

Supporting Information (SI)

Intermolecular interactions boost aggregation induced emission in carbazole Schiff base derivatives

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Figure S1: The characterization data of compounds **1-6**

Figure S2: UV-Vis (a) and fluorescence (b) spectra of compound **2** in six organic solvents with different polarities at a concentration of $2 \times 10^{-5} \text{ mol L}^{-1}$.

Figure S3: UV-Vis (a) and fluorescence (b) spectra of compound **3** in six organic solvents with different polarities at a concentration of $2 \times 10^{-5} \text{ mol L}^{-1}$.

Figure S4: UV-Vis (a) and fluorescence (b) spectra of compound **4** in six organic solvents with different polarities at a concentration of $2 \times 10^{-5} \text{ mol L}^{-1}$.

Figure S5: UV-Vis (a) and fluorescence (b) spectra of compound **5** in six organic solvents with different polarities at a concentration of $2 \times 10^{-5} \text{ mol L}^{-1}$.

Figure S6: UV-Vis (a) and fluorescence (b) spectra of compound **6** in six organic solvents with different polarities at a concentration of $2 \times 10^{-5} \text{ mol L}^{-1}$.

Figure S7: UV-Vis (a) and fluorescence (b) spectra of compound **2** in water/acetonitrile mixtures with different f_w at a concentration of $2.0 \times 10^{-5} \text{ M}$.

Figure S8: UV-Vis (a) and fluorescence (b) spectra of compound **3** in water/acetonitrile mixtures with different f_w at a concentration of $2.0 \times 10^{-5} \text{ M}$.

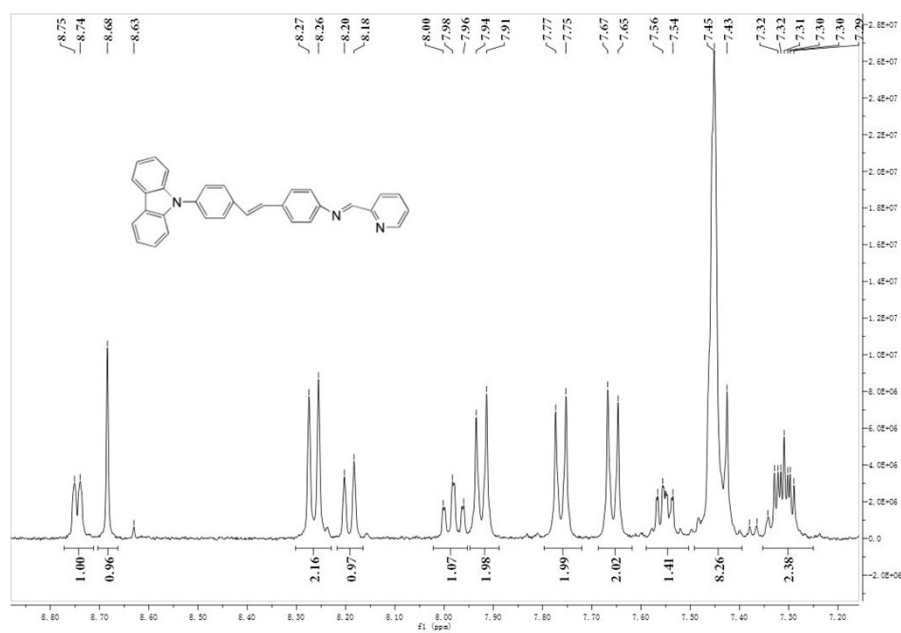
Figure S9: UV-Vis (a) and fluorescence (b) spectra of compound **4** in water/acetonitrile mixtures with different f_w at a concentration of $2.0 \times 10^{-5} \text{ M}$.

Figure S10: UV-Vis (a) and fluorescence (b) spectra of compound **5** in water/acetonitrile mixtures with different f_w at a concentration of $2.0 \times 10^{-5} \text{ M}$.

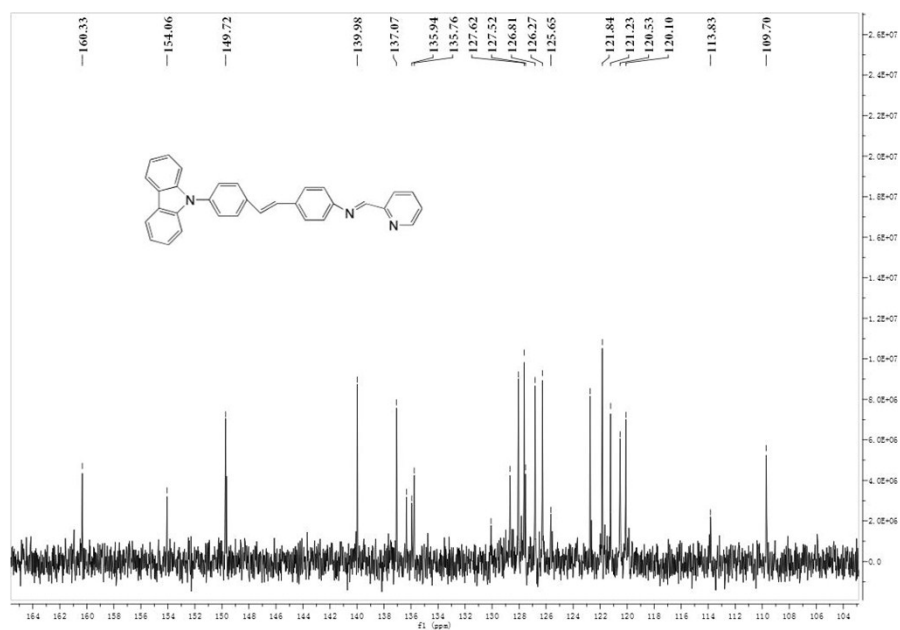
Figure S11: MTT assay of Hela cells treated with compounds **1-6** at different concentrations for 24 h

Table S1 Crystal data of compounds **1, 2, 3, 5** and **6**

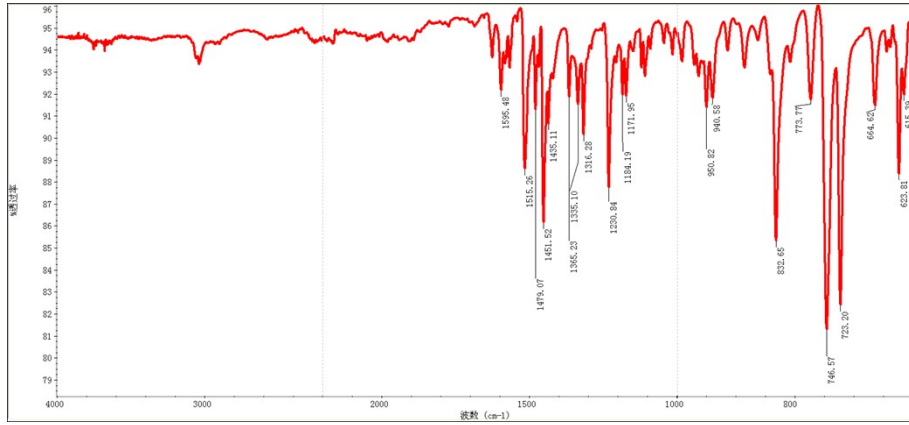
Figure S1a: ^1H NMR, ^{13}C NMR, IR and ESI MS spectra of compound **1**.



