Supporting information

Near-Infrared Biothiols-Specific Fluorescent Probe for Cancer Cell Recognition

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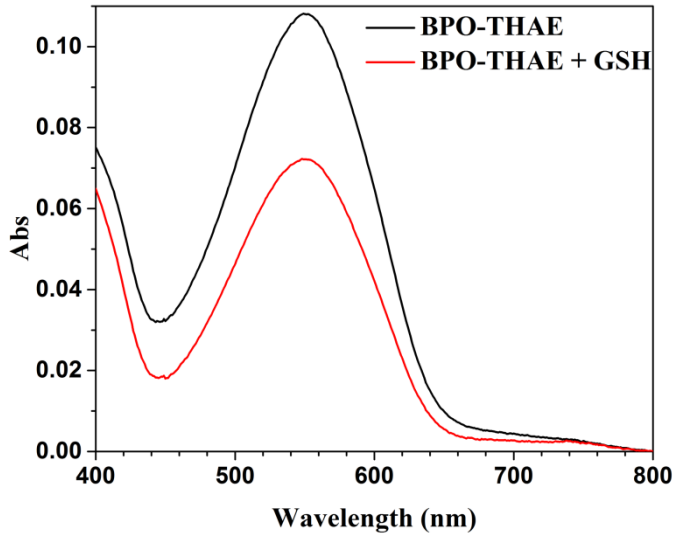


Fig. S1 Absorption spectra of **BPO-THAE** (10 μM) interacting with GSH (500 μM).

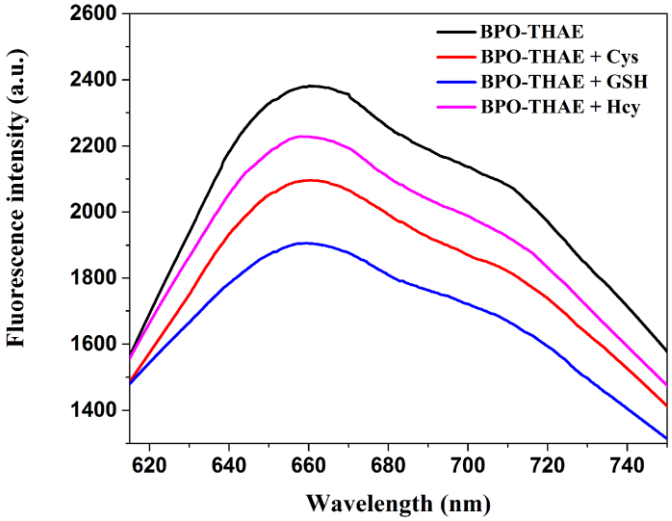


Fig. S2 Fluorescence spectra of **BPO-THAE** (10 μM) interacting with 500 μM Cys, GSH or Hcy.

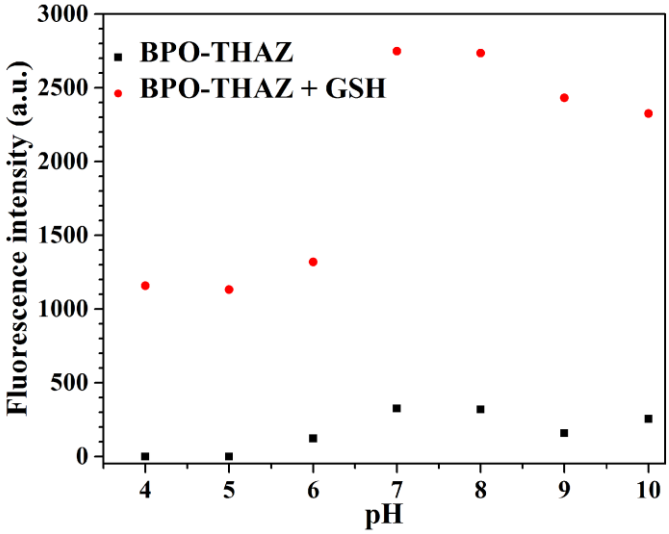


Fig S3 pH dependent fluorescence changes of **BPO-THAZ** (10 μM) in the absence and presence of 500 μM GSH.

