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Table S1 The frontier molecular orbital energy and HOMO-LUMO gaps of probes **1a-b** in their deprotonated/protonated forms at the ground state (S_0 state) and the lowest excited state (S_1 state).

probe		HOMO (eV)	LUMO (eV)	ΔE_{H-L} (eV)
1a	S0	-5.608	-3.945	1.663
	S1	-5.527	-4.133	1.394
1a -H^+	S0	-4.813	-3.316	1.497
	S1	-4.850	-3.519	1.331
1b	S0	-5.692	-4.018	1.674
	S1	-5.718	-4.309	1.409
1b -H^+	S0	-4.888	-3.427	1.461
	S1	-4.939	-3.632	1.307

Table S2 Selected parameters for the vertical excitation (UV-vis absorptions) of probes **1a-b** in their deprotonated/protonated forms based on the optimized ground state geometries.

probe	Electronic transitions	Excitation energy		$\lambda_{exp.}$/nm	f^a	Composition^b	CI^c
		E/eV	λ/nm				
1a	$S_0 \rightarrow S_1$	2.56	484	455	1.8002	H→L	0.70767
1a -H^+	$S_0 \rightarrow S_1$	2.27	547	578	1.7470	H-2→L	0.17620
						H→L	0.69478
1b	$S_0 \rightarrow S_1$	2.32	484	448	1.7774	H→L	0.70692
1b -H^+	$S_0 \rightarrow S_1$	2.22	560	558	1.8101	H-2→L	0.12722
						H→L	0.70153

[a] Oscillator strength. [b] H stands for HOMO and L stands for LUMO. [c] Coefficient of the wavefunction for each excitations.

Table S3 Selected parameters for emission related of probes **1a-b** in their deprotonated/protonated forms based on the optimized lowest singlet excited state geometries.

probe	Electronic transitions	Excitation energy		$\lambda_{exp.}$/nm	f^a	Composition^b	CI^c
		E/eV	λ/nm				
1a	$S_0 \rightarrow S_1$	2.11	586	594	1.4680	H-1→L	0.12808
						H→L	0.70156
1a -H^+	$S_0 \rightarrow S_1$	1.97	628	654	1.2398	H-2→L	0.19990
						H→L	0.68657
1b	$S_0 \rightarrow S_3$	2.62	474	594	1.0084	H-5→L	-0.12584
						H-3→L	0.32928
						H-1→L	0.61414
1b -H^+	$S_0 \rightarrow S_2$	2.11	587	659	1.8209	H→L	0.71262

[a] Oscillator strength. [b] H stands for HOMO and L stands for LUMO. [c] Coefficient of the wavefunction for each excitations.

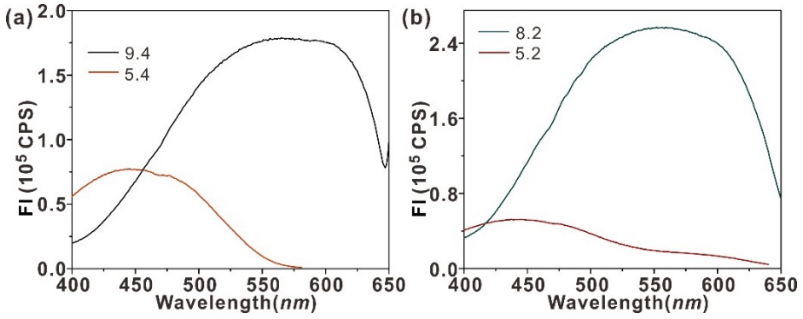

Fig. S1 Excitation spectra of probes **1a-b** (10 μM) in basic and acidic conditions. (a) Probe **1a**. (b) Probe **1b**.

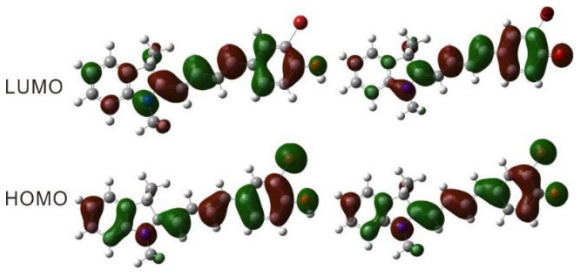

Fig. S2 The frontier molecular orbitals (FMOs) plots of probe **1b** in their protonated (the left column) and deprotonated (the right column) forms.

