

## Supporting Information

# Portable fluorescence sensing system for timely onsite perfluorooctane sulfonate detection based on aggregate induced emission fluorescence sensor

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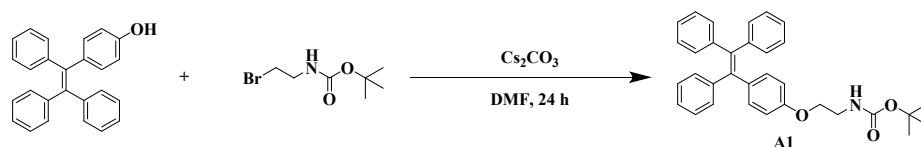
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## Synthesis of TPE-PA1

### Synthesis of A1

4-hydroxy tetraphenylethylene (TPE-OH) (0.75 g, 2.14 mmol) and 2-(boc-amino) ethyl bromide (1.15 g, 5.14 mmol) were dissolved in 25 mL dimethyl sulfoxide, then cesium carbonate (1.25 g, 6.42 mmol) was added. The mixture was stirred at room temperature overnight. After that, 5 mL water was added. Then the mixture was extracted with ethyl acetate twice, washed with saturated sodium chloride aqueous solution. The organic phase was dried with anhydrous sodium sulfate and the solvent was removed under reduce pressure. The obtained product A1 was dried in a vacuum oven.

$^1\text{H NMR}$  (600 MHz,  $\text{CDCl}_3$ )  $\delta$  (ppm): 7.11 (m, 9H), 7.03 (m, 6H), 6.95 (d, 2H), 6.69 (d, 2H), 4.10 (t, 2H), 3.29 (t, 2H), 1.42 (s, 9H)

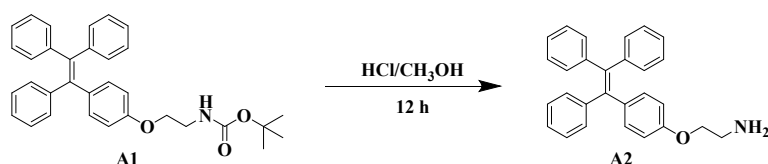


### Synthesis of A2

A1 (1.00 g) was dissolved in 10 mL HCl/CH<sub>3</sub>OH solutions, and stirred overnight at room temperature. The solvent was removed under reduced pressure. Then 10 mL fresh methanol was added to dissolve the solid product, and the solvent was removed again under reduced pressure. This process was repeat twice. The product was dissolved in 10 mL methanol, and then potassium carbonate (1.00 g) was added. The mixture was stirred overnight at room temperature. The solid was removed by

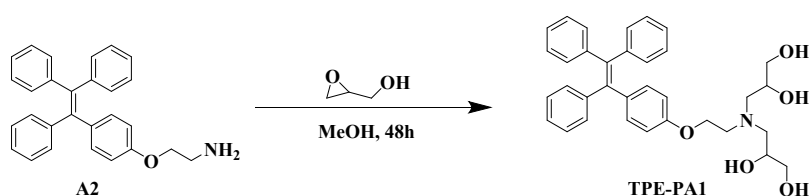
filtration, and the desired product was purified by flash chromatography using petroleum ether/ethyl acetate (1:1) as eluent.

$^1\text{H}$  NMR (600MHz,  $\text{CDCl}_3$ )  $\delta$  (ppm): 7.11 (m, 9H), 7.03 (m, 6H), 6.95 (d, 2H), 6.69 (d, 2H), 4.10 (t, 2H), 3.29 (t, 2H), 1.7 (s, 2H)



### Synthesis of A3 (TPE-PA1)

Compound A2 (1.00 g, 2.55 mmol) and glycidyl ether (0.31 mL, 5.10 mmol) were dissolved in 10 mL methanol, then the solution was heated at 40°C for 12 h. After that, the solution was concentrated, and precipitate in diethyl ether twice. The solid product was collected and dried in a vacuum oven. The  $^1\text{H}$  NMR and FT-IR spectra were shown in figure 1.



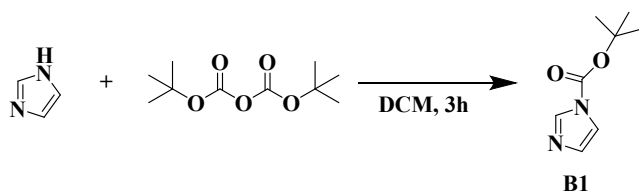
### Synthesis of TPE-PA2

### Synthesis of B1

Imidazole (5.00 g, 73.44 mmol) was dissolved in 25 mL dichloromethane. Dibutyldicarbonate (14.43 g, 66.10 mmol) was slowly dropped into the solution under vigorous stirring at room temperature. The solution was stirred for another 3 hours, and then washed with water for three times to remove the unreacted imidazole. After that,

the aqueous phase was discarded, the organic phase was dried with magnesium sulfate, and the solvent was removed under reduce pressure. The obtained product B1 was dried in a vacuum oven.

