Electronic Supplementary Material (ESI) for RSC Advances.

Supporting Information For:

High-contrast mechanochromism and polymorphism-dependent fluorescence of difluoroboron β-diketonate complexs based on the effects of AIEE and halogen

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Table S1 Photophysical data of 2a, 2b and 2c.(The emission wavelength was exited at maximum absorption)

	Solvent		λabs (nm)		λem (nm)
	Cyclohexane		351 408		520
	Toluene		359 414	C	586
2a	THF		359 415		564
	DCM		359 421		591
	DMSO	Toluene	367 422		607
	Cyclohexane		361 388		514
	Toluene		368		501
		C	398		580
2b	THF		365 421		570
	DCM		368 422		582
	DMSO		375 403		528
	Cyclohexane		361 402		516
	Toluene		368		495
		C	407		584
2c	THF		366 421		572
	DCM		366 421		591
	DMSO		376 418		525

Table S2 Different solid state emission data of 2a, 2b and 2c.(The emission wavelength was exited at 360 nm)

	Solid State	λem (nm)
2a	as synthesized	562
	grinding	582
	fuming	563
	heating	568
2b	as synthesized	547
	grinding	617
	fuming	554
	heating	565
2c	as synthesized	539
	grinding	598
	fuming	548
	heating	563

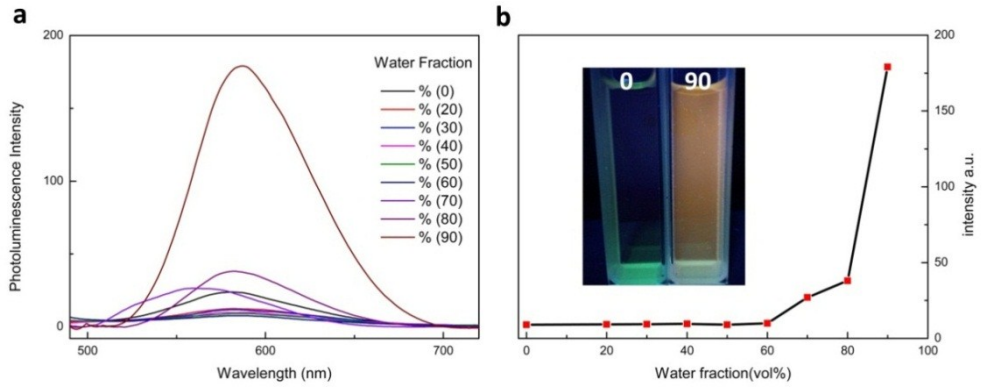

Figure S1 a) PL spectra of 2b in THF and THF/water mixtures. b) Plot of PL peak intensity vs. water fraction (f_w) of the aqueous mixture. Luminogen concentration: 1×10^{-5} mol/L; excitation wavelength: 420 nm. Inset: Solution of 2b in THF (f_w = 0%) and its suspension in a THF/water mixture with f_w = 90%; photographs taken under UV illumination.

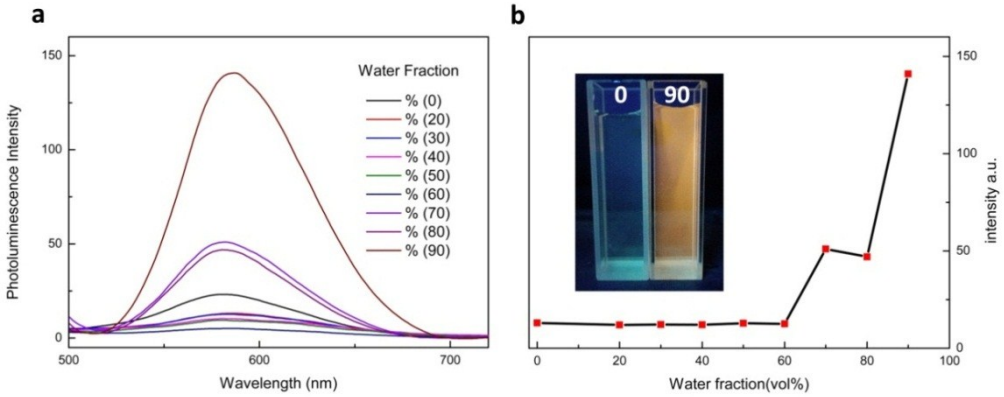

Figure S2 a) PL spectra of 2c in THF and THF/water mixtures. b) Plot of PL peak intensity vs. water fraction (f_w) of the aqueous mixture. Luminogen concentration: 1×10^{-5} mol/L; excitation wavelength: 420 nm. Inset: Solution of 2c in THF (f_w = 0%) and its suspension in a THF/water mixture with f_w = 90%; photographs taken under UV illumination.

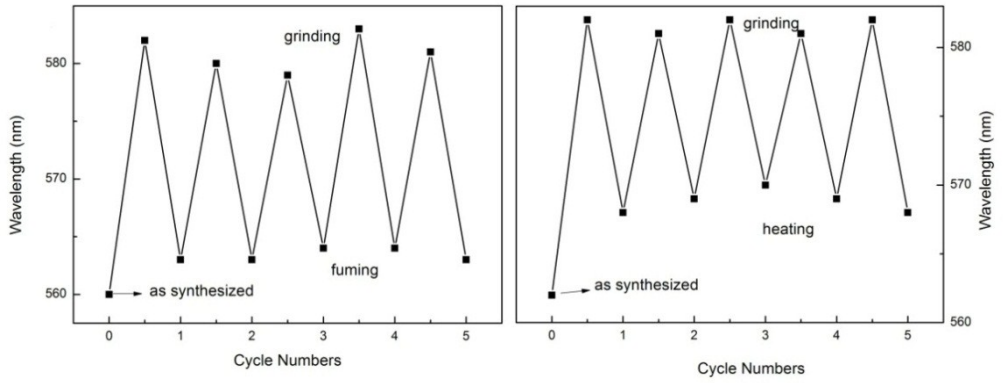

Figure S3 Maximum fluorescent emission of 2a upon treated by repeating grinding and fuming with DCM (left), or heating at 150 °C (right), respectively.

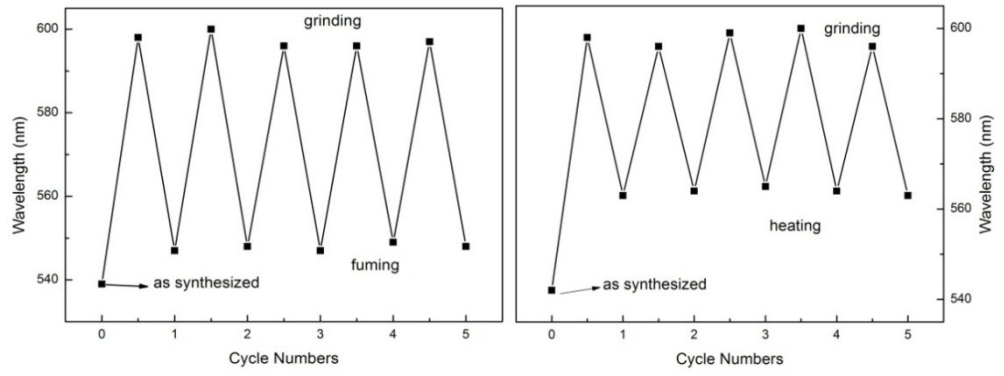

Figure S4 Maximum fluorescent emission of 2b upon treated by repeating grinding and fuming with DCM (left), or heating at 150 °C (right), respectively.