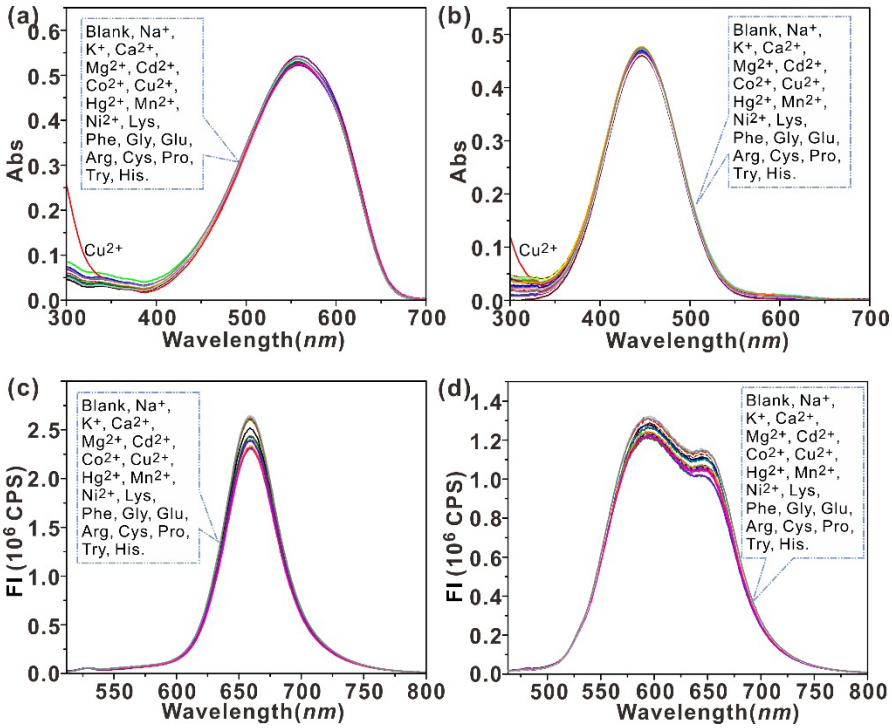

Fig. S3 Optical responses of **1b** (10 μM) towards different analytes. (a, b) Absorption spectra. (c, d) Emission spectra. (a, c) Tested in basic buffer solutions with pH = 8.2. (b, d) Tested in acidic buffer solutions with pH = 5.2. Used analytes: K^+ (100 mM), Na^+ (100 mM), Ca^{2+} (0.5 mM), Cd^{2+} (0.3 mM), Cu^{2+} (0.3 mM), Mg^{2+} (0.5 mM), Co^{2+} (0.3 mM), Hg^{2+} (0.3 mM), Mn^{2+} (0.3 mM), Ni^{2+} (0.3 mM), Cys (0.1 mM), Phe (0.1 mM), Gly (0.1 mM), Glu (0.1 mM), Arg (0.1 mM), Lys (0.1 mM), Pro (0.1 mM), Try (0.1 mM) and His (0.1 mM).

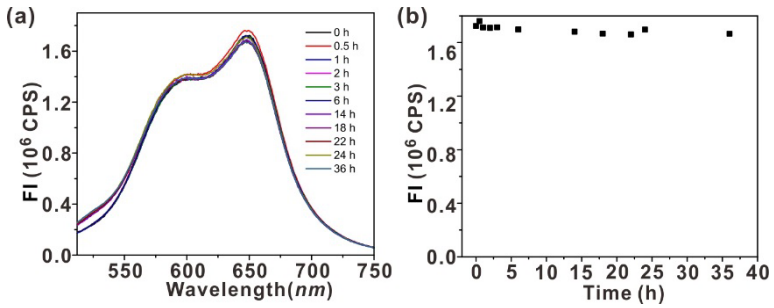

Fig. S4 Fluorescence intensity changes of probe **1a** (10 μM) in the absence of 10% FBS serum in the buffer solution. (a) Fluorescent spectra; (b) Time-dependent fluorescence intensity changes at 651 nm of probe **1a.**

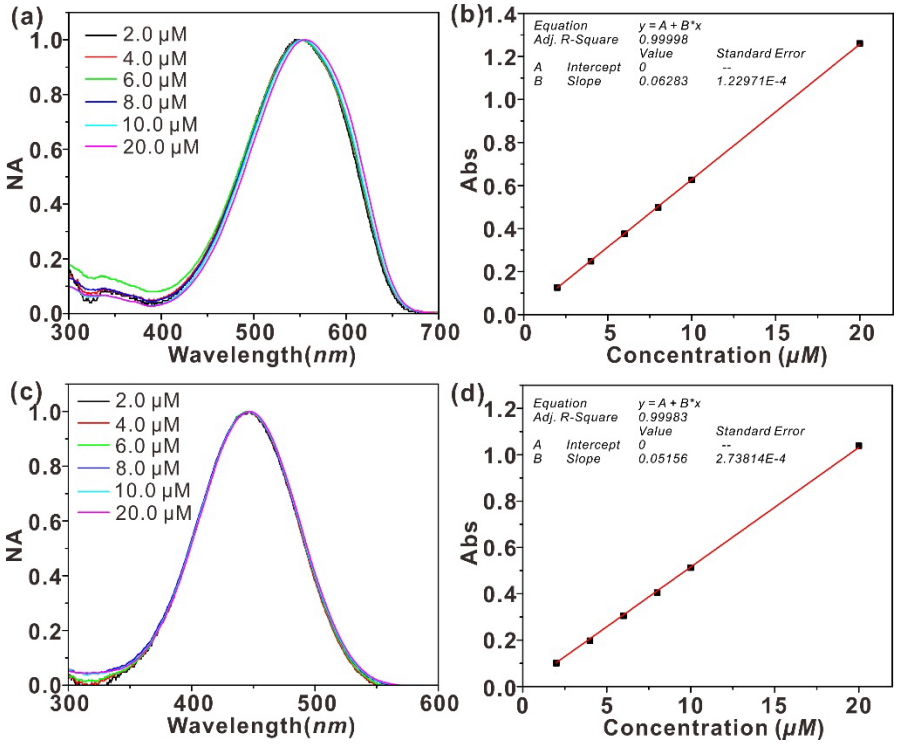

Fig. S5 Concentration related absorptions of probe **1b** (2, 4, 6, 8, 10 and 20 μM) in basic and acidic conditions. (a, c) Normalized absorption spectra. (b, d) The linear relationship of absorption intensity and concentration. (a, b) Tested in basic buffer solutions with pH = 9.2. (c, d) Tested in acidic buffer solutions with pH = 4.8.

