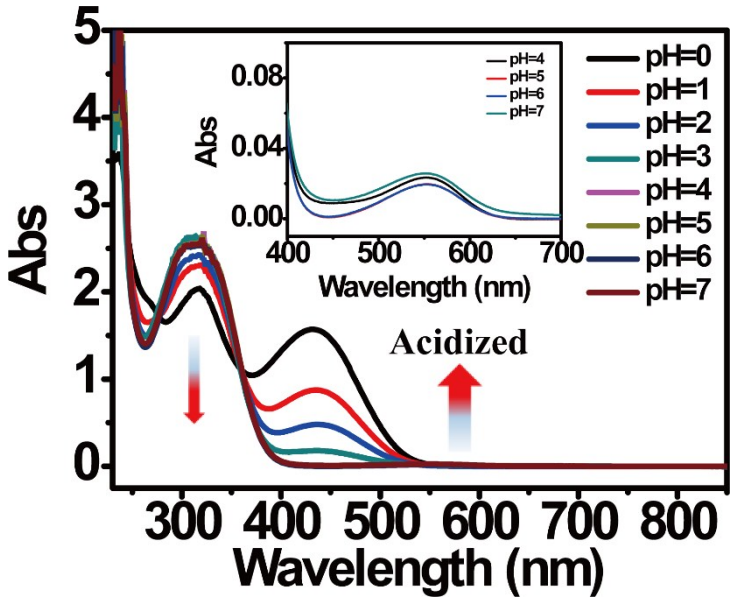

Fig. S5 Absorption spectra of TPE-Sp-CN solution (1×10^{-4} M) added with 0.2 mL water sample of pH from 0 to 7. Inset: the amplified absorption spectra from 400 nm to 700 nm. The absorption at about 552 nm originated from TPE-MC-CN which was induced by water.

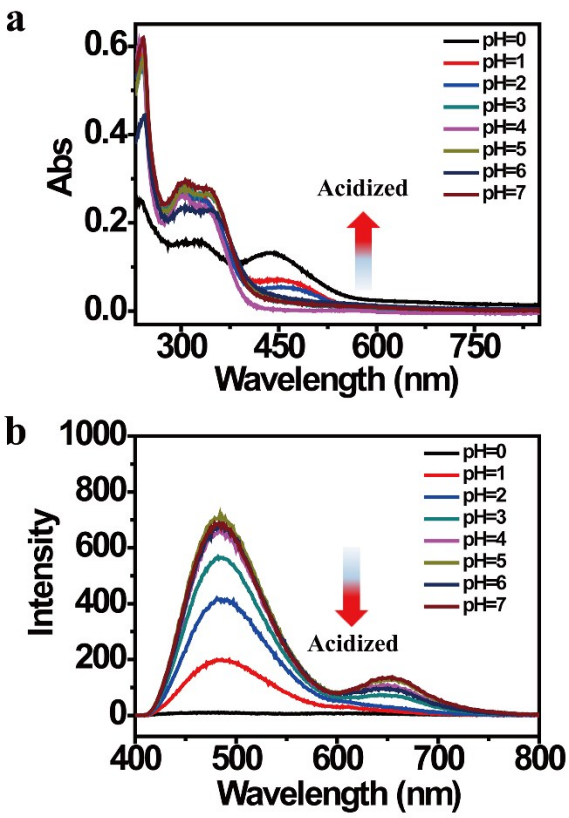

Fig. S6 (a) Absorption spectra (b) and PL spectra of TPE-Sp-CN solution (1×10^{-5} M) with 90% water with pH from 0 to 7. The obvious red shift of absorption spectra compared with that in Fig. S5 meant that aggregation process happened.

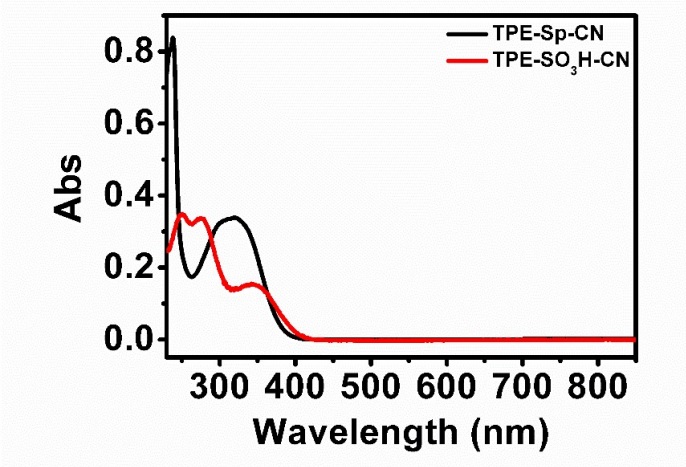

Fig. S7 The contrast of absorption spectra of TPE-Sp-CN and TPE-SO_3H-CN. Solution concentration were 1×10^{-5} M. The different absorption in UV range meant that the decolor of solution was due to addtion reaction rather than ring-closing process.

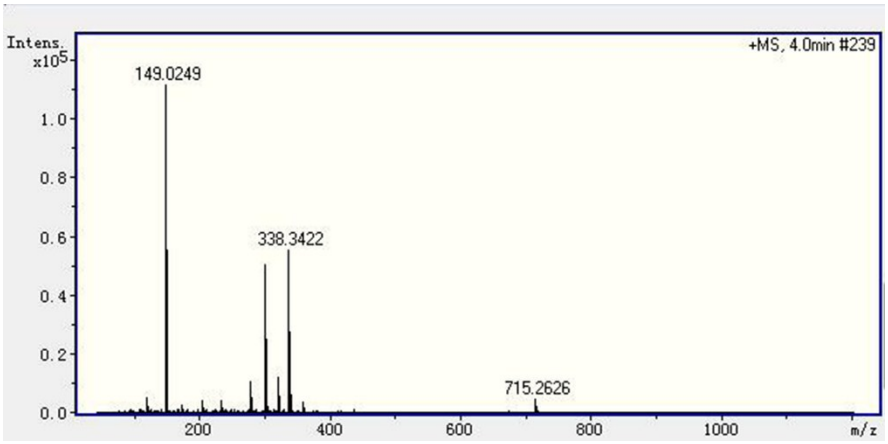

Fig. S8 MS spectrum of TPE-SO_3H-CN. m/z: 715.2626 $[M]^+$, calcd: 715.2625.

