Supporting Information

A new class of teraryl-based AIEgen for highly selective imaging of intracellular lipid droplets and its detection in advanced-stage human cervical cancer tissues

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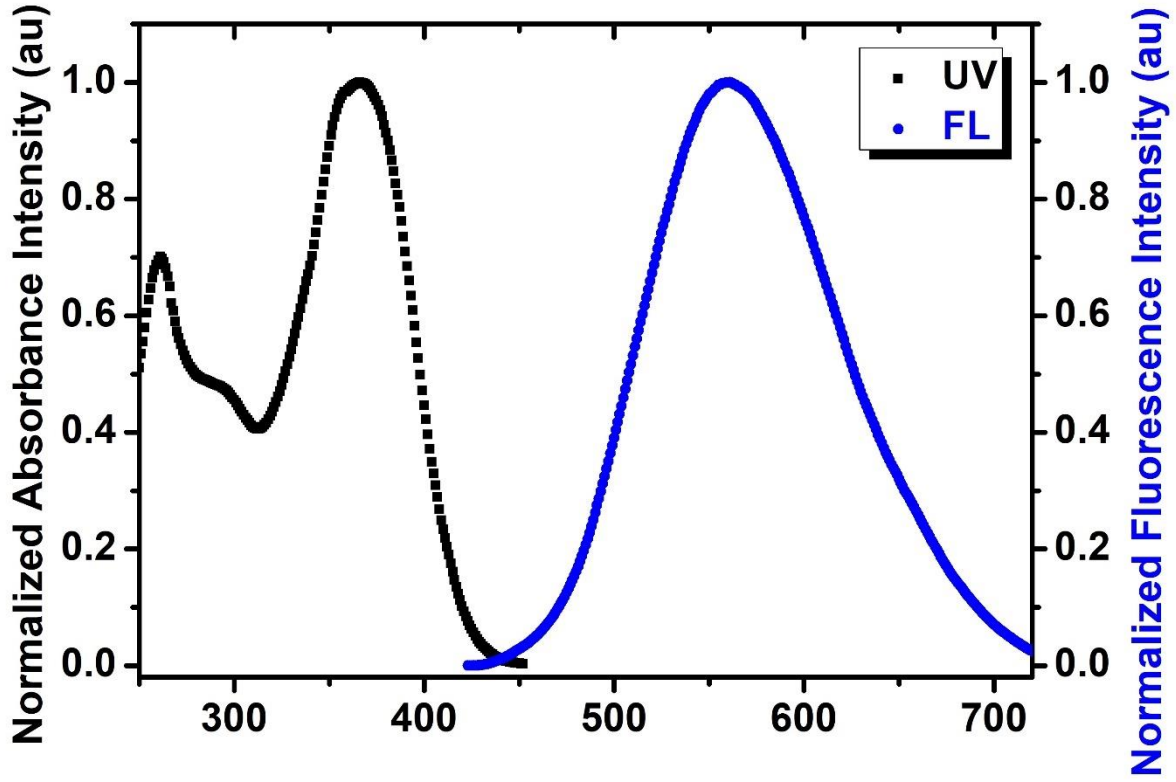

Fig. S1. Normalized UV and fluorescence spectra of **6a** (10μM) in DMSO.

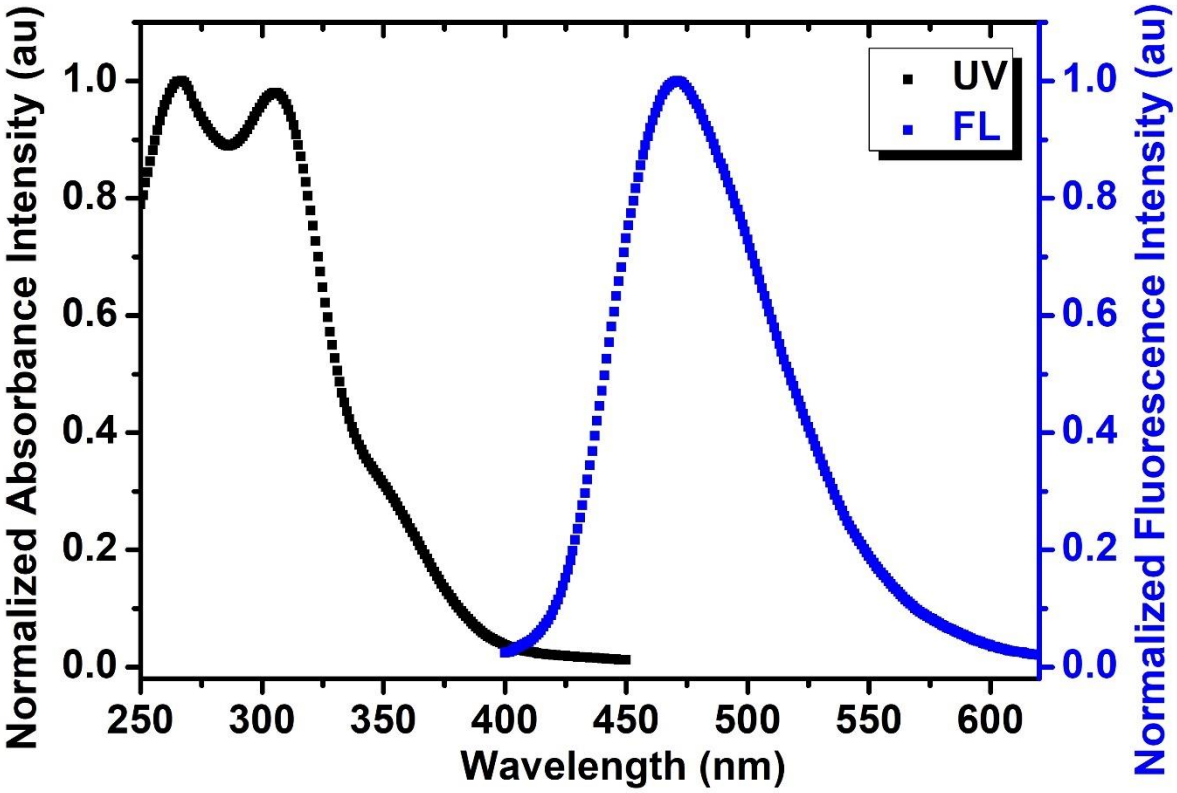

Fig. S2. Normalized UV and fluorescence spectra of **6b** (10μM) in DMSO.

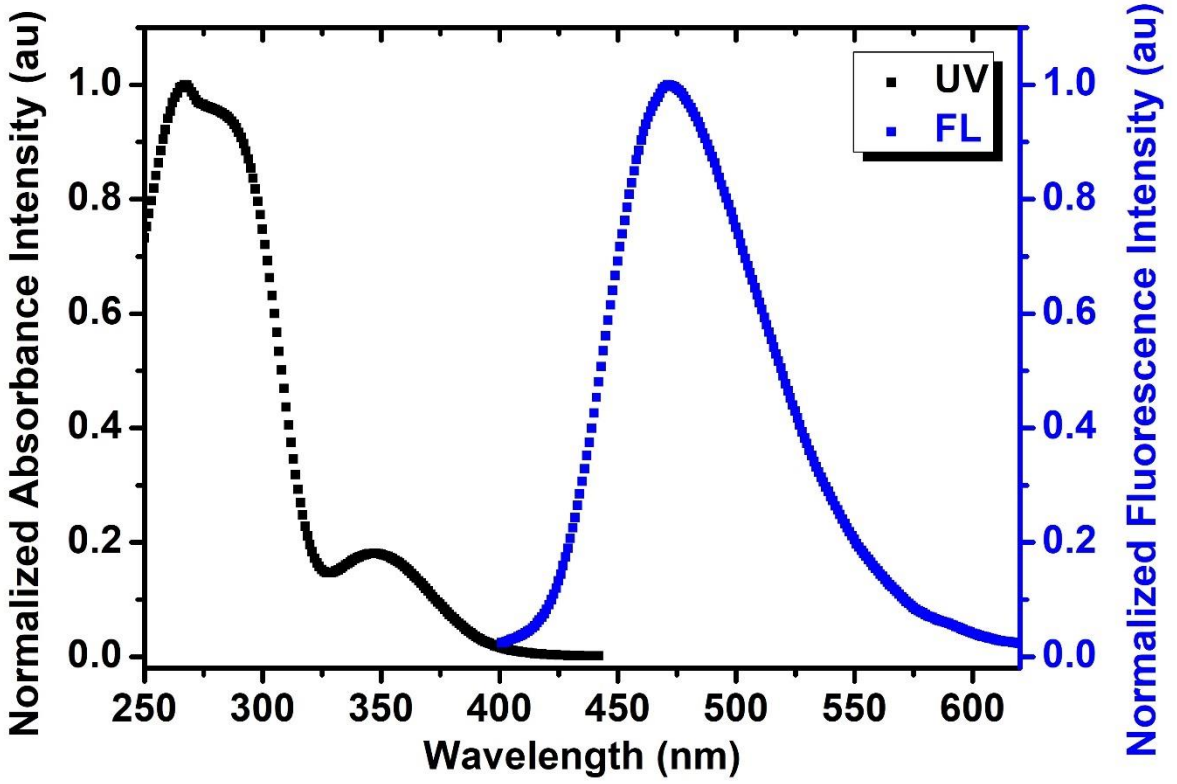

Fig. S3. Normalized UV and fluorescence spectra of **6c** (10μM) in DMSO.

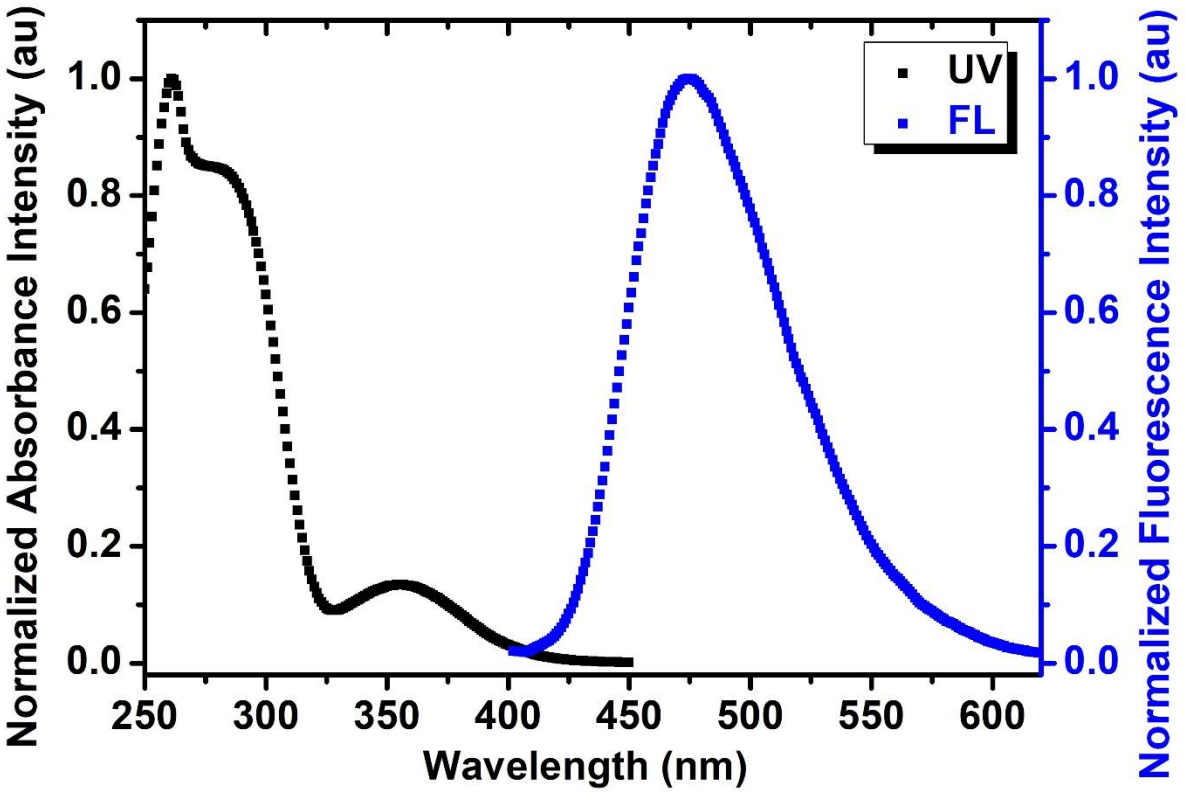

Fig. S4. Normalized UV and fluorescence spectra of **6d** (10μM) in DMSO.

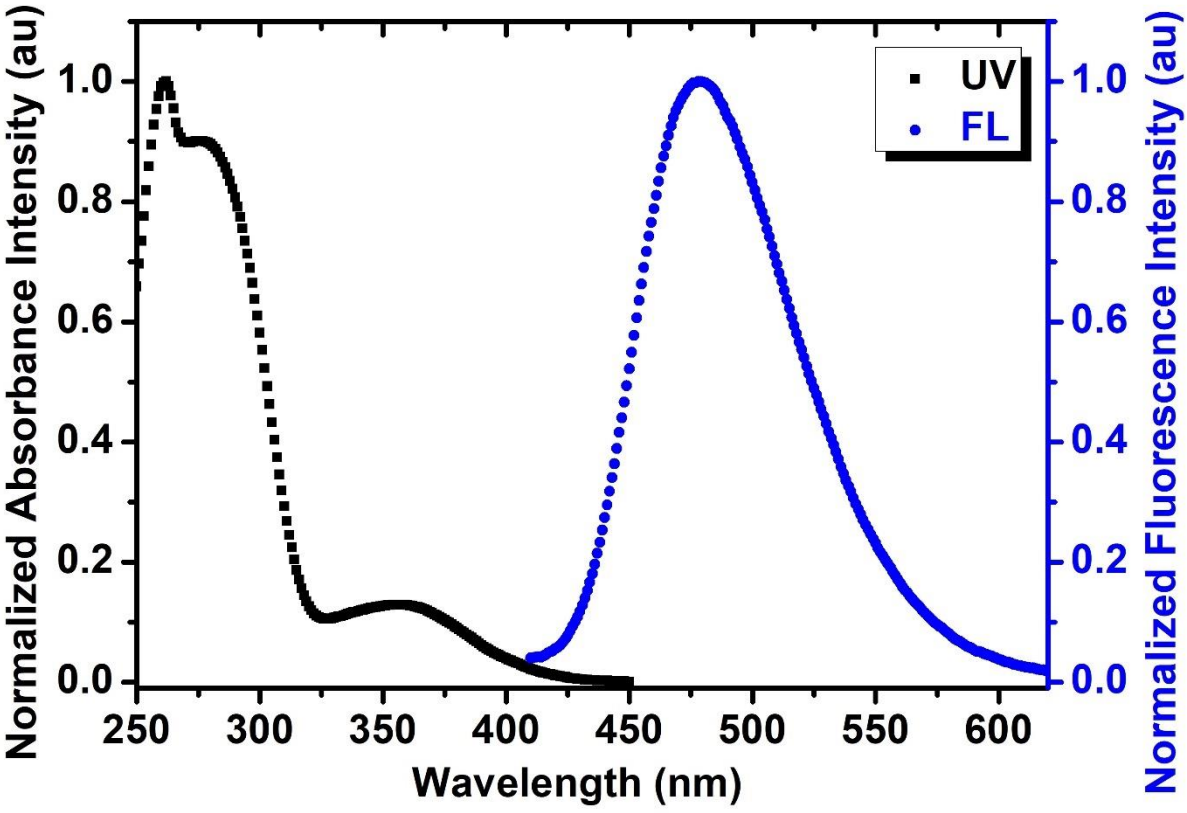

Fig. S5. Normalized UV and fluorescence spectra of **6e** (10μM) in DMSO.

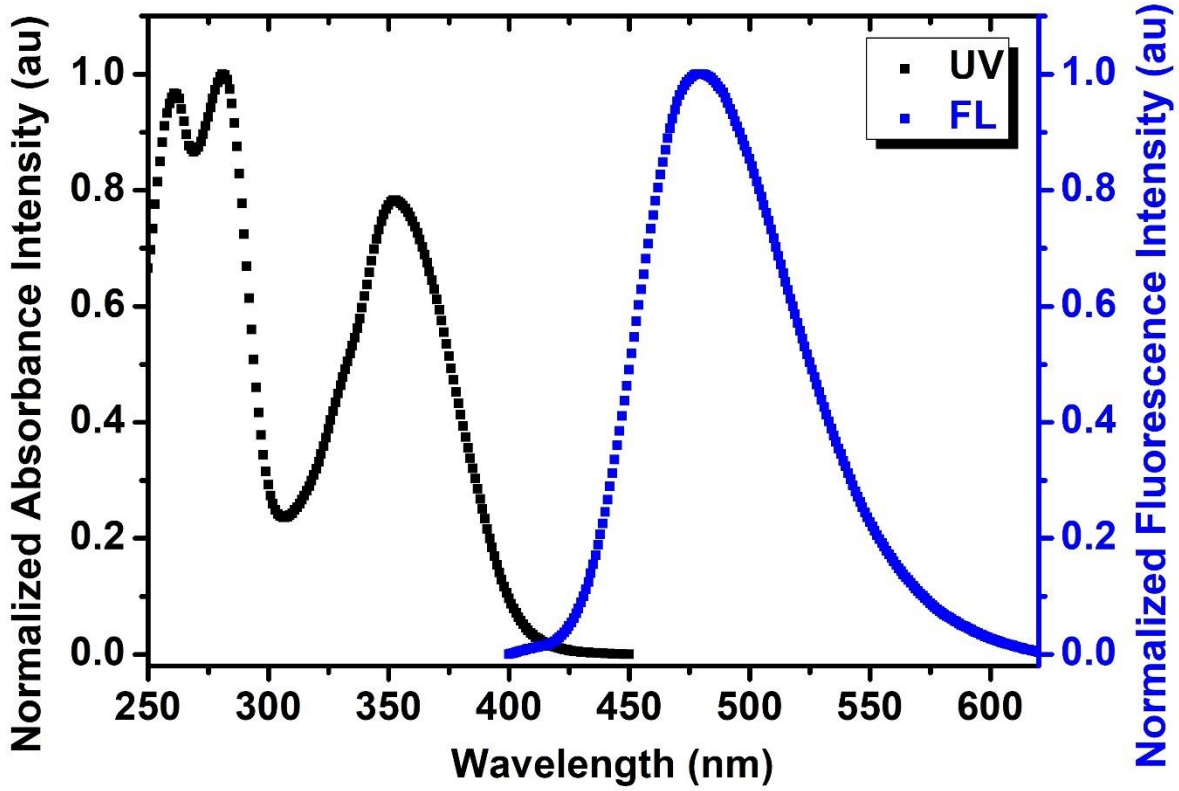

Fig. S6. Normalized UV and fluorescence spectra of **6f** (10μM) in DMSO.

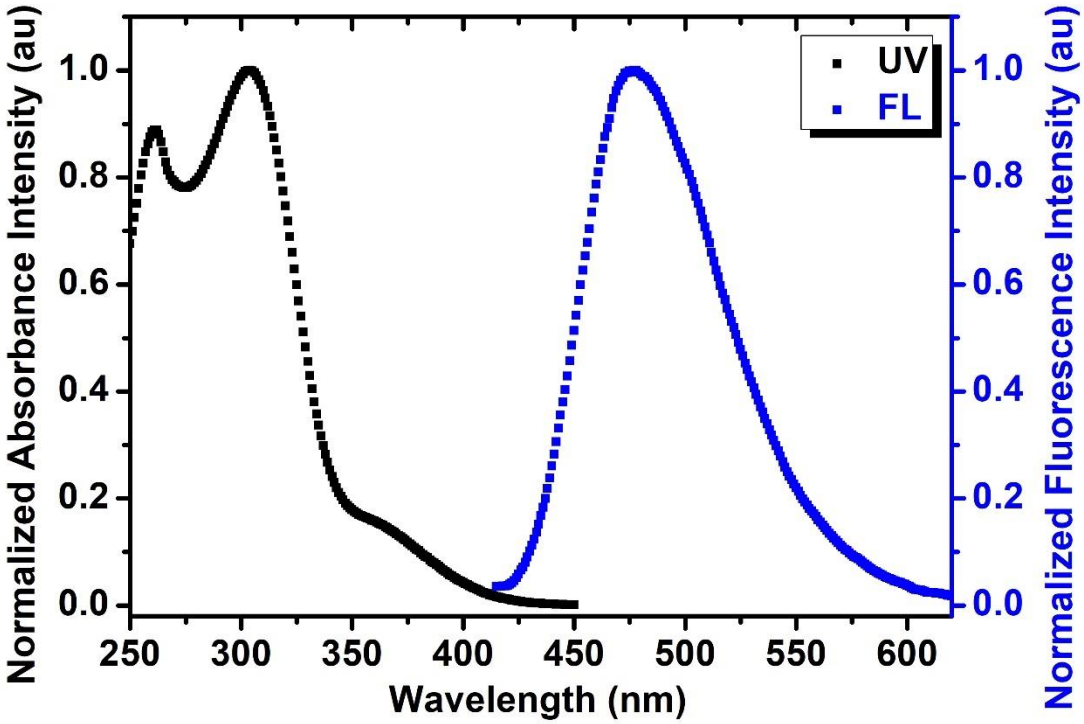

Fig. S7. Normalized UV and fluorescence spectra of **6g** (10μM) in DMSO.

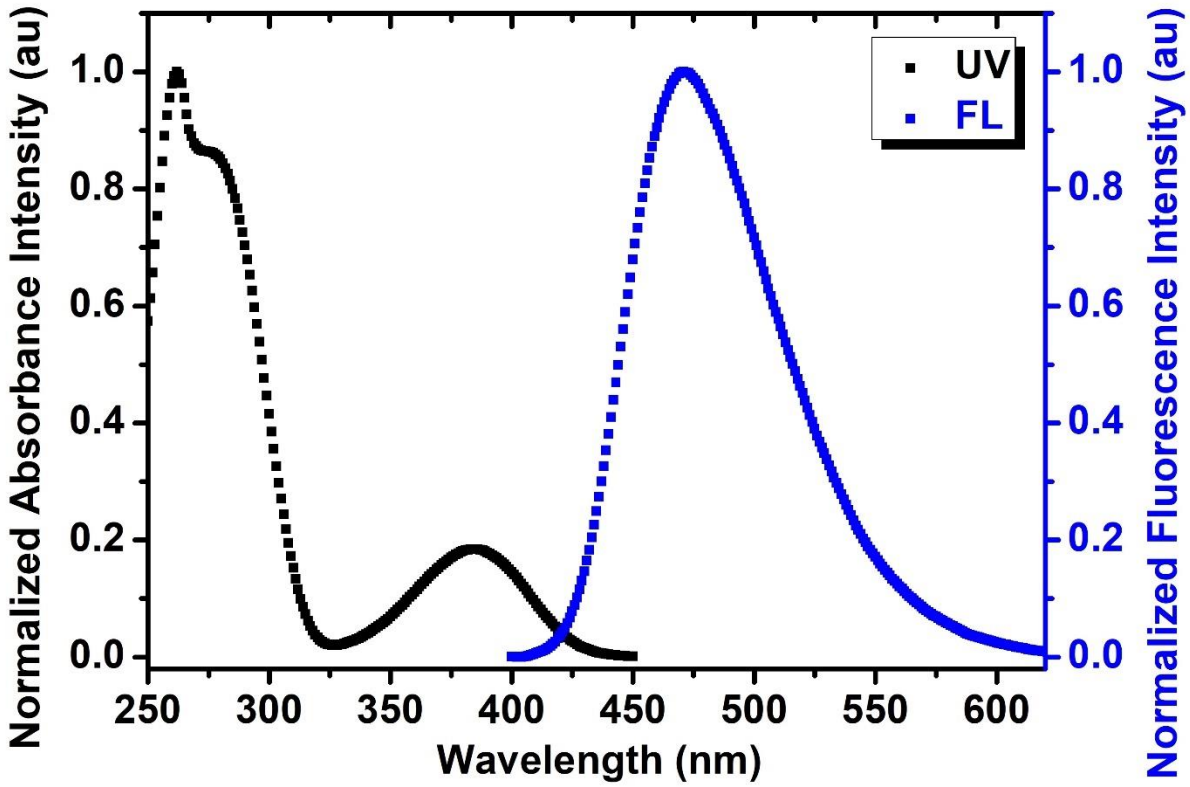

Fig. S8. Normalized UV and fluorescence spectra of **6h** (10μM) in DMSO.

