

Supporting Information for

Aliphatic Hyperbranched Polyphosphate: a Novel Multicolor RTP Material with AIE Character

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Table S1. The specific data during P1~P3 synthesis.

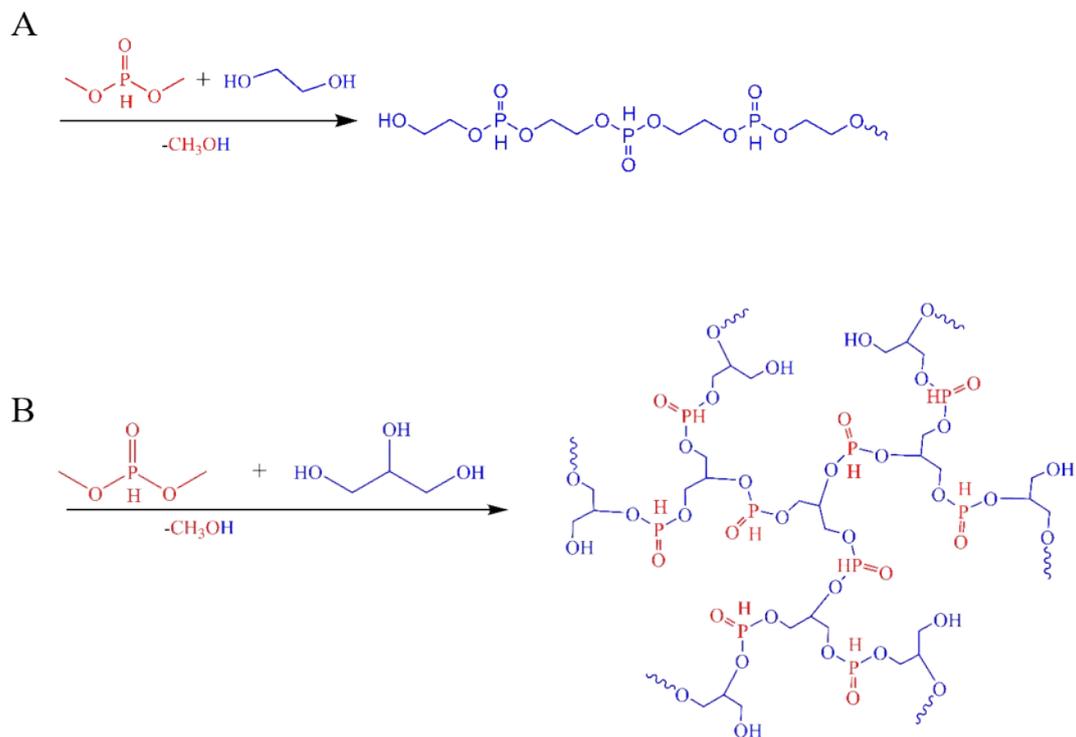
	P1	P2	P3
Reactant A	TEP	DEP	DEP
Reactant B	EG	EG	GI
A/B(mol/mol)	1:1.6	1:1.2	1:0.8
m _A /g (n _A /mol)	27.32 (0.15)	22.01 (0.2)	22.01 (0.20)
m _B /g (n _B /mol)	14.90 (0.24)	14.90 (0.24)	14.73 (0.16)
-OCH ₂ CH ₃ /-OH (mol/mol)	3:3.2	1:1.2	1:1.2

Where m_A: the mass of reactant A

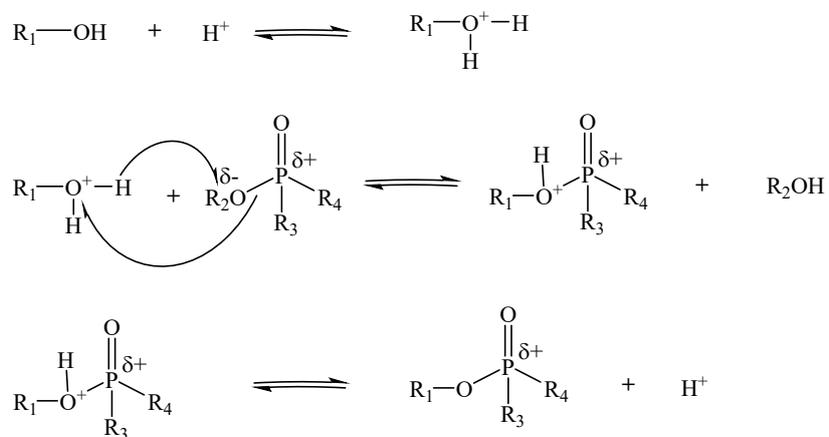
n_A: the amount of substance of reactant A