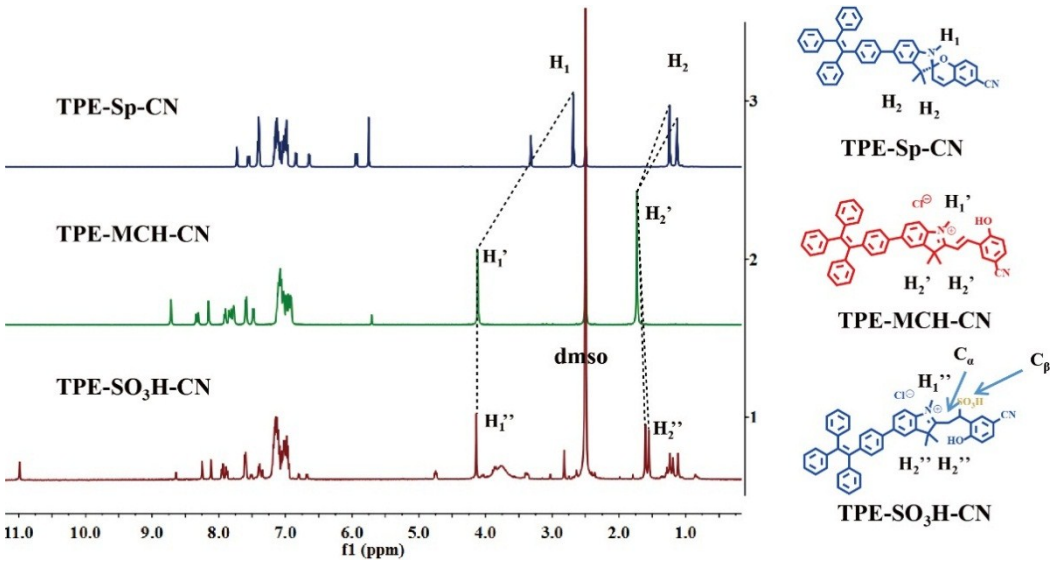

Fig. S9 ^{1}H NMR characterization of addition product TPE-SO_3H-CN. 1: ^{1}H NMR spectrum of TPE-SO_3H-CN. 2: ^{1}H NMR spectrum of TPE-MCH-CN. 3: ^{1}H NMR spectrum of TPE-Sp-CN. DMSO-d_6 were used as deuterated solvent. TPE-SO_3H-CN sample was obtained by centrifugation of the detection solution.

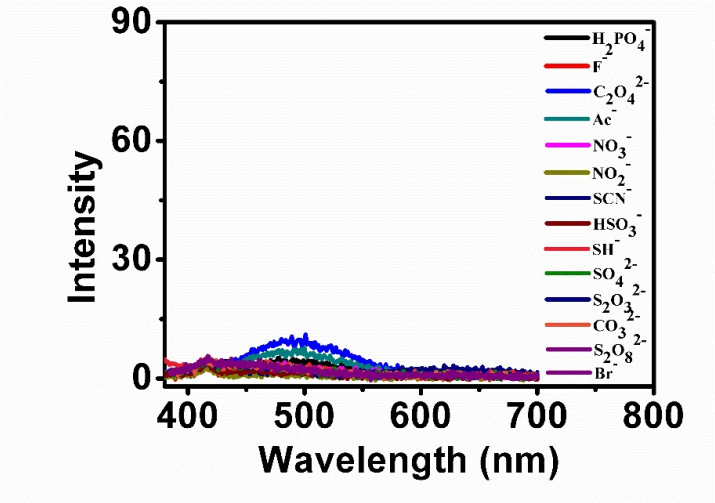

Fig. S10 PL spectra of low concentration TPE-MCH-CN in fourteen anions conditions. TPE-MCH-CN concentration: 1×10^{-5} M, HCl concentration: 5×10^{-3} M, anions concentration: 1×10^{-3} M.

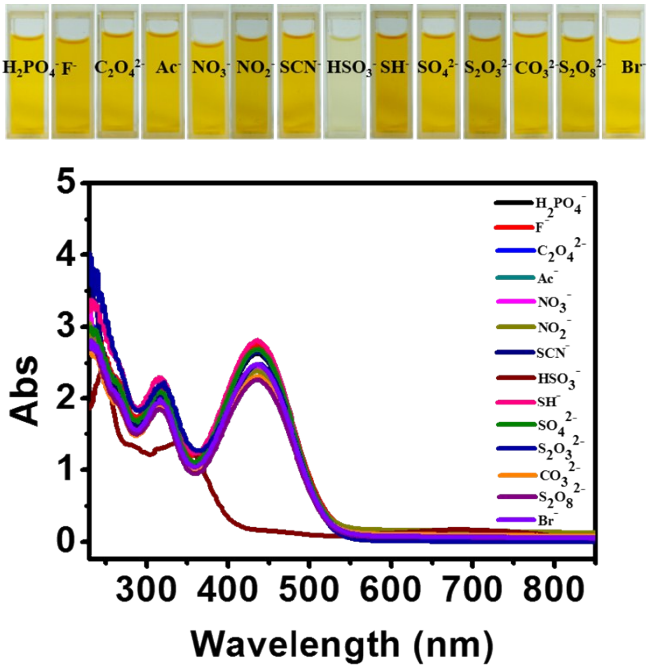

Fig. S11 Absorption spectra of high concentration TPE-MCH-CN in fourteen anions conditions. TPE-MCH-CN concentration: 1×10^{-4} M, HCl concentration: 5×10^{-3} M, anions concentration: 1×10^{-3} M. Corresponding pictures were taken under ambient light.

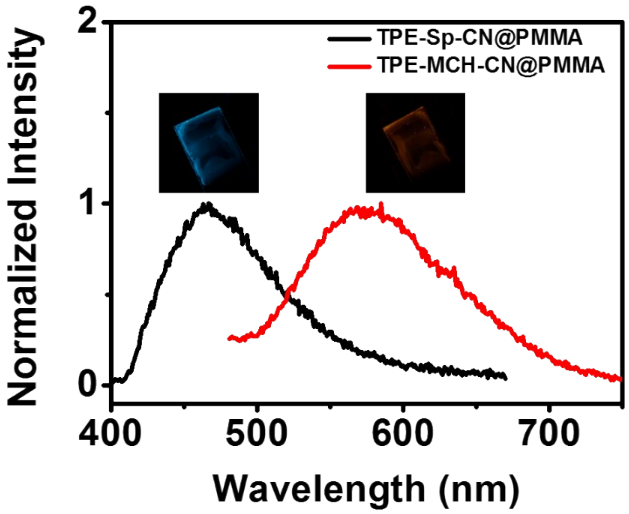

Fig. S12 PL spectra of TPE-Sp-CN doped PMMA film (TPE-Sp-CN@PMMA) and TPE-MCH-CN doped PMMA film (TPE-MCH-CN@PMMA). TPE-MCH-CN@PMMA was obtained by treating TPE-Sp-CN@PMMA with HCl gas. Mass ratio: TPE-Sp-CN: PMMA=1/100.

