Electronic Supplementary Material (ESI) for New Journal of Chemistry.

Synthesis of Indenophenanthridine *via* [4+2] Annulation Strategy: "Turn-Off'' Fe^{3+} Ion Sensor, Practical Application in Live Cell Imaging and Reversible Acidochromism Studies†

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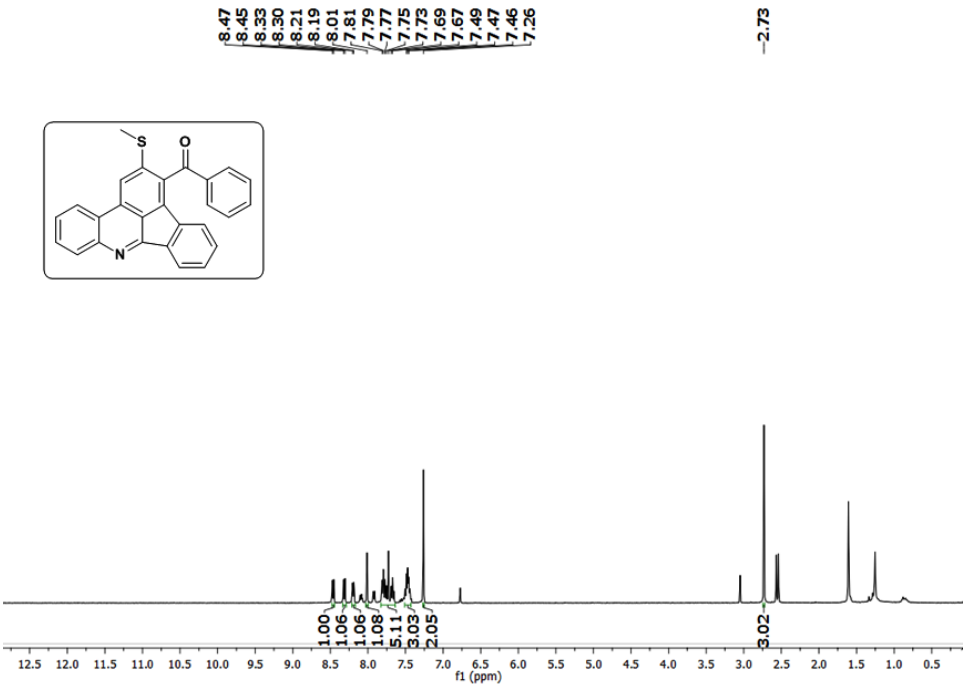

