Electronic Supplementary Material (ESI) for Journal of Materials Chemistry C.

Reversible Mechanochromic Luminescence of Phenothiazine-based 10,10´-Bianthracene Derivatives with Different Length of Alkyl Chains

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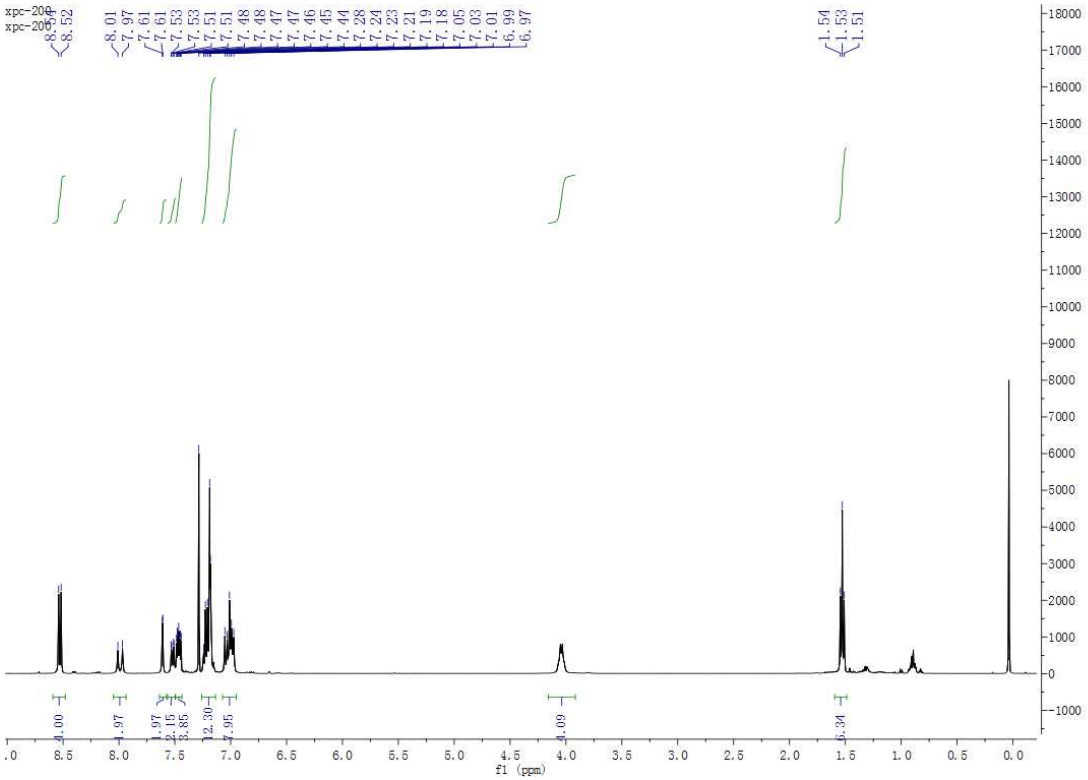

Fig. S1 ^{1}H NMR spectrum of **PVBA2** in $CDCl_3$.

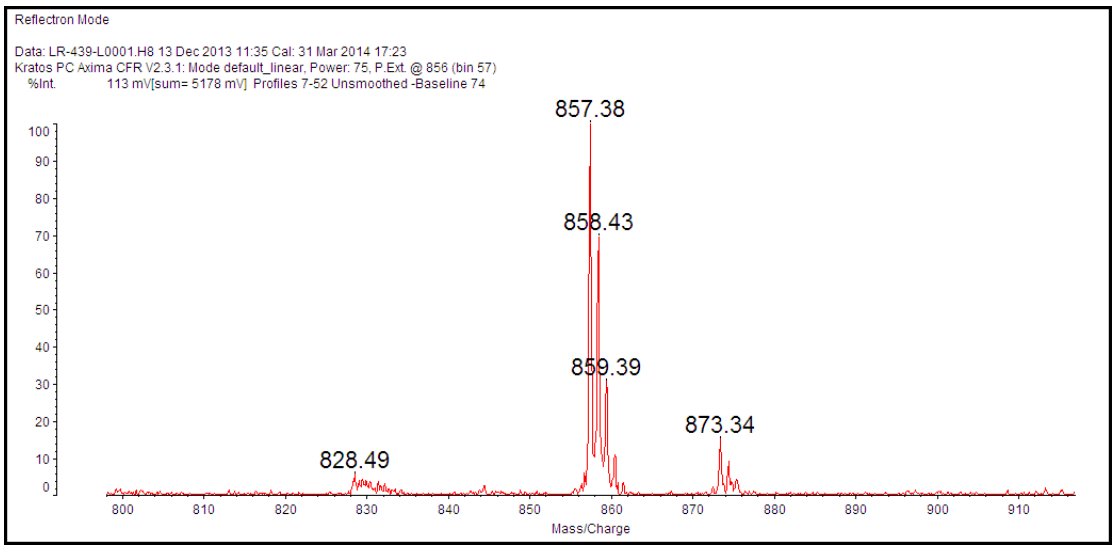

Fig. S2 MALDI-TOF spectrum of **PVBA2** in $CDCl_3$.

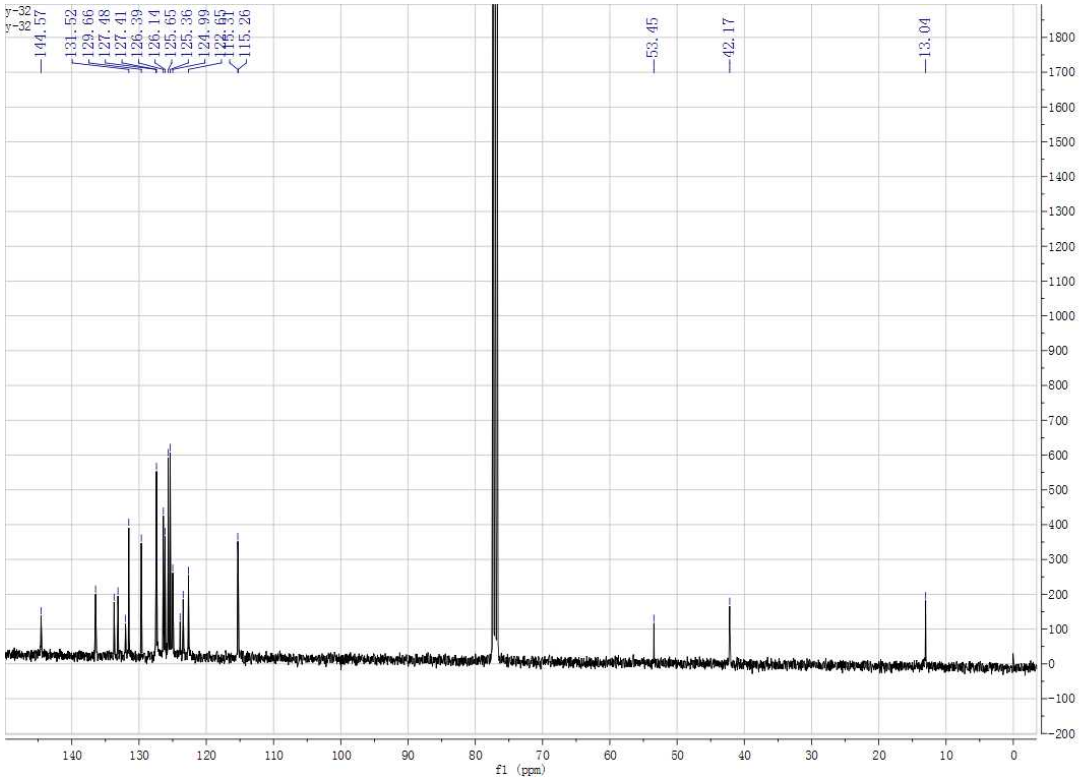

Fig. S3 ^{13}C NMR spectrum of **PVBA2** in $CDCl_3$.

