Electronic Supporting Information

Indene-1,3-dionemethylene-4*H*-pyran derivatives containing alkoxy chains of various lengths: Aggregation-induced emission enhancement, mechanofluorochromic properties and solvent-induced emission changes

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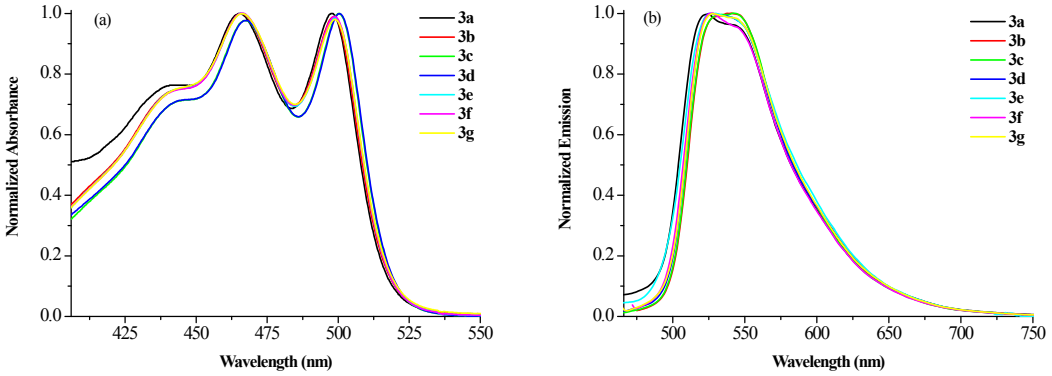
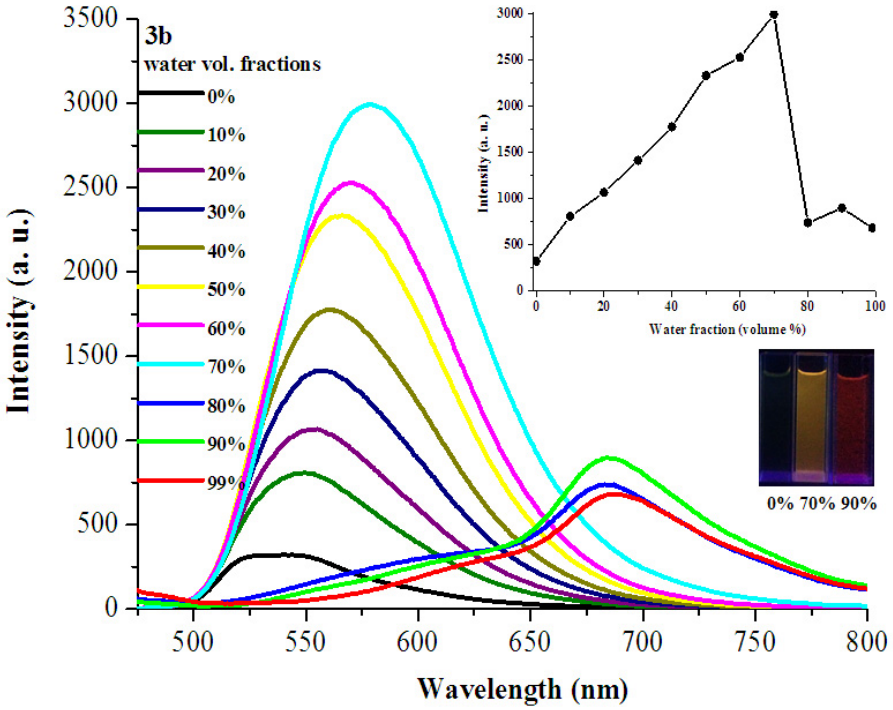
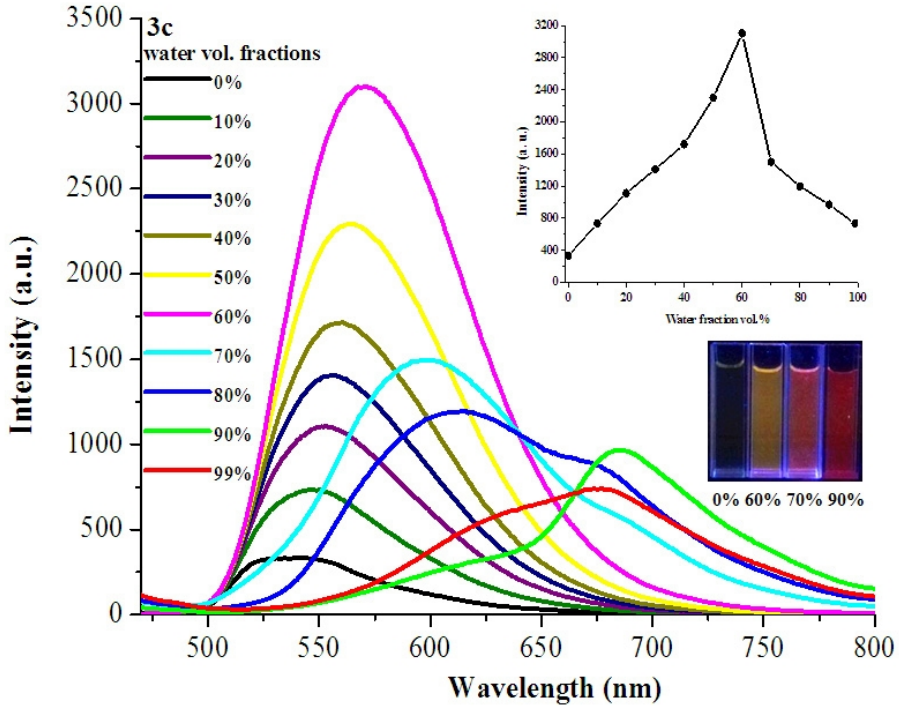


Fig. S1 Absorption spectra (a) and fluorescence spectra (b) of **3a-3g** (1×10^{-5} mol/L) in THF solution.

Table S1 Physical properties of IDMP derivatives in THF solution (s = shoulder peak).

Compound	λ_{abs} (nm)	λ_{em} (nm)
3a	442(s), 465, 498	524, 544
3b	442 (s), 466, 498	529, 542
3c	444 (s), 467, 500	531, 544
3d	444 (s), 467, 500	526, 545(s)
3e	442 (s), 466, 498	530, 547(s)
3f	441 (s), 466, 498	527, 545(s)
3g	442 (s), 467, 499	527, 543


3b
water vol. fractions
0%
10%
20%
30%
40%
50%
60%
70%
80%
90%
99%
Intensity (a. u.)
Wavelength (nm)
Intensity (a. u.)
Water fraction (volume %)
0% 70% 90%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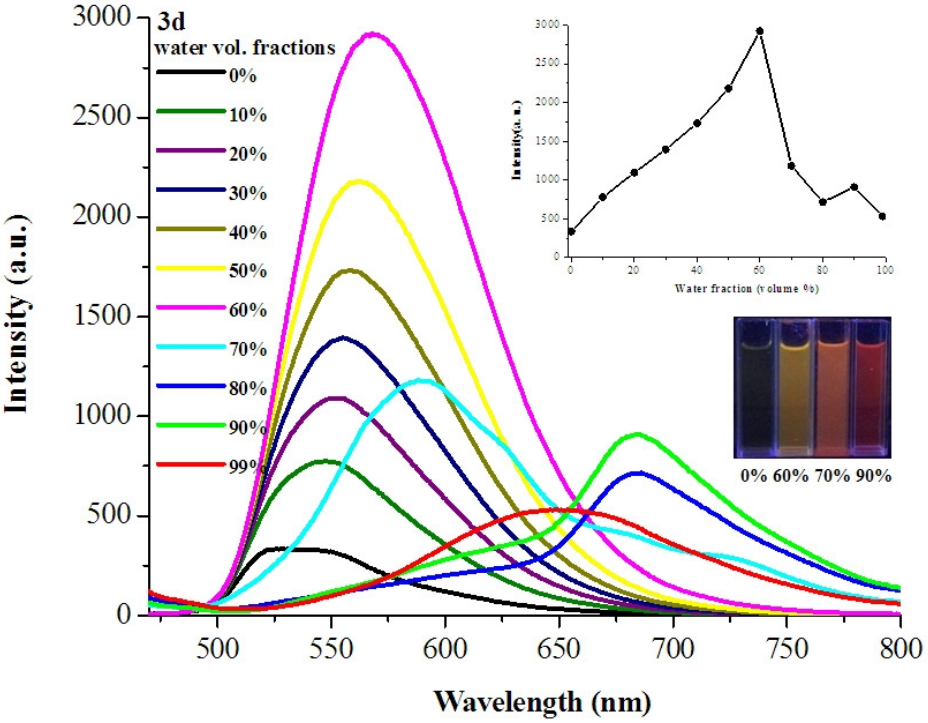
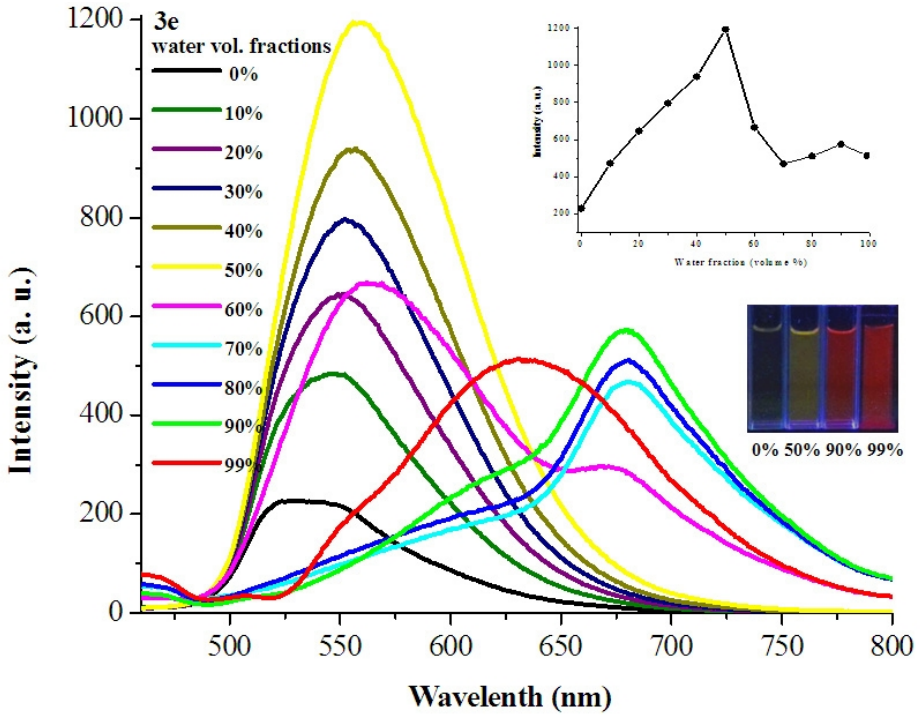
water vol. fractions
0%
10%
20%
30%
40%
50%
60%
70%
80%
90%
99%
Intensity (a.u.)
Wavelength (nm)
Intensity (a. u.)
Water fraction vol.%
0% 60% 70% 90%


3d
water vol. fractions
0%
10%
20%
30%
40%
50%
60%
70%
80%
90%
99%
Intensity (a.u.)
Wavelength (nm)
Water fraction (volume %)
0% 60% 70% 90%


3e
water vol. fractions
0%
10%
20%
30%
40%
50%
60%
70%
80%
90%
99%
Intensity (a. u.)
Wavelenth (nm)
Water fraction (volume %)
0% 50% 90% 99%

