Supporting Information

Novel AIEgens with 3,5-dibromobenzaldehyde skeleton: molecular design, synthesis, tunable emission and detection application

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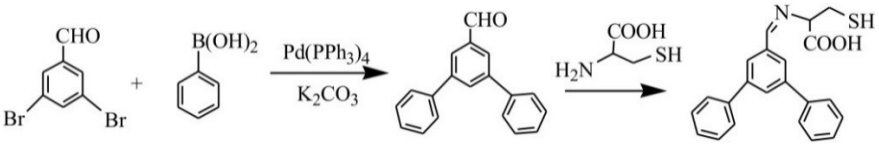
Synthesis of S1



Scheme S1 Synthesis of S1

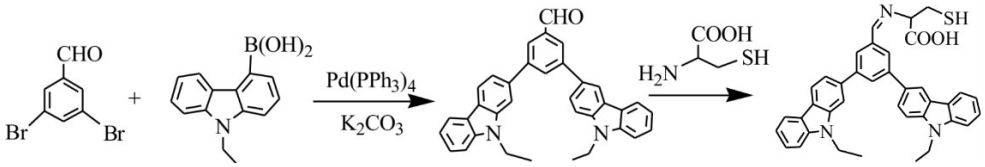
S1: ^{1}H NMR (400MHz, d_6-DMSO) δ (ppm): 10.12 (s, 1H), 8.14-7.80 (m, 9H), 7.60-7.45 (m, 6H), 4.31-4.25 (t, 1H), 3.07-2.89 (m, 2H), 2.36-2.41 (t, 1H).

^{13}C NMR (100MHz, d_6-DMSO) δ (ppm): 171.15, 160.03, 135.24, 134.01, 132.27, 127.11, 126.13, 122.79, 120.45, 119.45, 60.07 and 24.47.

ESI-MS (m/z): calcd for $C_{22}H_{19}NO_2S$ $[M]^+$, 361.5; found, 361.1.

Elemental analysis: calcd for $C_{22}H_{19}NO_2S$: C, 73.10; H, 5.30; N, 3.88; S, 8.85. Found: C, 73.12; H, 5.31; N, 3.92; S, 8.84.

Synthesis of S2



Scheme S2 Synthesis of S2

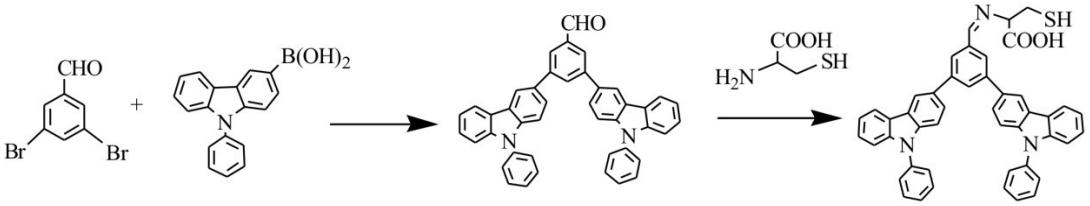
S2: ^{1}H NMR (400MHz, d_6-DMSO) δ (ppm): 9.88 (s, 1H), 7.79-7.60 (m, 10H), 7.93-7.91 (d, 3H), 7.40-7.45 (m, 4H), 7.33-7.37 (m, 3H), 4.35-4.29 (t, 1H), 3.77-3.61 (m, 4H), 3.14-3.26 (2H), 1.34-1.30 (t, 6H).

^{13}C NMR (100MHz, d_6-DMSO) δ (ppm): 173.39, 162.46, 134.45, 133.06, 128.98, 127.05, 125.70, 122.41, 120.40, 117.32, 65.32, 51.79, 27.14, 13.97 and 13.74.

ESI-MS (m/z): calcd for $C_{38}H_{33}N_3O_2S$ $[M]^+$, 595.4; found, 595.1.

Elemental analysis: calcd for $C_{38}H_{33}N_3O_2S$: C, 76.61; H, 5.58; N, 7.05; S, 5.38. Found: C, 76.63; H, 5.57; N, 7.02; S, 5.40.

Synthesis of S3



Scheme S3 Synthesis of S3

S3: ^{1}H NMR (400MHz, d_6-DMSO) δ (ppm): 9.82 (s, 1H), 8.23-8.16 (m, 4H), 8.01-7.88 (m, 2H), 7.67-7.48 (m, 10H), 7.41-7.23 (m, 12H), 4.1 (t, 1H), 3.11-2.94 (m, 2H).

^{13}C NMR (100MHz, d_6-DMSO) δ (ppm): 167.49, 158.31, 140.61, 137.33, 130.63, 128.12, 127.16, 126.63, 123.18, 120.97, 114.03, 111.97, 110.03, 66.43, and 26.14.