Figure S.1: ^{1}H NMR spectrum of compound **4a**

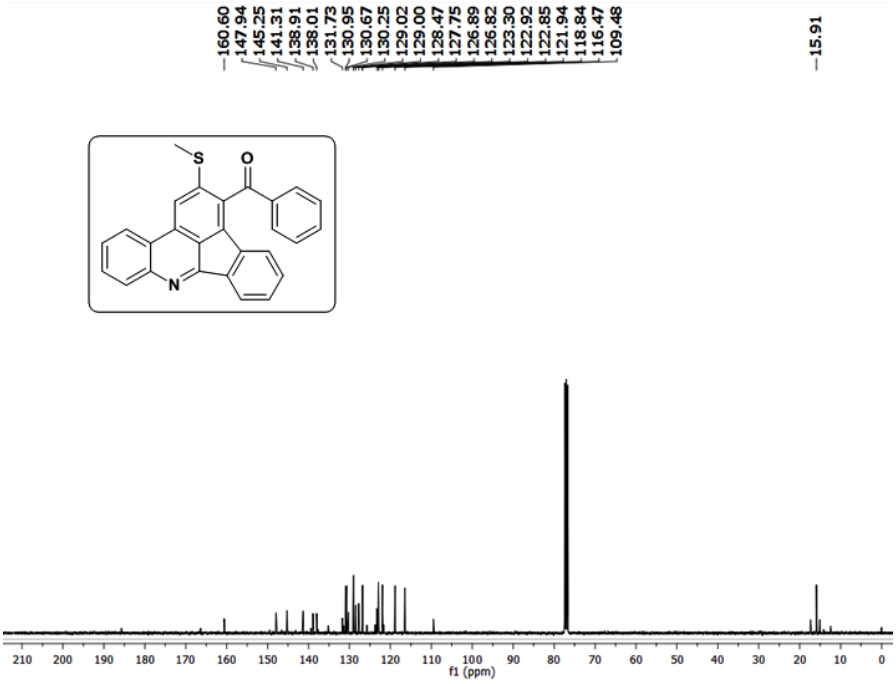

Figure S.2: C^{13} spectrum of compound **4a**

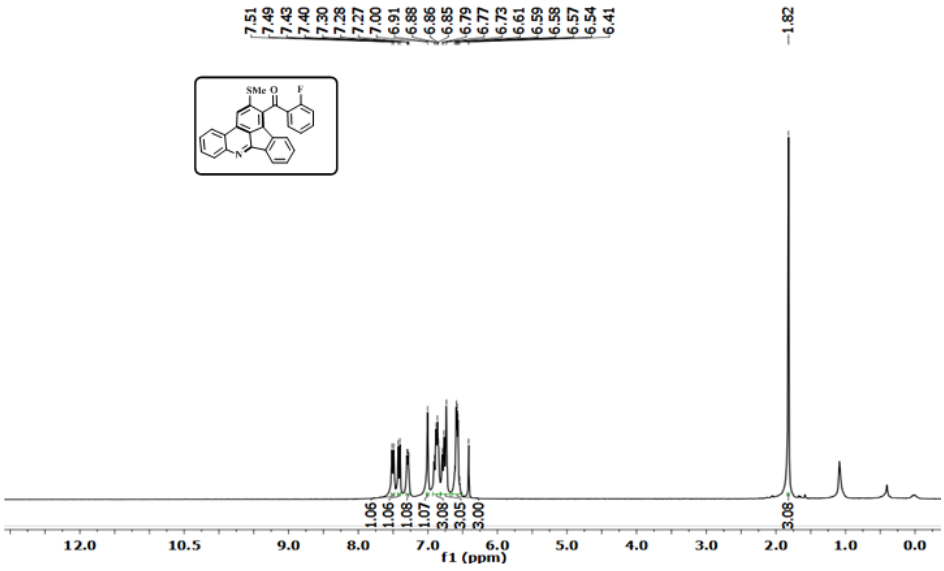

Figure S.3: ^{1}H NMR spectrum of compound **4b**

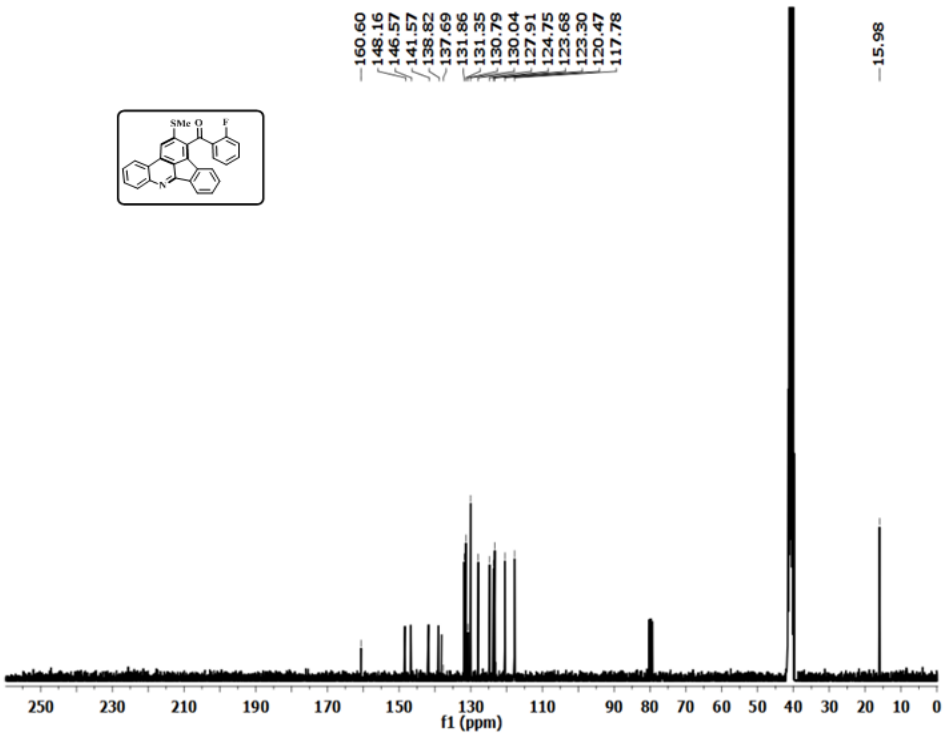

Figure S.4: C^{13} spectrum of compound **4b**

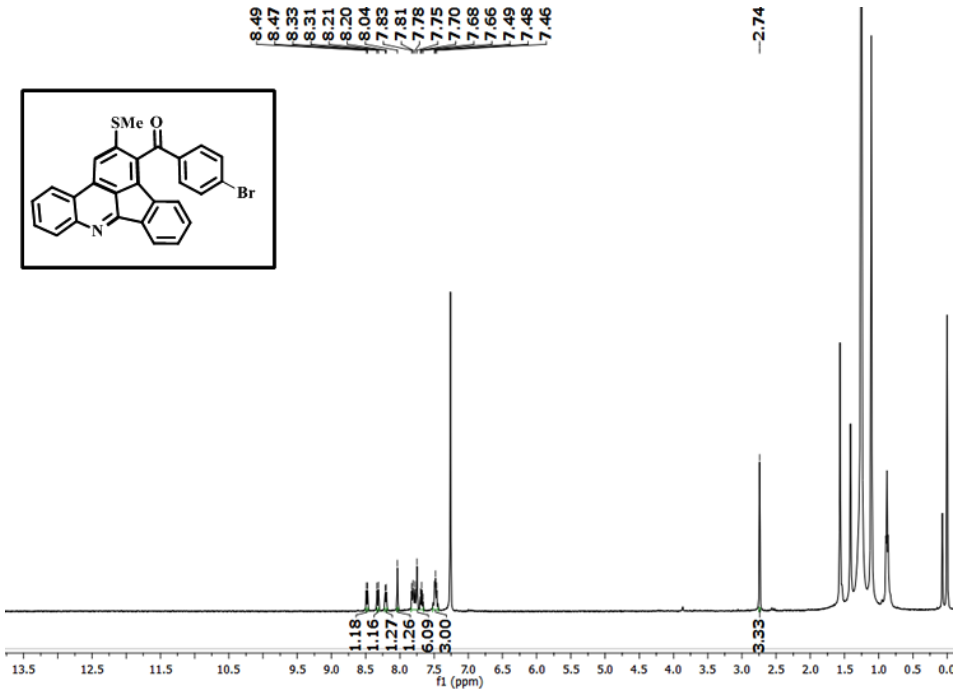

Figure S.5: ^{1}H NMR spectrum of compound **4c**

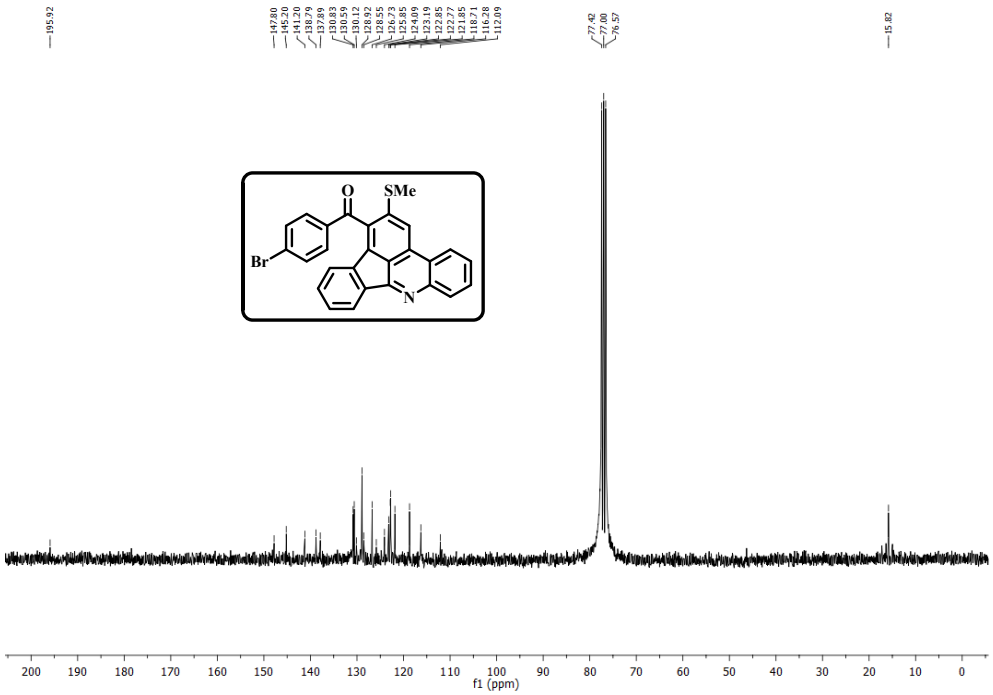

Figure S.6: C^{13} NMR spectrum of compounds **4c**

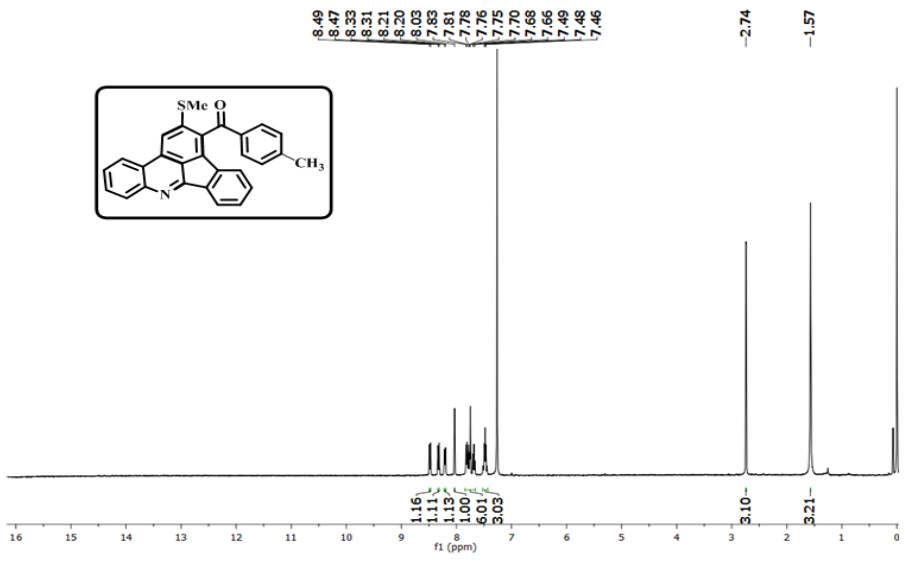

Figure S.7: ^{1}H NMR spectrum of compound **4d**