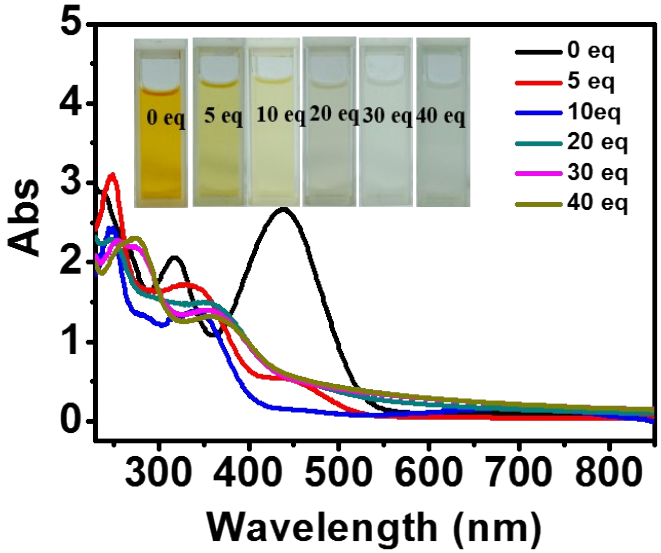

Fig. S13 Absorption spectra of TPE-MCH-CN solution with different HSO_3^- concentrations. TPE-MCH-CN concentration: 1×10^{-4} M, HCl concentration: 5×10^{-3} M, HSO_3^- concentration: 0 M ~ 4×10^{-3} M. Corresponding pictures were taken under ambient light.

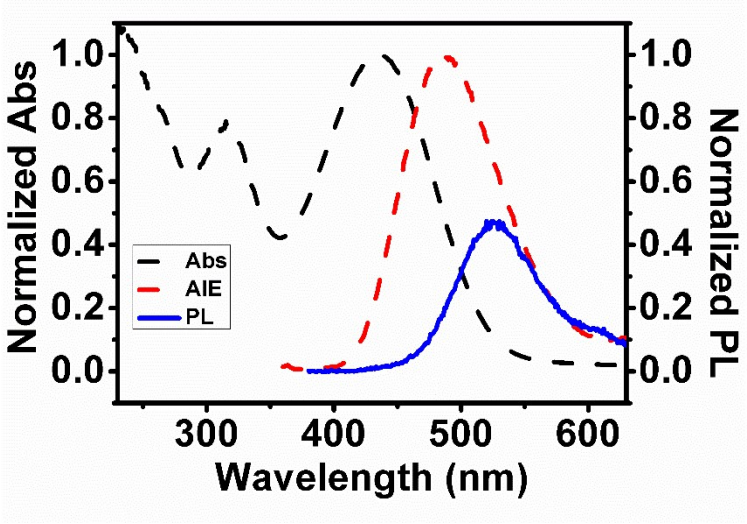

Fig. S14 The normalized absorption spectrum of TPE-MCH-CN solution (black dash line), normalized PL spectrum of TPE-Sp-CN aggregates (red dash line), and PL spectrum (blue solid line) of anion detection solution (TPE-Sp-CN: 1×10^{-4} M, HCl: 5×10^{-3} M, KF: 1×10^{-3} M).

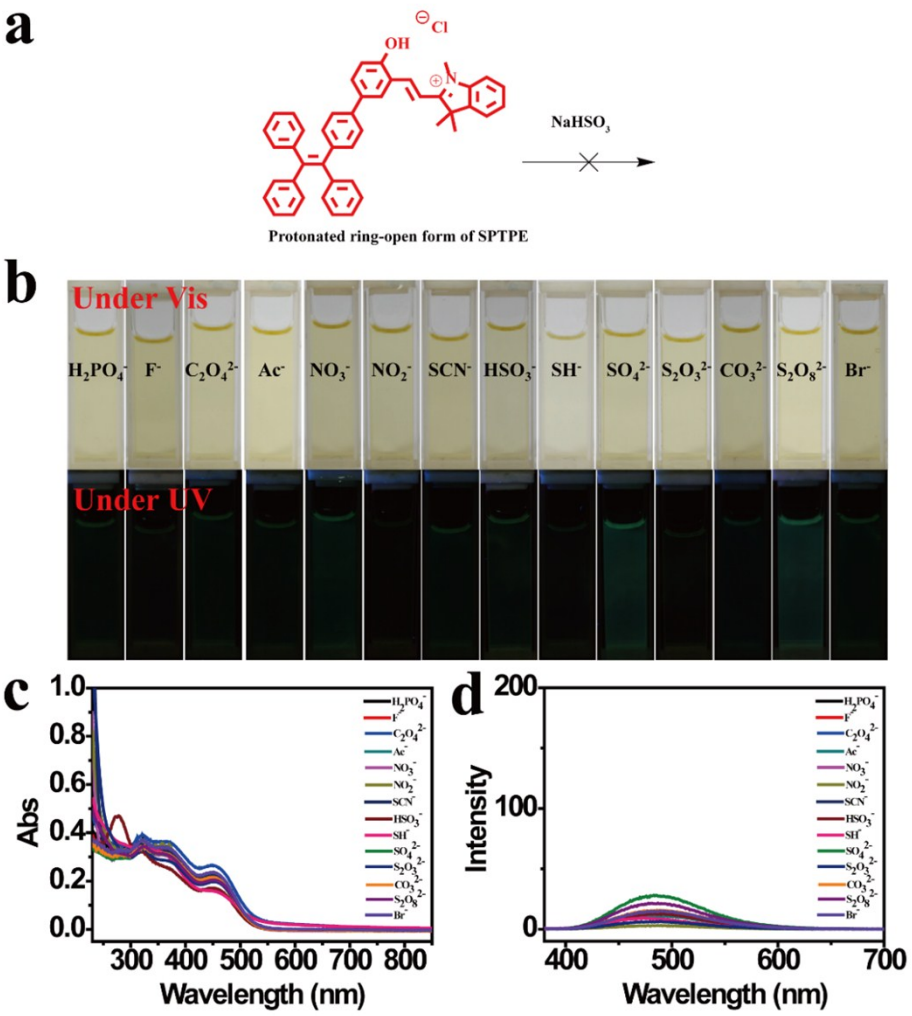

Fig. S15 (a) The structure of protonated ring-open form of SPTPE. (b) The images of SPTPE in fourteen anions detection solution under visible light (up) and 365 nm UV light (down). (c) Absorption spectra and (d) PL spectra of SPTPE in fourteen anions detection solution. Detection solution: 1×10^{-5} M SPTPE, 5×10^{-3} M HCl and 1×10^{-3} M anions.