m_B: the mass of reactant B

n_B: the amount of substance of reactant B



Scheme S1. (A) The synthetic route of P2; (C) The synthetic route of P3



Scheme S2. The possible transesterification polymerization reaction mechanism.

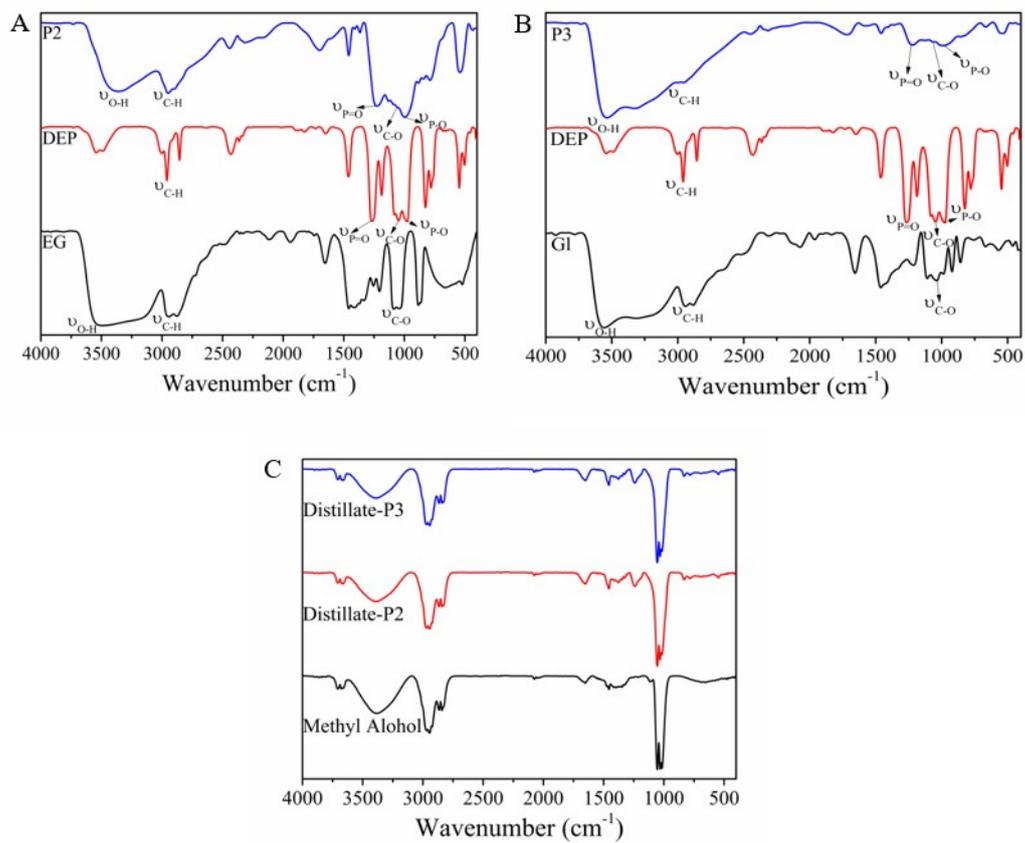


Figure S1. (A) FTIR spectra of EG, DEP and P2; (B) FTIR spectra of GI, DEP and P3; (C) FTIR spectra of standard methyl alcohol and distillates during P2 and P3 synthesis process.