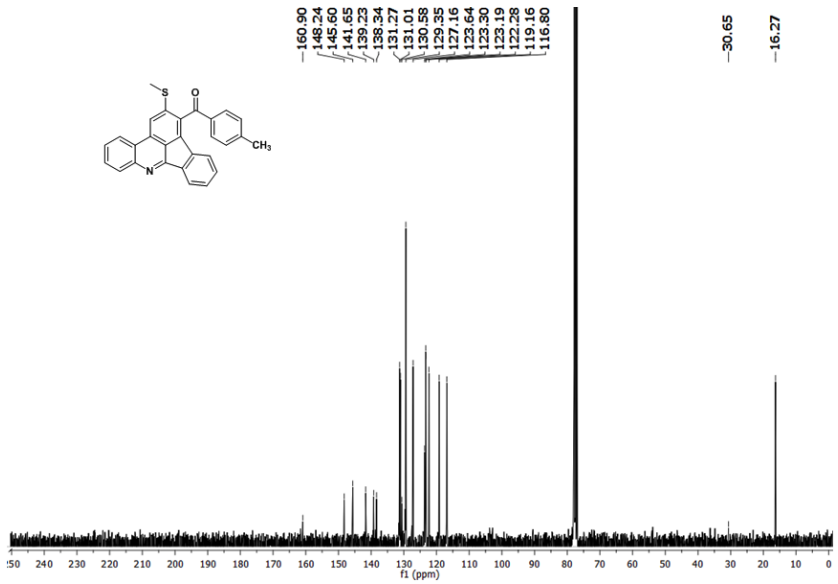

Figure S.8: C^{13} spectrum of compound **4d**

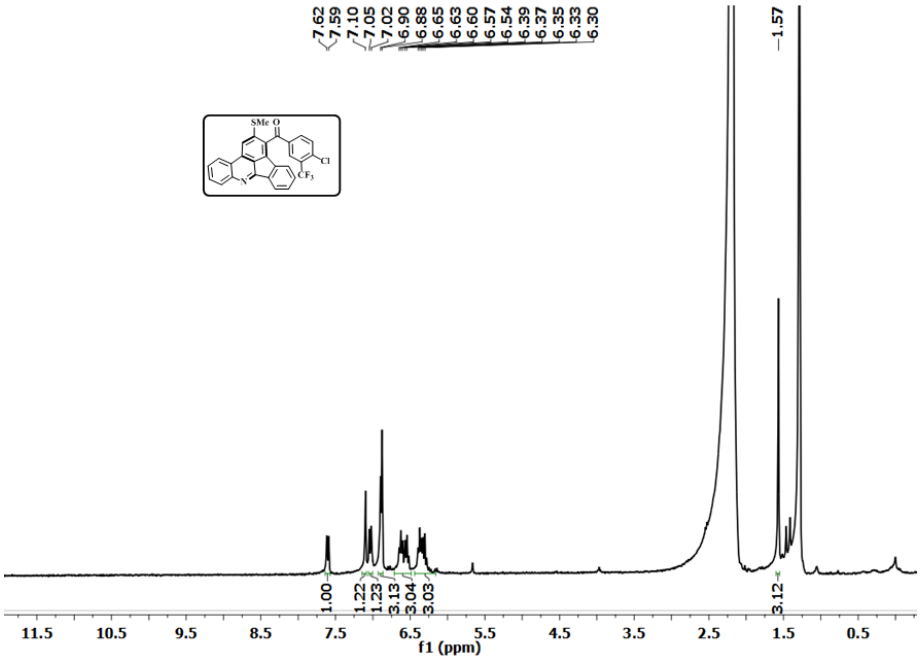

Figure S.9: ^{1}H NMR spectrum of compound **4e**

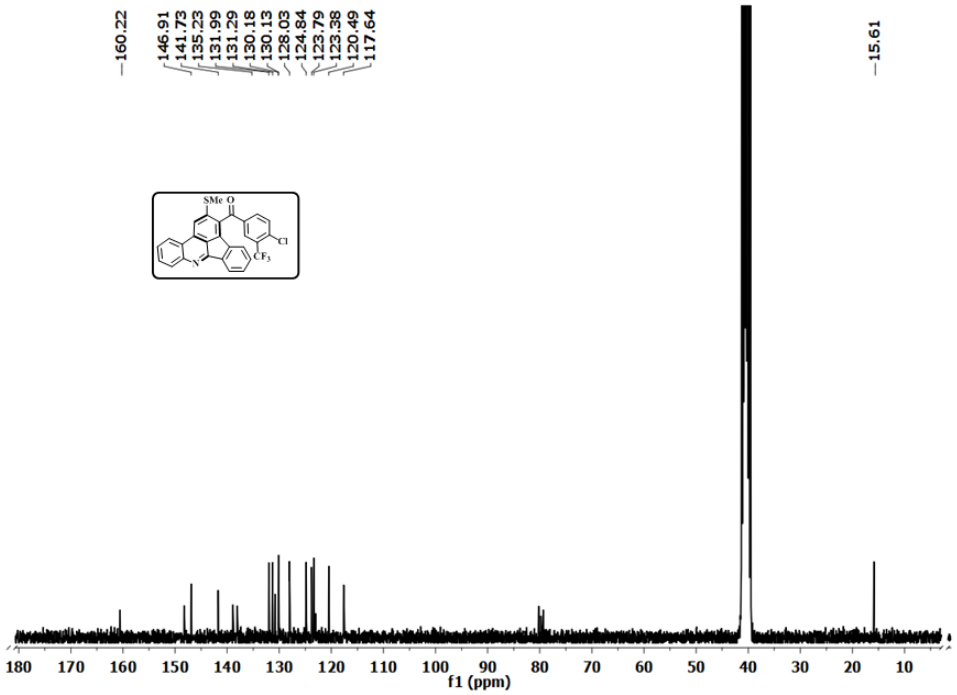

Figure S.10: ^{13}C NMR spectrum of compound **4e**

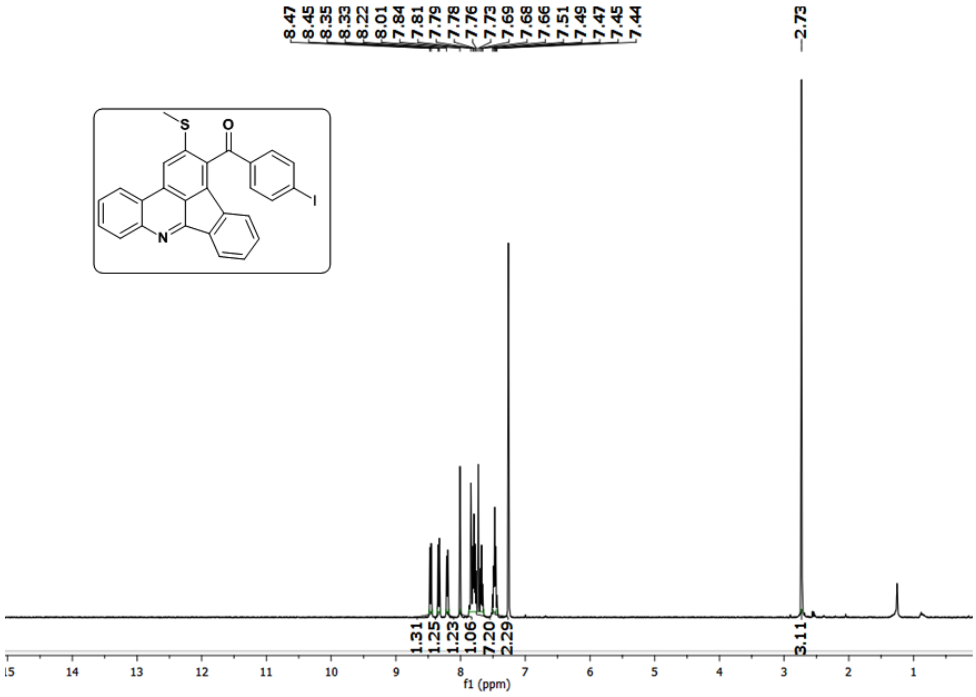

Figure S.11: ^{1}H NMR spectrum of compound **4f**

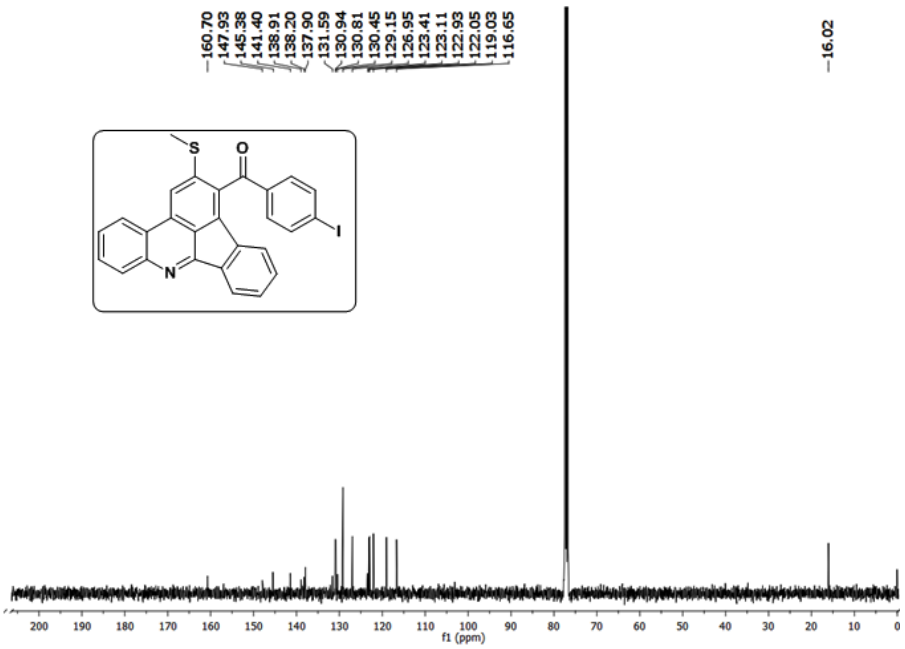

Figure S.12: ^{13}C NMR spectrum of compound **4f**

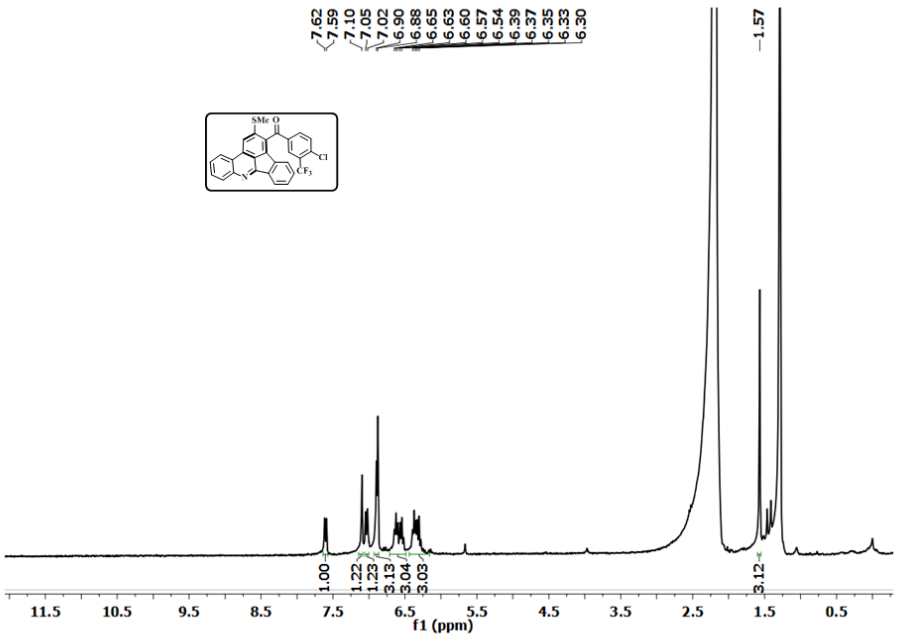

Figure S.13: ^{1}H NMR spectrum of compound **4g**

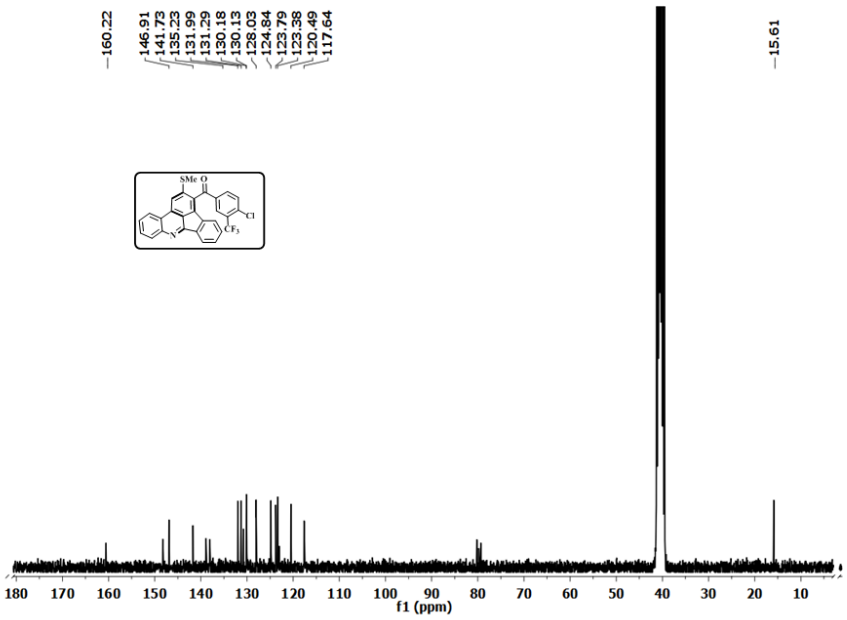

