

Supporting Information

AIE-active polysulfates via a sulfur (VI) fluoride exchange (SuFEx) click reaction and investigation of their two-photon fluorescence and cyanide detection in water and in living cells

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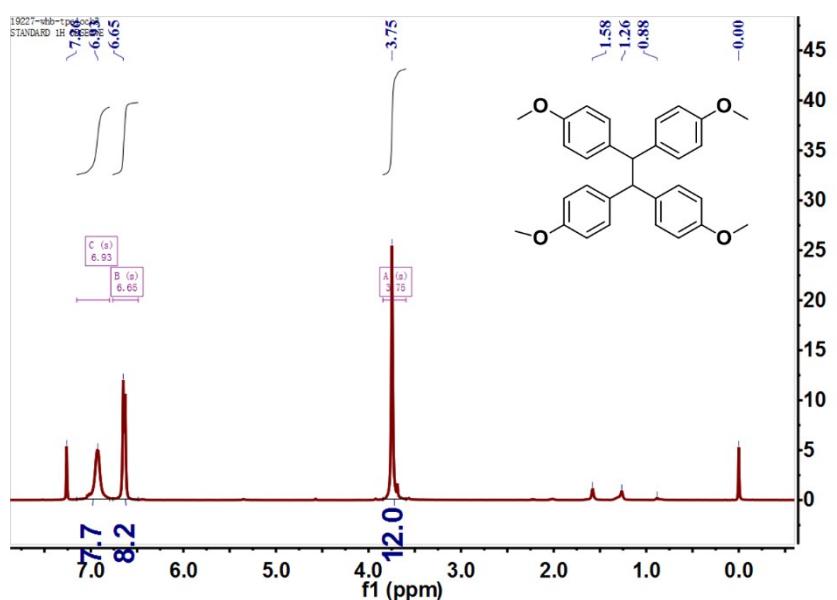


Fig. S1 ^1H NMR spectral of TPE4OCH $_3$ (CDCl $_3$).

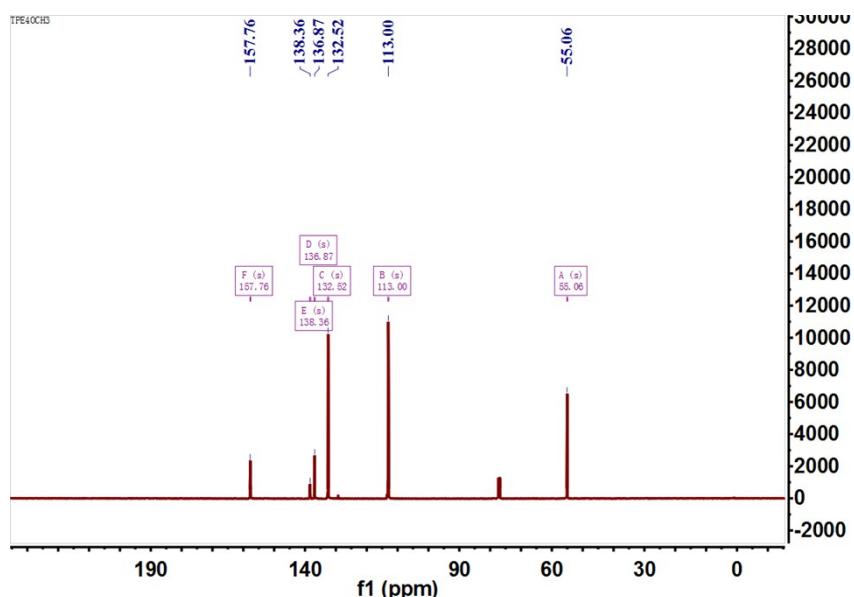


Fig. S2 ^{13}C NMR spectral of TPE4OCH $_3$ (CDCl $_3$).

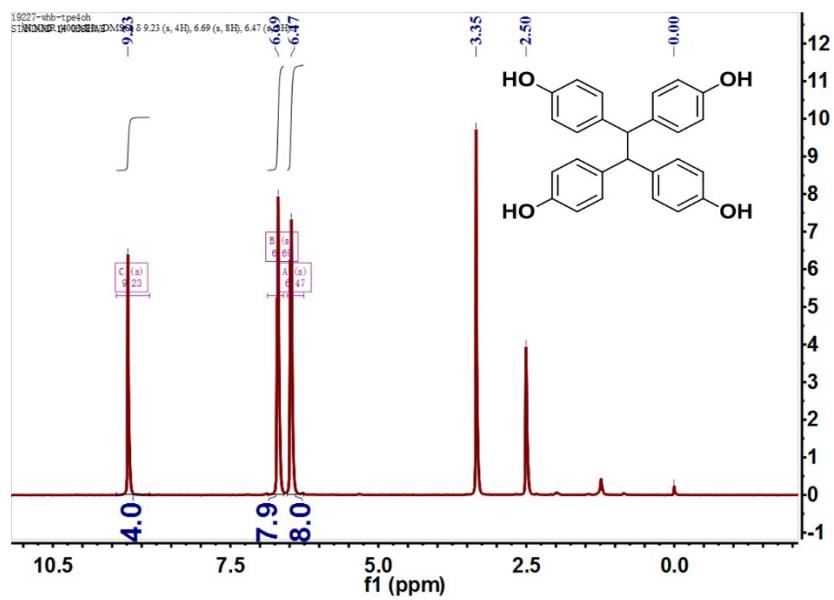


Fig. S3 ¹H NMR spectral of TPE4OH (DMSO-d₆).