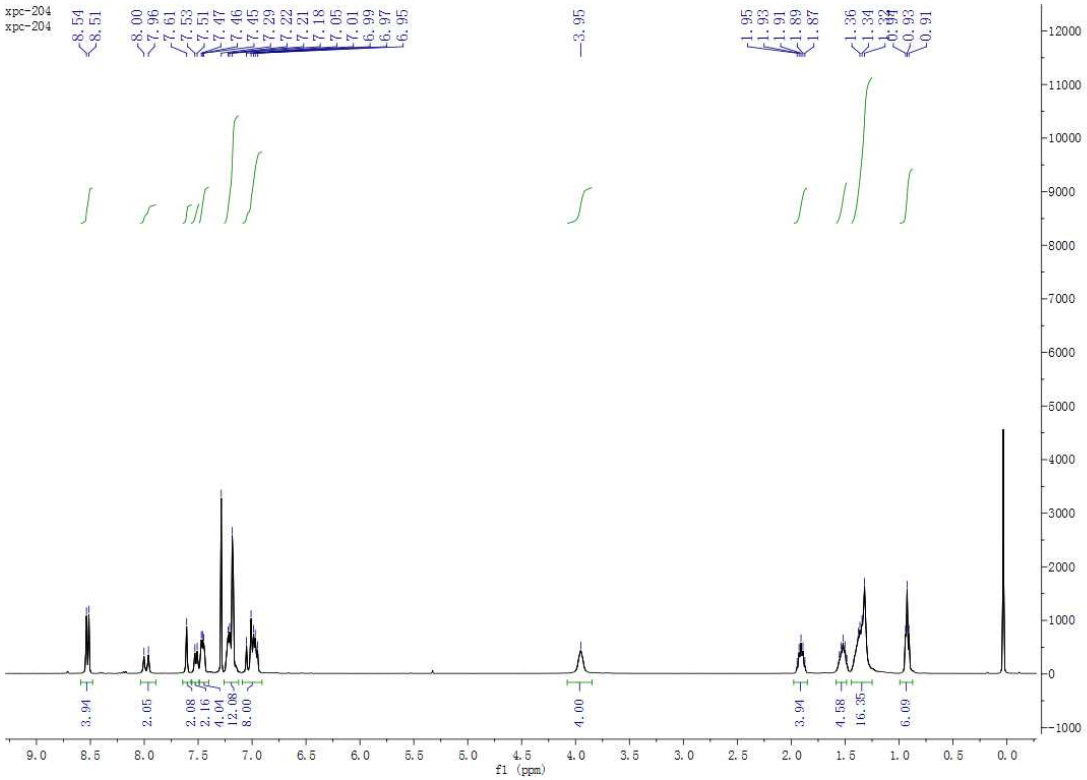

Fig. S4 ^{1}H NMR spectrum of **PVBA8** in $CDCl_3$.

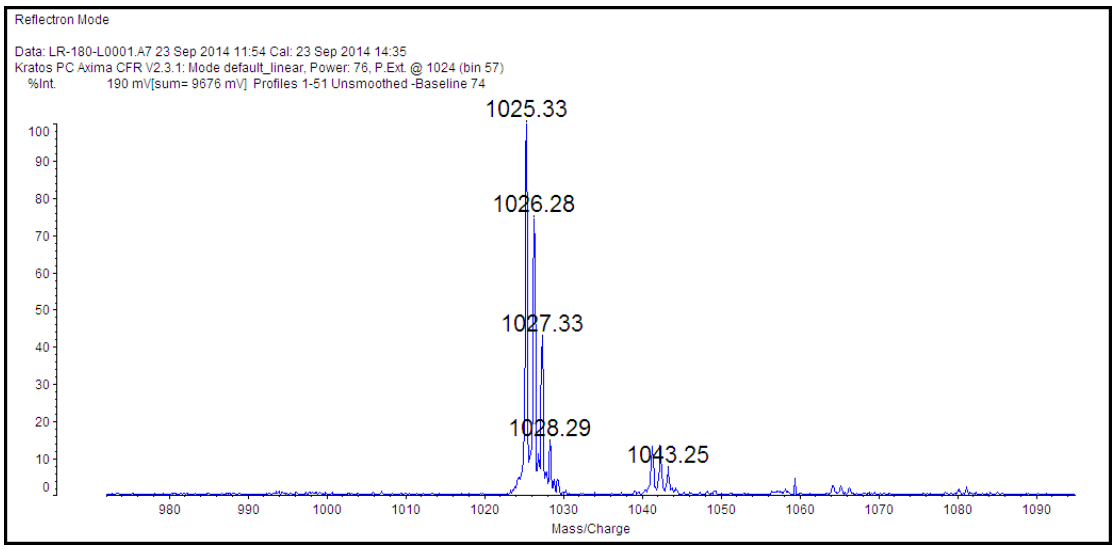

Fig. S5 MALDI-TOF spectrum of **PVBA8** in $CDCl_3$.

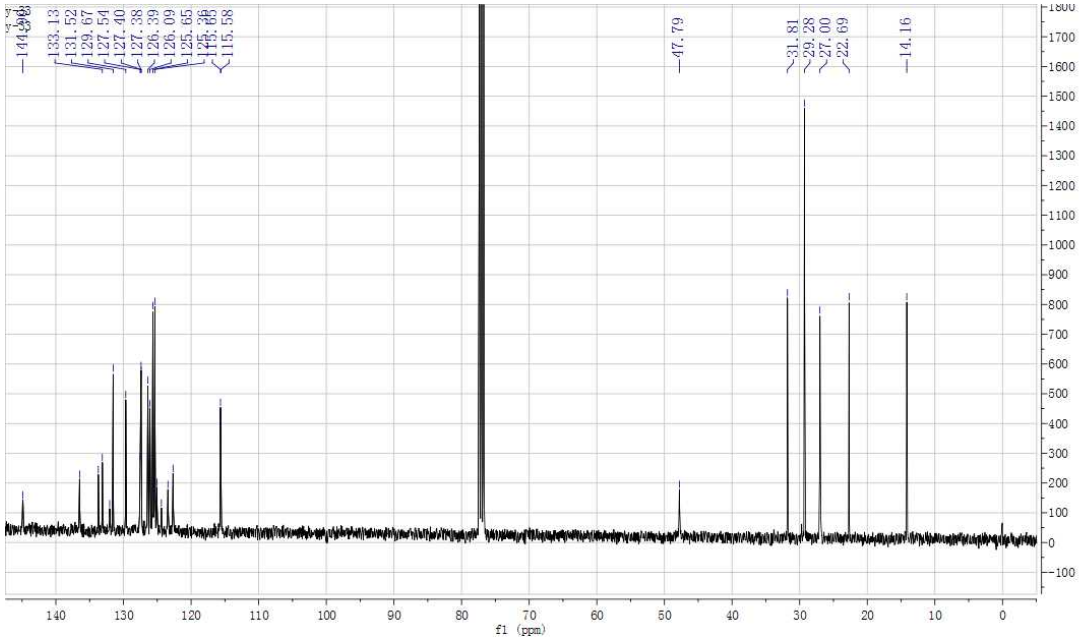

Fig. S6 ^{13}C NMR spectrum of **PVBA8** in $CDCl_3$.