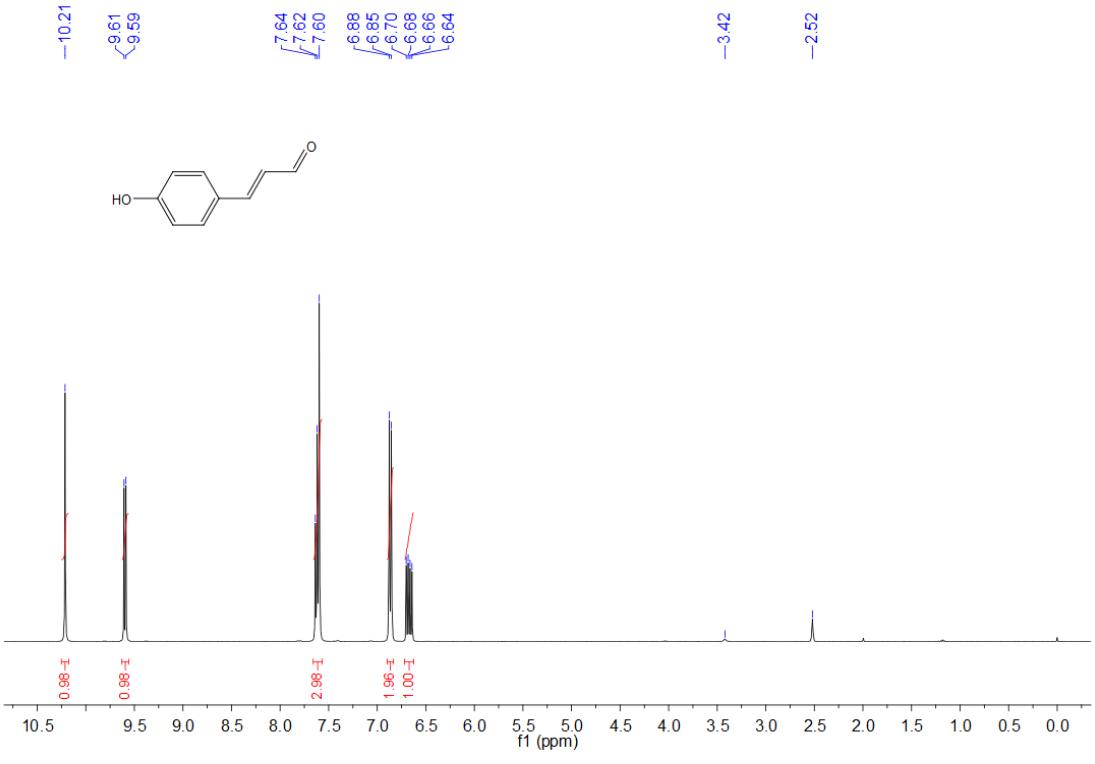

Fig. S6 ^{1}H NMR of **4a** in DMSO-d_6.

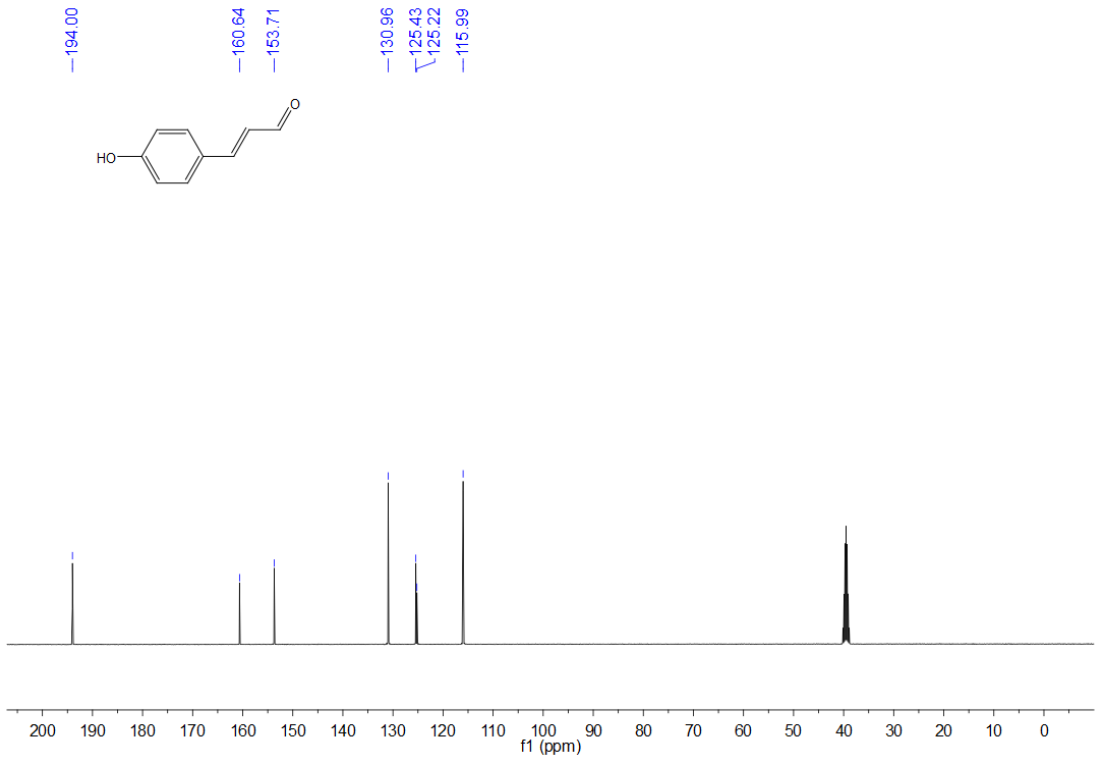

Fig. S7 ^{13}C NMR of **4a** in DMSO-d_6.

