Electronic Supplementary Material (ESI) for RSC Advances.

Tetraphenylethene Modified β-Ketoiminate Boron Complexes Bearing Aggregation-Induced Emission and Mechanofluorochromism

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Table S1. Photophysical data of **TTPE-H** in different solvents.

solvent	Viscosity (cP at 20 °C)	λ_{abs} (nm)	ε^{max} (M^{-1} cm^{-1})	λ_{em} (nm)	$\Delta\nu_{st}$[a] (cm^{-1})	Φ_f[b]	τ[c] (ns)	K_f[d]/K_{nr}[e] (10^9 s^{-1})
Hexane	0.31	401	46100	480	4104	0.015	1.87	0.0080/0.5267
Cyclohexane	1.00	303, 403	48300	485	4195	0.009	1.66	0.0054/0.5970
Toluene	0.59	303, 405	43600	495	4489	0.007	1.52	0.0046/0.6533
THF	0.55	305, 402	46300	508	5191	0.004	—[f]	—/—
DCM	0.44	302, 402	45100	528	5936	0.005	—[f]	—/—
DMF	0.92	302, 401	44600	532	6141	0.003	—[f]	—/—
DMSO	2.24	304, 403	45000	542	6364	0.005	—[f]	—/—
Ethylene glycol	23.5	305, 405	31800	518	5386	0.105	0.79	0.1329/1.1329
Glycerol	1412	406	28500	501	4670	0.165	0.98	0.1684/0.8520

[a]$\Delta\nu_{st} = \nu_{abs}-\nu_{em}$. [b]The fluorescence quantum yield (Φ_f) was measured using quinine sulfate as a standard (Φ=0.546 in 0.5 mol L^{-1} H_2SO_4) as standard. [c]Fluorescence lifetime. [d]Radiative rate constant $K_f = \Phi_f/\tau$. [e]Nonradiative rate constant $K_{nr} = (1 - \Phi_f)/\tau$. [f]Too short to be measured (<0.1 ns).

Table S2. Photophysical data of **TTPE-CN** in different solvents.

solvent	Viscosity (cP at 20 °C)	λ_{abs} (nm)	ε^{max} (M^{-1} cm^{-1})	λ_{em} (nm)	$\Delta\nu_{st}$[a] (cm^{-1})	Φ_f[b]	τ[c] (ns)	K_f[d]/K_{nr}[e] (10^9 s^{-1})
Hexane	0.31	408	22800	498	4429	0.025	1.58	0.0158/0.6171
Cyclohexane	1.00	302, 410	21900	519	5122	0.005	1.32	0.0038/0.7538
Toluene	0.59	301, 409	38500	529	5546	0.004	1.09	0.0037/0.9138
THF	0.55	304, 402	38300	565	7177	0.003	—[f]	—/—
DCM	0.44	304, 405	37900	583	7539	0.001	—[f]	—/—
DMF	0.92	303, 397	35900	607	8714	0.002	—[f]	—/—
DMSO	2.24	397	35100	612	8850	0.002	—[f]	—/—
Ethylene glycol	23.5	309, 414	19300	533	5393	0.172	0.83	0.2072/0.9976
Glycerol	1412	418	15600	514	4468	0.204	1.09	0.1872/0.7303

[a]$\Delta\nu_{st} = \nu_{abs}-\nu_{em}$. [b]The fluorescence quantum yield (Φ_f) was measured using quinine sulfate as a standard (Φ=0.546 in 0.5 mol L^{-1} H_2SO_4) as standard. [c]Fluorescence lifetime. [d]Radiative rate constant $K_f = \Phi_f/\tau$. [e]Nonradiative rate constant $K_{nr} = (1 - \Phi_f)/\tau$. [f]Too short to be measured (<0.1 ns).

Table S3. Photophysical data of **TTPE-H** and **TTPE-CN** in water/THF mixtures with different water fractions (f_w, 1.0×10^{-5} mol L^{-1}).

Compound	f_w	λ_{abs} (nm)	λ_{em} (nm)	Φ_f[a]	T[b] (ns)	K_f[c]/K_{nr}[d](10^9 s^{-1})
TTPE-H	0%	402	508	0.0042	—[e]	—/—
	20%	403	509	0.0043	—[e]	—/—
	40%	403	507	0.0047	—[e]	—/—
	60%	403	510	0.0053	—[e]	—/—
	70%	403	513	0.0056	—[e]	—/—
	80%	411	508	0.0375	0.78	0.0481/1.2340
	85%	409	508	0.0983	0.96	0.1024/0.9393
	90%	408	513	0.2355	1.32	0.1784/0.5792
TTPE-CN	0%	402	565	0.0034	—[e]	—/—
	20%	403	579	0.0018	—[e]	—/—
	40%	403	580	0.0019	—[e]	—/—
	60%	404	583	0.0024	—[e]	—/—
	70%	403	583	0.0026	—[e]	—/—
	80%	408	556	0.0224	0.77	0.0291/1.2696
	85%	408	553	0.0699	0.99	0.0706/0.9395
	90%	410	553	0.2082	1.39	0.1498/0.5696

[a]The fluorescence quantum yield (Φ_f) was measured using fluorescein (Φ=0.79 in 0.1 M sodium hydroxide water solution) as standard. [b]Fluorescence lifetime, the fluorescence decays can be fitted with a single exponential function. [c]Radiative rate constant $K_f = \Phi_f/\tau$. [d]Nonradiative rate constant $K_{nr} = (1 - \Phi_f)/\tau$. [e]Too short to be measured (<0.1 ns).