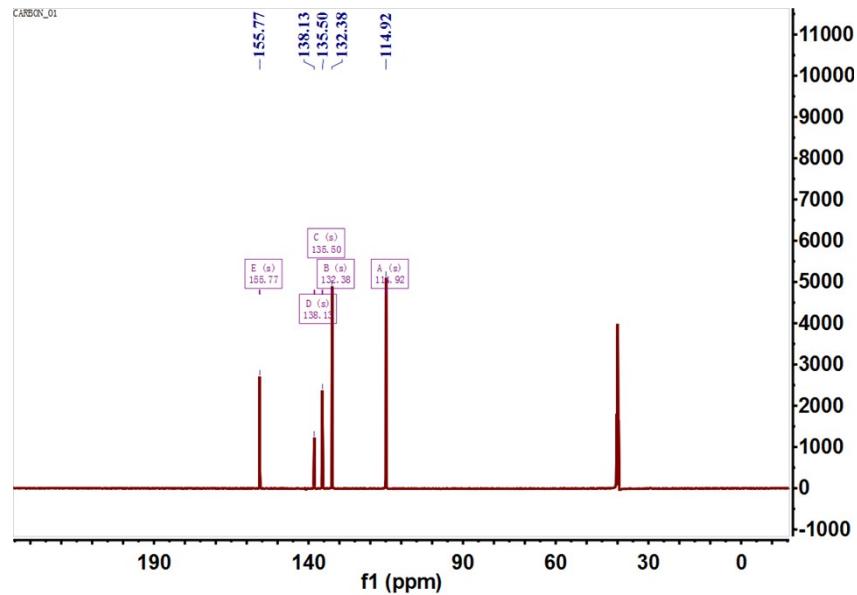


Fig. S4 ¹³C NMR spectral of TPE4OH (DMSO-d₆).

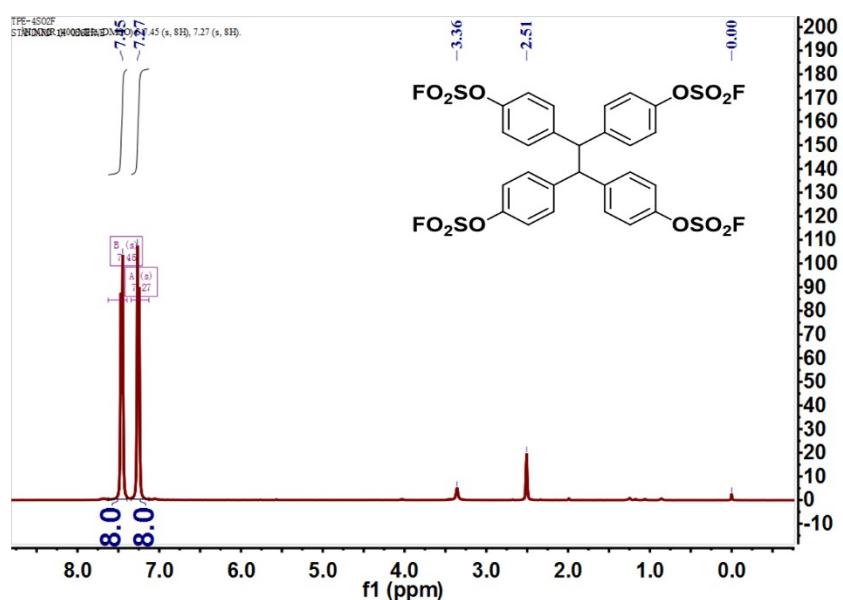


Fig. S5 ¹H NMR spectral of TPE4SO₂F (DMSO-d₆).

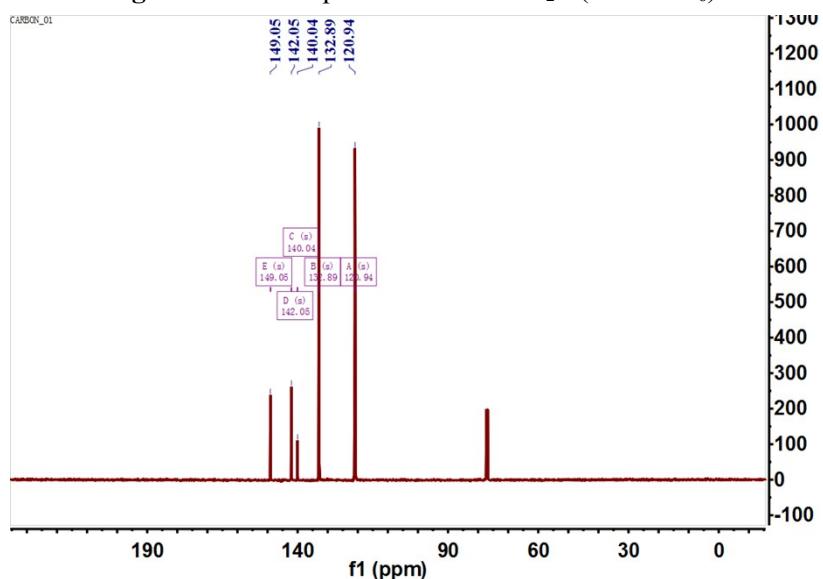


Fig. S6 ¹³C NMR spectral of TPE4SO₂F (CDCl₃).

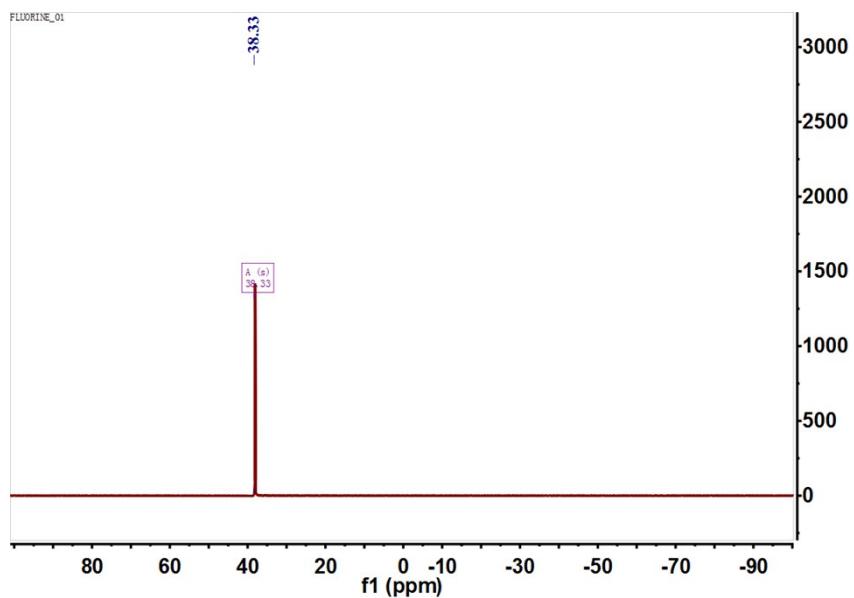
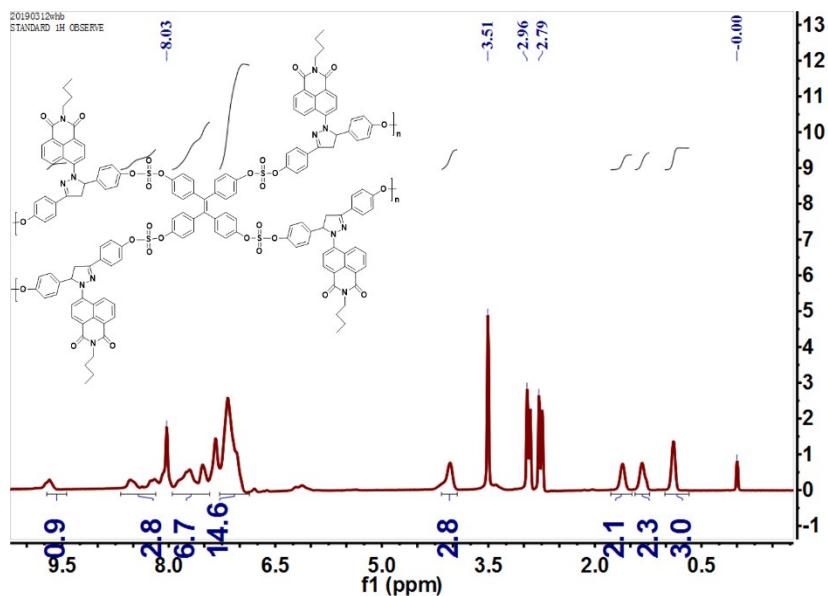