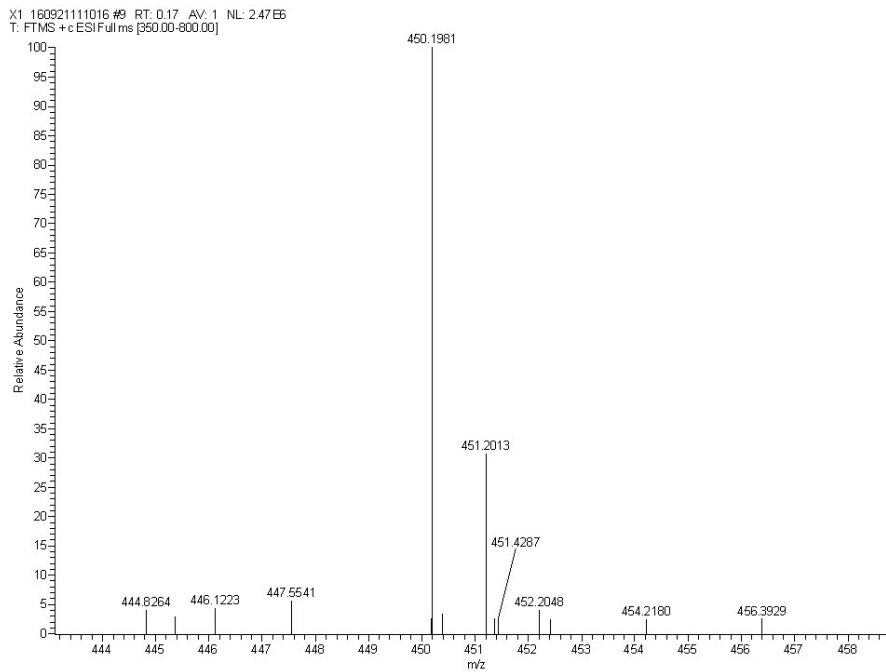
The ^1H NMR (400MHz) spectrum of compound **1** in $\text{DMSO-}d_6$



The ^{13}C NMR (100 MHz) spectrum of compound **1** in $\text{DMSO-}d_6$

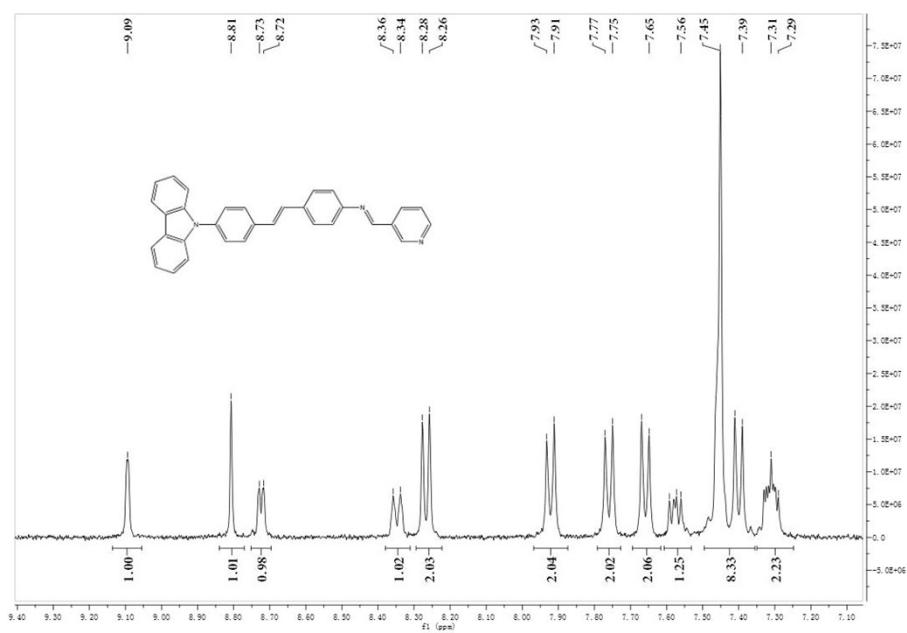


IR spectrum of compound 1

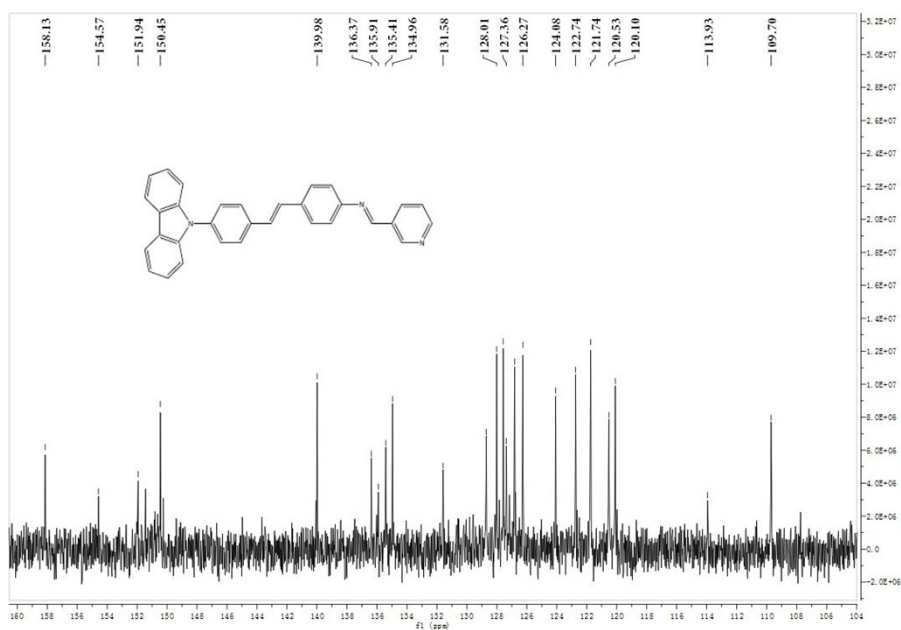


ESI MS of compound 1

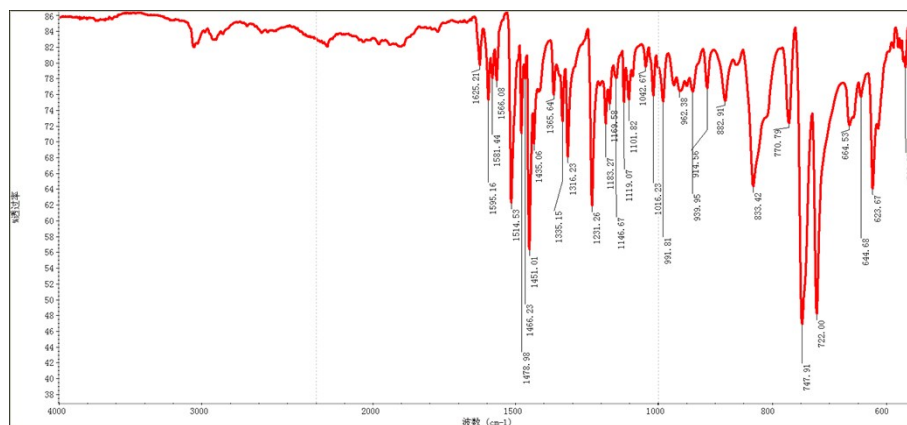
Figure S1b: ^1H NMR, ^{13}C NMR, IR and ESI MS spectra of compound **2**.