Figure S.14: ^{13}C NMR spectrum of compound **4g**

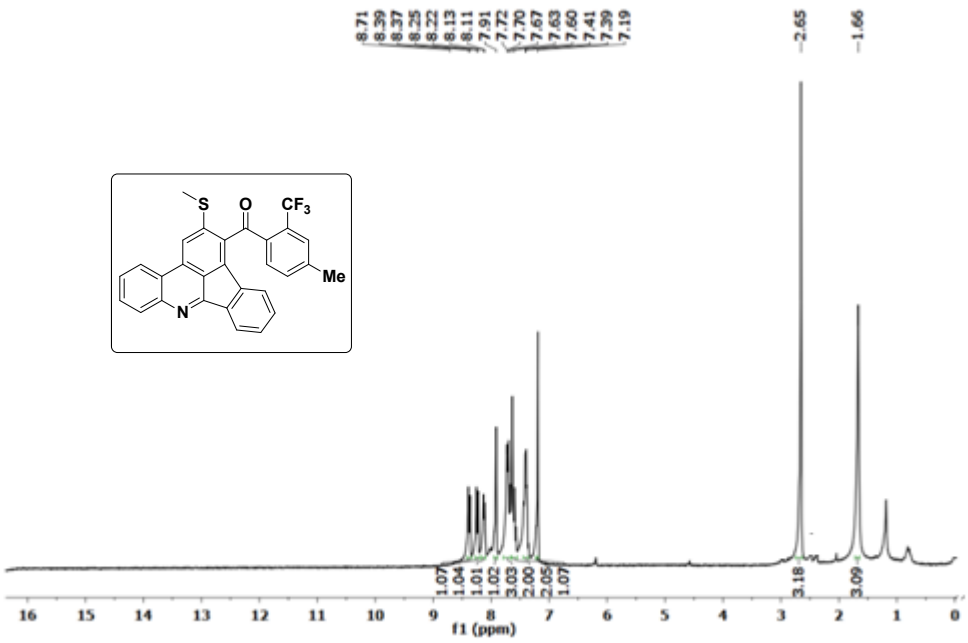

Figure S.15: ^{1}H NMR spectrum of compound **4h**

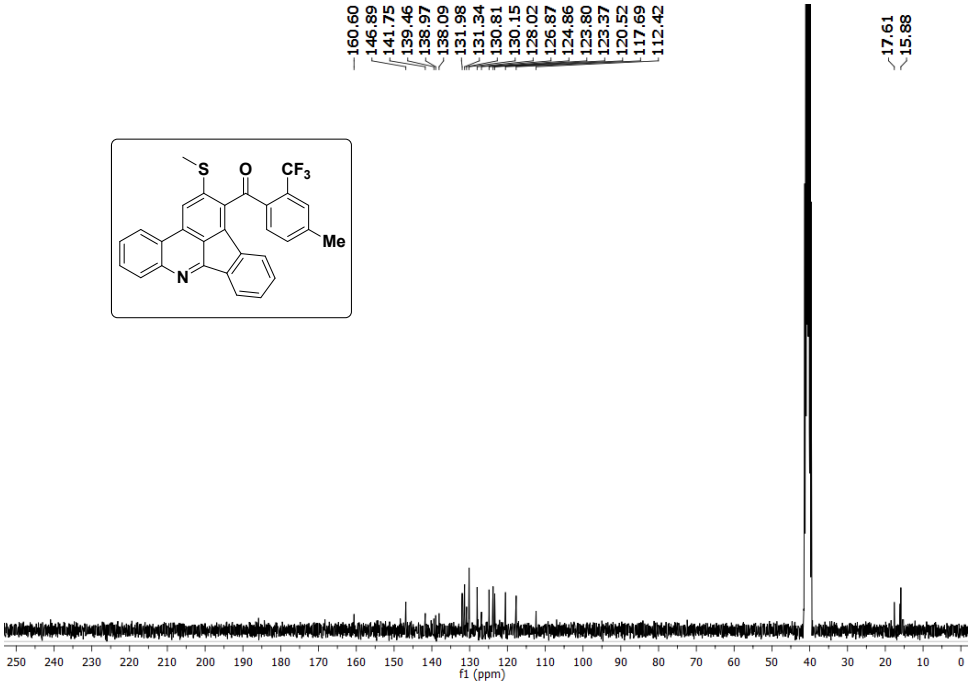

Figure S.16: ^{13}C NMR spectrum of compound **4h**

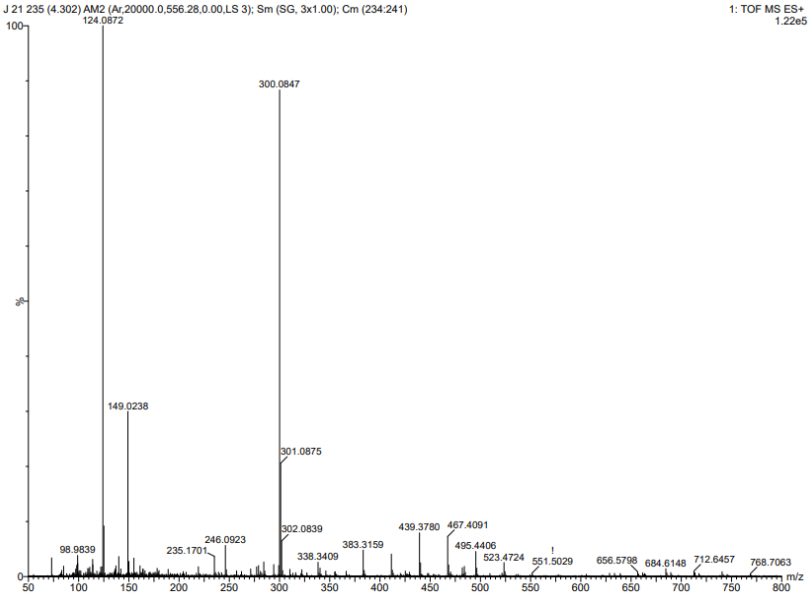

Figure S.17: HRMS spectrum of compound **4a**

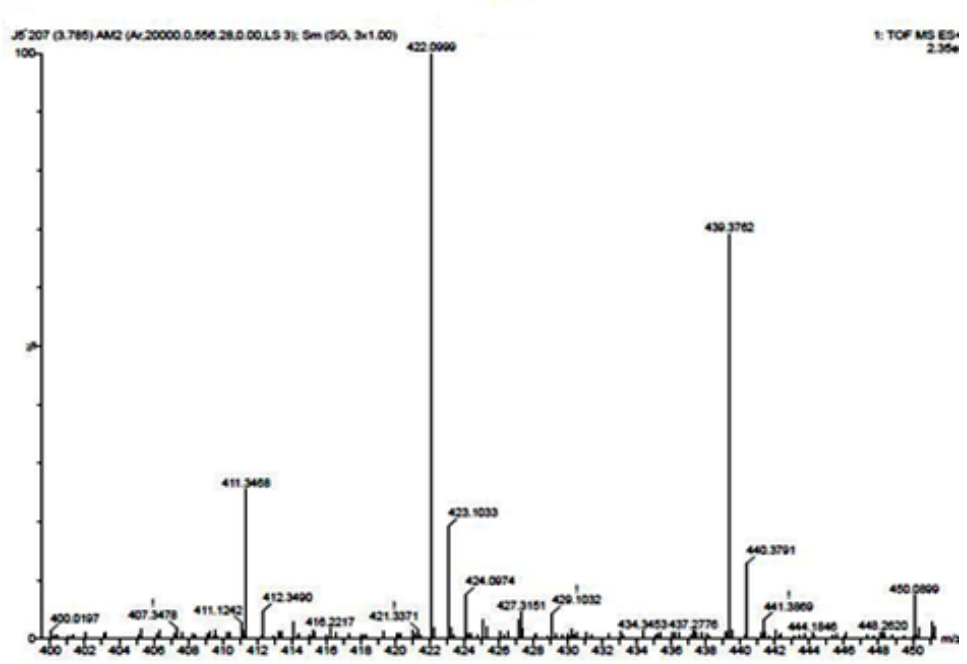

Figure S.18: HRMS spectrum of compound **4b**

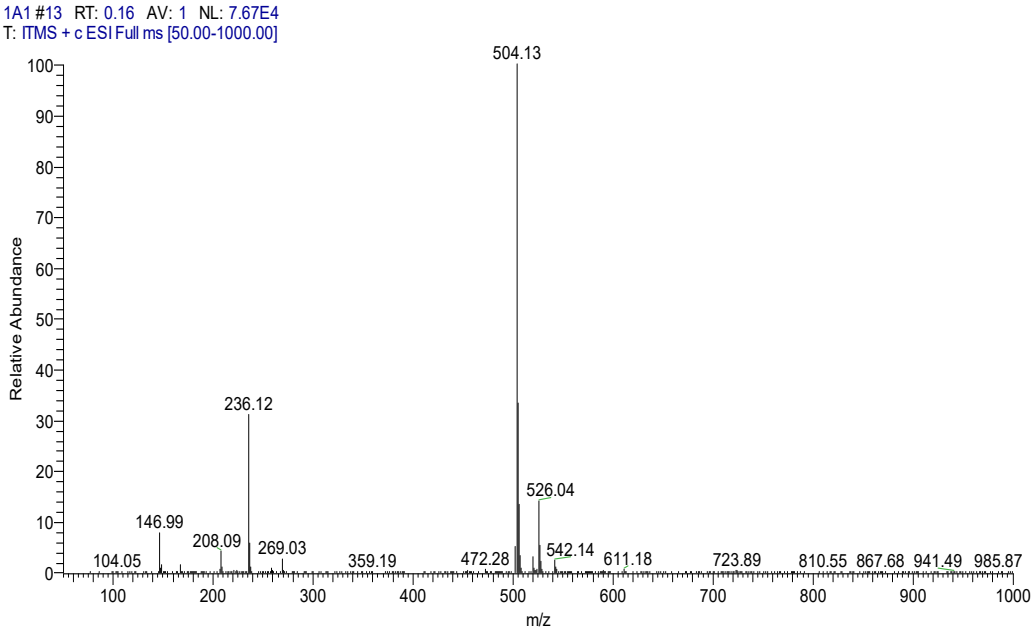

Figure S.19: ESI-MS spectrum of compound **4c**

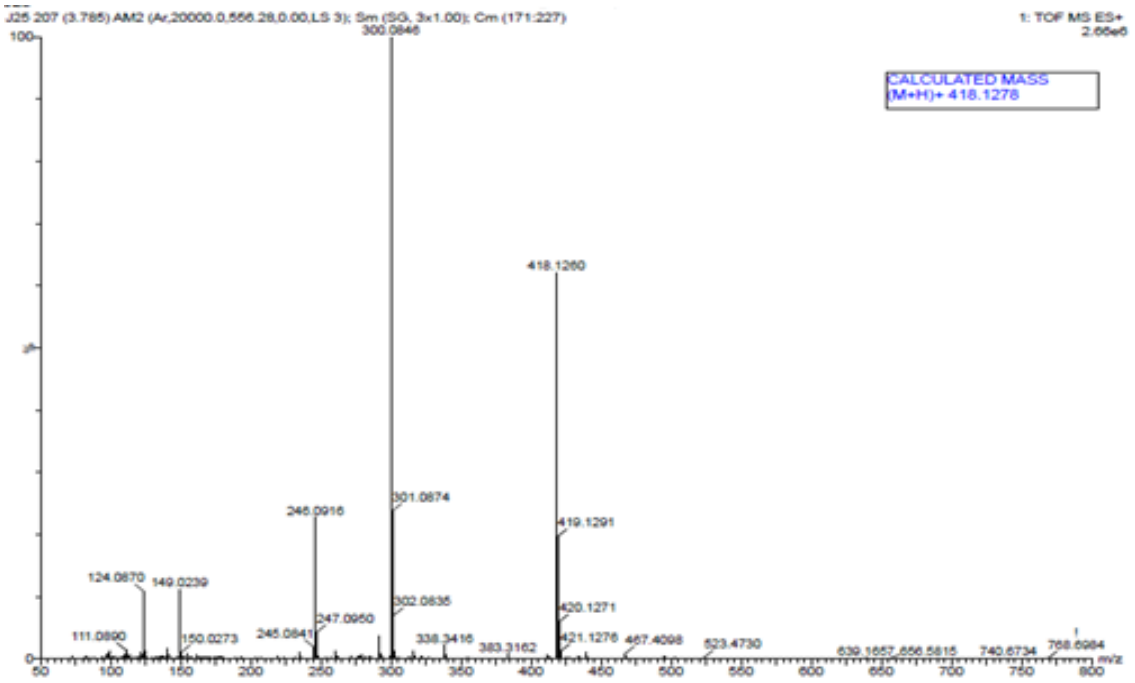

Figure S.20: HRMS spectrum of compound **4d**

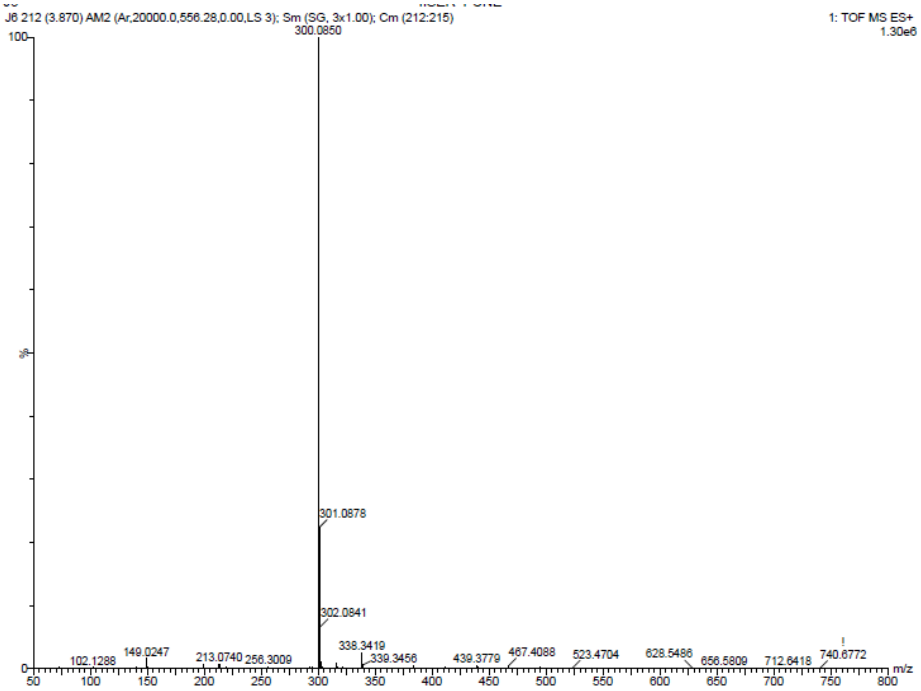