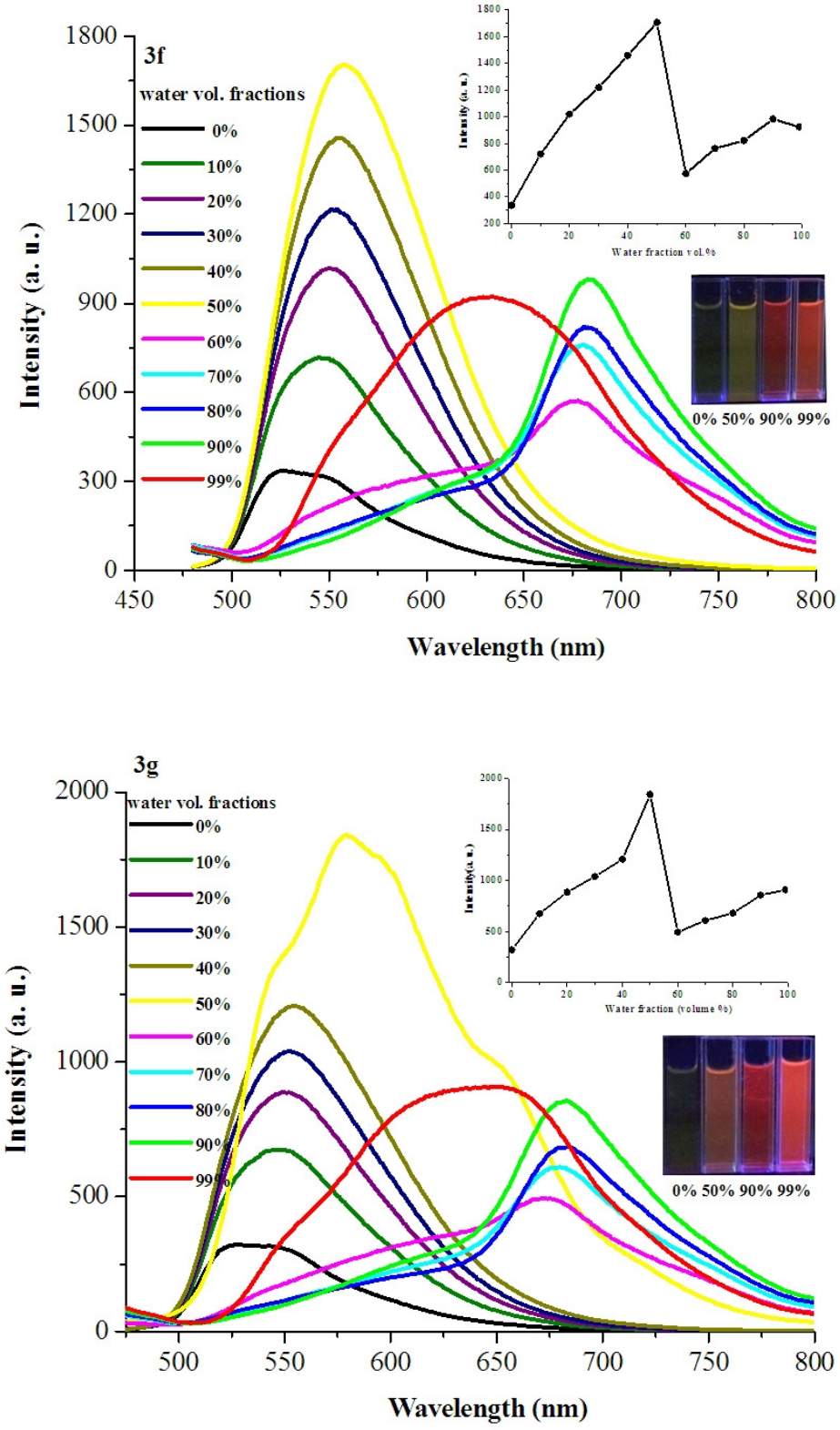


Fig. S2 Fluorescence spectra of **3b**-**3g** (1×10^{-5} mol/L) in THF/water mixtures with different f_w values. The insets depict the changes in fluorescence peak intensity and emission images of the compounds in different water fraction mixtures under a 365-nm UV lamp.

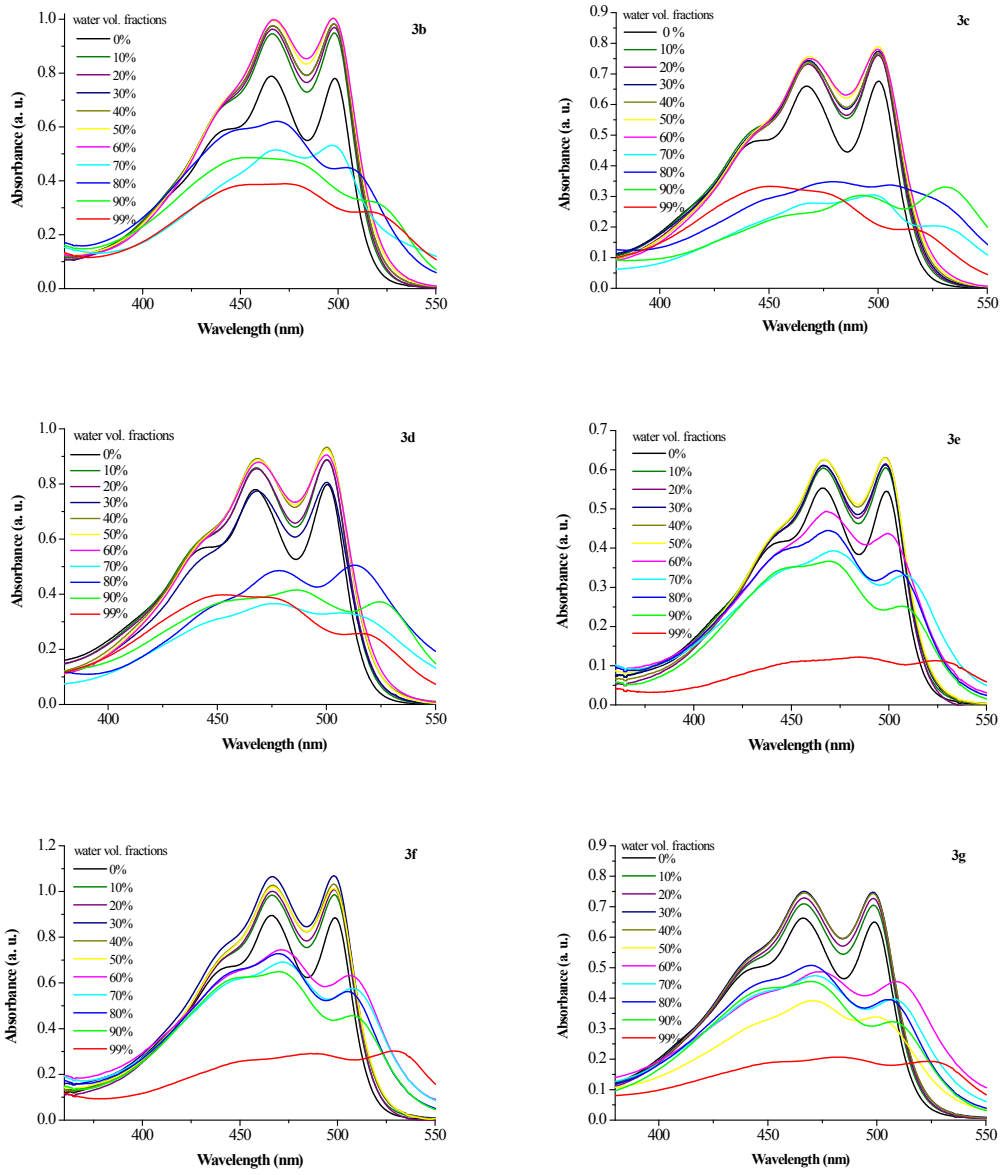


Fig. S3 UV-vis spectra of **3b-3g** (1×10^{-5} mol/L) in THF/water mixtures with different f_w values.

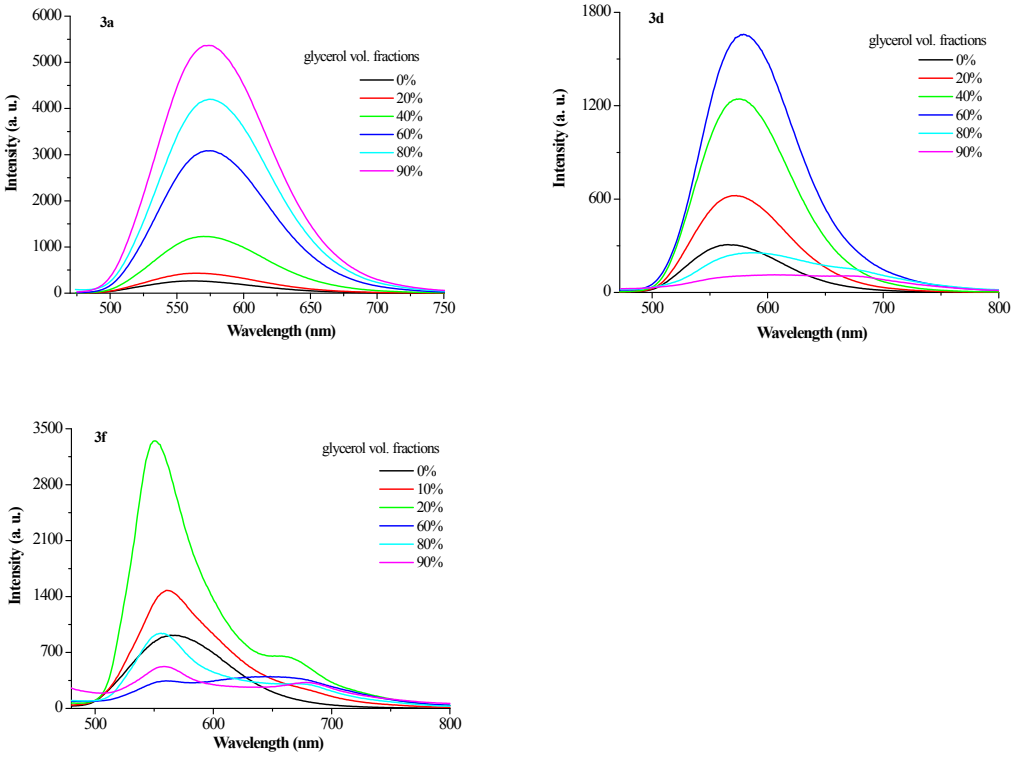


Fig. S4 Fluorescence spectra of **3a**, **3d** and **3f** in methanol/glycerol mixtures (1×10^{-5} mol/L, containing 0.5 vol % THF) with different glycerol volume fractions.

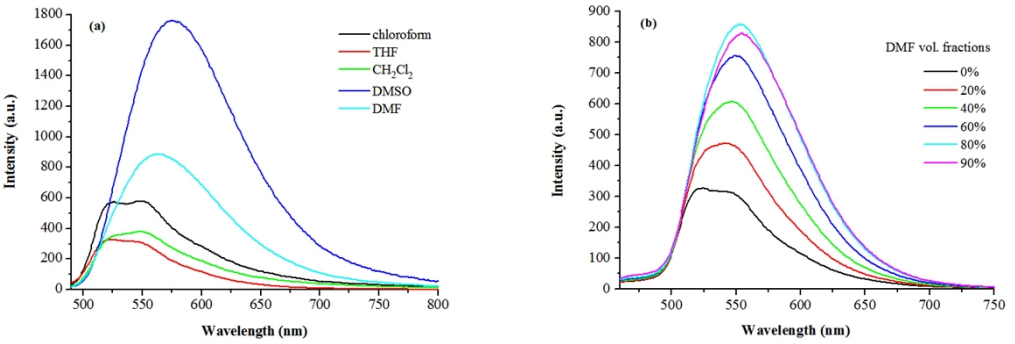


Fig. S5 (a) Fluorescence spectra of **3a** (1×10^{-5} mol/L) in various solvents. (b) Fluorescence spectra of **3a** (1×10^{-5} mol/L) in THF/DMF mixtures with different DMF volume fractions.