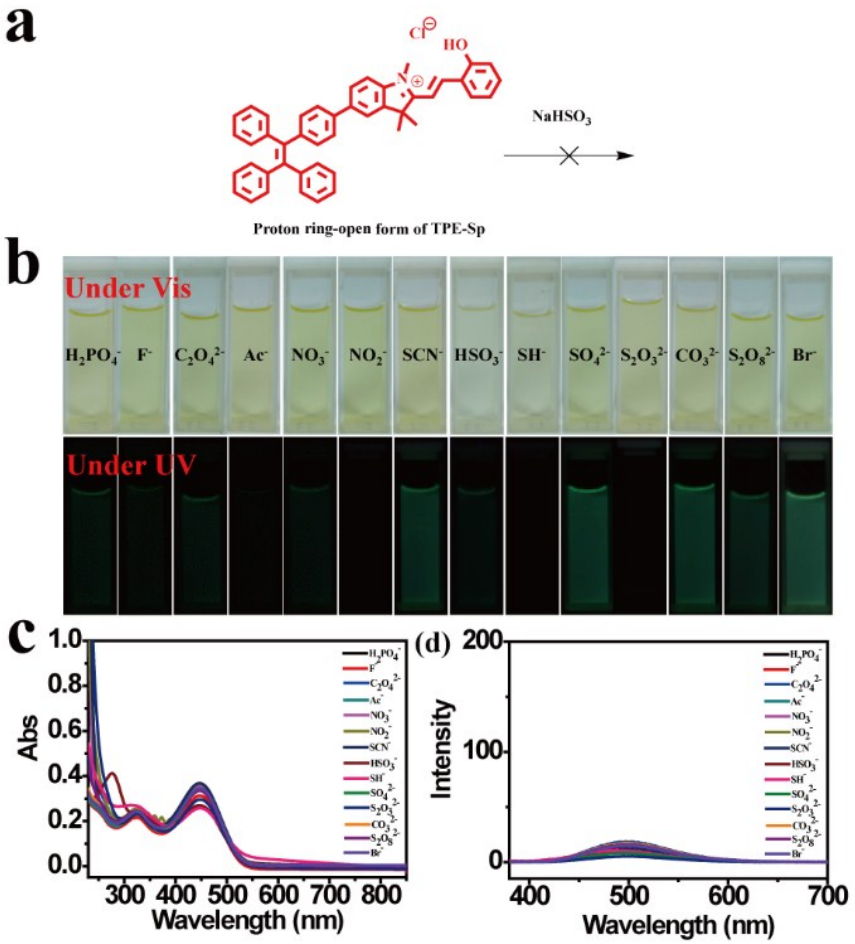

Fig. S16 (a) The structure of protonated ring-open form of TPE-Sp. (b) The images of TPE-Sp in fourteen anions detection solution under visible light (up) and 365 nm UV light (down). (c) Absorption spectra and (d) PL spectra of TPE-Sp in fourteen anions detection solution. Detection solution: 1×10^{-5} M TPE-Sp, 5×10^{-3} M HCl and 1×10^{-3} M anions.

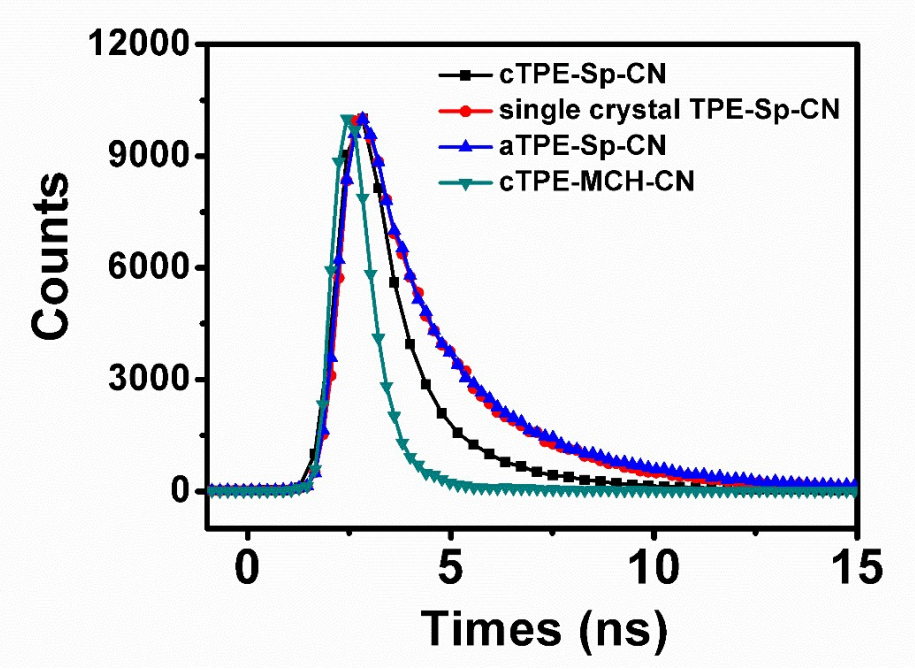

Fig. S17 Time-resolved decay spectra of cTPE-Sp-CN, single crystal TPE-Sp-CN, aTPE-Sp-CN and cTPE-MCH-CN.

Table S1. The quantum yields, lifetimes, irradiation rate and non-irradiation rates of cTPE-Sp-CN, single crystal TPE-Sp-CN, aTPE-Sp-CN and cTPE-MCH-CN.

Sample	φ_F (%)	τ_1	τ_2	k_r	K_{nr}
cTPE-Sp-CN	**2.76%**	0.80 ns(50.91%)	2.30 ns(49.09%)	$1.7965\times10^{7}s^{-1}$	$6.329\times10^{8}s^{-1}$
Single crystal TPE-Sp-CN	**6.15%**	1.40 ns(34.02%)	3.04ns(65.98%)	$2.477\times10^{7}s^{-1}$	$3.781\times10^{8}s^{-1}$
aTPE-Sp-CN	**34.62%**	1.47ns(41.29%)	3.61ns(58.71%)	$1.2698\times10^{8}s^{-1}$	$2.398\times10^{8}s^{-1}$
cTPE-MCH-CN	**4.52%**	0.41ns(84.94%)	1.14ns(15.06%)	$8.694\times10^{7}s^{-1}$	$1.8365\times10^{9}s^{-1}$