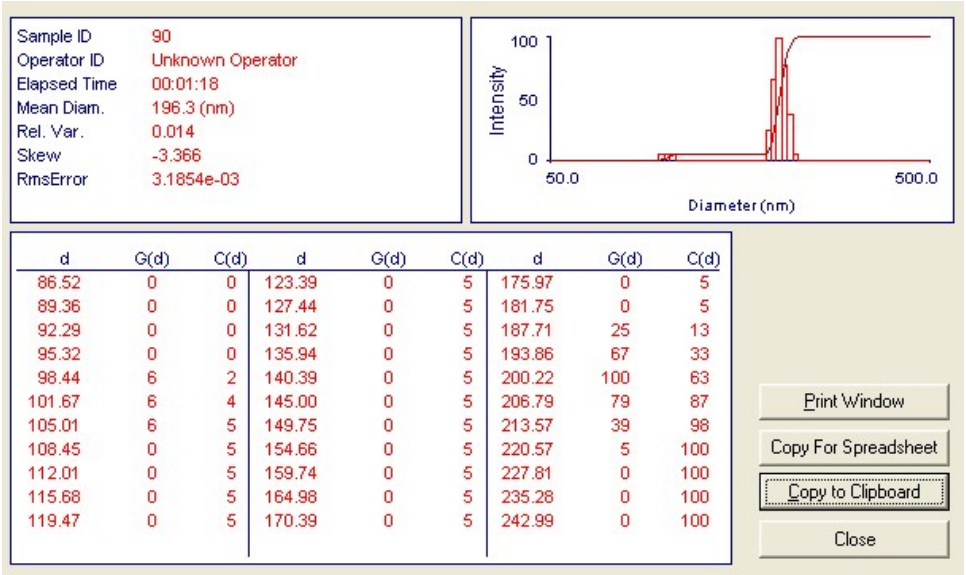
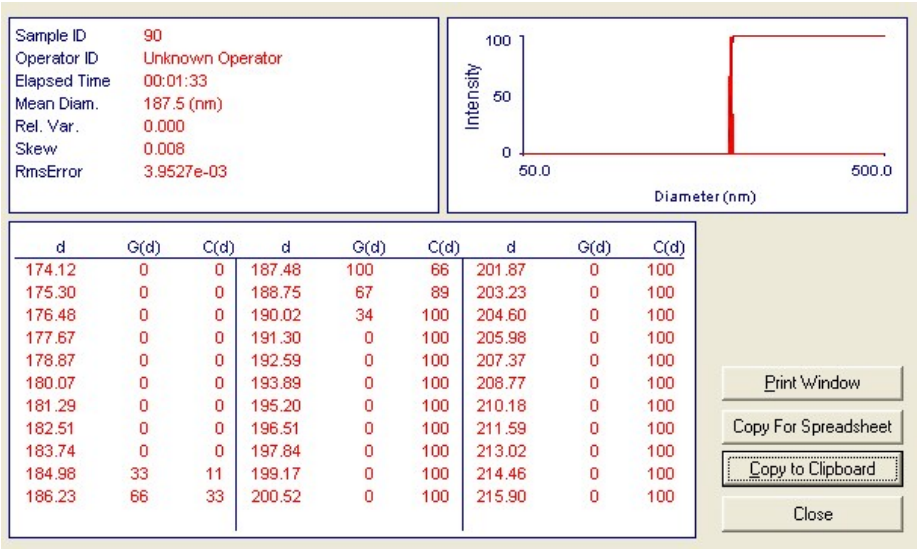
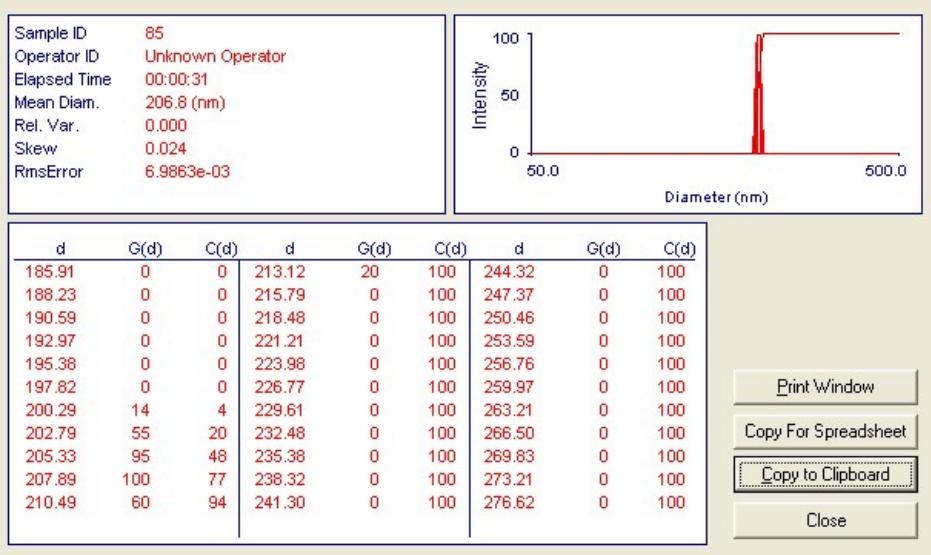


Fig. S1 DLS data of **TTPE-H** (1.0×10^{-5} mol L^{-1}) in ethylene glycol–THF mixture with ethylene glycol fraction of 90%.



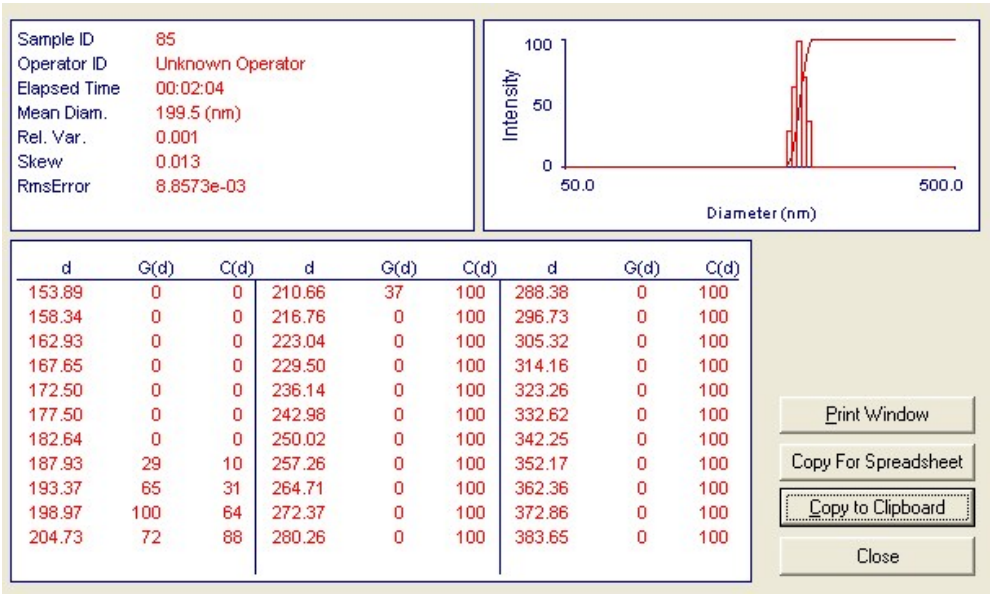
d	G(d)	C(d)	d	G(d)	C(d)	d	G(d)	C(d)
174.12	0	0	187.48	100	66	201.87	0	100
175.30	0	0	188.75	67	89	203.23	0	100
176.48	0	0	190.02	34	100	204.60	0	100
177.67	0	0	191.30	0	100	205.98	0	100
178.87	0	0	192.59	0	100	207.37	0	100
180.07	0	0	193.89	0	100	208.77	0	100
181.29	0	0	195.20	0	100	210.18	0	100
182.51	0	0	196.51	0	100	211.59	0	100
183.74	0	0	197.84	0	100	213.02	0	100
184.98	33	11	199.17	0	100	214.46	0	100
186.23	66	33	200.52	0	100	215.90	0	100

Fig. S2 DLS data of **TTPE-CN** (1.0×10^{-5} mol L^{-1}) in ethylene glycol–THF mixture with ethylene glycol fraction of 90%.