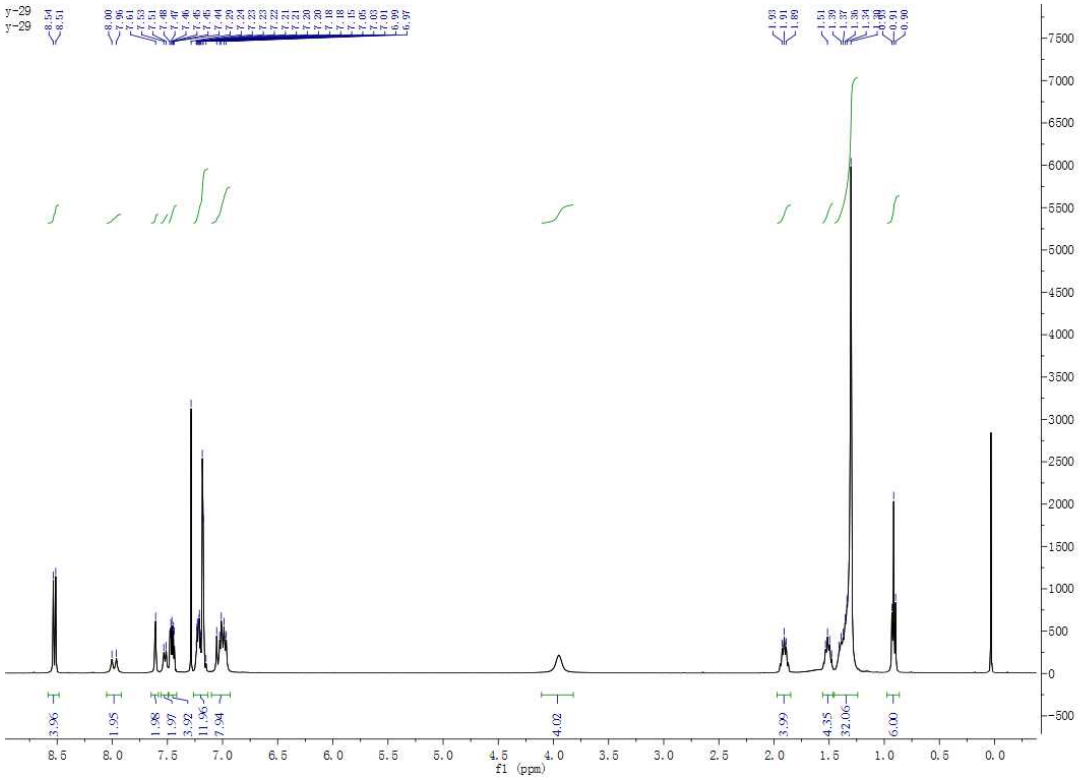

Fig. S7 ^{1}H NMR spectrum of **PVBA12** in $CDCl_3$.

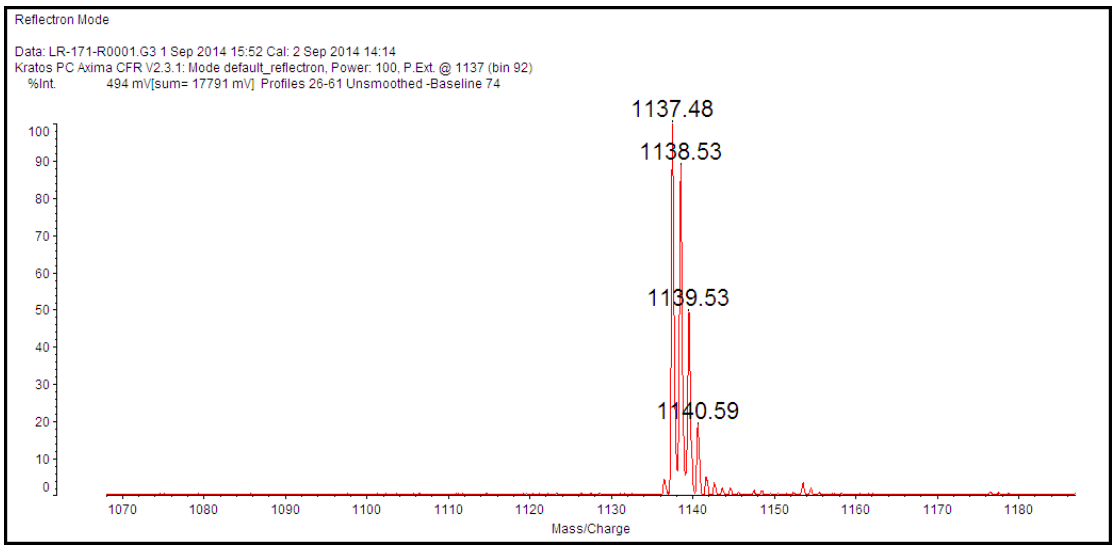

Fig. S8 MALDI-TOF spectrum of **PVBA12** in $CDCl_3$.