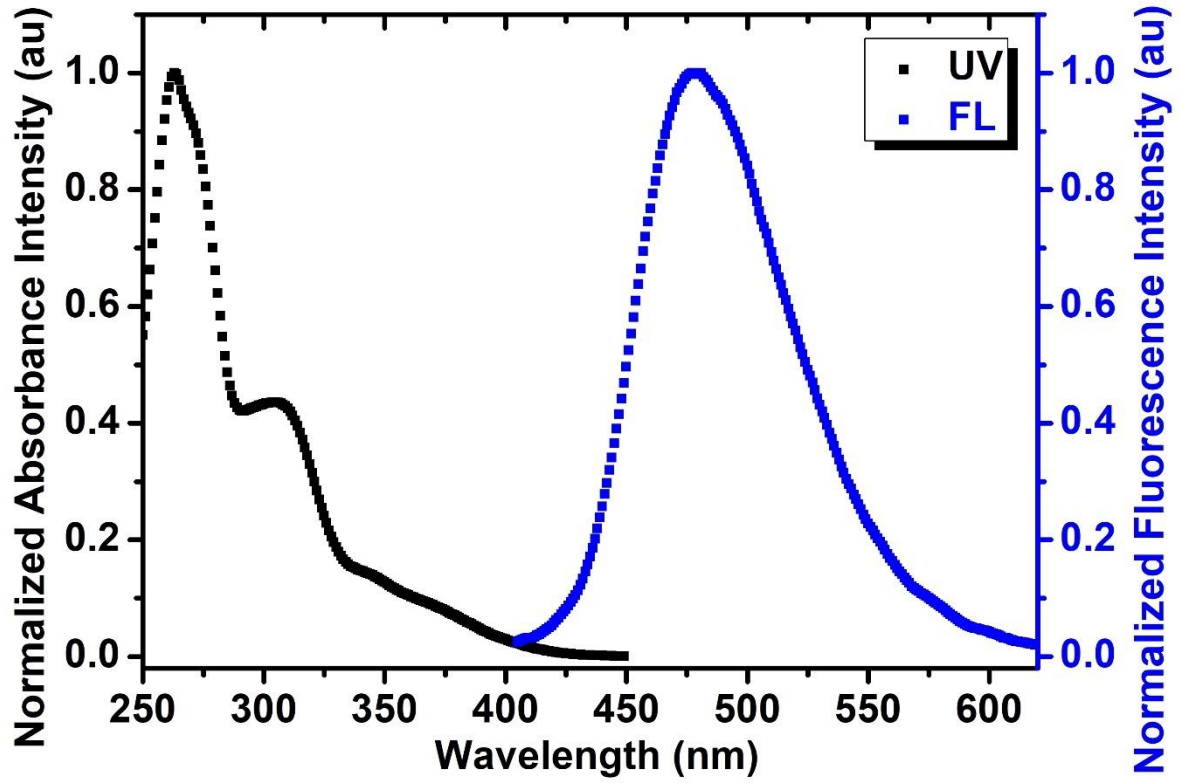

Fig. S9. Normalized UV and fluorescence spectra of **6i** (10μM) in DMSO.

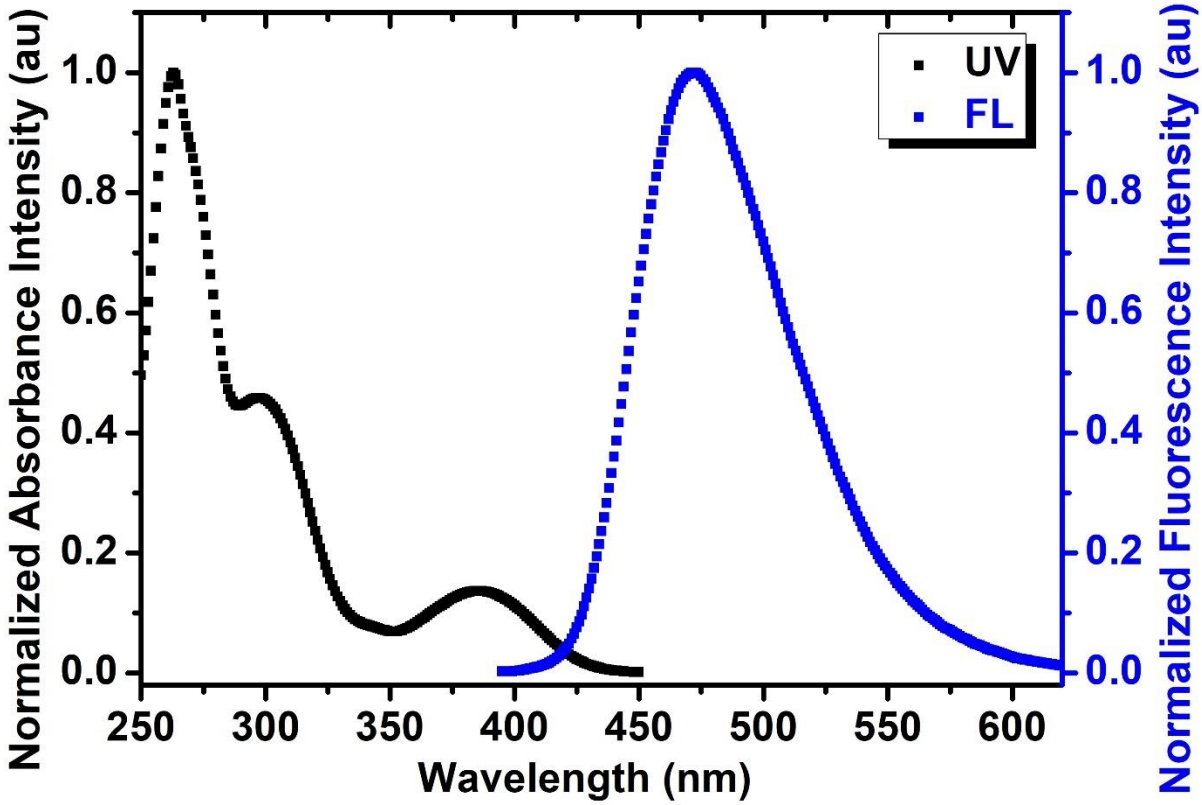

Fig. S10. Normalized UV and fluorescence spectra of **6j** (10μM) in DMSO.

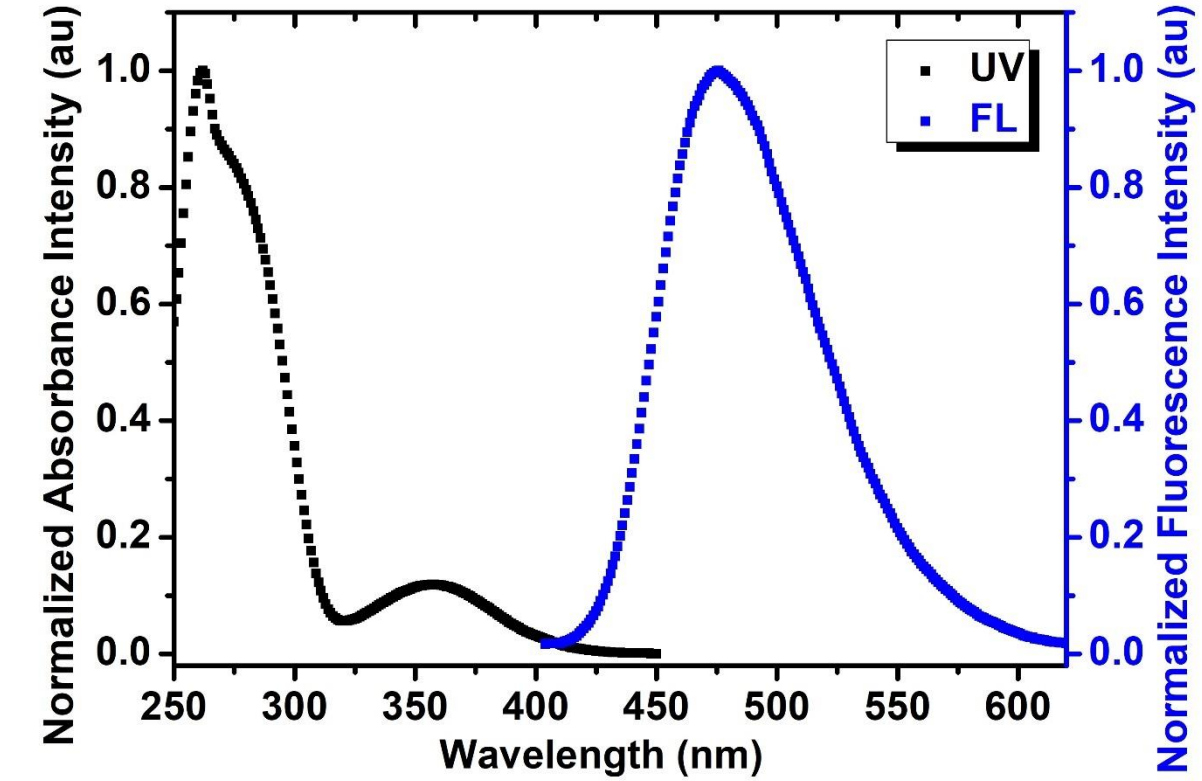

Fig. S11. Normalized UV and fluorescence spectra of **6k** (10μM) in DMSO.

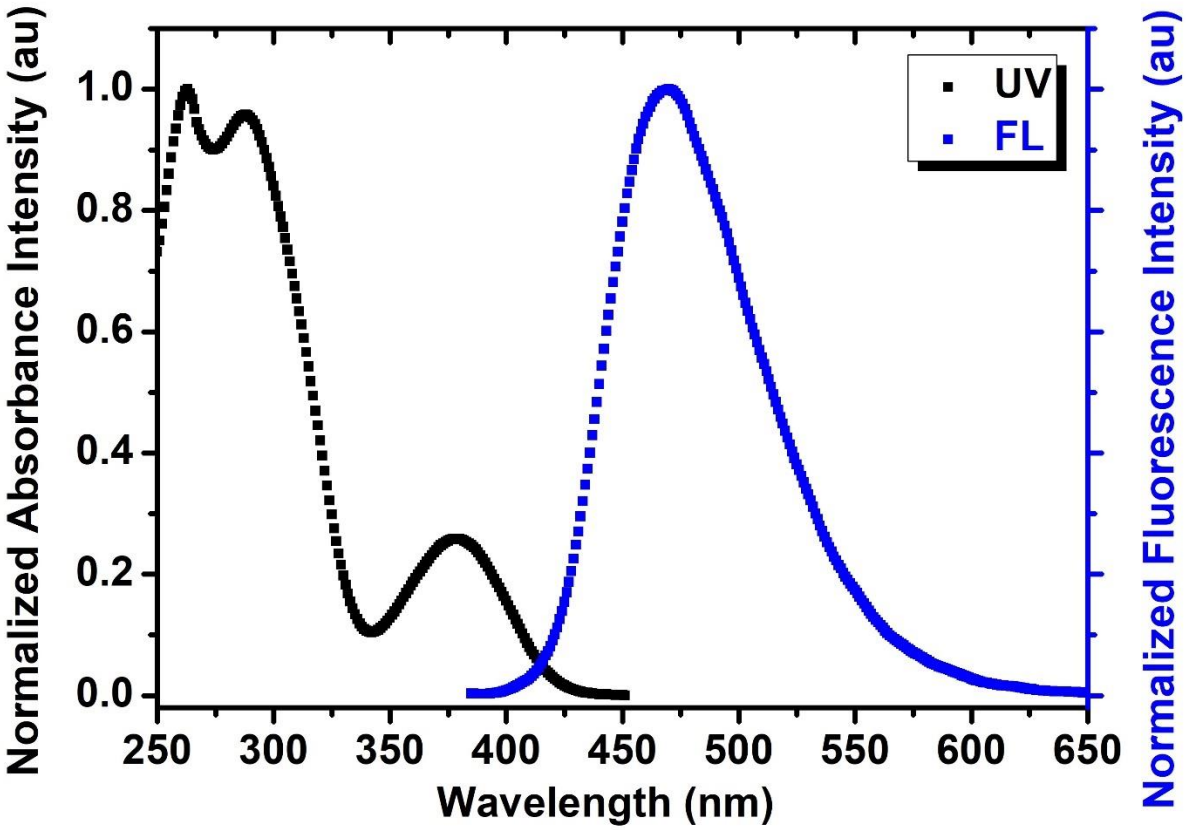

Fig. S12. Normalized UV and fluorescence spectra of **6l** (10μM) in DMSO.

Table S1. Solvatochromic data of **6a** in various solvents.

Entry	Polarity Index (Δf)	Solvents	λ_{max}, abs (nm)[a]	λ_{max}, em (nm)[b]	Stokes shift (nm)[c]	CIE (x,y)
6a	0.0134	Toluene	350	442	90	0.14, 0.07
	0.0231	Dioxane	350	454	105	0.14, 0.11
	0.201	EA	352	493	140	0.19, 0.36
	0.2096	THF	353	516	160	0.27, 0.48
	0.286	Acetone	356	535	180	0.35, 0.52
	0.2745	DMF	363	553	190	0.41, 0.52
	0.2640	DMSO	365	560	195	0.41, 0.51

[a]Absorption maxima, [b]Fluorescence maxima in different solvents.. [c]Stokes shift (nm) = (λ_{em} -λ_{abs})

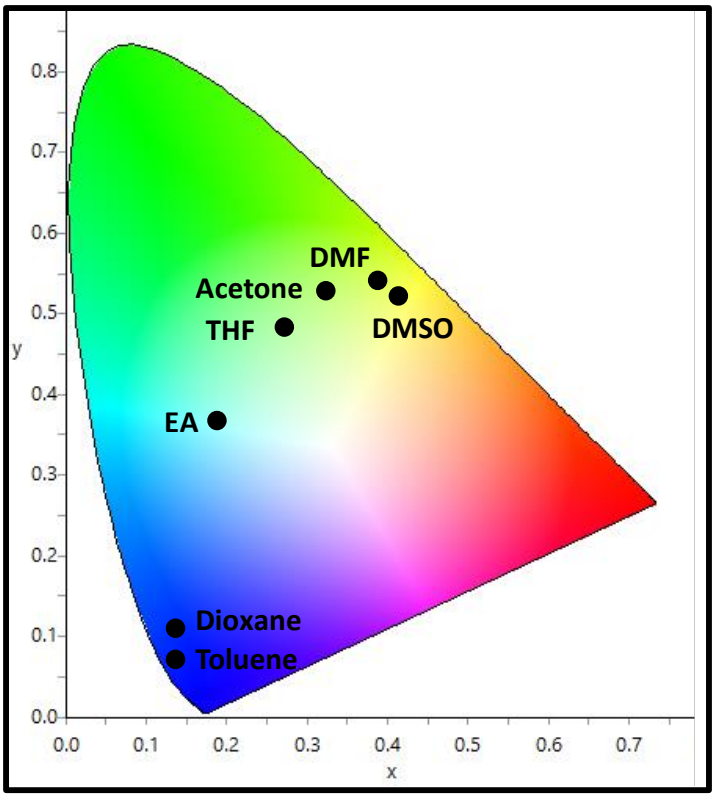

Fig. S13. CIE representation of the solvatochromic effect for compound **6a** using color calculator software.

Fluorescence life time decay of all the synthesized derivatives (6a-l)

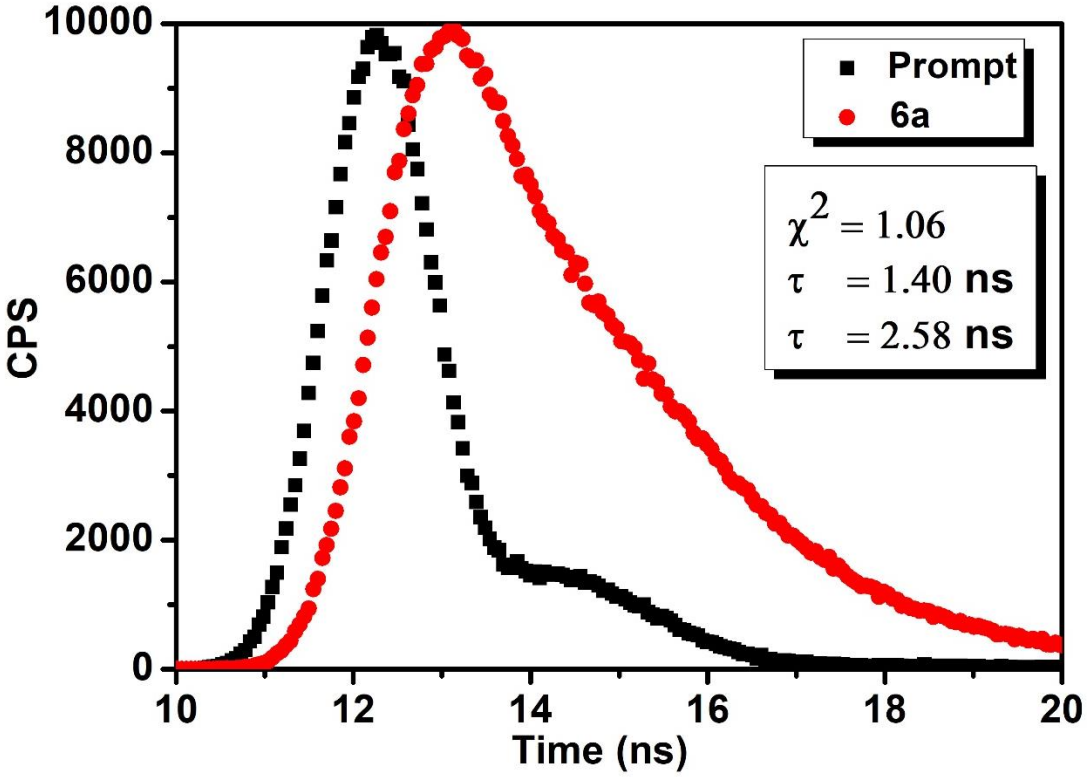

Fig. S14. Fluorescence life time spectrum of **6a** (~10^{-5} M) in DMSO.

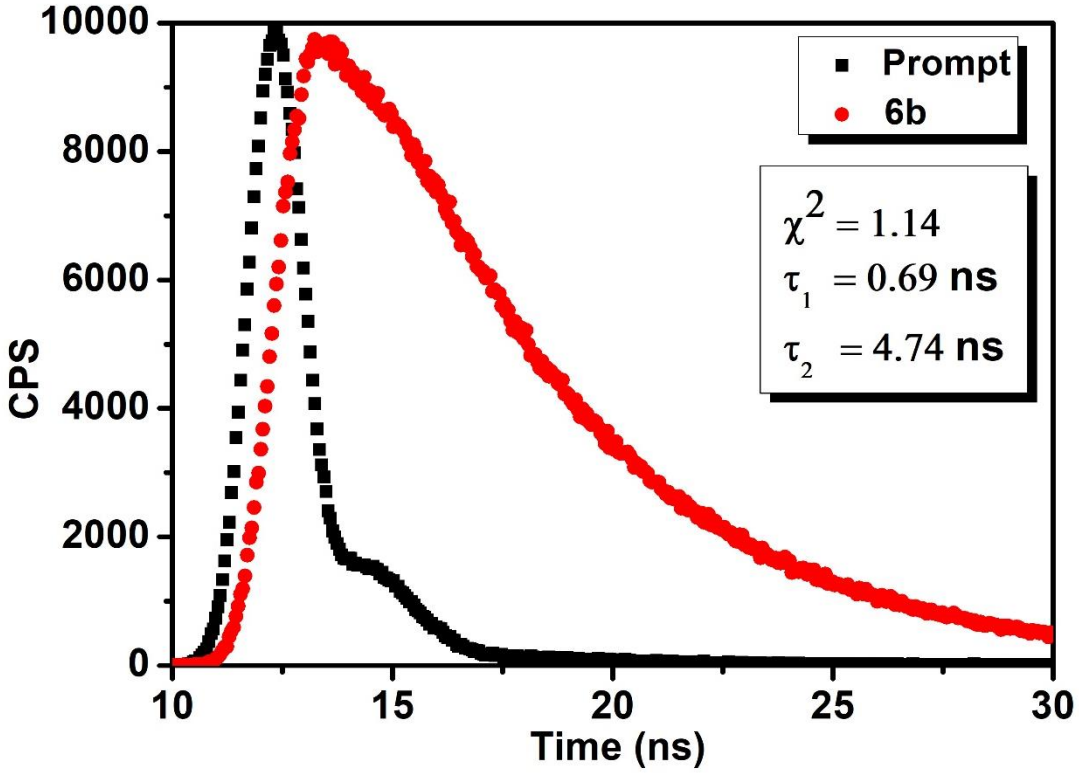

Fig. S15. Fluorescence life time spectrum of **6b** (~10^{-5} M) in DMSO.

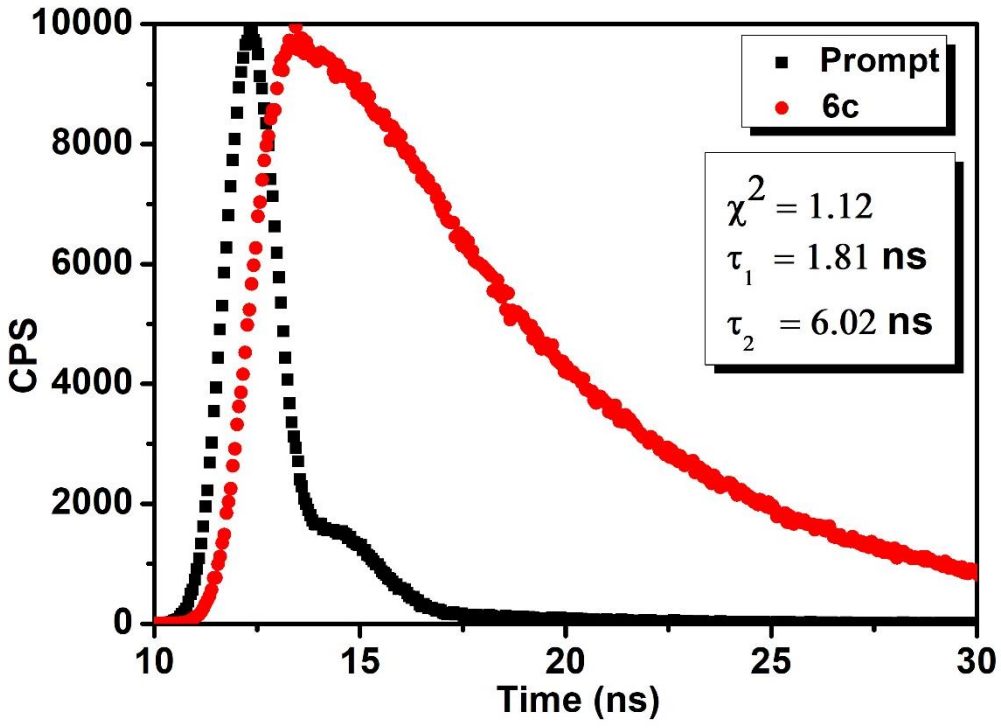

Fig. S16. Fluorescence life time spectrum of **6c** (~10^{-5} M) in DMSO.