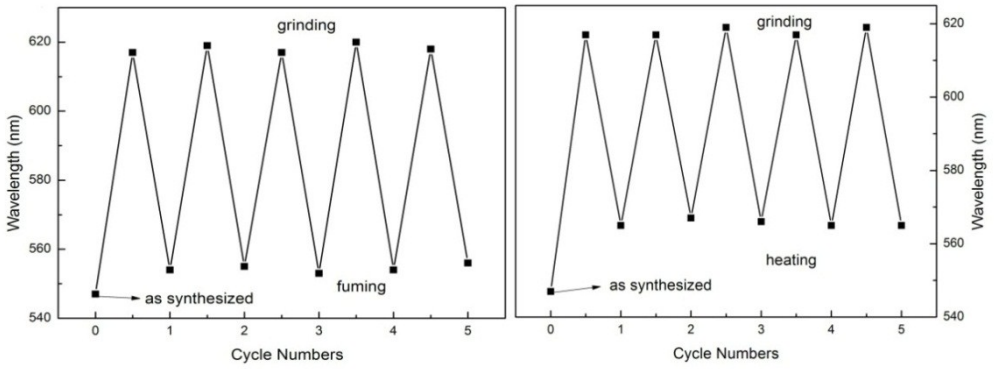

Figure S5 Maximum fluorescent emission of 2c upon treated by repeating grinding and fuming with DCM (left), or heating at 150 °C (right), respectively.

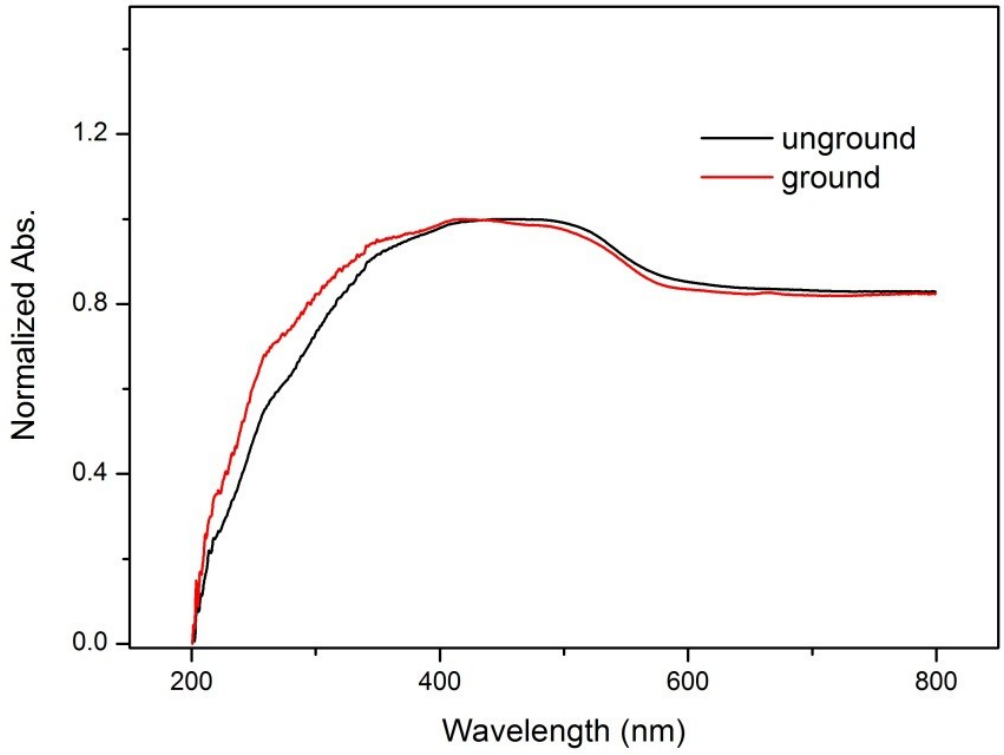

Figure S6 UV-visible curves of 2a in different solid state measured in a reflection mode.

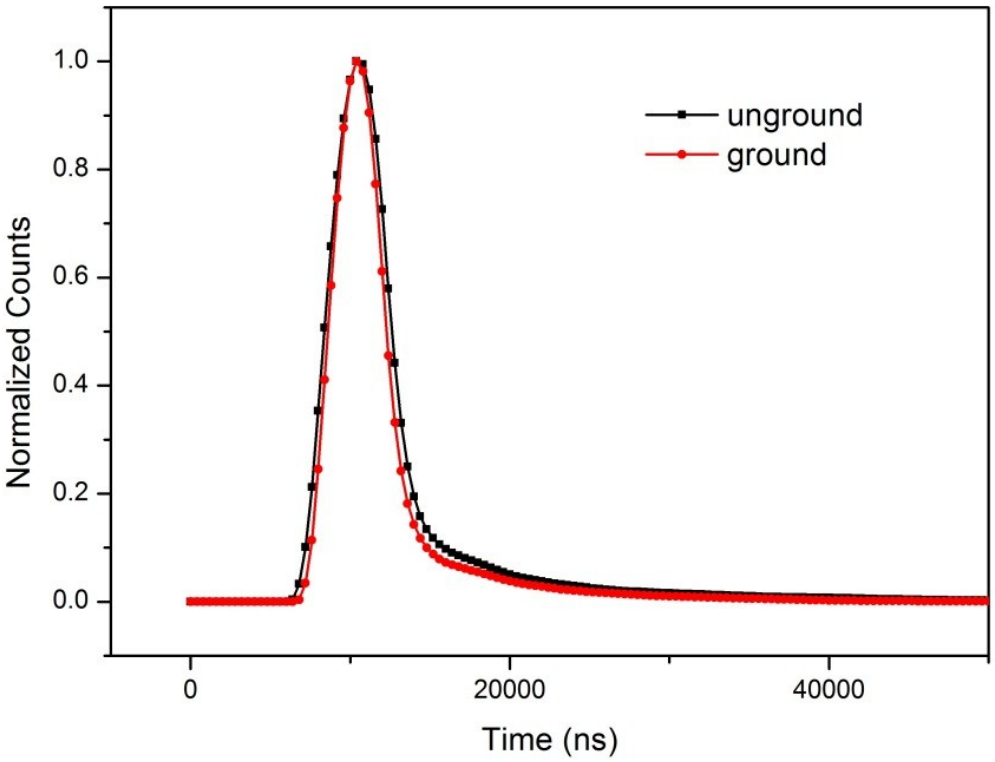

Figure S7 Time-resolved emission decay curves of the sample 2a.

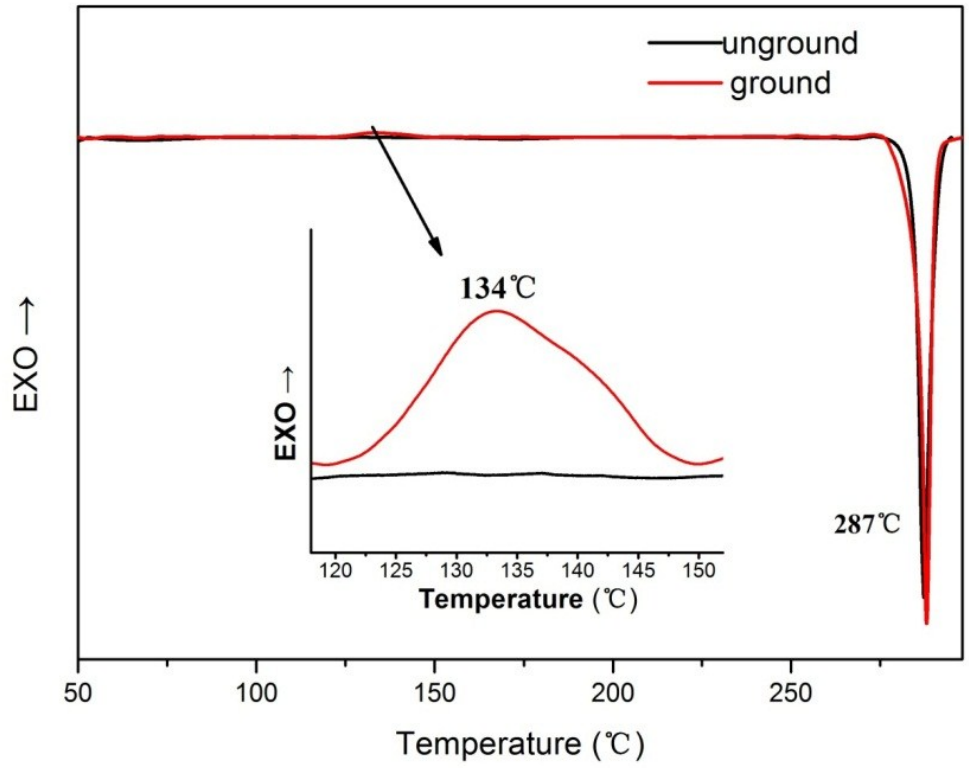

Figure S8 DSC thermograms of 2b in different state.