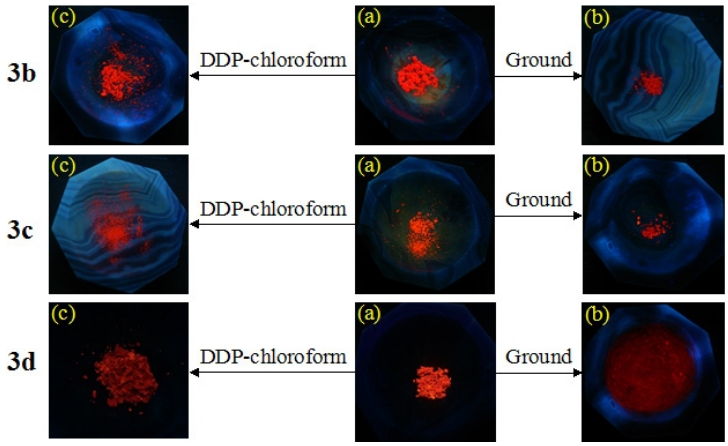


Fig. S6 Fluorescence images of **3b**–**3d** solid samples taken under a 365-nm UV lamp: (a) as-synthesized samples; (b) ground samples; (c) DDP-chloroform samples.

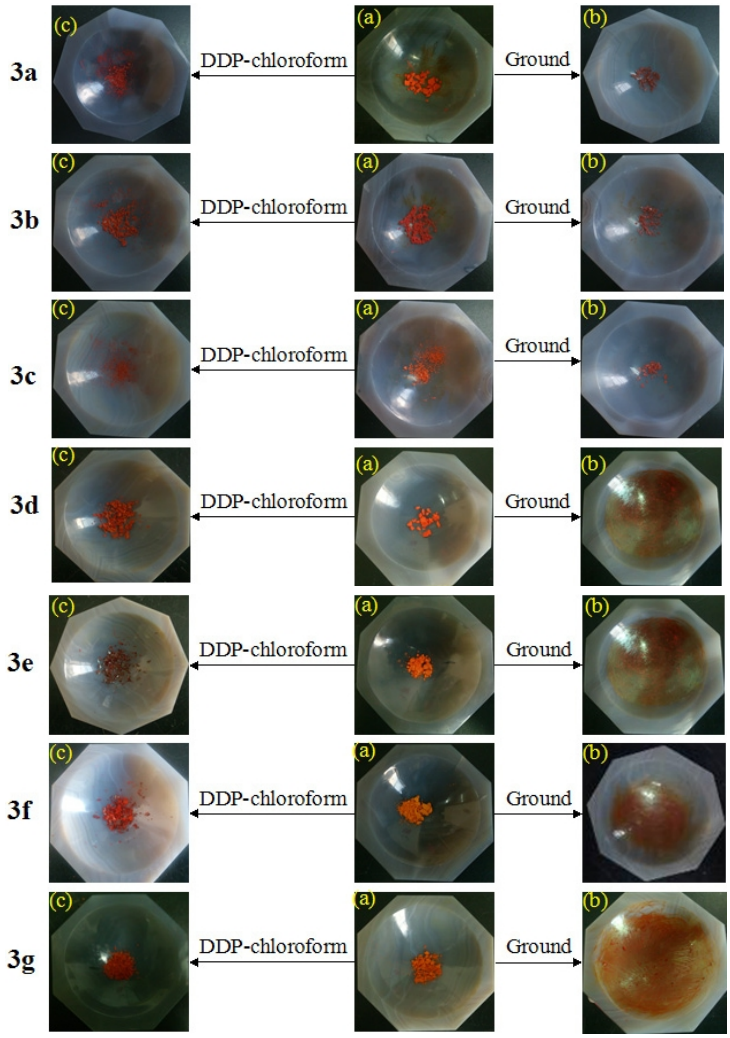


Fig. S7 Images of **3a-3g** solid samples taken under natural light: (a) as-synthesized samples; (b) ground samples; (c) DDP-chloroform samples.

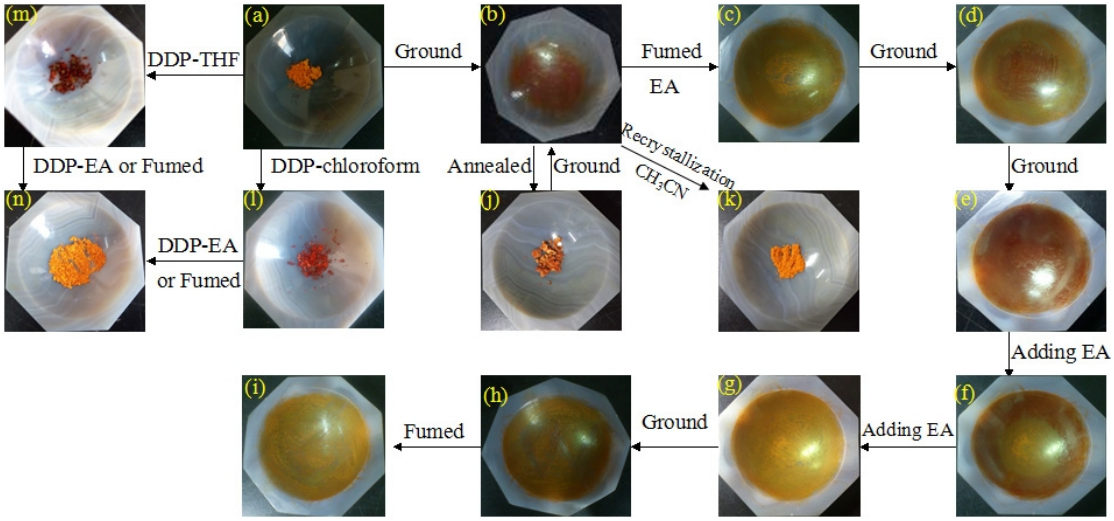


Fig. S8 Fluorescence images of **3f** solid samples taken under natural light: (a) as-synthesized samples; (b) ground samples; (c) fumed samples; (d) the central part of fumed samples was ground; (e) all fumed samples were ground; (f) several drops of EA were dropped onto the ground samples; (g) all ground samples were soaked with EA; (h) and (i) **3f** is used to write "W" with a metal spatula and then fumed using EA; (j) annealed samples; (k) recrystallized samples using CH_3CN as a solvent; (l) DDP-chloroform samples; (m) DDP-THF samples; (n) DDP-EA samples or fumed samples using EA.

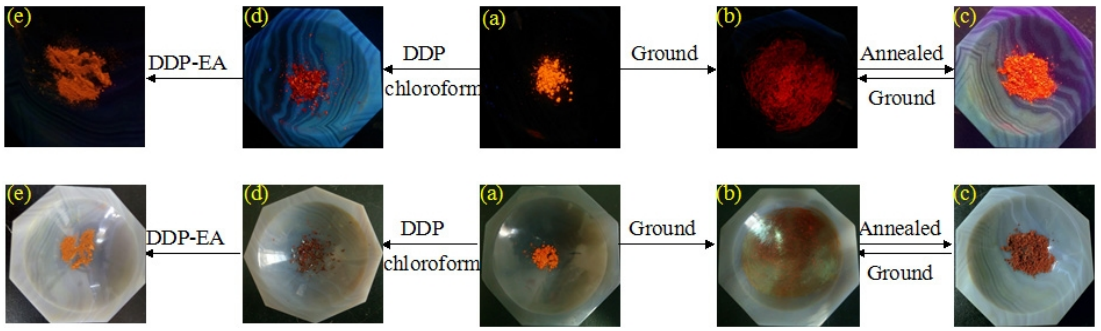


Fig. S9 Fluorescence images of **3e** solid samples taken under a 365 nm UV lamp (top) and natural light (bottom), respectively: (a) as-synthesized samples; (b) ground samples; (c) annealed samples; (d) DDP-chloroform samples; (e) DDP-EA samples.

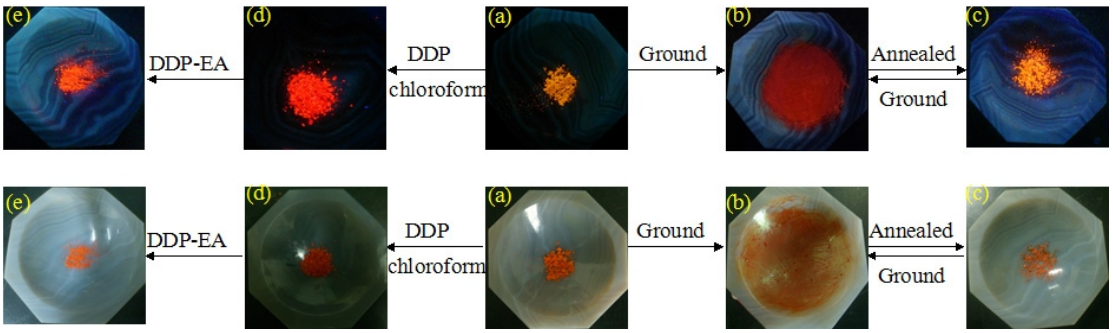


Fig. S10 Fluorescence images of **3g** solid samples taken under a 365-nm UV lamp (top) and natural light (bottom), respectively: (a) as-synthesized samples; (b) ground samples; (c) annealed samples; (d) DDP-chloroform samples; (e) DDP-EA samples.

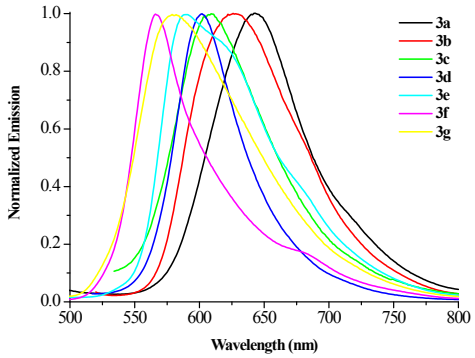


Fig. S11 Fluorescence spectra of as-synthesized **3a-3g** solids.

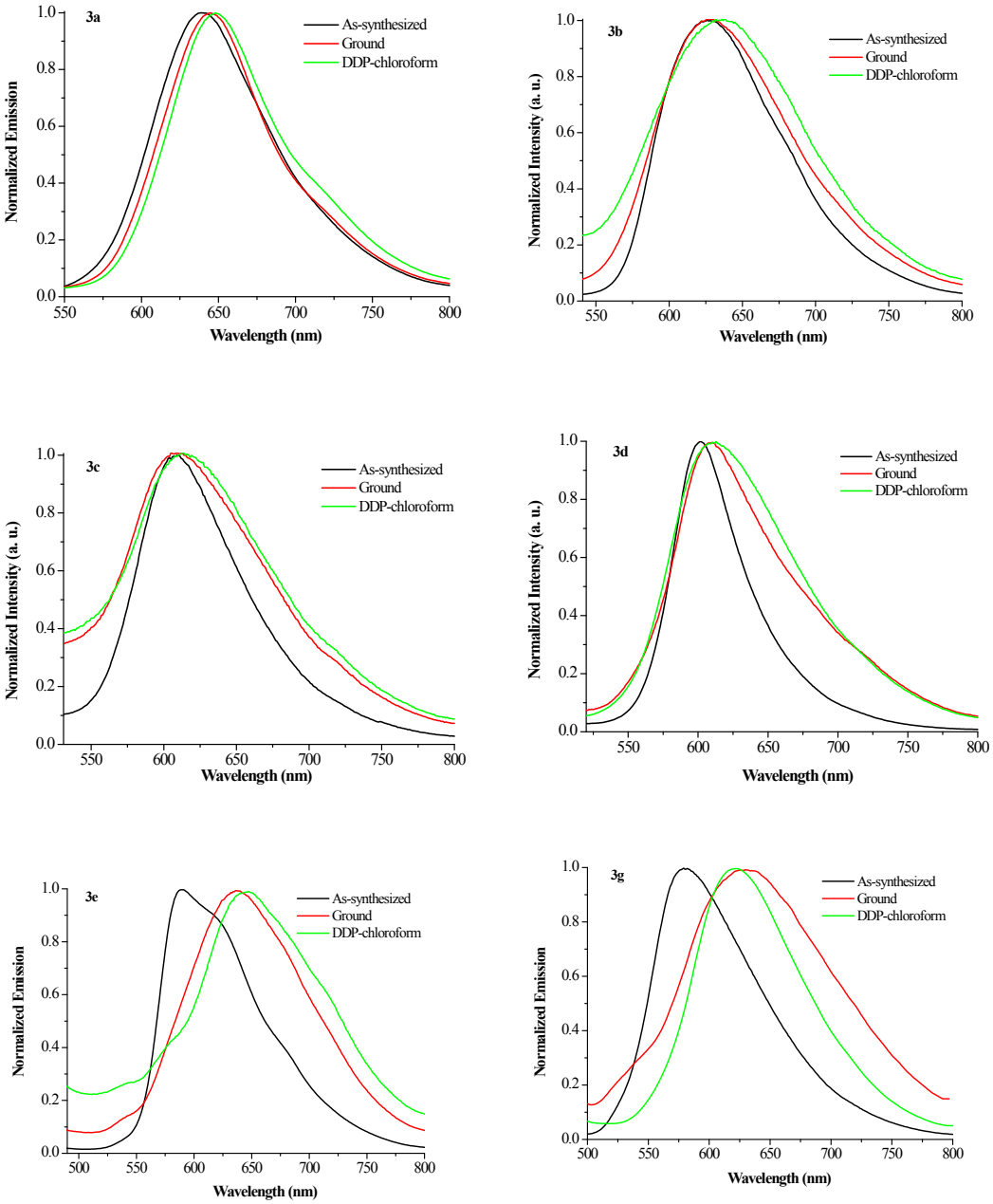


Fig. S12 Fluorescence spectra of **3a-3e** and **3g** solid samples under different conditions.