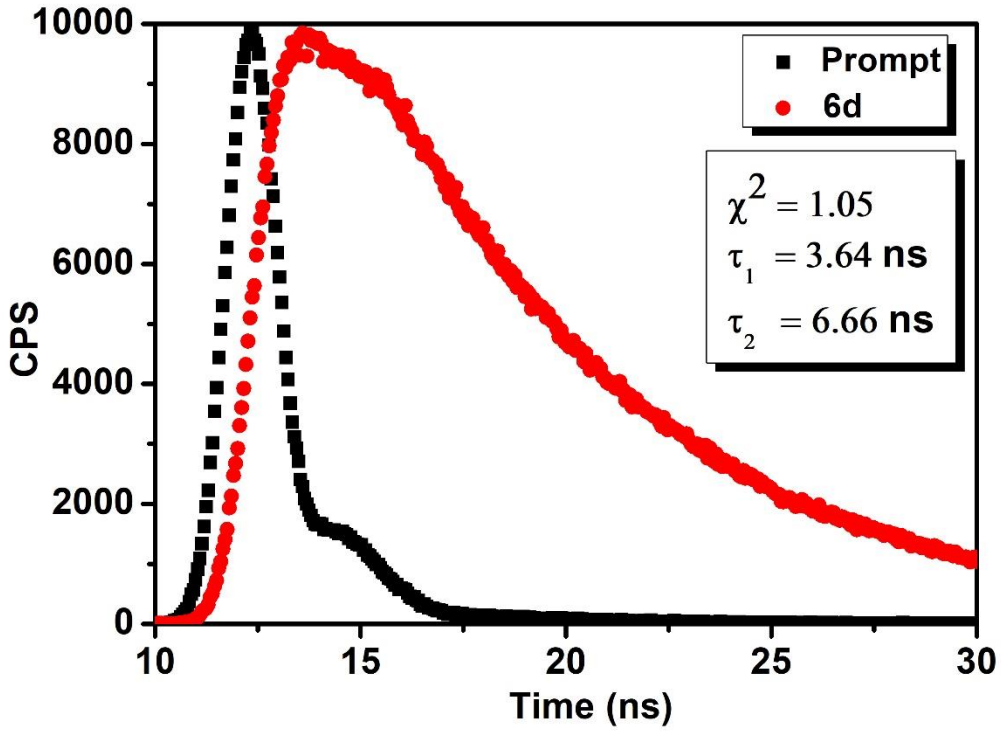

Fig. S17. Fluorescence life time spectrum of **6d** (~10^{-5} M) in DMSO.

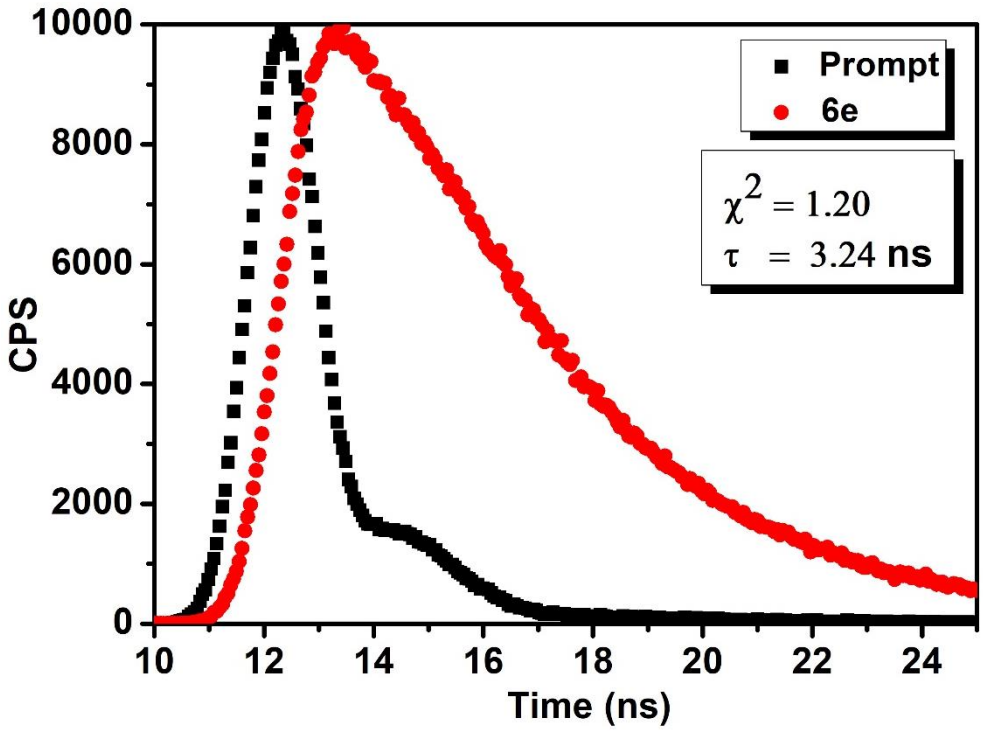

Fig. S18. Fluorescence life time spectrum of **6e** (~10^{-5} M) in DMSO.

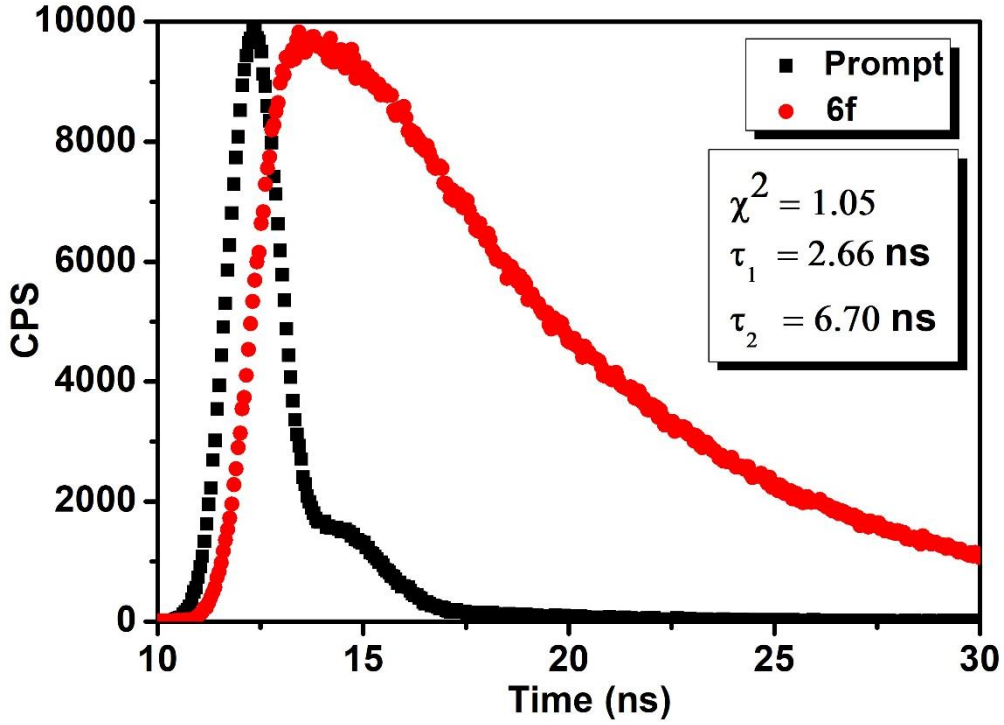

Fig. S19. Fluorescence life time spectrum of **6f** (~10^{-5} M) in DMSO.

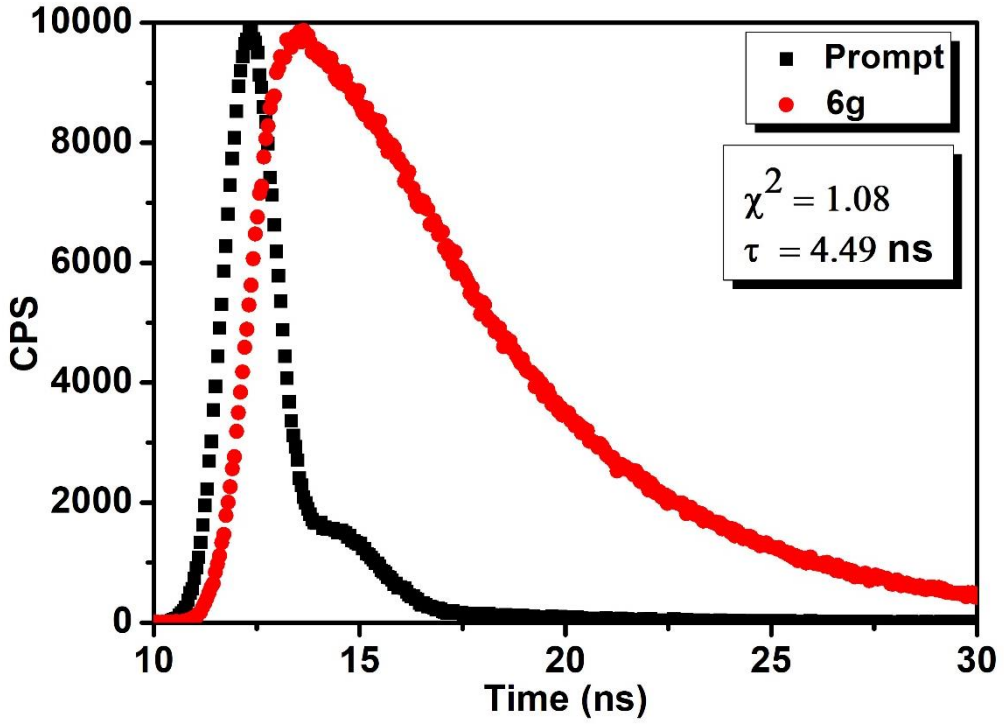

Fig. S20. Fluorescence life time spectrum of **6g** (~10^{-5} M) in DMSO.

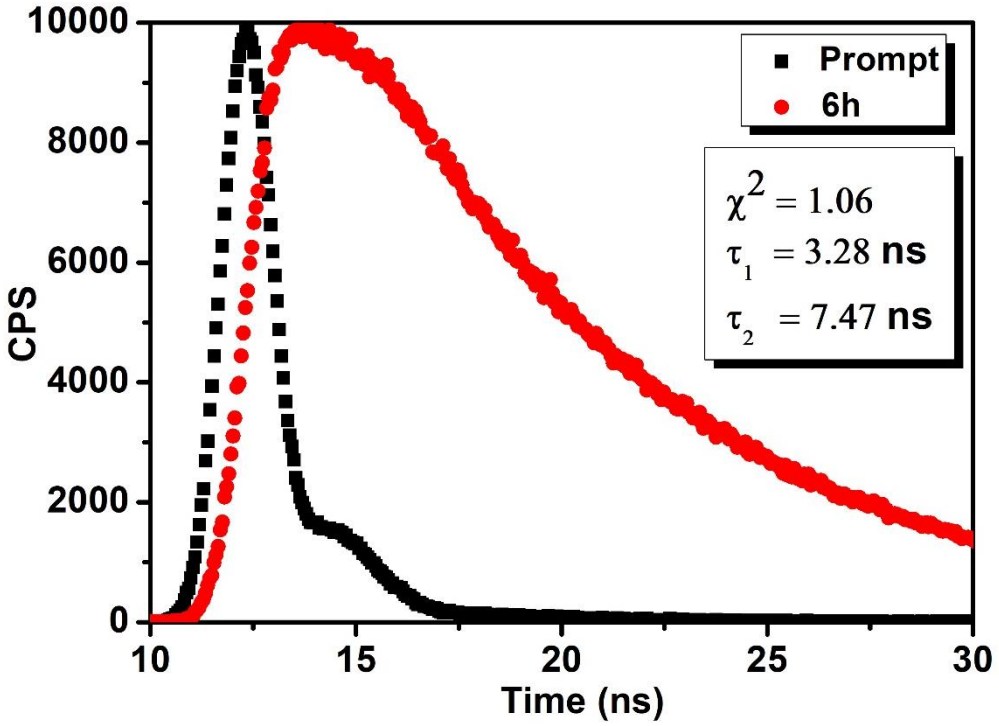

Fig. S21. Fluorescence life time spectrum of **6h** (~10^{-5} M) in DMSO.

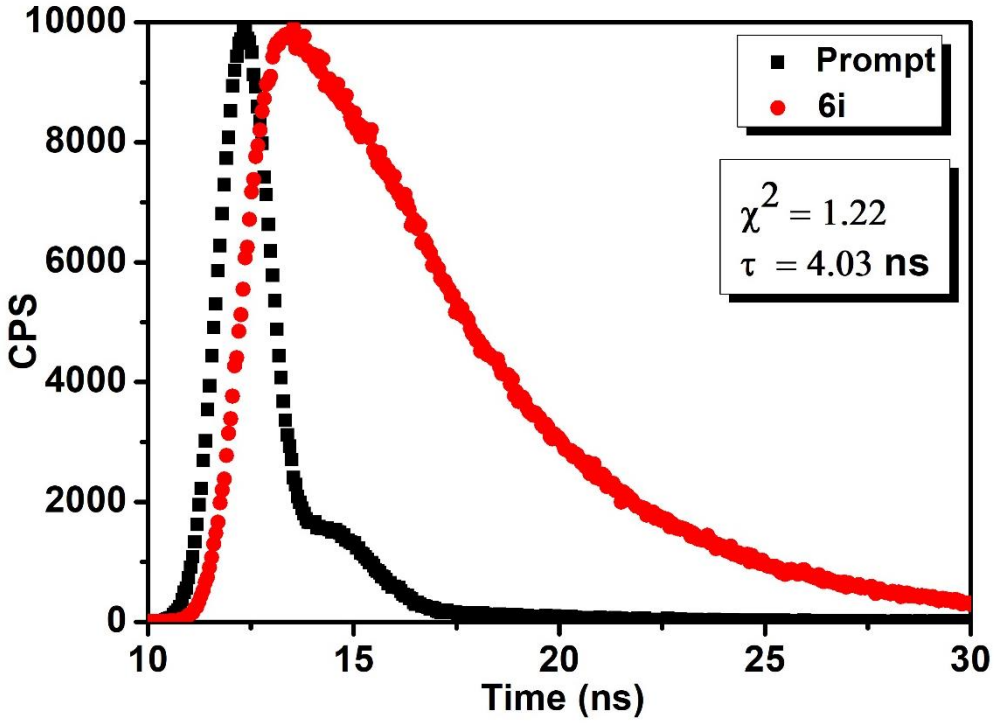

Fig. S22. Fluorescence life time spectrum of **6i** (~10^{-5} M) in DMSO.

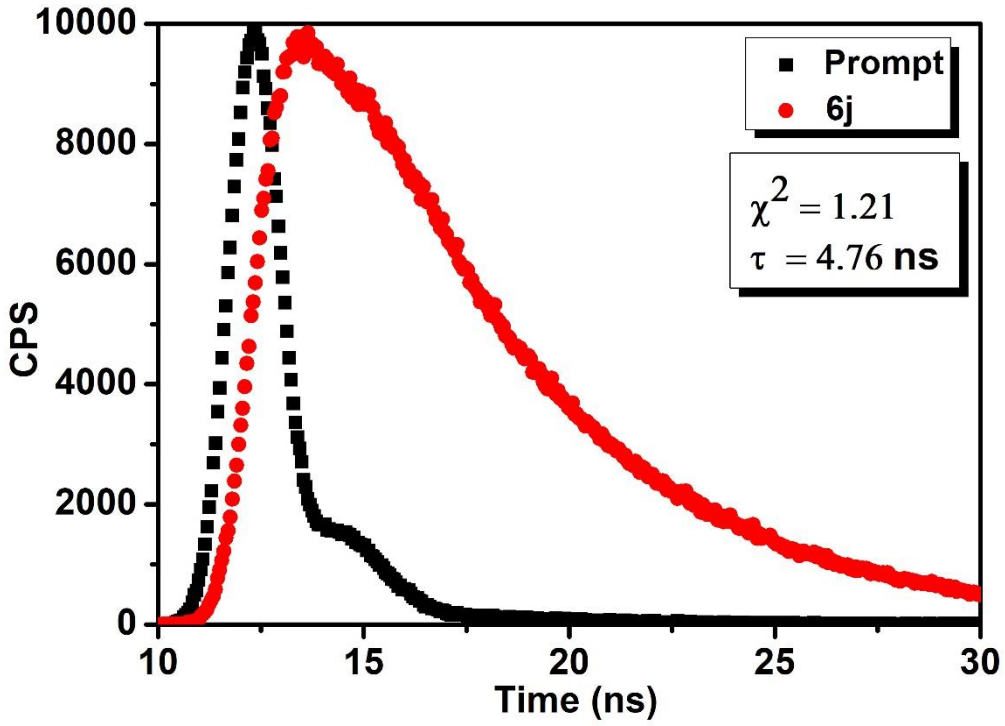

Fig. S23. Fluorescence life time spectrum of **6j** (~10^{-5} M) in DMSO.

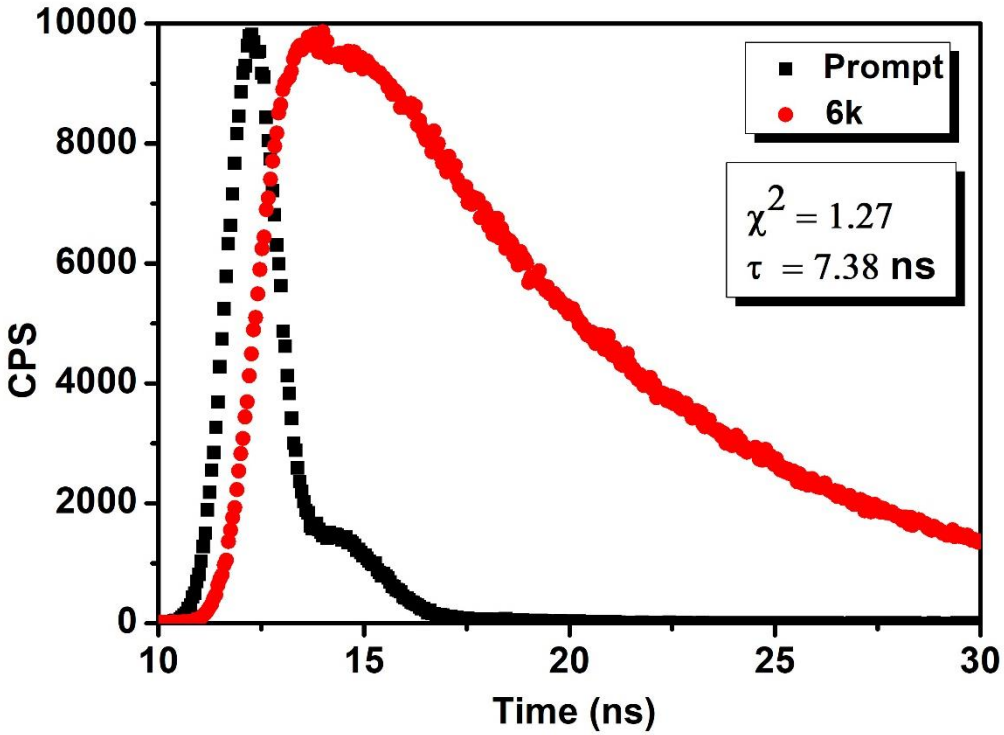

Fig. S24. Fluorescence life time spectrum of **6k** (~10^{-5} M) in DMSO.

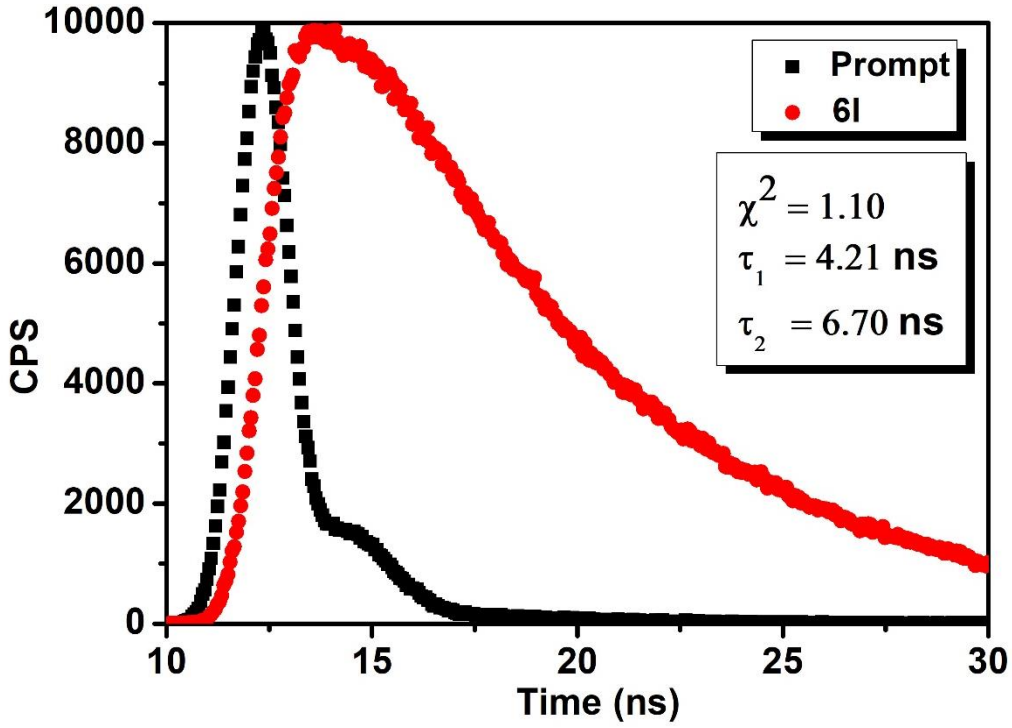

Fig. S25. Fluorescence life time spectrum of **6l** (~10^{-5} M) in DMSO.

Table S2: Average life time (ns) of synthesized derivatives **6a-l.**

Entry	Average Life time (ns)	Solvent
6a	1.57	DMSO
6a	12.67	99:1Water: DMSO
6b	4.59	DMSO
6c	5.76	DMSO
6d	6.29	DMSO

6e	3.24	DMSO
6f	6.41	DMSO
6g	4.49	DMSO
6h	7.12	DMSO
6i	4.03	DMSO
6j	4.6	DMSO
6k	7.38	DMSO
6l	6.18	DMSO

Solid State Fluorescence Spectra of all the Synthesized Compounds

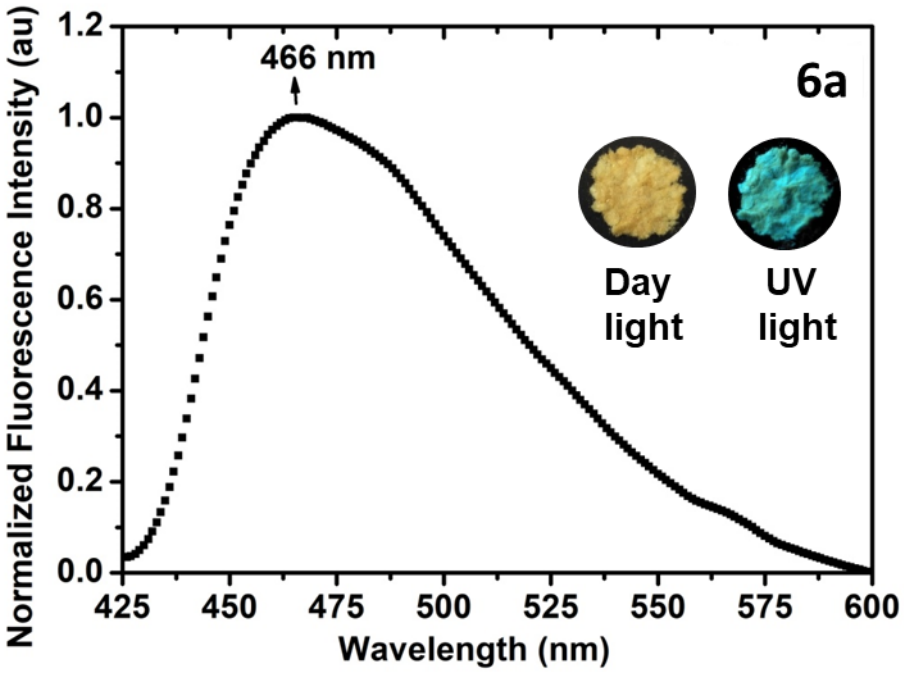

Fig. S26. Solid state fluorescence spectrum of compound **6a** and image in day light and UV light (hand held UV lamp 365 nm).