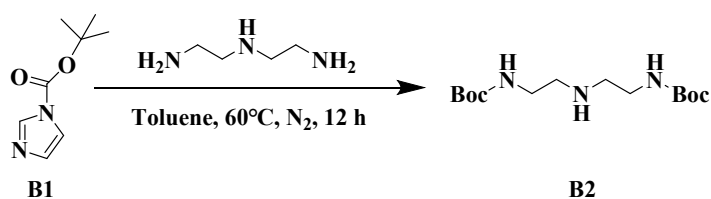
$^1\text{H}$  NMR (600 MHz,  $\text{CDCl}_3$ )  $\delta$  (ppm): 8.07 (s, 1H), 7.40 (d, 1H), 7.03 (d, 1H), 1.63 (s, 9H)



### Synthesis of B2

DETA (2.50 g, 24.23 mmol) and B1 (7.38 g, 43.86 mmol) were dissolved in 6 mL toluene under nitrogen atmosphere. The solution was heated at 60 °C for 3 hours. After cooling to room temperature, toluene was removed under reduced pressure. The solid residue was re-dissolved in 10 mL dichloromethane, and washed with water for three times to remove the unreacted Boc-Imidazole. After that, the organic phase was dried with magnesium sulfate, and the solvent was removed under reduce pressure. The product was dried overnight at room temperature in vacuum. A light yellow oil product B2 was obtained.

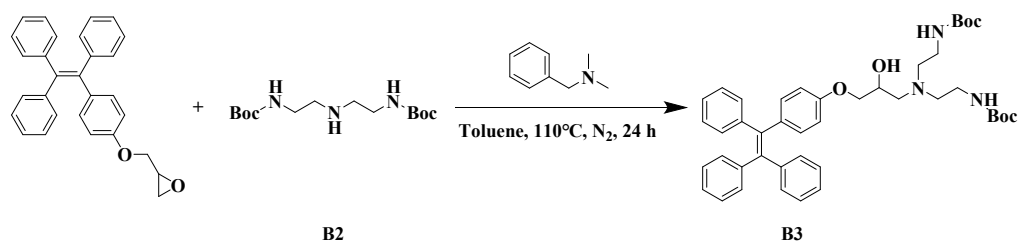
$^1\text{H}$  NMR (600 MHz,  $\text{CDCl}_3$ )  $\delta$  (ppm): 4.84 (s, 2H), 3.15 (d, 4H), 2.65 (t, 4H), 1.37 (s, 18H)



### Synthesis of B3

B2 (0.75 g, 2.47 mmol), TPE-epoxide (1.00 g, 2.47 mmol) and benzenemethanamine (3  $\mu$ L) were dissolved in 8 mL toluene. The solution was refluxed for about 24 hours under nitrogen atmosphere. After cooling to room temperature, the solvent was removed under reduced pressure and the crude product was purified by flash chromatography using ethyl acetate/petroleum ether as eluent. The obtained white solid product B3 was dried at room temperature in vacuum.

$^1\text{H}$  NMR (600MHz,  $\text{CDCl}_3$ )  $\delta$  (ppm): 7.11 (m, 9H), 7.03 (m, 6H), 6.95 (d, 2H), 6.69 (d, 2H), 5.16 (s, 1H), 4.20 (m, 3H), 3.26 (t, 4H), 2.62 (m, 6H), 1.42 (s, 18H)

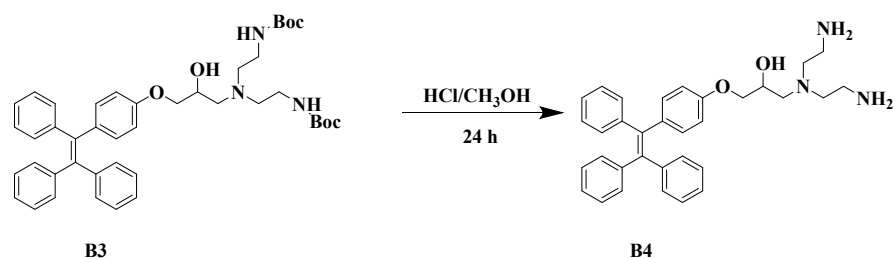


### Synthesis of B4

B3 (1.38 g, 1.84 mmol) was dissolved in 20 mL concentrated HCl/methanol solution. After stirred for about 24 hours, the white solid product was collected and wash with methanol for three times. The solid was dissolved in 20 mL dichloromethane, and then the pH of the solution was adjusted to  $\sim$ 12 by dilute potassium carbonate aqueous solution. The organic phase was collected. After removing of the solvent, a light yellow solid product B4 was obtained.