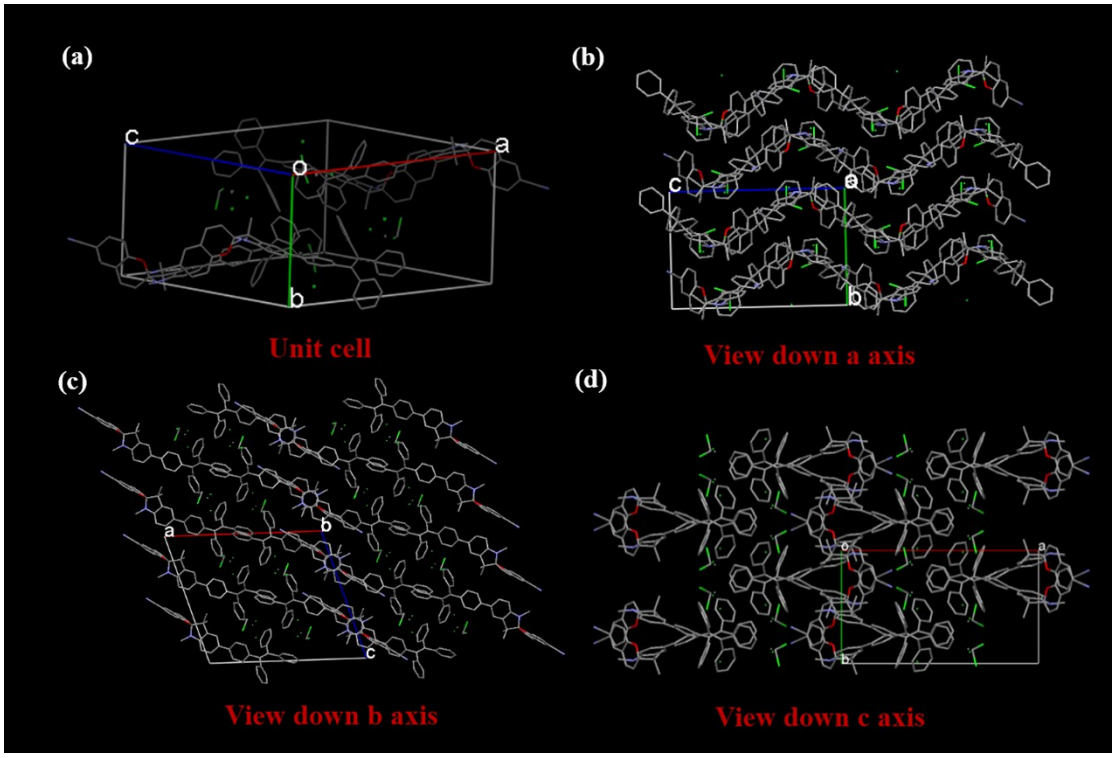

Fig. S18 (a) The unit cell of single crystal TPE-Sp-CN, and the packing patterns viewed down (b) a axis, (c) b axis and (d) c axis, respectively.

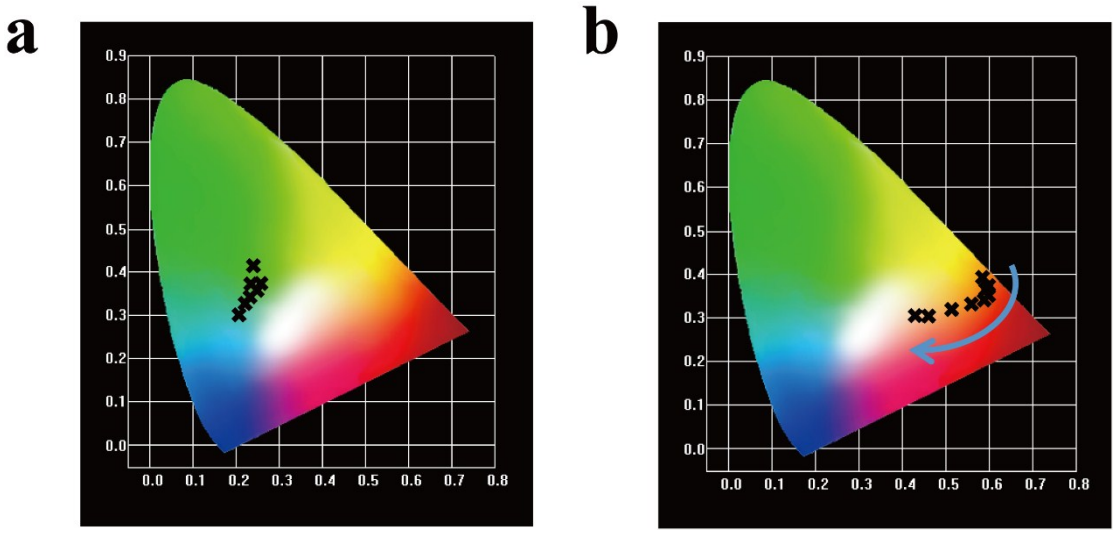

Fig. S19 (a) The CIE graph of single crystal of TPE-Sp-CN emission under pressure from 0.00 GPa to 3.99 GPa; (b) The CIE graph of cTPE-MCH-CN emission under pressure from 0.00 GPa to 6.05 GPa.

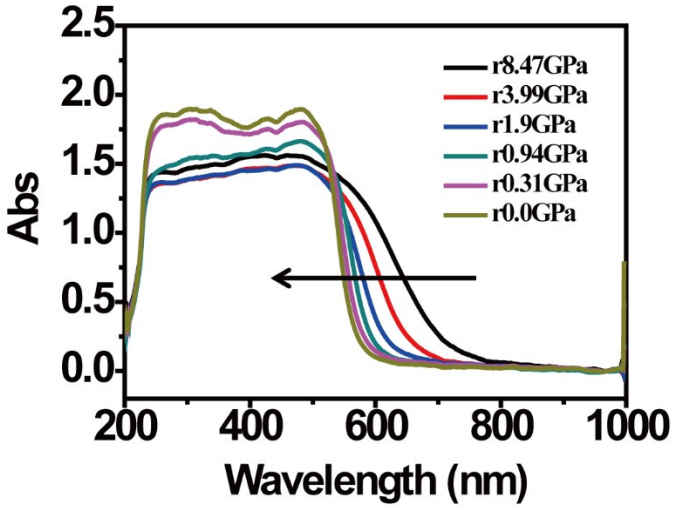

Fig. S20 The insitu absorption spectra of cTPE-MCH-CN in pressure releasing process.

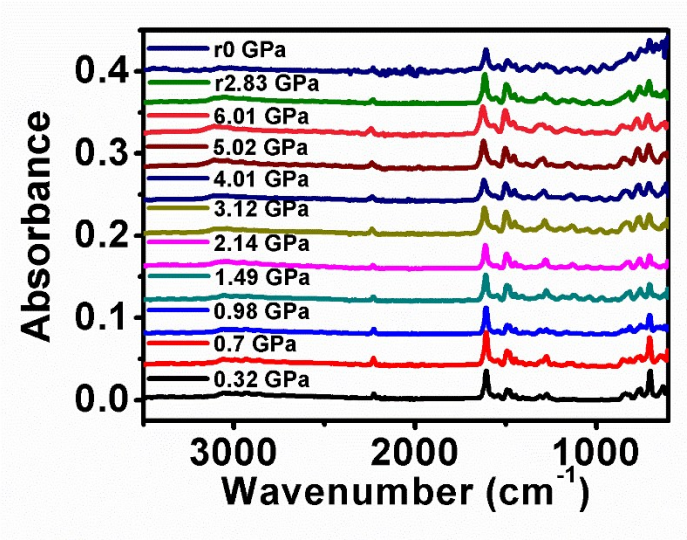

Fig. S21 The insitu IR spectra of cTPE-MCH-CN in pressurization and depressurization process.