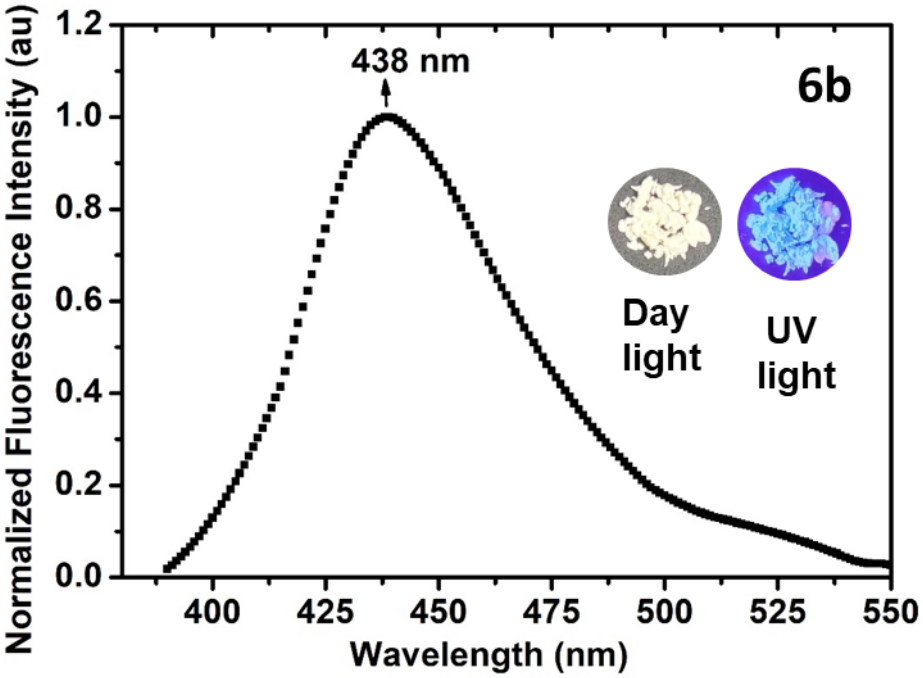

Fig. S27. Solid state fluorescence spectrum of compound **6b** and image in day light and UV light (hand held UV lamp 365 nm).

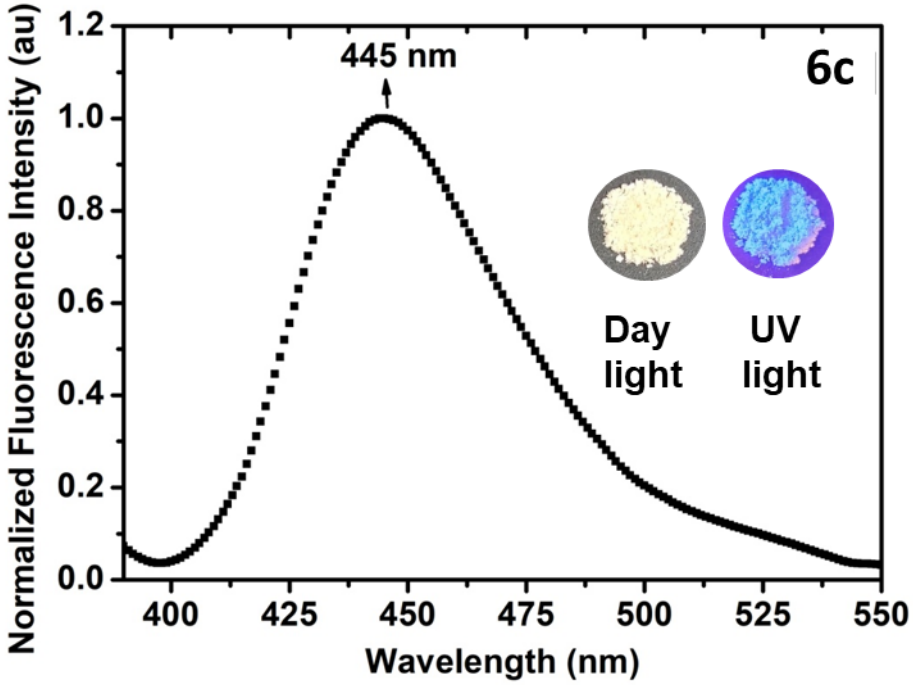

Fig. S28. Solid state fluorescence spectrum of compound **6c** and image in day light and UV light (hand held UV lamp 365 nm).

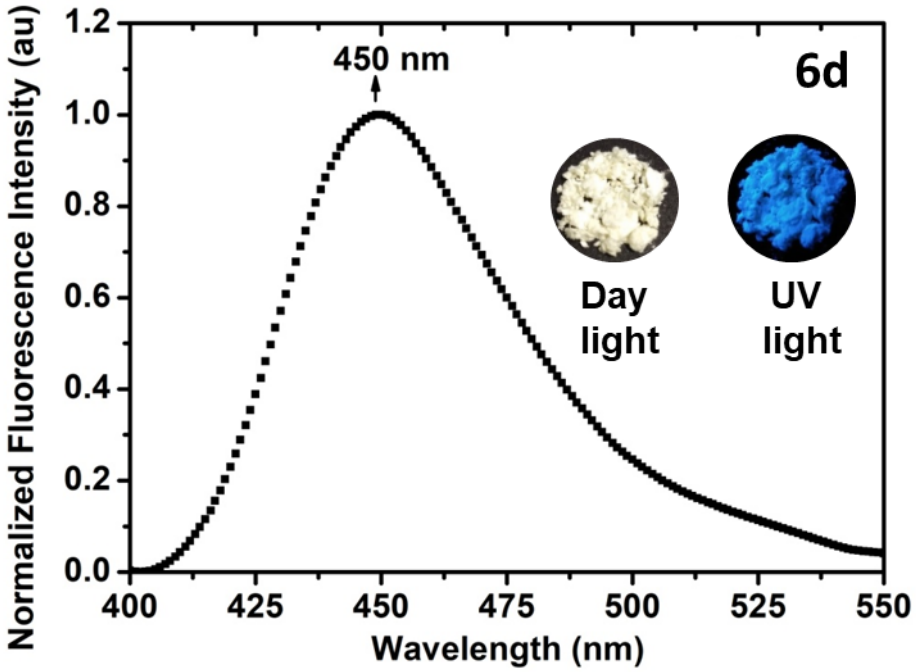

Fig. S29. Solid state fluorescence spectrum of compound **6d** and image in day light and UV light (hand held UV lamp 365 nm).

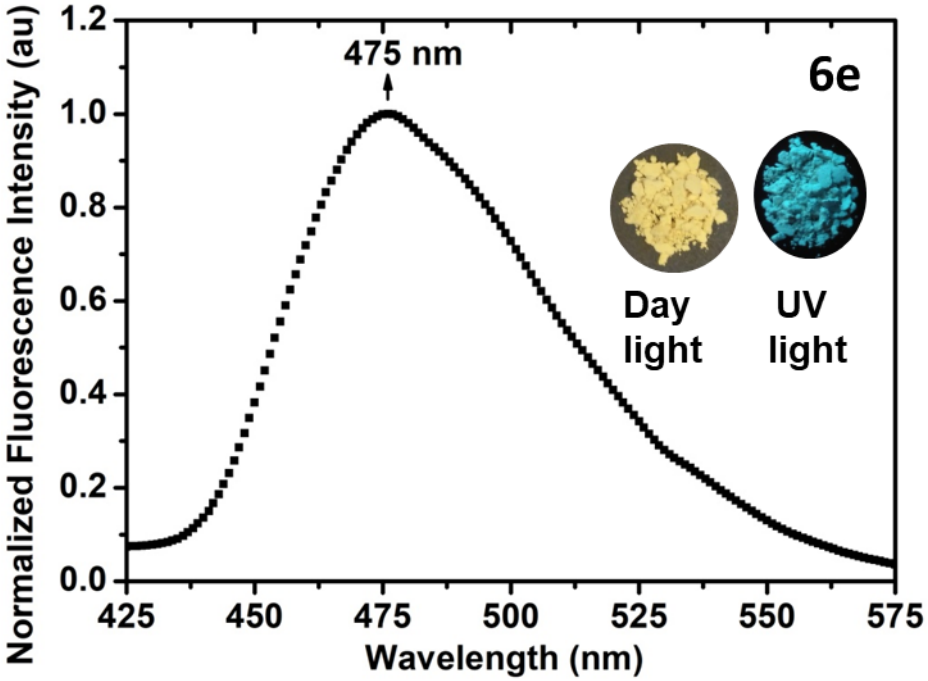

Fig. S30. Solid state fluorescence spectrum of compound **6e** and image in day light and UV light (hand held UV lamp 365 nm).

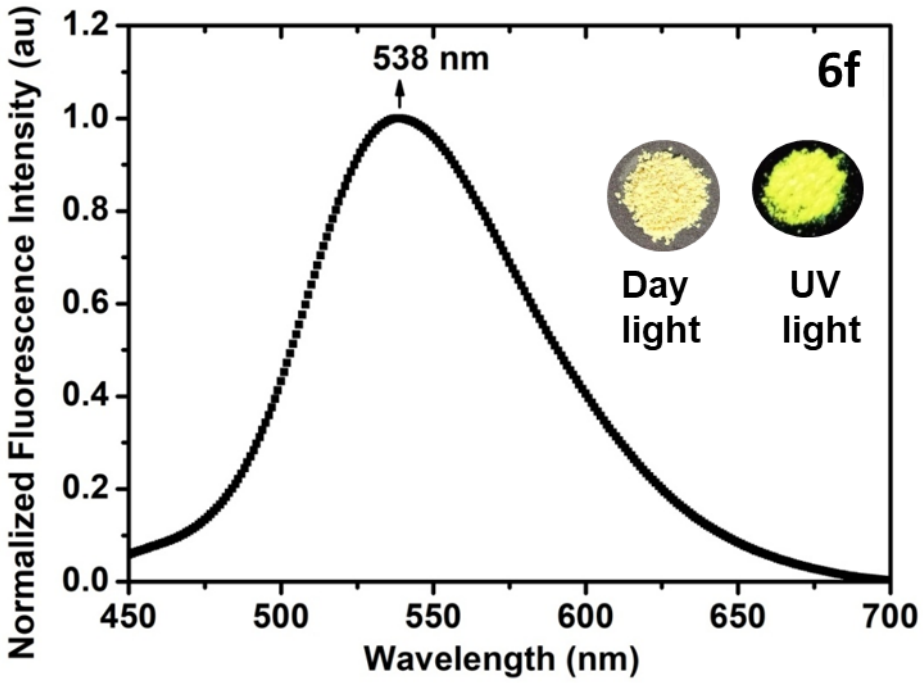

Fig. S31. Solid state fluorescence spectrum of compound **6f** and image in day light and UV light (hand held UV lamp 365 nm).

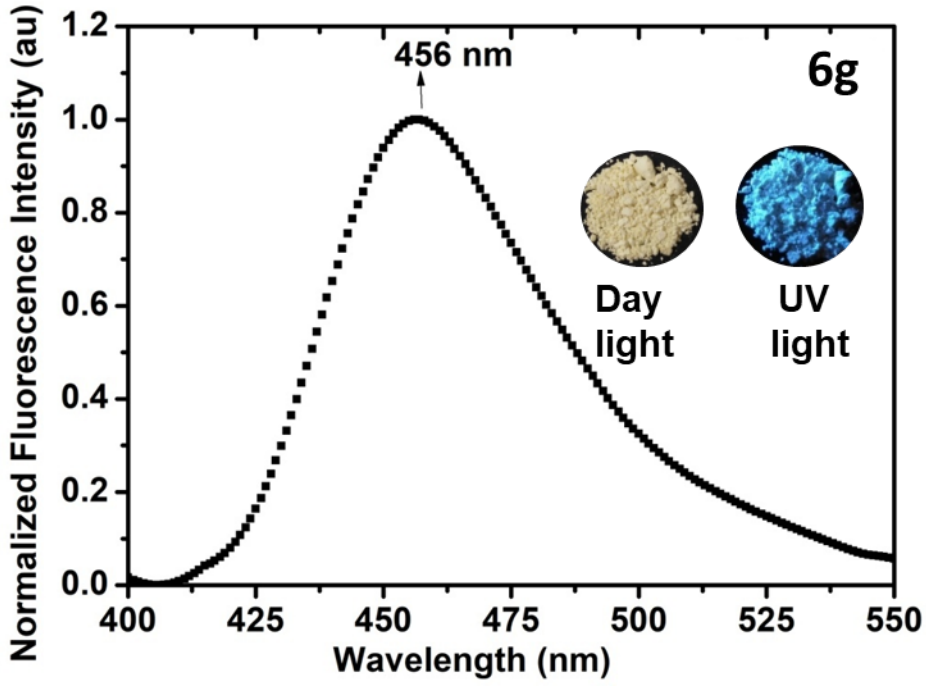

Fig. S32. Solid state fluorescence spectrum of compound **6g** and image in day light and UV light (hand held UV lamp 365 nm).

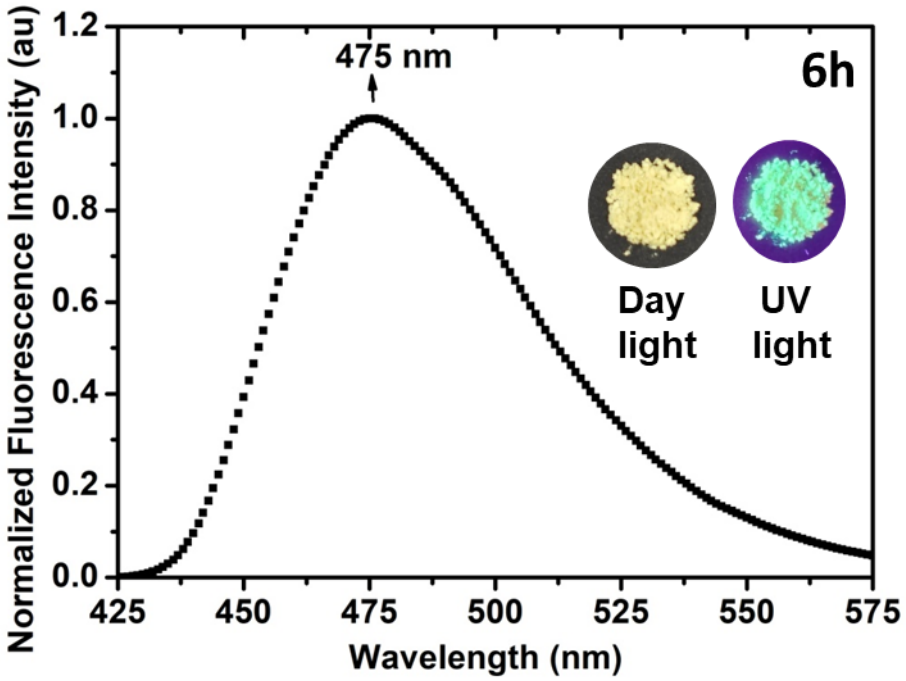

Fig. S33. Solid state fluorescence spectrum of compound **6h** and image in day light and UV light (hand held UV lamp 365 nm).

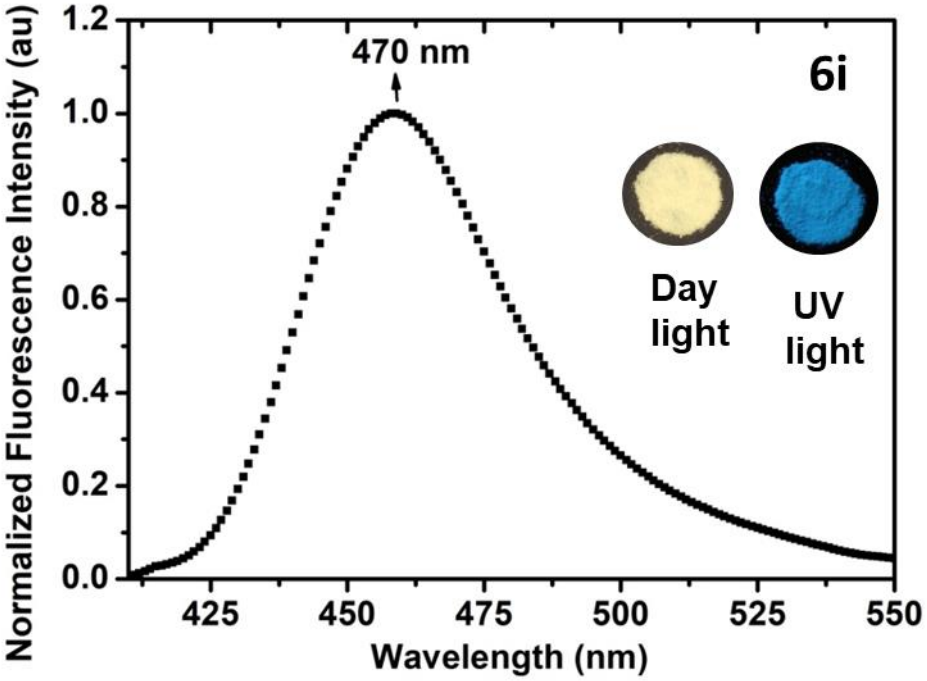

Fig. S34. Solid state fluorescence spectrum of compound **6i** and image in day light and UV light (hand held UV lamp 365 nm).

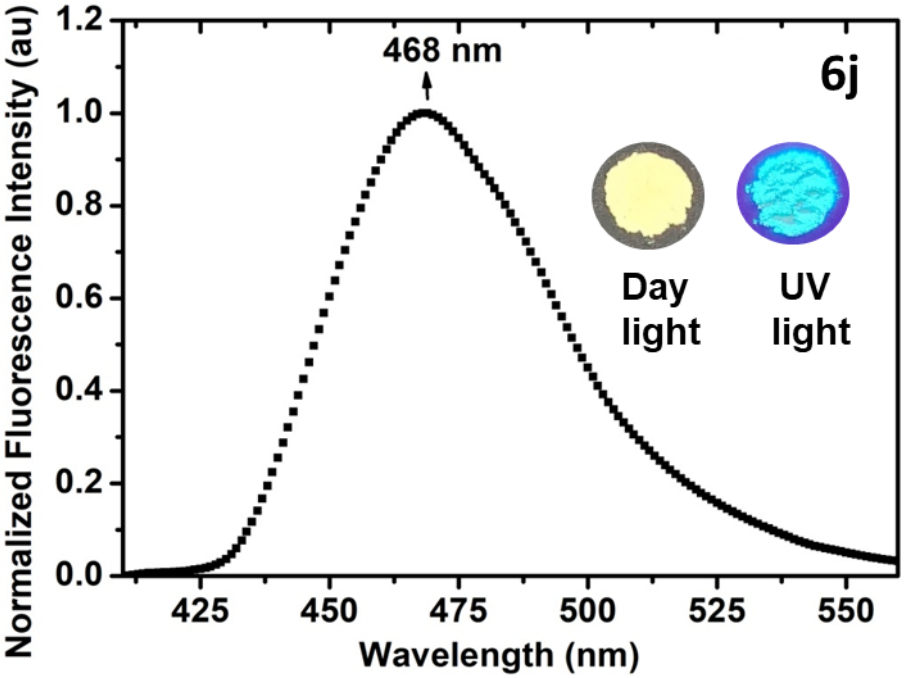

Fig. S35. Solid state fluorescence spectrum of compound **6j** and image in day light and UV light (hand held UV lamp 365 nm).

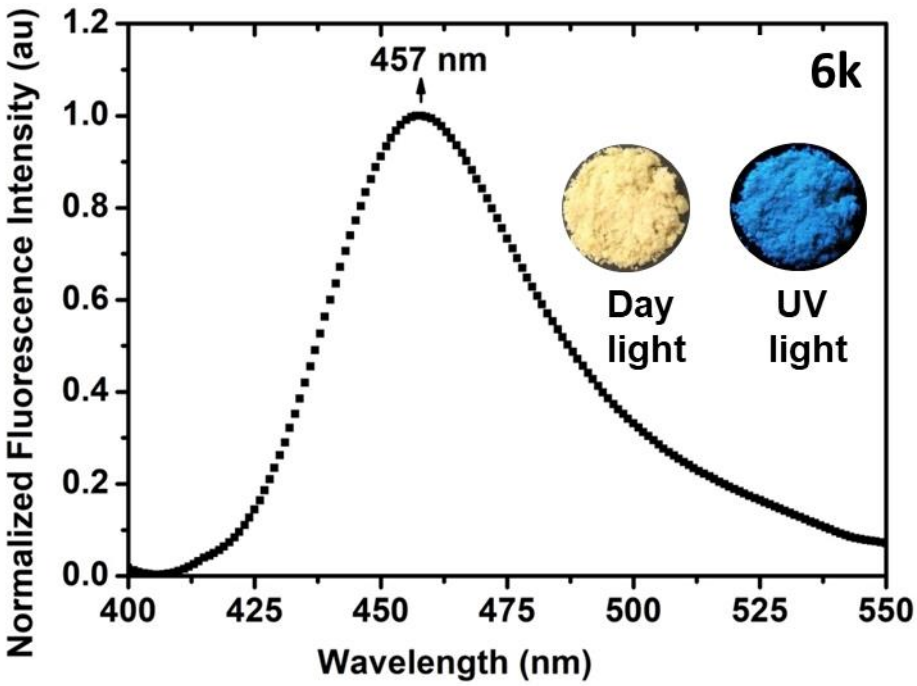

Fig. S36. Solid state fluorescence spectrum of compound **6k** and image in day light and UV light (hand held UV lamp 365 nm).

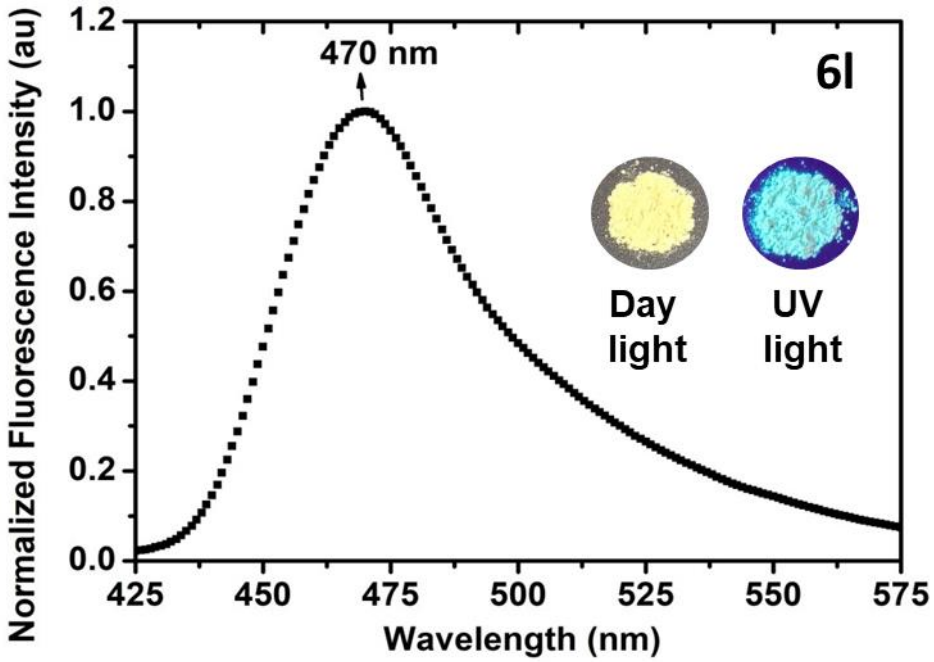

Fig. S37. Solid state fluorescence spectrum of compound **6l** and image in day light and UV light (hand held UV lamp 365 nm).

DFT Study (HOMO-LUMO images) of all the compounds

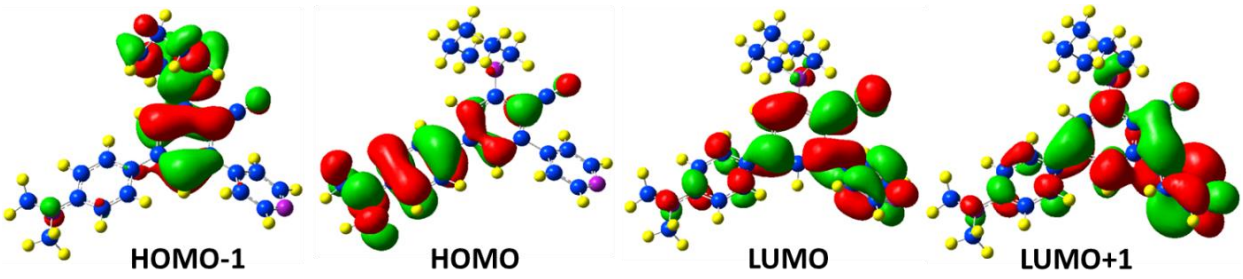

Fig. S38. Computed molecular orbital HOMO, LUMO, HOMO−1 and LUMO+1 for **6a**.