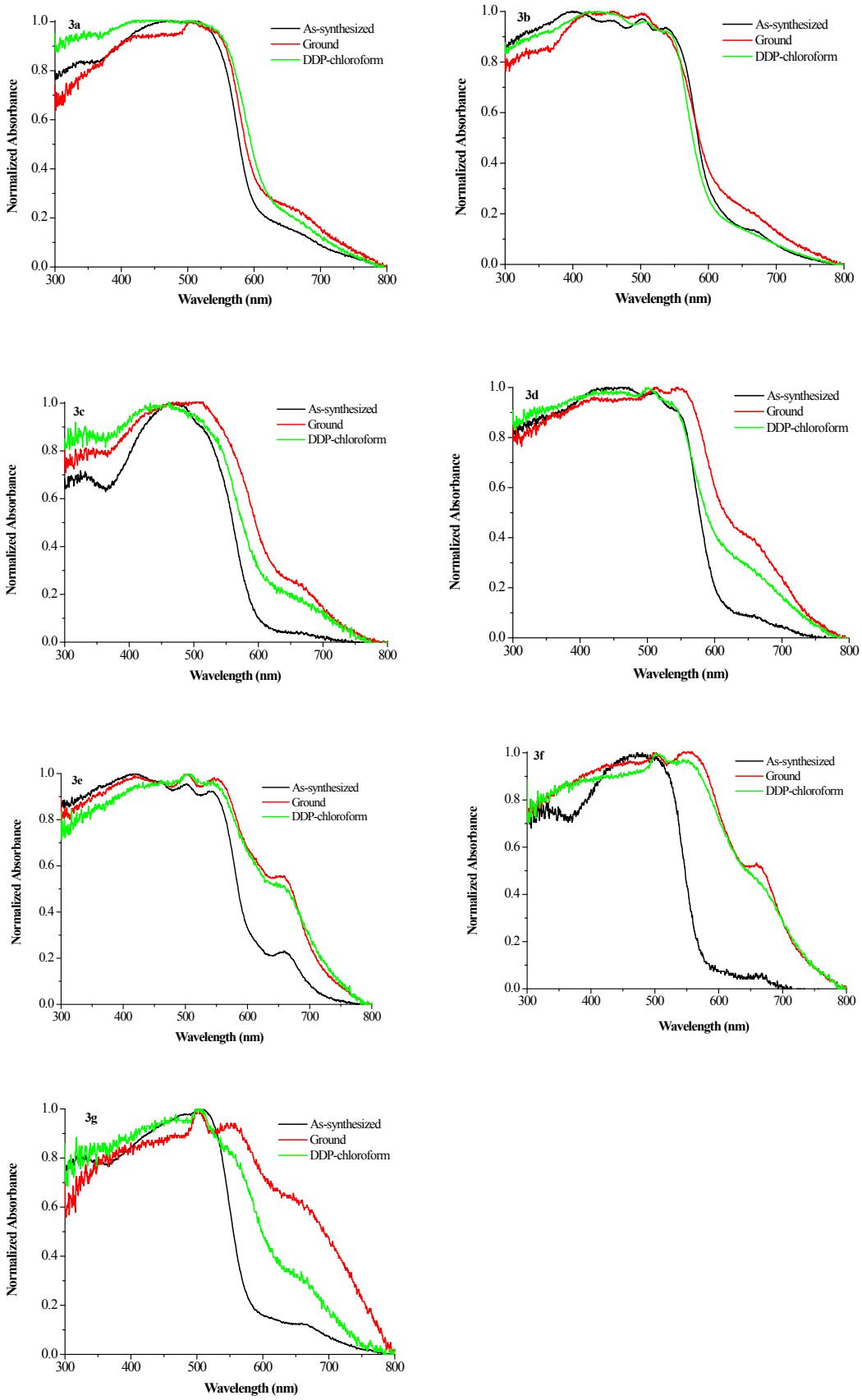


Fig. S13 UV-vis absorption spectra of **3a-3g** solid samples under different conditions.

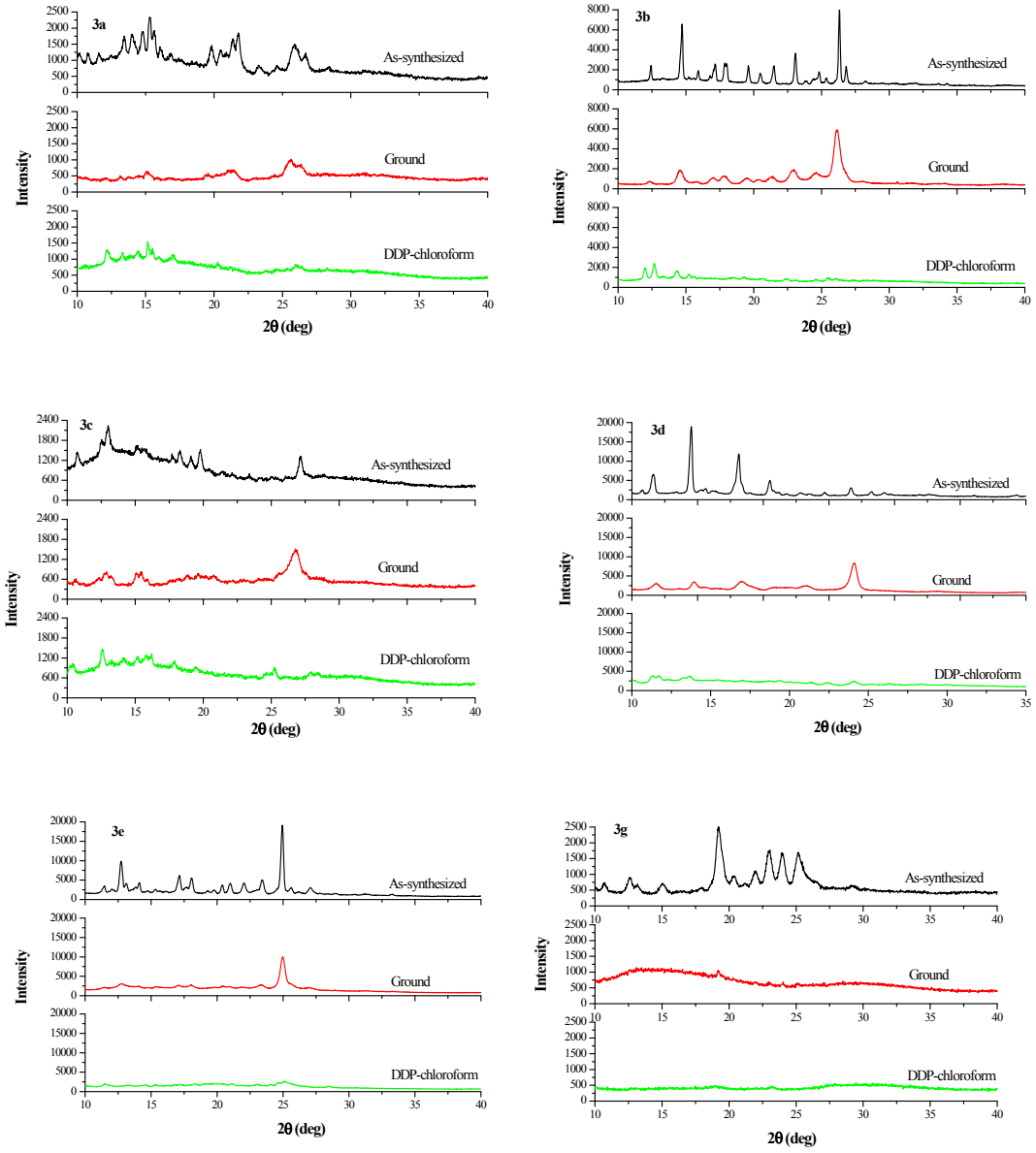


Fig. S14 XRD curves of **3a-3e** and **3f** solid samples under different conditions.

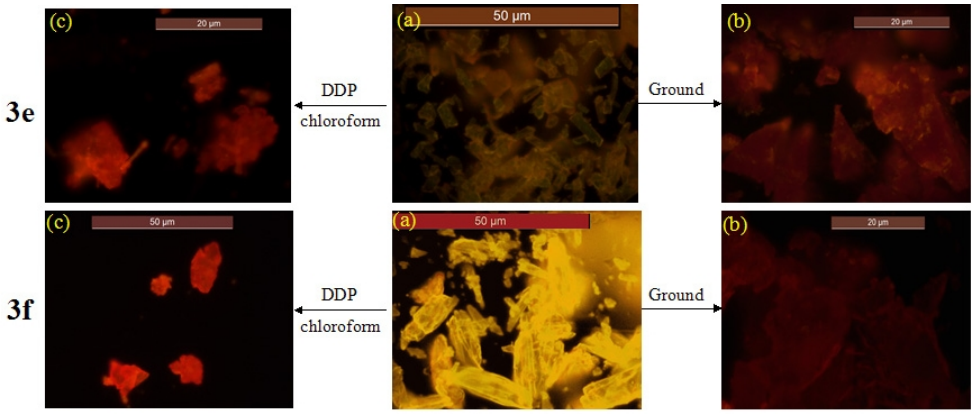


Fig. S15 The fluorescence microscope image of **3e** (top) and **3f** (bottom): (a) as-synthesized samples; (b) ground samples; (c) DDP-chloroform samples.

Table S2 Fluorescence decay parameters[a] and fluorescence quantum yields (Φ_F) of IDMP derivatives in the solid state.