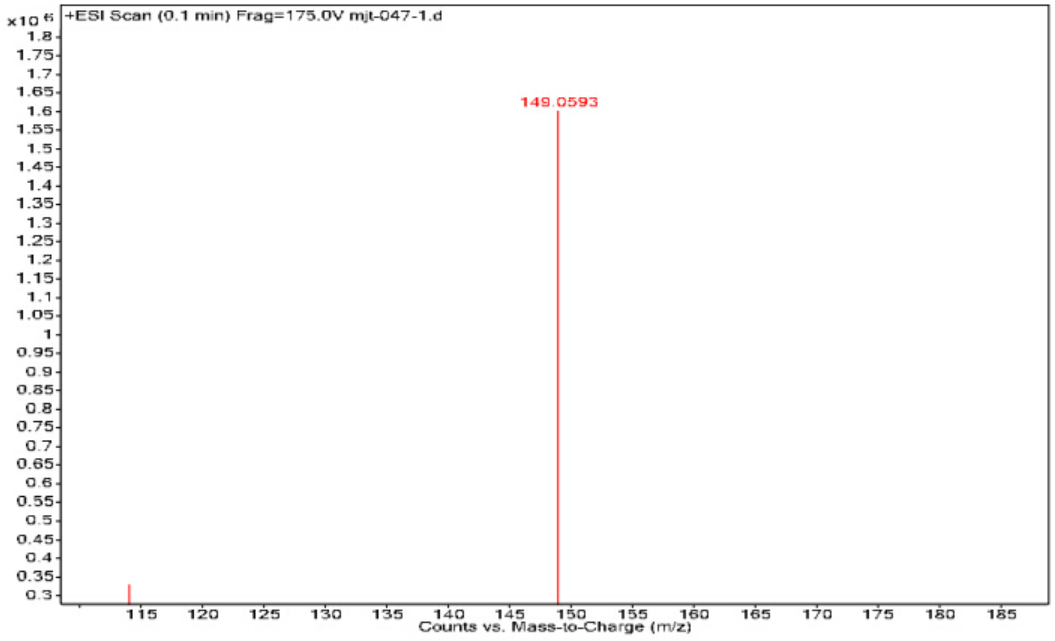

Fig. S8 HRMS of **4a**.

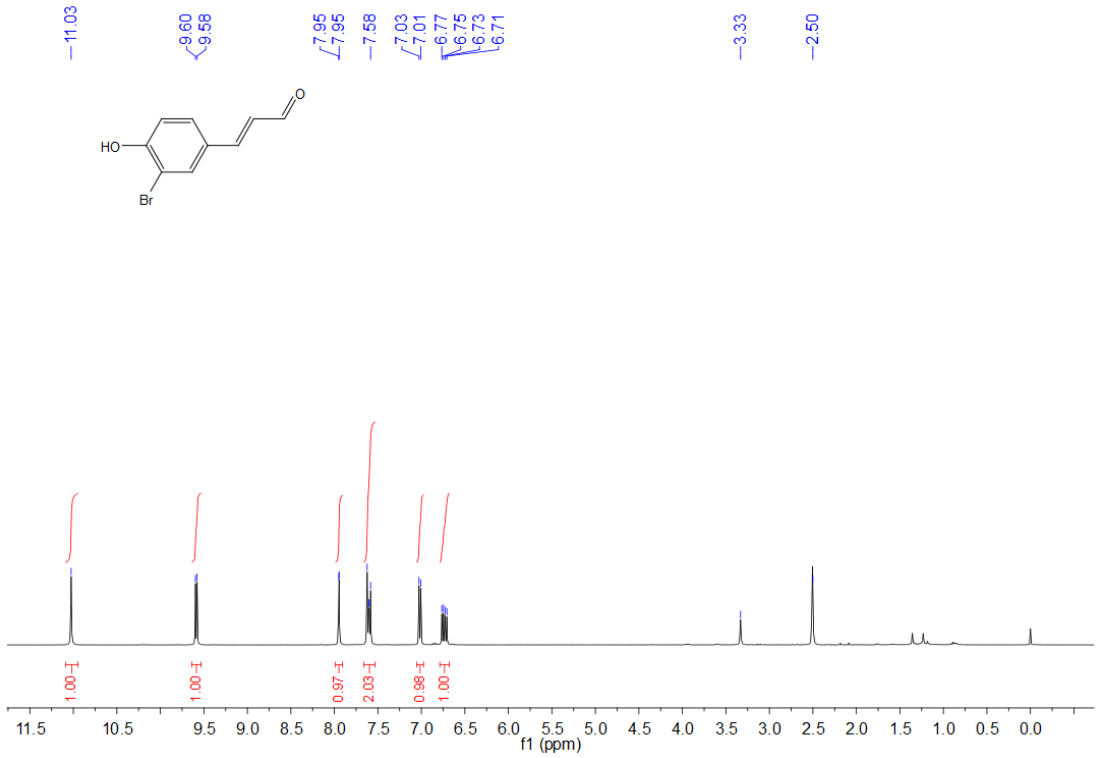

Fig. S9 ^{1}H NMR of **4b** in DMSO-d_6.