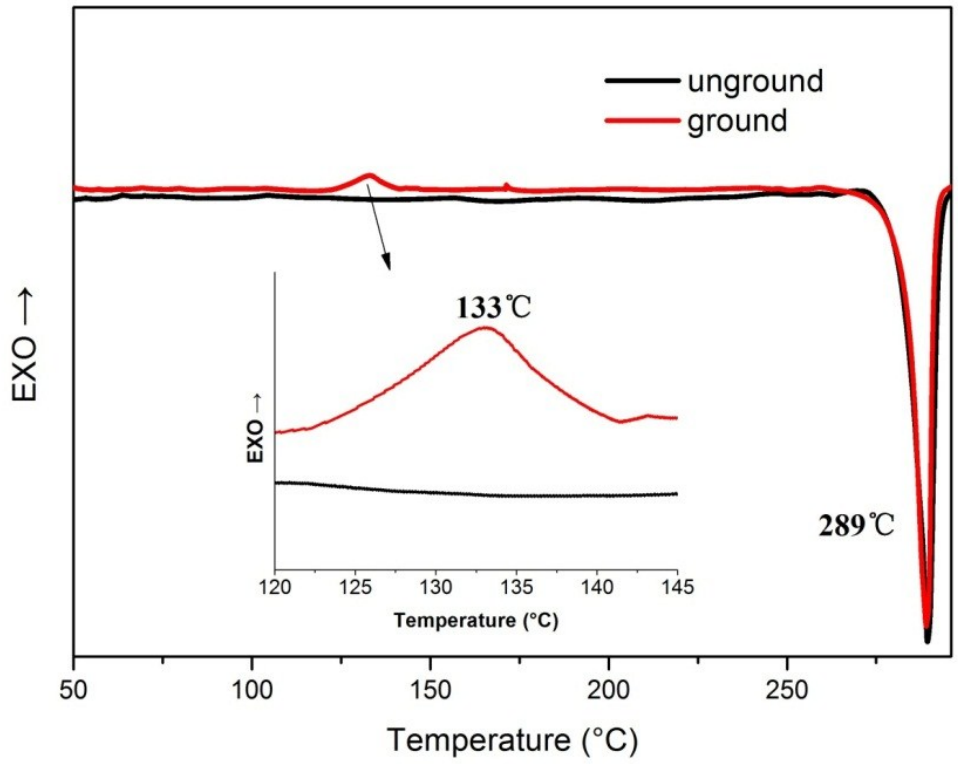

Figure S9 DSC thermograms of 2c in different state.

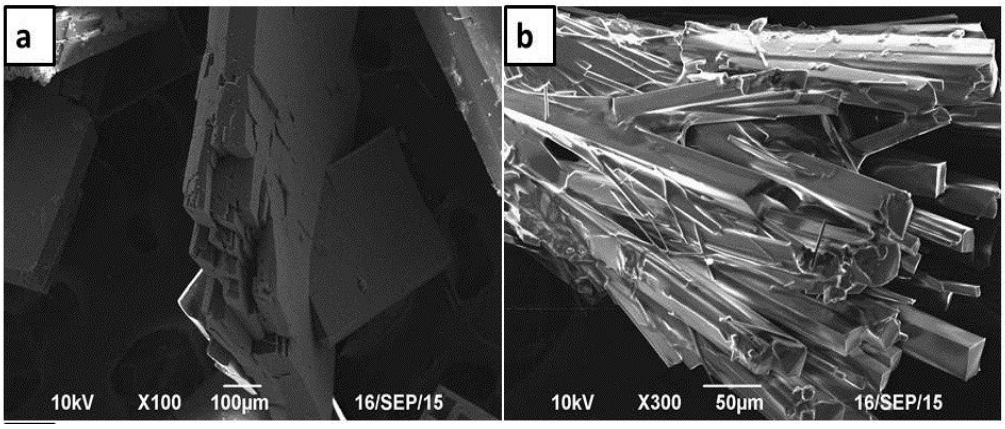

Figure S10 SEM images of (a) pointed-plate-like and (b) needlelike structures of 2c.

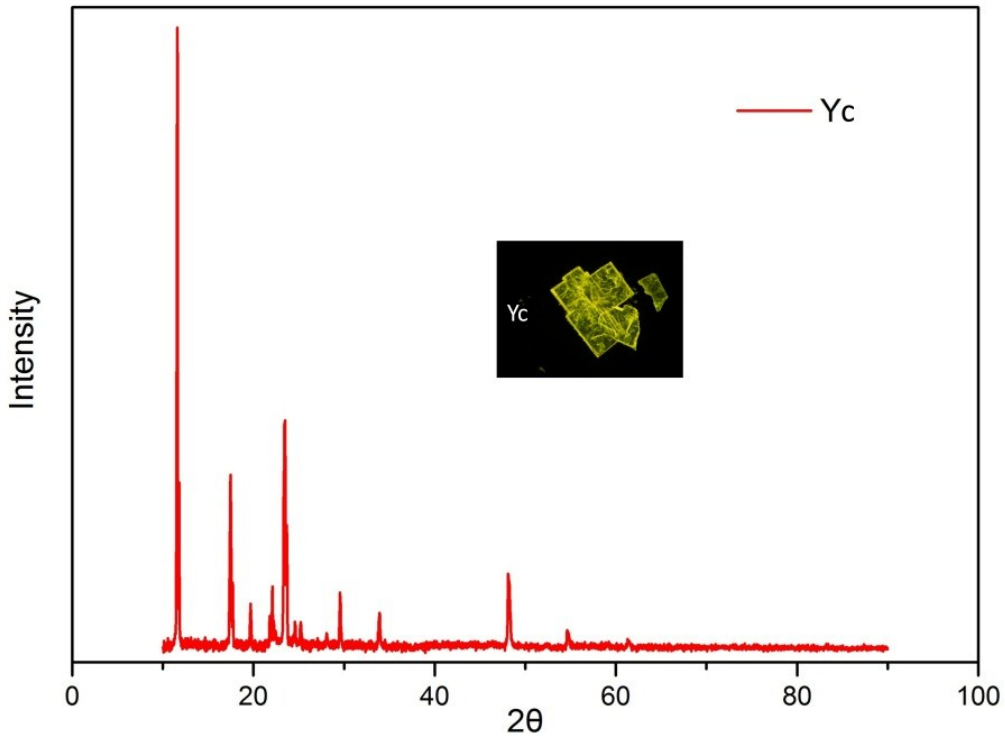

Figure S11 XRD patterns of plate-like structure of 2c, inset: fluorescence microscope photos of plate-like structure of 2c.