Fig. S7 ^{19}F NMR spectral of TPE4SO₂F (CDCl₃).



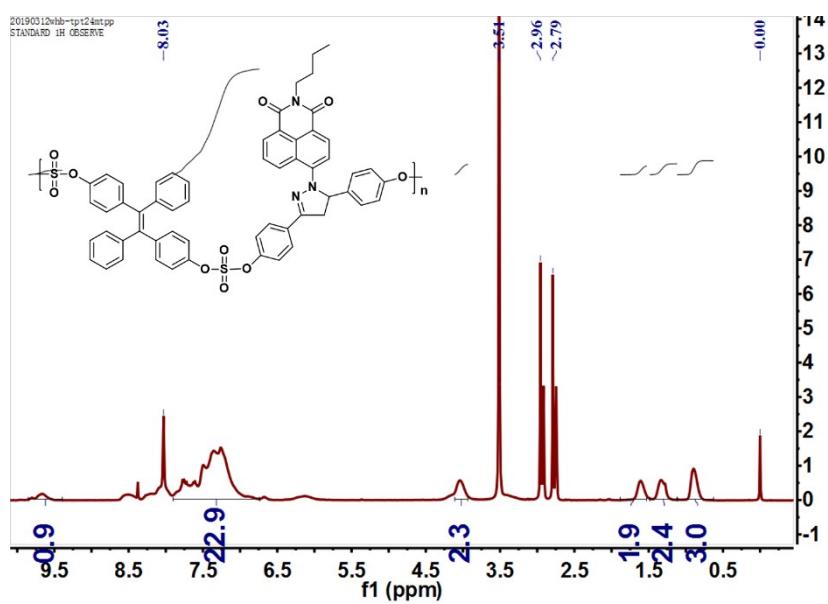


Fig. S9 ^1H NMR spectral of P2 (DMF- d_7).

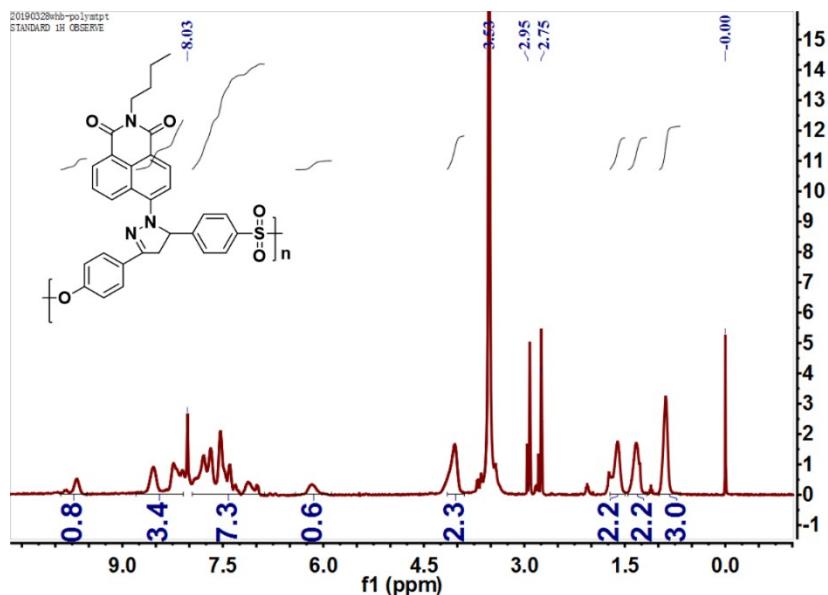


Fig. S10 ^1H NMR spectral of P3 (DMF- d_7).

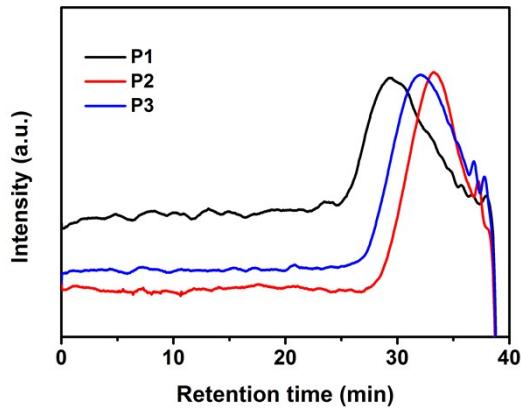


Fig. S11 GPC analysis of the P1, P2 and P3 (obtained at 70 °C) with DMF as a mobile phase at a flow rate of 1 mL min⁻¹ and with column temperature of 30 °C.