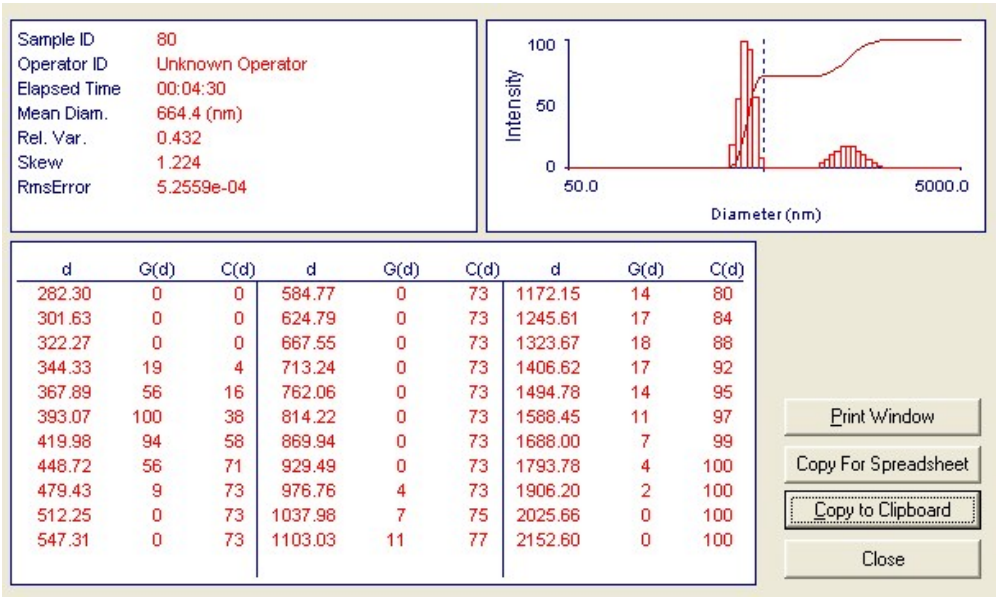
d	G(d)	C(d)	d	G(d)	C(d)	d	G(d)	C(d)
185.91	0	0	213.12	20	100	244.32	0	100
188.23	0	0	215.79	0	100	247.37	0	100
190.59	0	0	218.48	0	100	250.46	0	100
192.97	0	0	221.21	0	100	253.59	0	100
195.38	0	0	223.98	0	100	256.76	0	100
197.82	0	0	226.77	0	100	259.97	0	100
200.29	14	4	229.61	0	100	263.21	0	100
202.79	55	20	232.48	0	100	266.50	0	100
205.33	95	48	235.38	0	100	269.83	0	100
207.89	100	77	238.32	0	100	273.21	0	100
210.49	60	94	241.30	0	100	276.62	0	100

Fig. S3 DLS data of **TTPE-H** (1.0×10^{-5} mol L^{-1}) in ethylene glycol–THF mixture with ethylene glycol fraction of 85%.



d	G(d)	C(d)	d	G(d)	C(d)	d	G(d)	C(d)
153.89	0	0	210.66	37	100	288.38	0	100
158.34	0	0	216.76	0	100	296.73	0	100
162.93	0	0	223.04	0	100	305.32	0	100
167.65	0	0	229.50	0	100	314.16	0	100
172.50	0	0	236.14	0	100	323.26	0	100
177.50	0	0	242.98	0	100	332.62	0	100
182.64	0	0	250.02	0	100	342.25	0	100
187.93	29	10	257.26	0	100	352.17	0	100
193.37	65	31	264.71	0	100	362.36	0	100
198.97	100	64	272.37	0	100	372.86	0	100
204.73	72	88	280.26	0	100	383.65	0	100

Fig. S4 DLS data of **TTPE-CN** (1.0×10^{-5} mol L^{-1}) in ethylene glycol–THF mixture with ethylene glycol fraction of 85%.



d	G(d)	C(d)	d	G(d)	C(d)	d	G(d)	C(d)
282.30	0	0	584.77	0	73	1172.15	14	80
301.63	0	0	624.79	0	73	1245.61	17	84
322.27	0	0	667.55	0	73	1323.67	18	88
344.33	19	4	713.24	0	73	1406.62	17	92
367.89	56	16	762.06	0	73	1494.78	14	95
393.07	100	38	814.22	0	73	1588.45	11	97
419.98	94	58	869.94	0	73	1688.00	7	99
448.72	56	71	929.49	0	73	1793.78	4	100
479.43	9	73	976.76	4	73	1906.20	2	100
512.25	0	73	1037.98	7	75	2025.66	0	100
547.31	0	73	1103.03	11	77	2152.60	0	100

Fig. S5 DLS data of **TTPE-H** (1.0×10^{-5} mol L^{-1}) in ethylene glycol–THF mixture with ethylene glycol fraction of 80%.

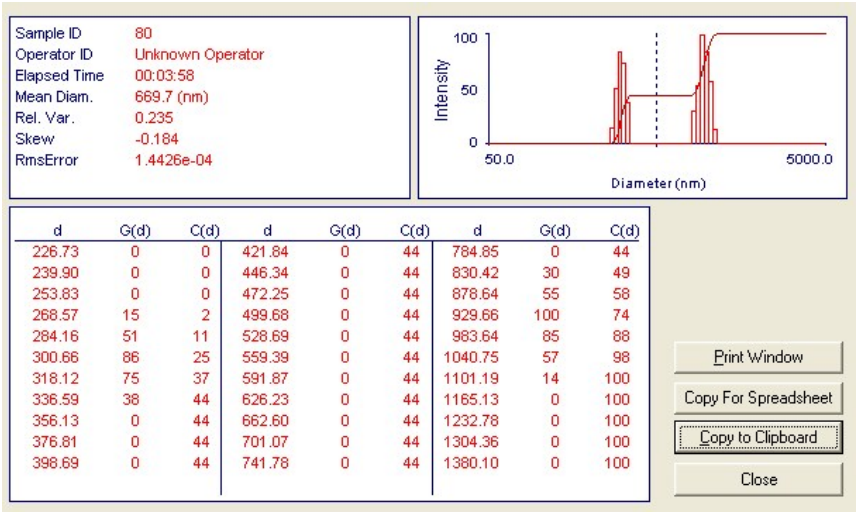


Fig. S6 DLS data of **TTPE-CN** (1.0×10^{-5} mol L^{-1}) in ethylene glycol–THF mixture with ethylene glycol fraction of 80%.

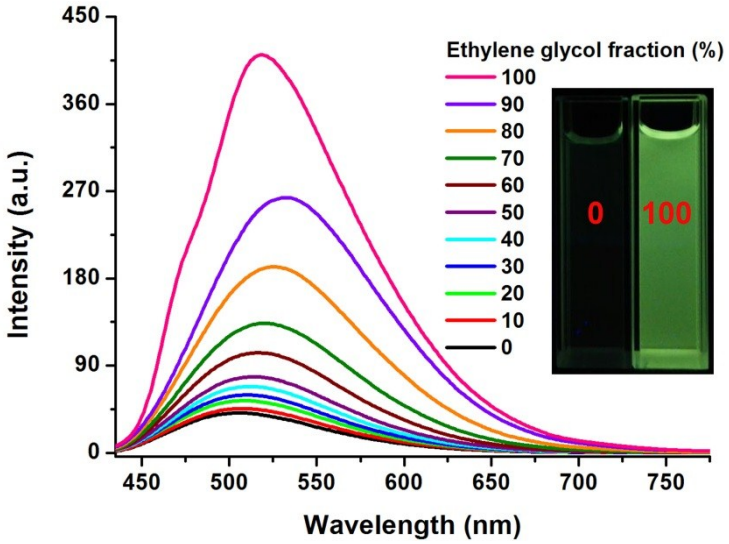


Fig. S7 PL spectra of **TTPE-H** in ethylene glycol–THF mixtures with different ethylene glycol fractions (from 0% to 100%, 1.0×10^{-5} mol L^{-1}, excited at 390 nm). Photographs are **TTPE-H** in THF and ethylene glycol under UV light (365 nm), respectively.