ESI-MS (m/z): calcd for $C_{46}H_{33}N_3O_2S$ $[M]^+$, 691.2; found, 691.1.

Elemental analysis: calcd for $C_{46}H_{33}N_3O_2S$: C, 79.86; H, 4.81; N, 6.07; S, 4.63. Found: C, 79.77; H, 4.84; N, 6.11; S, 4.62.

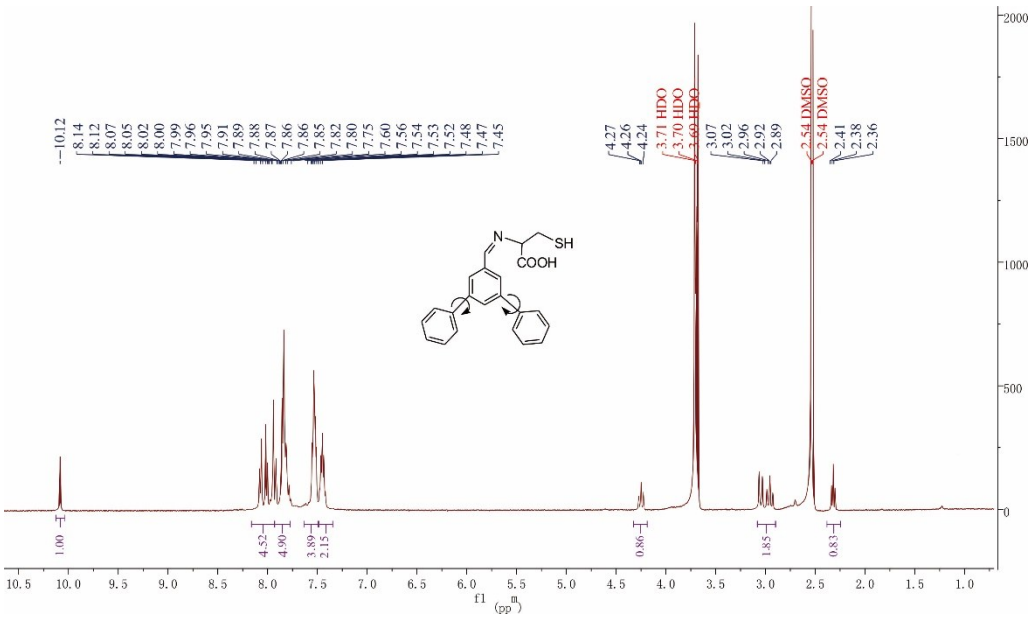


Fig. S1 The ^{1}H NMR spectrum of **S1** in d_6-DMSO