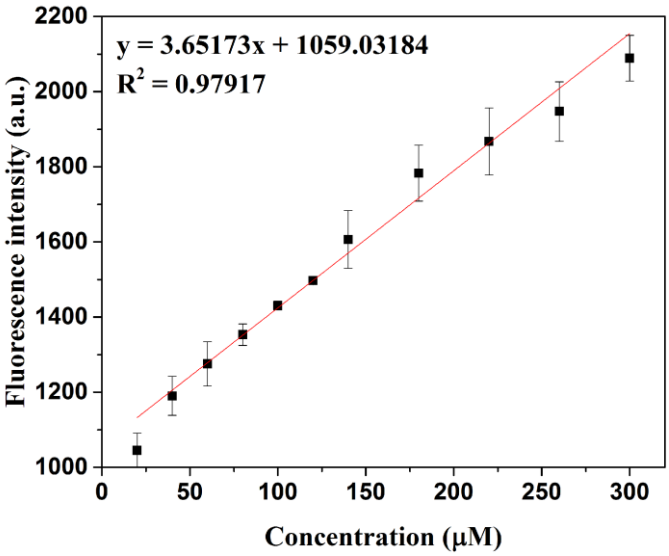


Fig S4 Linear fit of **BPO-THAZ** (10 μM) fluorescence intensity changes with different concentration of GSH at 660 nm.

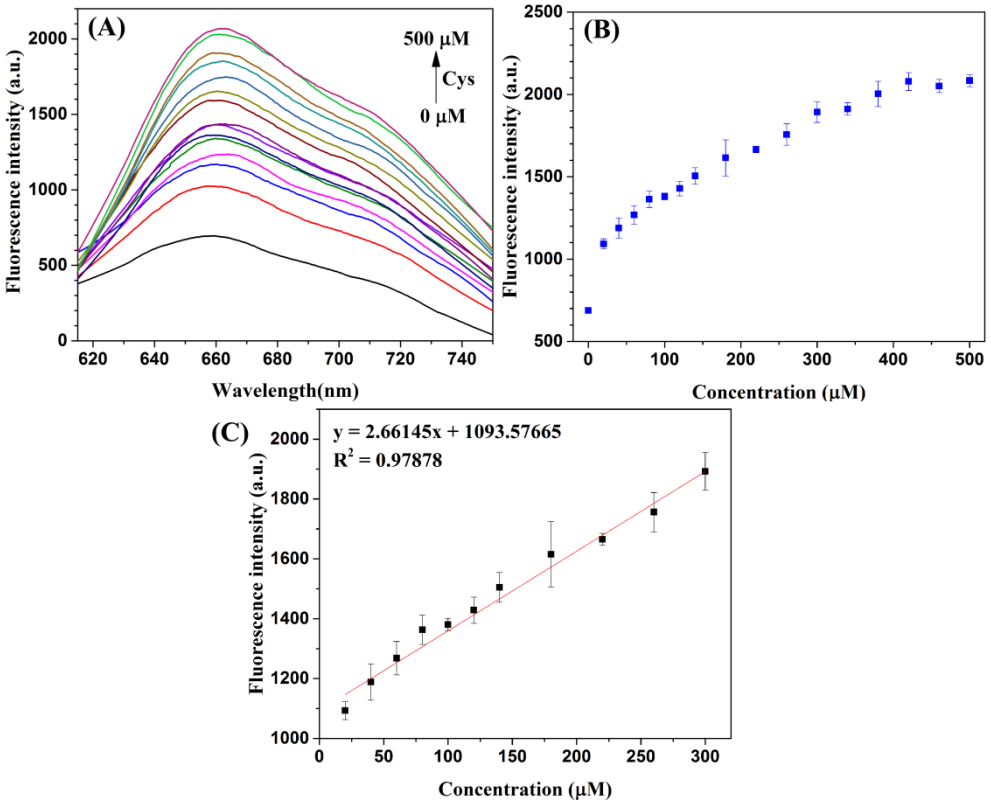


Fig. S5 (A) Fluorescence spectra of **BPO-THAZ** (10 μM) with addition of Cys (0–500 μM). (B) Plot of fluorescence intensity (**BPO-THAZ**, 10 μM) treated with various concentrations of Cys (0–500 μM). (C) Linear fit of fluorescence intensity changes with different concentration of Cys at 660 nm.