Sample	type	τ_1 (ns)	τ_2 (ns)	A_1	A_2	<τ> (ns)	Φ_F[b]
3a	As-synthesized	0.36	1.92	0.74	0.26	1.40	2.5%
	Ground	0.44	2.59	0.72	0.28	1.07	n.d.[c]
	DDP-chloroform	0.59	2.30	0.59	0.41	1.07	n.d.
3b	As-synthesized	0.33	2.35	0.18	0.82	1.99	4.3%
	Ground	0.46	1.85	0.42	0.58	1.27	n.d.
	DDP-chloroform	0.73	2.43	0.57	0.43	1.46	n.d.
3c	As-synthesized	0.48	1.90	0.75	0.25	0.84	2.7%
	Ground	0.28	1.54	0.62	0.38	0.76	n.d.
	DDP-chloroform	0.15	1.49	0.54	0.45	0.75	n.d.
3d	As-synthesized	0.74	2.22	0.89	0.11	0.90	5.9%
	Ground	0.43	1.62	0.50	0.50	1.03	n.d.
	DDP-chloroform	0.48	1.99	0.70	0.30	0.93	n.d.
3e	As-synthesized	0.09	1.68	0.84	0.16	0.34	7.1%
	Ground	0.42	2.30	0.52	0.48	1.32	3.7%
	DDP-chloroform	0.29	1.82	0.56	0.44	0.96	1.7%
3f	As-synthesized	0.12	0.94	0.81	0.19	0.28	3.9%
	Ground	0.22	1.88	0.68	0.32	0.75	2.8%
	DDP-chloroform	0.39	2.38	0.51	0.49	1.37	2.7%
3g	As-synthesized	0.33	1.76	0.85	0.15	0.54	4.0%
	Ground	0.29	2.06	0.57	0.43	1.05	2.3%
	DDP-chloroform	0.59	2.12	0.54	0.46	1.29	2.5%

[a]Determined from $I = A_1\exp(-t/\tau_1)+A_2\exp(-t/\tau_2)$, where τ_1 and τ_2 are the lifetimes of the shorter- and longer-lived species, and A_1 and A_2 are their respective amplitudes, respectively. The weighted mean lifetime <τ> was calculated by the following equation: $\langle\tau\rangle = (A_1\tau_1+A_2\tau_2)/(A_1+A_2)$. [b]Solid-state emission quantum yields (ΦF) were determined by a FluoroMax-4 (Horiba Jobin Yvon) fluorometer equipped with an integrated sphere. [c]n.d. = no detection.

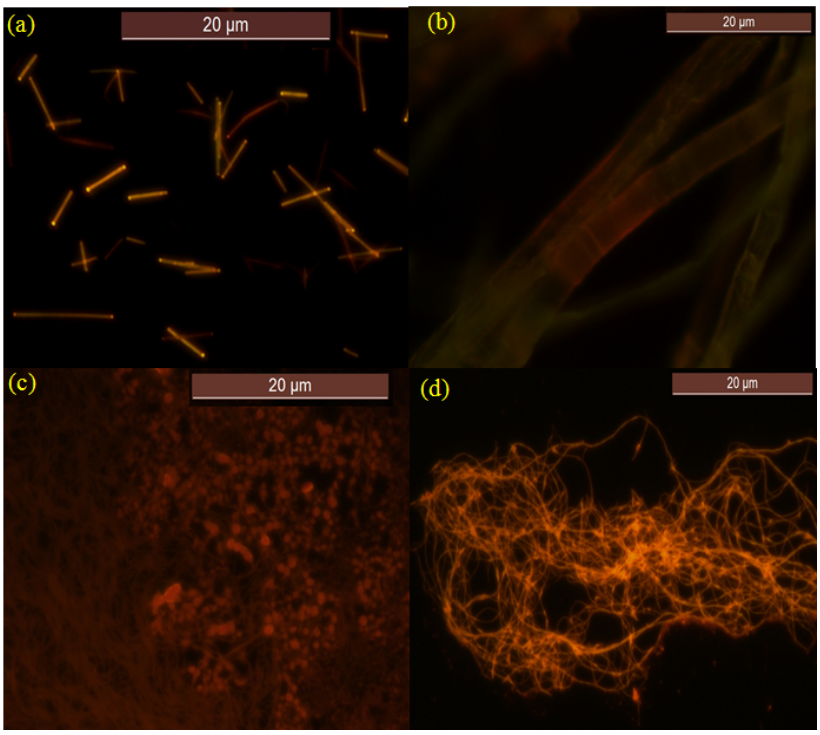


Fig. S16 The fluorescence microscope images of **3d, 3e** and **3g** in THF-water mixture (1×10^{-5} mol/L) at different f_w values: (a) **3d**, f_w = 70%; (b) **3e**, f_w = 70%; (c) **3g**, f_w = 30%; (d) **3g**, f_w = 70%.

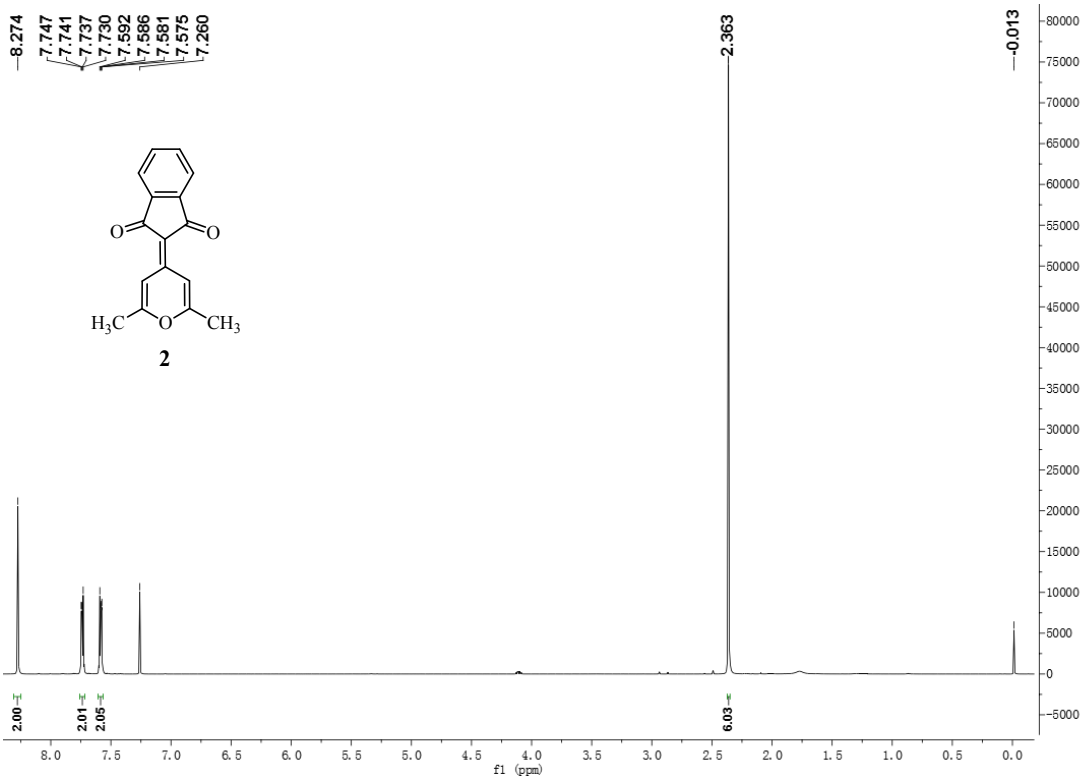


Fig. S17 ^{1}H NMR of compound **2** ($CDCl_3$, 500 MHz).

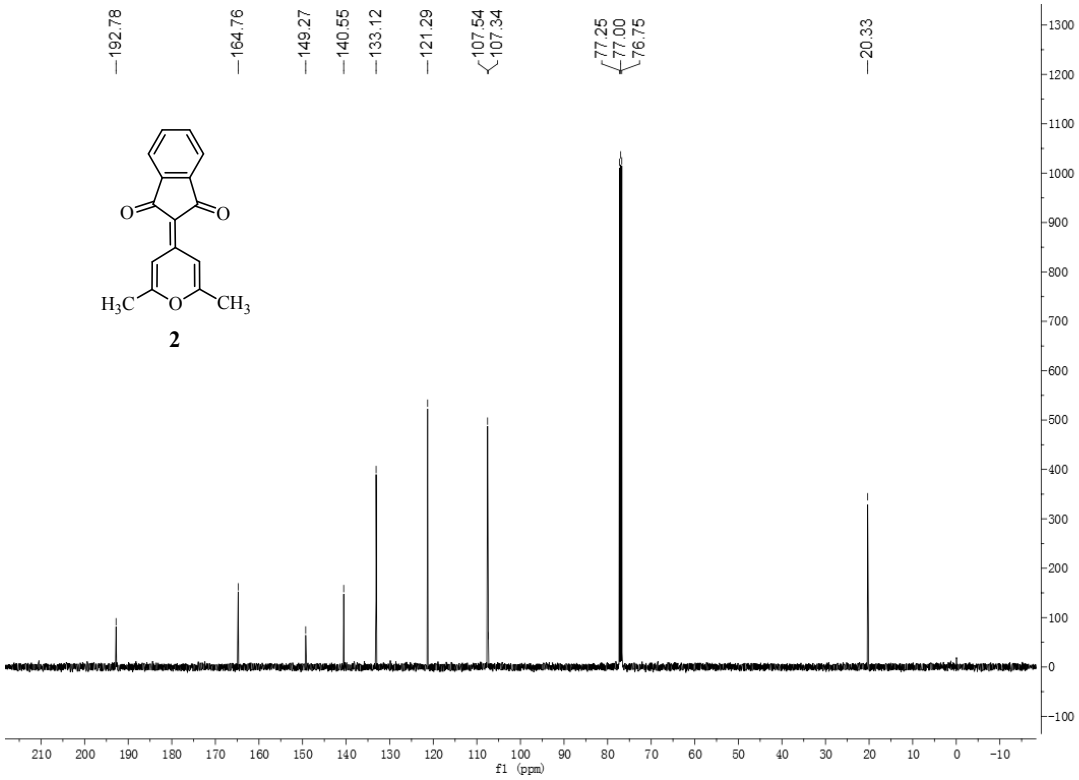


Fig. S18 ^{13}C NMR of compound **2** ($CDCl_3$, 125 MHz).

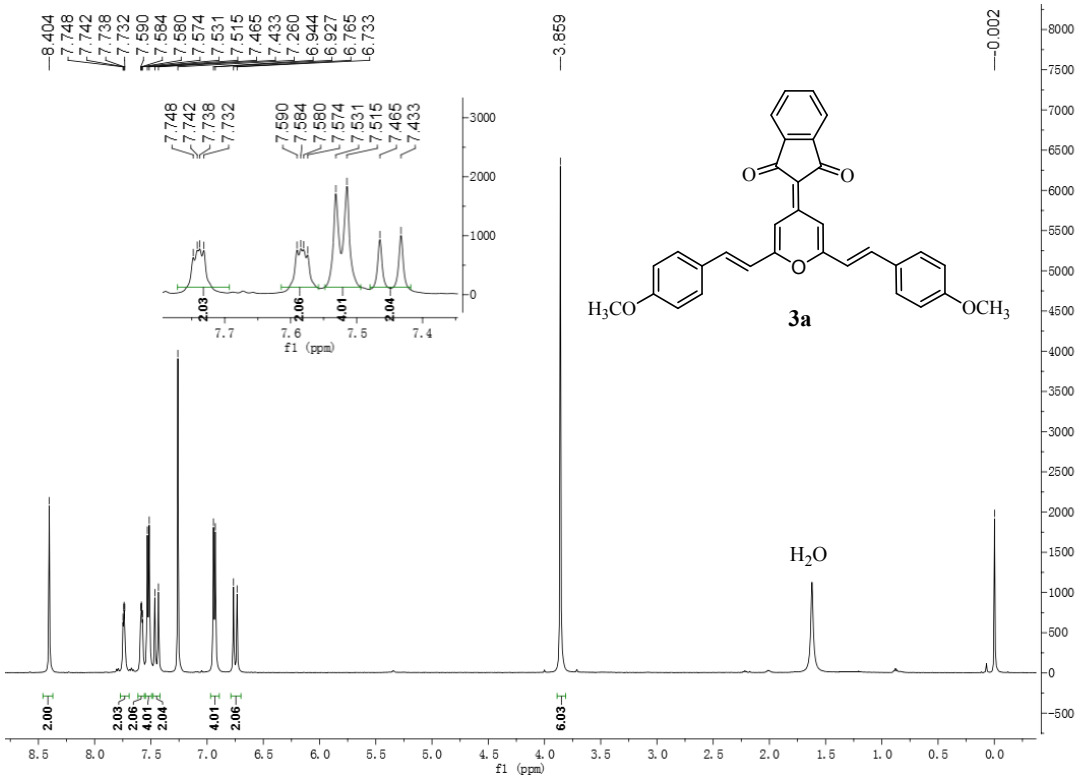


Fig. S19 ^{1}H NMR of **3a** ($CDCl_3$, 500 MHz).