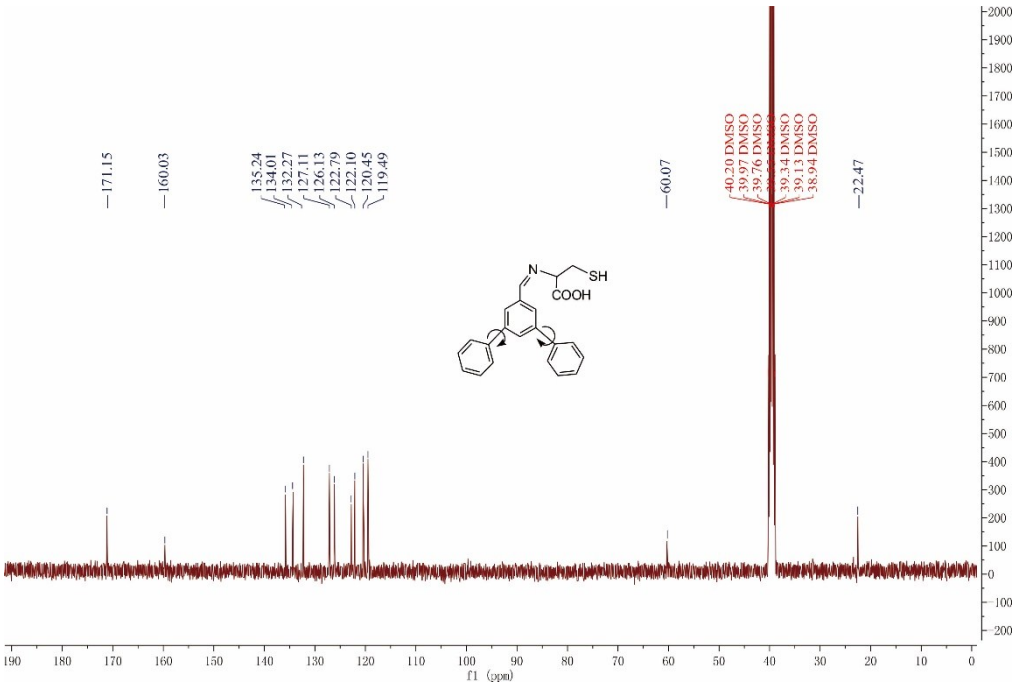


Fig. S2 The ^{13}C NMR spectrum of **S1** in d_6-DMSO

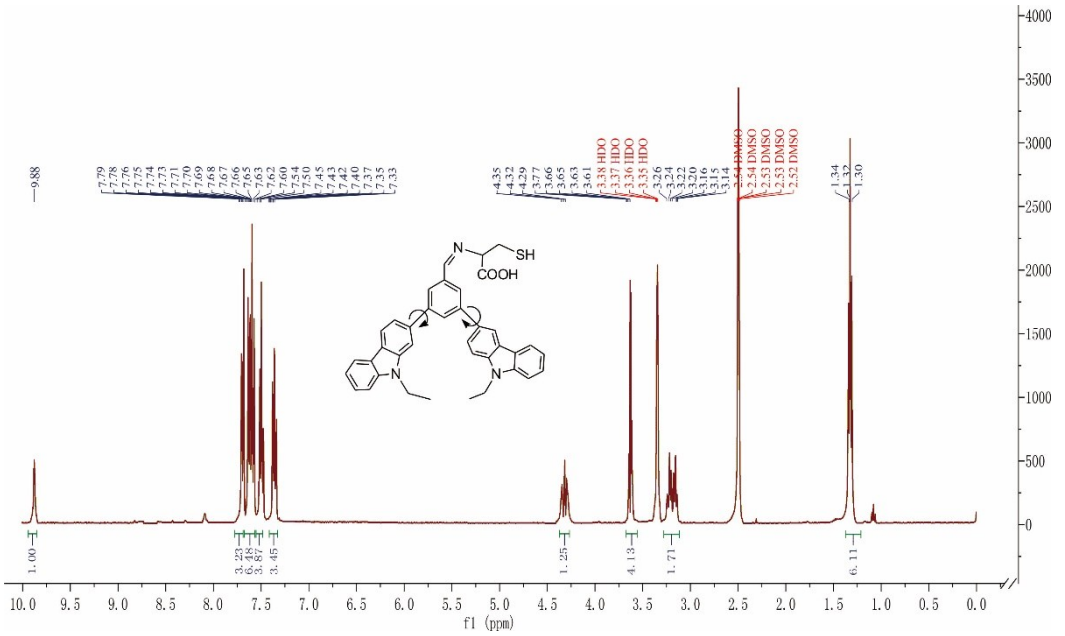


Fig. S3 The ^{1}H NMR spectrum of **S2** in d_6-DMSO

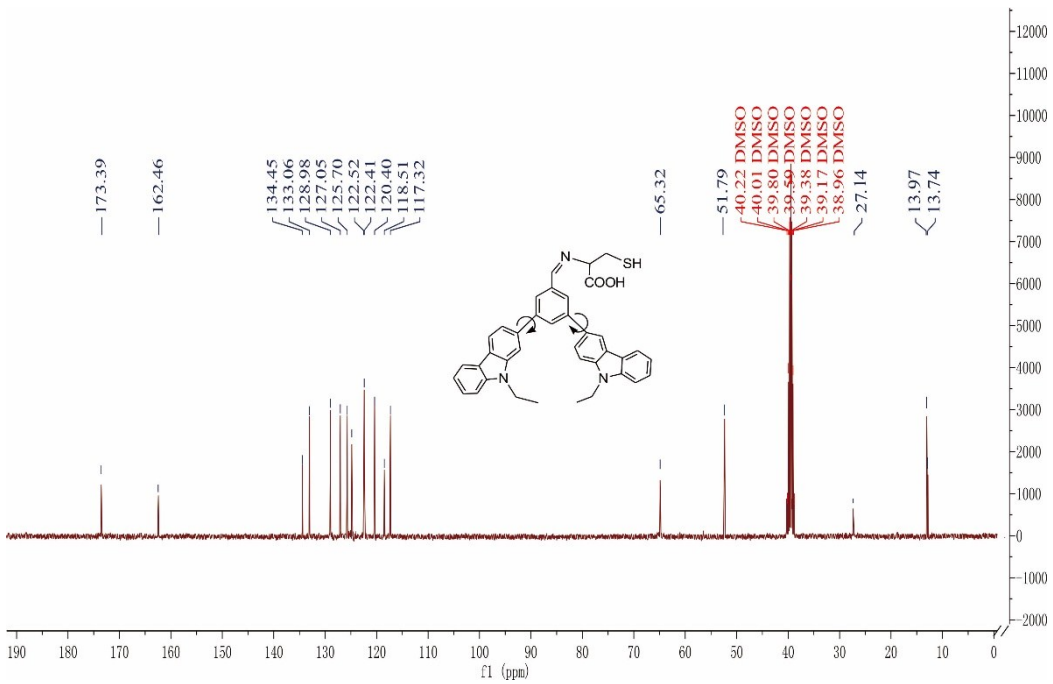


Fig. S4 The ^{13}C NMR spectrum of **S2** in d_6-DMSO

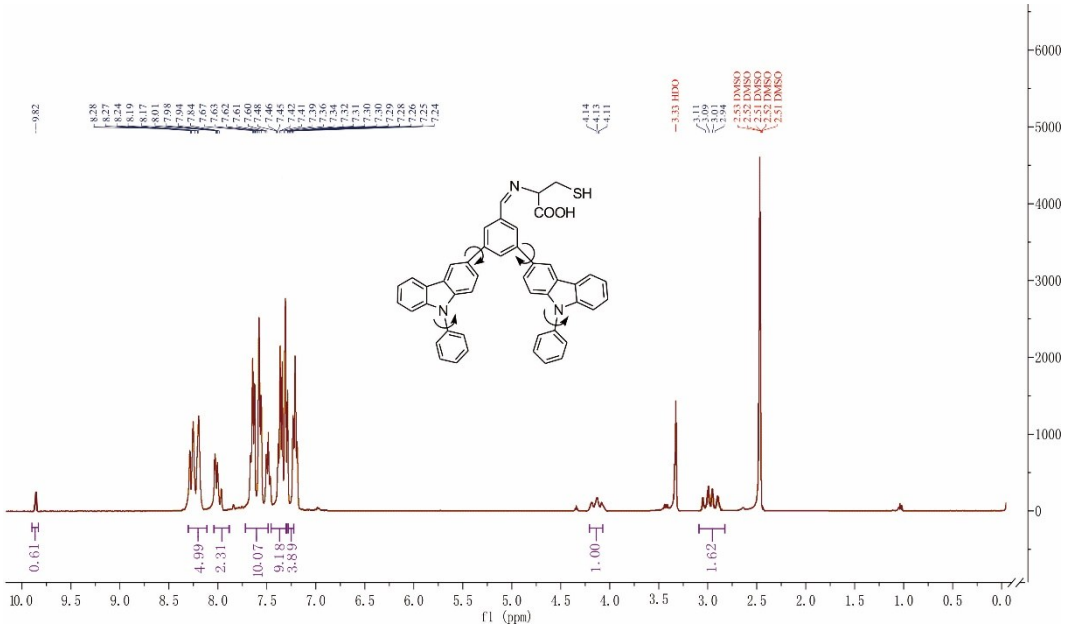