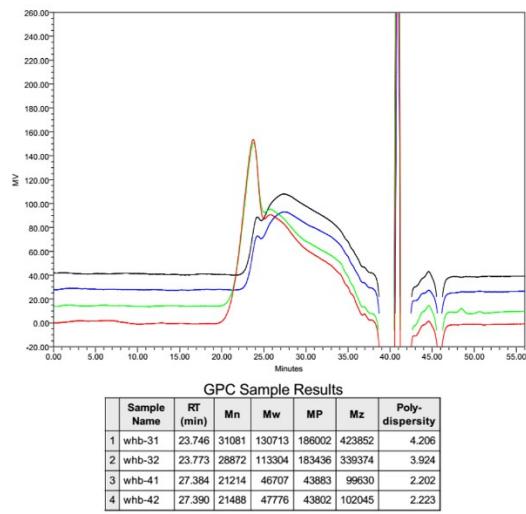


Fig. S12 GPC analysis of the P1 (obtained at 100 °C) with DMF as a mobile phase at a flow rate of 1 mL min⁻¹ and with column temperature of 30 °C.

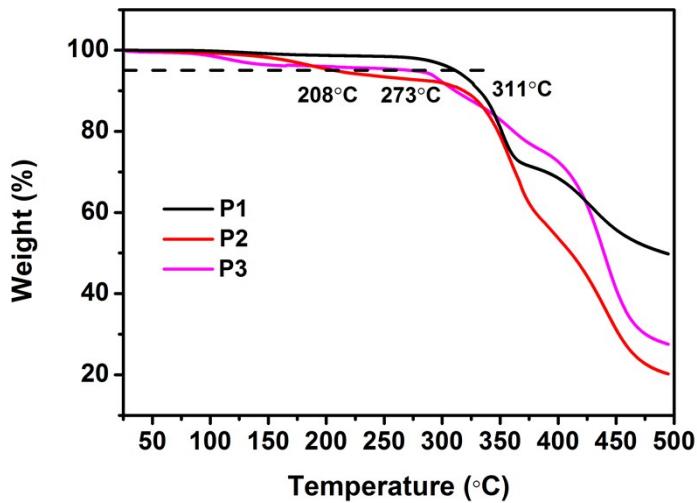


Fig. S13 TGA thermograms of the polymers.

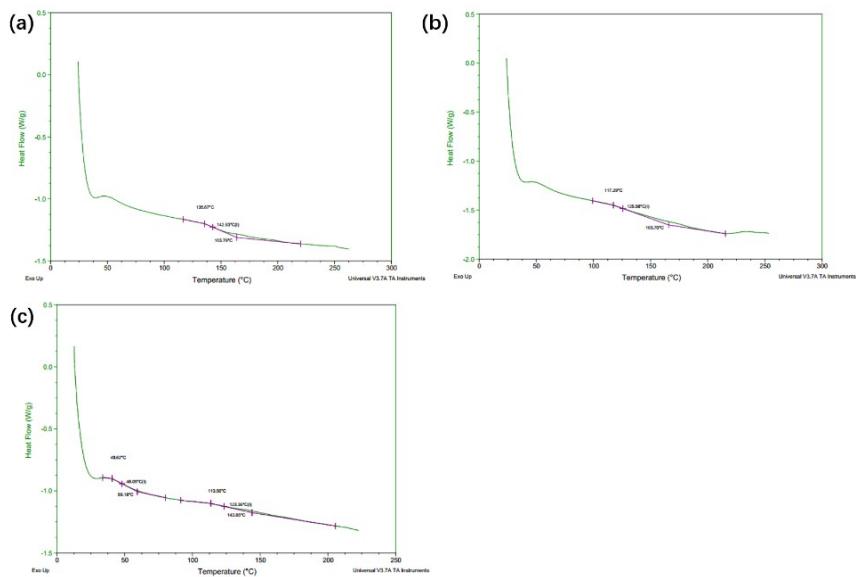


Fig.S14 DSC thermograms of the polymers. (a) P1, (b) P2 and (c) P3.

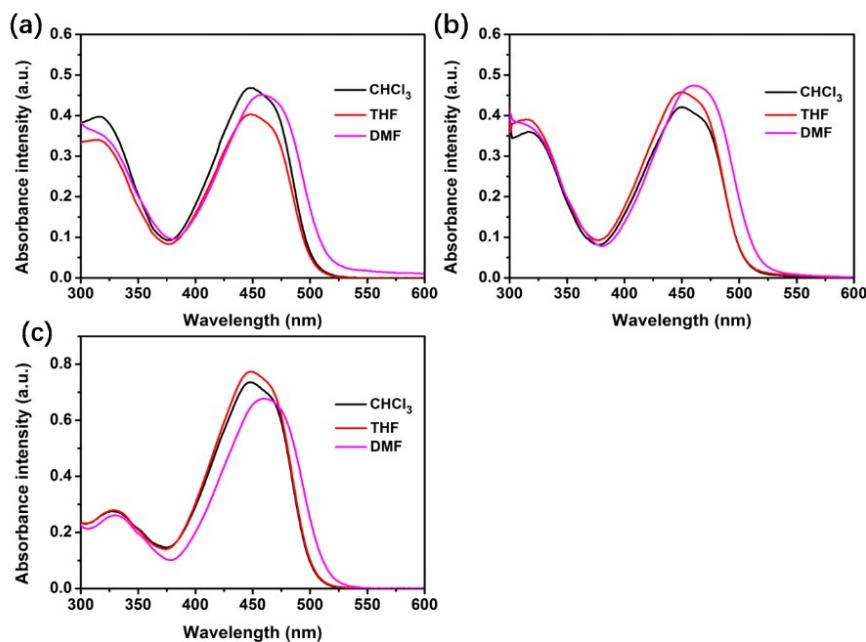


Fig. S15 The absorbance spectra of polymers in different solvents. (a) P1, (b) P2 and (c) P3. Concentration: 2 μ M.

