Electronic Supplementary Material (ESI) for Analytical Methods.
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Supplemental Information

Hyperbranched polymer based fluorescent probes for ppt level nerve agent simulant vapor detection

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Catalogue

1. NMR data

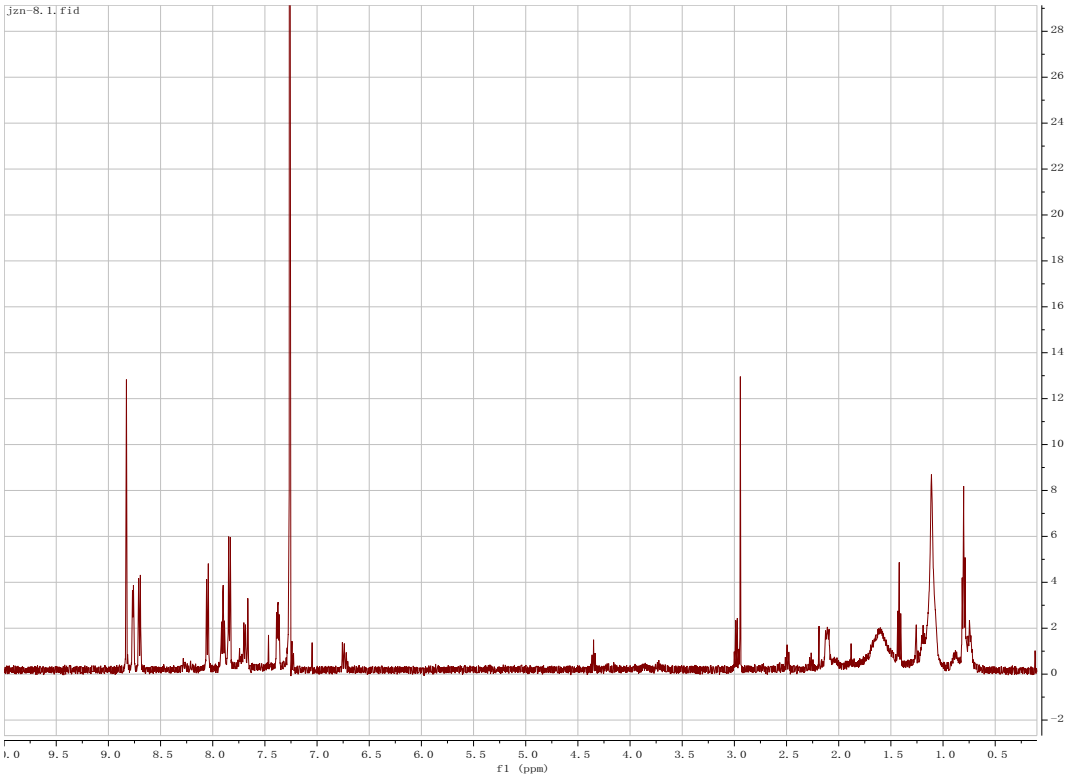


Figure S1. ^{1}H NMR spectrum of HPFP in $CDCl_3$.