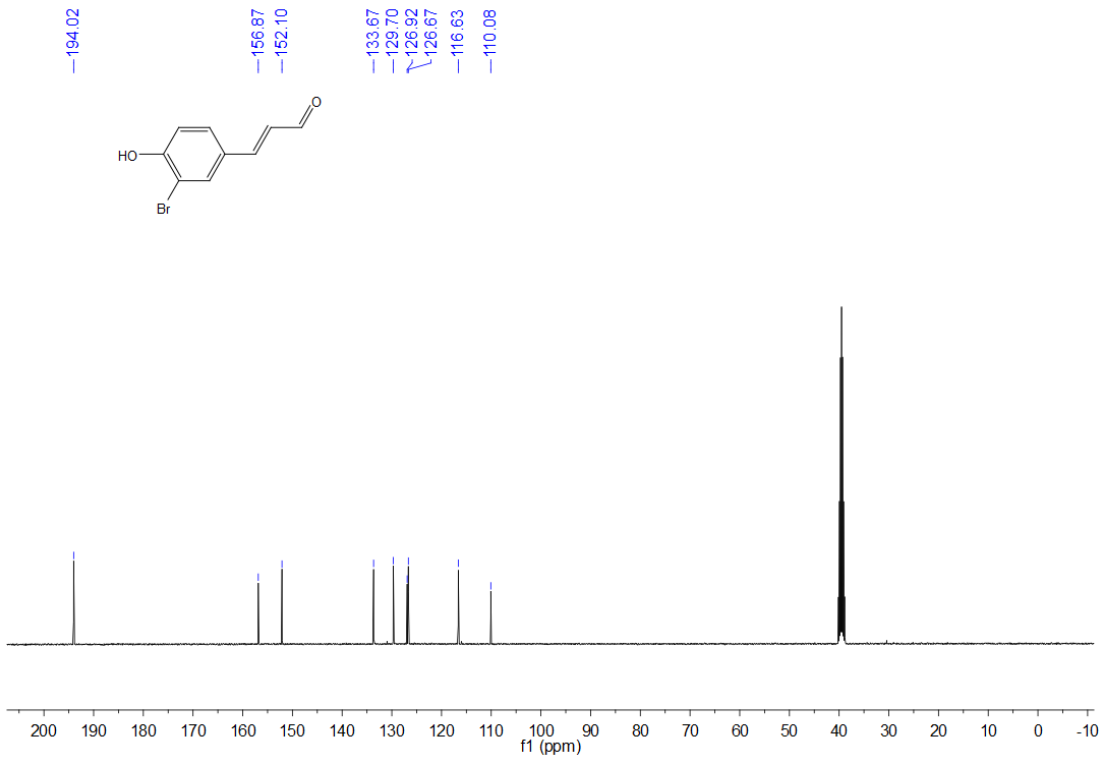

Fig. S10 ^{13}C NMR of **4b** in DMSO-d_6.

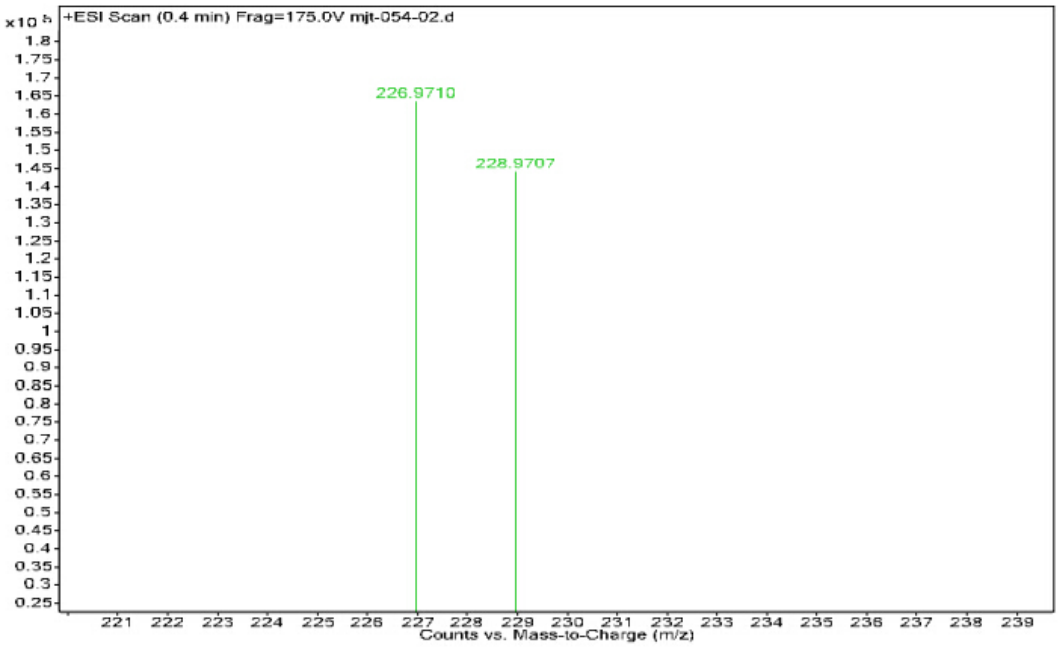

Fig. S11 HRMS of **4b**.