Fig. S5 The ^{1}H NMR spectrum of **S3** in d_6-DMSO

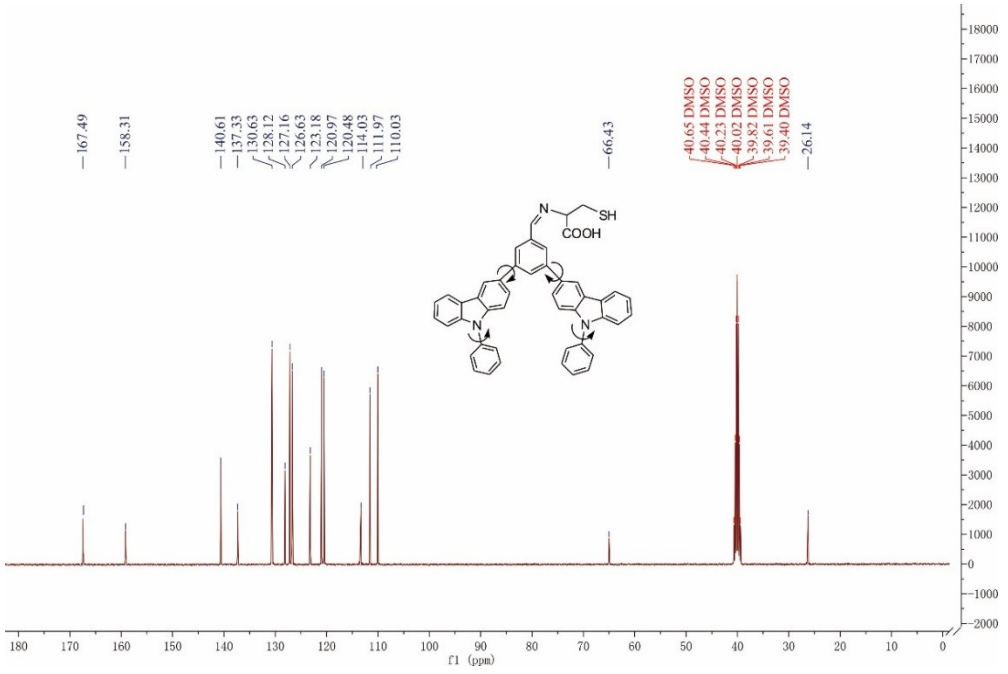


Fig. S6 The ^{13}C NMR spectrum of **S3** in d_6-DMSO

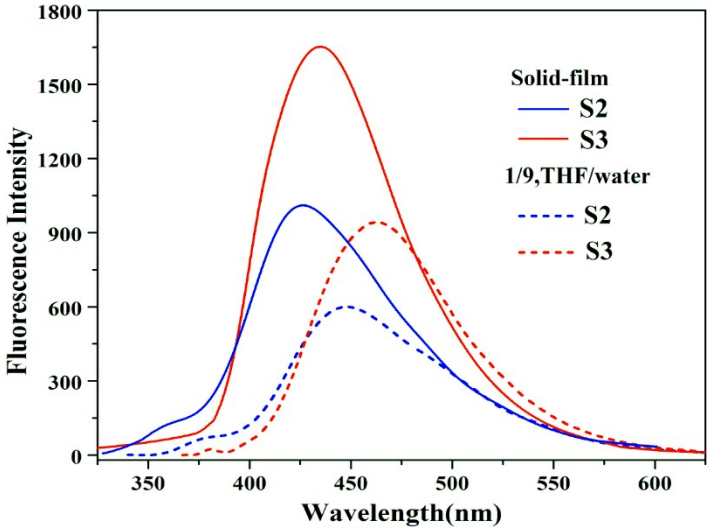


Fig. S7. The fluorescence spectra of S2 and S3 (10 μM) in solid-film state and THF-water mixtures (v/v, 1/9).