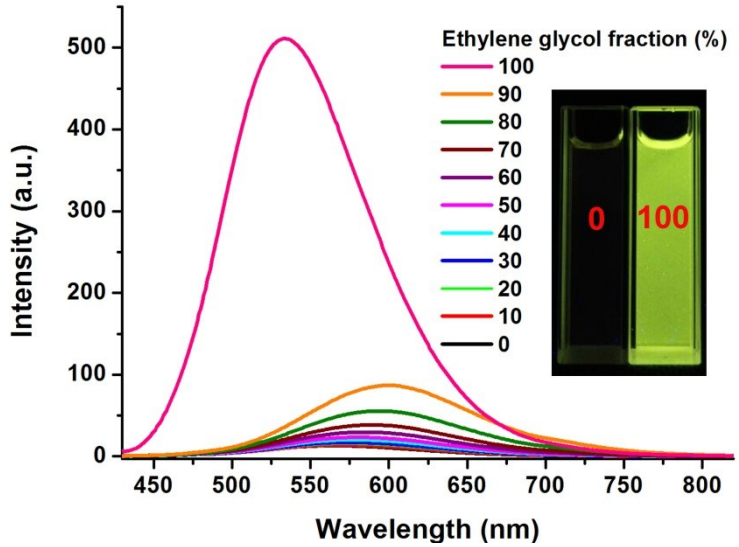


Fig. S8 spectra of **TTPE-CN** in ethylene glycol–THF mixtures with different ethylene glycol fractions (from 0% to 100%, 1.0×10^{-5} mol L^{-1}, excited at 410 nm). Photographs are **TTPE-H** in THF and ethylene glycol under UV light (365 nm), respectively.

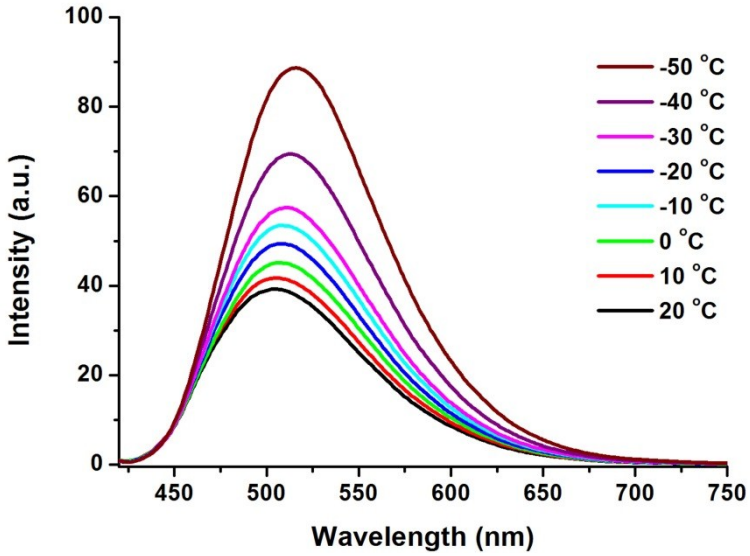


Fig. S9 PL spectra of **TTPE-H** in THF at different temperature (excited at 390 nm, 1.0×10^{-5} mol L^{-1}).

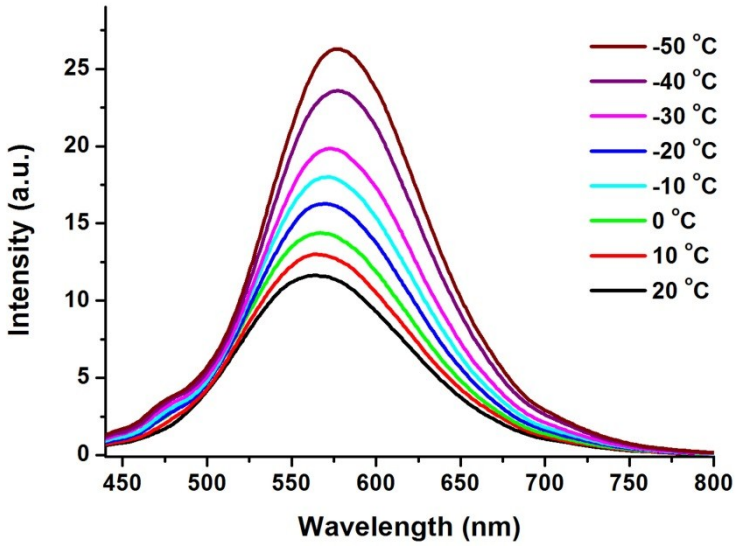


Fig. S10 PL spectra of **TTPE-CN** in THF at different temperature (excited at 410 nm, 1.0×10^{-5} mol L^{-1}).

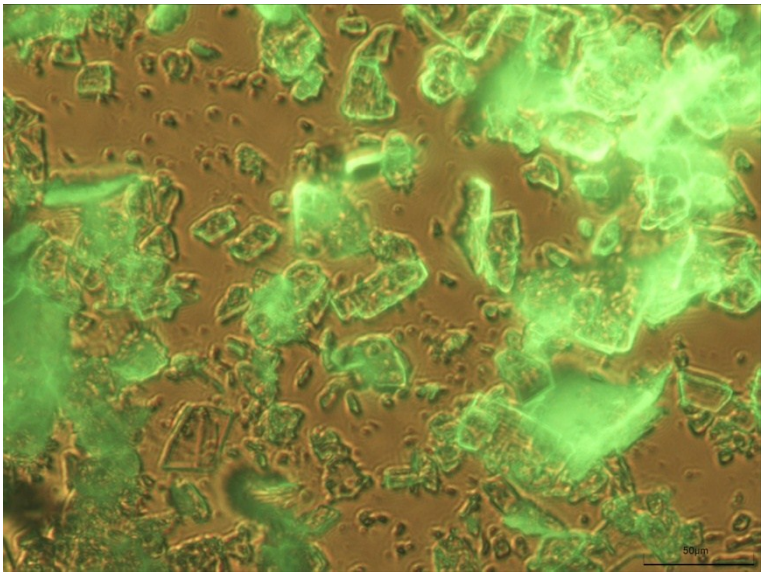


Fig. S11 Fluorescence microscopy image of **TTPE-H** powders. The excitation wavelength for measurements was 330–385 nm.

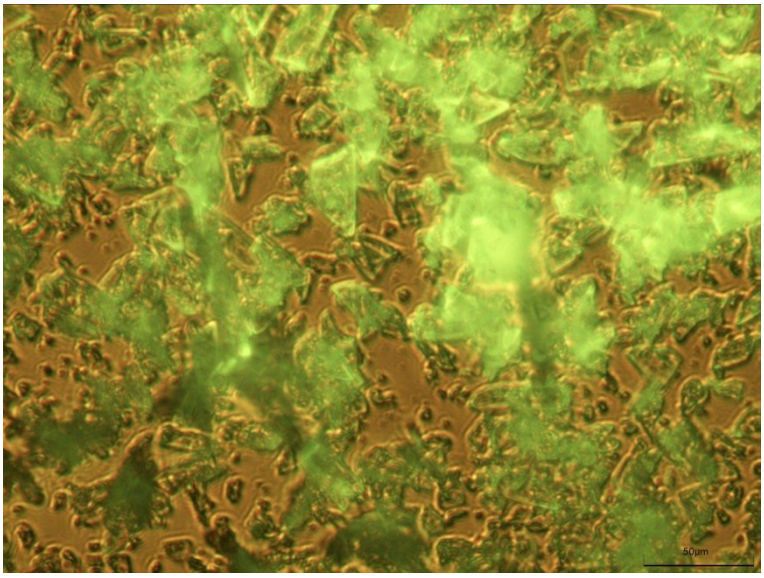


Fig. S12 Fluorescence microscopy image of **TTPE-CN** powders. The excitation wavelength for measurements was 330–385 nm.