Figure S.21: HRMS spectrum of compound **4e**

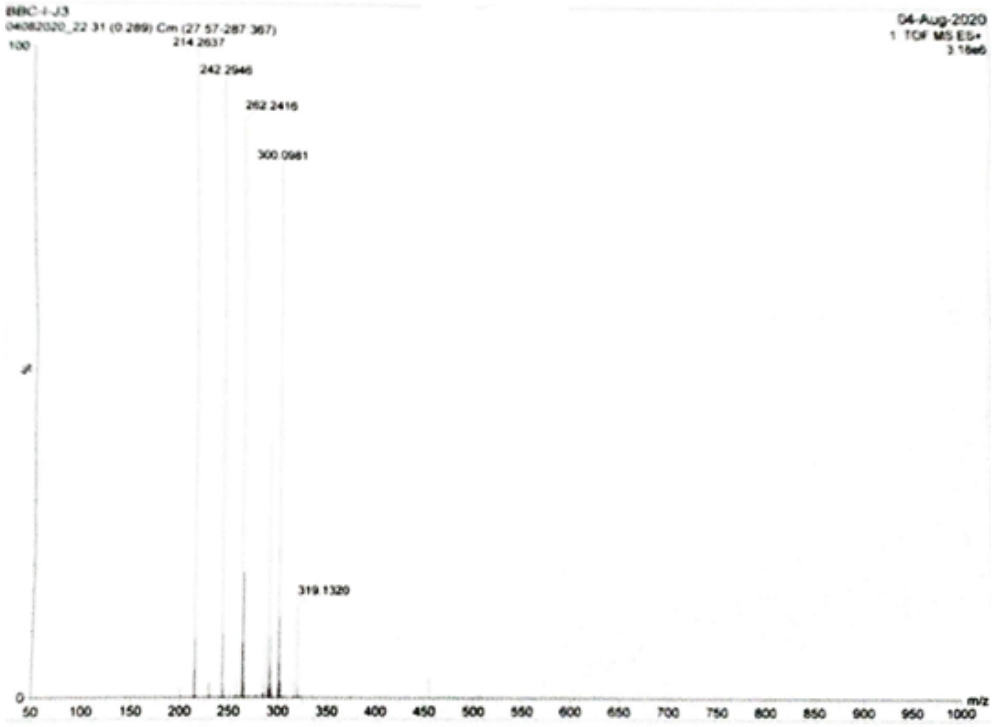

Figure S.22: HRMS spectrum of compound **4f**

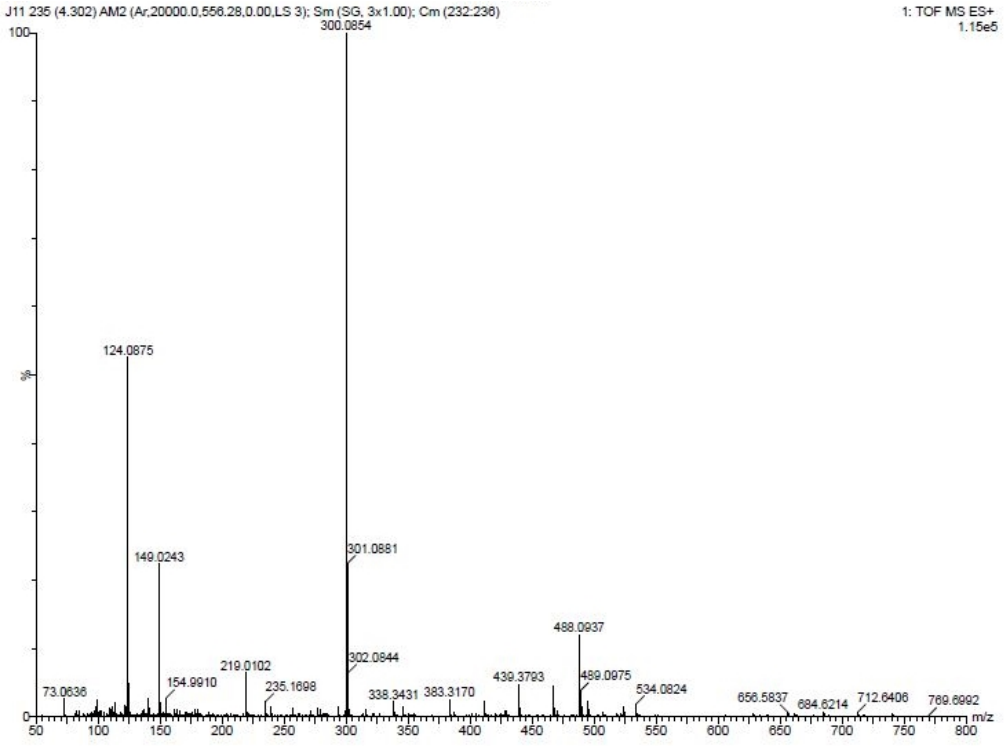

Figure S.23: HRMS spectrum of compound **4g**

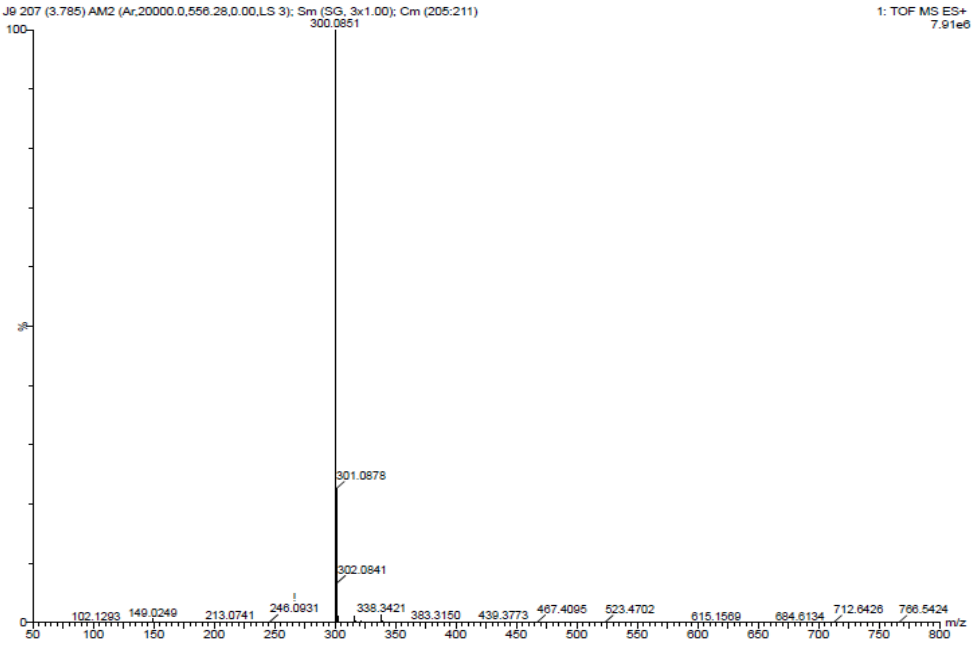

Figure S.24: HRMS spectrum of compound **4h**

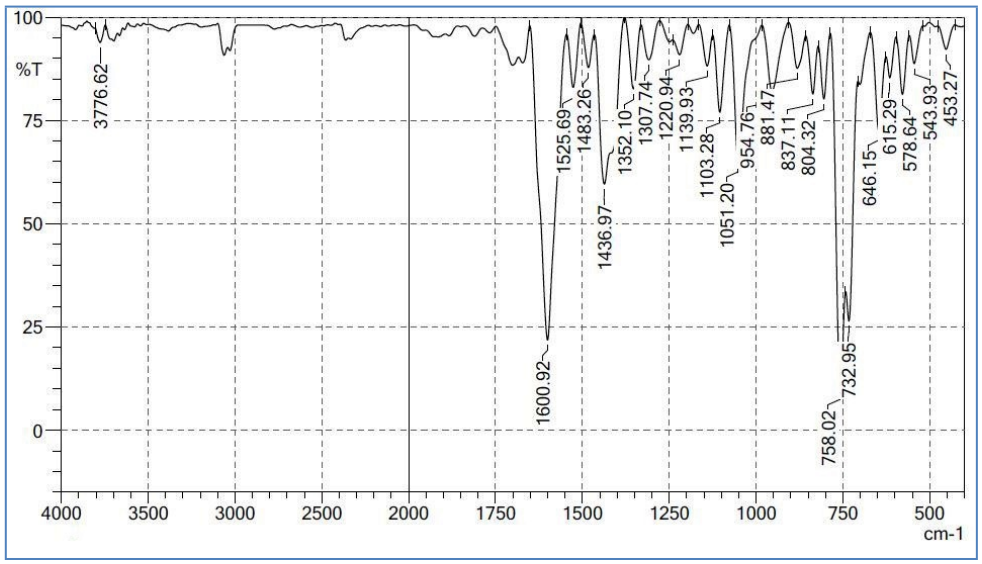

Figure S.25: IR Spectrum of compound **4b**

Table S.1: Relative quantum yield of compound **4a- h**

Entry	**Compound**	**Quantum yield ΦS (%)**
1.	4a	0.17
2.	4b	0.23
3.	4c	0.13
4.	4d	0.08
5.	4e	0.20
6.	4f	0.13
7.	4g	0.22
8.	4h	0.12