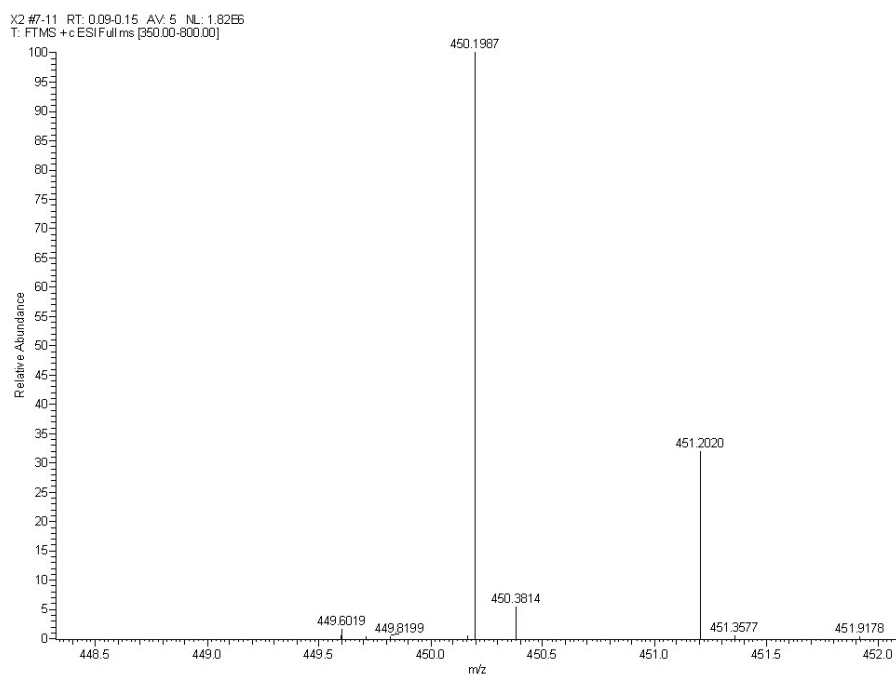
The ^1H NMR (400MHz) spectrum of compound **2** in $\text{DMSO-}d_6$



The ^{13}C NMR (100 MHz) spectrum of compound **2** in $\text{DMSO-}d_6$

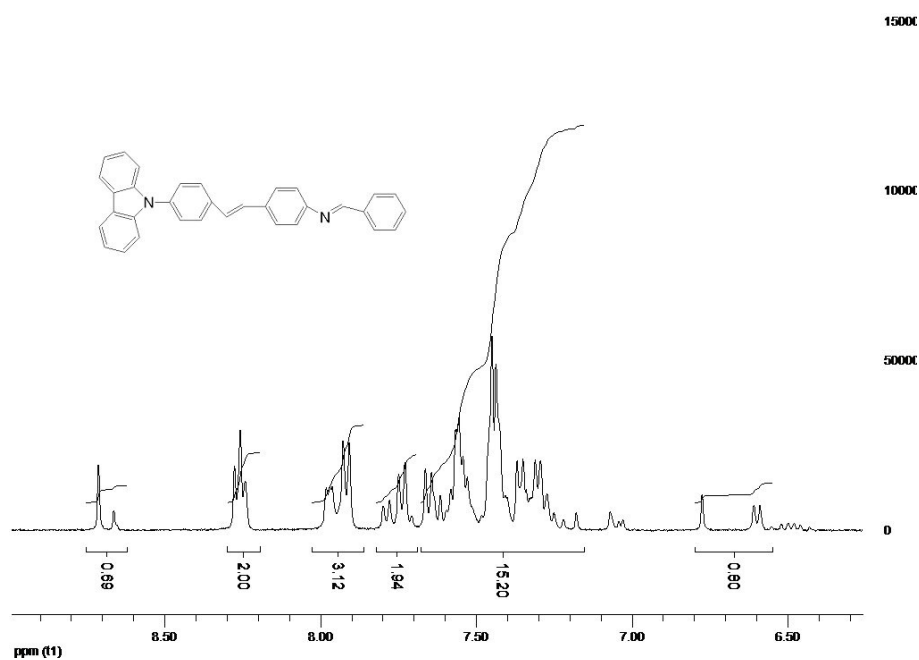


IR spectrum of compound 2

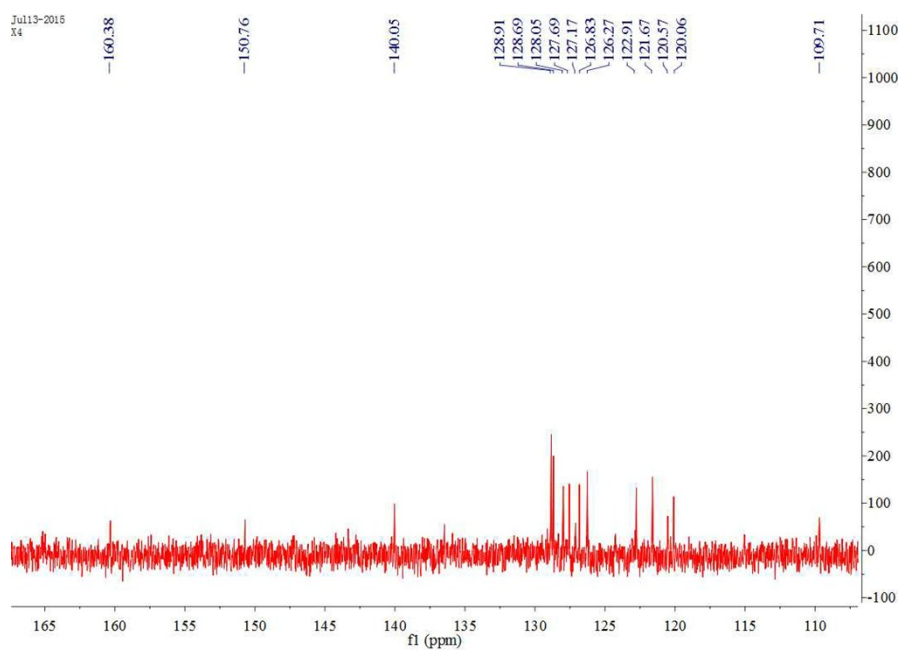


ESI MS of compound 2

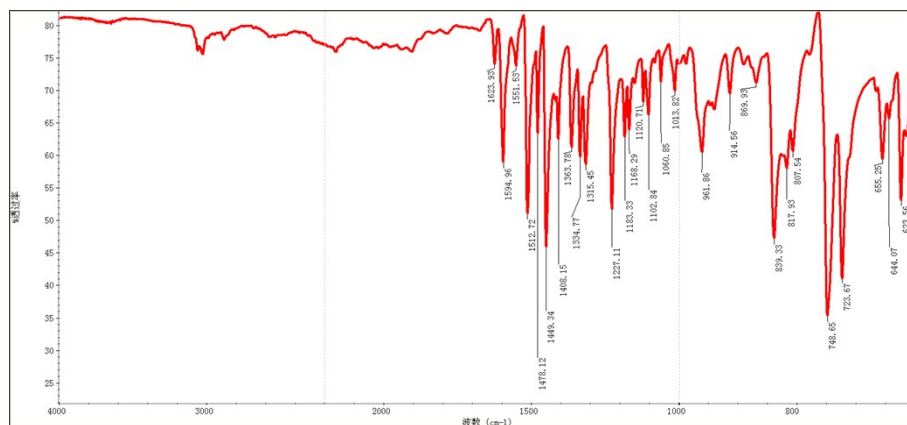
Figure S1c: ^1H NMR, ^{13}C NMR, IR and ESI MS spectra of compound **3**.