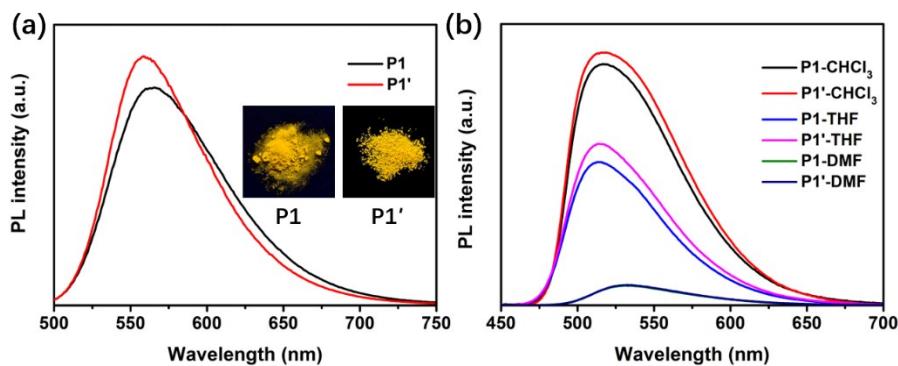


Fig. S16 (a) The solid fluorescent spectra of the branched polymer with different molecular weight (P1: 17950 g mol⁻¹ and P1': 31080 g mol⁻¹) and the inset pictures are the corresponding images under the UV light at 365 nm. Excitation wavelength: 470 nm. (b) The fluorescent spectra of P1 and P1' in different solvents. Excitation wavelength: 450 nm.

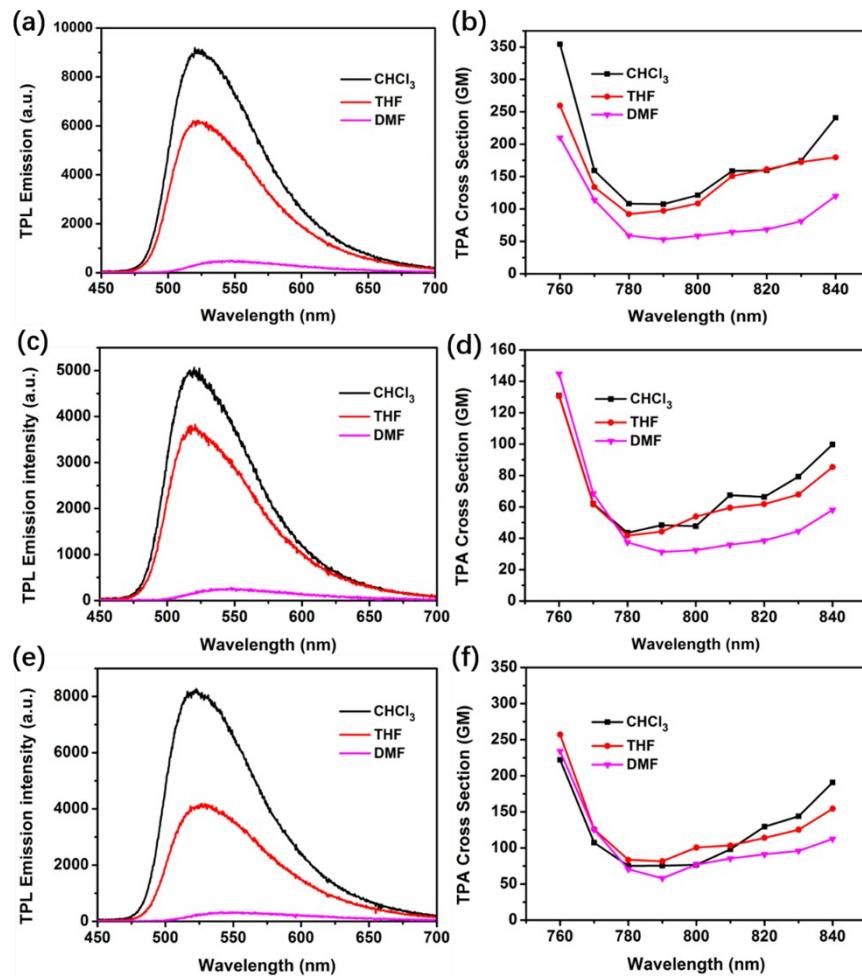


Fig. S17 TPF spectra and TPA spectra of polymers: (a, b) P1, (c, d) P2 and (e, f) P3 in different solvent at same concentration. Excitation wavelength: 840 nm.

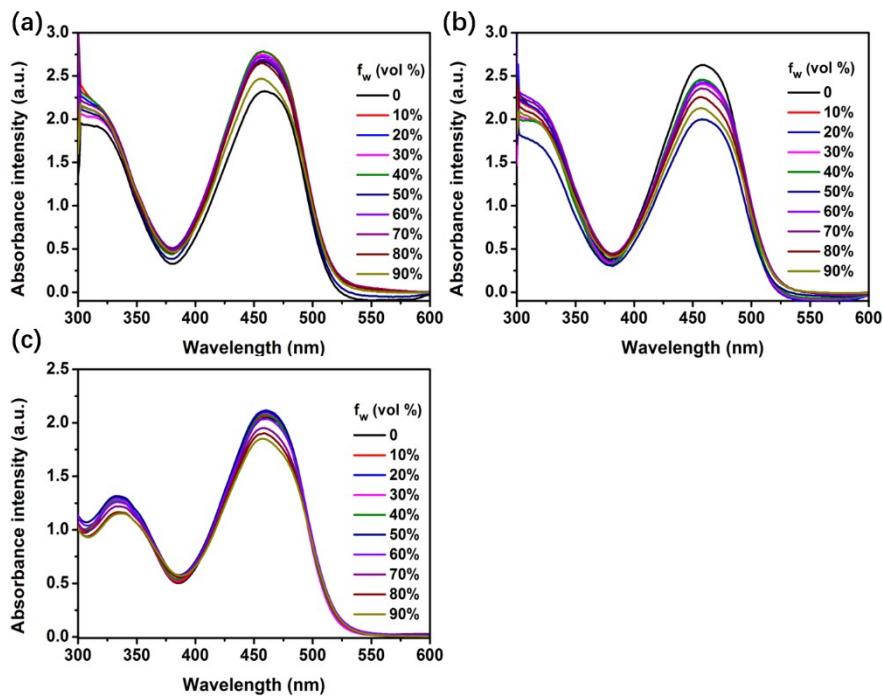


Fig. S18 (a) The absorbance spectra of polymers in DMF/water with different water fractions. (a) P1, (b) P2 and (c) P3. Concentration: 10 μ M.