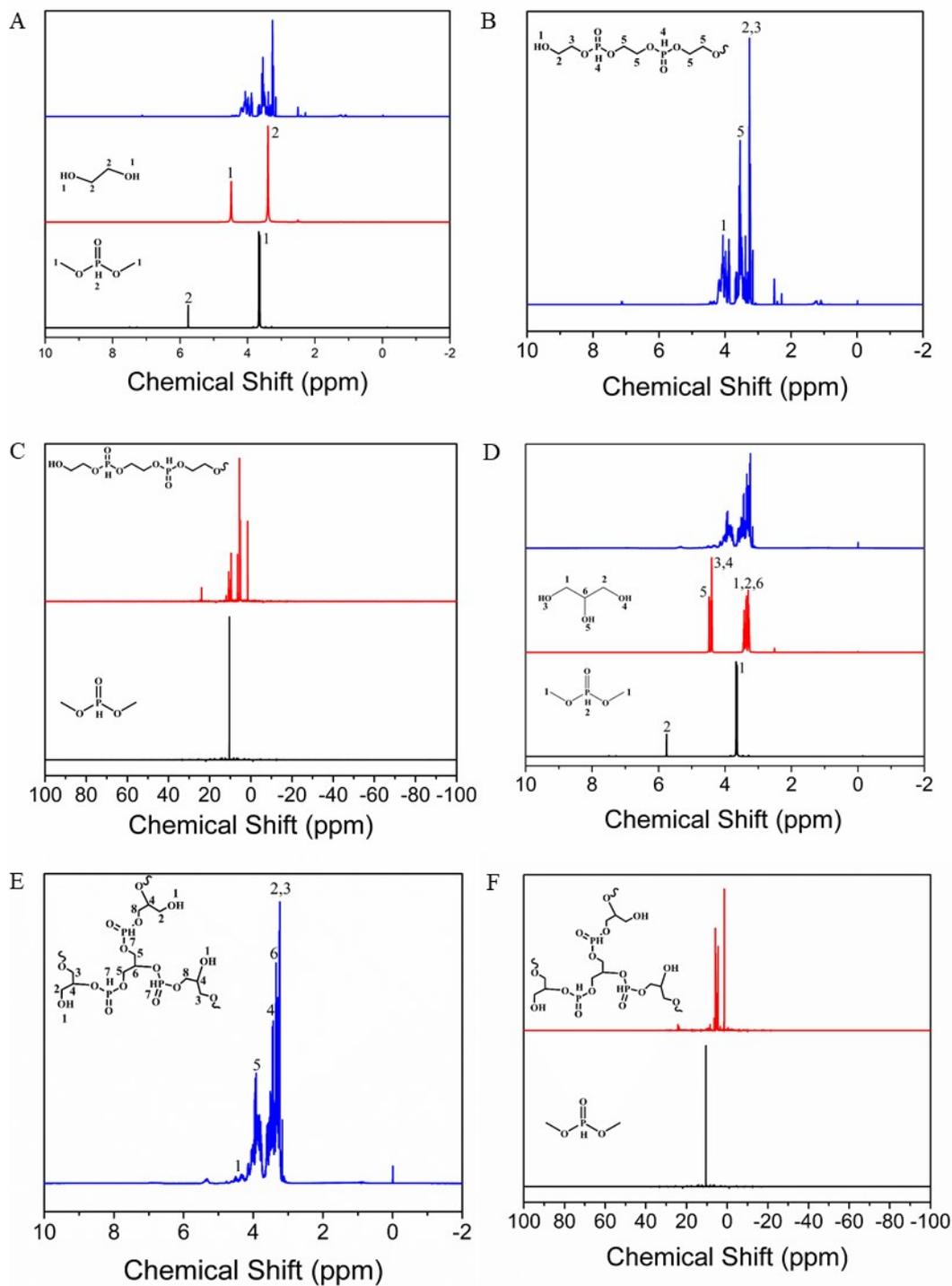


Figure S2. (A) ^1H NMR spectra of DEP, EG and P2; (B) ^1H NMR spectra of P2; (C) ^{31}P NMR spectra of DEP and P2; (D) ^1H NMR spectra of DEP, G1 and P3; (E) ^1H NMR spectra of P3; (F) ^{31}P NMR spectra of DEP and P3.