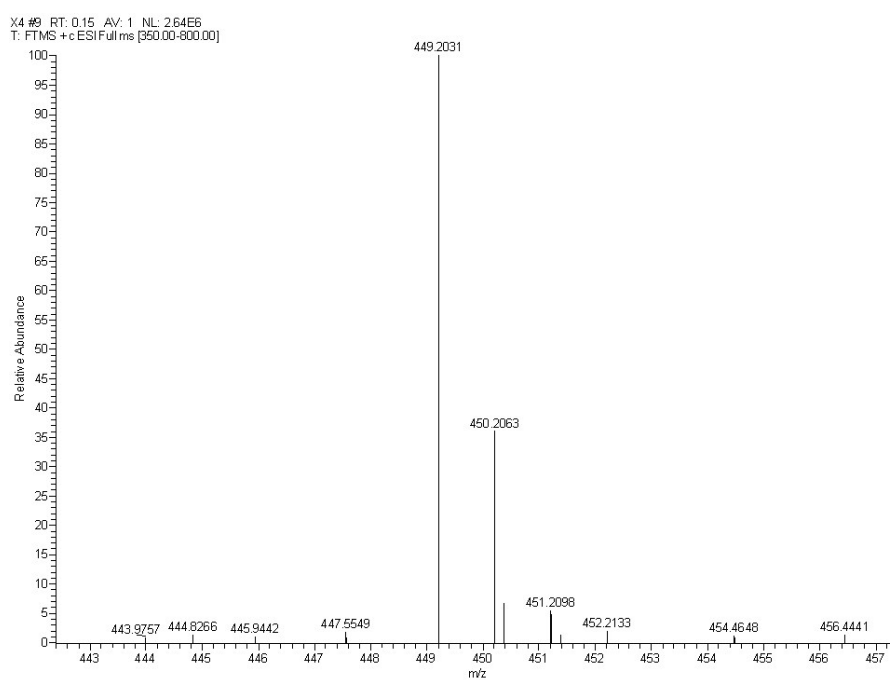
The ^1H NMR (400MHz) spectrum of compound **3** in $\text{DMSO}-d_6$



The ^{13}C NMR (100 MHz) spectrum of compound **3** in $\text{DMSO}-d_6$

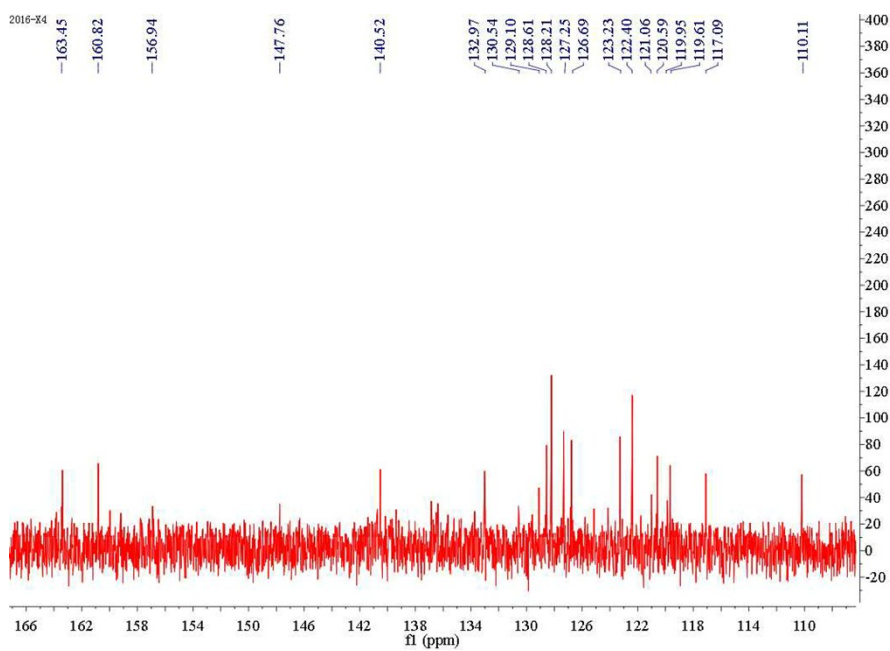
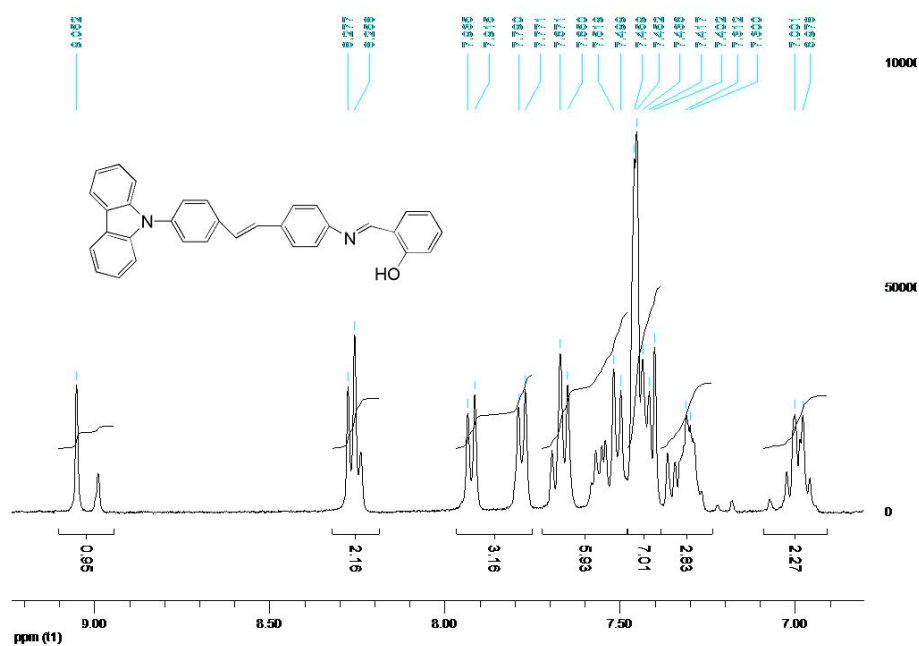


IR spectrum of compound 3

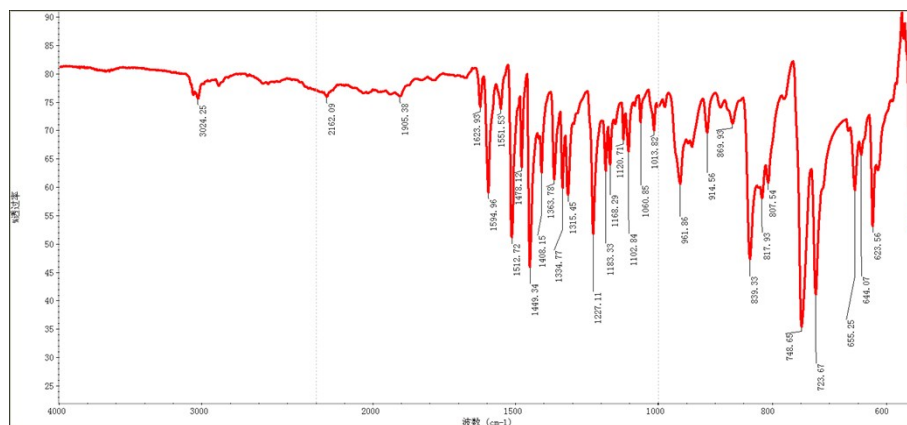


ESI MS of compound 3

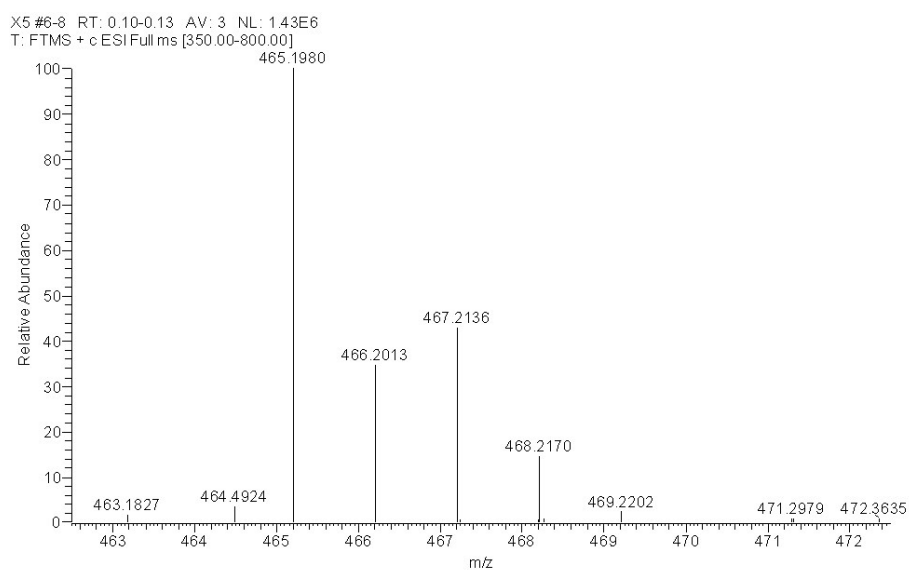
Figure S1d: ^1H NMR, ^{13}C NMR, IR and ESI MS spectra of compound 4.