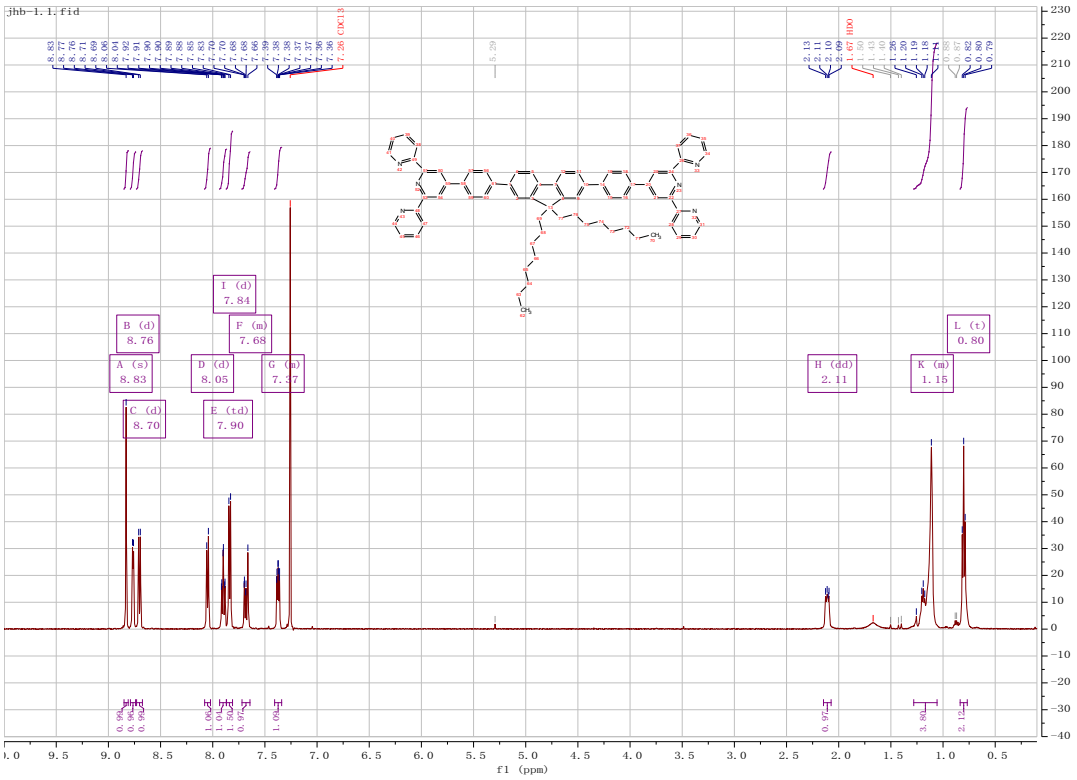


Figure S2. ^{1}H NMR spectrum of TPF in $CDCl_3$.

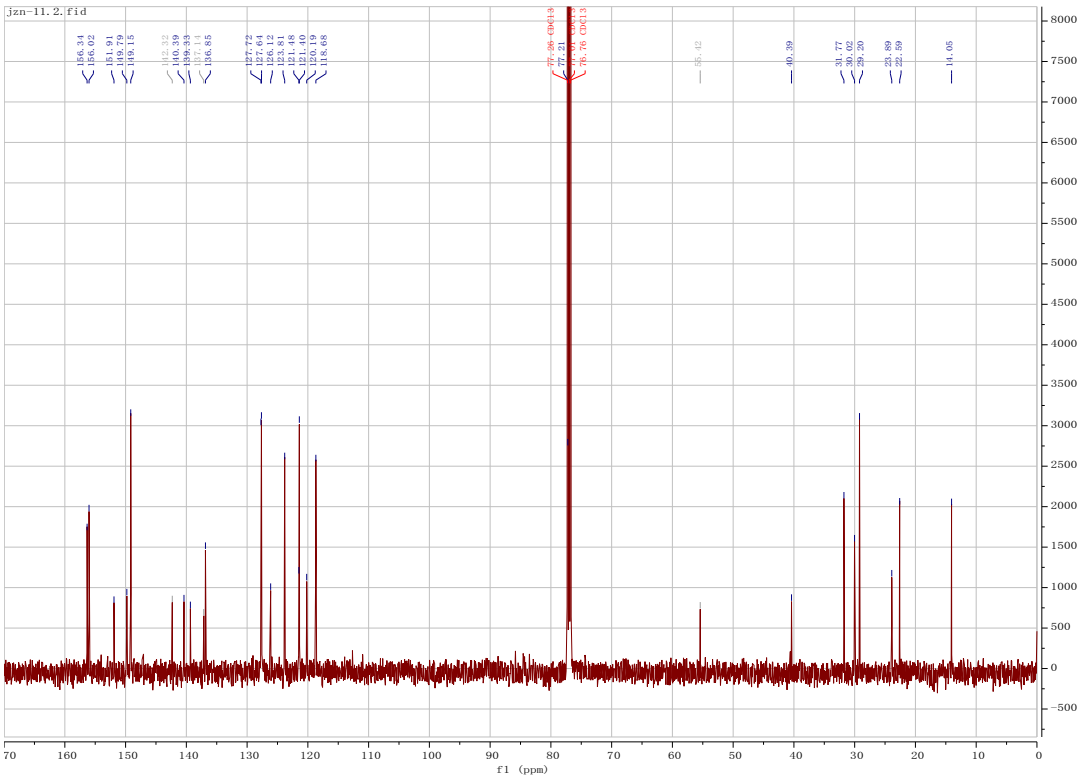


Figure S3. ^{13}C NMR spectrum of TPF in $CDCl_3$.