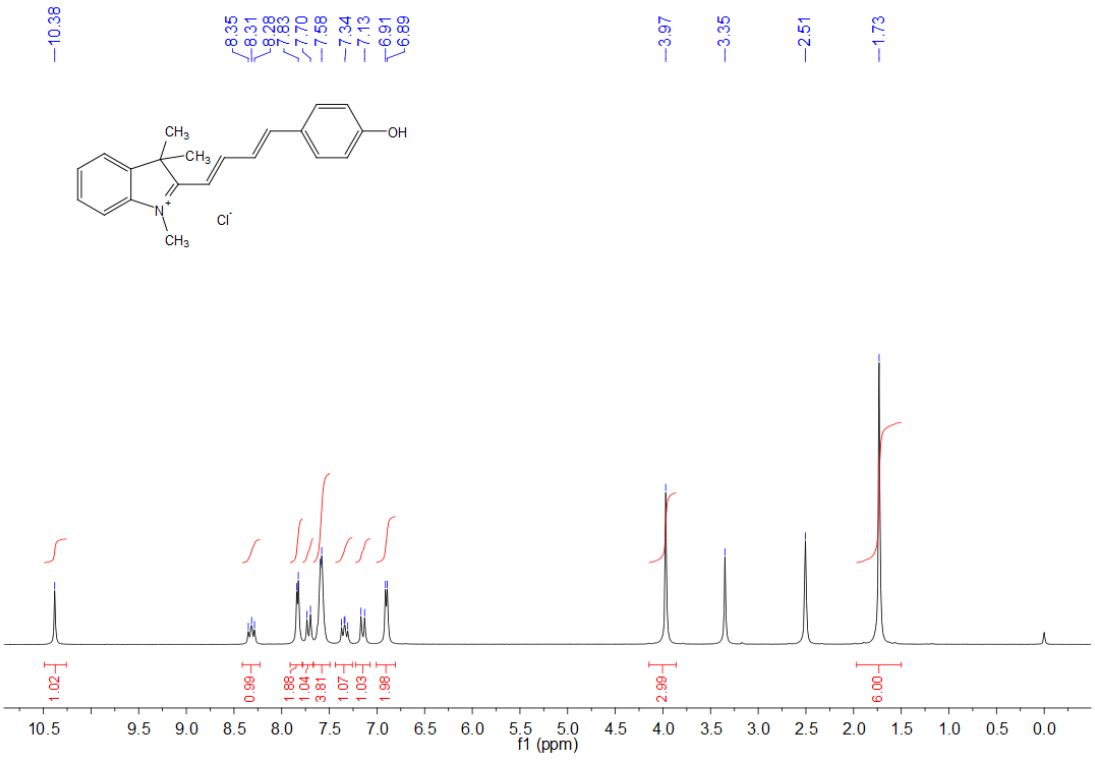

Fig. S12 ^{1}H NMR of **1a** in DMSO-d_6.

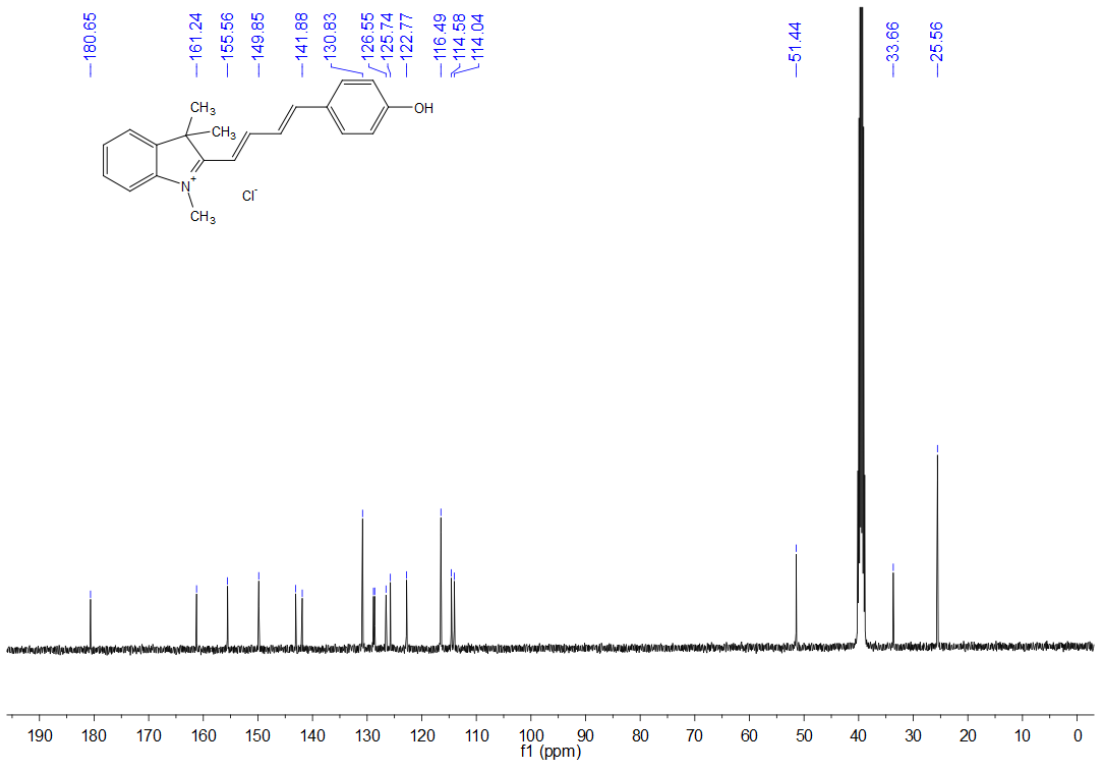

Fig. S13 ^{13}C NMR of **1a** in DMSO-d_6.