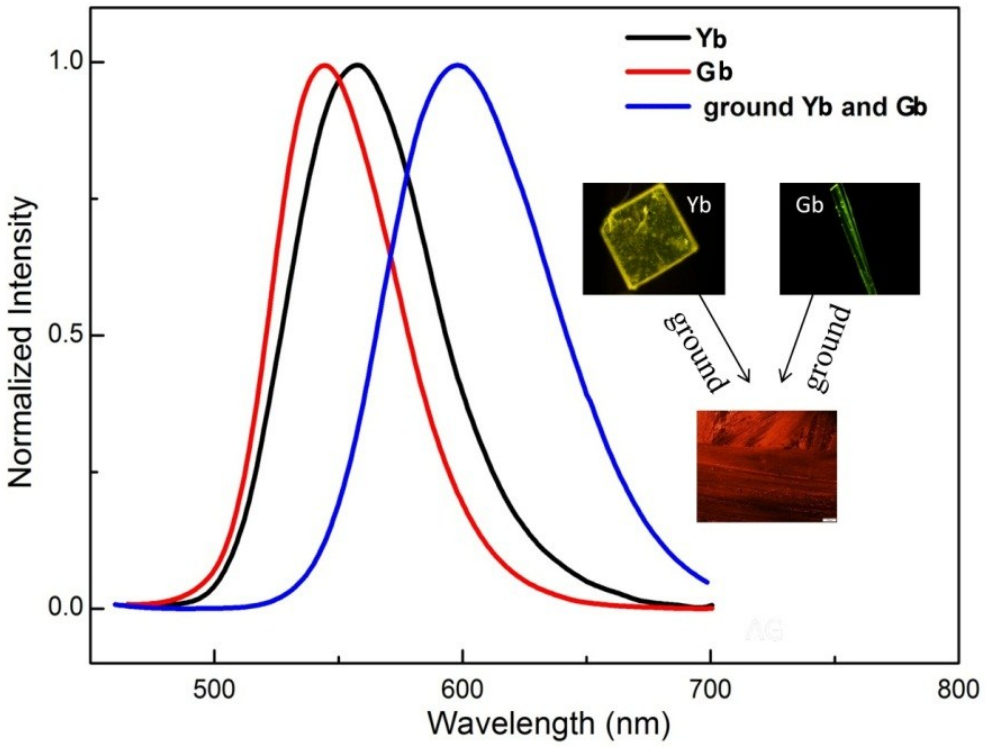

Figure S12 Fluorescence spectra of two different crystals structure of (Yb) pointed-plate-like, (Gb) needlelike structures and ground powder of 2b, inset: fluorescence microscope photos Yb, Gb and ground powder.

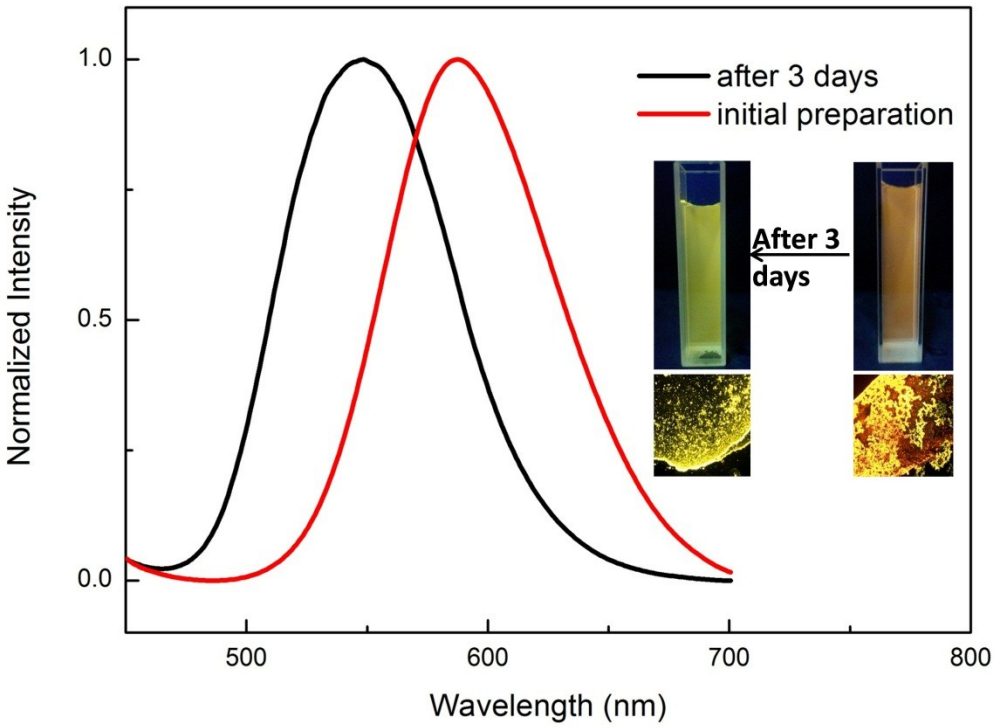

Figure S13 Fluorescence emission spectra of 2c in THF/water mixtures with f_w = 90% (concentration: 1×10^{-5} mol/L; excitation wavelength: 360 nm). Inset: photographs of suspension in a THF/water mixture with f_w = 90% taken under UV illumination (excitation wavelength: 360 nm). And corresponding Fluorescence microscope photos of the dry suspended particles (λ_{ex} = 405 nm).

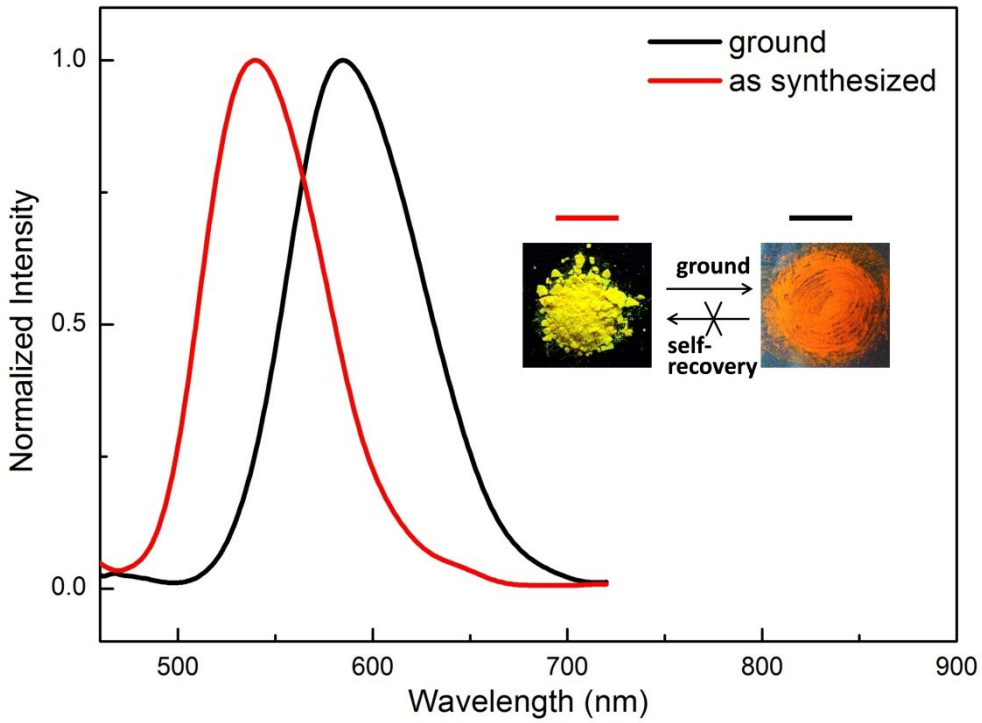

Figure S14 Fluorescence emission spectra of 2d in two different solid state (excitation wavelength: 360 nm). Inset: photographs of 2d in different solid state taken under UV illumination (excitation wavelength: 360 nm).