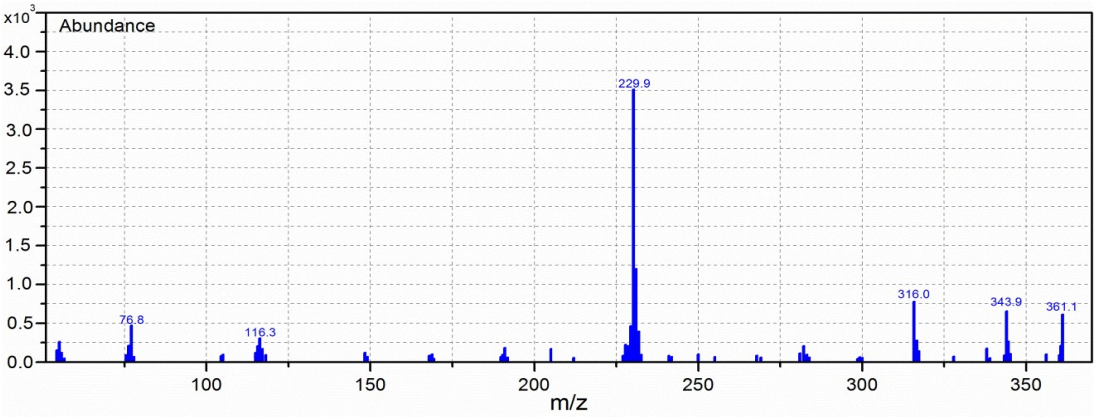


Fig. S8 ESI-Mass spectrum of S**1**

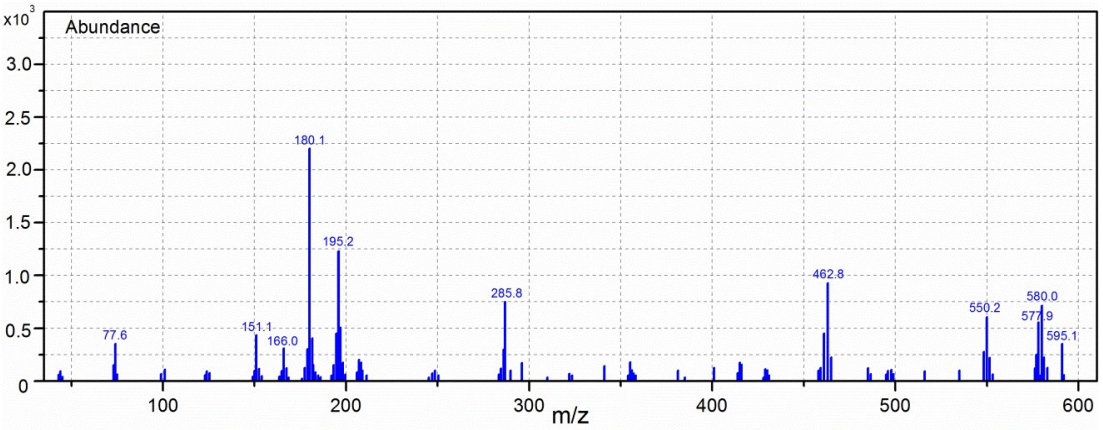


Fig. S9 ESI-Mass spectrum of **S2**