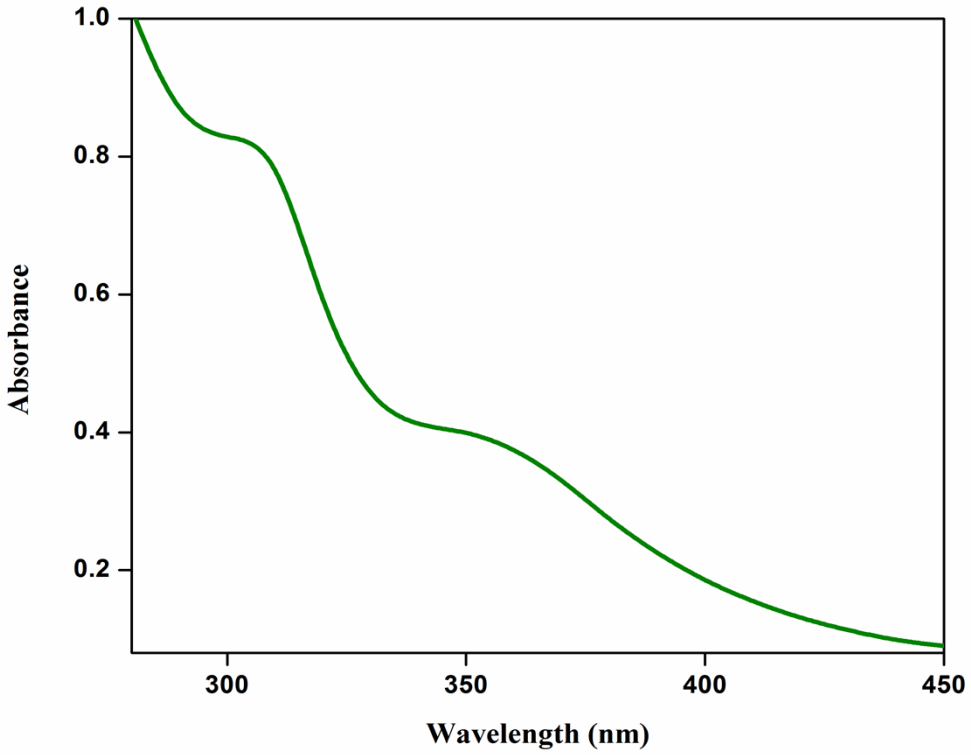

Figure S.26: UV spectra of compound **4b** (1×10^{-5}M) in DMSO

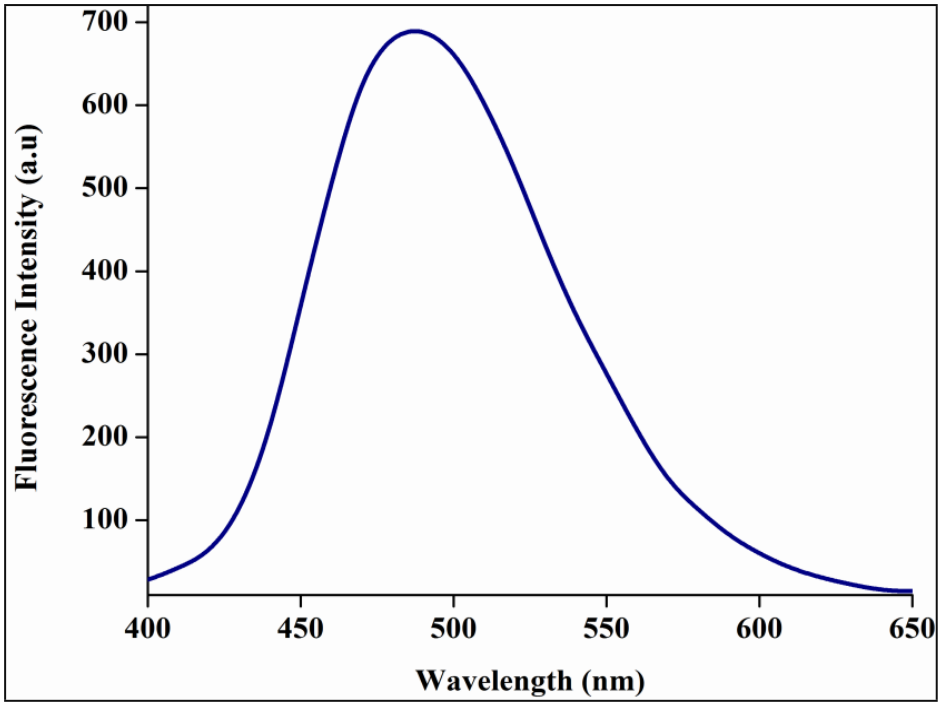

Figure S.27: Emission spectrum of **4b** (1×10^{-5}M) in DMSO

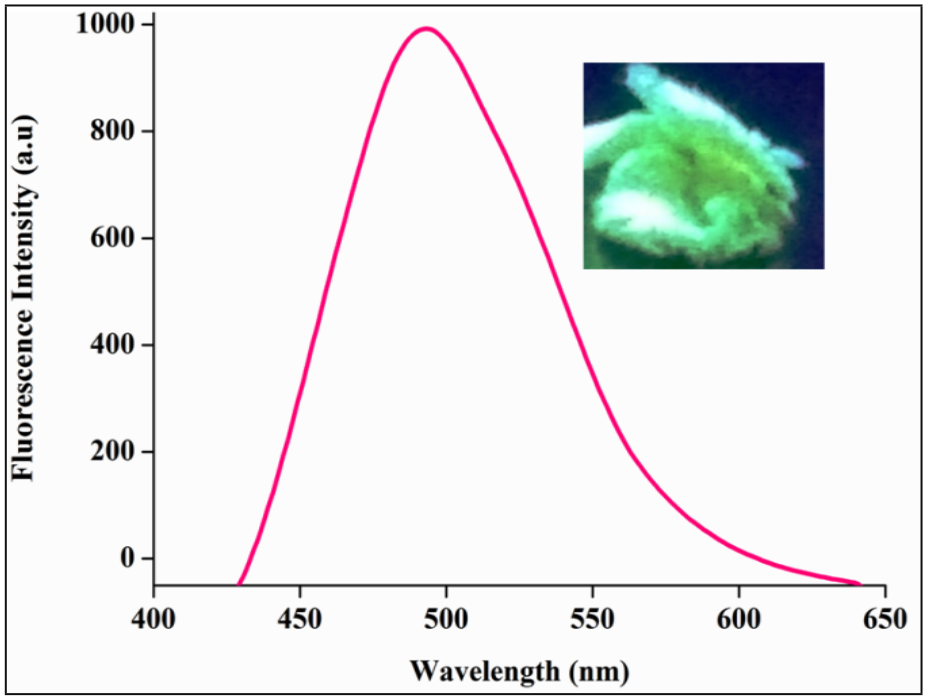

Figure S.28: Solid state emission spectrum of compound **4b**

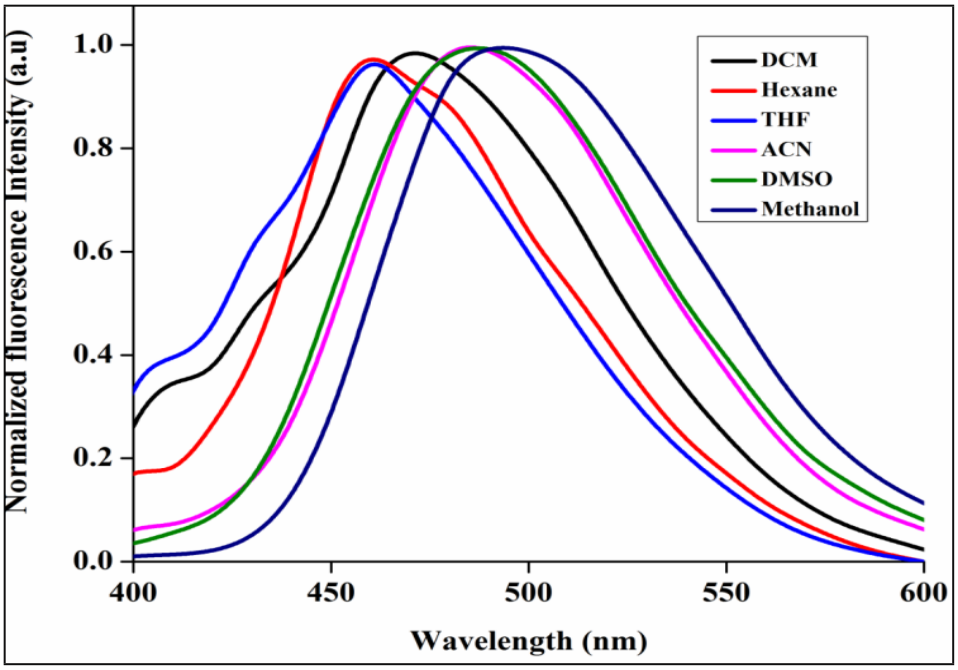

Figure S.29: Emission spectrum of compound 4**b** in various solvents

Table S.2: Solvatochromism studies results

S.No.	Solvent list	λ_{UV} max (nm)	ε ($M^{-1}cm^{-1}$)	λ_{PL} max (nm)	Stokes shift cm^{-1} & eV
1.	Hexane	310	32000	460	19,518.93, (1.30)
2.	CAN	310	61000	480	11,424.73, (1.41)
3.	THF	310	64000	470	10,981.47, (1.36)
4.	DCM	310	68000	470	10,981.47, (1.36)
5.	DMSO	310	84000	480	11,424.73, (1.41)
6.	MeOH	310	61000	500	12,258.06, (1.51)

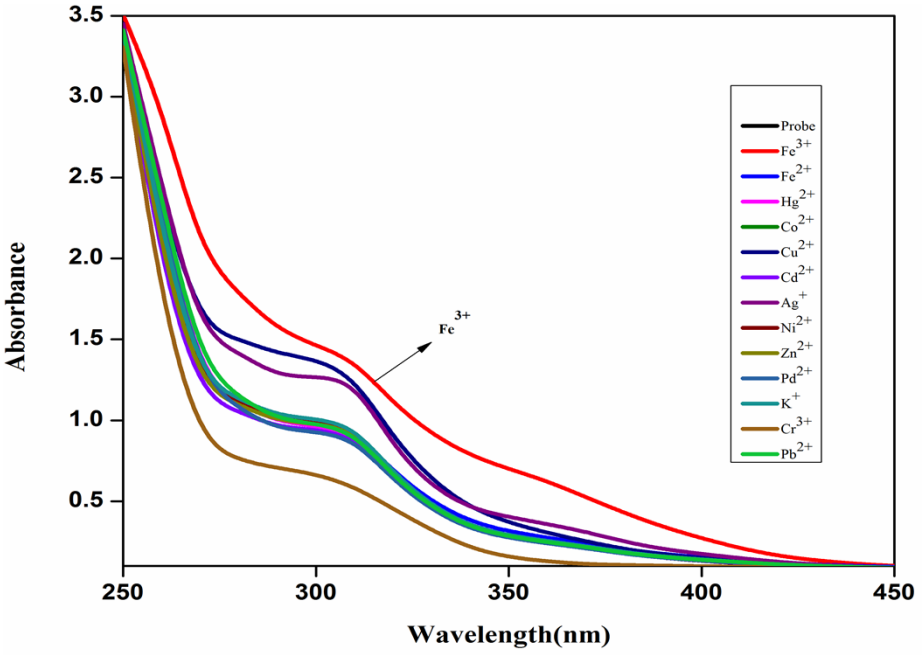

Figure S.30: UV-Vis spectra of **4b** (2×10^{-5} M) in different metal cations (150 µl)

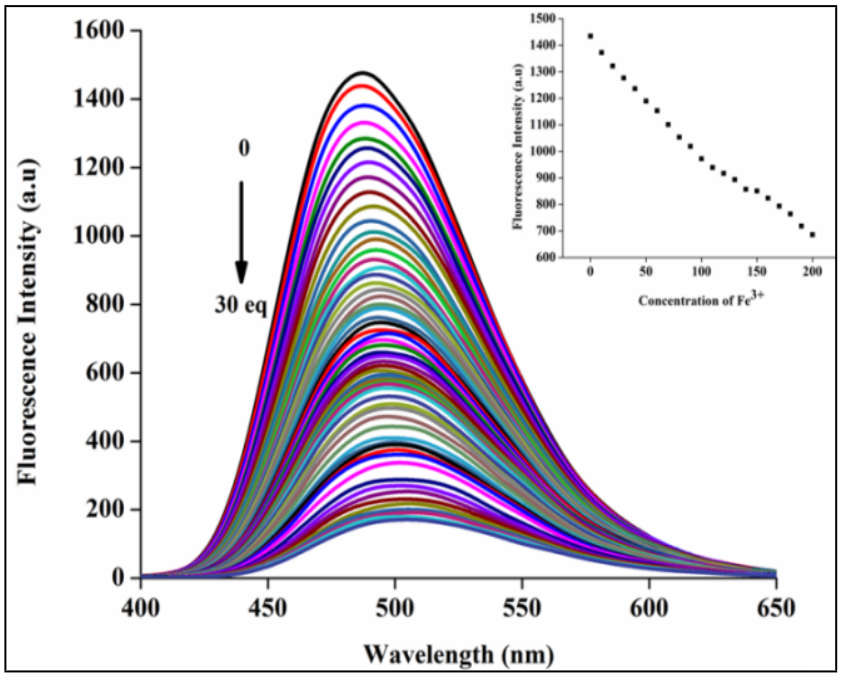

Figure S.31: Emission spectra of **4b** (2×10^{-5} M) in various concentrations of Fe^{3+} (0-300 µl) in DMSO and (inset) plot of P.L intensity vs metal ion concentration.