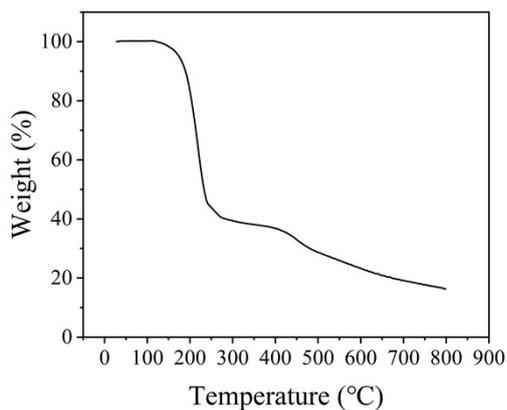


Figure S3. TGA cure of P1

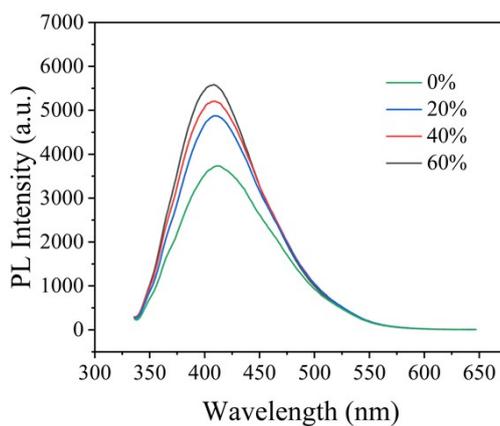


Figure S4. The PL intensity of P1 with different volume ratios of petroleum ether in ethanol / petroleum ether solvent mixtures (50 mg/mL).

Table S2. Stoke shifts of P1 solution under different concentration.

Concentration/mg·mL ⁻¹	λ_{ex}/nm	λ_{em}/nm	Stokes shift/nm
10	345	402	57
15	345	400	55
20	345	402	57
30	345	402	57
40	345	402	57
50	345	402	57