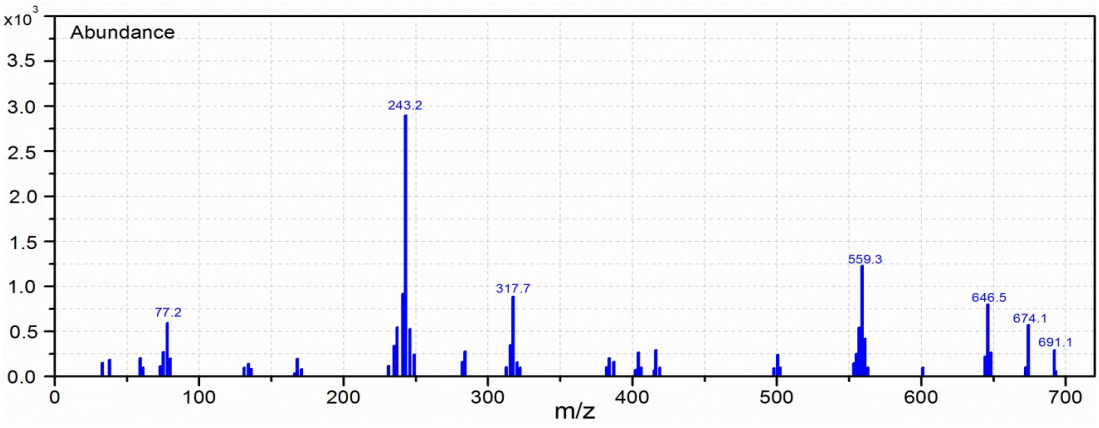


Fig. S10 ESI-Mass spectrum of **S3**

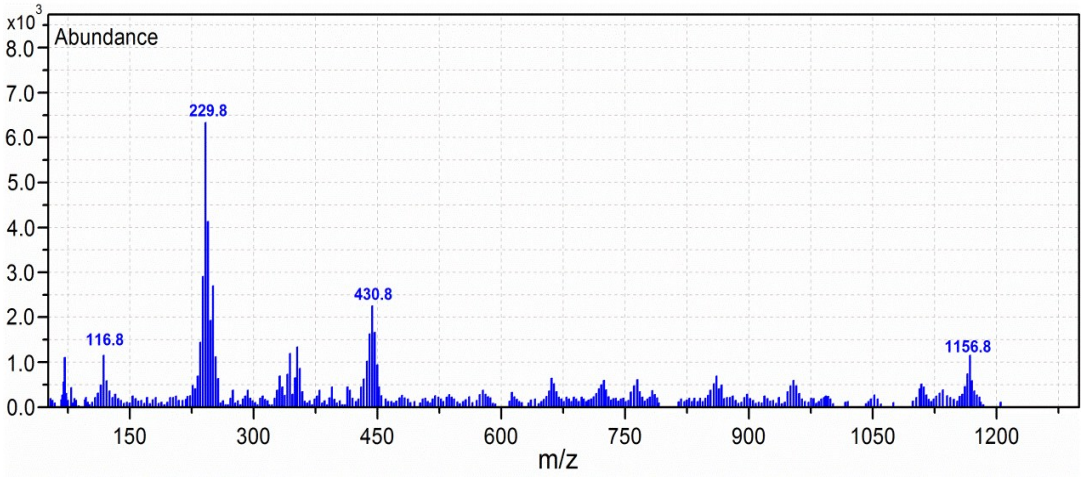


Fig. S11 ESI-Mass spectrum of S**1** after the addition of As^{3+} (240 ppb).