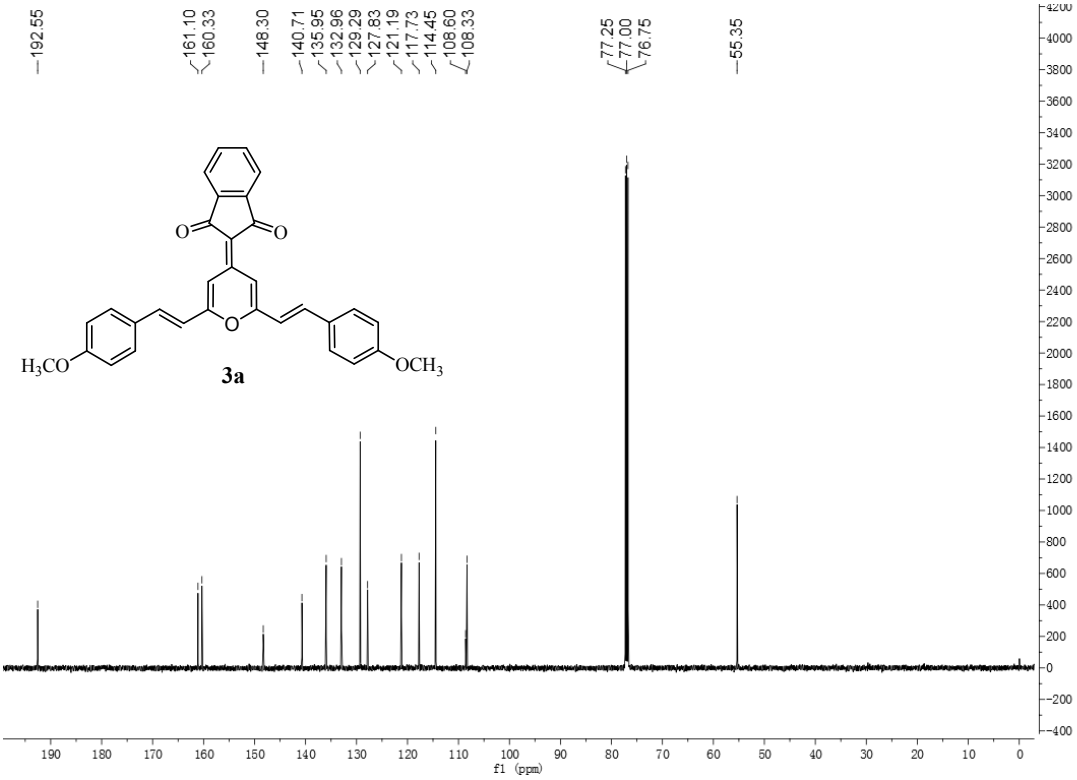


Fig. S20 ^{13}C NMR of **3a** ($CDCl_3$, 125 MHz).

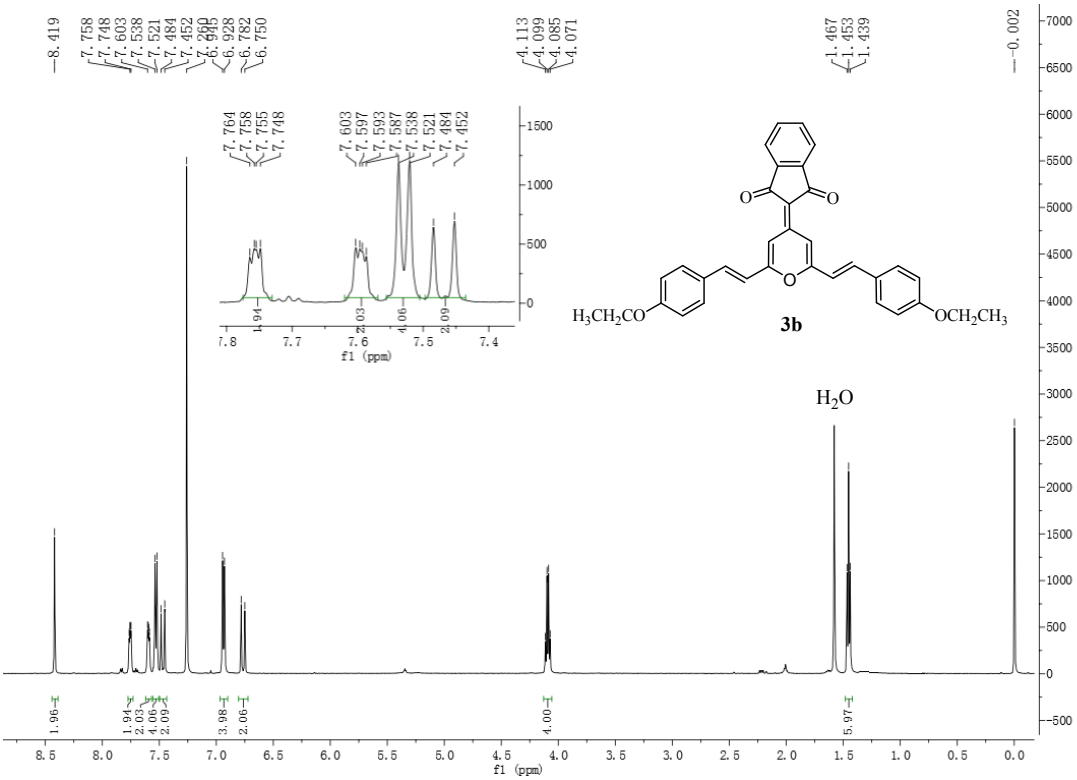


Fig. S21 ^{1}H NMR of **3b** ($CDCl_3$, 500 MHz).

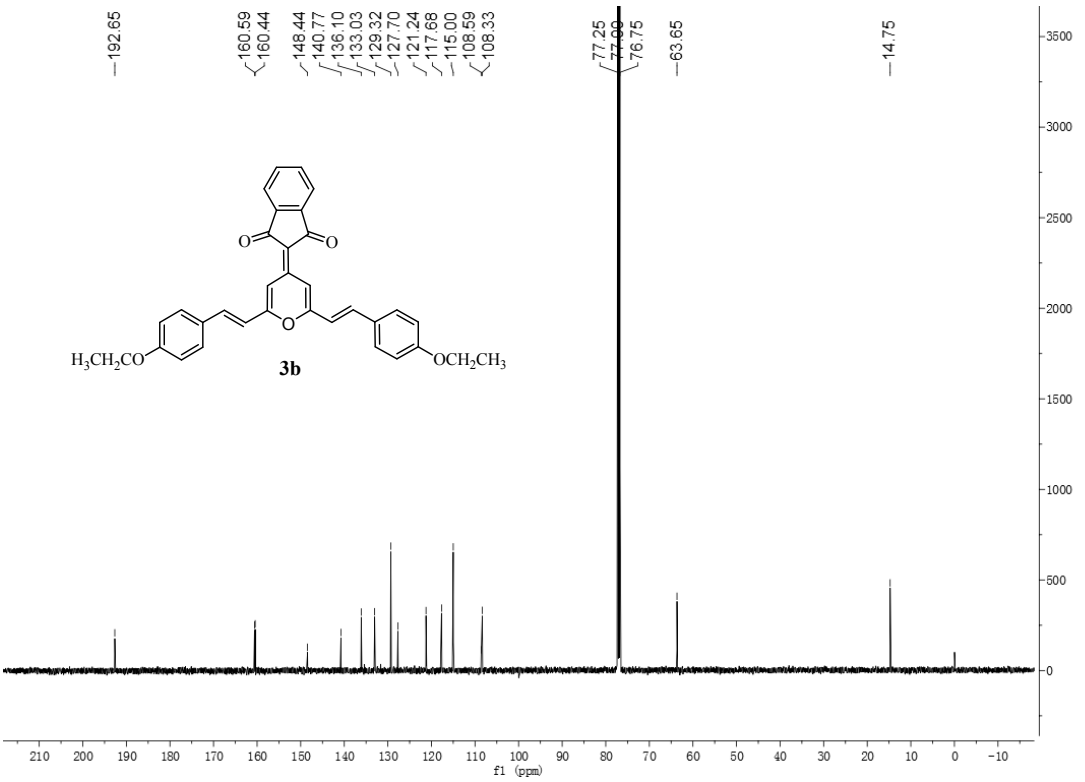


Fig. S22 ^{13}C NMR of **3b** ($CDCl_3$, 125 MHz).

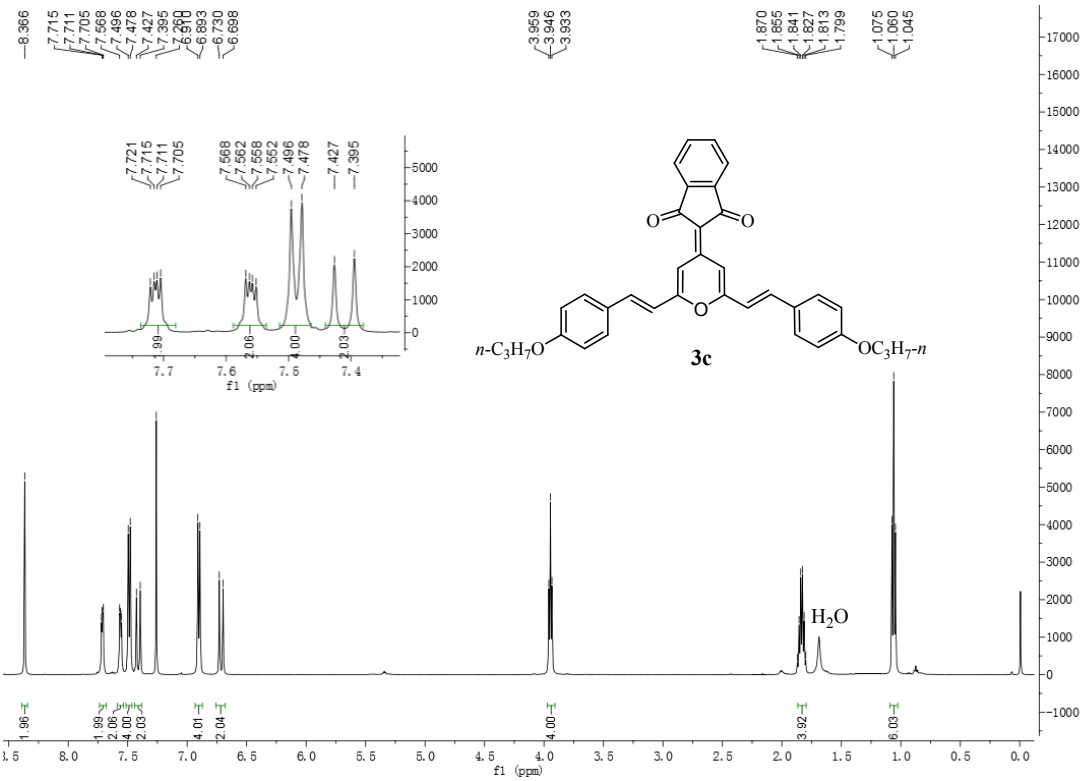


Fig. S23 ^{1}H NMR of **3c** ($CDCl_3$, 500 MHz).