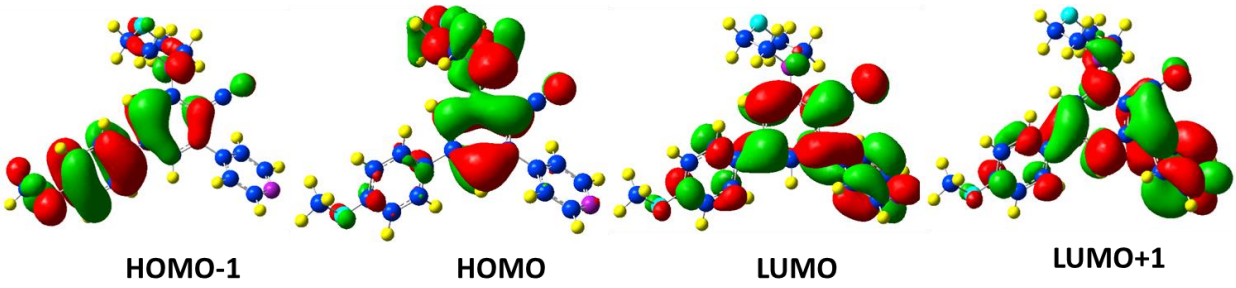

Fig. S39. Computed molecular orbital HOMO, LUMO, HOMO−1 and LUMO+1 for **6b**.

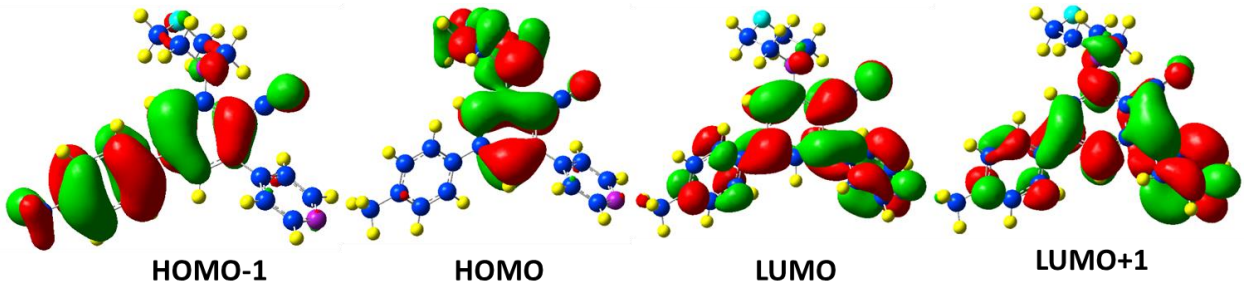

Fig. S40. Computed molecular orbital HOMO, LUMO, HOMO−1 and LUMO+1 for **6c**.

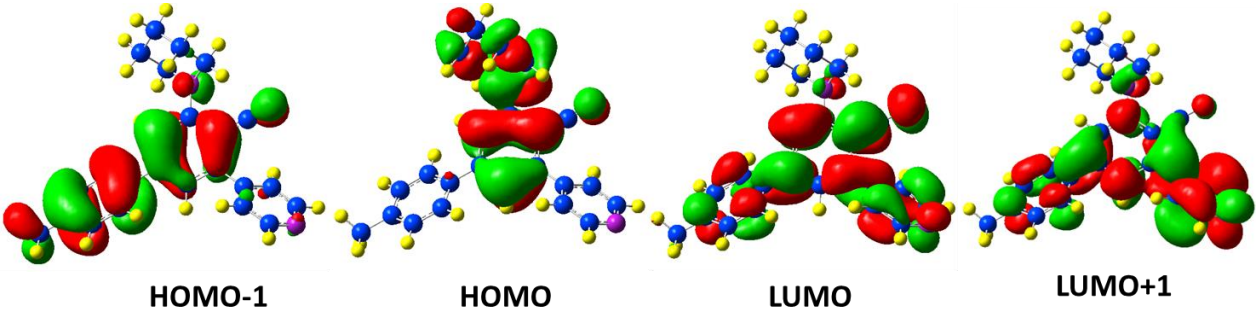

Fig. S41. Computed molecular orbital HOMO, LUMO, HOMO−1 and LUMO+1 for **6d**.

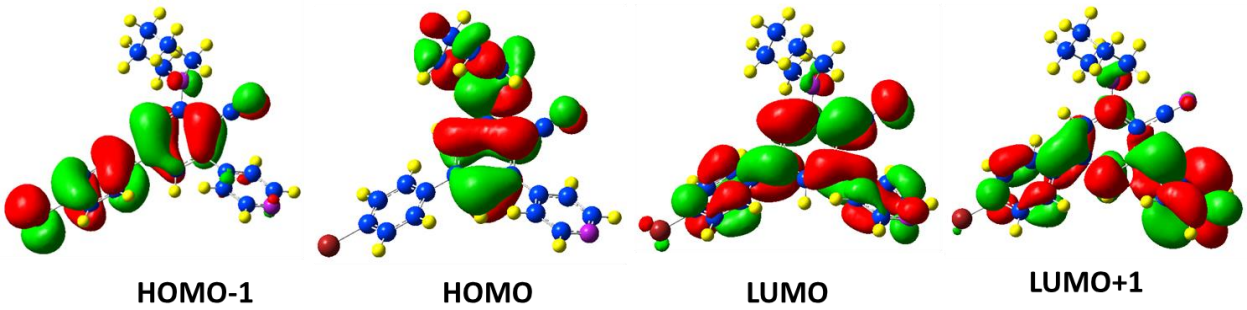

Fig. S42. Computed molecular orbital HOMO, LUMO, HOMO−1 and LUMO+1 for **6e**.

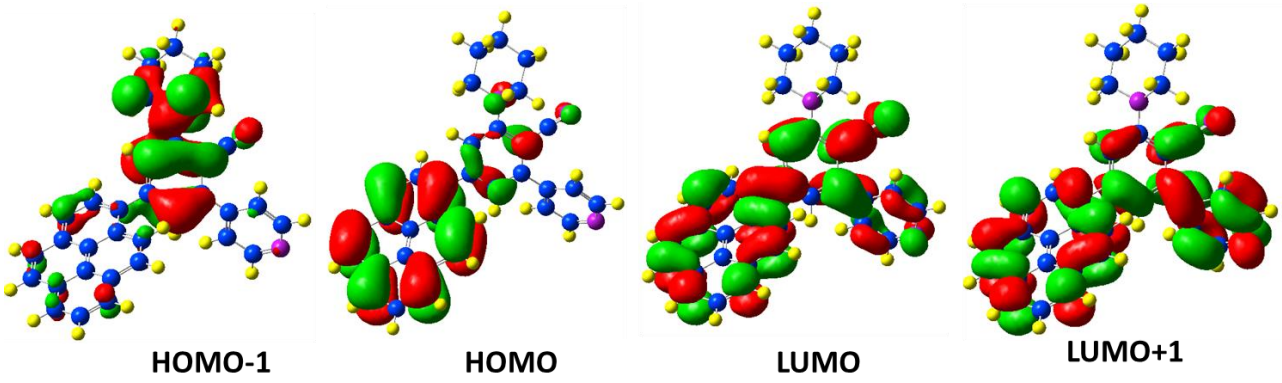

Fig. S43. Computed molecular orbital HOMO, LUMO, HOMO−1 and LUMO+1 for **6f**.

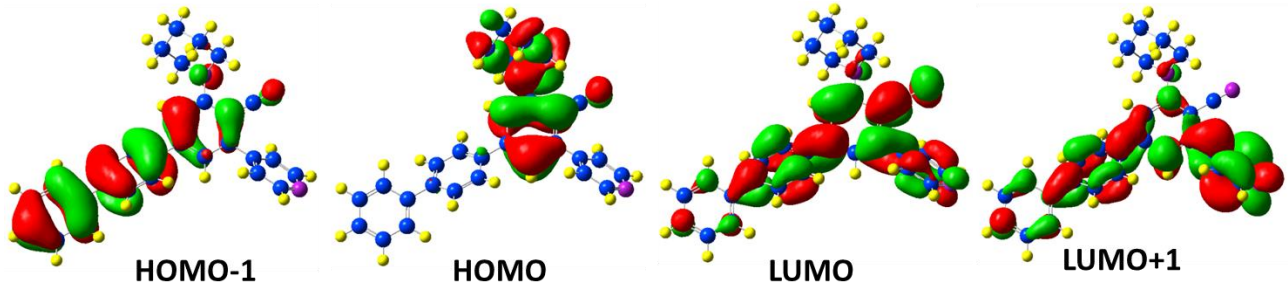

Fig. S44. Computed molecular orbital HOMO, LUMO, HOMO−1 and LUMO+1 for **6g**.

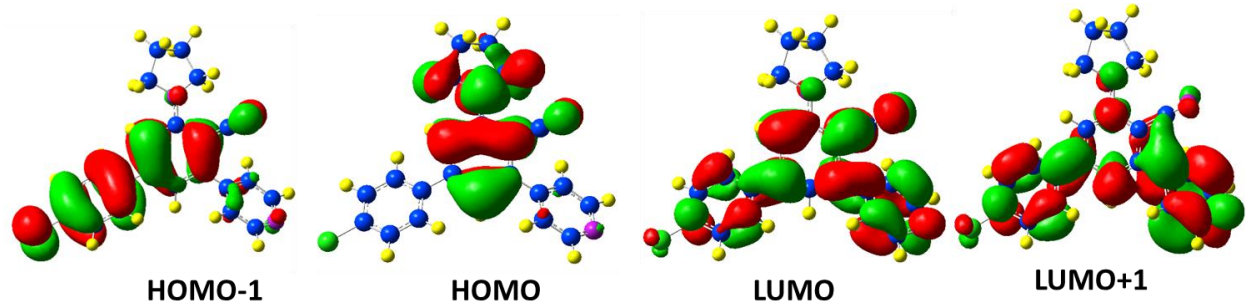

Fig. S45. Computed molecular orbital HOMO, LUMO, HOMO−1 and LUMO+1 for **6h**.

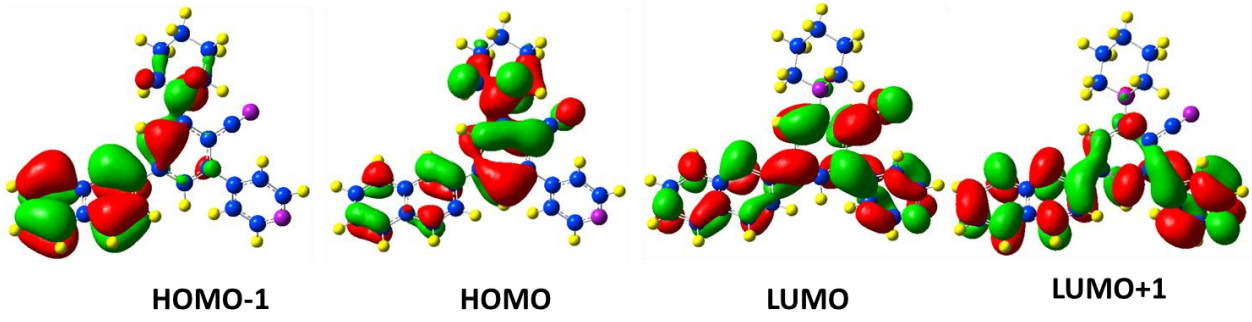

Fig. S46. Computed molecular orbital HOMO, LUMO, HOMO−1 and LUMO+1 for **6i**.

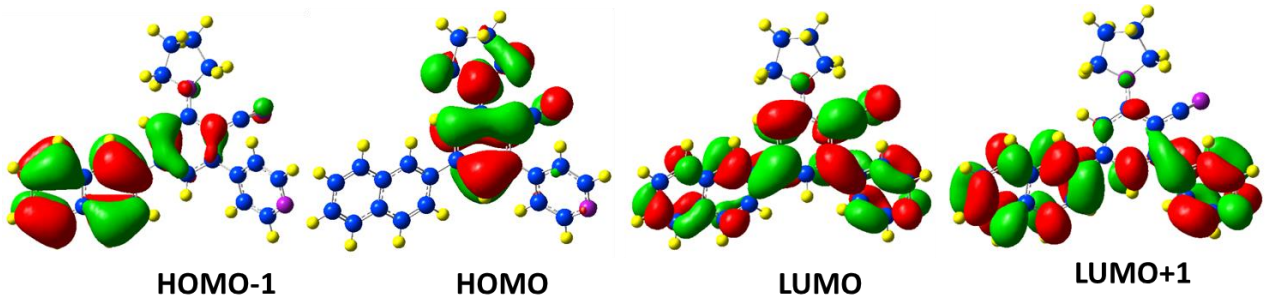

Fig. S47. Computed molecular orbital HOMO, LUMO, HOMO−1 and LUMO+1 for **6j**.

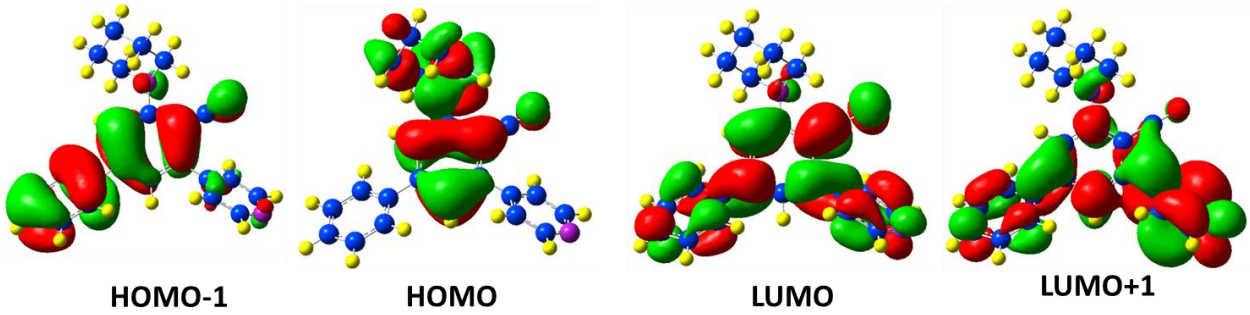

Fig. S48. Computed molecular orbital HOMO, LUMO, HOMO−1 and LUMO+1 for **6k**.

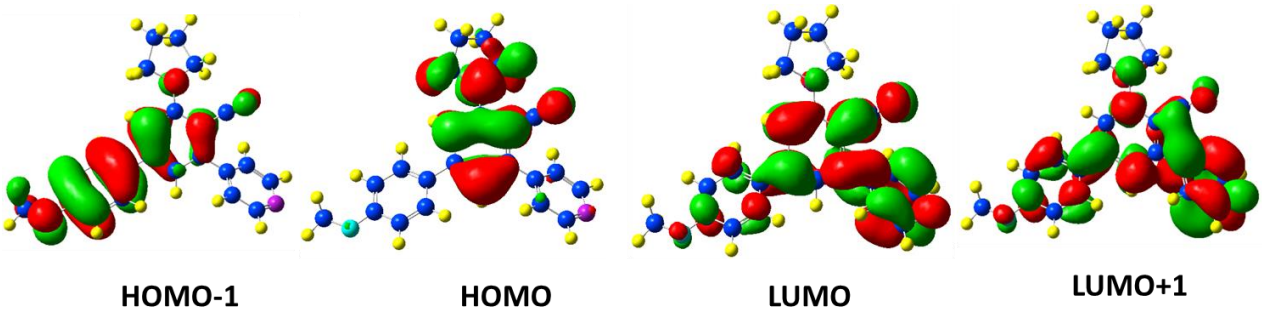

Fig. S49. Computed molecular orbital HOMO, LUMO, HOMO−1 and LUMO+1 for **6l**.

Table S3. Computed values of vertical excitations, oscillator strength (*f*), assignment, HOMO, LUMO and energy band gap for **6a-l**.

Entry	λ_{max} (nm)	*f*	Assignment (%)	HOMO (eV)	LUMO (eV)	E_g (eV)
6a	408	0.4489	HOMO →LUMO (96%)	-5.41	-1.99	3.42
6b	394	0.1224	HOMO→LUMO (96%)	-5.90	-2.16	3.74

6c	395	0.1143	HOMO→LUMO (98%)	-5.92	-2.18	3.74
6d	391	0.1072	HOMO→LUMO (97%)	-5.87	-2.08	3.79
6e	398	0.1022	HOMO→LUMO (98%)	-5.90	-2.18	3.72
6f	407	0.4616	HOMO→LUMO (90%)	-5.70	-2.28	3.42
6g	398	0.1118	HOMO →LUMO (97%)	-5.82	-2.11	3.71
6h	390	0.1345	HOMO→LUMO (98%)	-5.89	-2.14	3.75
6i	386	0.1395	HOMO→LUMO (90%)	-6.10	-2.28	3.82
6j	392	0.1429	HOMO→LUMO (97%)	-5.87	-2.16	3.71
6k	393	0.1022	HOMO →LUMO (98%)	-5.98	-2.11	3.87
6l	381	0.1485	HOMO→LUMO (90%)	-5.78	-1.97	3.81

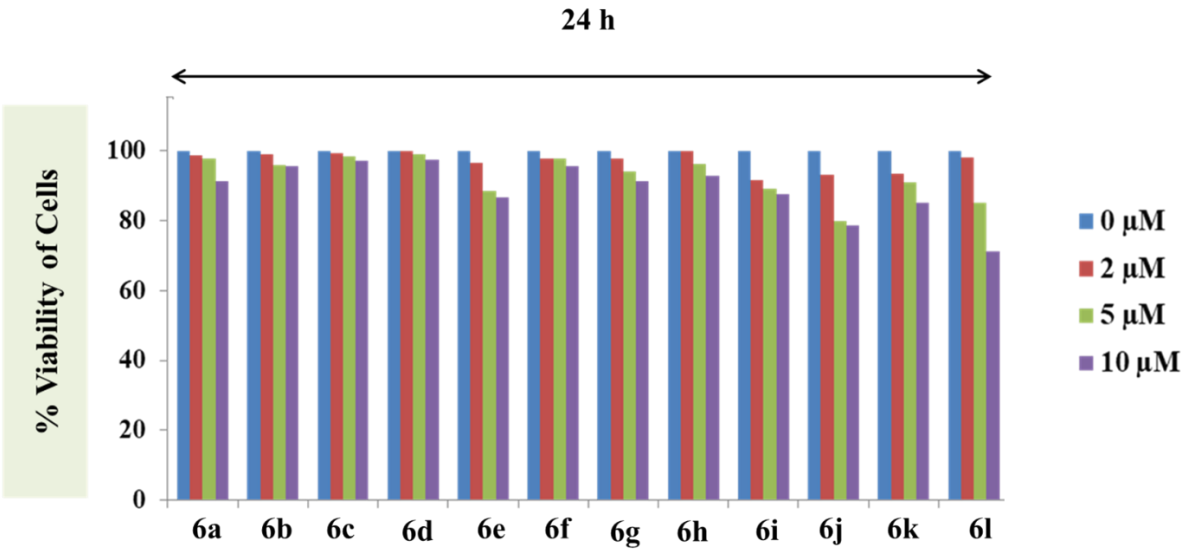

Fig. S50. Cell viability assessment of **6a-l** in 3T3-L1 adipocytes at different concentration.