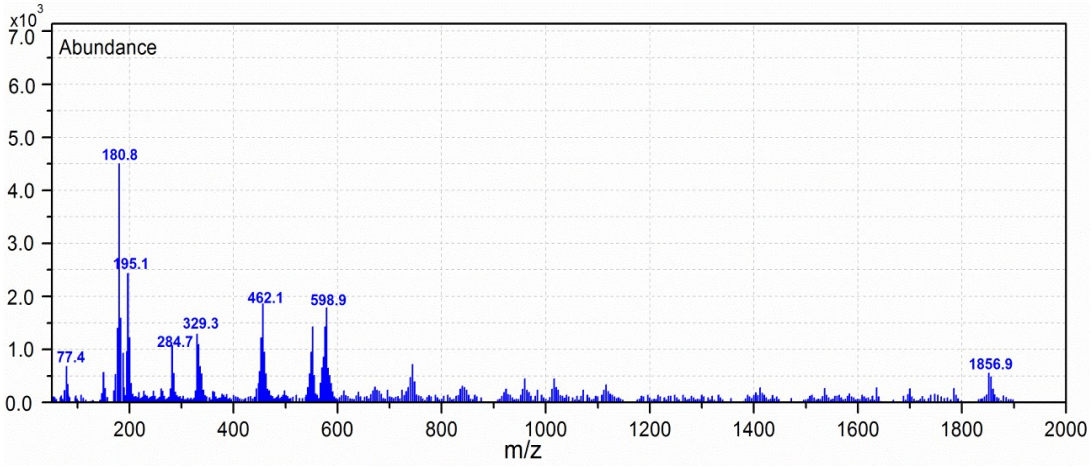


Fig. S12 ESI-Mass spectrum of S**2** after the addition of As^{3+} (240 ppb).

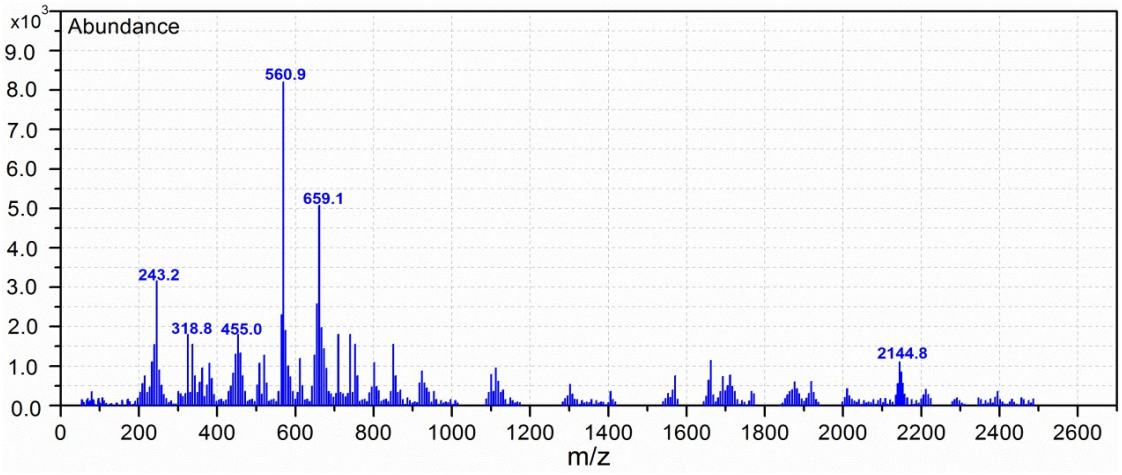


Fig. S13 ESI-Mass spectrum of S**3** after the addition of As^{3+} (240 ppb).

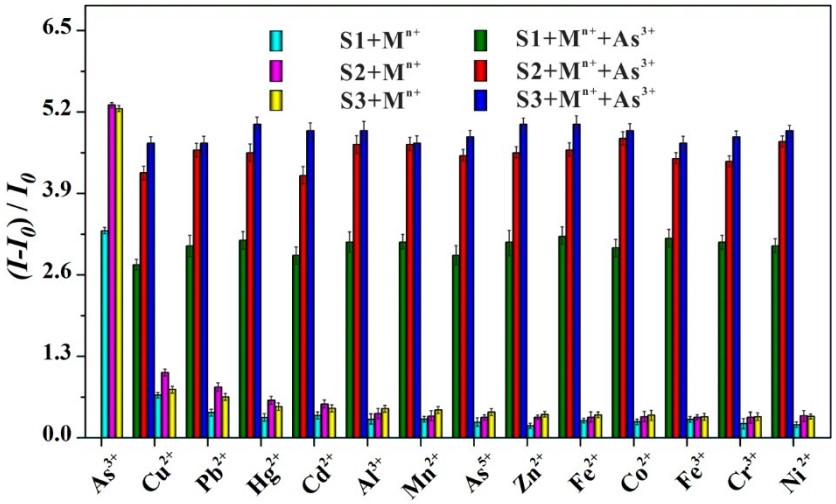


Fig. S14 The selectivity and anti-interference of S1, S2 and S3 toward As^{3+} in water-THF mixtures (v/v, 7/3). The cyan, magenta and yellow bars represent the fluorescence responses of S1, S2 and S3 (10 μM) to various cation ions (As^{3+}, 200 ppb; As^{5+}, Pb^{2+}, Cu^{2+}, 400 ppb; the other, 2000 ppb), respectively. The green, red and blue bars represent the fluorescence of above solution upon subsequent addition of 200 ppb of As^{3+}.