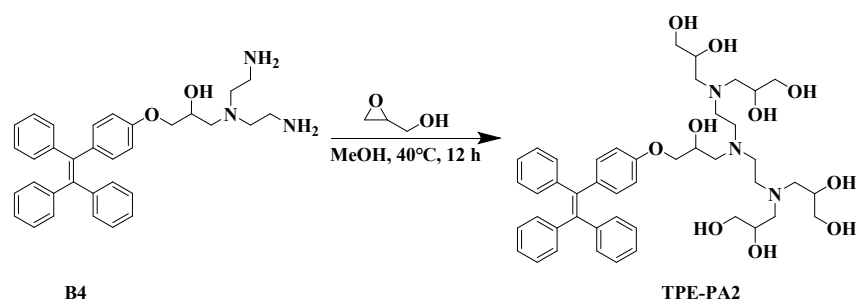
$^1\text{H}$  NMR (600 MHz,  $\text{CDCl}_3$ )  $\delta$  (ppm) 7.11 (m, 9H), 7.03 (m, 6H), 6.95 (d, 2H), 6.69 (d,

2H), 5.37 (s, 1H), 4.20 (m, 3H), 2.62 (m, 6H), 2.60 (m, 4H), 1.5(s, 2H)



### Synthesis of B5 (TPE-PA2)

B4 (0.7 g, 1.38 mmol) and glycidol (1.04 mL, 16.55 mmol) were dissolved in 10 mL methanol, and the solution was heated at 40 °C for 24 hours. After cooling to room temperature, the solution was concentrated, and dropped into cold diethyl ether. The precipitate was collected and dried at room temperature in vacuum. The final yellowish viscous liquid product TPE-PA2 was obtained. The <sup>1</sup>H NMR and FT-IR, spectra were shown in figure 1.



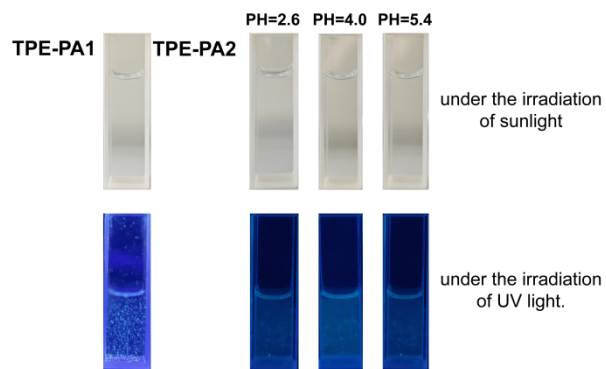


Figure S1 The photos of TPE-PA1/acetic acid solution and TPE-PA2/AA buffer solutions under the irradiation of sunlight and UV light.