^{1}H & ^{13}C NMR Spectra of Compounds 6a-l

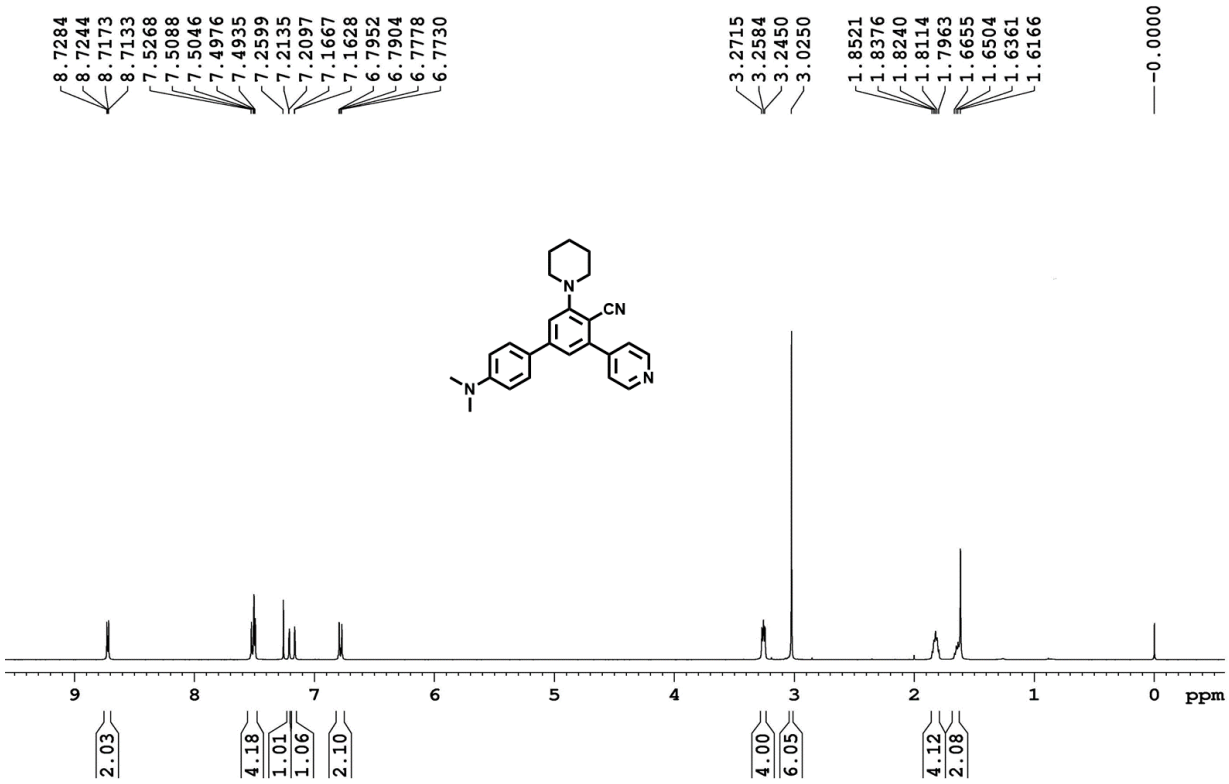

Fig. S51. ^{1}H NMR spectrum of **6a** in $CDCl_3$

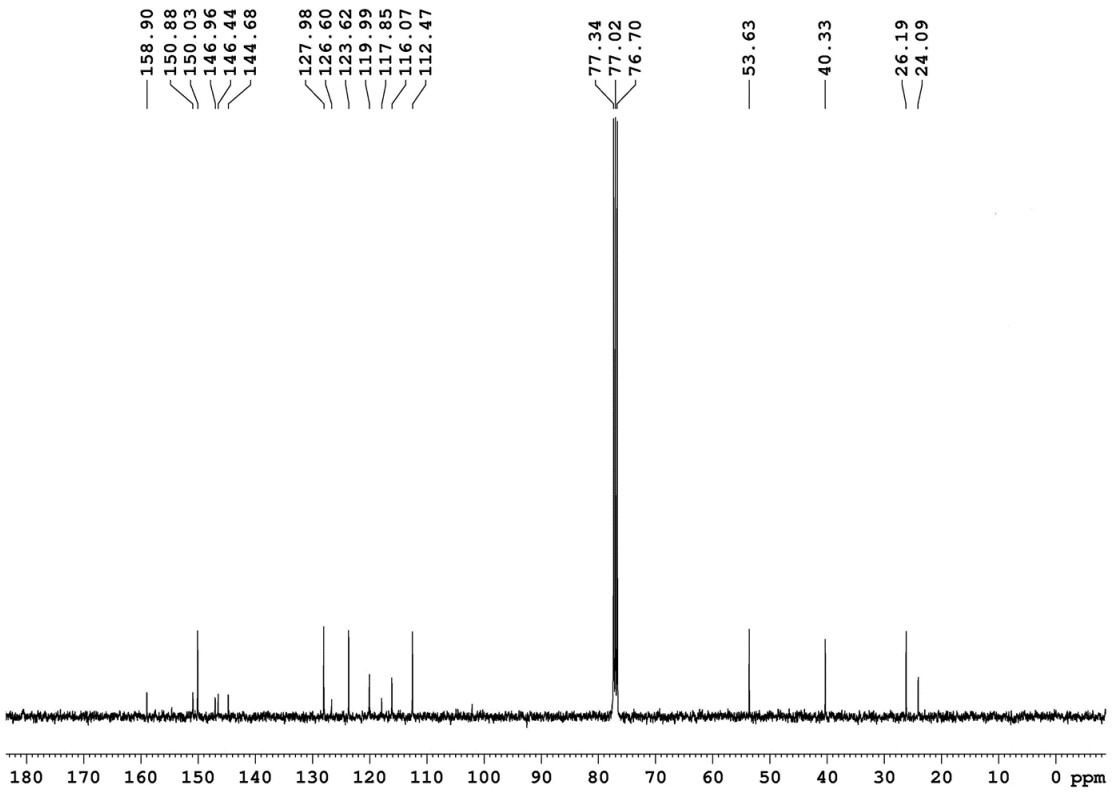

Fig S52. ^{13}C NMR spectrum of **6a** in $CDCl_3$

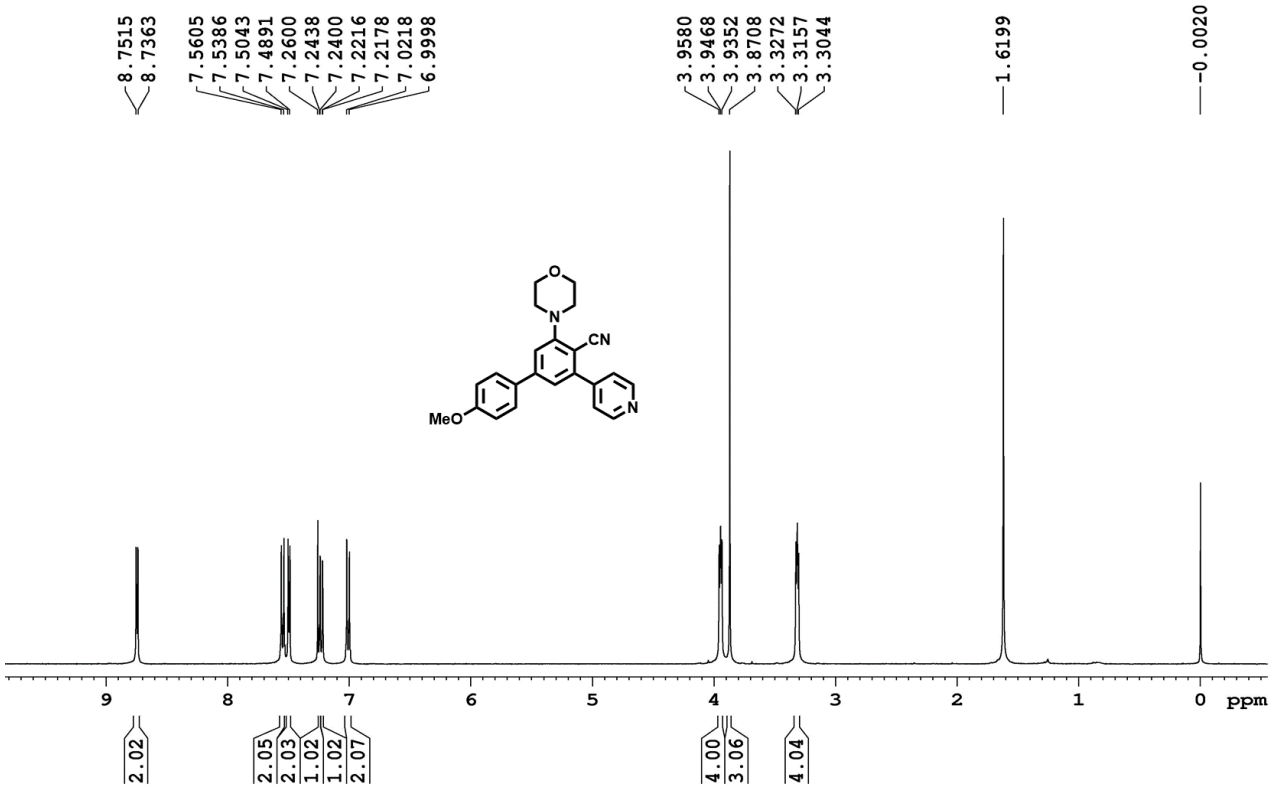

Fig. S53. ^{1}H NMR spectrum of **6b** in $CDCl_3$

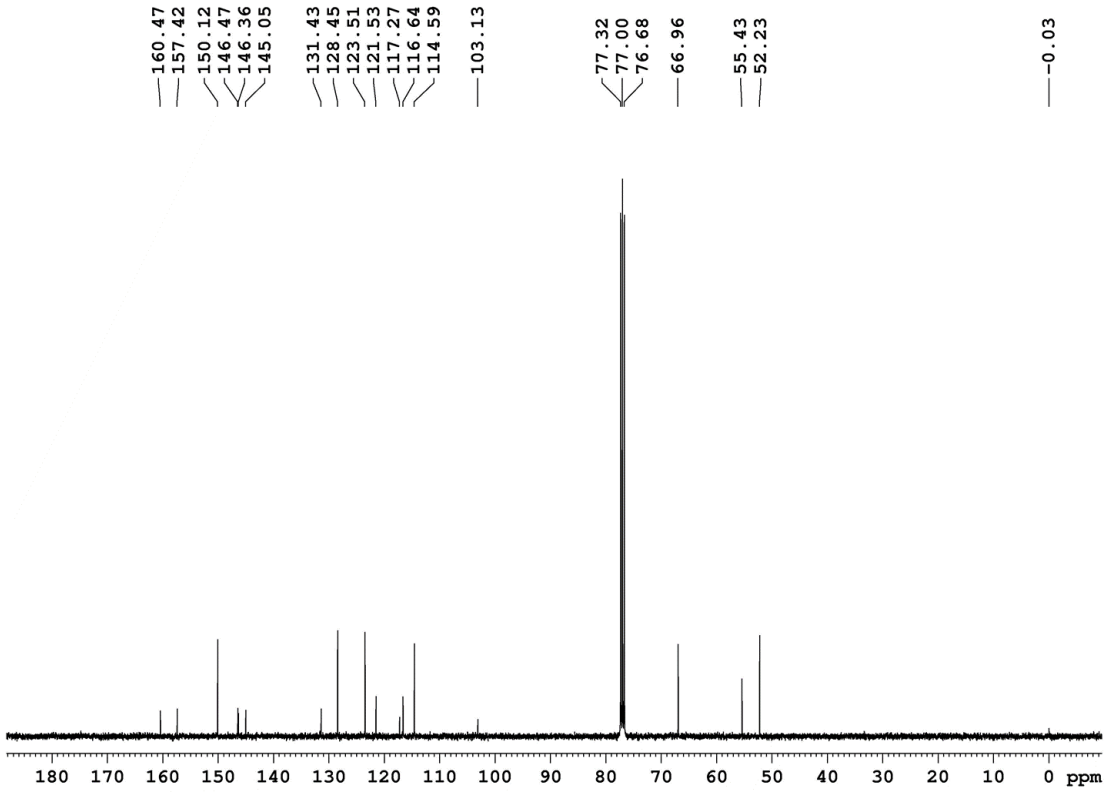

Fig. S54. ^{13}C NMR spectrum of **6b** in $CDCl_3$

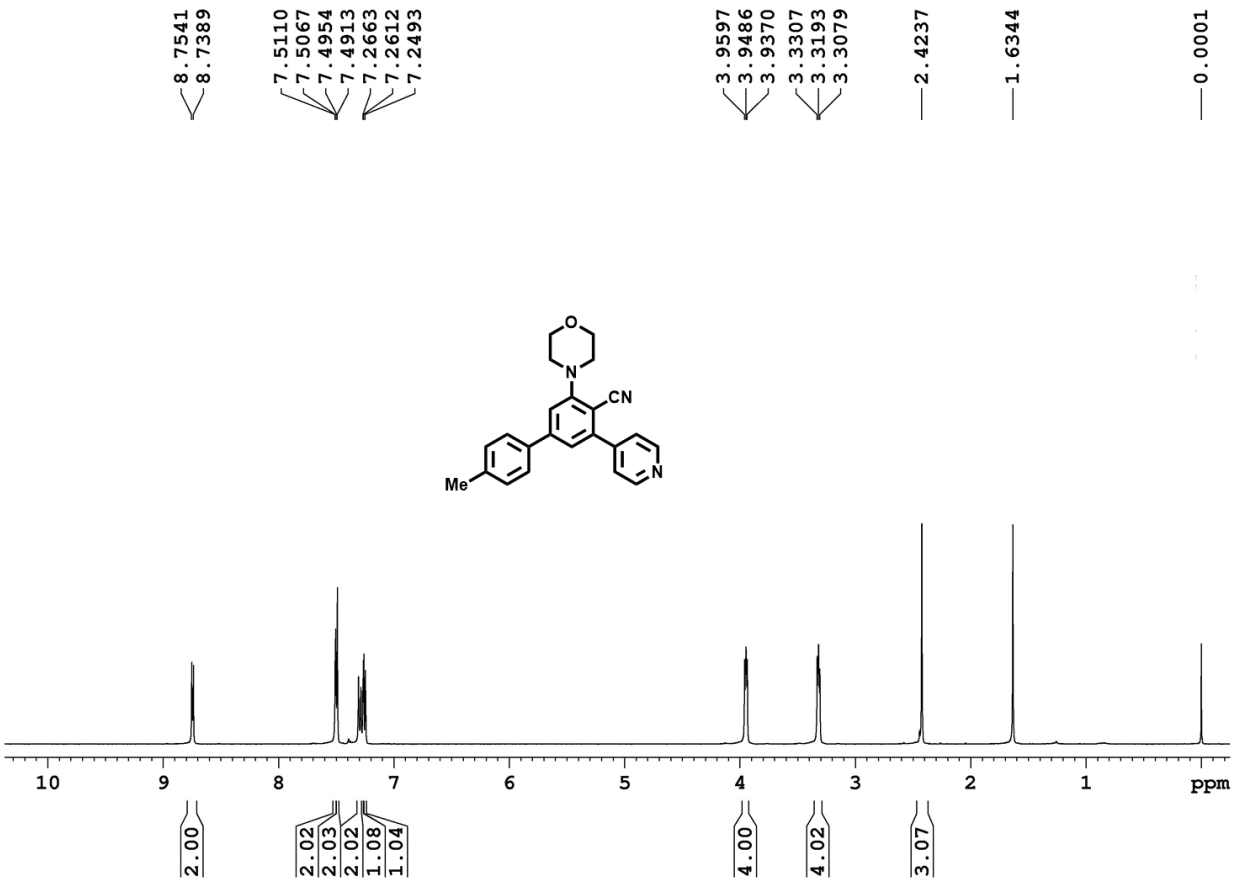

Fig. S55. ^{1}H NMR spectrum of **6c** in $CDCl_3$

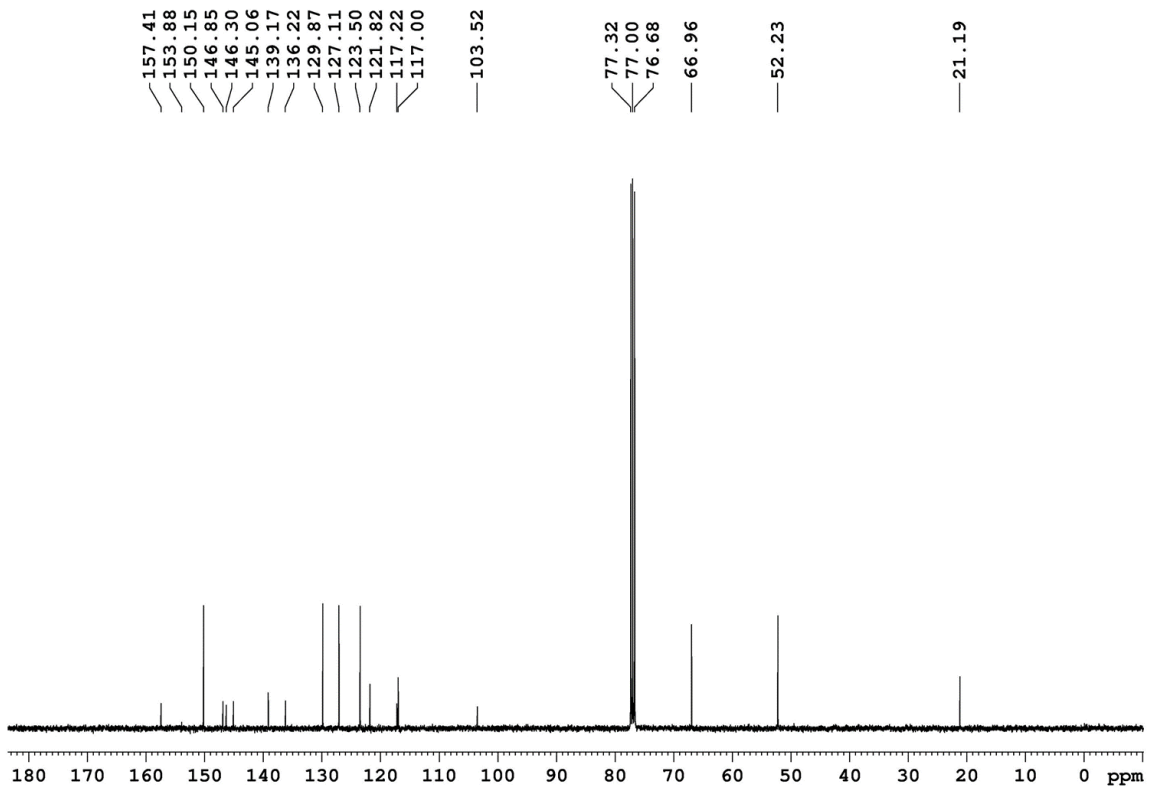

Fig. S56. ^{13}C NMR spectrum of **6c** in $CDCl_3$

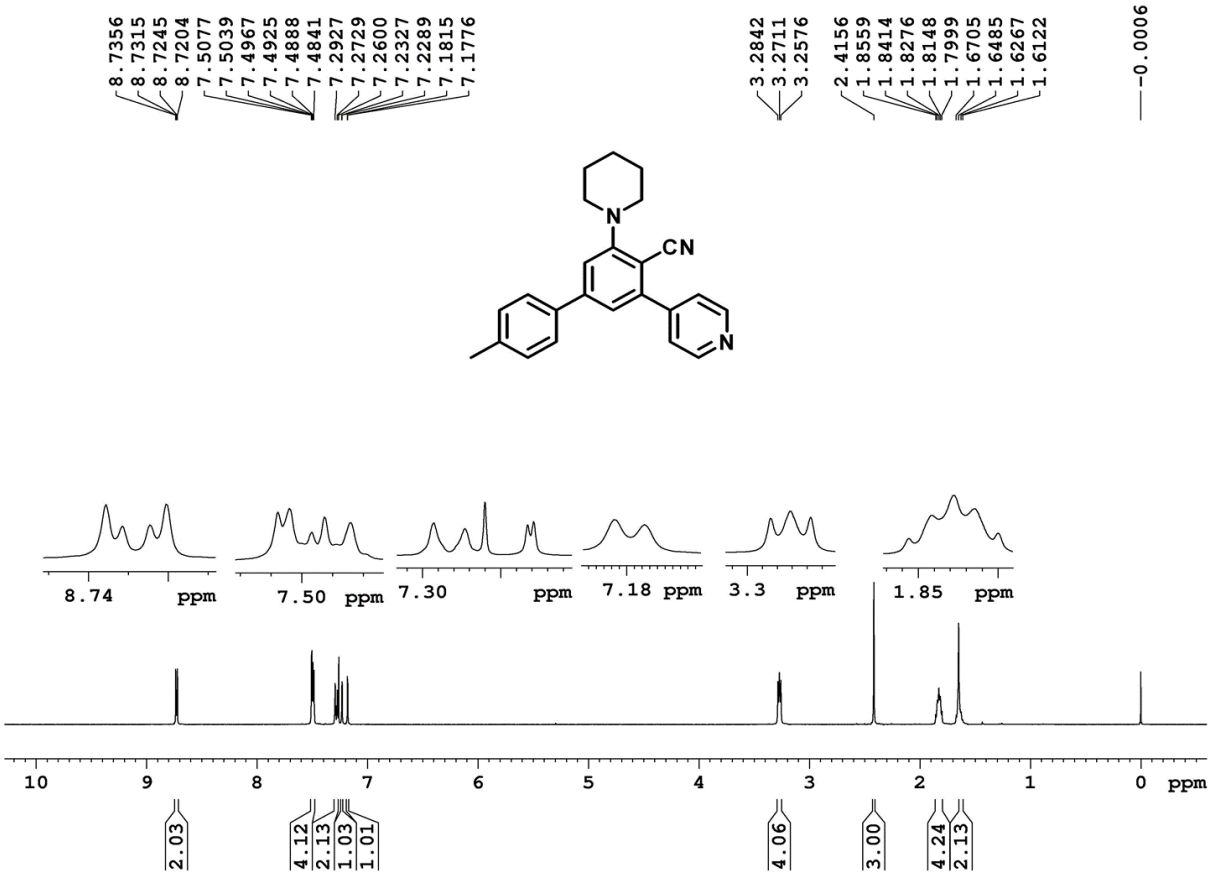

Fig. S57. ^{1}H NMR spectrum of **6d** in $CDCl_3$

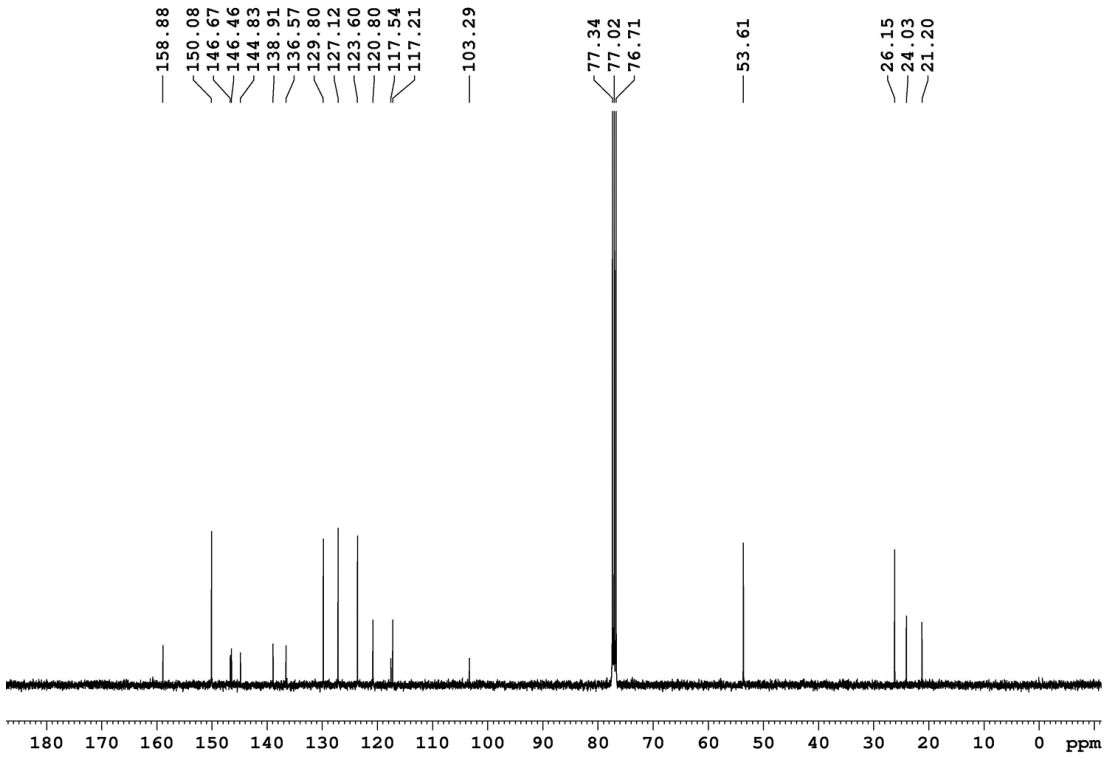