2. Stability and Sensing Properties

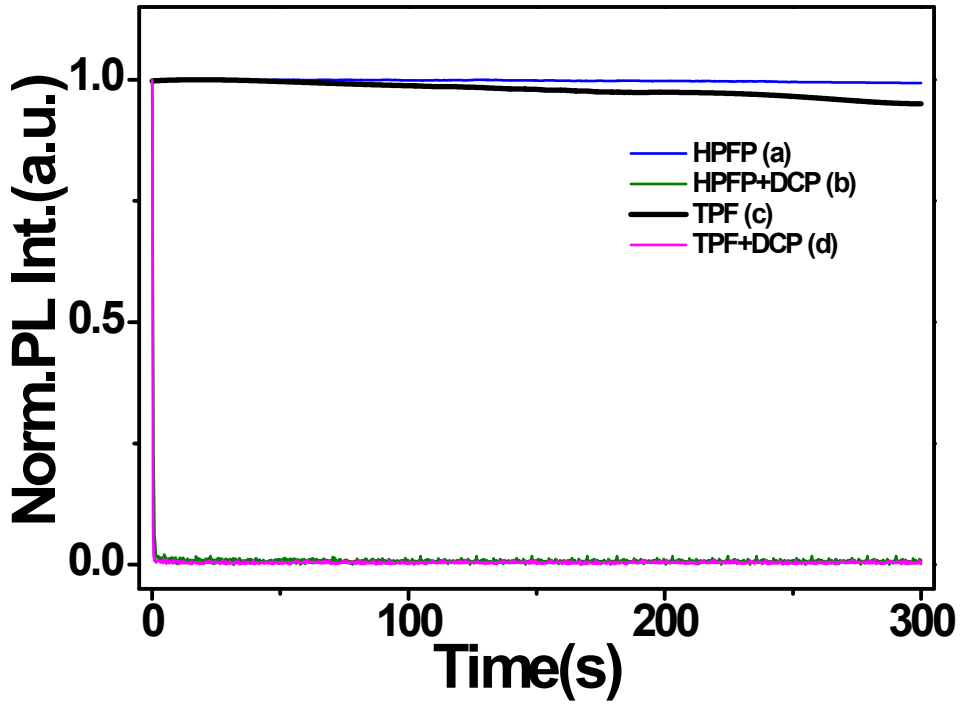


Figure S4. Stability and sensing properties of HPFP and TPF films in air and in saturated DCP vapor for 300 s (a: HPFP in air; b: HPFP in saturated DCP vapor; c: TPF in air; d: TPF in saturated DCP vapor).

3. Detection of possible interferents

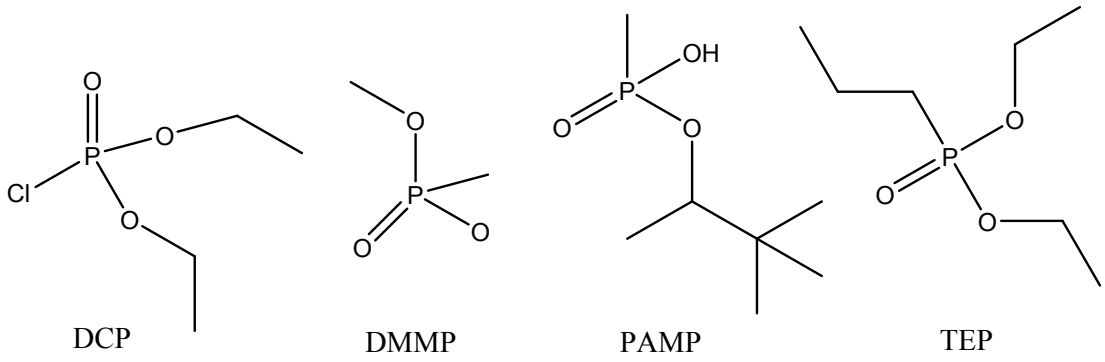


Figure S5. Chemical structures of DCP and the available organophosphonate compounds.