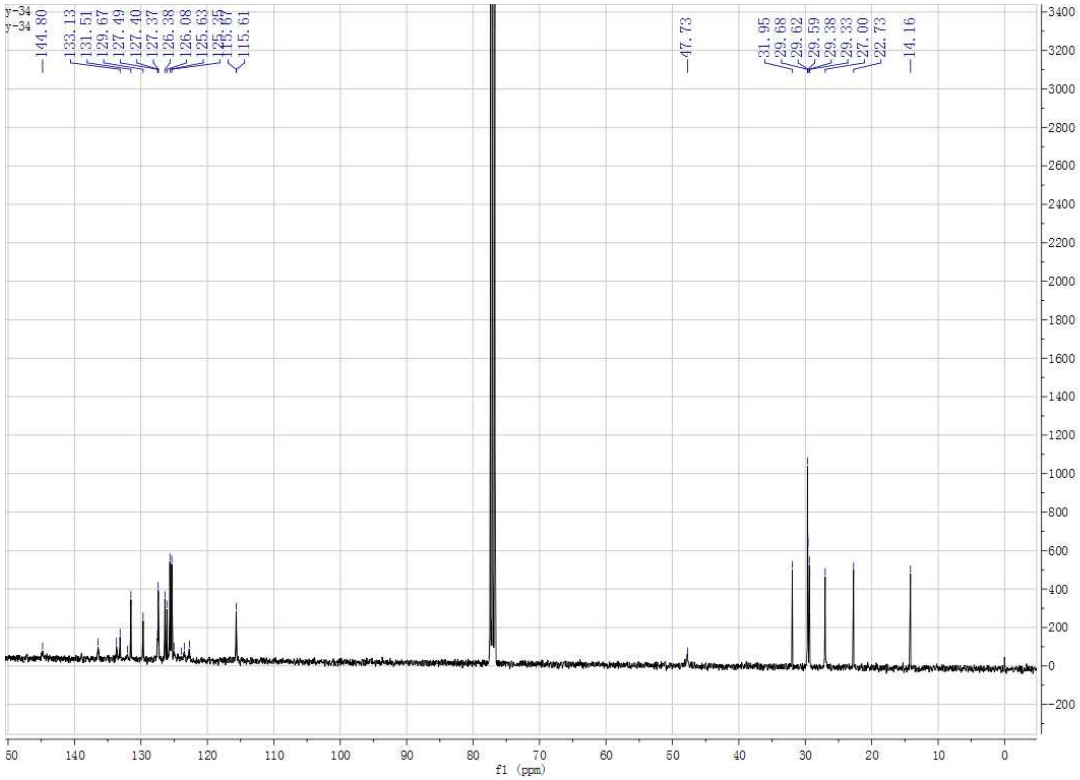

Fig. S9 ^{13}C NMR spectrum of **PVBA12** in $CDCl_3$.

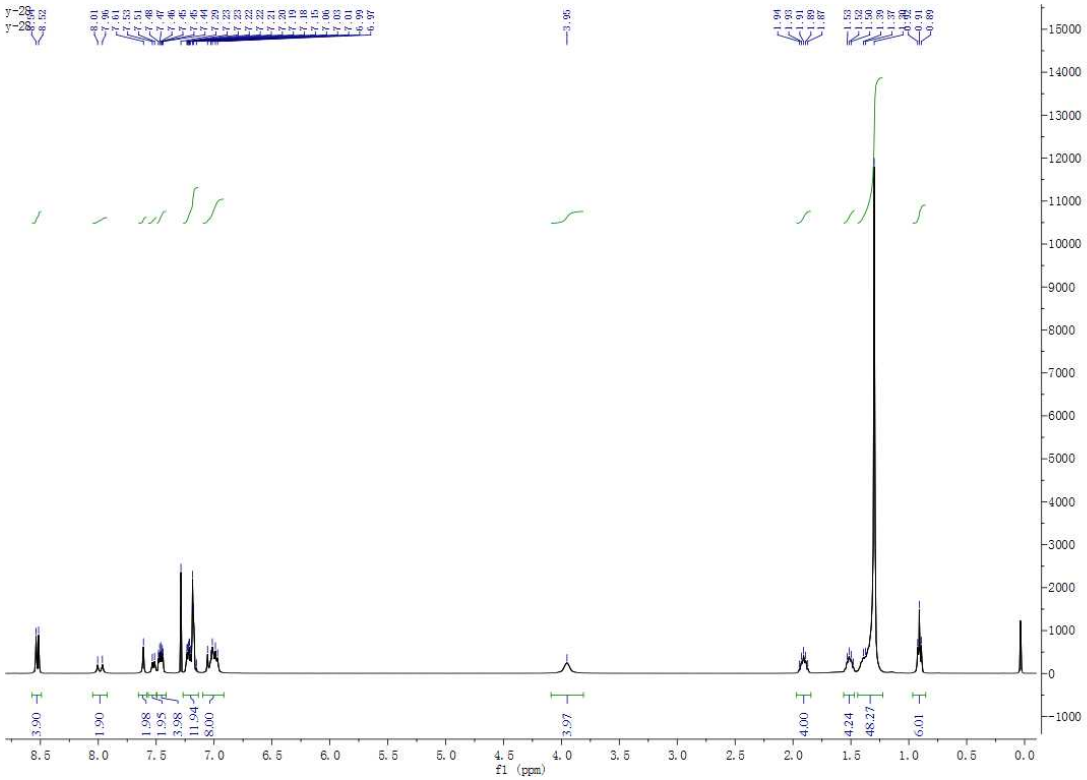

Fig. S10 ^{1}H NMR spectrum of **PVBA16** in $CDCl_3$.

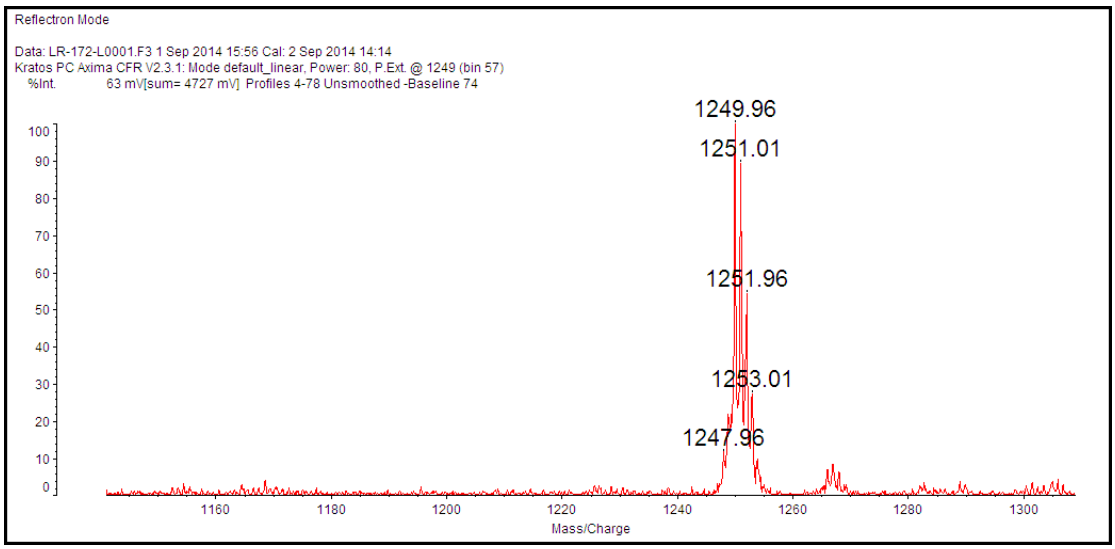

Fig. S11 MALDI-TOF spectrum of **PVBA16** in $CDCl_3$.