The ^{13}C NMR (100 MHz) spectrum of compound 4 in $\text{DMSO}-d_6$

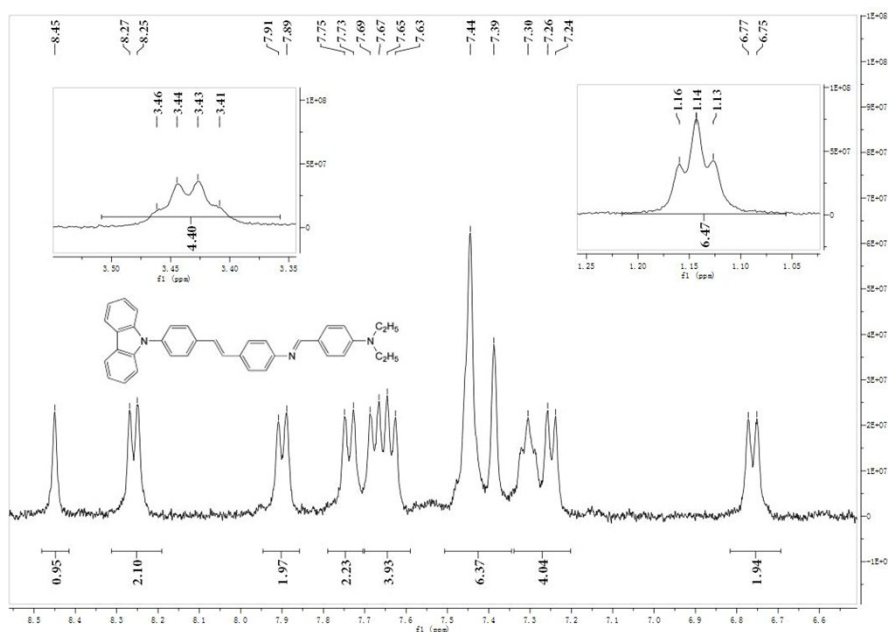


IR spectrum of compound 4

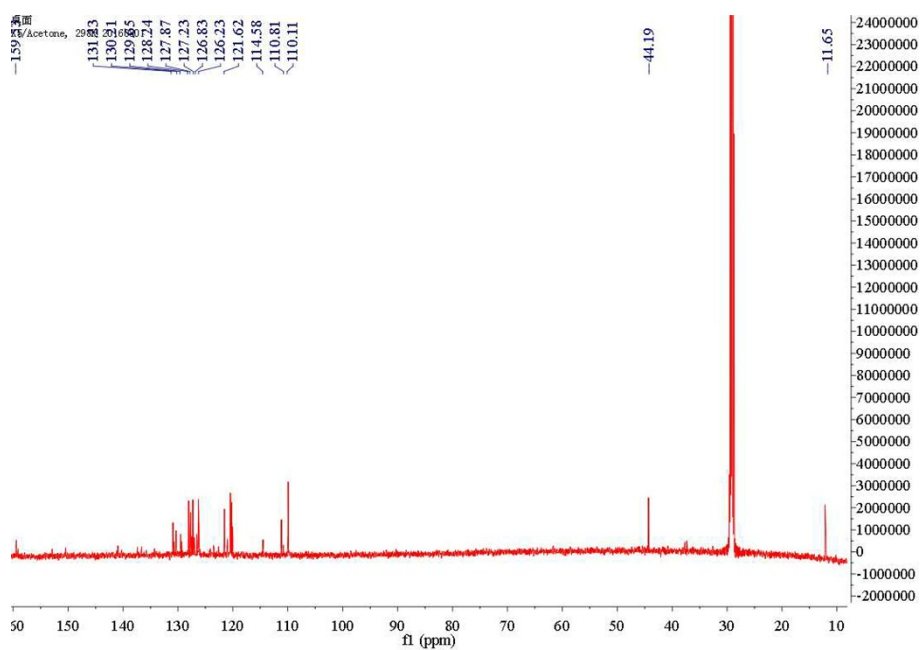


ESI MS of compound 4

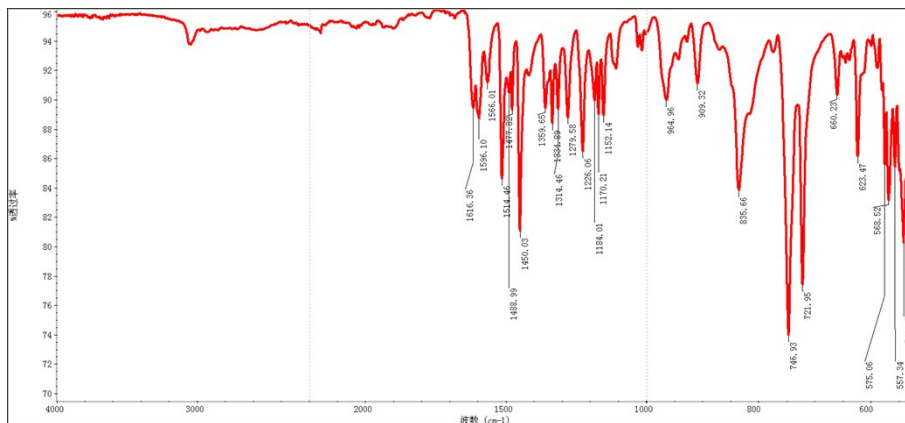
Figure S1e: ^1H NMR, ^{13}C NMR, IR and ESI MS spectra of compound 5.



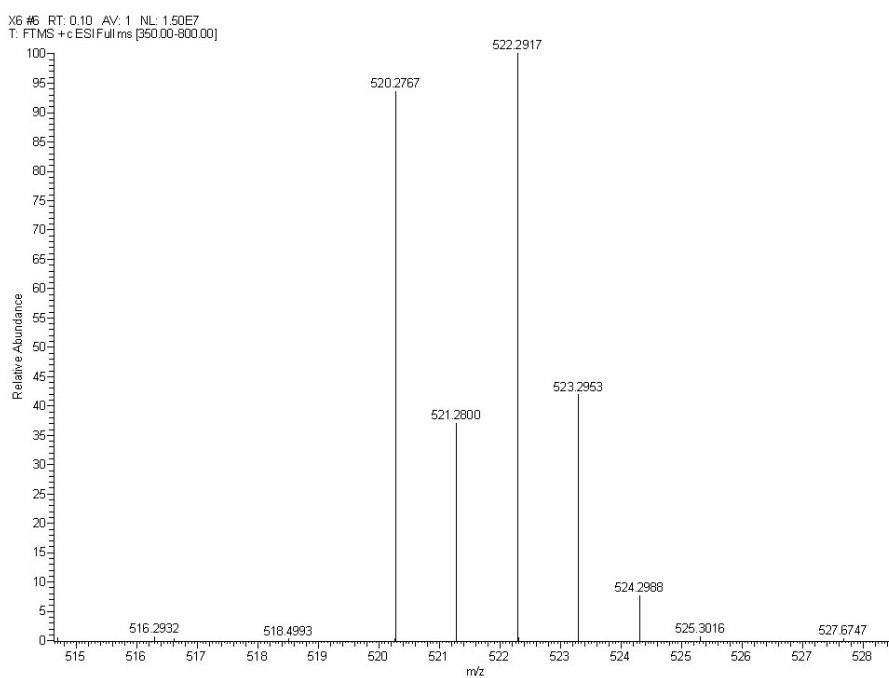
The ¹H NMR (400MHz) spectrum of compound **5** in DMSO-*d*₆