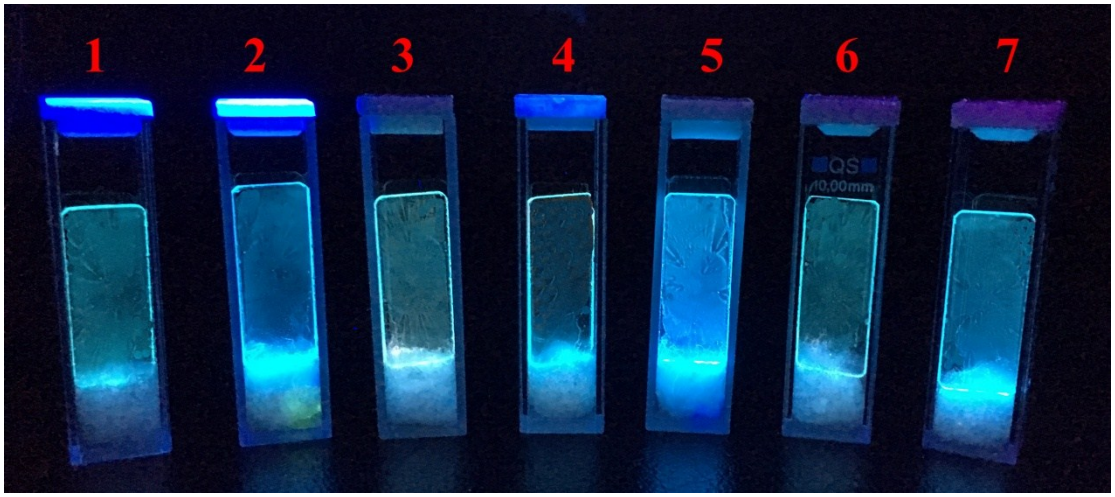


Figure S6. HPFP films excited by UV lamp 365 nm after exposure in solvent vapor (1 H2O, 2 THF, 3 Acetone, 4 Ethyl Acetate, 5 Toluene, 6 Ethyl Alcohol, 7 Chloroform).

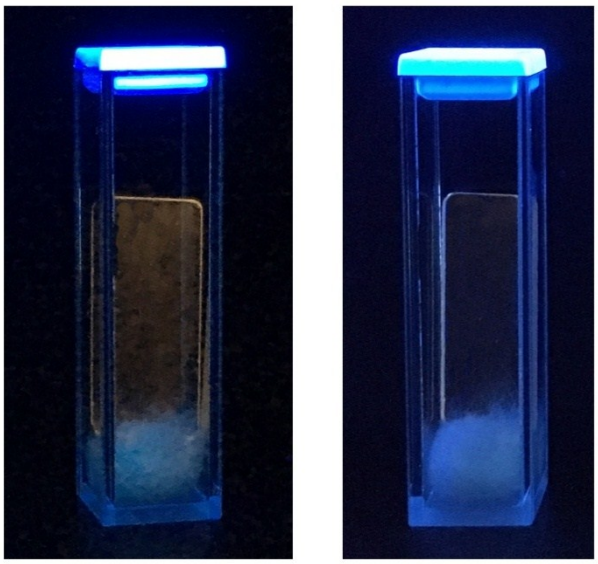


Figure S7. HPFP films excited by UV lamp 365 nm after exposure in DCP (left) and HCl (right) vapor.

4. Fluorescence spectra

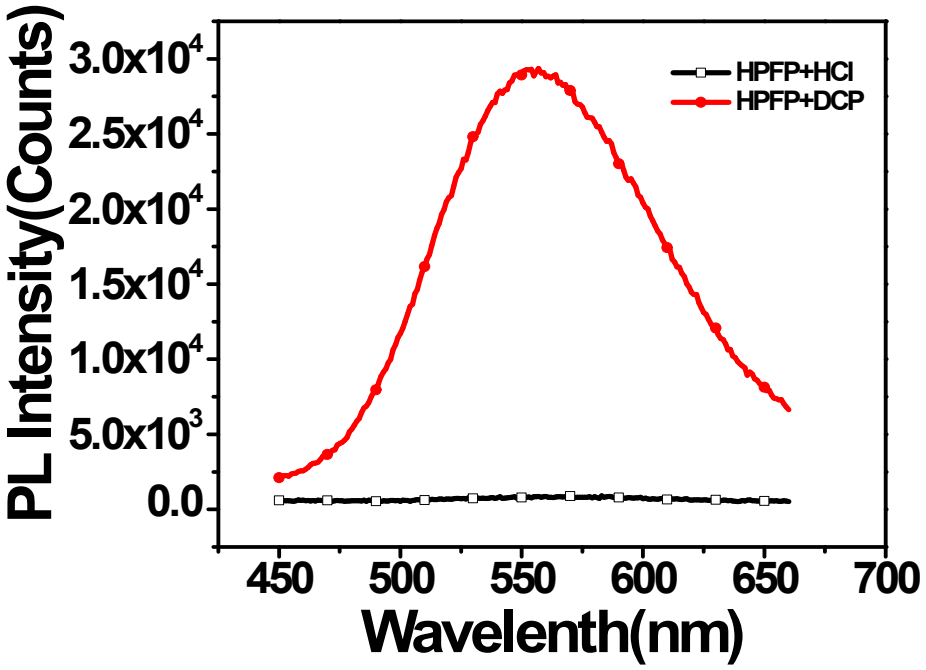
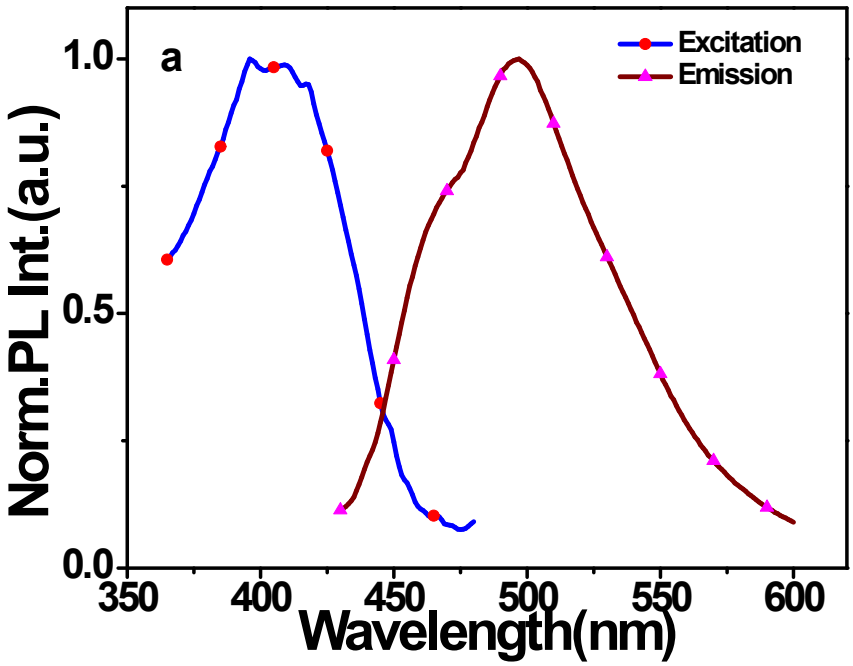