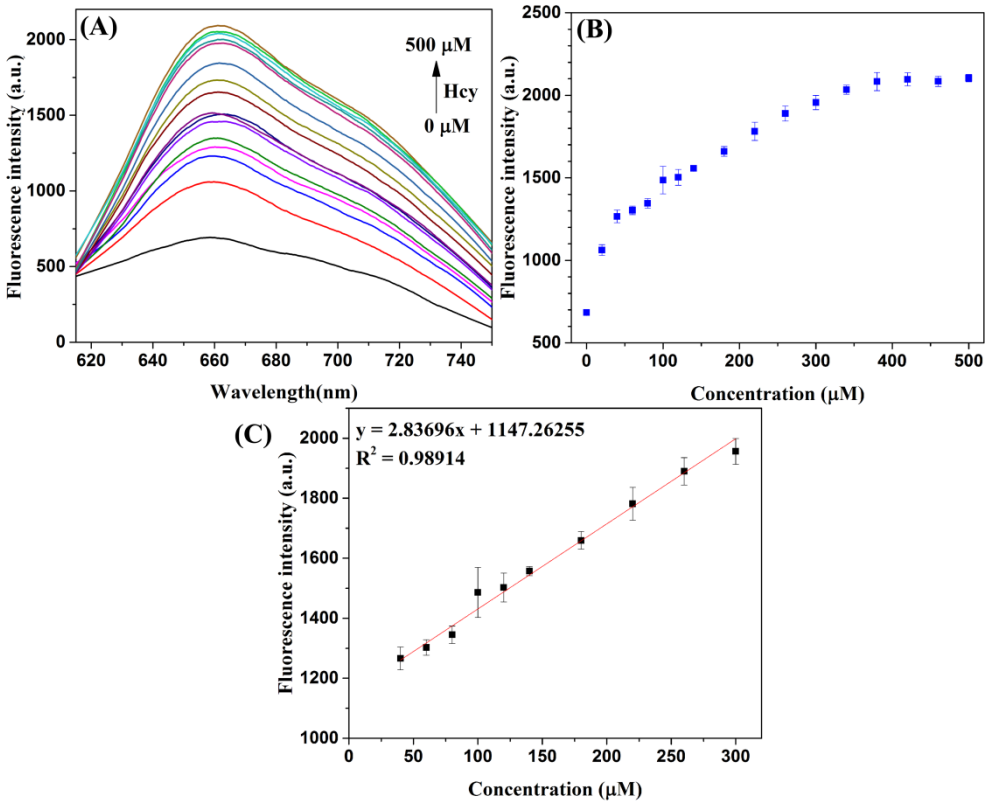


Fig S6 (A) Fluorescence spectra of **BPO-THAZ** (10 mM) with addition of Hcy (0–500 μM). (B) Plot of fluorescence intensity (**BPO-THAZ**, 10 μM) treated with various concentrations of Hcy (0–500 μM). (C) Linear fit of fluorescence intensity changes with different concentration of Hcy at 660 nm.

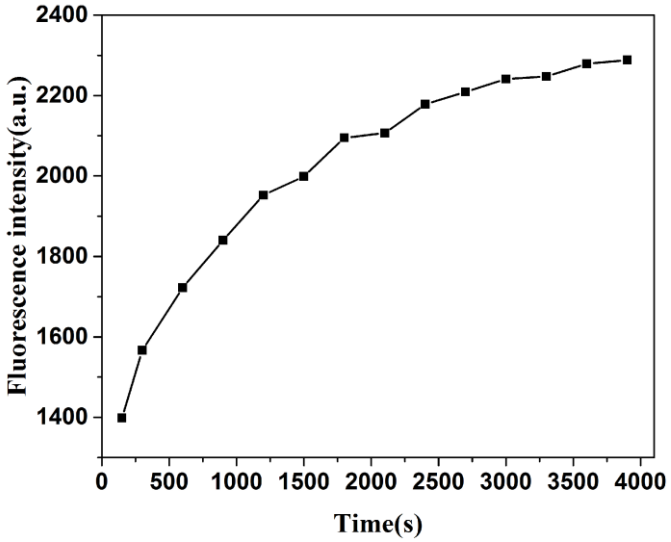


Fig. S7 Time dependent fluorescence changes of **BPO-THAZ** (10 μM) in the presence of 500 μM GSH.

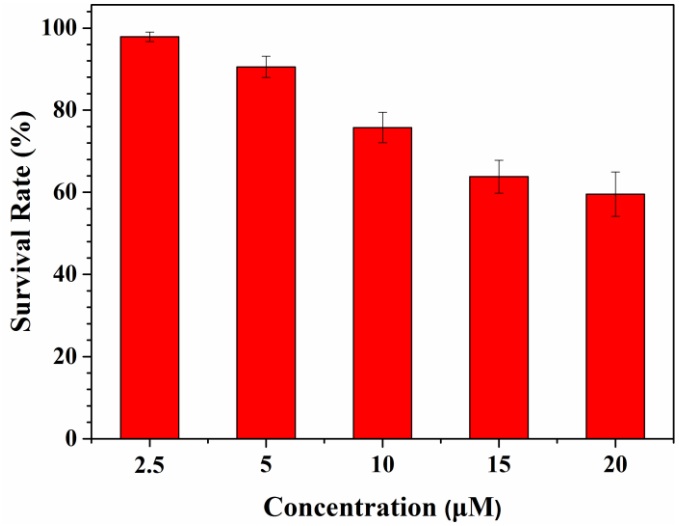


Fig. S8 Cell viability of **BPO-THAZ** by a standard MTT assay.