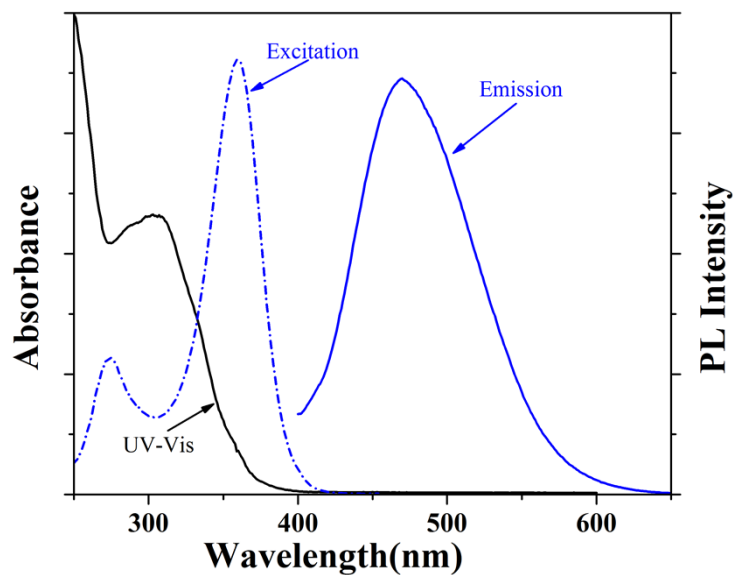


Figure S2 The UV-Vis, fluorescence emission and excitation spectra of TPE-PA2

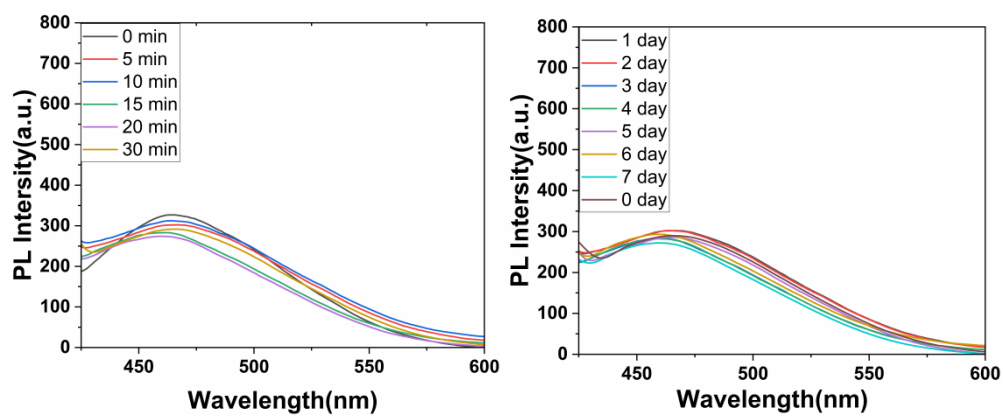


Figure S3 The fluorescence emission spectra of TPE-PA2 solution under the irradiation of UV light (left) or stored under natural condition (right) for various durations.

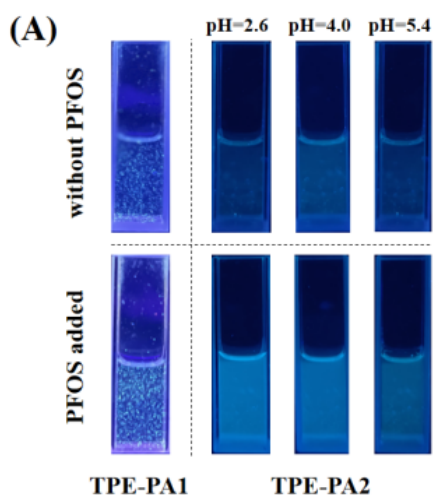


Figure S4 The fluorescence picture of TPE-PAs before and after the addition of PFOS



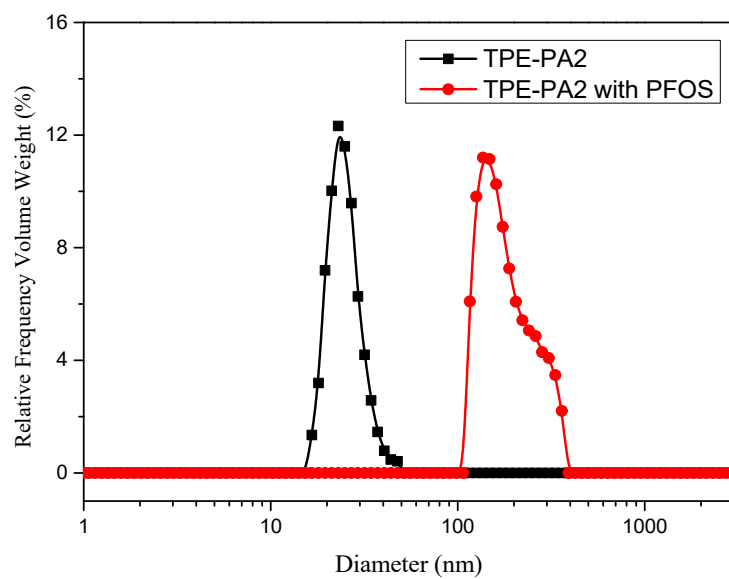


Figure S5 DLS curves of TPE-PA2/AA buffer solution before and after mixing with PFOS

Table S1 Performance of different fluorescence sensors for determination of PFOS.