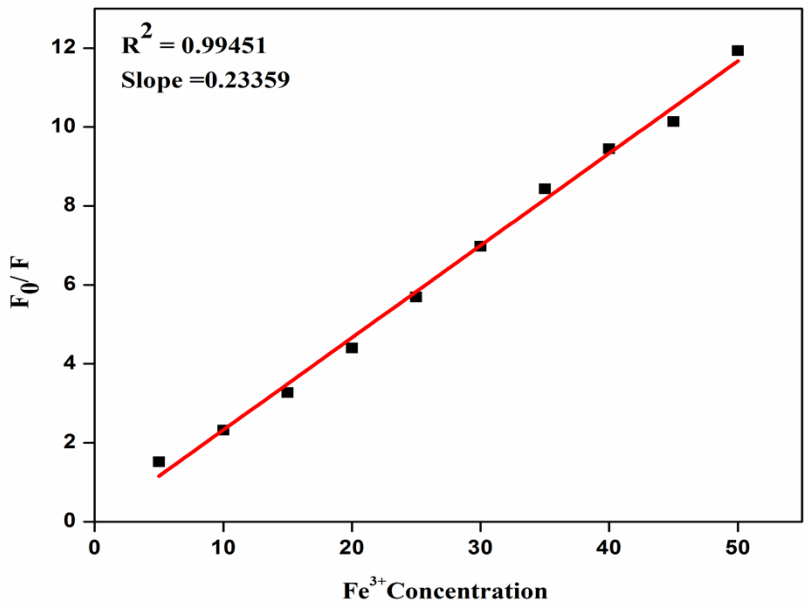

Figure S.32: Stern-Volmer plot for **4b** with Fe^{3+} in DMSO

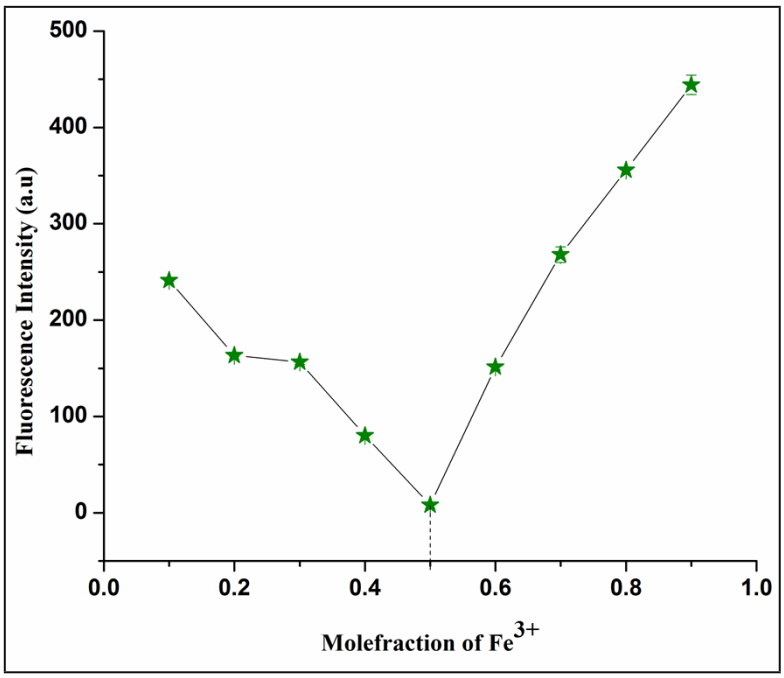

Figure S.33: Job's plot

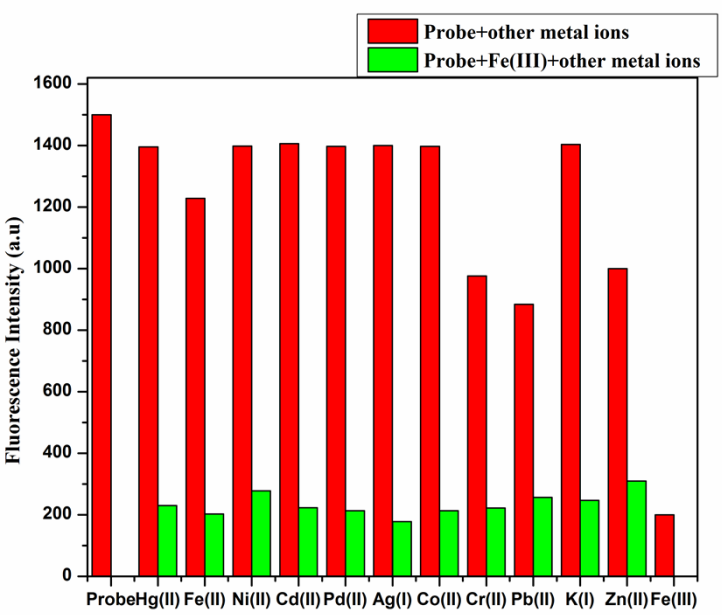

Figure S.34: The selectivity of **4b** (2 $\times 10^{-5}$M) in the presence of various metal ions in DMSO

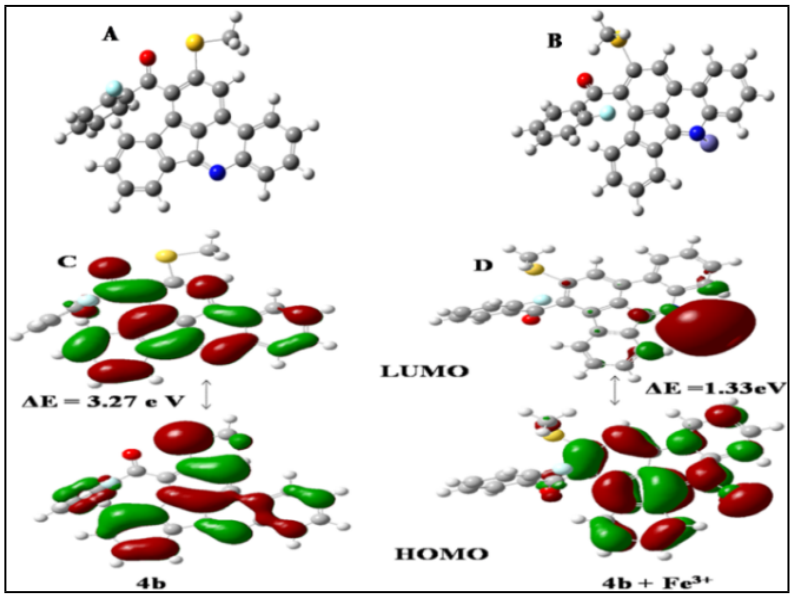

Figure S.35: Optimized structure of A (**4b**) & B (**4b** + **Fe**$^{3+}$) and Frontier orbital diagram of probe C (**4b**) & D (**4b** +**Fe**$^{3+}$).

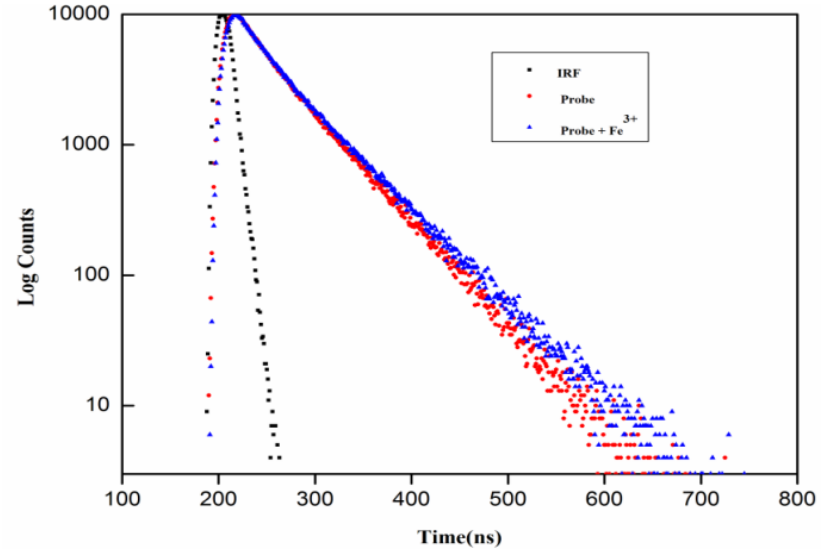

Figure S.36: Time–correlated single photon counting spectrometer for probe 4b and 4b+ Fe^{3+}

λ_{ex} = 350 nm and λ_{em} = 480 nm

Table S.3 Fluorescence lifetime Parameters of compound **4b** and **4b+ Fe^{3+}**

System	λ_{ex}	λ_{em}	τ_1(ns) (Rel%)	τ_2(ns) (Rel%)	$\tau_{average}$(ns)	χ^2
4b	350 nm	480 nm	1.57 (24.5)	3.06 (75.50)	2.7	1.19
4b+Fe^{3+}	350 nm	480 nm	1.34 (24.73)	3.34 (75.27)	2.8	1.13

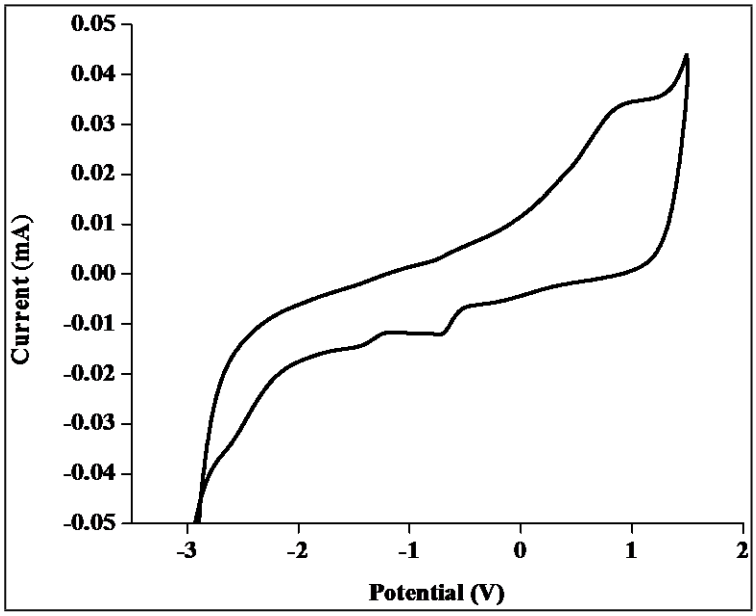

Figure S.37: Cyclic voltammogram of probe **4b** in DMSO with 0.1 M of $LiclO_4$

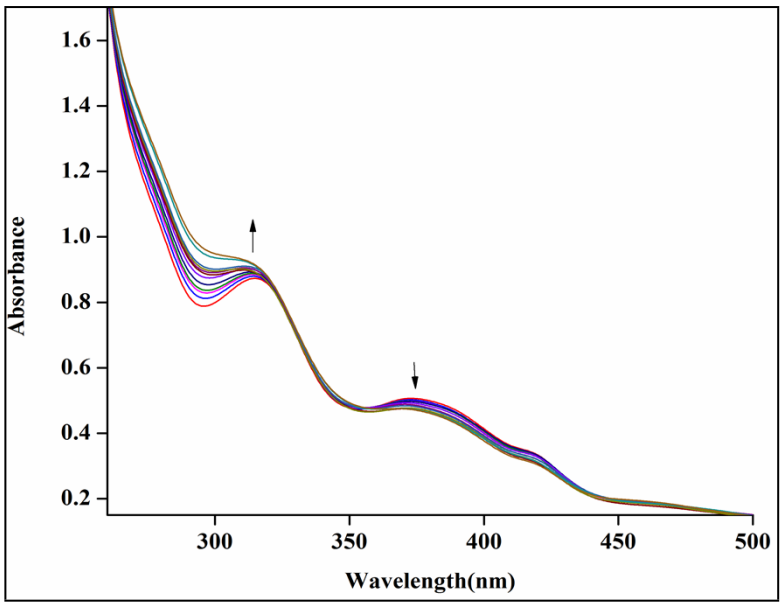

Figure S.38: UV-Vis spectra of probe **4b** (1×10^{-5} M) with addition various concentrations of TFA in DMSO