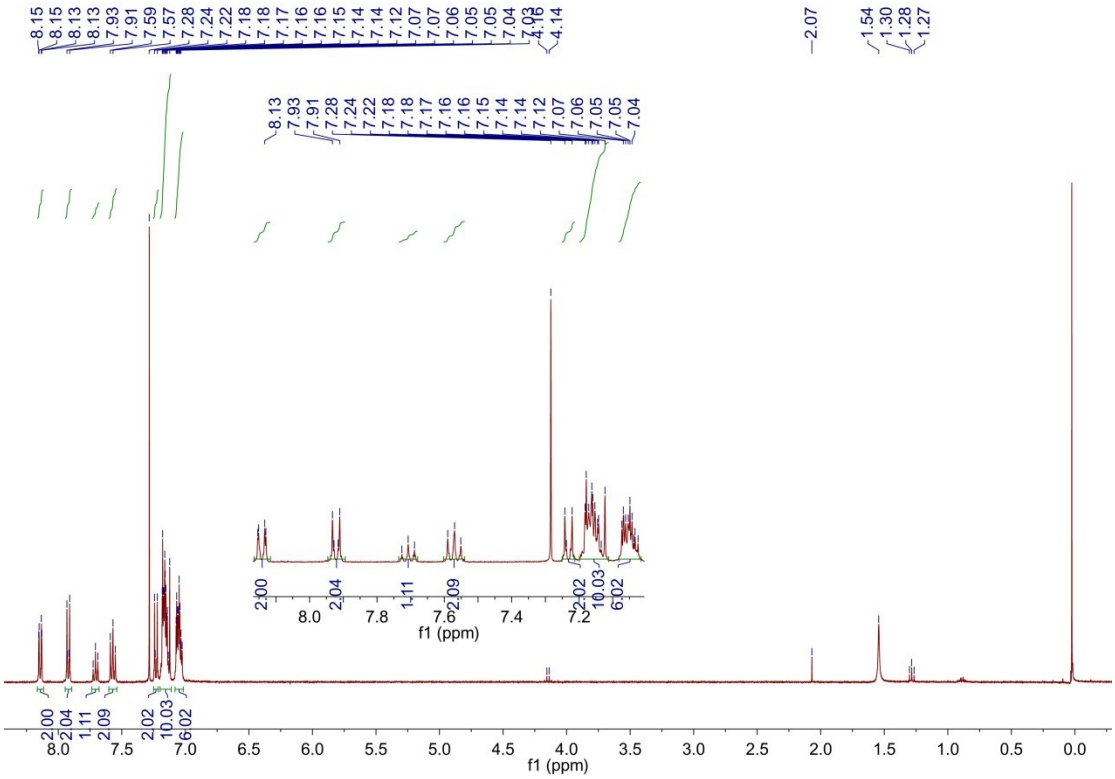

Figure S15 ^{1}H NMR (400 MHz) spectrum of compound 2a in $CDCl_3$.

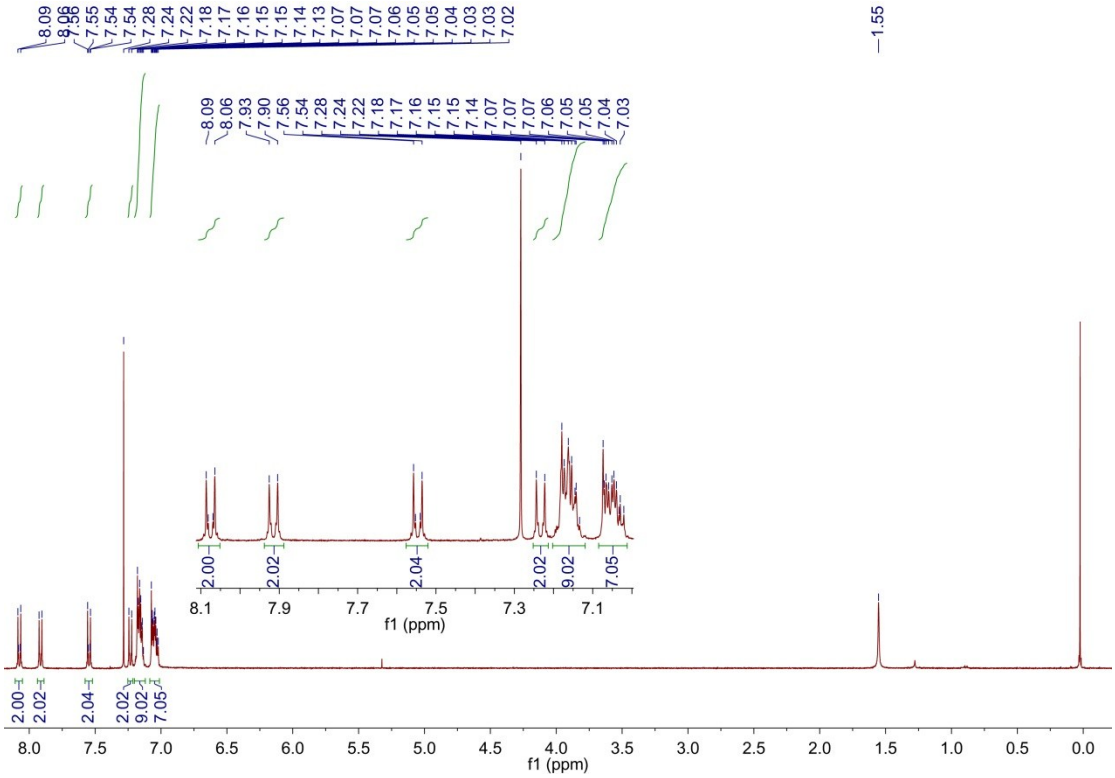

Figure S16 ^{1}H NMR (400 MHz) spectrum of compound 2b in $CDCl_3$.

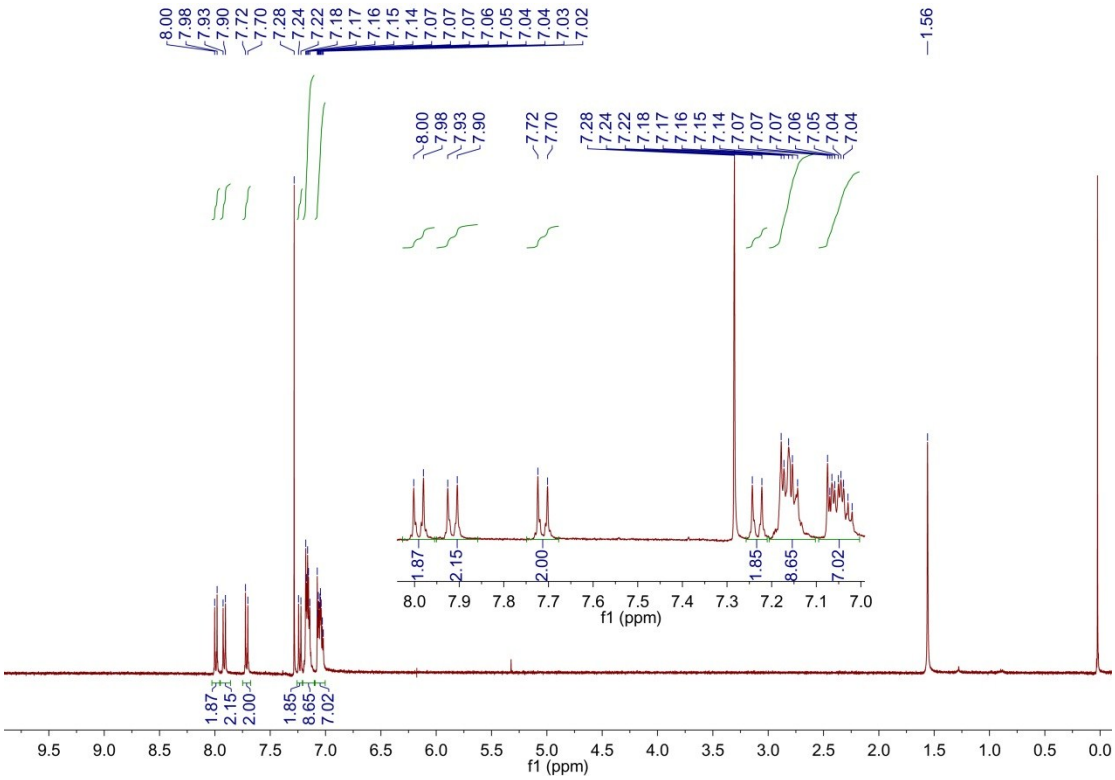

Figure S17 ^{1}H NMR (400 MHz) spectrum of compound 2c in $CDCl_3$.