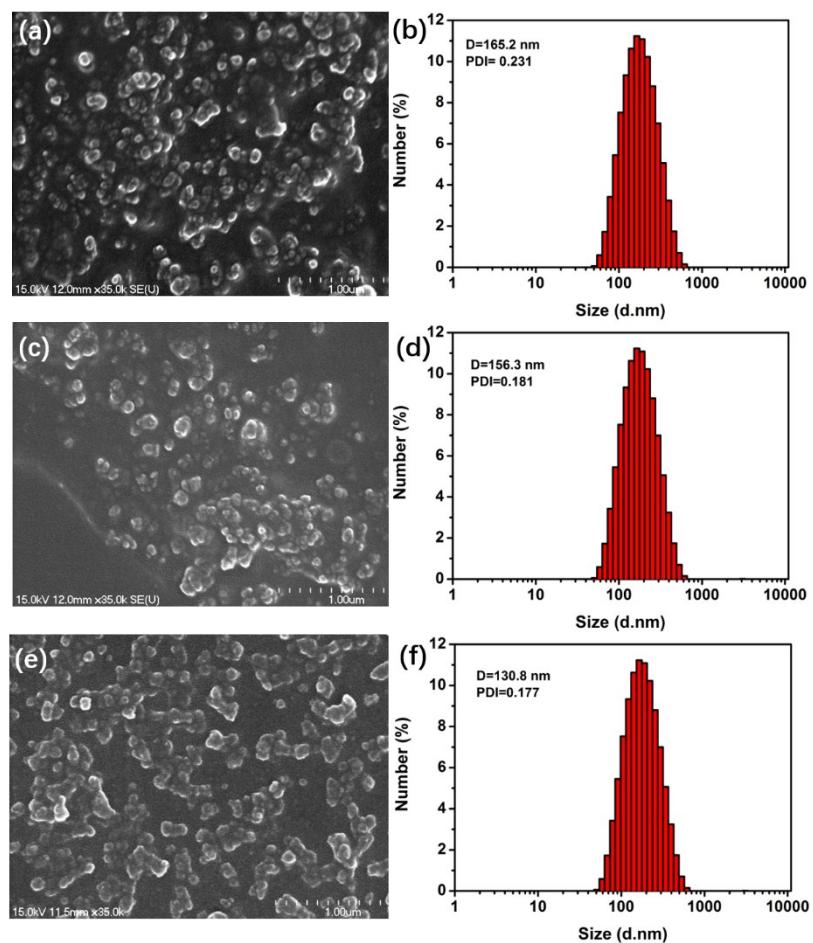


Fig. S19 SEM image of nanoparticles and size distribution of particles measured by DLS analysis in 90% DMF/water mixture solution. (a, b) P1, (c, d) P2 and (e, f) P3.

Scale bar: 1 μ m. Concentration: 10 μ M.

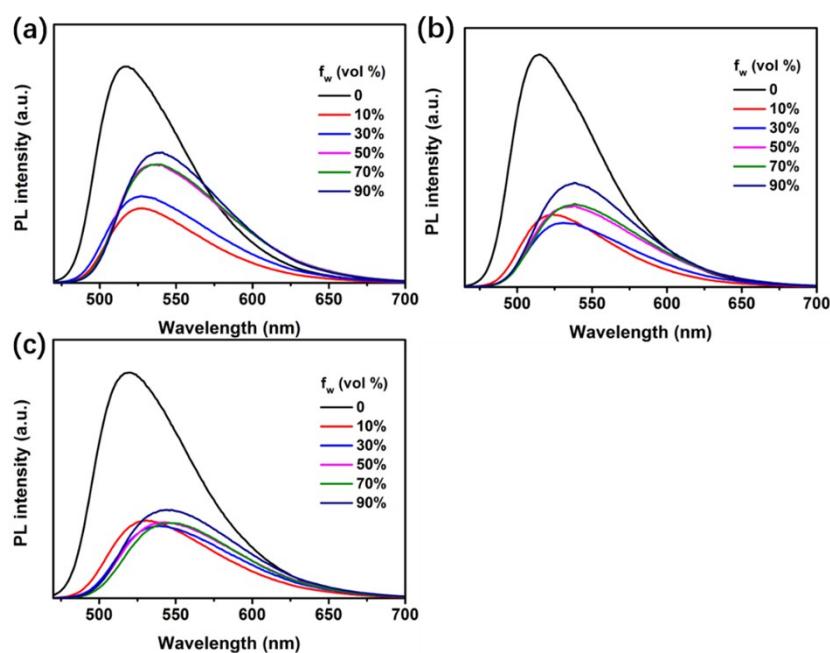


Fig.S20 Emission spectra and plots of maximum emission intensity and wavelength of the polymers in THF/water with different water fractions, (a) P1, (b) P2 and (c) P3. Excitation wavelength: 440 nm, concentration: 10 μ M.