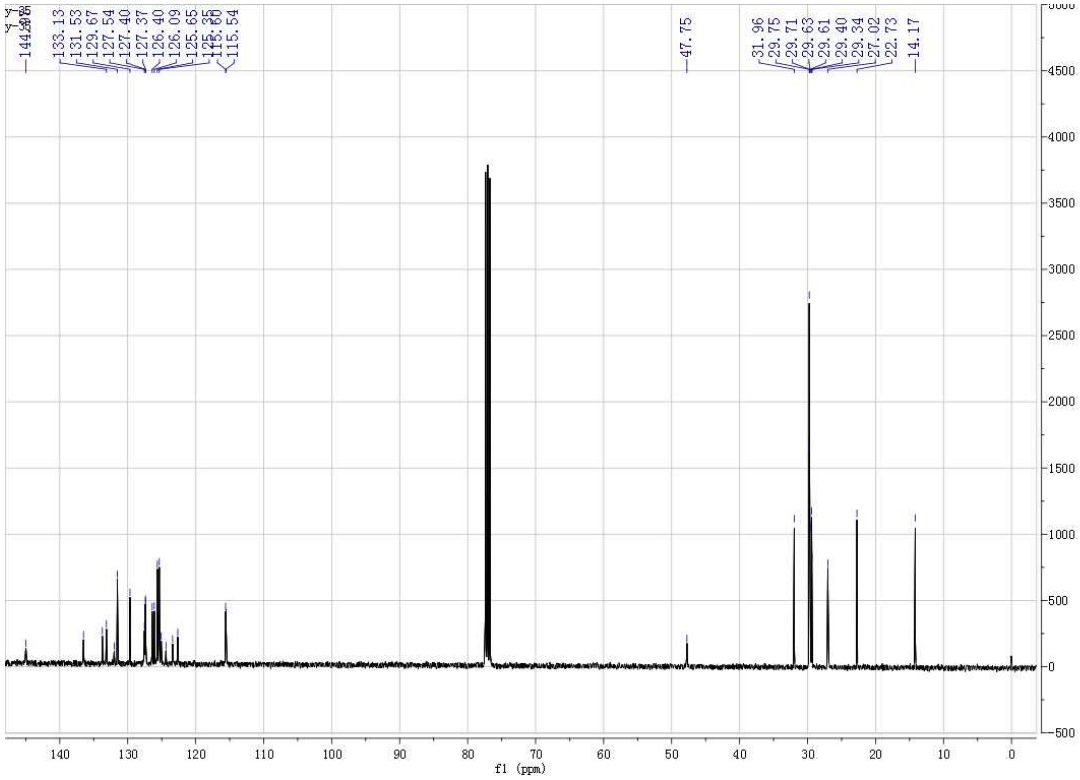

Fig. S12 ^{13}C NMR spectrum of **PVBA16** in $CDCl_3$.

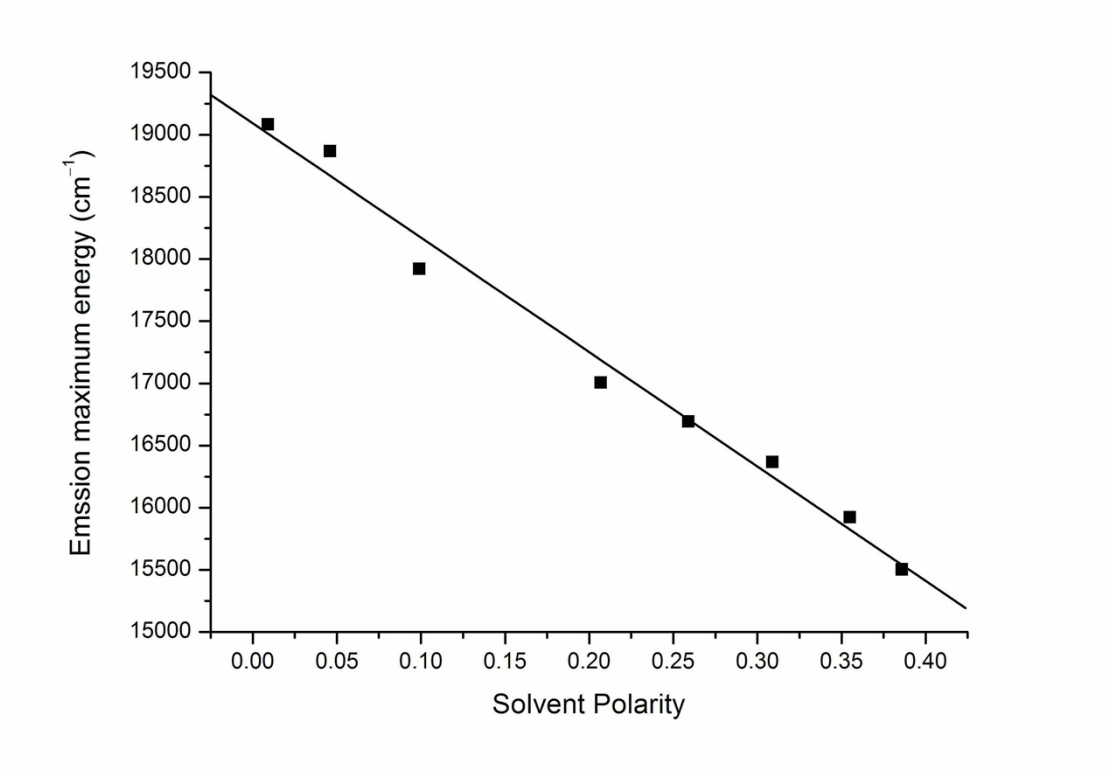

Fig. S13 Plot of emission maximum energy of **PVBA8** vs solvent polarity.