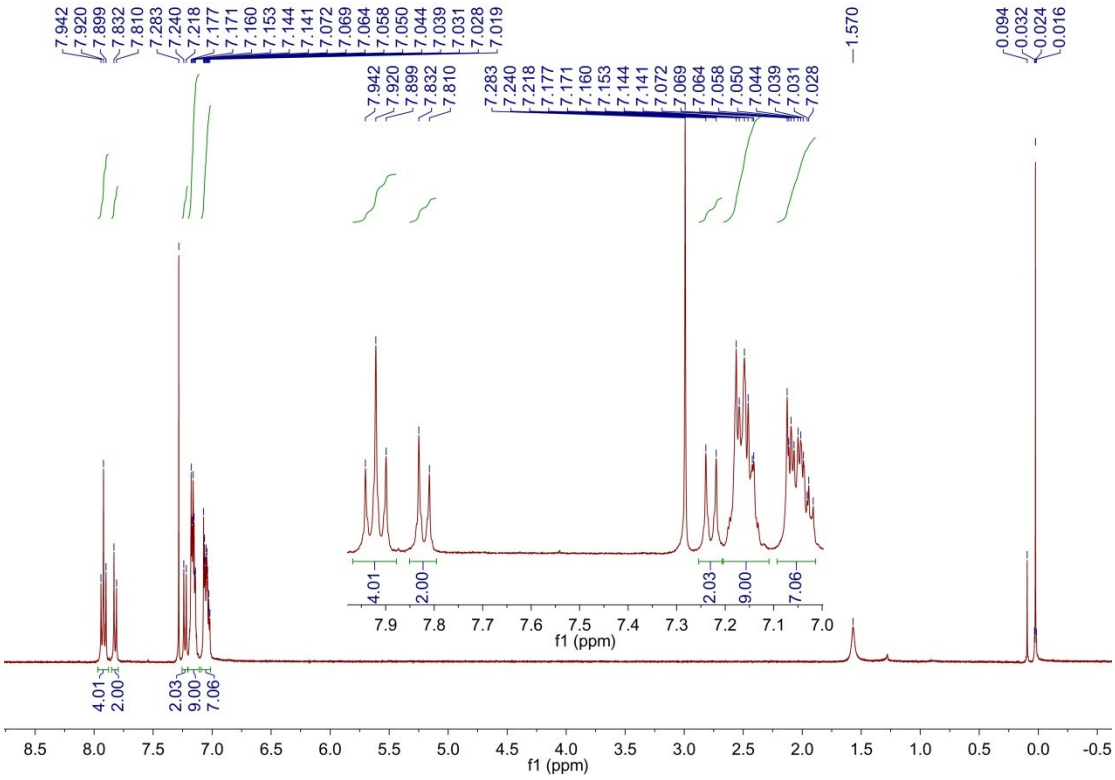

Figure S18 ^{1}H NMR (400 MHz) spectrum of compound 2d in $CDCl_3$.

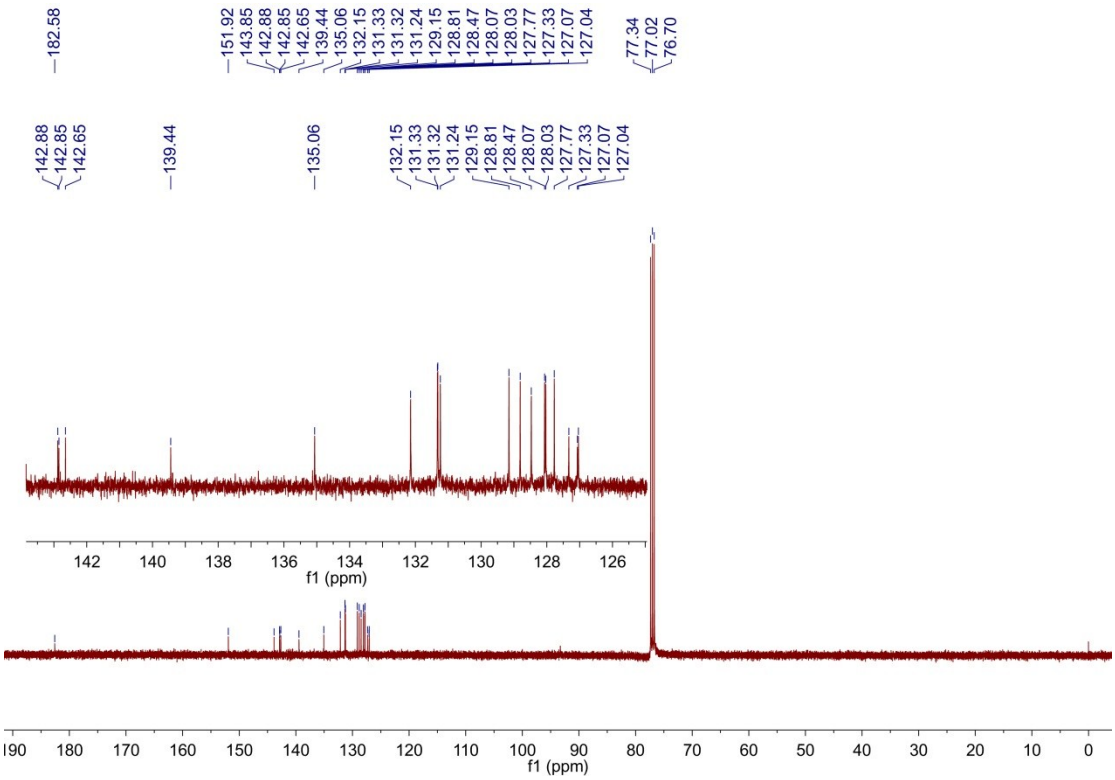

Figure S19 ^{13}C NMR (100 MHz) spectrum of compound 2a in $CDCl_3$.

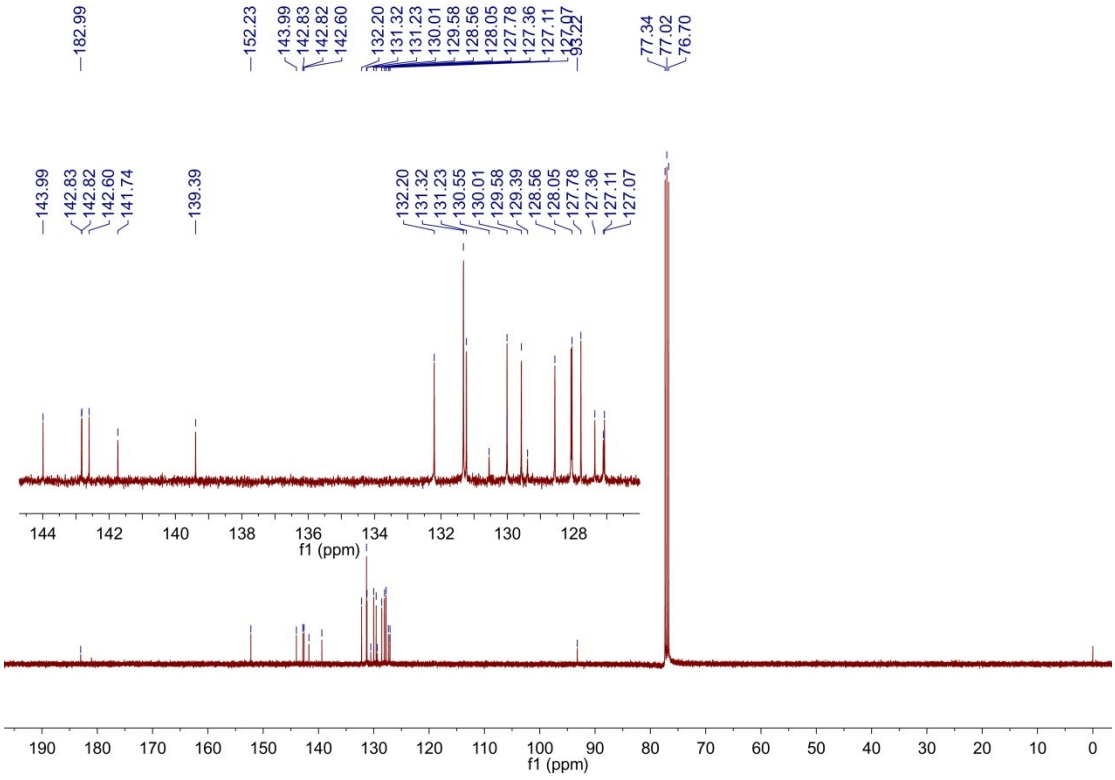

Figure S20 ^{13}C NMR (100 MHz) spectrum of compound 2b in $CDCl_3$.