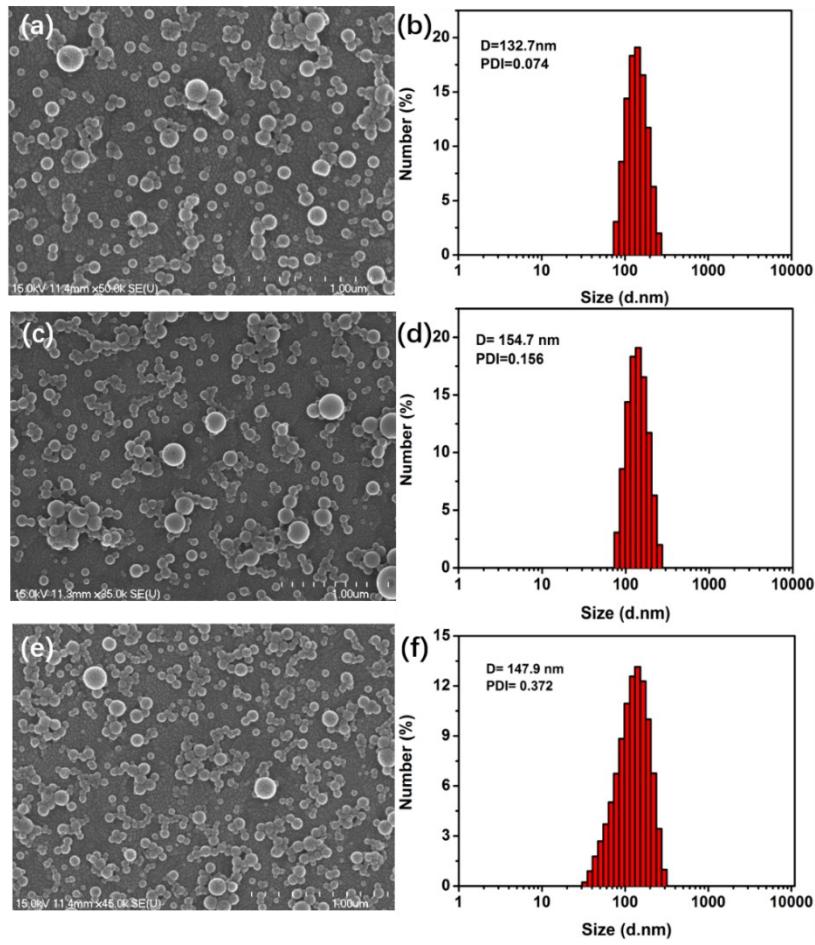


Fig. S21 The SEM images and size distribution of polymer nanoparticles in THF/water (1/9, v/v) mixture: (a, b) P1, (c, d) P2 and (e, f) P3. Scale bar: 1 μ m. Concentration: 10 μ M.

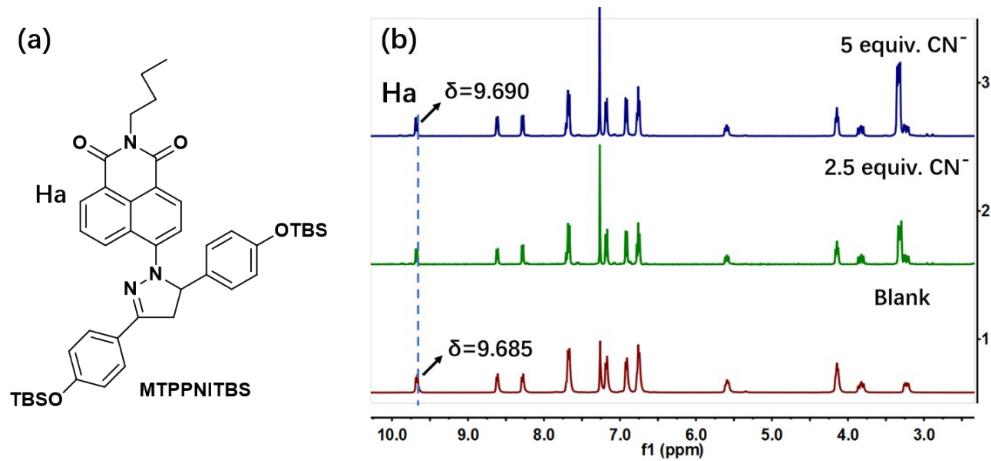


Fig. S22 (a) The structure of MTPPNITBS and (b) the partial ^1H NMR (400 MHz) spectra of the MTPPNITBS in CDCl_3 in the absence and presence of 2.5 and 5 equiv. of CN^- .

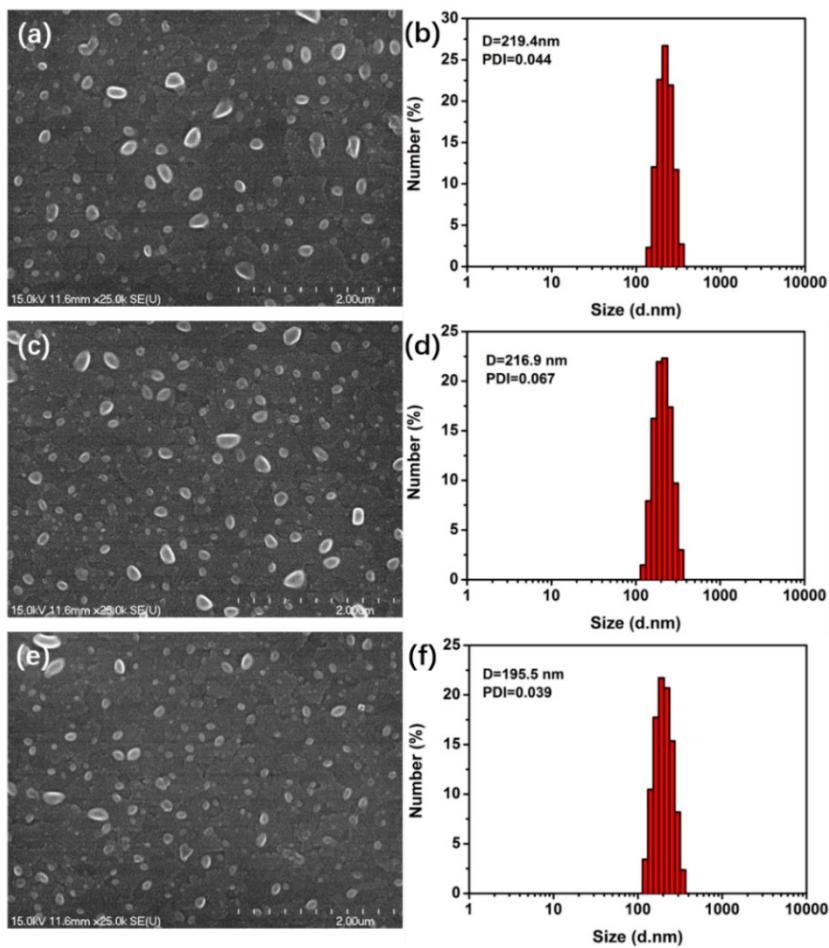


Fig. S23 SEM image and size distribution of particles measured by DLS analysis after 24 h in THF/water (3/7, v/v). (a, b) P1, (c, d) P2 and (e, f) P3. Scale bar: 2 μM. Concentration: 2 μM.