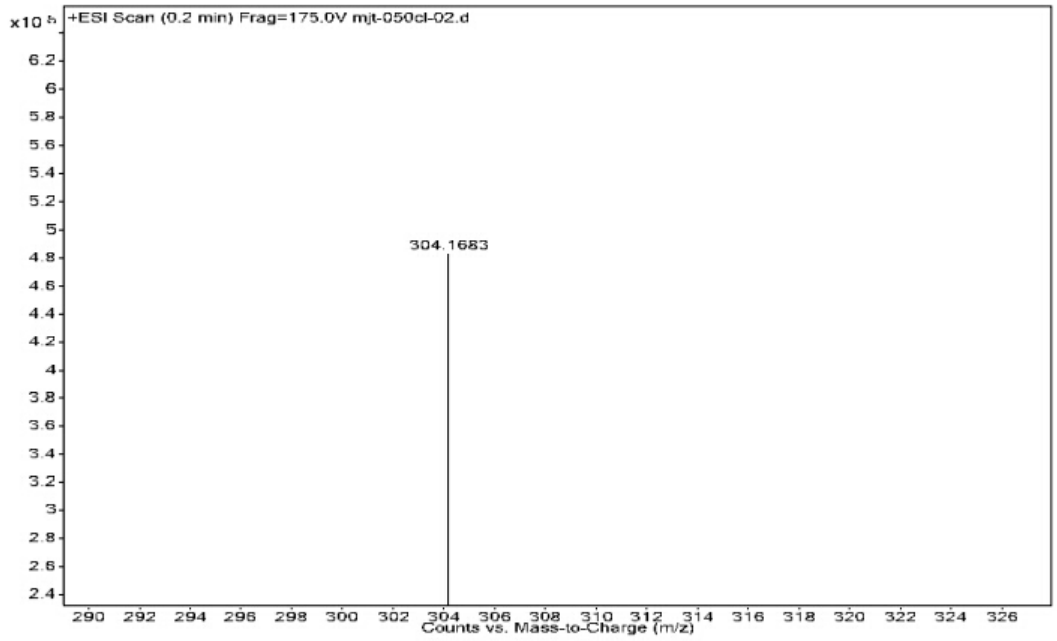

Fig. S14 HRMS of **1a**.

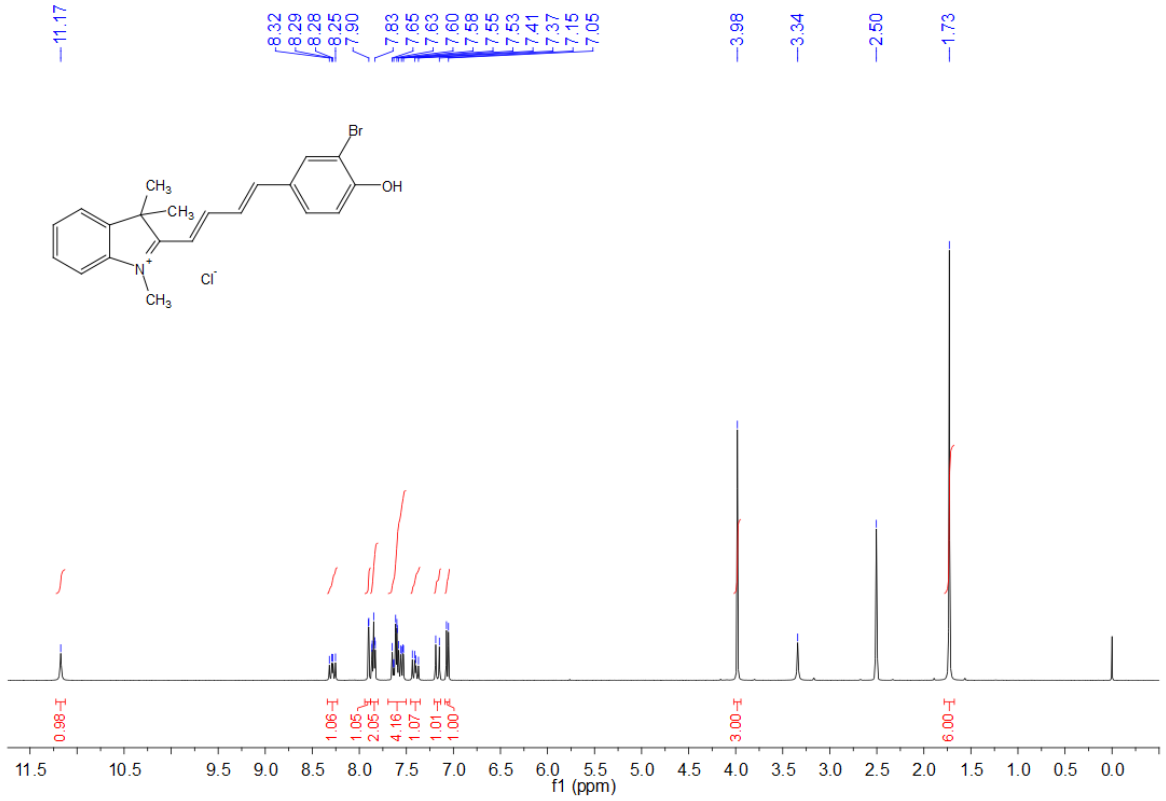

Fig. S15 ^{1}H NMR of **1b** in DMSO-d_6.