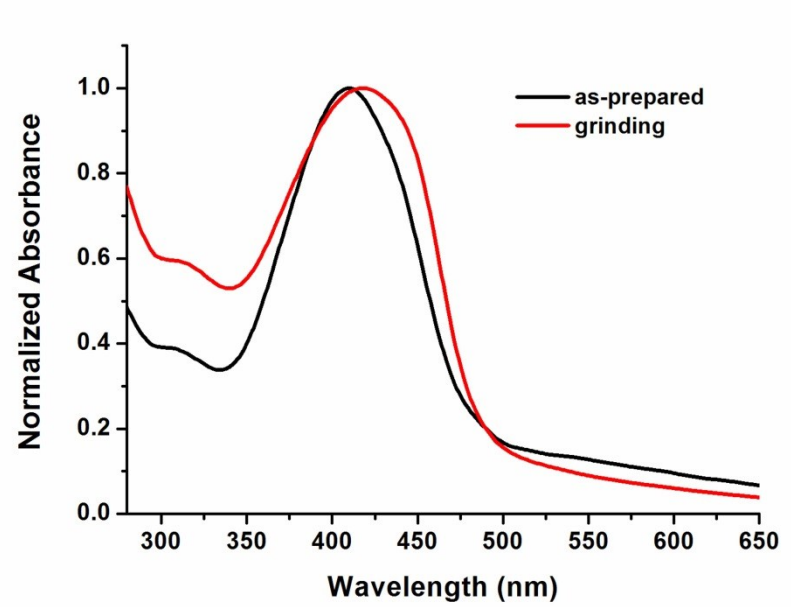


Fig. S13 Normalized UV-vis absorption spectra of **TTPE-H** in different solid-states: as-prepared and grinding.

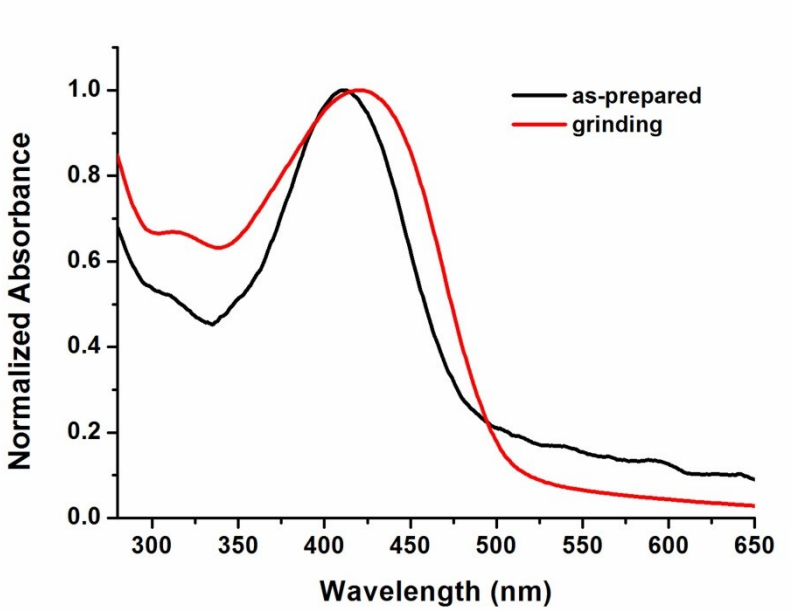


Fig. S14 Normalized UV-vis absorption spectra of **TTPE-CN** in different solid-states: as-prepared and grinding.

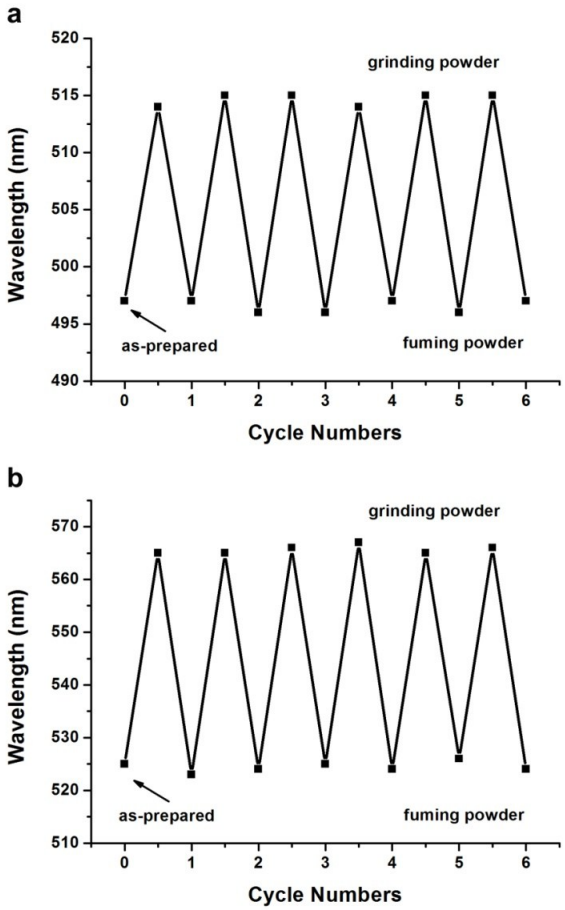


Fig. S15 Maximum fluorescent emission of **TTPE-H** (a) and **TTPE-CN** (b) upon repeating treated by grinding and fuming with DCM.

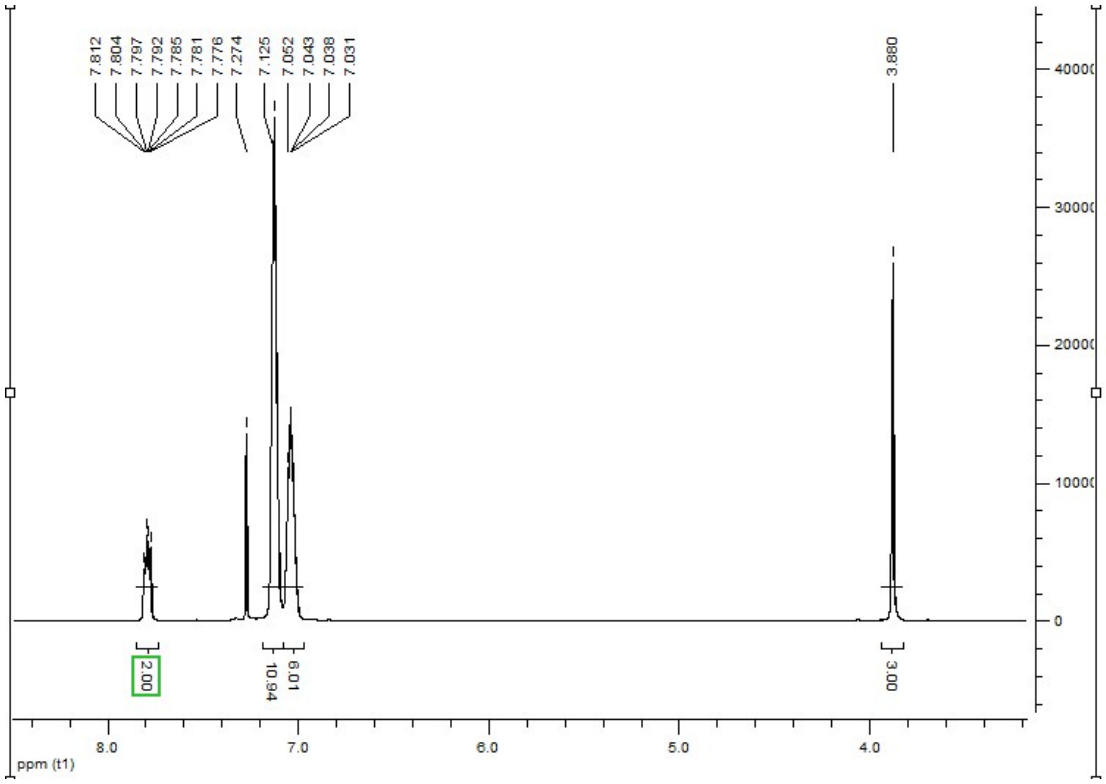


Fig. S16 ^{1}H NMR (400 MHz) spectrum of compound **3**.