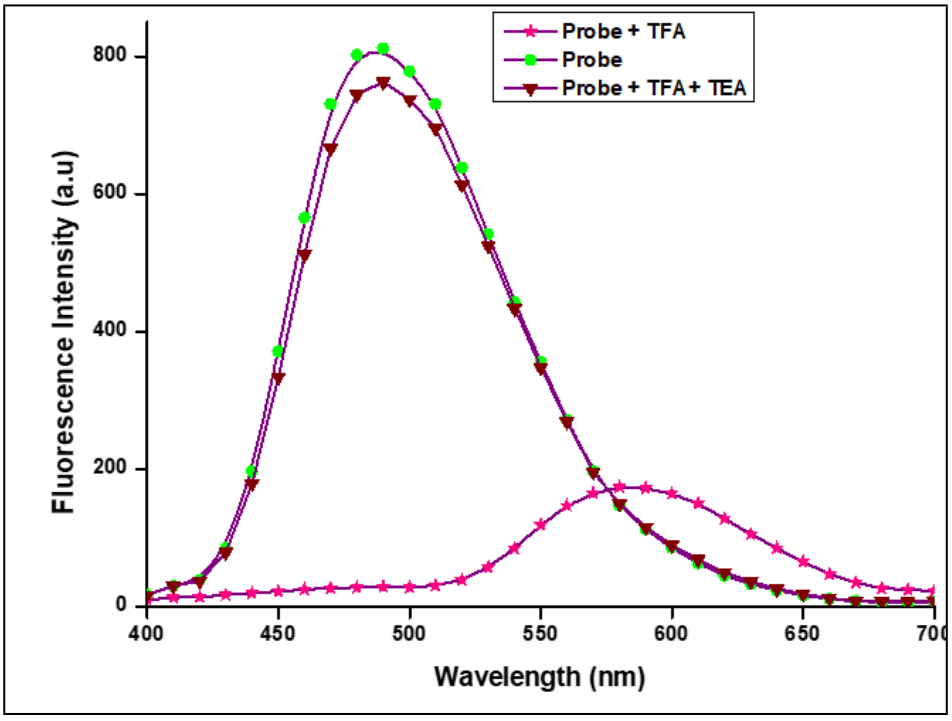

Figure S.39: Reversible emission spectra of probe **4b** (1×10^{-5} M) with the addition of different volumes of TFA and TEA in DMSO

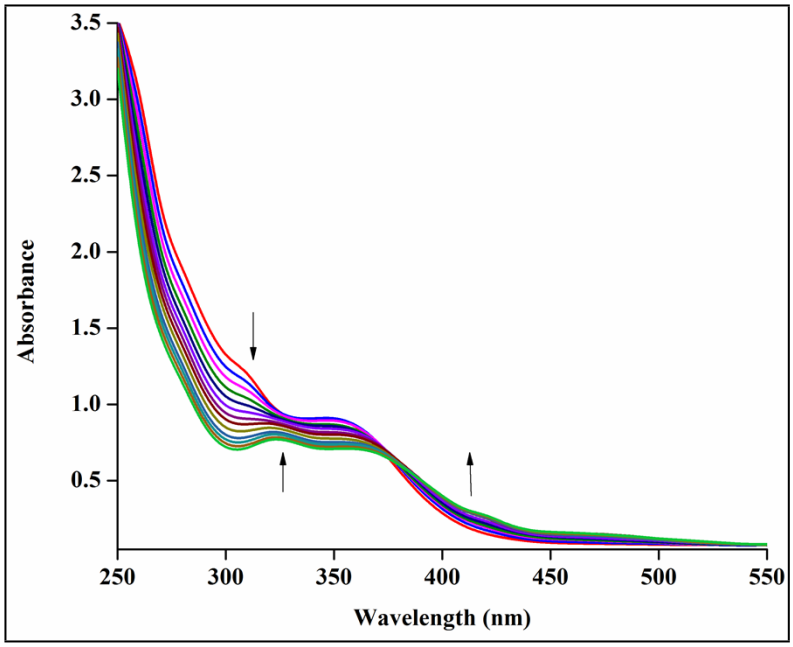

Figure S.40: Reversible UV-vis spectra of probe **4b** (1×10^{-5} M) with the addition of a different volumes of TFA and TEA in DMSO

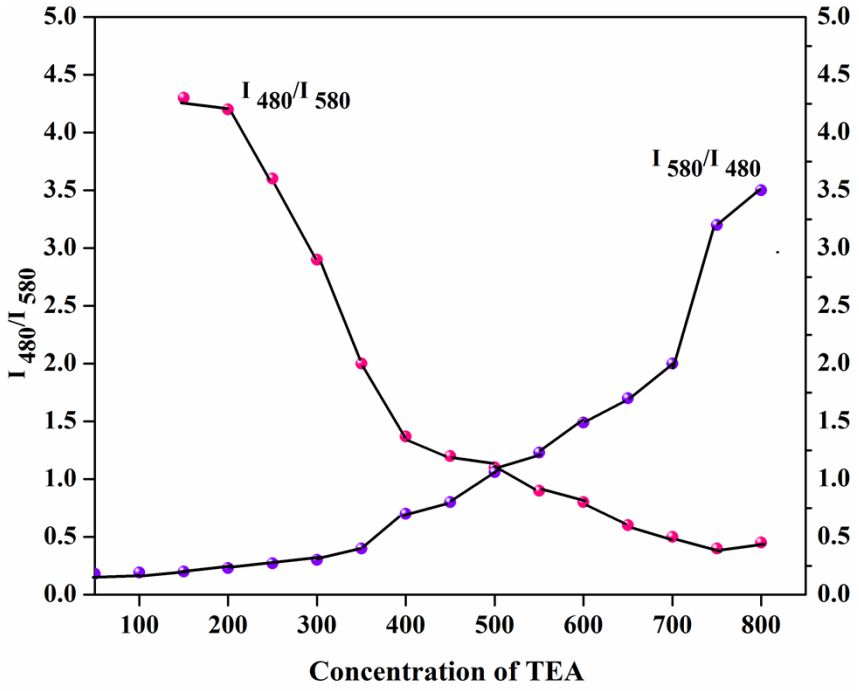

Figure S.41: Sigmoidal graph.

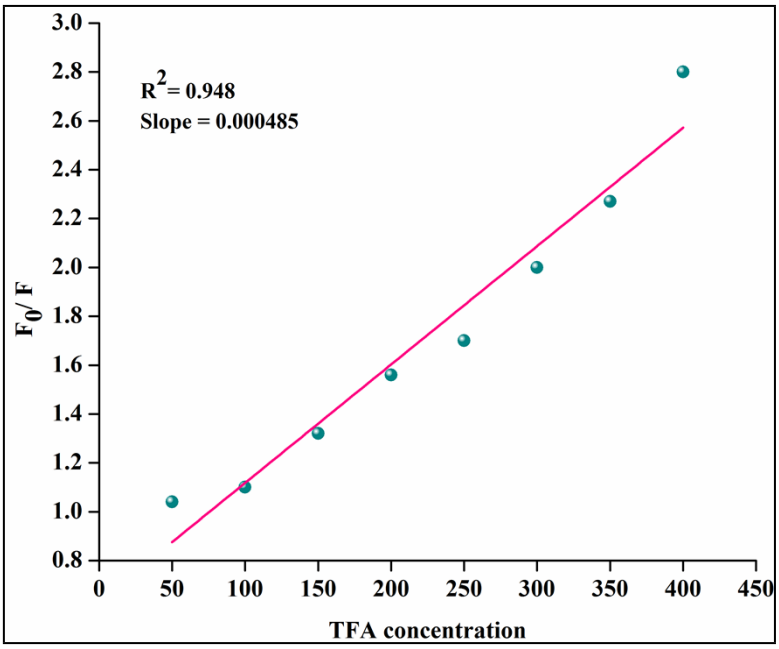

Figure S.42: Stren-Volmer plot of acidochromism studies of probe **4b**

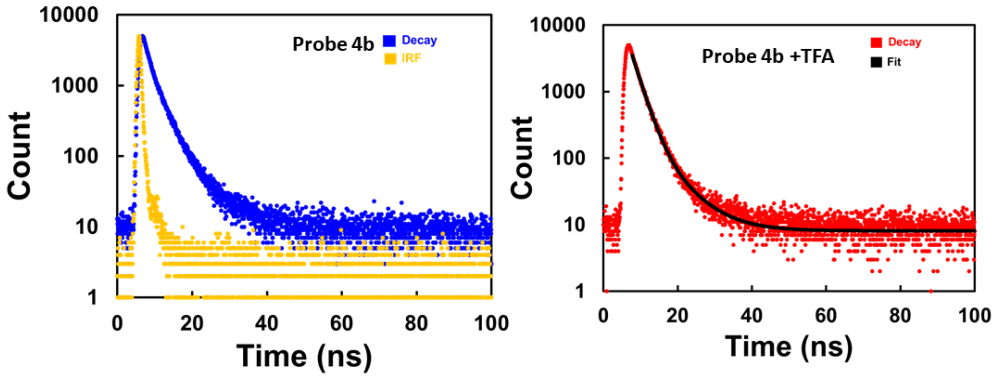

Figure S.43: Time–correlated single photon counting spectrometer for probe 4b and 4b+ TFA

λ_{ex} = 375 nm and λ_{em} = 480 nm for probe 4b and λ_{ex} = 375 nm and λ_{em} = 580 nm for probe 4b+TFA

	λ_{ex}	λ_{em}	τ_1 (Rel%)	τ_2 (Rel%)	T average (ns)	χ^2
2F-IND	375 nm	480 nm	2.06 ns (56.42)	5.52(43.58)	3.5	1.229
2F-IND + TFA	375 nm	580 nm	2.35 ns (82.71)	6.94 ns (17.29)	3.1	1.192

Table S.4: Fluorescence lifetime Parameters of compound **4b** and **4b+ TFA**