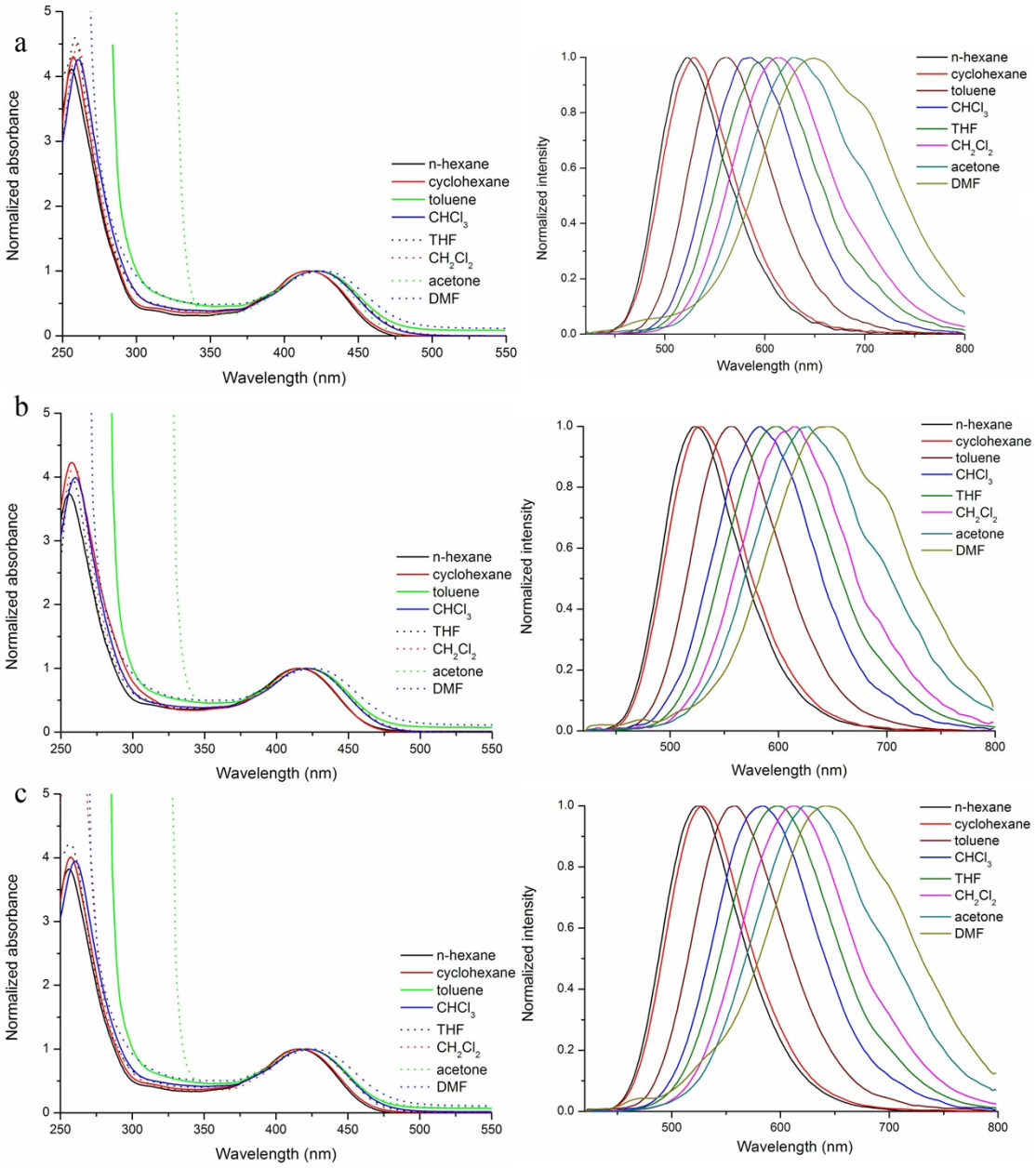

Fig. 14 UV-vis absorption (left) and fluorescence (right) of **PVBA2** (a), **PVBA12** (a) and **PVBA16** (c). The concentration of the samples was 10^{-5} M.

Table S1. The UV-vis absorption and fluorescent data of **PVBA2** and **PVBA8.**

	PVBA2			**PVBA8**		
	λ_{abs}	λ_{max}	Φ^a	λ_{abs}	λ_{max}	Φ^a
n-hexane	416	522	0.36	416	524	0.40
Cyclohexane	416	529	0.37	417	530	0.50
Toluene	422	561	0.23	422	558	0.33
$CHCl_3$	422	585	0.17	421	588	0.18
THF	422	603	0.16	422	600	0.16
CH_2Cl_2	422	614	0.14	422	611	0.18
Acetone	421	629	0.05	420	628	0.05
DMF	426	652	0.01	426	643	0.02

[a] The fluorescence quantum yields were obtained by comparing with a standard (9,10-diphenyl anthracene in benzene, Φ = 0.85).

Table S2. The UV-vis absorption and fluorescent data of **PVBA12** and **PVBA16**.

	PVBA12			**PVBA16**		
	λ_{abs}	λ_{max}	Φ^a	λ_{abs}	λ_{max}	Φ^a
n-hexane	415	523	0.59	416	525	0.54
Cyclohexane	416	528	0.49	416	528	0.50
Toluene	422	557	0.33	422	558	0.32
$CHCl_3$	422	583	0.25	421	584	0.25
THF	421	598	0.33	421	598	0.26
CH_2Cl_2	421	614	0.18	422	612	0.19
Acetone	420	626	0.10	420	622	0.08
DMF	425	646	0.03	426	642	0.02

[a] The fluorescence quantum yields were obtained by comparing with a standard (9,10-diphenyl anthracene in benzene, Φ = 0.85).

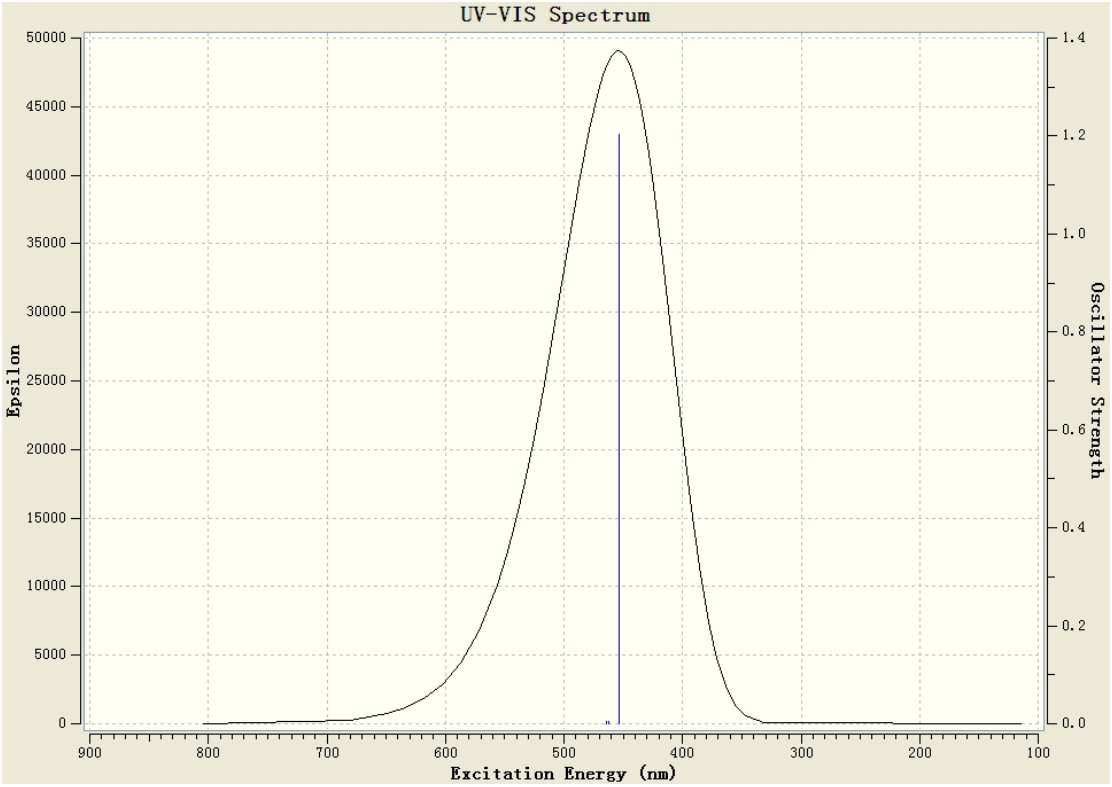

Fig. S15 Stimulated UV-vis absorption spectrum of **PVBA2**.

Table S3. Electronic transition data obtained by the TD/DFT-B3LYP/6-31G(d,p) calculation for **PVBA2**.