Fig. S58. ^{13}C NMR spectrum of **6d** in $CDCl_3$

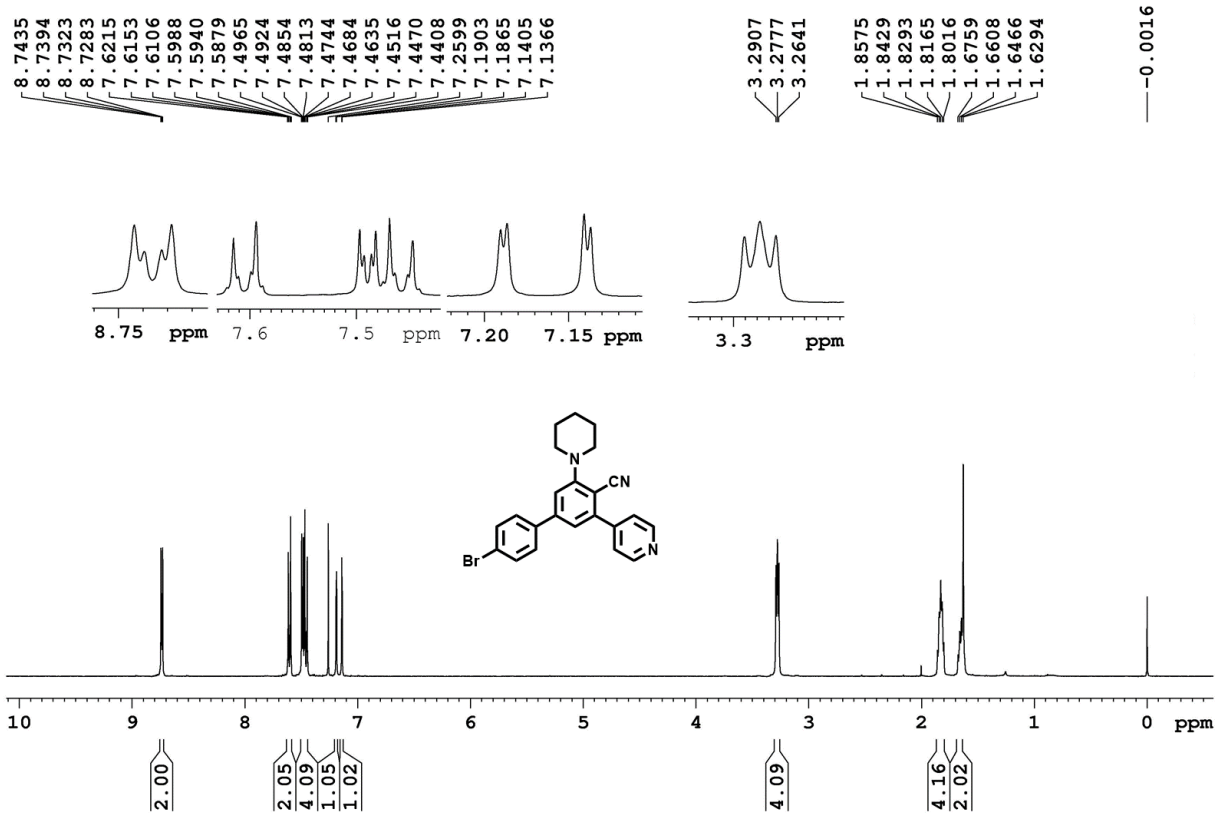

Fig. S59. ^{1}H NMR spectrum of **6e** in $CDCl_3$

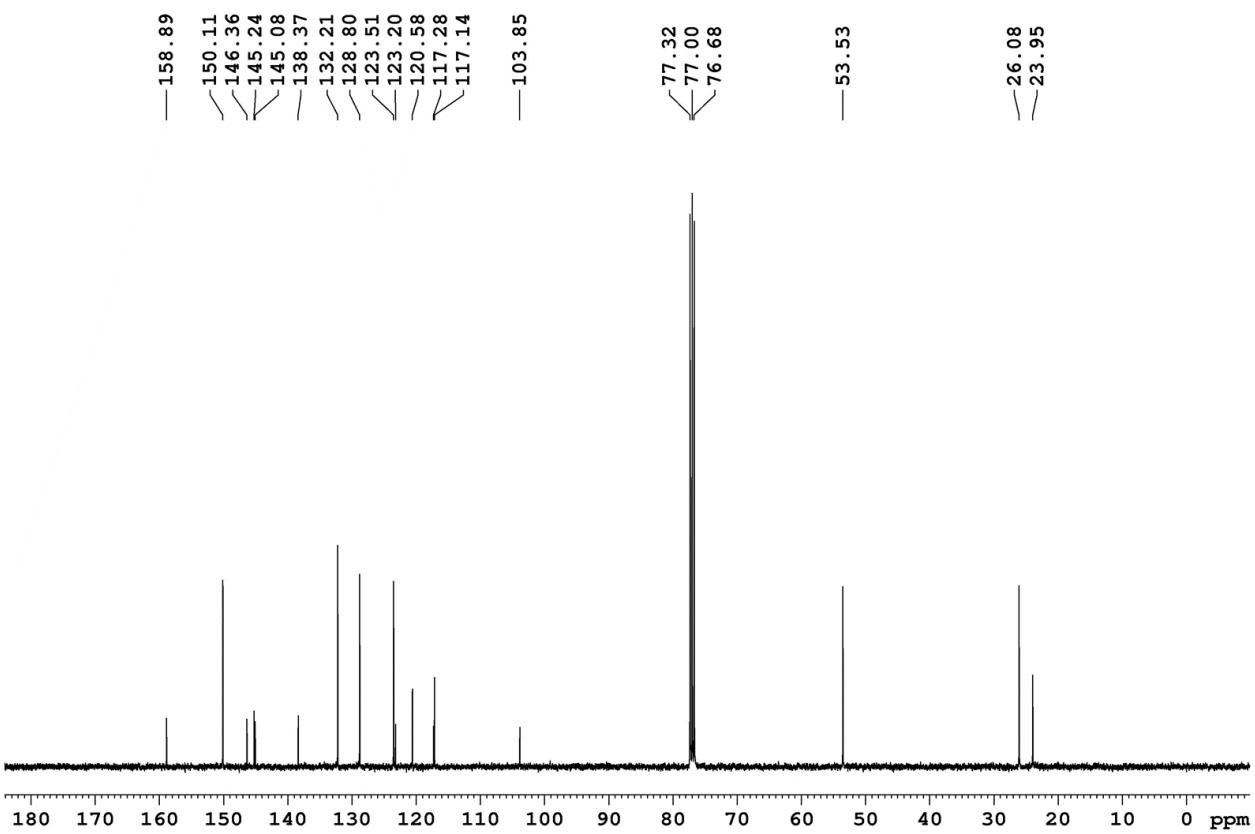

Fig. S60. ^{13}C NMR spectrum of **6e** in $CDCl_3$

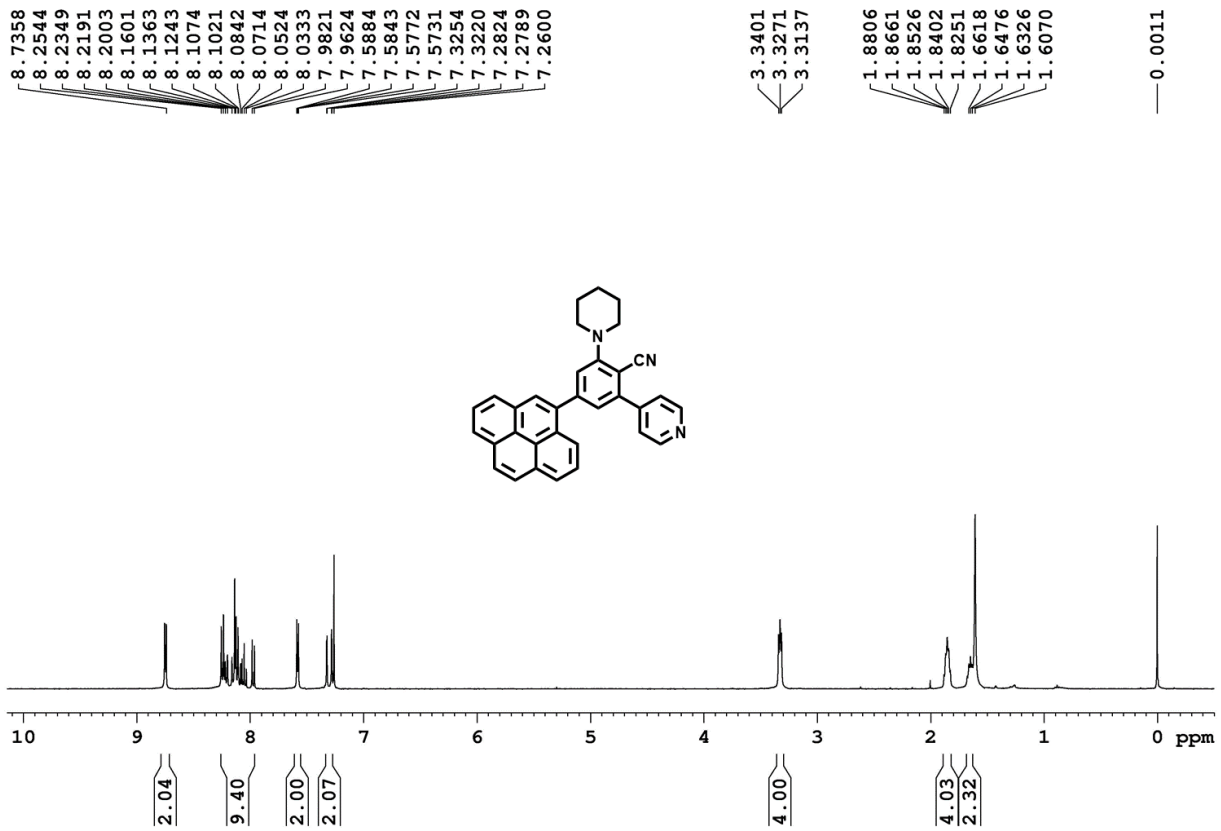

Fig. S61. ^{1}H NMR spectrum of **6f** in $CDCl_3$

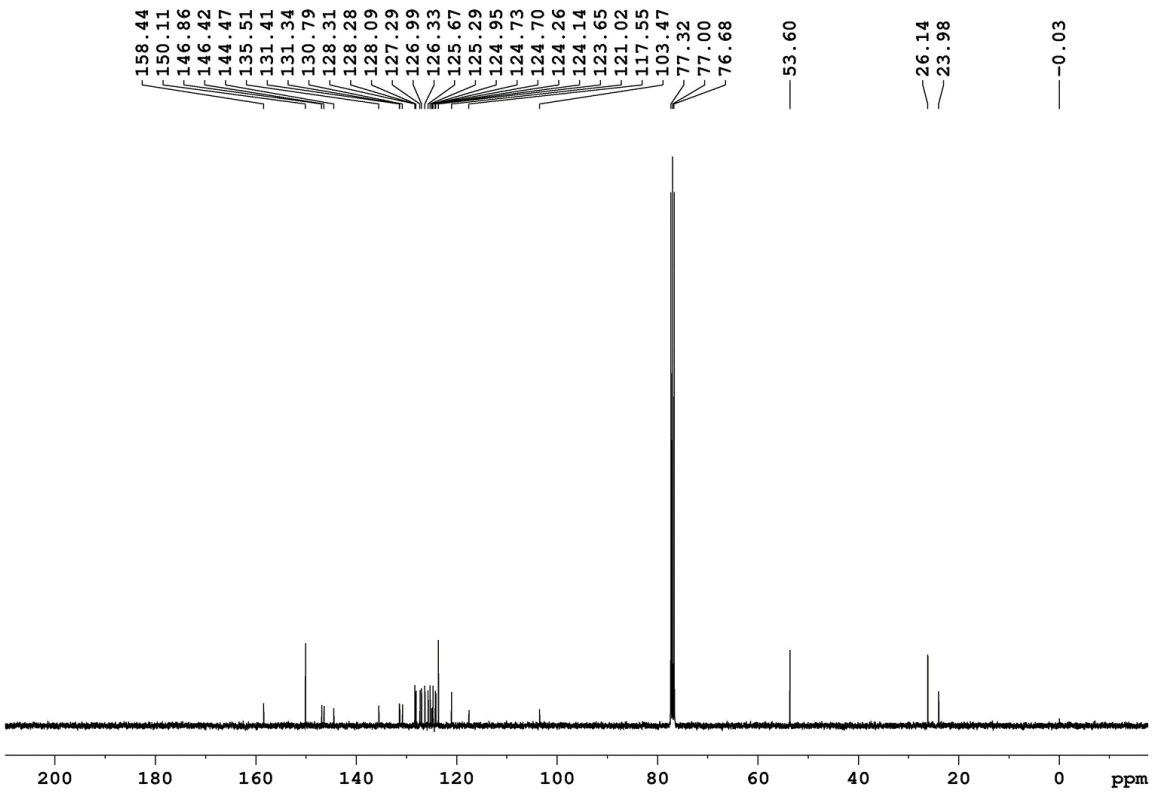

Fig. S62. ^{13}C NMR spectrum of **6f** in $CDCl_3$

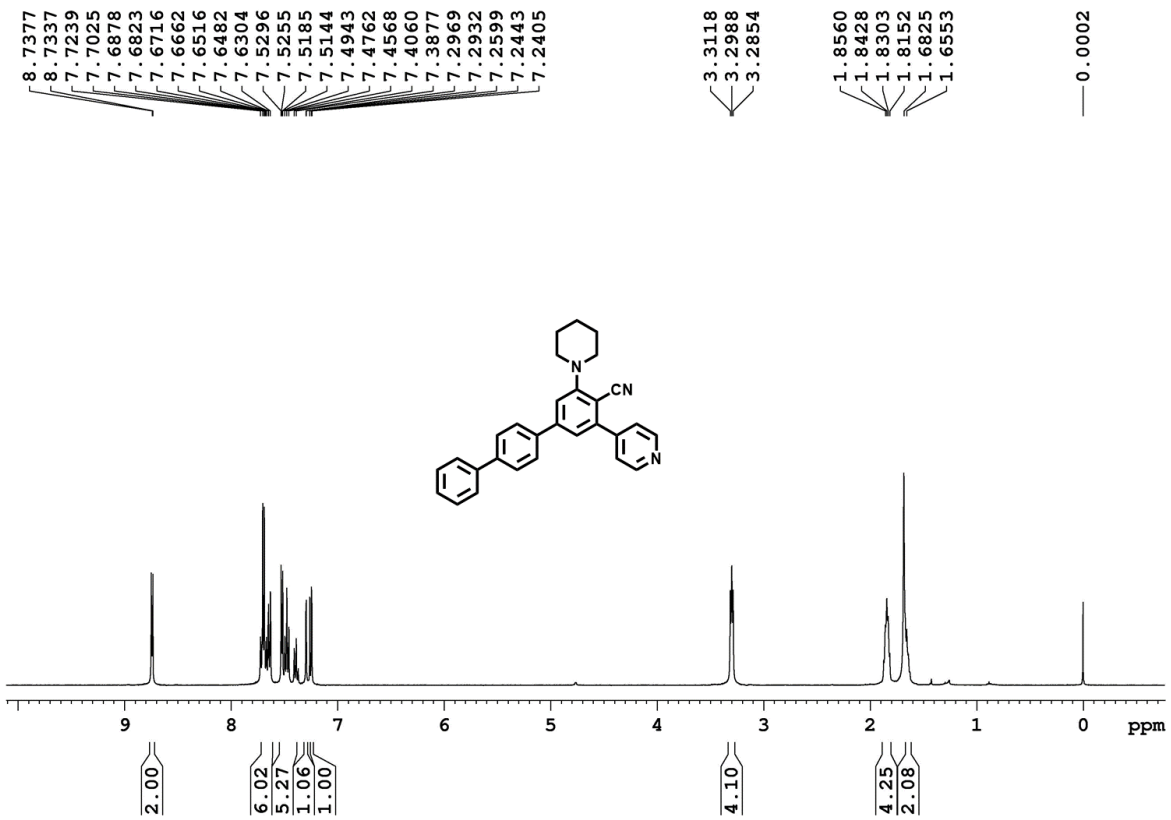

Fig. S63. ^{1}H NMR spectrum of **6g** in $CDCl_3$

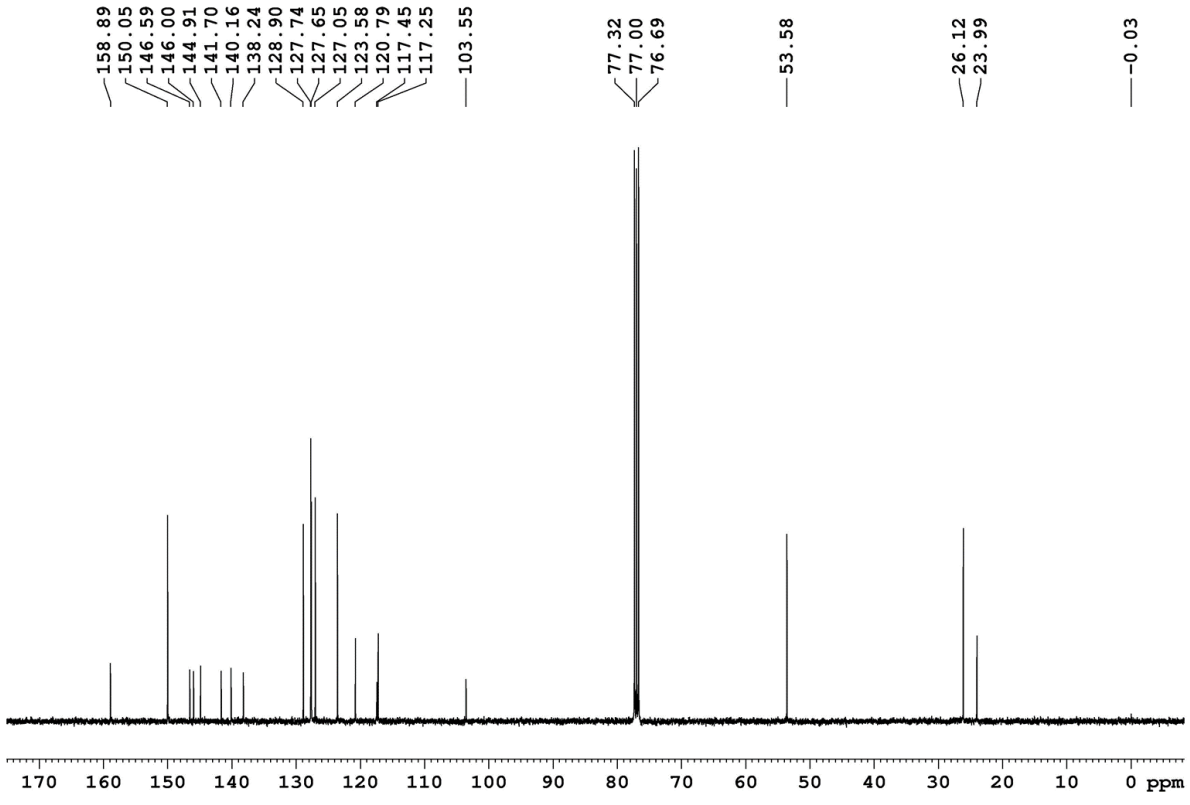

Fig. S64. ^{13}C NMR spectrum of **6g** in $CDCl_3$

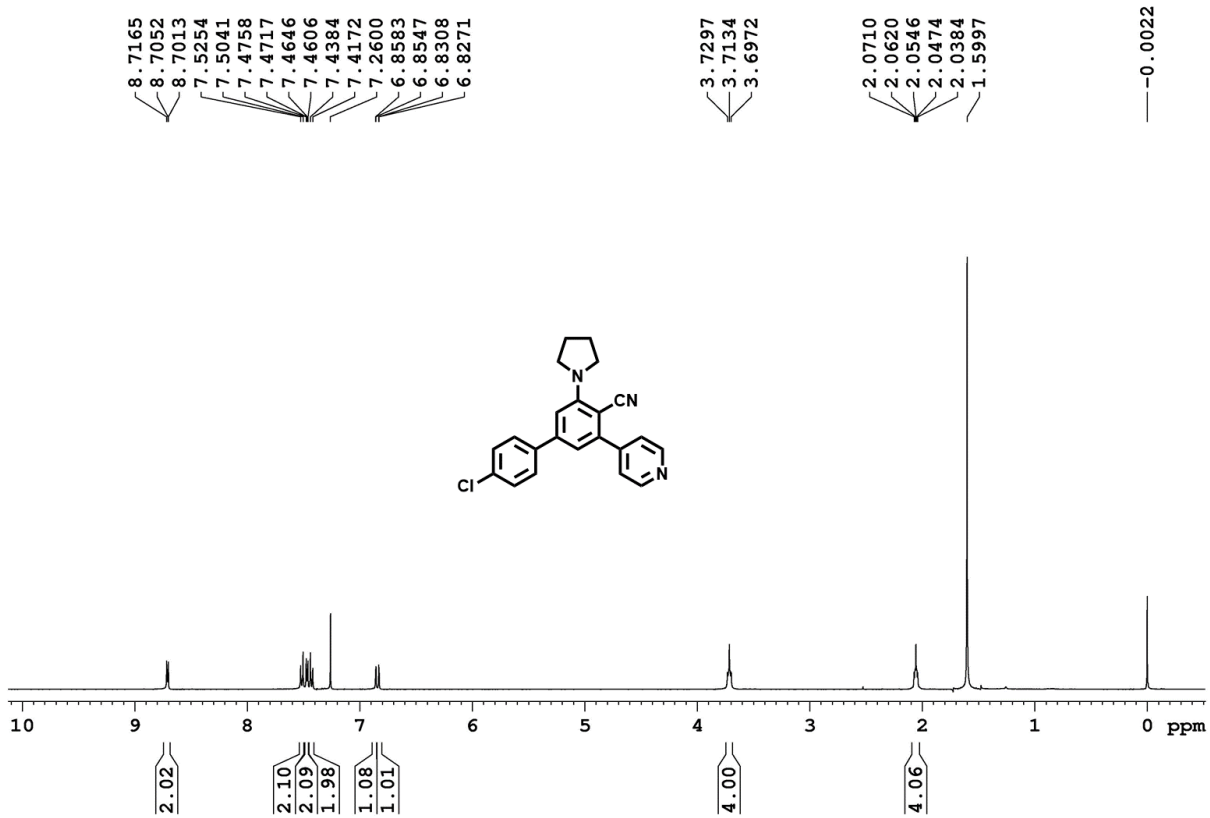

Fig. S65. ^{1}H NMR spectrum of **6h** in $CDCl_3$

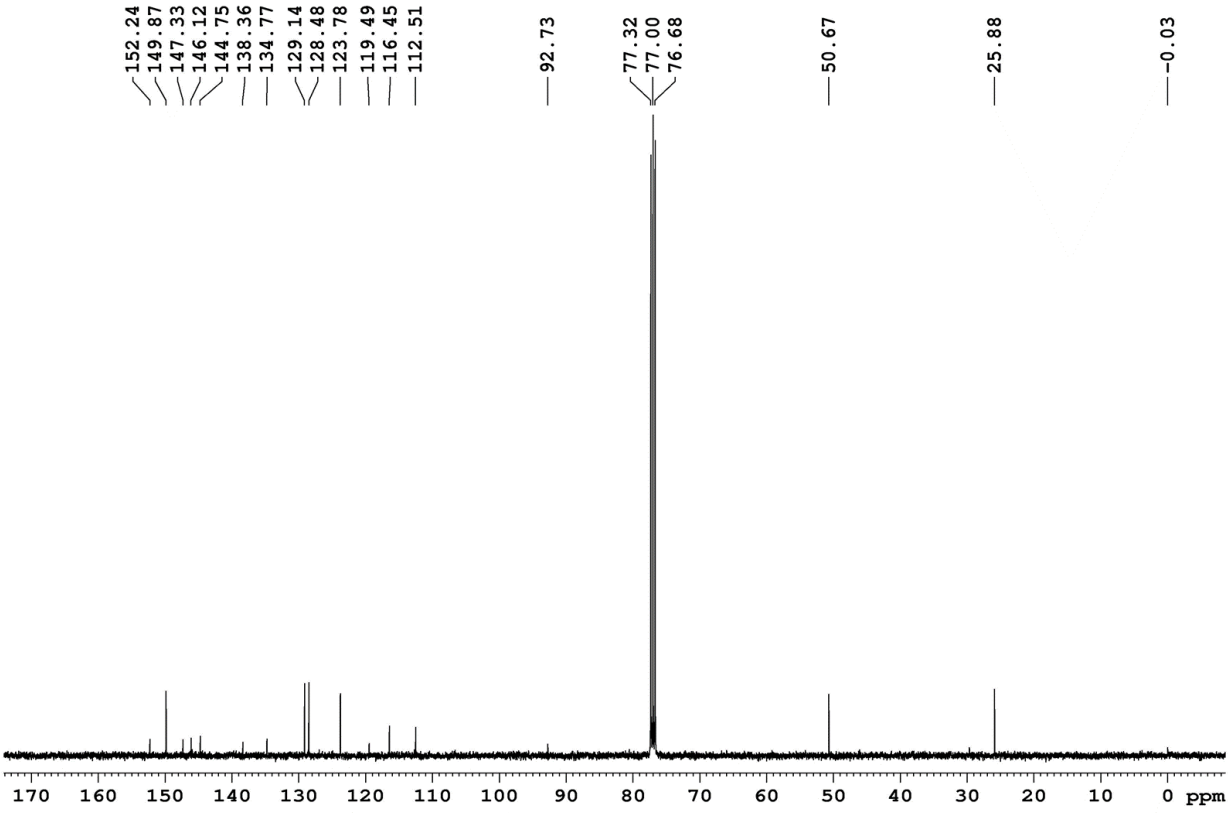

Fig. S66. ^{13}C NMR spectrum of **6h** in $CDCl_3$