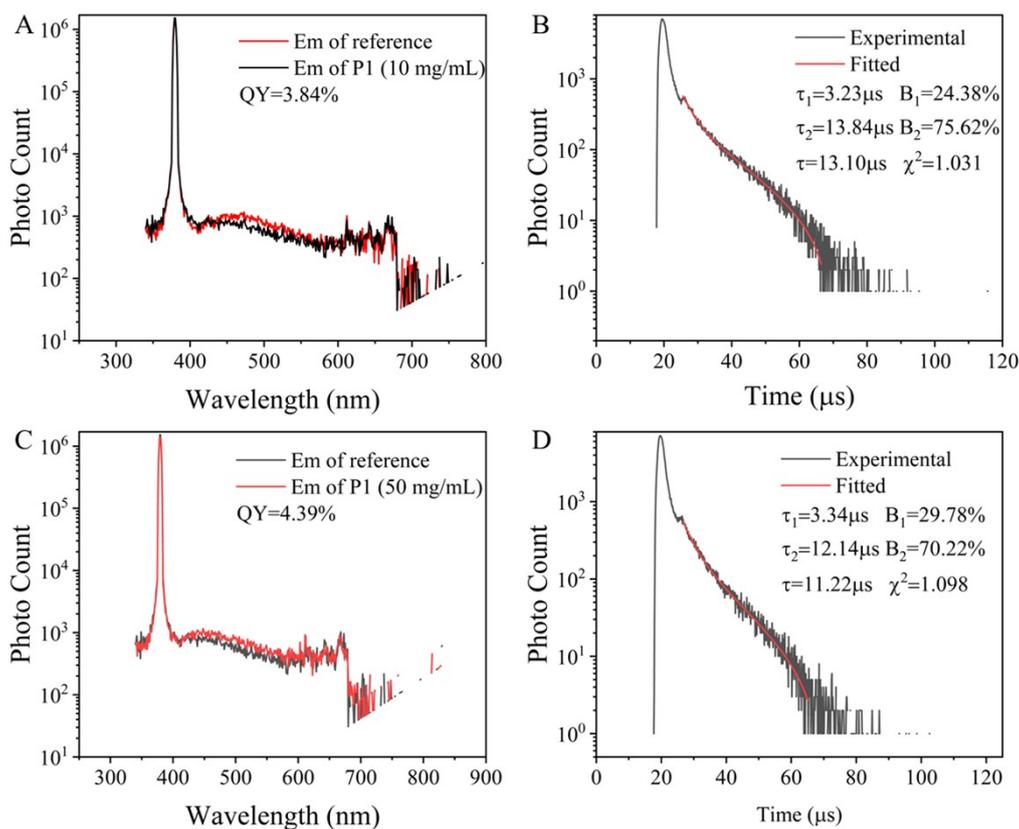


Figure S5. (A) Absolute photoluminescence quantum yield of P1 (10 mg/mL); (B) Transient photoluminescence decay curve of P1 (10 mg/mL); (C) Absolute photoluminescence quantum yield of P1 (50 mg/mL); (D) Transient photoluminescence decay curve of P1 (50 mg/mL).

Table S3 k_r and k_{nr} of P1

Concentration/mg·mL ⁻¹	QY/%	$\tau/\mu\text{s}$	$k_r/\times 10^3\cdot\text{s}^{-1}$	$k_{nr}/\times 10^4\cdot\text{s}^{-1}$
10	3.84	13.10	2.93	7.34
50	4.39	11.22	3.91	8.52
Pure state	22.42	12.82	17.48	6.05

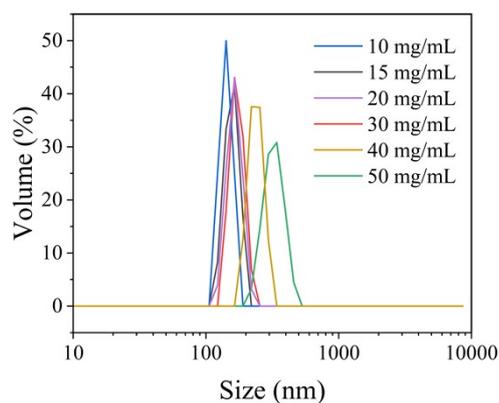


Figure S6. Aggregates size distributions of the P1 at different concentration in aqueous solution measured at room temperature.

Table S4. DFT calculation results of HOMO-LUMO energy levels of the conformations with 1~4 first generation P1 molecules, 1st~3rd generation P1 with one molecule, 1~4 first generation P3 molecules and 1~3 second generation P3 molecules.

Gnenration number	Molecule number	E	E	Energy gap (a.u.)	Energy gap (eV)	
		(HOMO) (a.u.)	(LUMO) (a.u.)			
P1	1	-0.27636	0.04041	0.31677	8.619755	
	2	-0.2533	0.02997	0.28327	7.708173	
	3	-0.24659	0.02251	0.2691	7.322588	
	4	-0.24334	0.01937	0.26271	7.148707	
	2	1	-0.25754	0.01596	0.2735	7.442318
	3	1	-0.25124	0.01749	0.26873	7.31252
	P4	1	-0.26256	0.03748	0.30004	8.164508
2		-0.24998	0.02477	0.27475	7.476332	
3		-0.23629	0.03263	0.26892	7.31769	
4		-0.24217	0.01573	0.2579	7.01782	
2		1	-0.2668	0.03069	0.29749	8.095119
2		2	-0.26476	0.02628	0.29104	7.919606
3		3	-0.25444	0.01682	0.27126	7.381364