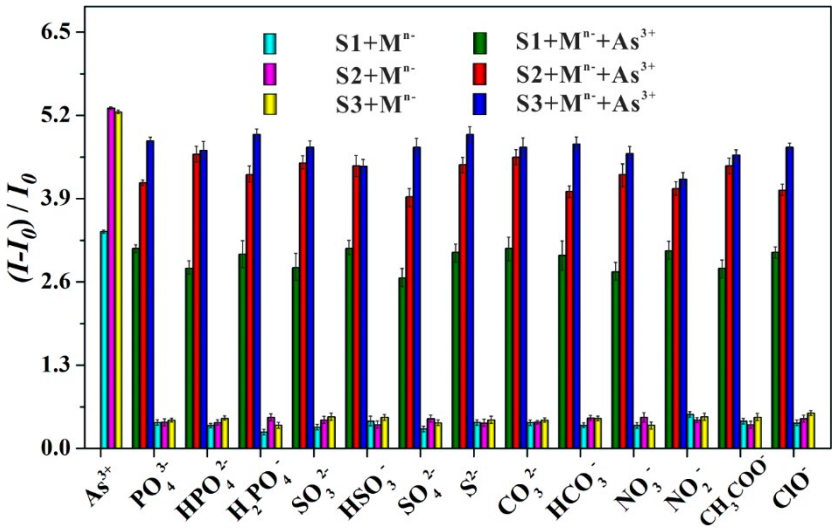


Fig. S15 The selectivity and anti-interference of S1, S2 and S3 toward As^{3+} in water-THF mixtures (v/v, 7/3). The cyan, magenta and yellow bars represent the fluorescence responses of S1, S2 and S3 (10 μM) to various anions (the concentration for various anion was 2000 ppb), respectively. The green, red and blue bars represent the fluorescence of above solution upon subsequent addition of 200 ppb of As^{3+}.

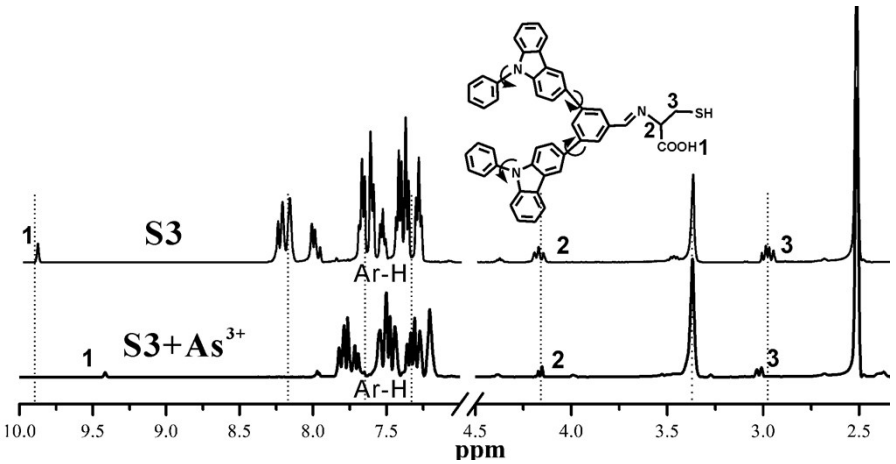


Fig. S16 The ^1H NMR spectra of **S3** in d_6-DMSO before (a) and after (b) addition of 240 ppb of As^{3+}.

Table S1 Comparison of the LOD for the detection of $As^{3+}$by fluorescence chemsensors

Method	LOD(ppb)
Coumarin-Appended Benzothiazolines[1, 2]	0.14-0.23
Functionalized gold nanoparticles[3]	2.58-2.84
Schiff base system[4]	4.10
Cationic polymers and aptamers probe[5]	5.30
GO/Fe_3O_4@GSH[6]	0.1
Rhodamine based fluorescence reagent[7]	0.22
Glutathione-capped CdTe quantum dots[8]	1.50
IC-HG-AFS[9]	1.0-3.0
Gold cluster-based fluorescent sensor[10]	4.01
Nano-sized arsenic-imprinted polymer[11]	37.50
Pulsed Laser-Induced Desorption[12]	1.87
S1	6.74
S2	2.63
S3	1.32

References

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