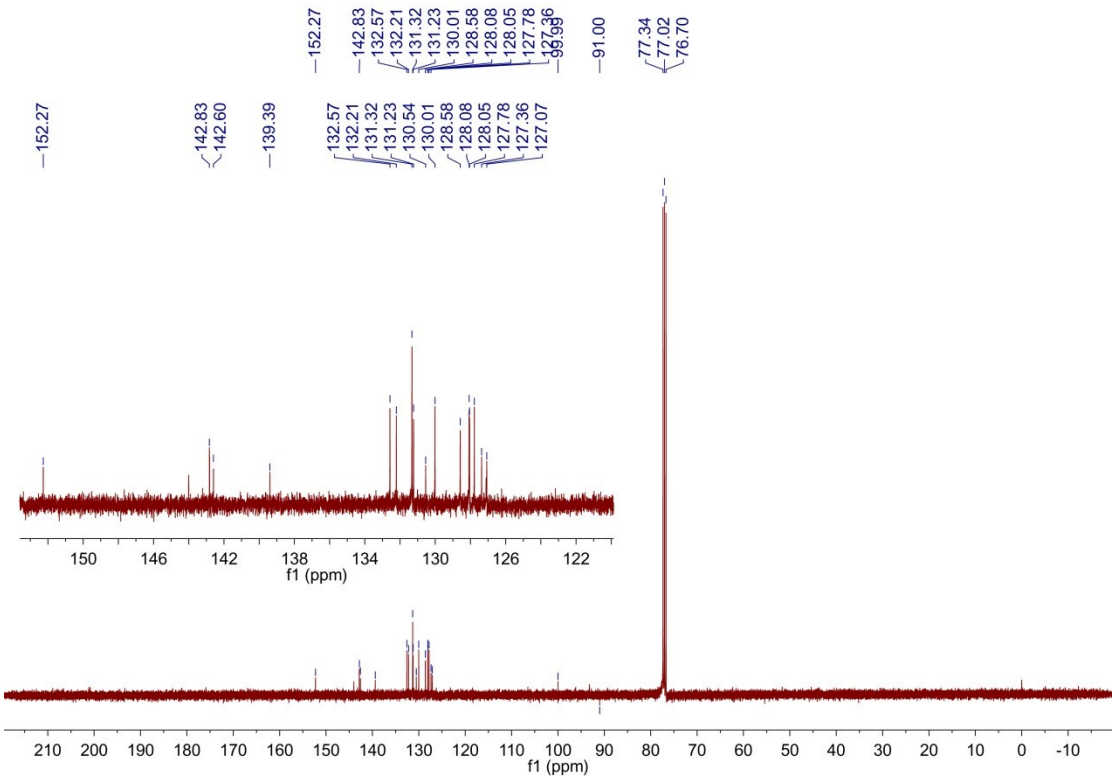

Figure S21 ^{13}C NMR (100 MHz) spectrum of compound 2c in $CDCl_3$.

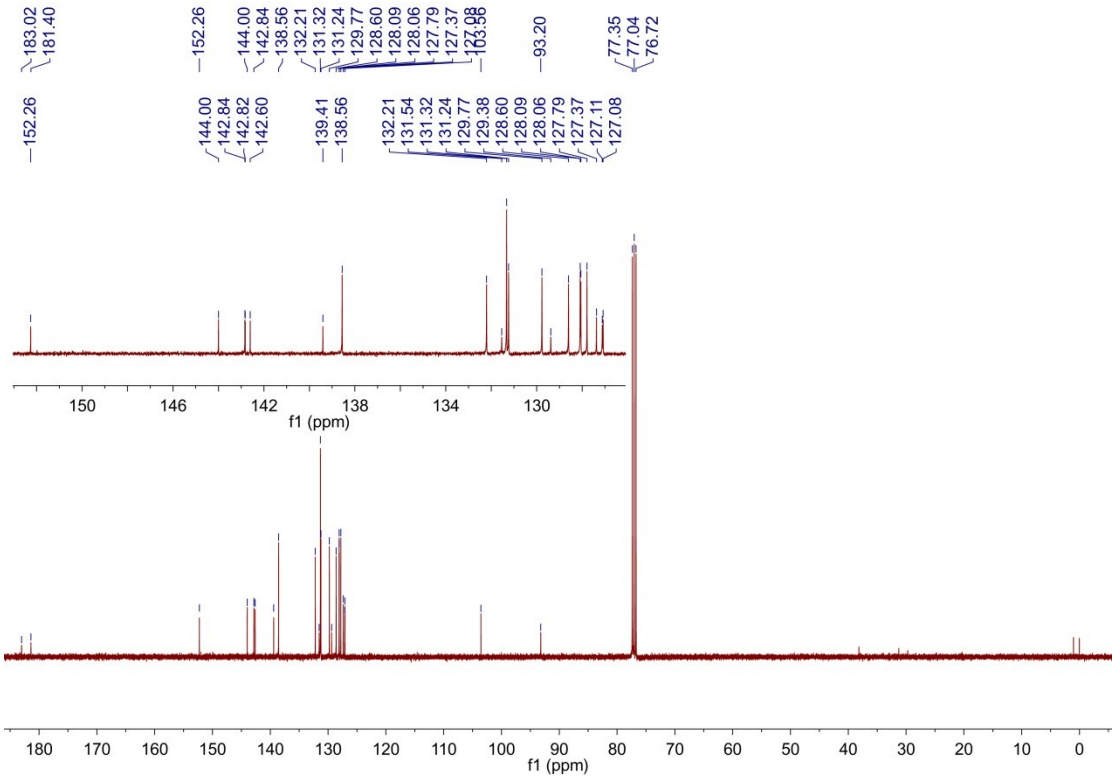

Figure S22 ^{13}C NMR (100 MHz) spectrum of compound 2d in $CDCl_3$.

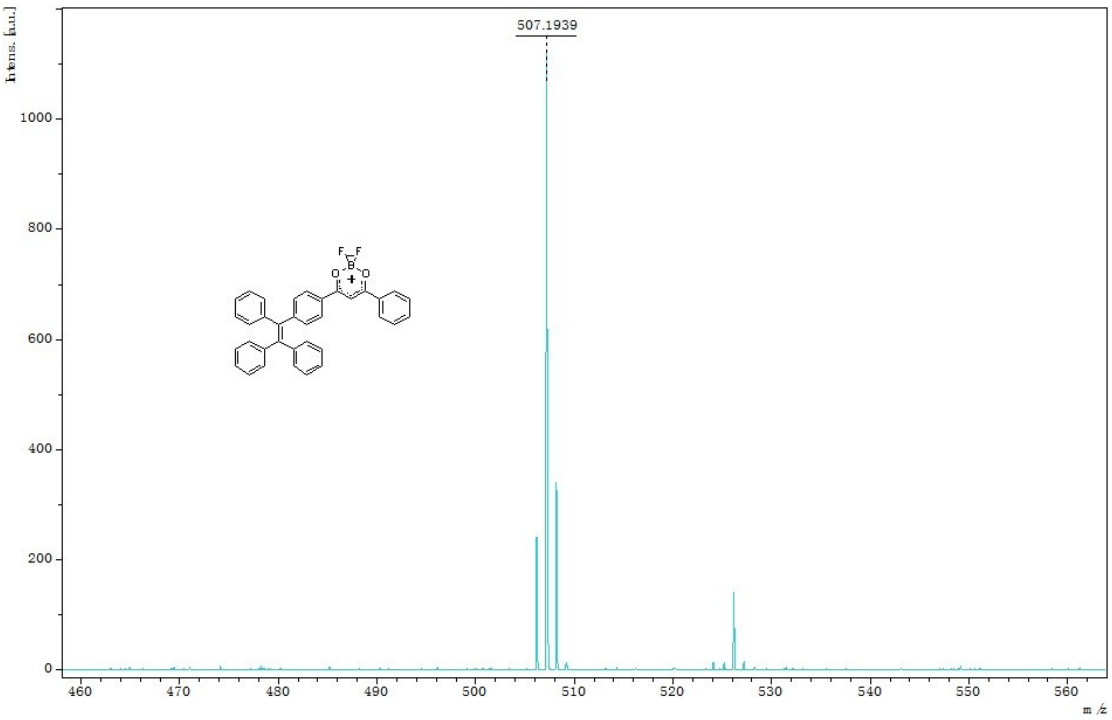

Figure S23 MALDI/TOF MS spectrum of compound 2a.