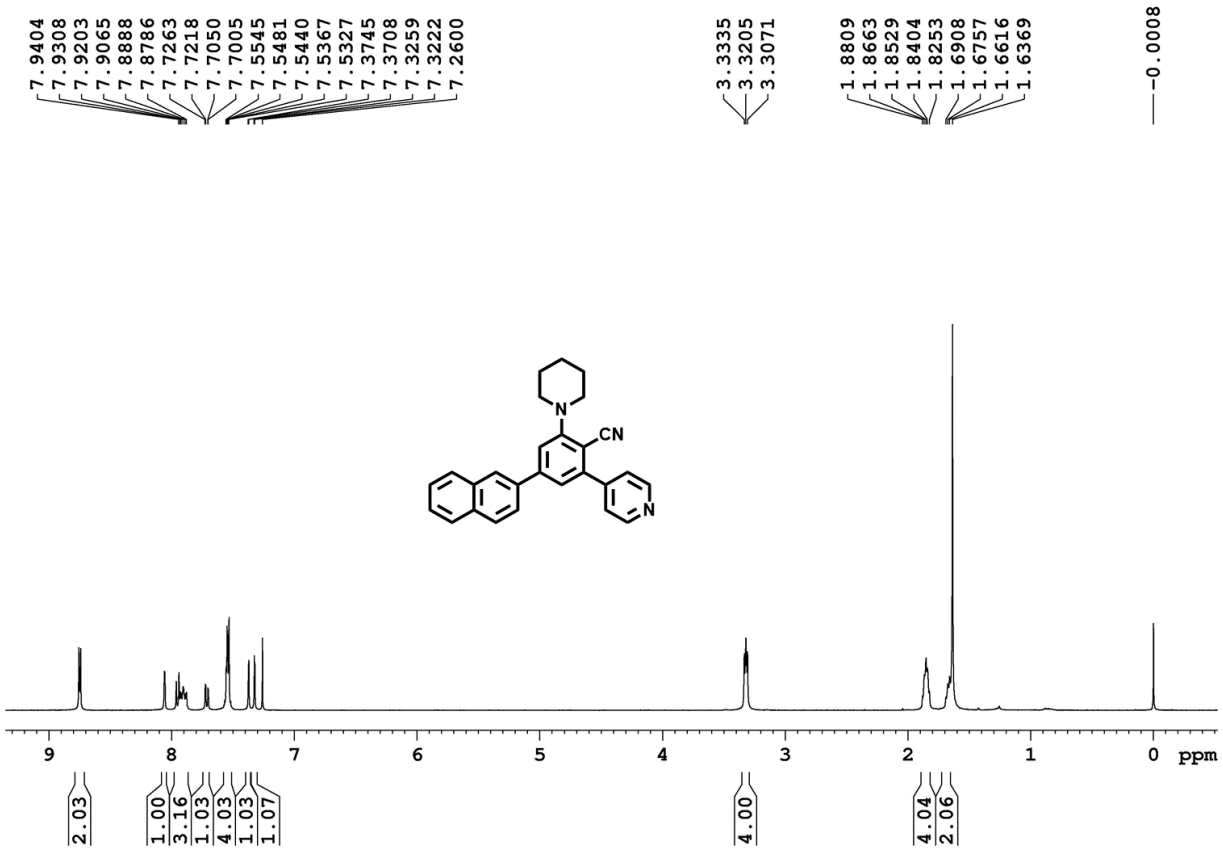

Fig. S67. ^{1}H NMR spectrum of **6i** in $CDCl_3$

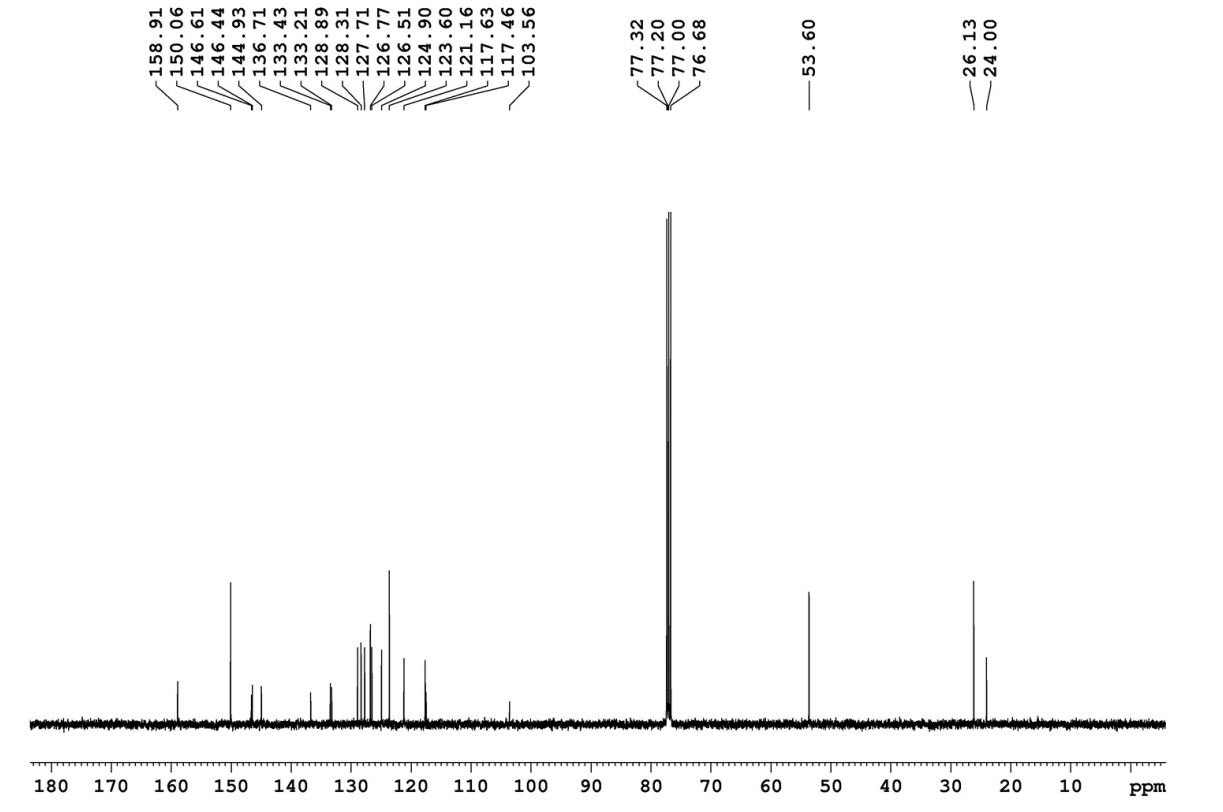

Fig. S68. ^{13}C NMR spectrum of **6i** in $CDCl_3$

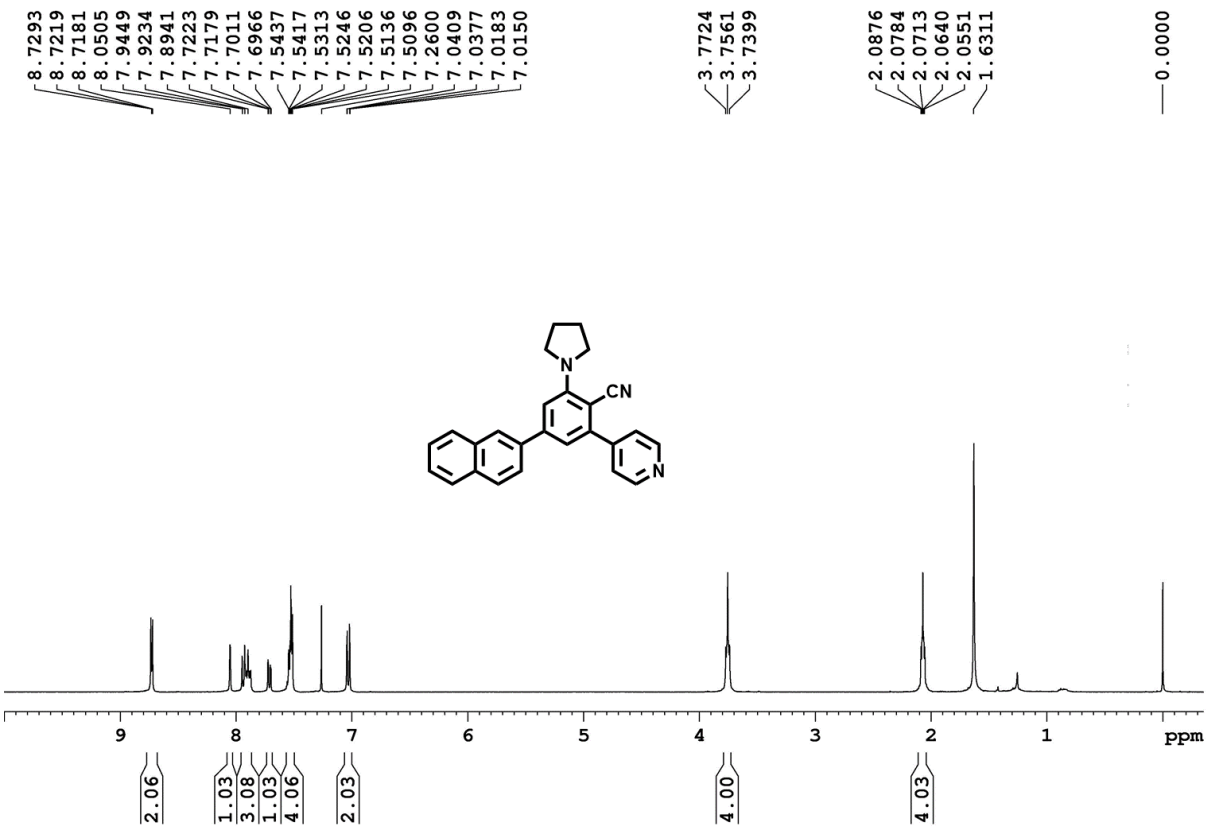

Fig. S69. ^{1}H NMR spectrum of **6j** in $CDCl_3$

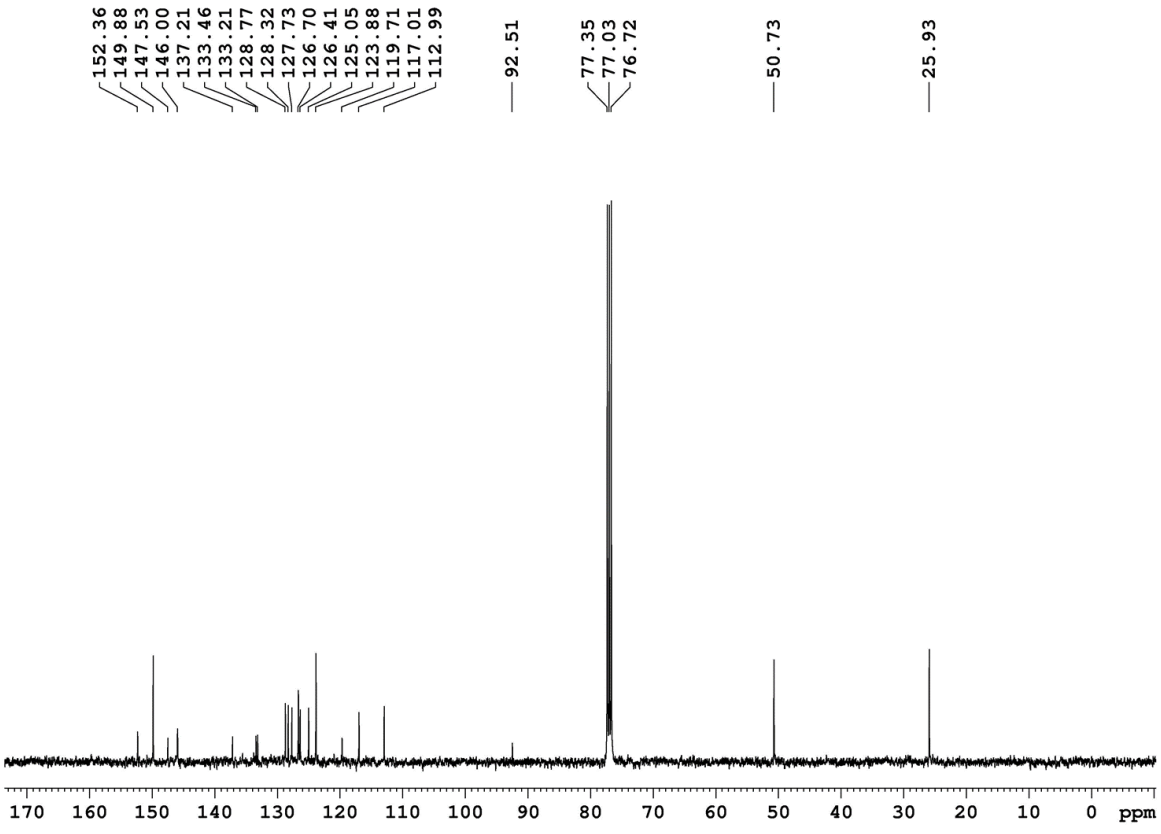

Fig. S70. ^{13}C NMR spectrum of **6j** in $CDCl_3$

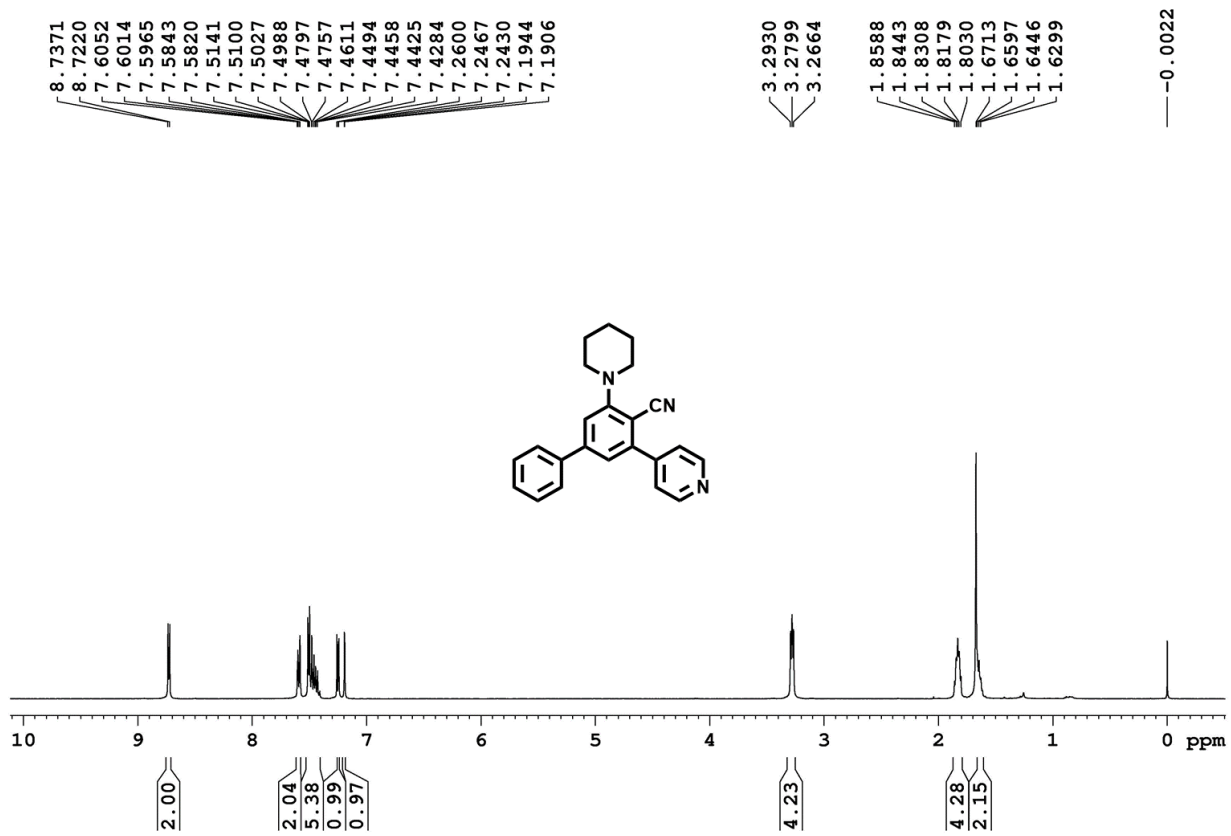

Fig. S71. ^{1}H NMR spectrum of **6k** in $CDCl_3$

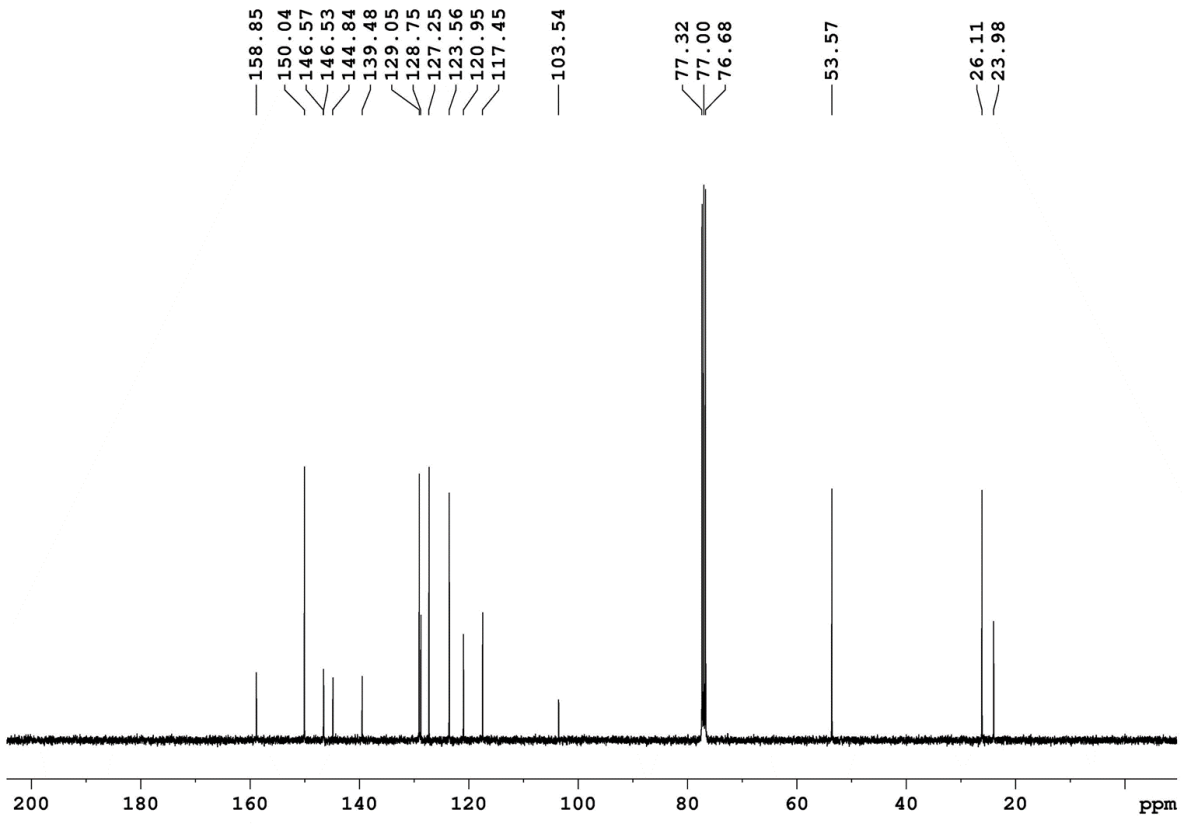

Fig.S72. ^{13}C NMR spectrum of **6k** in $CDCl_3$

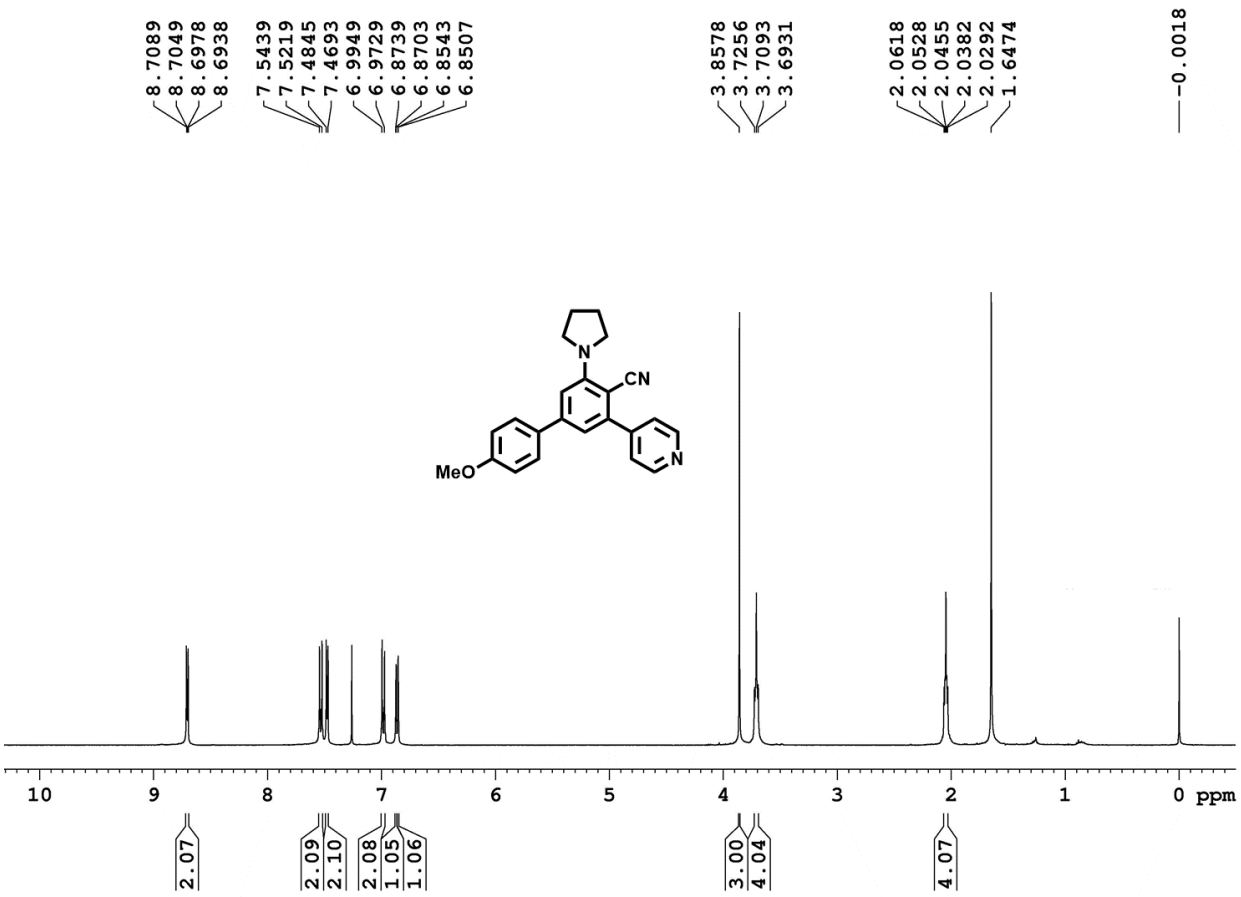

Fig. S73. ^{1}H NMR spectrum of **6l** in $CDCl_3$

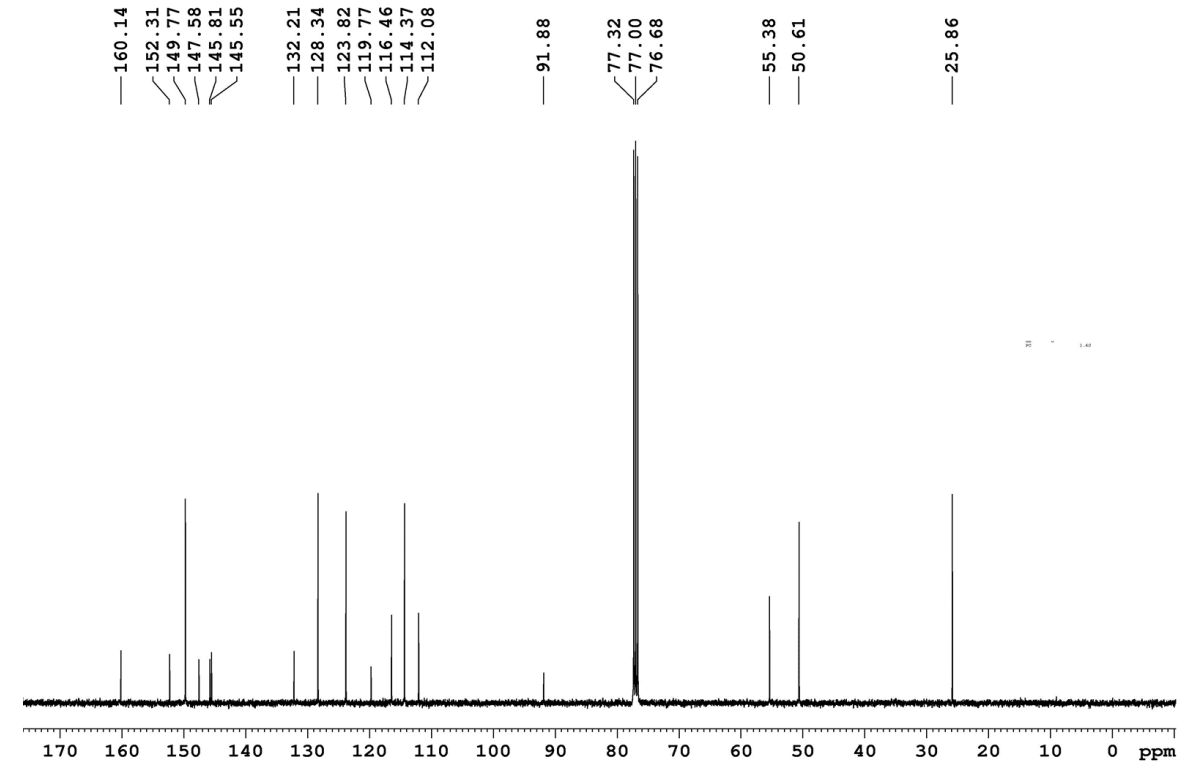

Fig. S74. ^{13}C NMR spectrum of **6l** in $CDCl_3$