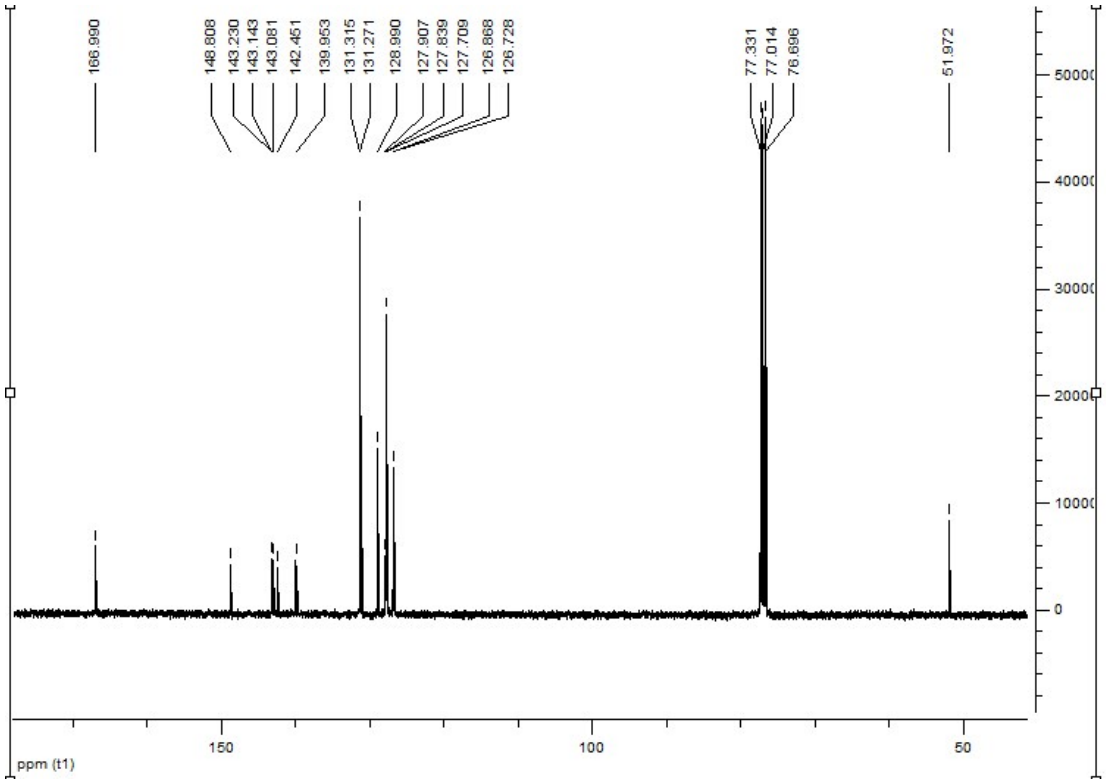


Fig. S17 ^{13}C NMR (100 MHz) spectrum of compound **3**.

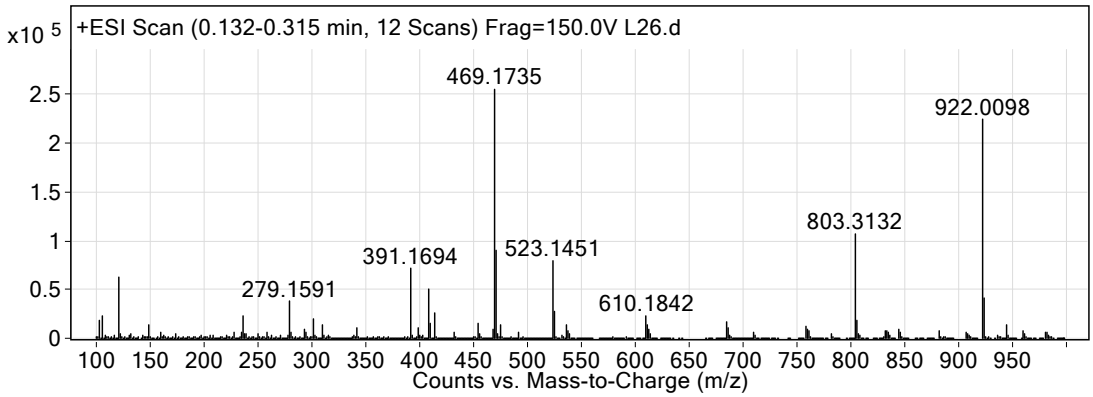


Fig. S18 TOF LC/MS spectrum of compound **3**.

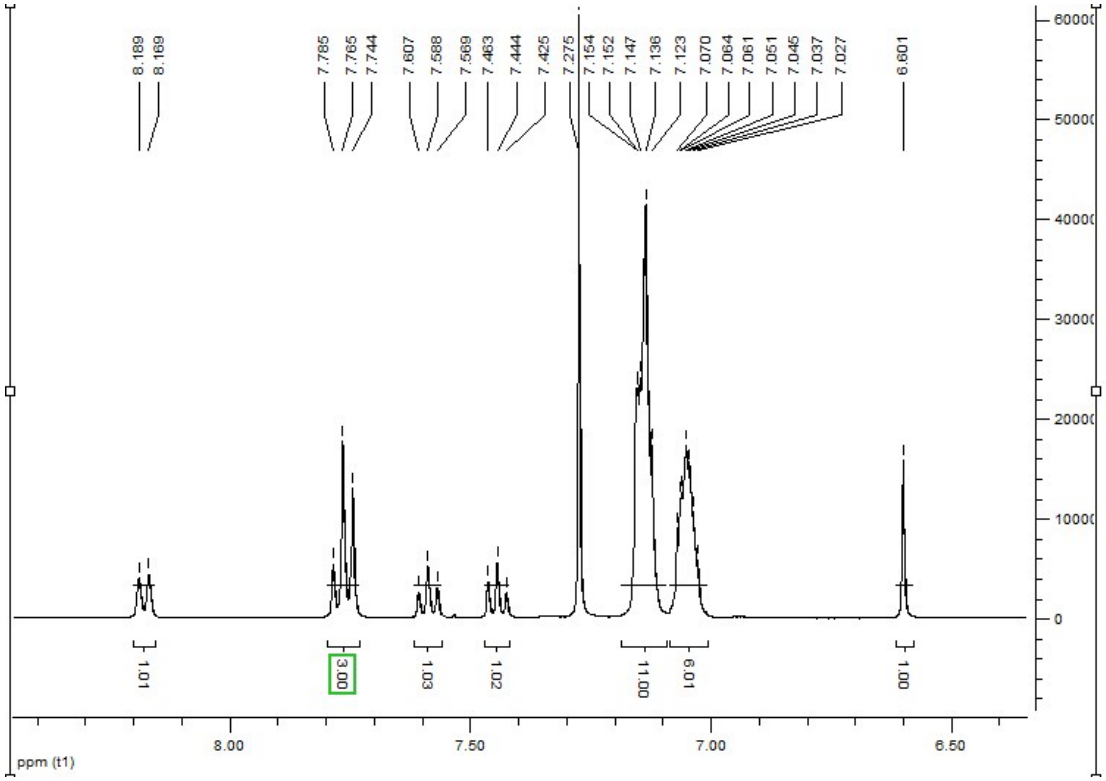


Fig. S19 ^{1}H NMR (400 MHz) spectrum of compound **TTPE-H**.