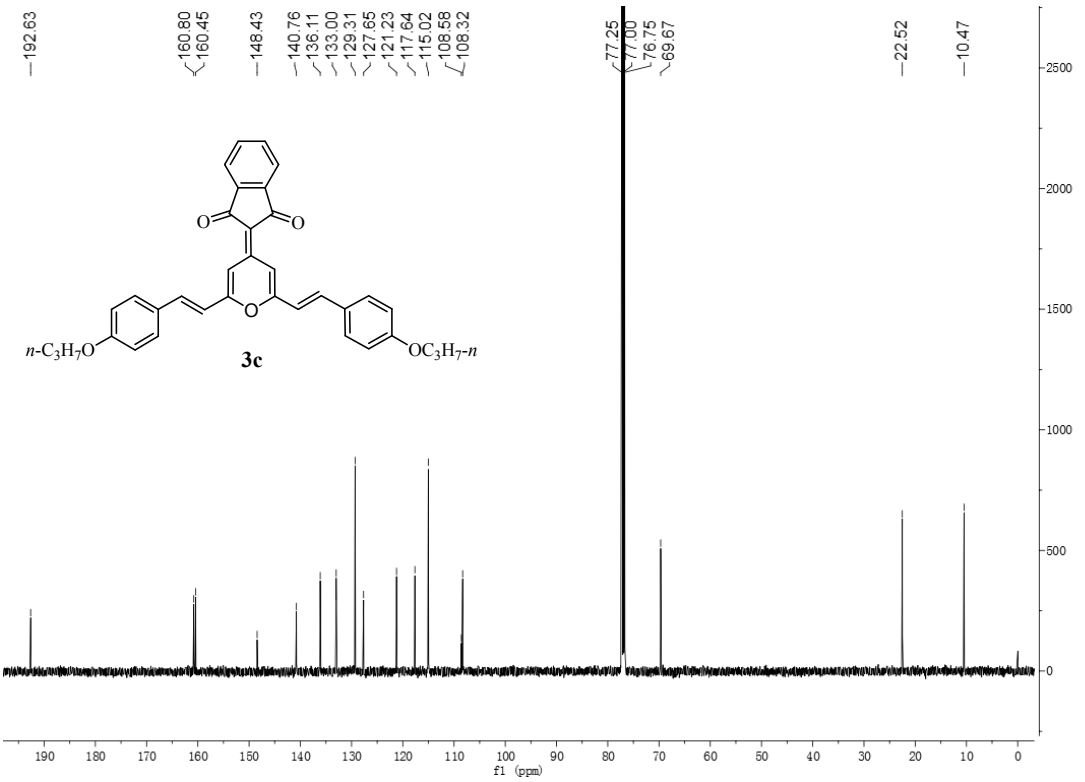


Fig. S24 ^{13}C NMR of **3c** ($CDCl_3$, 125 MHz).

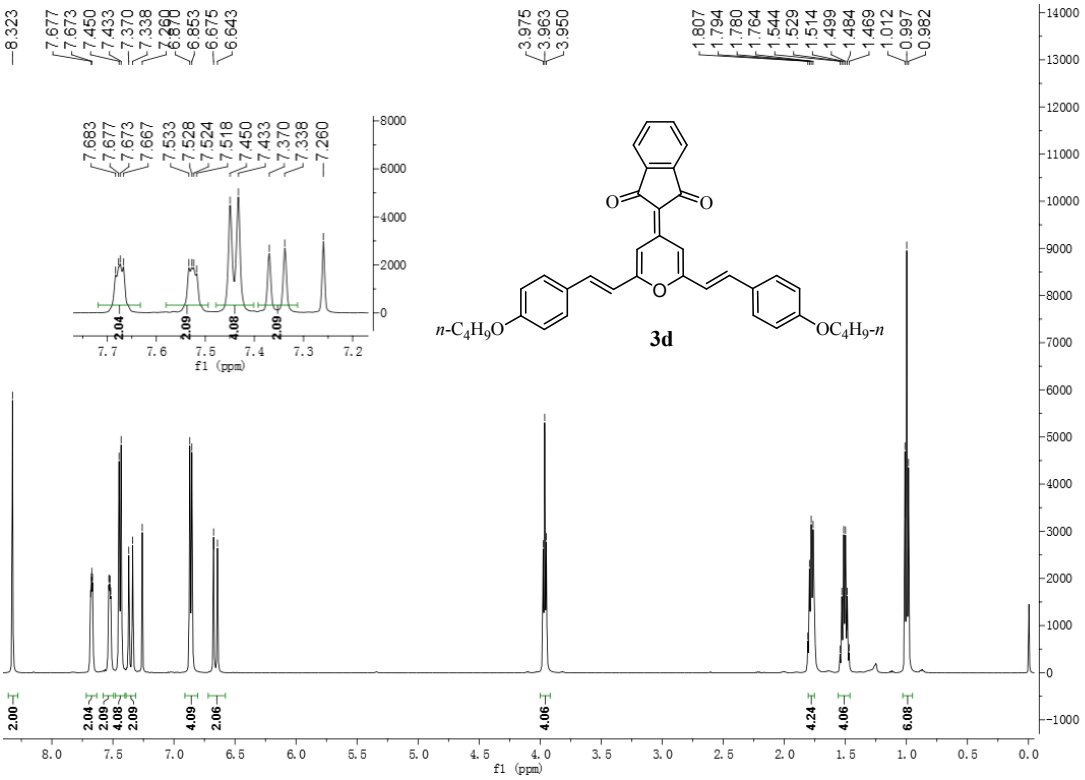


Fig. S25 ^{1}H NMR of **3d** ($CDCl_3$, 500 MHz).

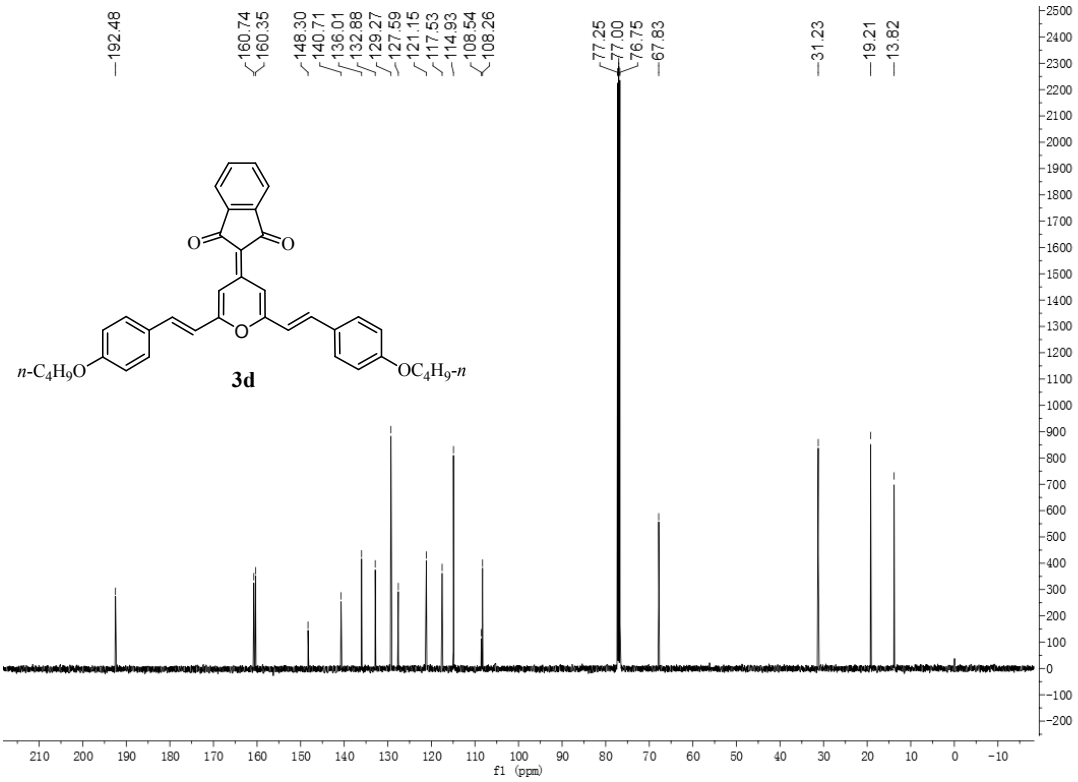


Fig. S26 ^{13}C NMR of **3d** ($CDCl_3$, 125 MHz).

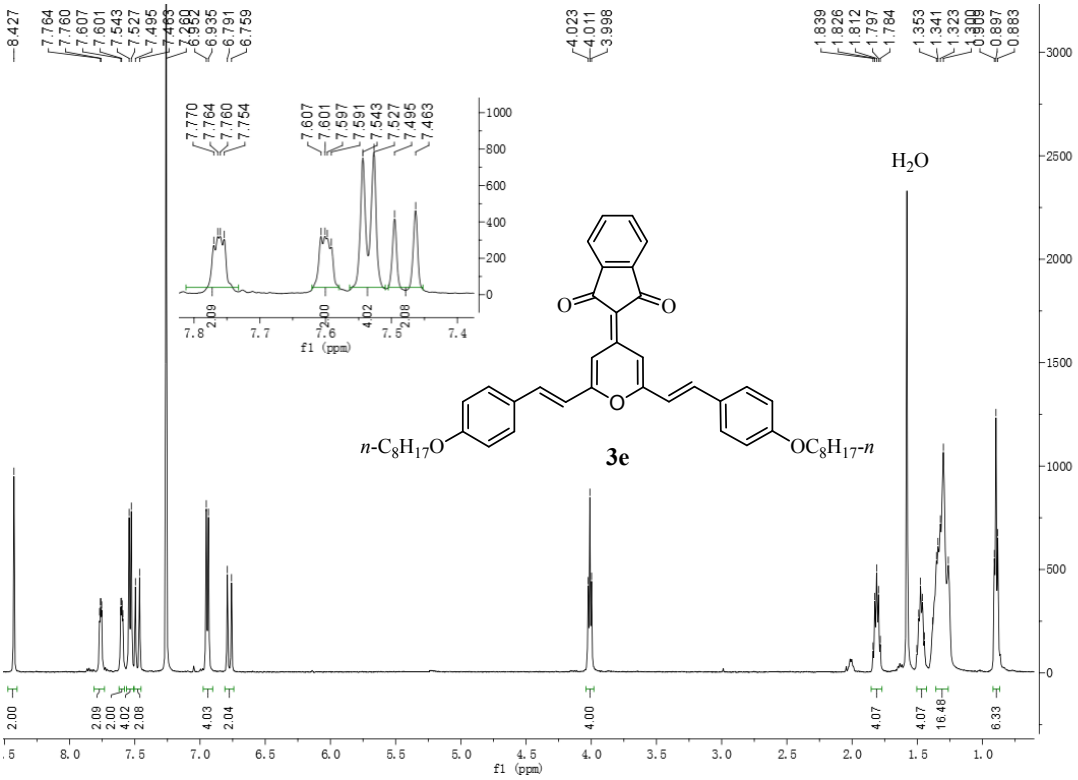


Fig. S27 ^{1}H NMR of **3e** ($CDCl_3$, 500 MHz).

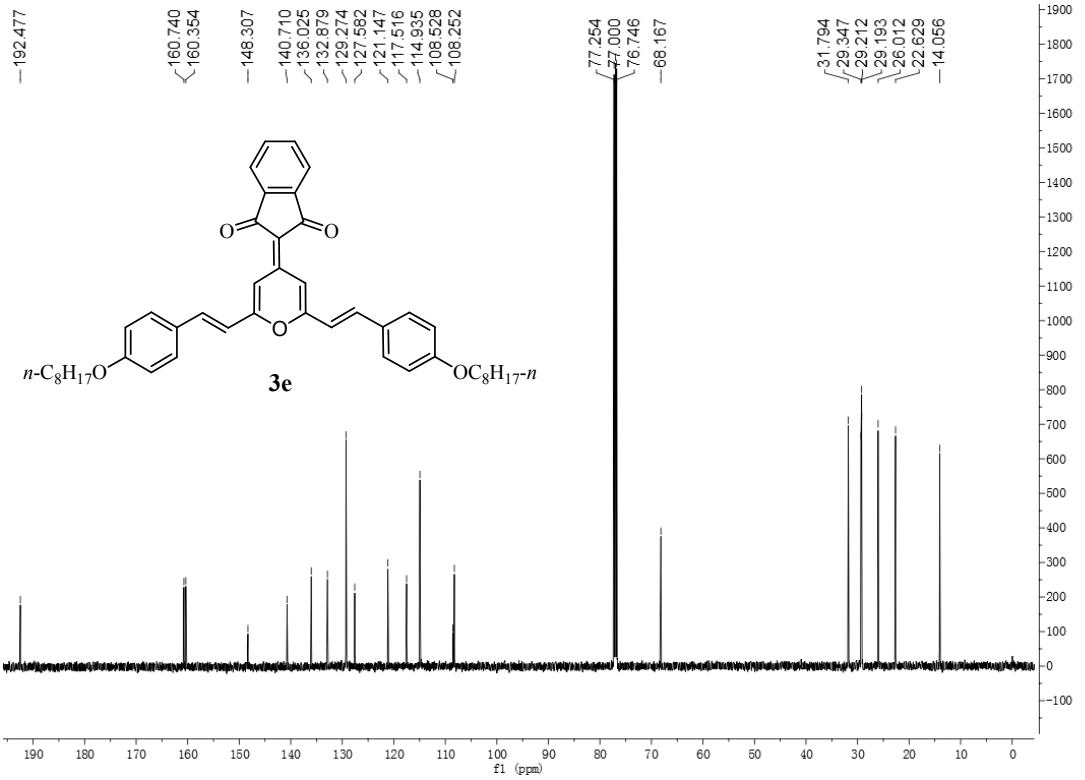


Fig. S28 ^{13}C NMR of **3e** ($CDCl_3$, 125 MHz).