Probe	Concentration range	Limit of detection	Sensor concentration	Ref.
Carbon dots - Berberine chloride hydrate (BH)	0.11–25 ppm	10.8 ppb	<0.03 mg/ml	[1]
Eosin Y - Polyethyleneimine (PEI)	0–1 ppm	7.5 ppb	0.692 ng/ml	[2]
MIP chitosan doped Carbon quantum dots	20–200 ppq	65 ppq (serum)/85 ppq (urine)	--	[3]
Cationic porphyrin	0.02–8 ppm	4 ppb	6.46 ng/ml	[4]
Carbon quantum dots	0–6 ppm	9.13 ppb	0.5 ng/ml	[5]
Nitrogen doped Carbon dots	0–1 ppm	13.9 ppb	--	[6]
Covalent organic framework UCNPs	90 ppq–9 ppb	75 ppq	0.1 mg/ml	[7]
supramolecular assembly with fluorescent gold-nanoclusters	1.07–53.8 ppm	0.72 ppm	50 ug/ml	[8]
The sensor (PFOS-MIPPDA/AuNPs/GCE)	5.38-4.3 ppb	2.26 ppb	--	[9]
Fluorescent Probe	0-10.76 ppm	5.92 ppm	1.48 ug/ml	[10]
Portable fluorescence sensing system	0.05-30 ppm	0.047 ppm	0.12 mg/ml	This work

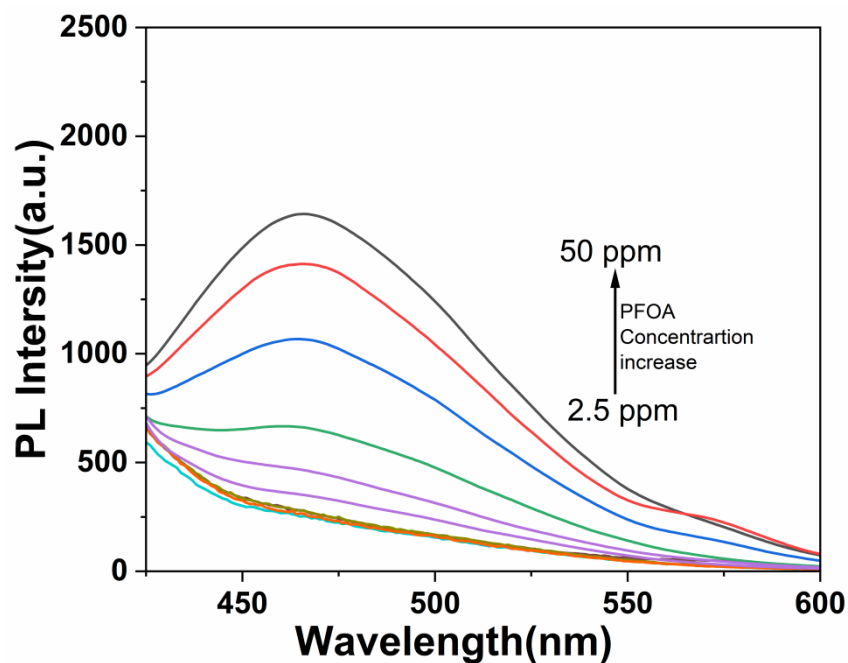


Figure S6 Emission spectra of TPE-PA2/AA buffer solution (pH = 2.6) in the presence of different concentrations of PFOA

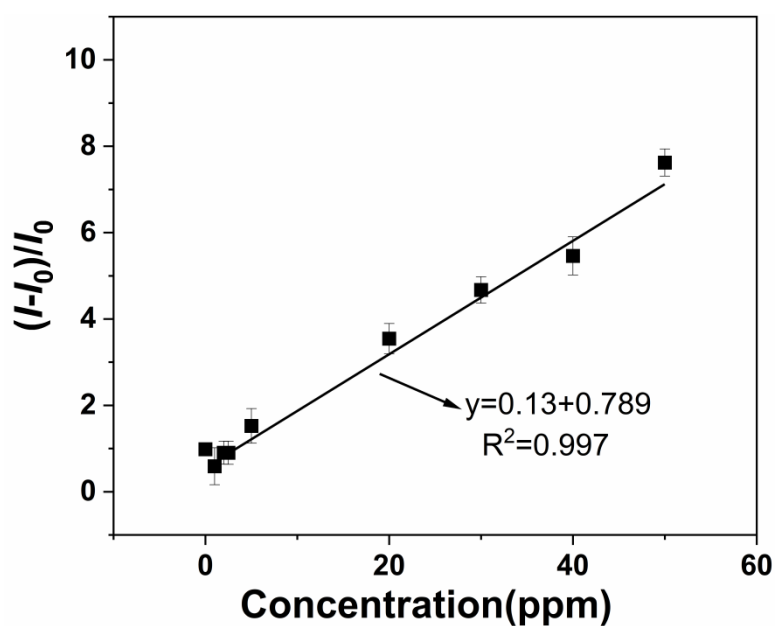


Figure S7 Plot of the changes in fluorescence intensity of TPE-PA2/AA buffer solution at 460 nm versus the PFOA concentration.

## References

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