The ¹³C NMR (100 MHz) spectrum of compound **5** in CD₃COCD₃

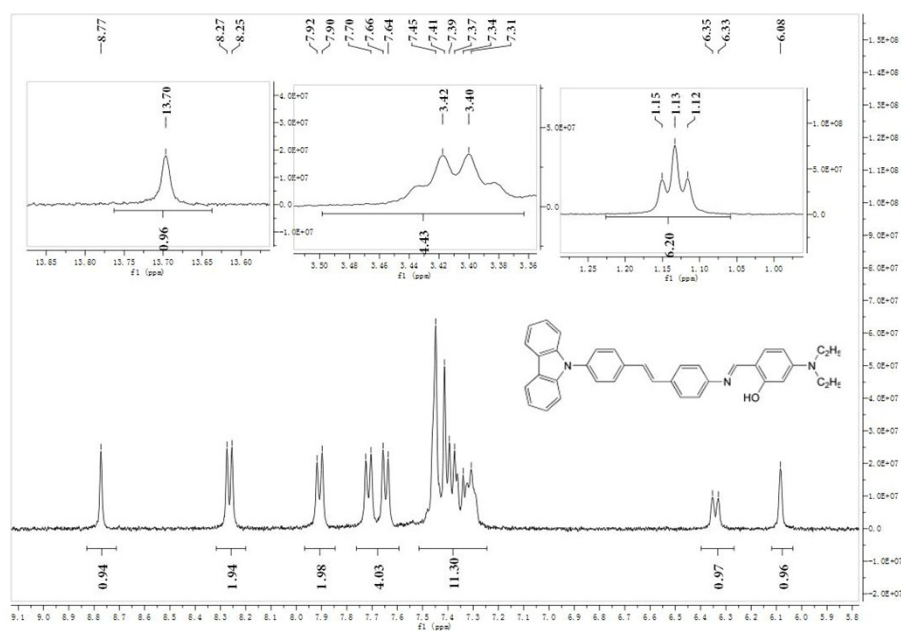


IR spectrum of compound 5

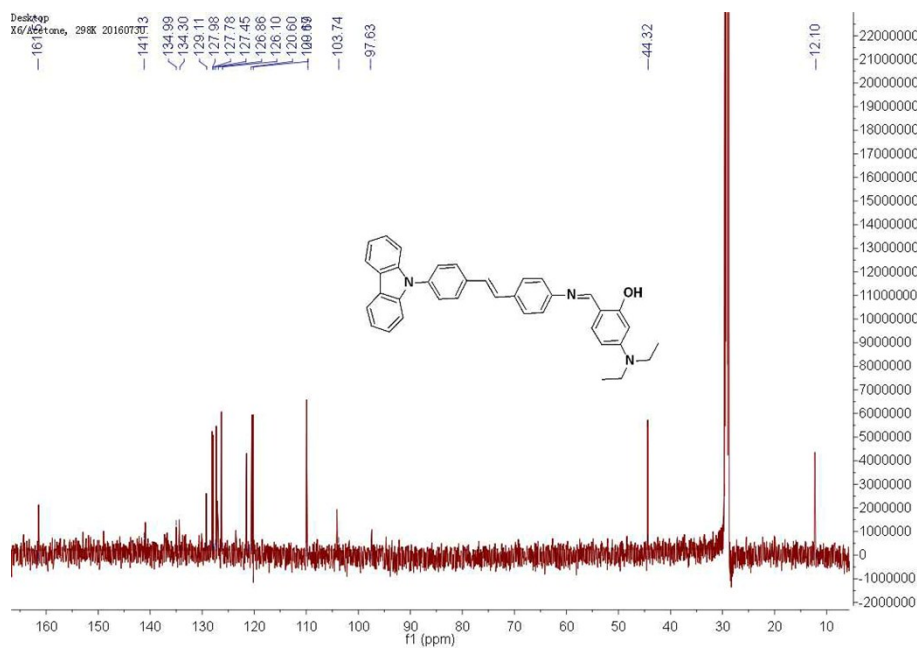


ESI MS of compound 5

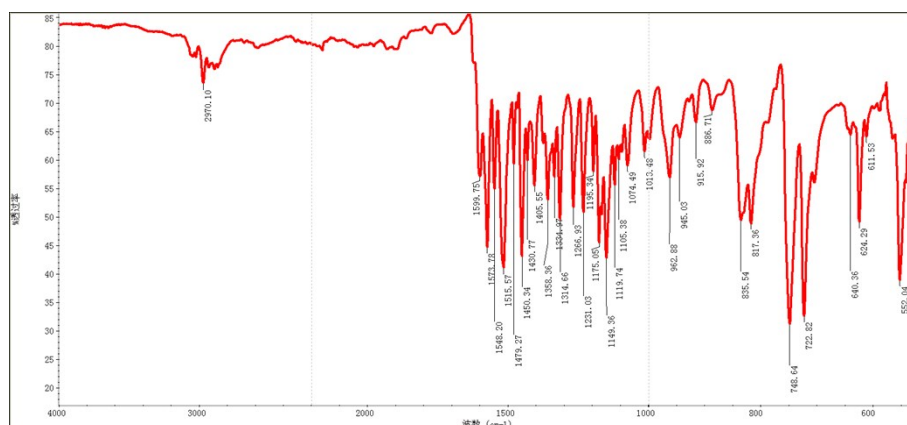
Figure S1f: ^1H NMR, ^{13}C NMR, IR and ESI MS spectra of compound **6**.



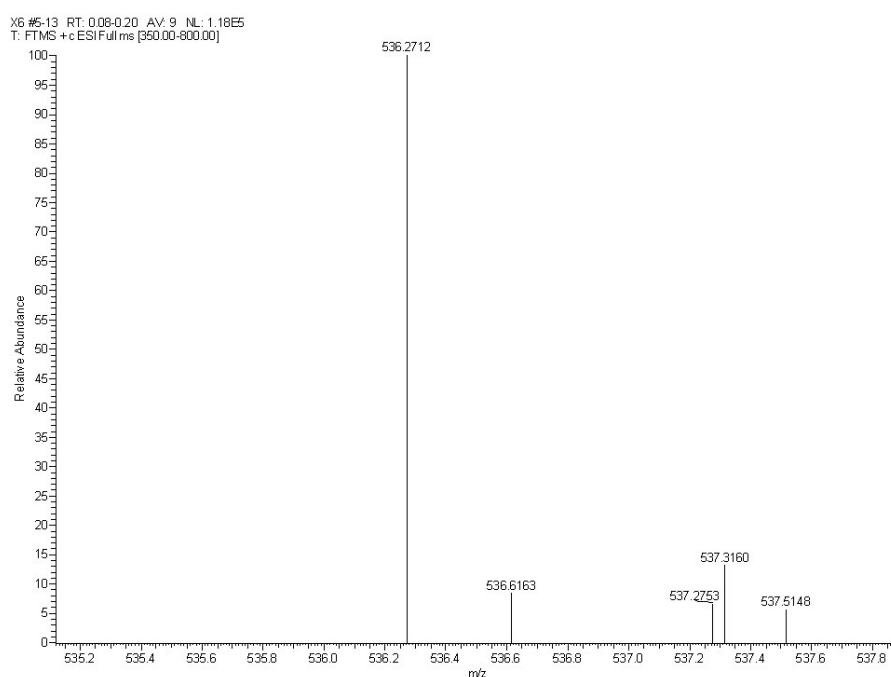
The ^1H NMR (400MHz) spectrum of compound **6** in $\text{DMSO-}d_6$



The ^{13}C NMR (100 MHz) spectrum of the compound **6** in CD_3COCD_3



IR spectrum of compound 6



ESI MS of compound 6

Figure S2: UV-Vis (a) and fluorescence (b) spectra of compound 2 in six organic solvents with different polarities at a concentration of $2 \times 10^{-5} \text{ mol L}^{-1}$.