Transition assignment	E (eV)	λ_{abs} (nm)	Oscillator strength
HOMO-3→ LUMO (2.9%) HOMO-3→ LUMO+1 (7.6%) HOMO→ LUMO (29.3%) HOMO→ LUMO+1 (60.2%)	2.6705	464.28	0.0045
Transition assignment	E (eV)	λ_{abs} (nm)	Oscillator strength
HOMO-2→ LUMO (8.3%) HOMO-2→ LUMO+1 (3.3%) HOMO-1→ LUMO (67.4%) HOMO-1→ LUMO+1 (21.0%)	2.6819	462.31	0.0038
Transition assignment	E (eV)	λ_{abs} (nm)	Oscillator strength
HOMO-1→ LUMO (4.8%) HOMO-1→ LUMO+1 (42.0%) HOMO→ LUMO (40.8%) HOMO→ LUMO+1 (12.4%)	2.7319	453.84	1.2038

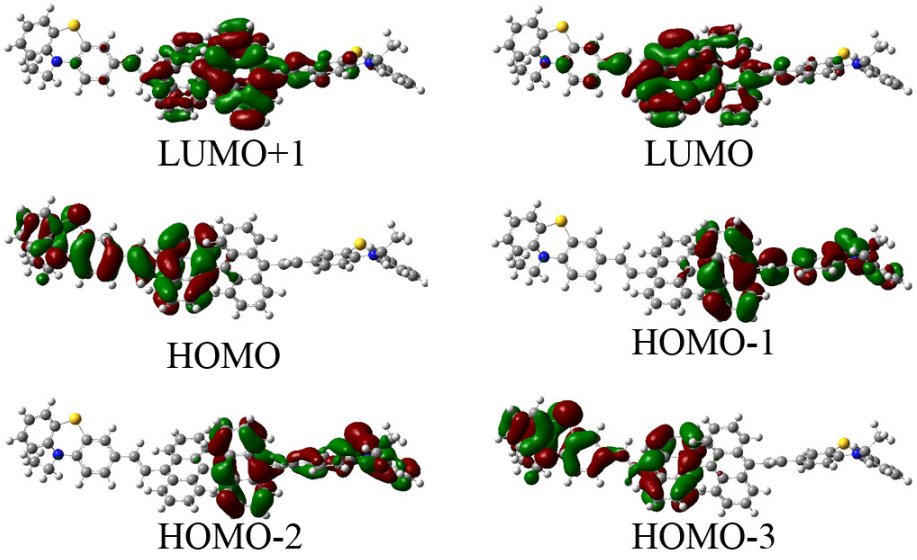

Fig. S16 electron density distributions of the frontier molecular orbitals of **PVBA2**.

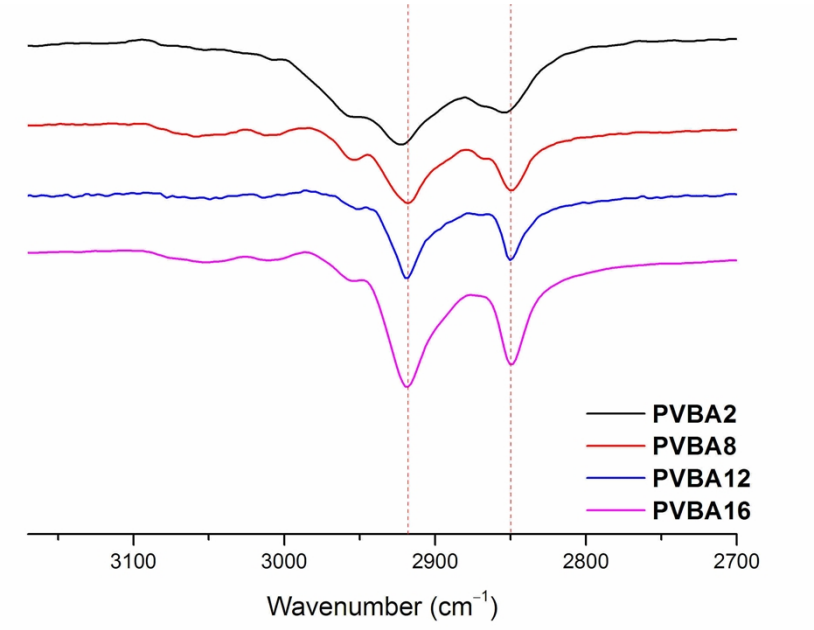

Fig. S17 IR spectra of the pristine solids.