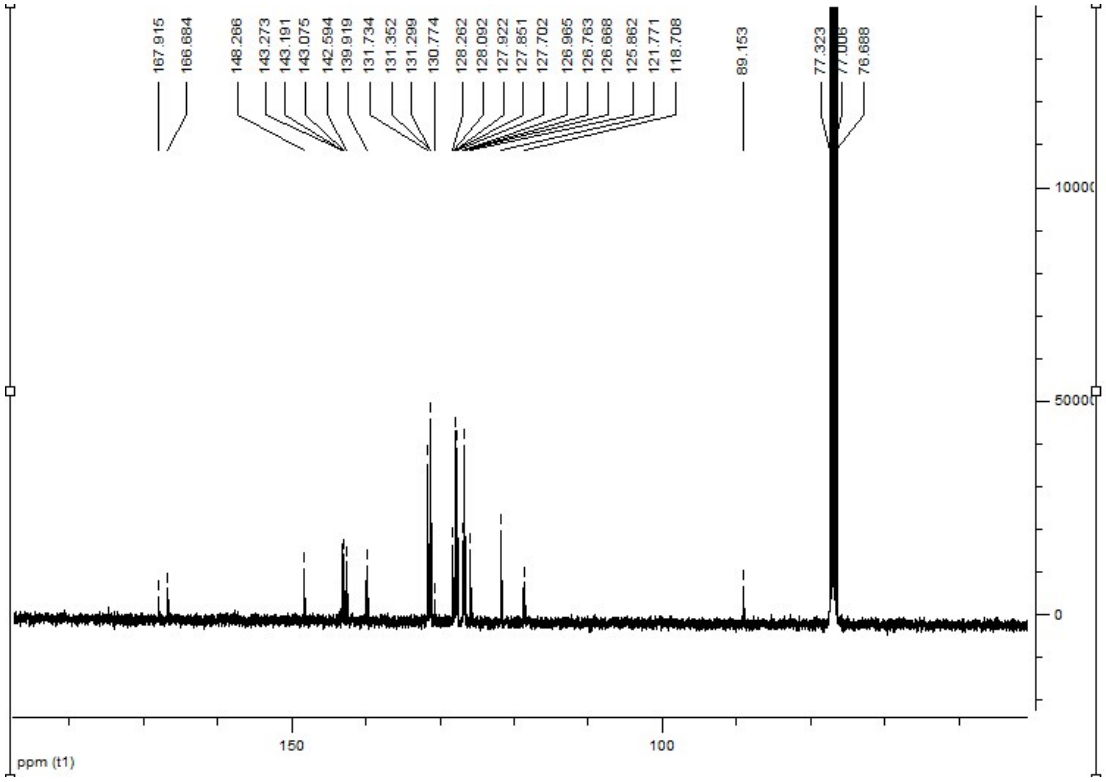


Fig. S20 ^{13}C NMR (100 MHz) spectrum of compound **TTPE-H**.

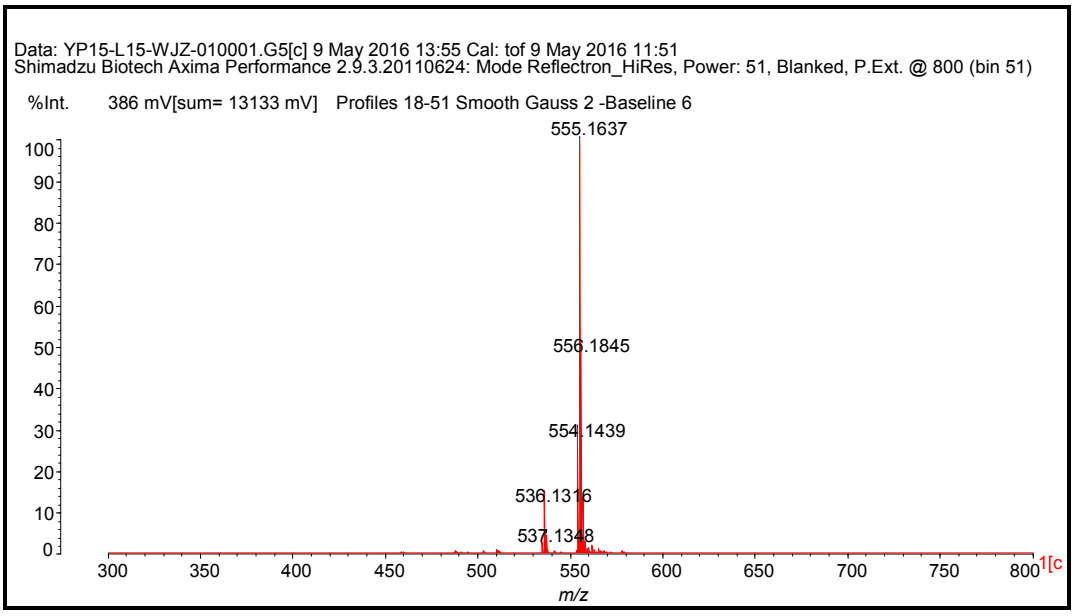


Fig. S21 MALDI/TOF MS spectrum of compound **TTPE-H**.