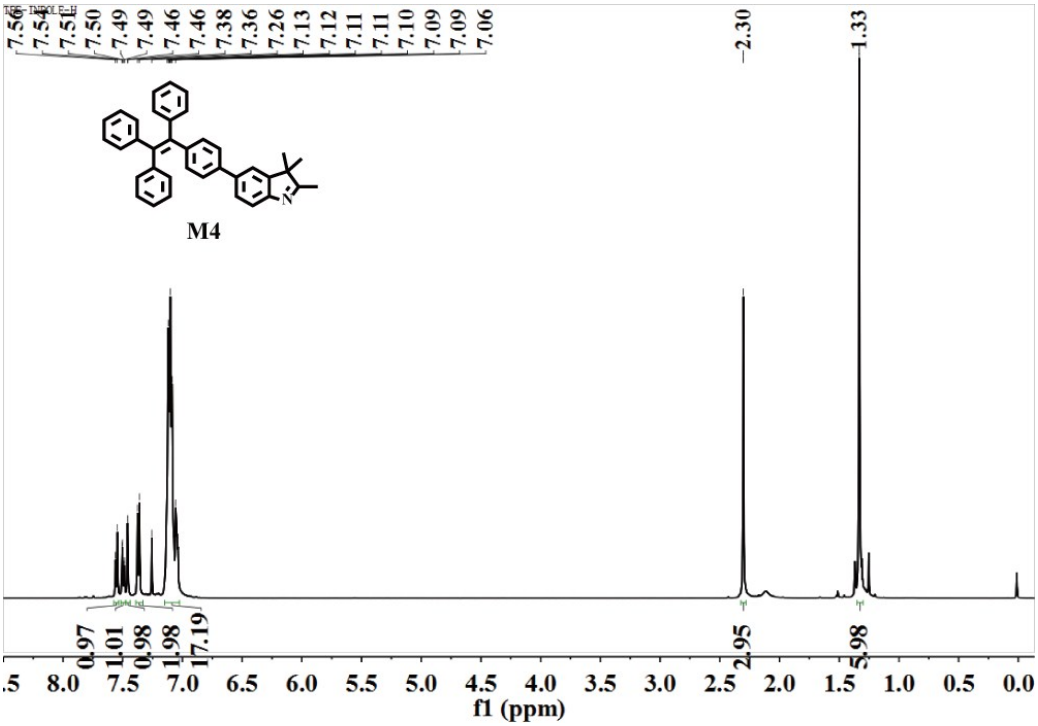

Fig. S22 ^{1}H NMR spectrum of M4 in $CDCl_3$.

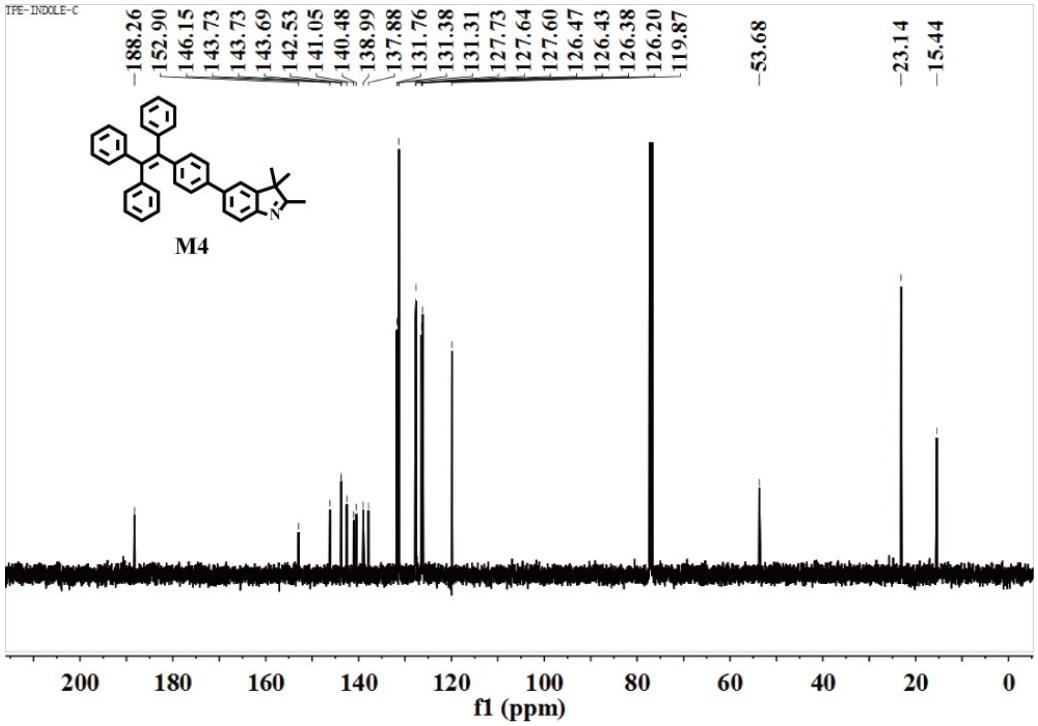

Fig. S23 ^{13}C NMR spectrum of M4 in $CDCl_3$.

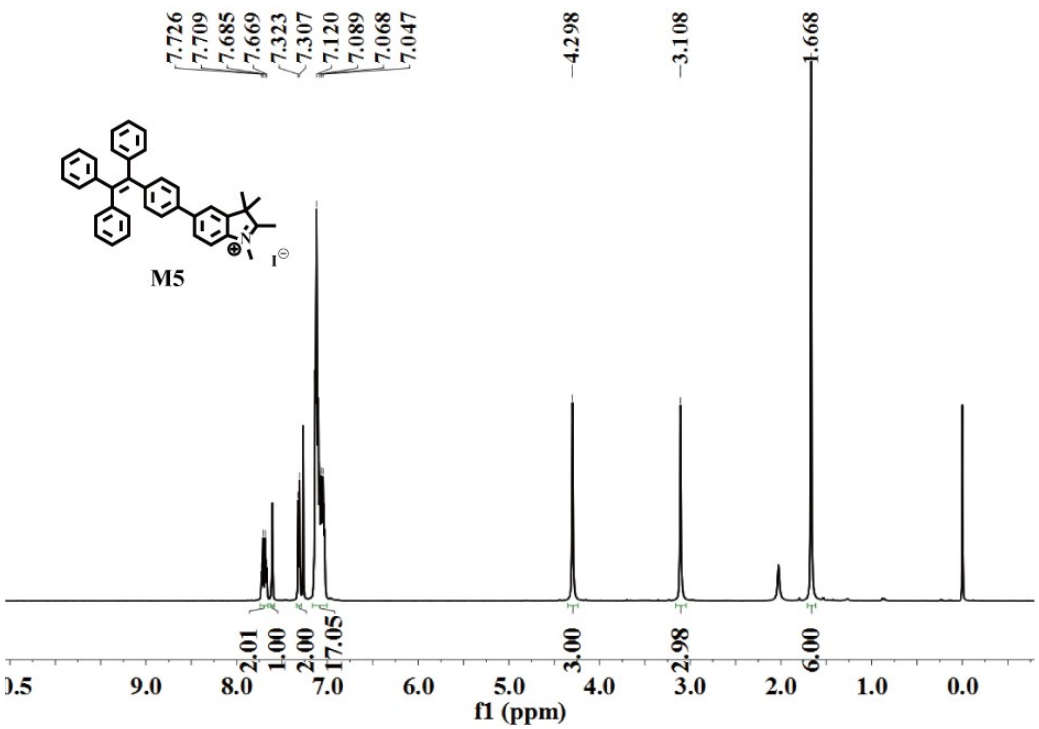

Fig. S24 ^{1}H NMR spectrum of M5 in $CDCl_3$.