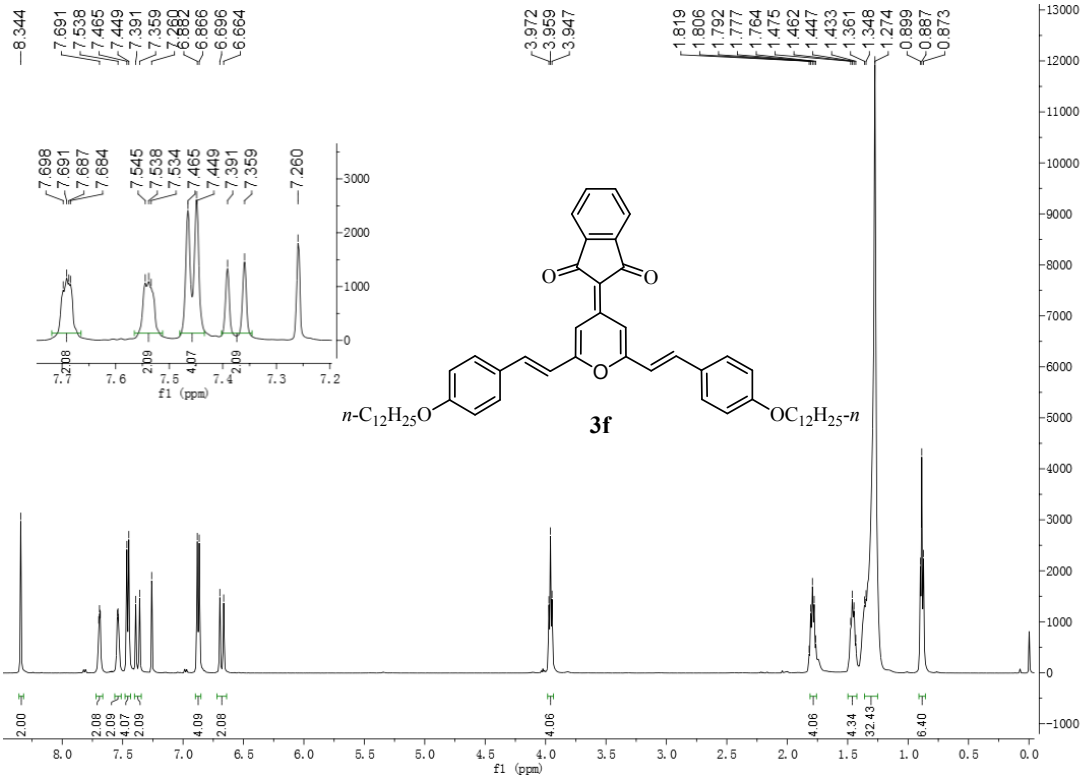


Fig. S29 ^{1}H NMR of **3f** ($CDCl_3$, 500 MHz).

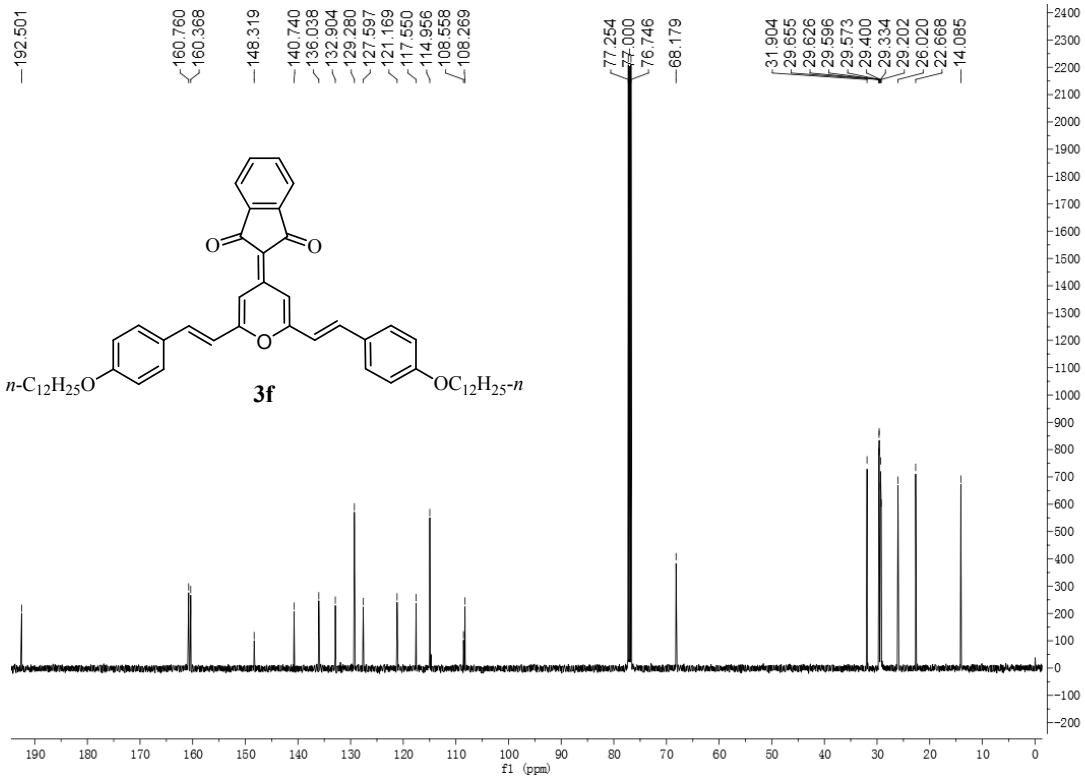


Fig. S30 ^{13}C NMR of **3f** ($CDCl_3$, 125 MHz).

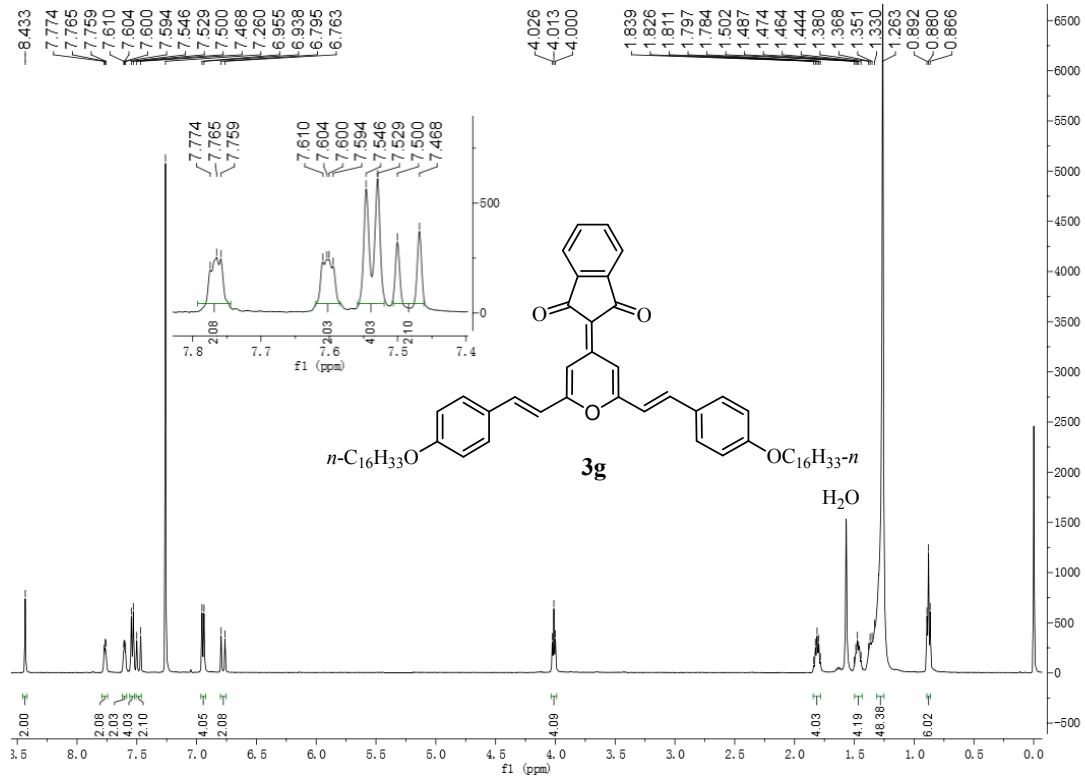


Fig. S31 ^{1}H NMR of **3g** ($CDCl_3$, 500 MHz).

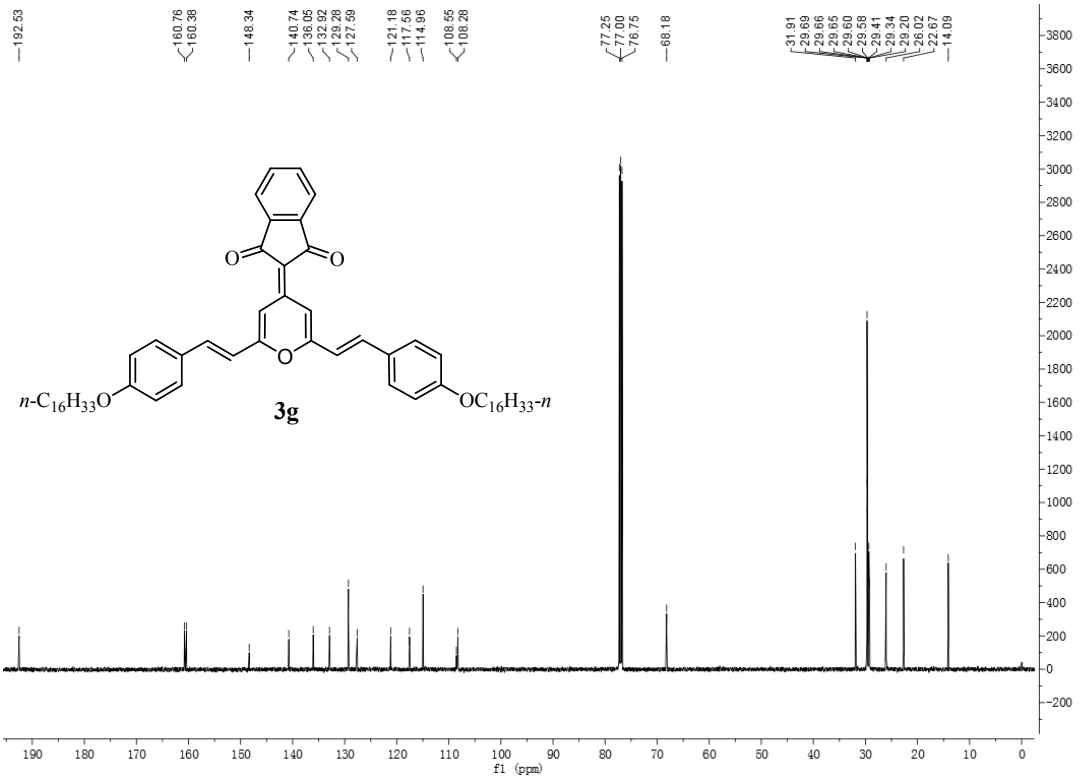


Fig. S32 ^{13}C NMR of **3g** ($CDCl_3$, 125 MHz).