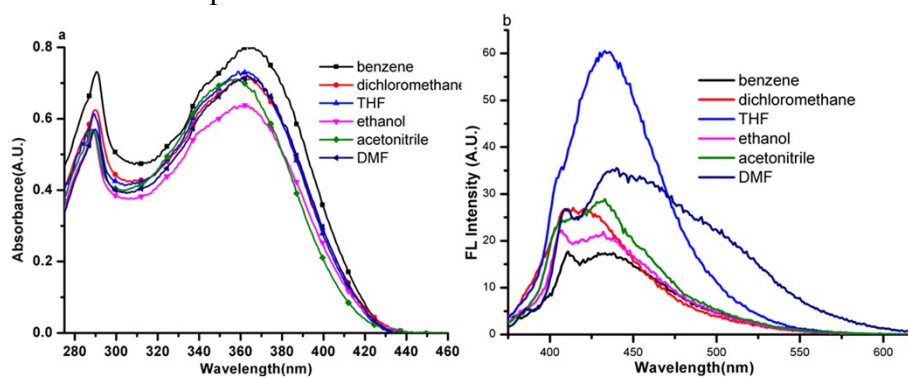


Figure S3: UV-Vis (a) and fluorescence (b) spectra of compound **3** in six organic solvents with different polarities at a concentration of $2 \times 10^{-5} \text{ mol L}^{-1}$.

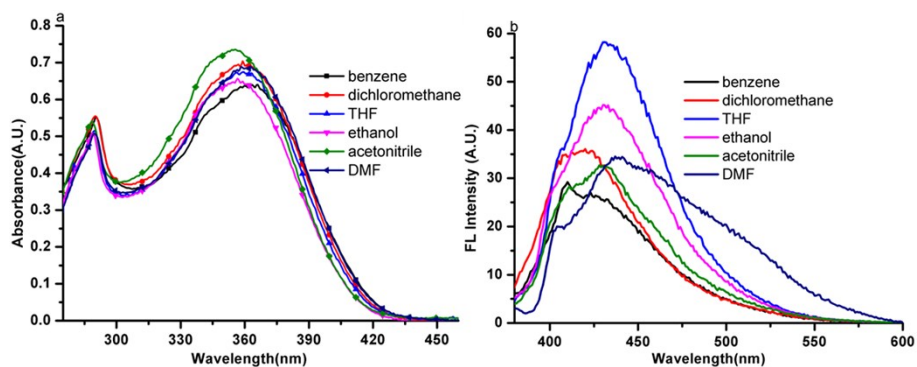


Figure S4: UV-Vis (a) and fluorescence (b) spectra of compound **4** in six organic solvents with different polarities at a concentration of $2 \times 10^{-5} \text{ mol L}^{-1}$.

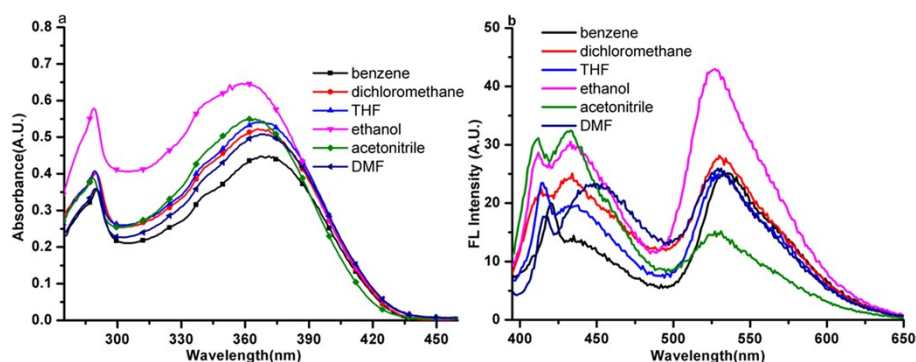


Figure S5: UV-Vis (a) and fluorescence (b) spectra of compound **5** in six organic solvents with different polarities at a concentration of $2 \times 10^{-5} \text{ mol L}^{-1}$.

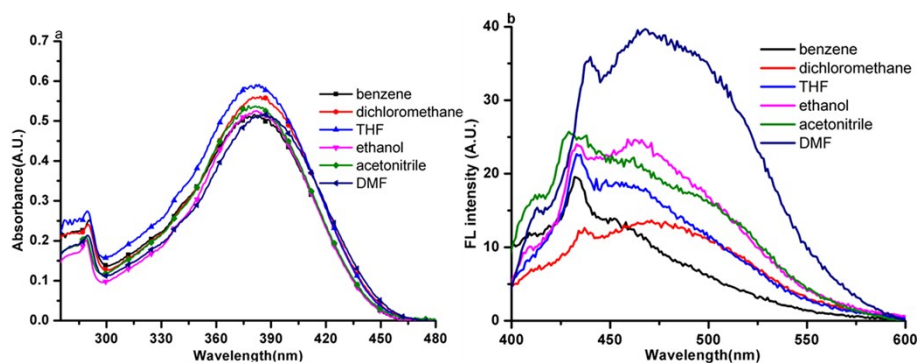


Figure S6: UV-Vis (a) and fluorescence (b) spectra of compound **6** in six organic solvents with different polarities at a concentration of $2 \times 10^{-5} \text{ mol L}^{-1}$.

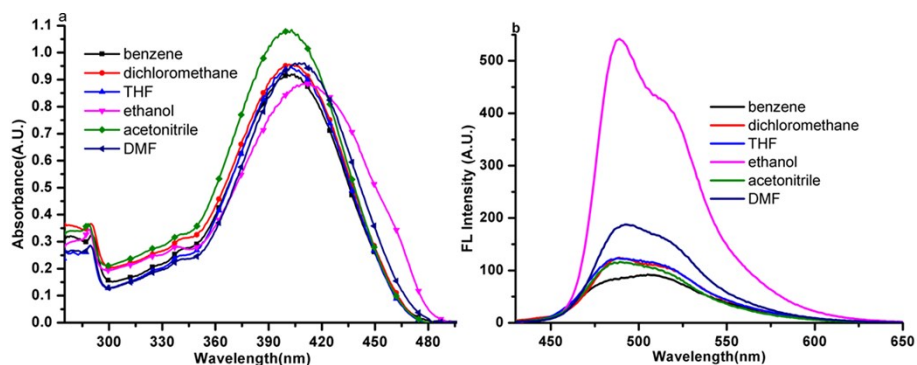


Figure S7: UV-Vis (a) and fluorescence (b) spectra of compound **2** in water/acetonitrile mixtures with different f_w at a concentration of 2.0×10^{-5} M.

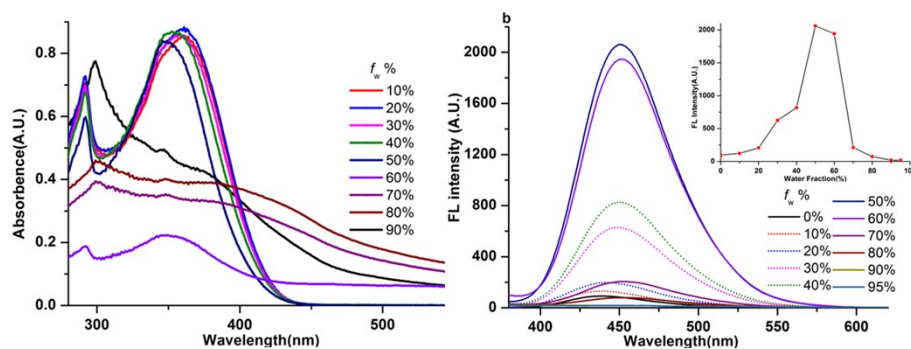


Figure S8: UV-Vis (a) and fluorescence (b) spectra of compound **3** in water/acetonitrile mixtures with different f_w at a concentration of 2.0×10^{-5} M.