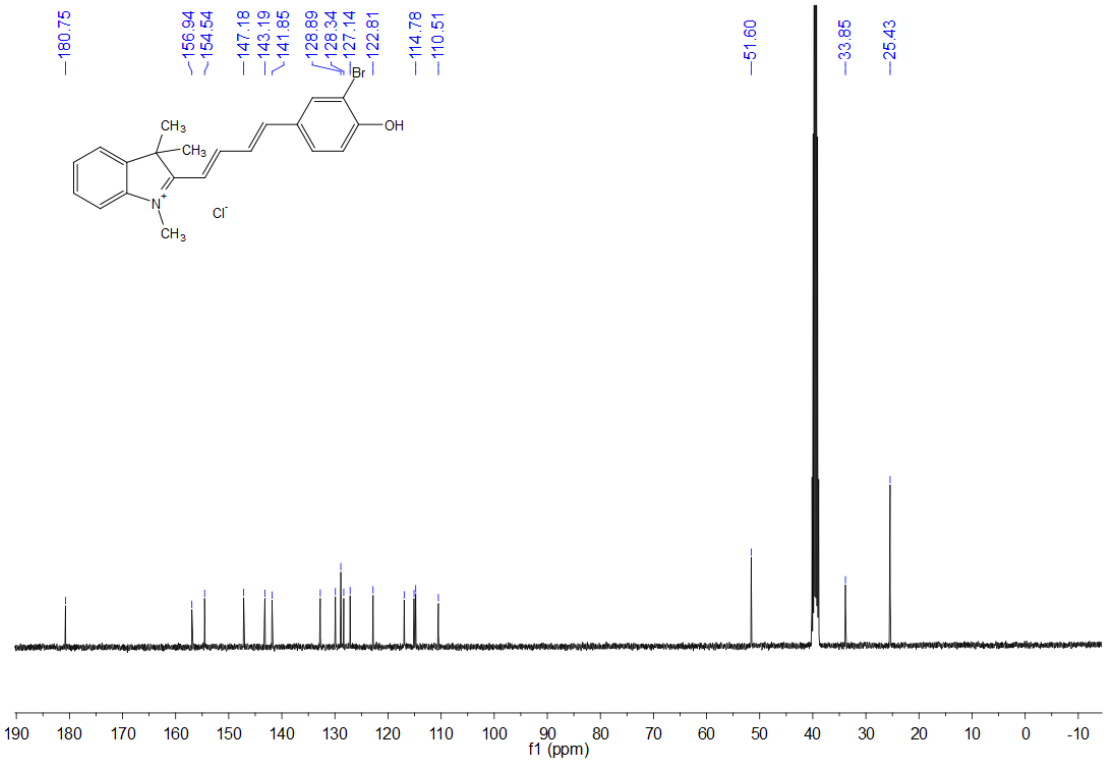

Fig. S16 ^{13}C NMR of **1b** in DMSO-d_6.

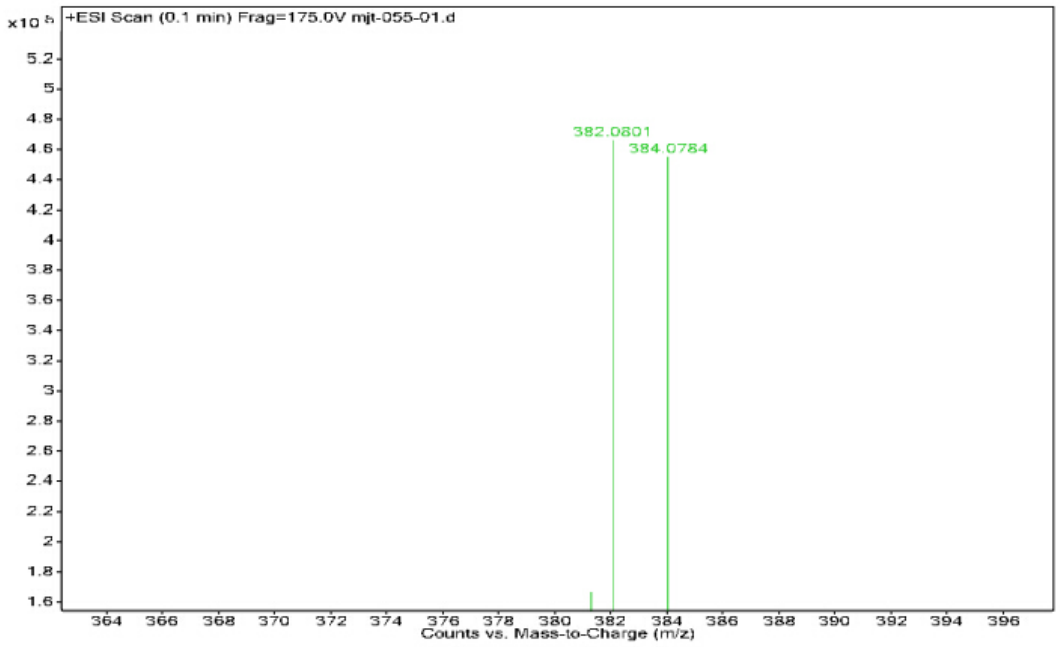

Fig. S17 HRMS of **1b**.