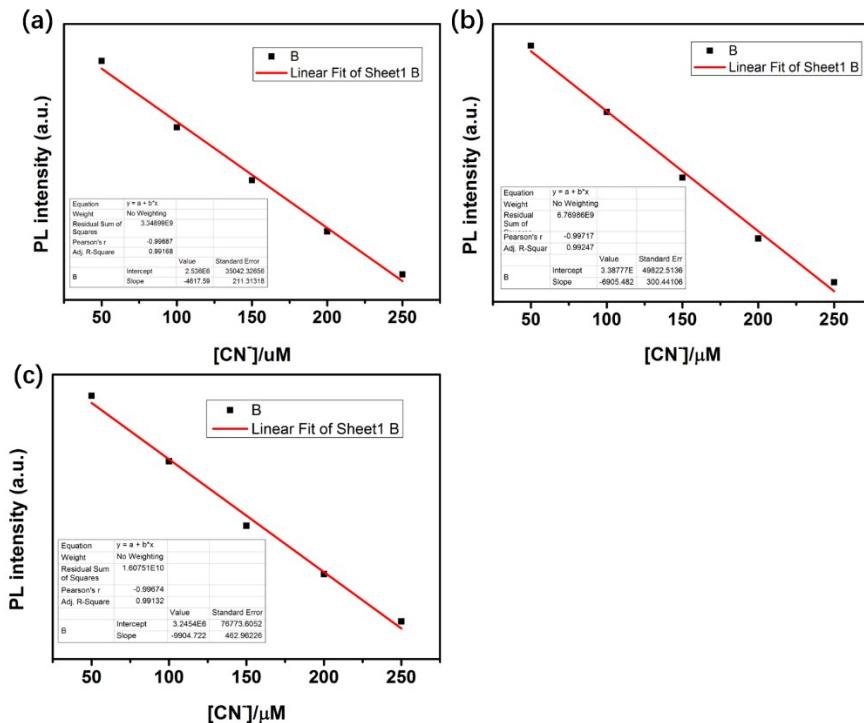


Fig. S24 The emission intensity changes at 550 nm of the polymers in THF/water (3/7, v/v) as a function of the concentration of cyanide ions. (a) P1, (b) P2 and (c) P3. Concentration: 2 μM .

Table S1 Comparisons of reported cyanide ion probes and our probes.

Probe	Solvent	Sensitivity	Selectivity	LOD	Ref
Dicyano-vinyl containing conjugated polymer	DMF	10 mins	F^- , Cl^- , Br^- , I^- , H_2PO_4^- , HSO_4^- , AcO^- , CN^-	0.54 μM	Wang et al ¹
BODIPY-based dye	THF/H ₂ O (10/1, v/v)	1 min	F^- , Cl^- , Br^- , I^- , H_2PO_4^- , HSO_4^- , AcO^- , NO_3^- , ClO_4^- , CN^-	1.10 μM	Wang et al ²
Orange emitting fluorescence	THF	No data	F^- , Cl^- , Br^- , I^- , H_2PO_4^- , HSO_4^- , AcO^- , NO_2^- , ClO_4^- , OH^- , SCN^- , N_3^- , S^{2-} , SH^- , CN^-	5.48 μM	Prasad et al ³
Hybrid coumarin-hemicyanine	MeOH/H ₂ O (1/1, v/v)	3 mins	F^- , Cl^- , Br^- , I^- , H_2PO_4^- , HPO_4^{2-} , HSO_4^- , AcO^- , NO_2^- , ClO^- , OH^- , SCN^- , NO_3^- , S^{2-} , Cys , NH_4^+ , CN^-	9.8 μM	Guo et al ⁴
Imidazole-functionalized polyfluorene Derivative	THF	No data	F^- , Cl^- , Br^- , I^- , HSO_4^- , HSO_3^- , SO_3^{2-} , SO_4^{2-} , AcO^- , NO_2^- , ClO_4^- , CN^-	11.92 μM	Li et al ⁵
Ratiometric fluorescent probe	CH ₃ CN/H ₂ O (95/5, v/v)	No data	F^- , Cl^- , I^- , $\text{C}_2\text{O}_4^{2-}$, AcO^- , ClO_4^- , H_2PO_4^- , HSO_3^- , SO_3^{2-} , SO_4^{2-} , CN^-	4 μM	Li et al ⁶
Aniline trimer based chemical sensor	DMSO/ H ₂ O (7/3, v/v)	No data	F^- , Cl^- , Br^- , I^- , HSO_4^- , SCN^- , PO_4^{3-} , NO_3^- , ClO_4^- , PF_6^- , BF_4^- , AcO^- , CN^-	0.2 μM	Yeh et al ⁷

Polysulfates	THF/ H ₂ O (3/7, v/v)	10 mins	F ⁻ , Cl ⁻ , Br ⁻ , I ⁻ , NO ₃ ⁻ , HSO ₄ ⁻ , BF ₄ ⁻ , AcO ⁻ , ClO ₄ ⁻ , PF ₆ ⁻ , SCN ⁻ , S ₂ O ₃ ²⁻ , EtOCSS ⁻ , CN ⁻	0.137 μM, 0.131 μM 0.145 μM	This work
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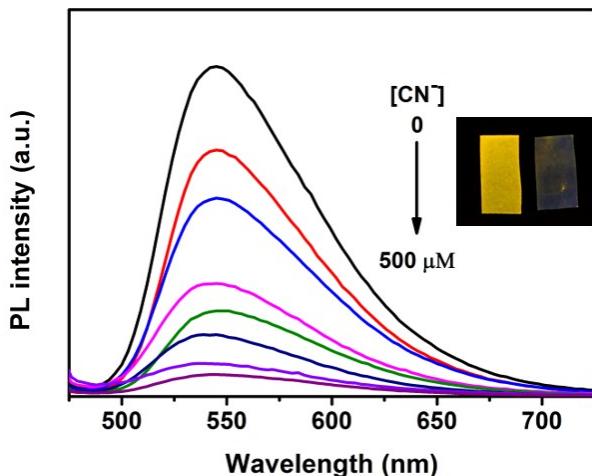


Fig. S25 The solid fluorescence changes of P1 test paper treated by cyanide ions at different concentrations (0, 50, 100, 150, 200, 300, 400 and 500 μM). The inset pictures are the corresponding images of papers before and after treated with 500 μM cyanide ions (from left to right) under UV light at 365 nm. The concentration of P1 stock solution in THF is 279 μM.

Reference

1. X. Wu, B. Xu, H. Tong and L. Wang, *Macromolecules*, 2011, **44**, 4241-4248.
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