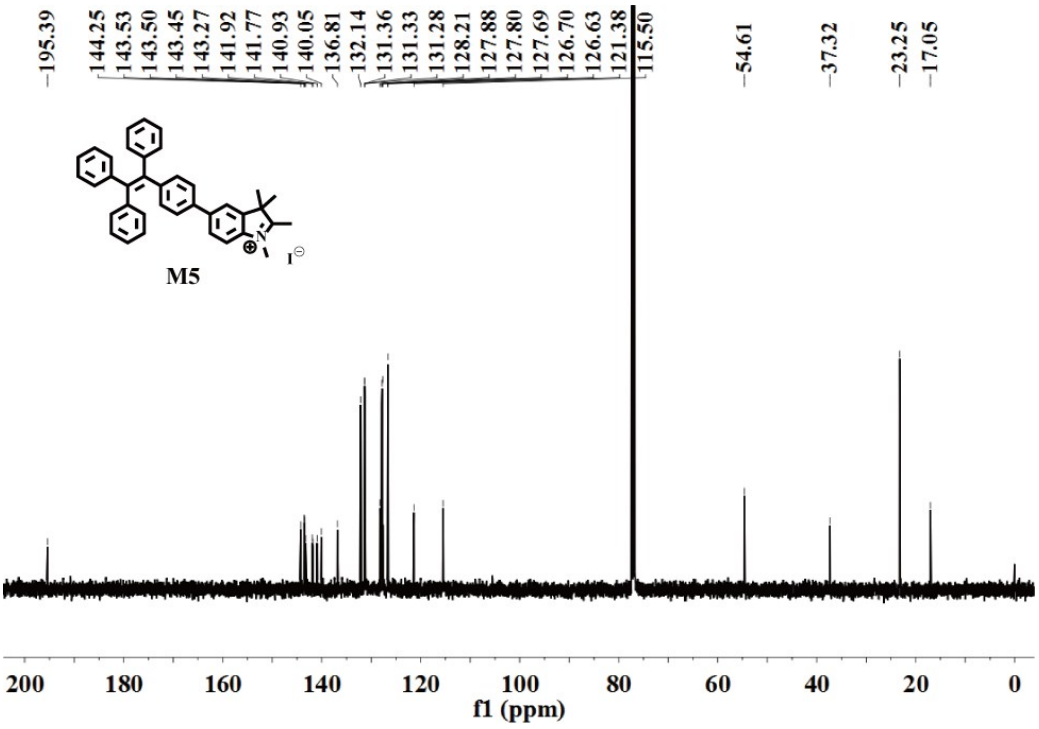

Fig. S25 ^{13}C NMR spectrum of M5 in $CDCl_3$.

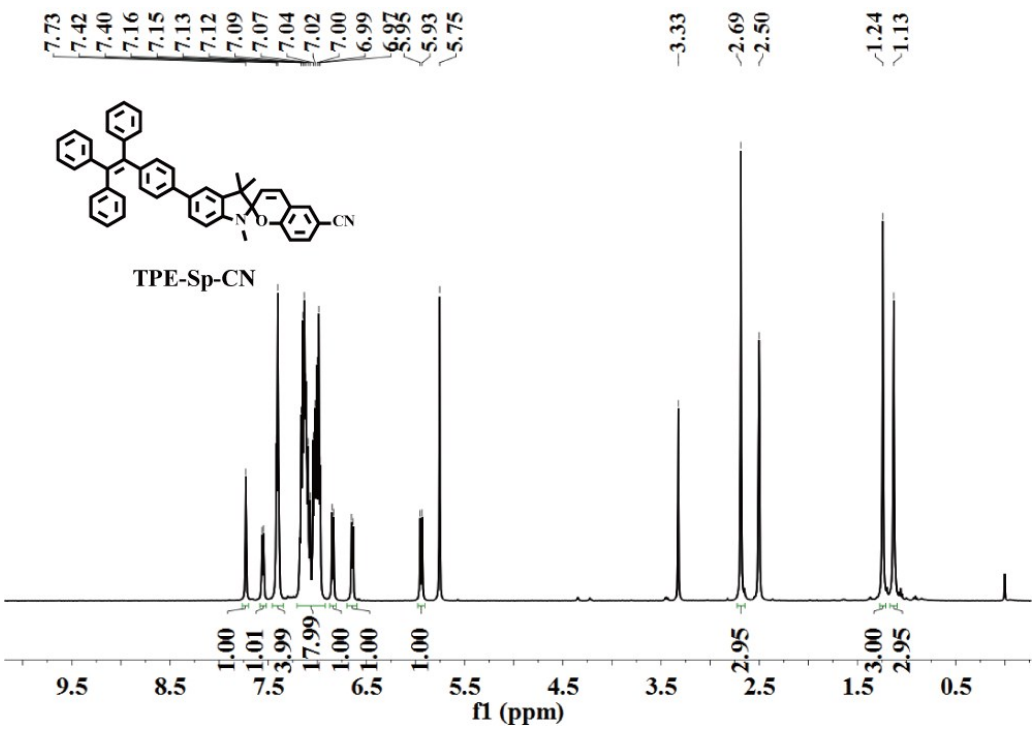

Fig. S26 [1]H NMR spectrum of TPE-Sp-CN in DMSO-d_6.