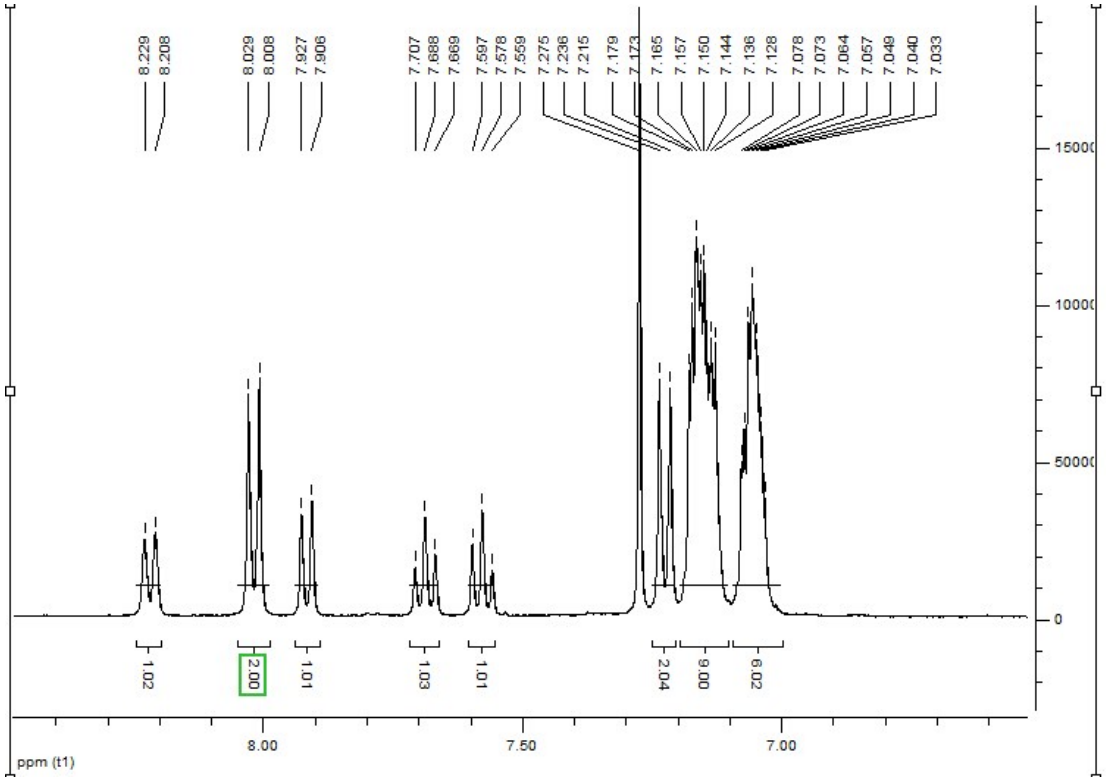


Fig. S22 ^{1}H NMR (400 MHz) spectrum of compound **TTPE-CN**.

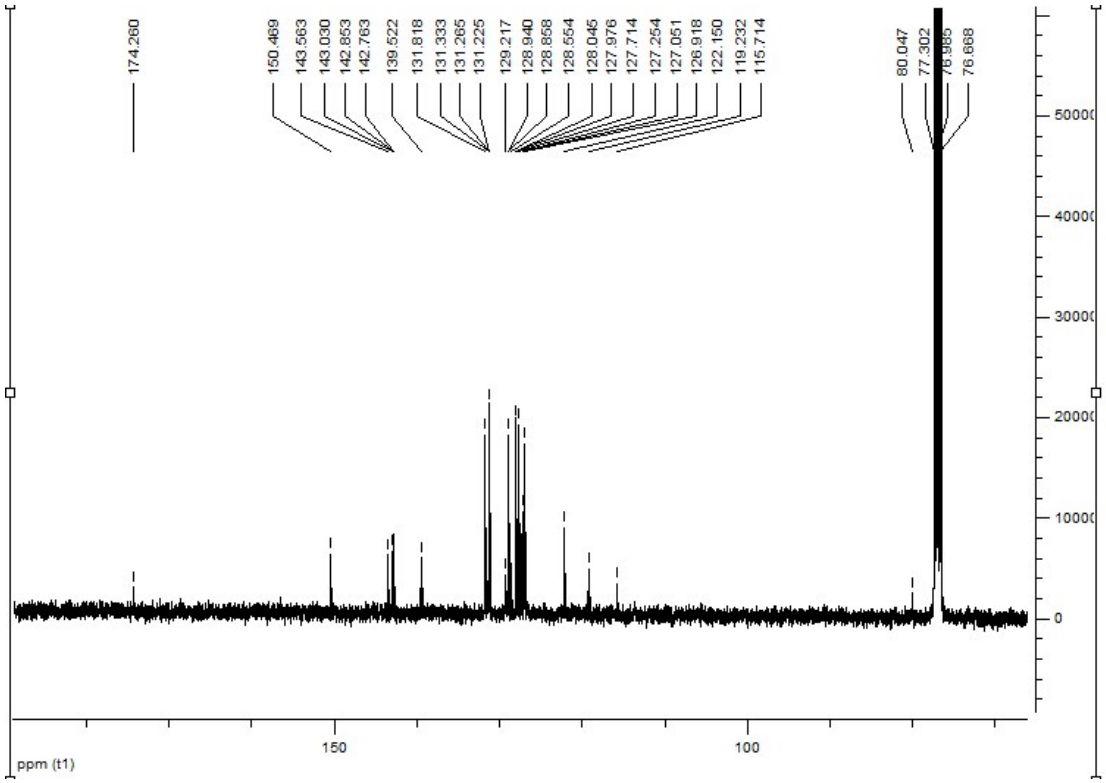


Fig. S23 ^{13}C NMR (100 MHz) spectrum of compound **TTPE-CN**.

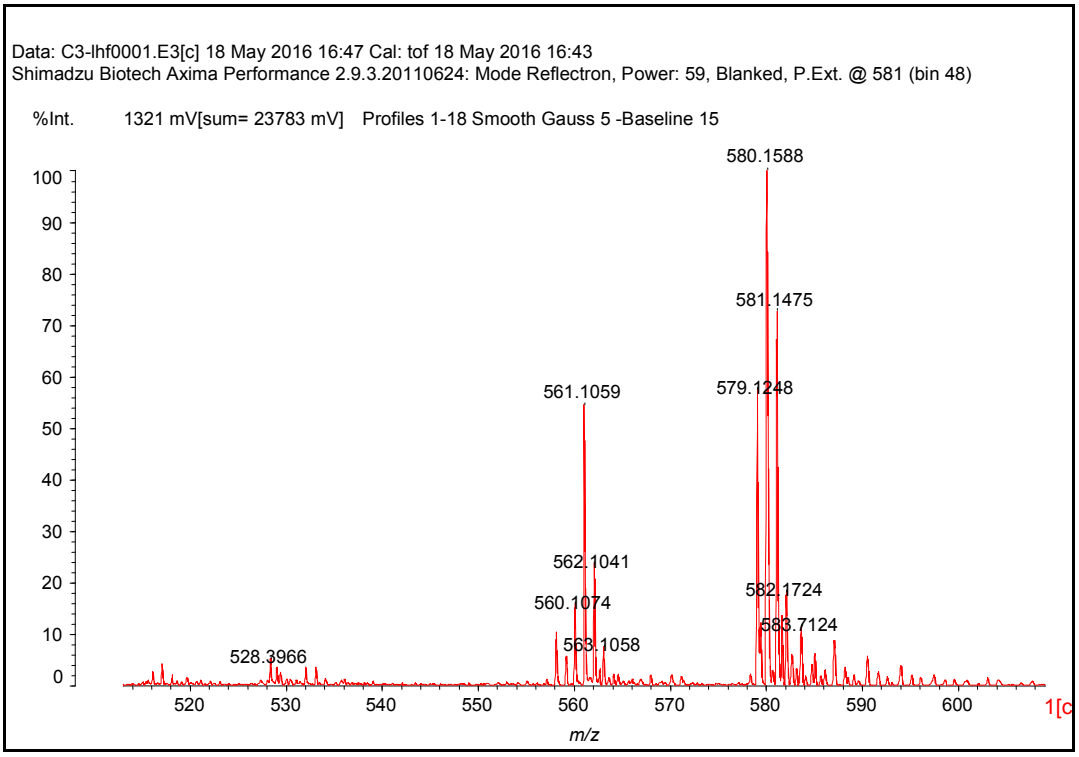


Fig. S24 MALDI/TOF MS spectrum of compound **TTPE-CN**.