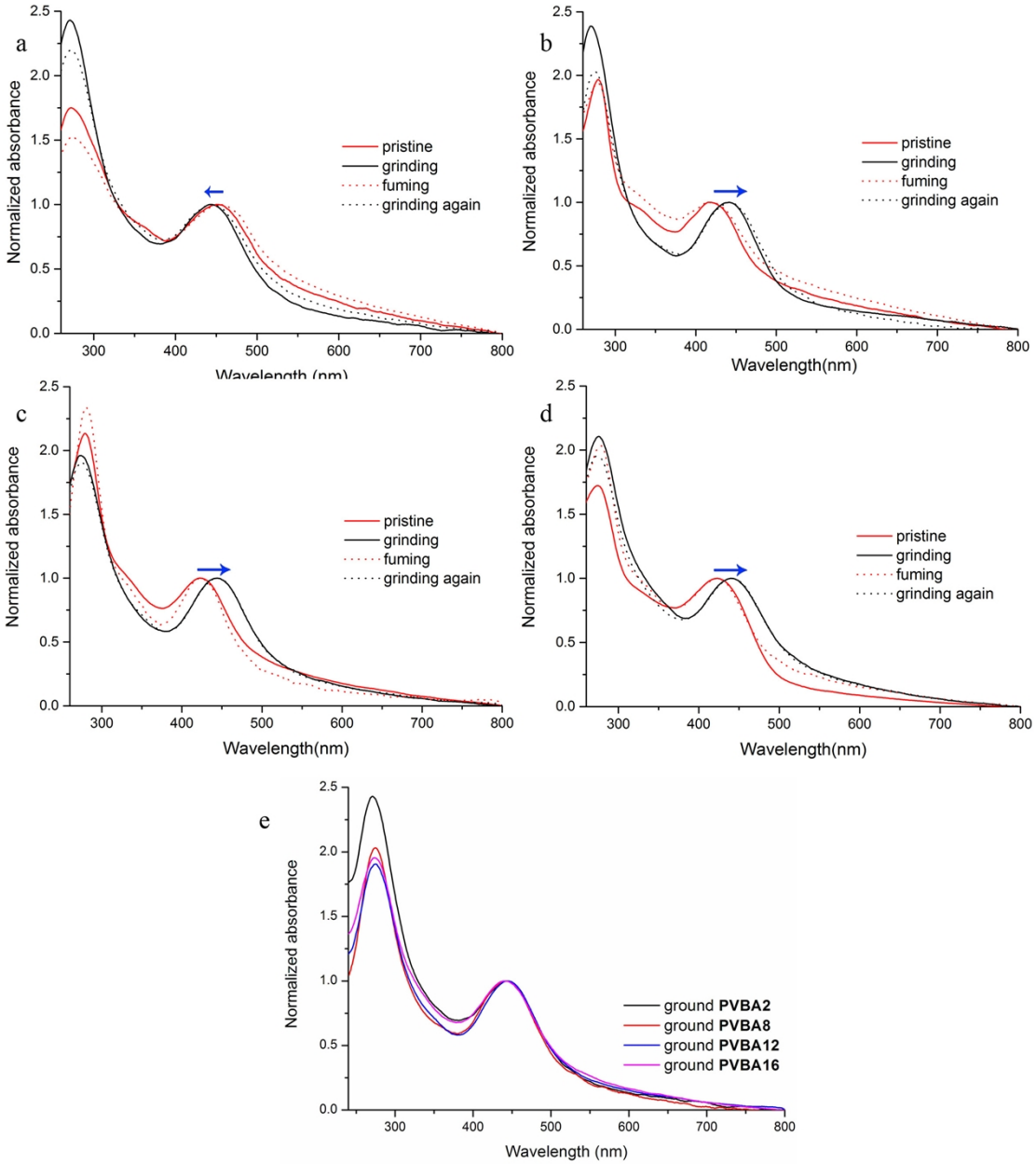

Fig. S18 Absorption spectra of (a) **PVBA2**, (b) **PVBA8**, (c) **PVBA12** and (d) **PVBA16** solids under external stimuli, (e) all ground powders.

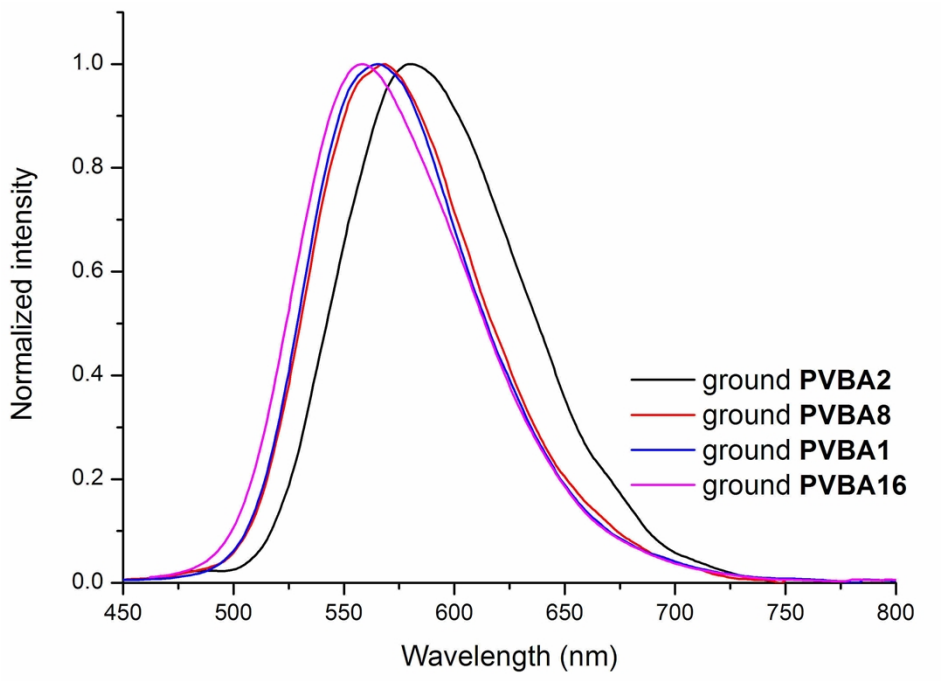

Fig. S19 Fluorescence spectra of ground **PVBAn**.

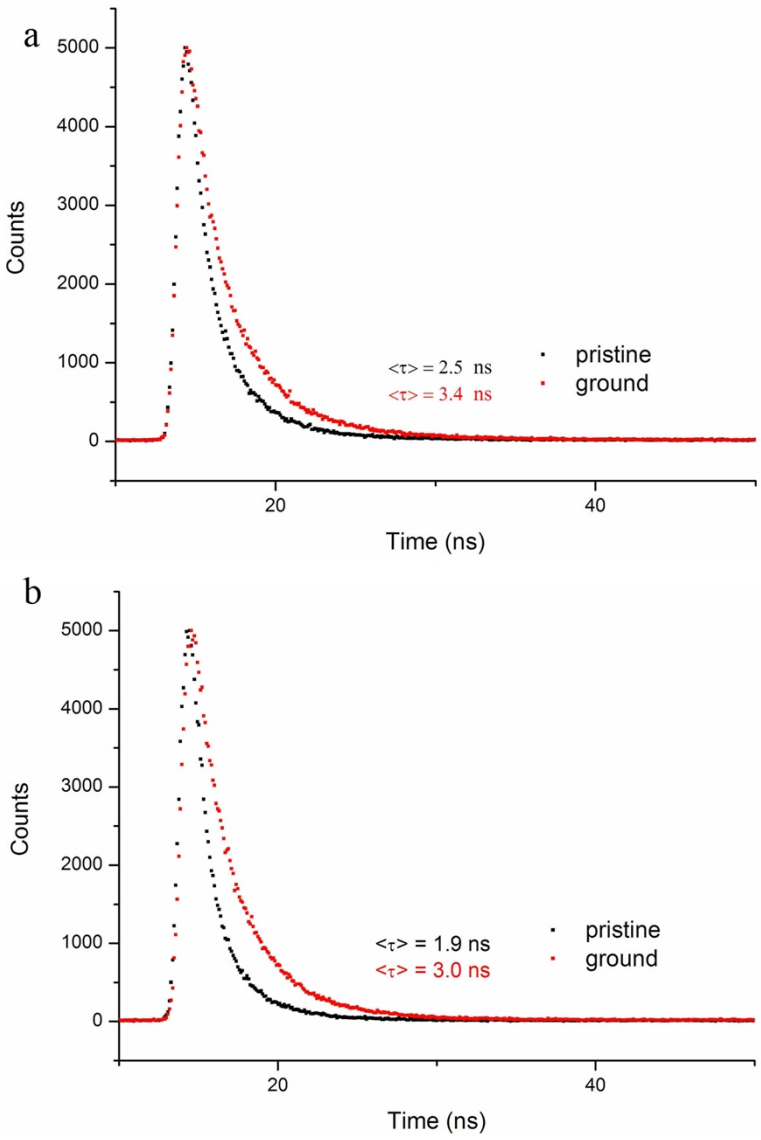

Fig. S20 Time resolved fluorescence spectra of (a) **PVBA2** and (b) **PVBA8** before and after grinding.

Table S4. Recovery times at different temperature for **PVBAn**.

PVBA2		**PVBA8**		**PVBA12**		**PVBA16**	
Time (s)	T (^{o}C)	Time (s)	T (^{o}C)	Time (s)	T (^{o}C)	Time (s)	T (^{o}C)
390	160	360	110	607	60	400	40
210	170	210	120	286	70	180	50
115	180	140	130	90	80	70	60
60	190	80	140	38	90	35	70
20	200	50	150	13	100	25	80
6	210	35	160	3	110	18	90
2	220	25	170	1	120	10	100
		15	180			2	110