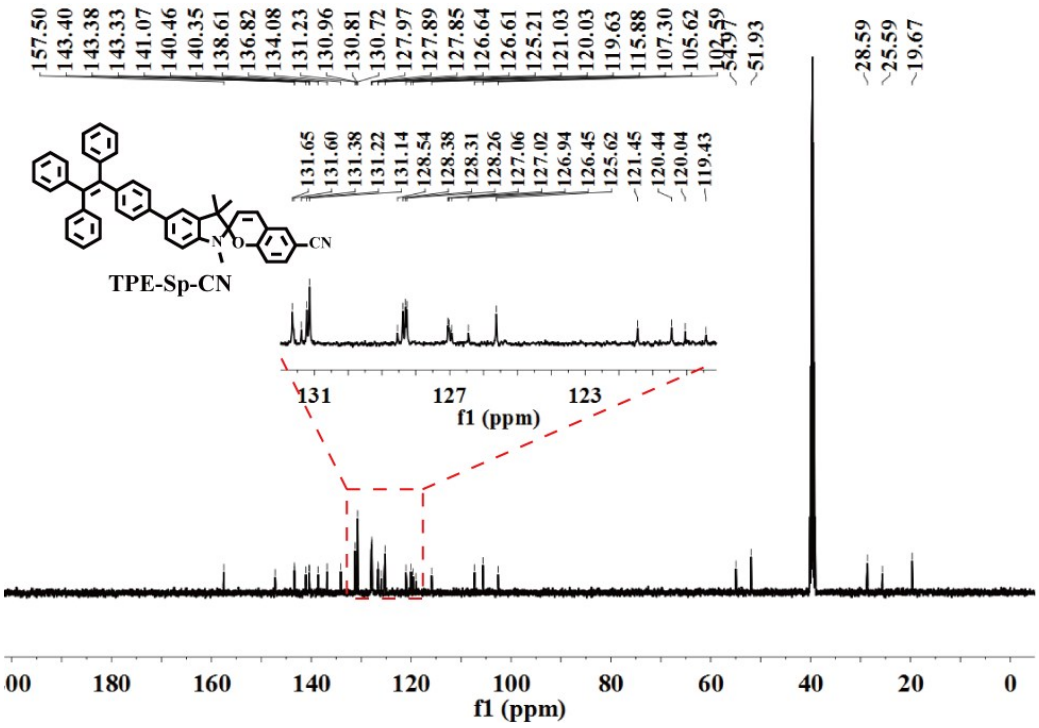

Fig. S27 [13]C NMR spectrum of TPE-Sp-CN in DMSO-d_6.

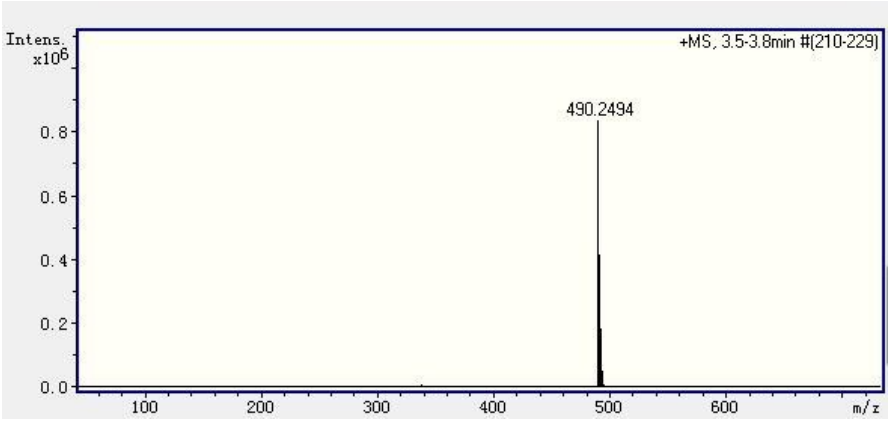

Fig. S28 MS spectrum of M4.

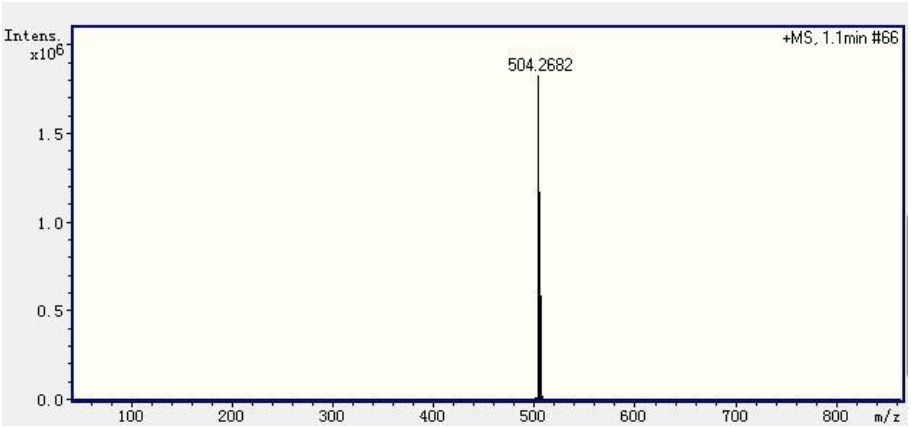

Fig. S29 MS spectrum of M5.

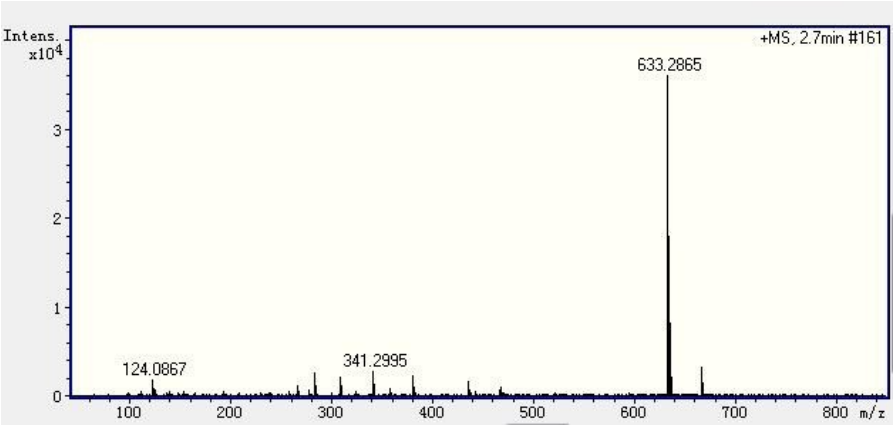

Fig. S30 MS spectrum of TPE-Sp-CN.

Table S2. Crystal data and structure refinement for TPE-Sp-CN.

Identification code	TPE-Sp-CN
Empirical formula	$C_{47}H_{38}Cl_2N_2O$
Formula weight	717.69
Temperature	273(2) K
Wavelength	0.71073 Å
Crystal system, space group	Monoclinic, *P*21/c
Unit cell dimensions	*a*= 20.728(9) Å *α*= 90°
	b= 11.337(5) Å *β*= 107.633(8)°
	c= 17.818(8) Å *γ*= 90°
Volume	3990(3) $Å^3$
Z, Calculated density	4, 1.195 g/cm^{-3}
Absorption coefficient	0.200 mm^{-1}
F(000)	1504.0
Crystal size	0.22× 0.20× 0.18 mm
Theta range for data collection	1.03 to 25.00°
Limiting indices	$-22\leq h\leq 24$, $-11\leq k\leq 13$, $-21\leq l\leq 20$
Reflections collected / unique	22165 / 6987 [R_{int}= 0.1070]
Completeness to theta = 25.00	99.3%
Absorption correction	Multi-scan
Max. and min. transmission	0.9649 and 0.9574
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	6987 / 61 / 501
Goodness-of-fit on F^2	0.890
Final *R* indices [I>2σ(*I*)][a]	*R*1= 0.0866, *wR*2= 0.2215
R indices (all data)	*R*1= 0.2198, w*R*2= 0.2971
Extinction coefficient	0.0053(11)
Largest diff. peak and hole	0.533 and -0.324 e.$Å^{-3}$