Figure S8. Emission spectra of HPFP films after interaction with DCP and HCl.



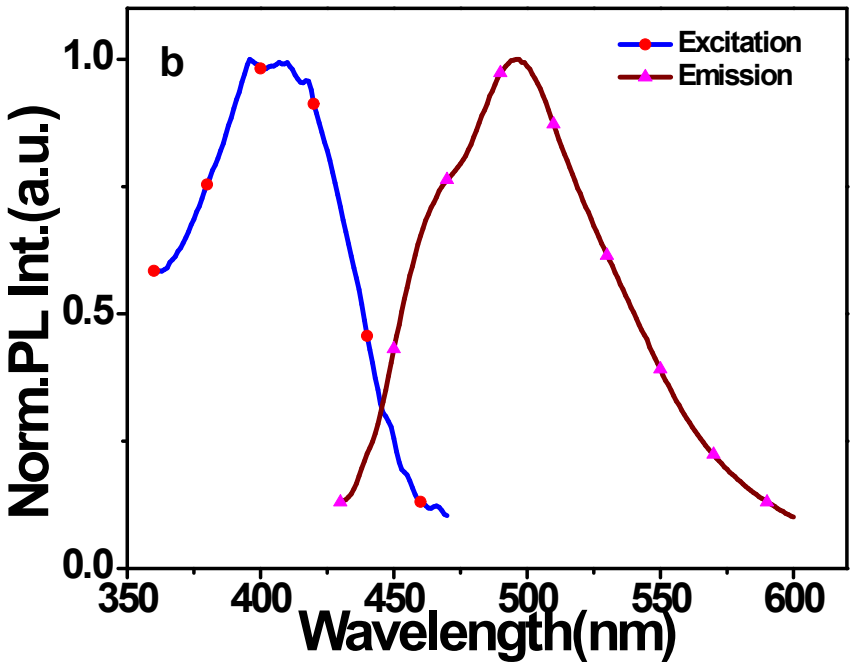


Figure S9. Excitation and emission spectra of borate ester end capped pyrene-fluorene polymer before (a) and after (b) exposure to DCP vapor.

5. Elemental Analysis data

Table S1. Elemental Analysis data

Sample		TPF	TPF+DCP	TPF+HCl
Percentage Composition	N	8.20%	5.55%	5.68%
	C	84.48%	60.64%	60.31%
	H	6.94	6.68%	6.23%
	P		1.19%	
	Cl		13.03%	15.87%

6. Detail methodology and parameters of DMol3

Table S2. Detail methodology and parameters of DMol3

DMol3	
Task	Geometry Optimization
Properties	Optics, Orbitals
Energy	1.0^{-5} Ha
Max. force	0.002 Ha/Å
Max. displacement	0.005 Å
Max. interations	1000
Max. step size	0.3 Å
Functional	GGA,BLYP
Integration accuracy	Fine
SCF tolerance	Fine
Core treatment	All Electron
Basis set	DNP+
Basis file	4.4
Orbital cutoff quality	Fine
Run in parallel on	12 cores