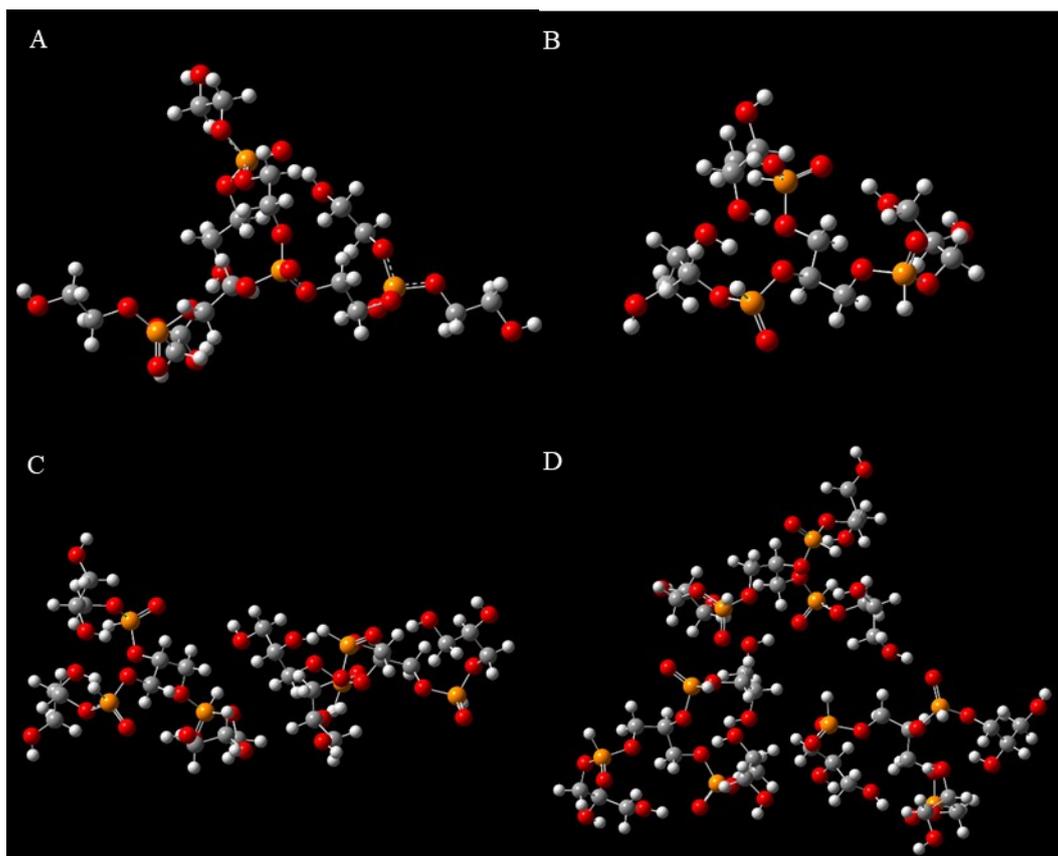


Figure S7. Optimized conformations of the second generation P1 with one molecule (A) and the second generation P3 with molecules increasing from 1 to 3 (B~D)