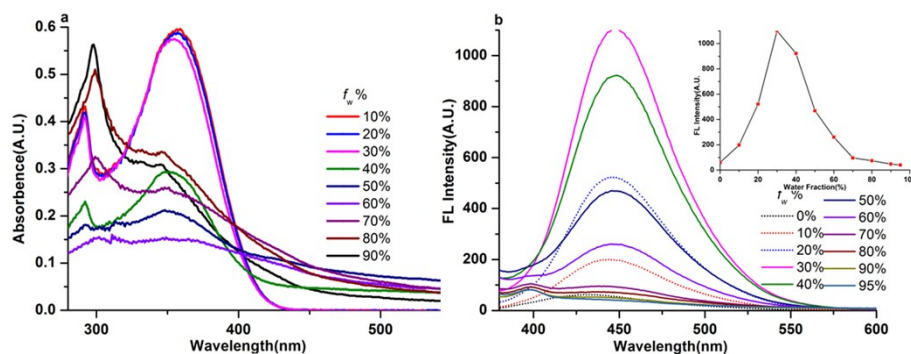


Figure S9: UV-Vis (a) and fluorescence (b) spectra of compound **4** in water/acetonitrile mixtures with different f_w at a concentration of 2.0×10^{-5} M.

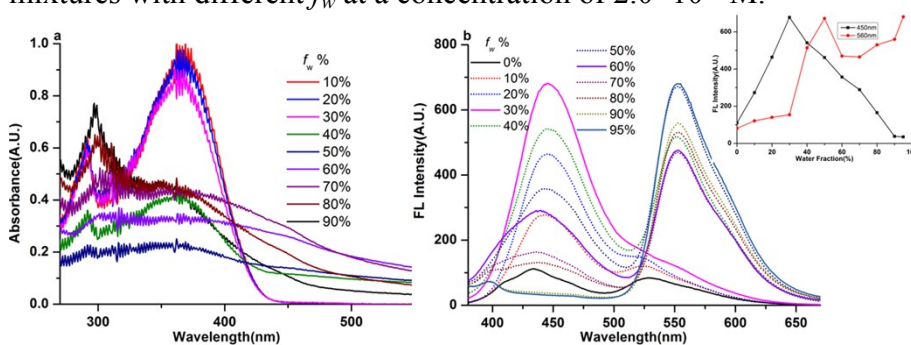


Figure S10: UV-Vis (a) and fluorescence (b) spectra of compound **5** in water/acetonitrile mixtures with different f_w at a concentration of 2.0×10^{-5} M.

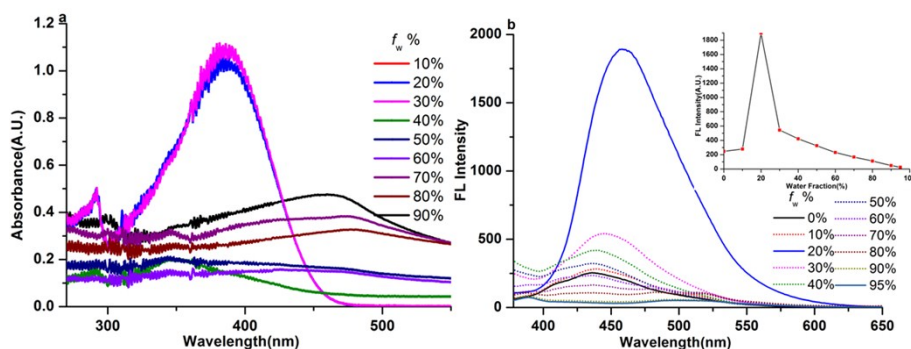


Figure S11: MTT assay of Hela cells treated with compounds **1-6** at different concentrations for 24 h

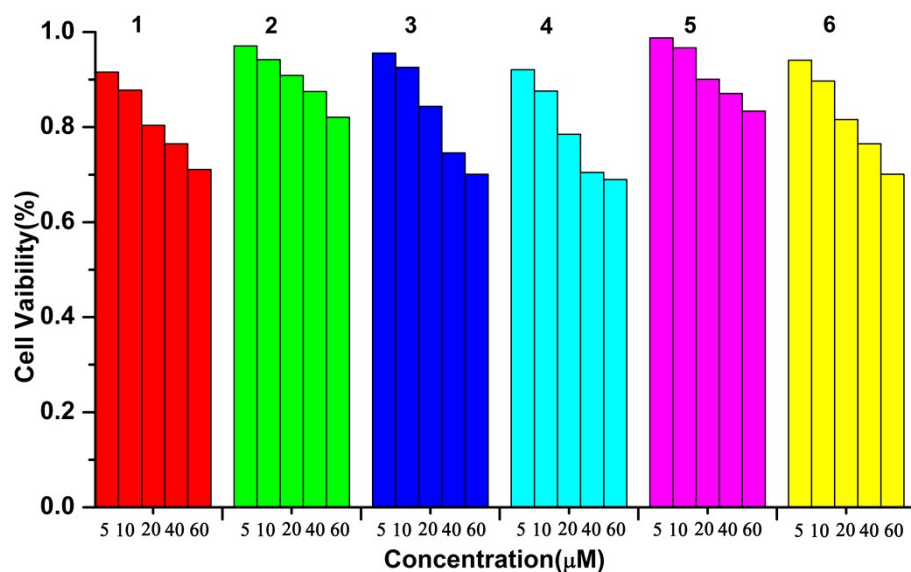


Table S1 Crystal data of compounds **1, 2, 3, 5** and **6**

Compounds	1	2	3	5	6
Empirical formula	C ₃₂ H ₂₃ N ₃	C ₃₂ H ₂₃ N ₃	C ₃₃ H ₂₄ N ₂	C ₃₇ H ₃₃ N ₃	C ₃₇ H ₃₃ N ₃ O
Formula weight	449.53	449.53	448.54	519.66	535.66
Crystal system	<i>monoclinic</i>	<i>monoclinic</i>	<i>monoclinic</i>	<i>triclinic</i>	<i>tetragonal</i>
Space group	C2/c	C2/c	C2/c	P-1	Pna21
a[Å]	17.791(4)	37.005(8)	36.888(6)	9.806(3)	16.383(5)
b[Å]	6.3822(15)	11.212(2)	11.0226(19)	17.473(4)	11.090(5)
c[Å]	42.441(10)	45.528(10)	46.003(8)	35.205(9)	31.475(5)
α[°]	90.00	90.00	90.00	104.3700	90.00
β[°]	93.833(3)	91.208(3)	92.876(2)	96.872(3)	90.00
γ[°]	90.00	90.00	90.00	90.00	90.00
V[Å ³]	4808.2(19)	18886(7)	18681(5)	5799(3)	5719(3)
Z	8	32	32	8	8
T[K]	296(2)	296(2)	296(2)	296(2)	293(2)
D _{calcd} [g·cm ⁻³]	1.242	1.265	1.276	1.191	1.244
F(000)	1888.0	7552.0	7552.0	2208.0	2272.0
μ[mm ⁻¹]	0.073	0.075	0.074	0.070	0.075
θrange[°]	0.96-25.00	1.10-25.00	0.89-25.00	1.20-25.00	1.29-25.00
Total no. data	4233	16569	16400	20014	10077
No. unique data	2611	7083	7368	4888	7322
R _{int}	0.0436	0.0809	0.0955	0.0766	0.0468
R ₁	0.0660	0.1690	0.0849	0.1070	0.0678
wR ₂	0.2339	0.2257	0.3329	0.3982	0.2224
GOF	1.081	1.008	0.977	0.842	1.059