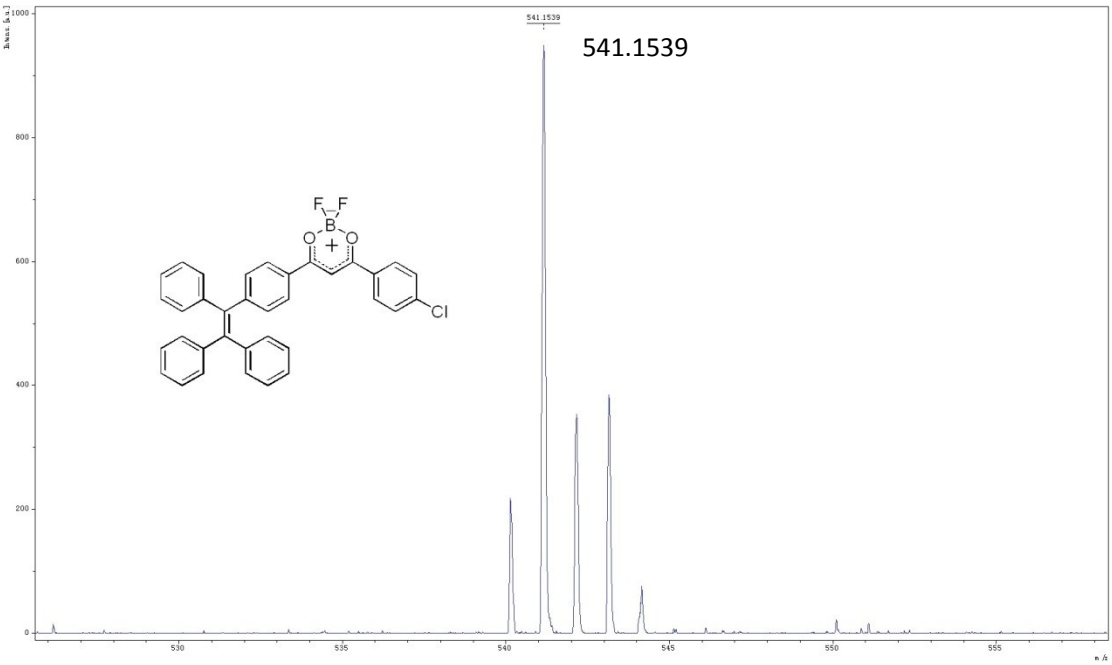

Figure S24 MALDI/TOF MS spectrum of compound 2b.

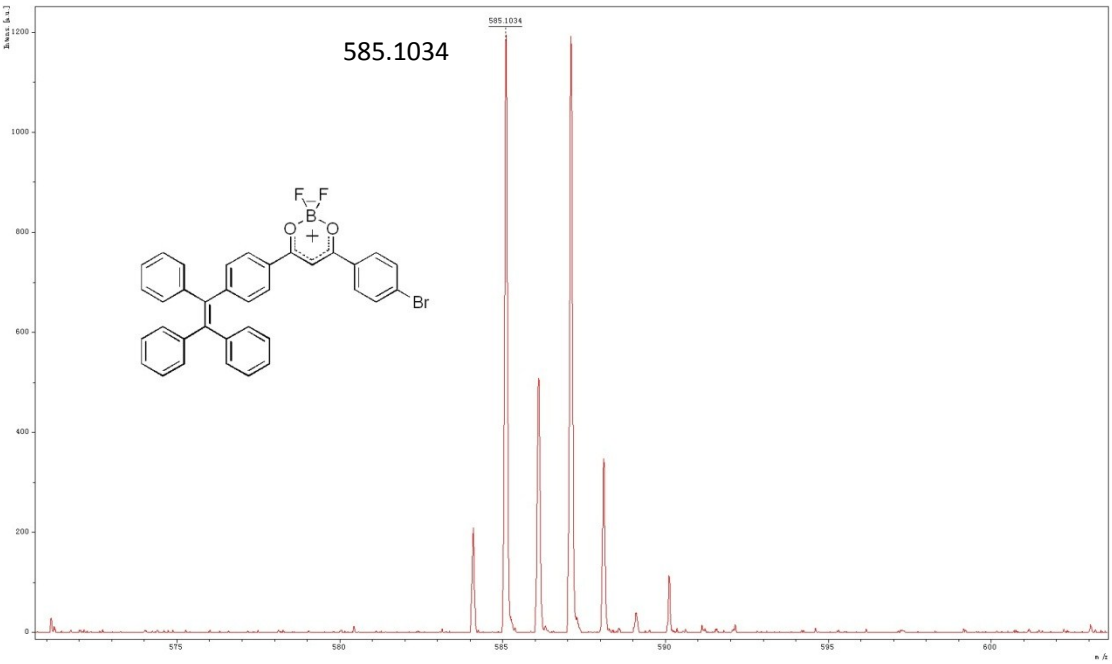

Figure S25 MALDI/TOF MS spectrum of compound 2c.

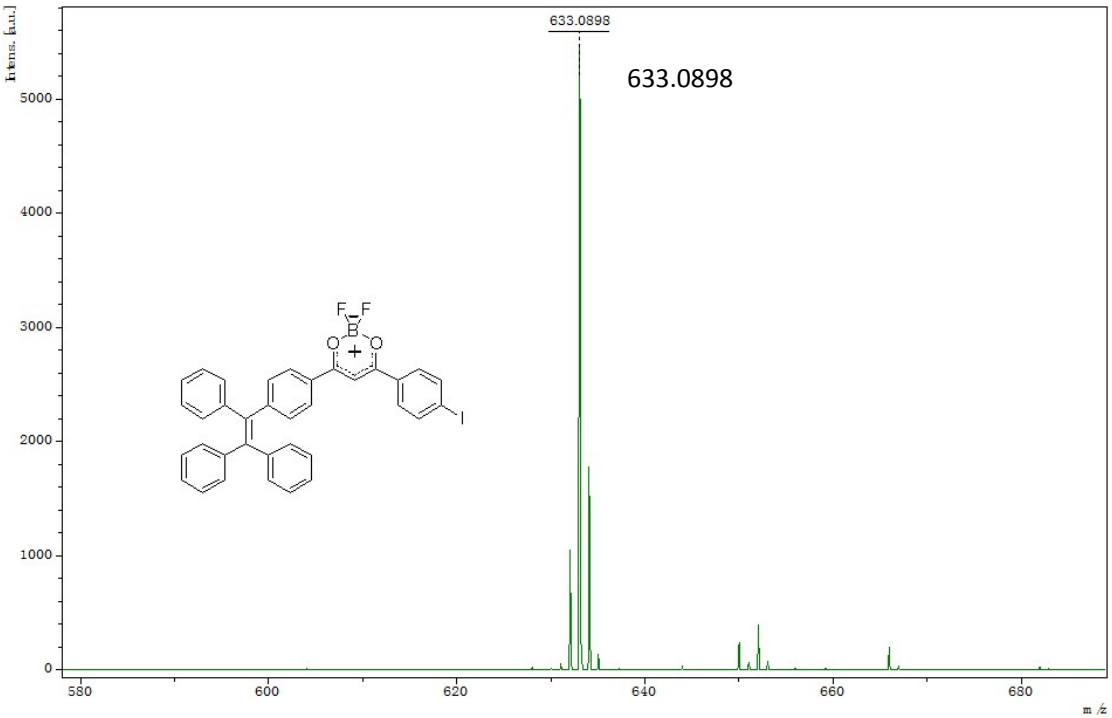

Figure S26 MALDI/TOF MS spectrum of compound 2d.