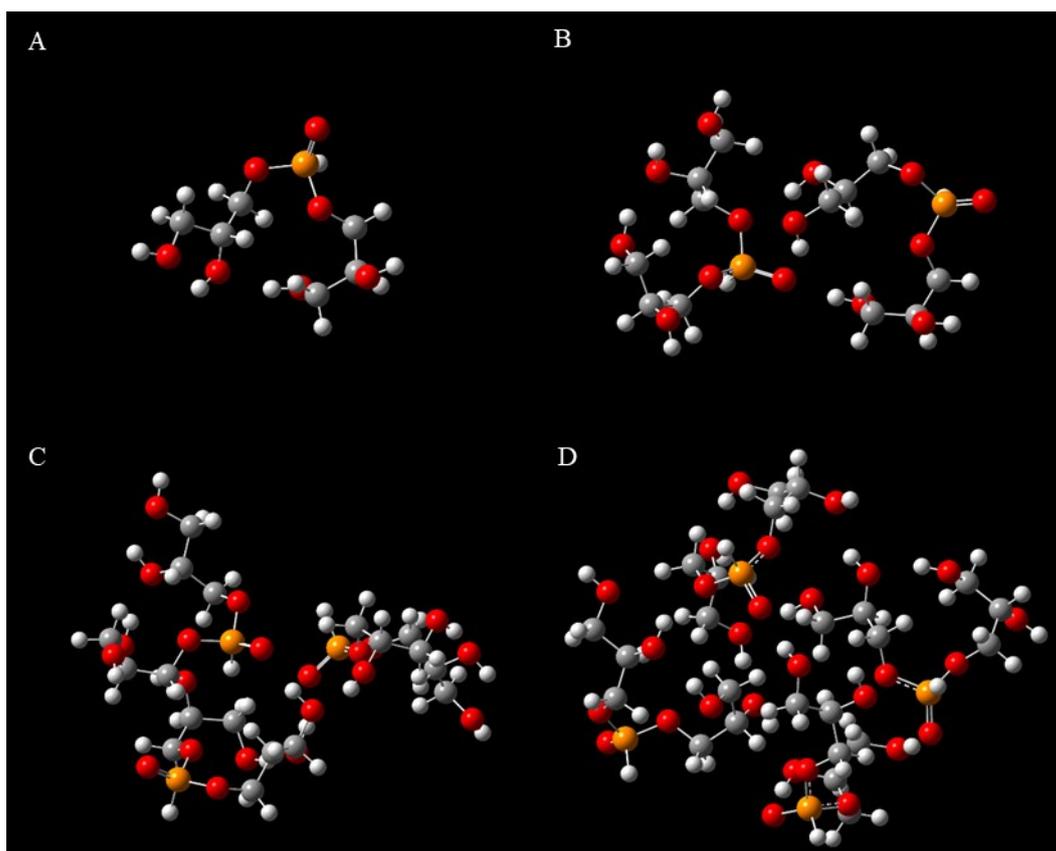


Figure S8. Optimized conformations of the first generation P3 with molecules increasing from 1 to 4 (A~D).

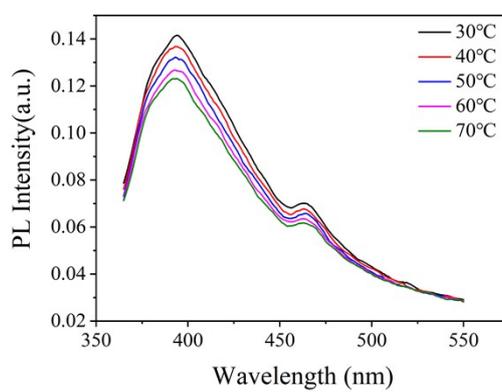


Figure S9. The emission spectra of P1 aqueous solution (50 mg/mL) at different temperature.

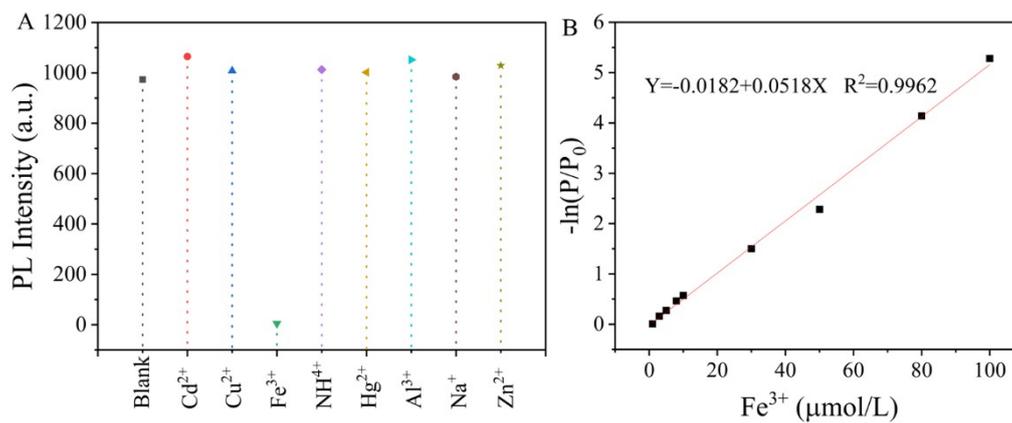


Figure S10. (A) Photoluminescence intensity of P1 (10mg/mL) in the presence of various metal ions (10^{-4} mol/L) in aqueous; (B) The dependence of $-\ln(P/P_0)$ on the concentration of Fe^{3+} in the range of $1 \times 10^{-6} \sim 1 \times 10^{-4}$ mol/L