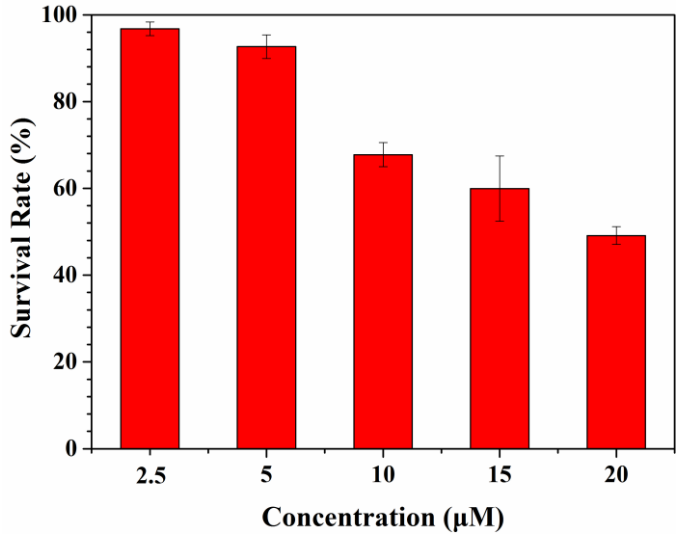


Fig. S9 Cell viability of **BPO-THAE** by a standard MTT assay.

Quantum Yields

The fluorescence quantum yield (Φ) was calculated using:

$$\Phi_x = \Phi_s * (A_s / A_x) * (D_x / D_s) *(n_x^2 / n_s^2)$$

where the subscripts s and x refer to the standard [fluorescein in 0.1 M NaOH (Φ_s = 0.85)] and the test samples, respectively. Thus, Φ_s and Φ_x were the respective quantum yields; n_s and n_x were the refractive indices of the solvents used; A_s and A_x were the absorption intensities at the respective excitation wavelengths of the standard and test samples; and Ds and D_x were integrals of the fluorescence intensities.

For BPO-THAZ: A_s = 0.00886, A_x = 0.04818, D_s = 2012539.252, D_x = 65558.925

For BPO-THAZ + GSH: A_s = 0.00886, A_x = 0.07118, D_s = 2012539.252, D_x = 272866.891

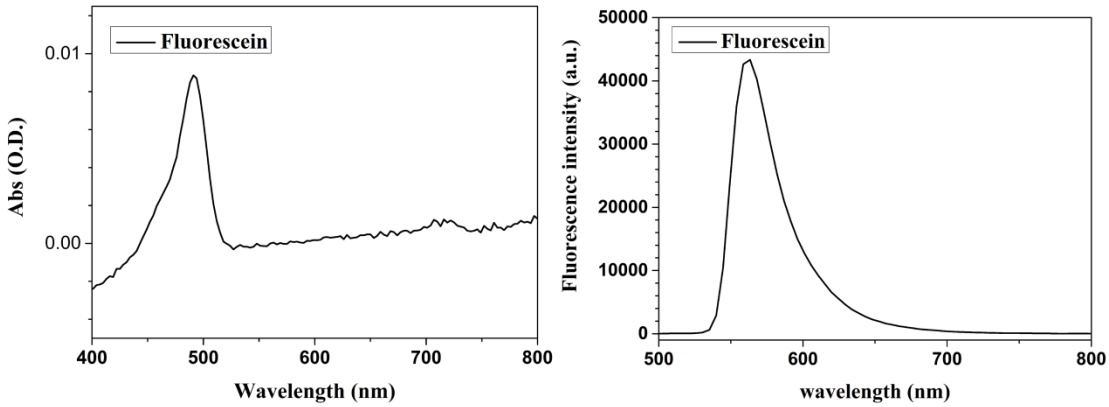


Fig. S10 The absorption and emission spectrum of fluorescein in 0.1 M NaOH solution for quantum yields testing.

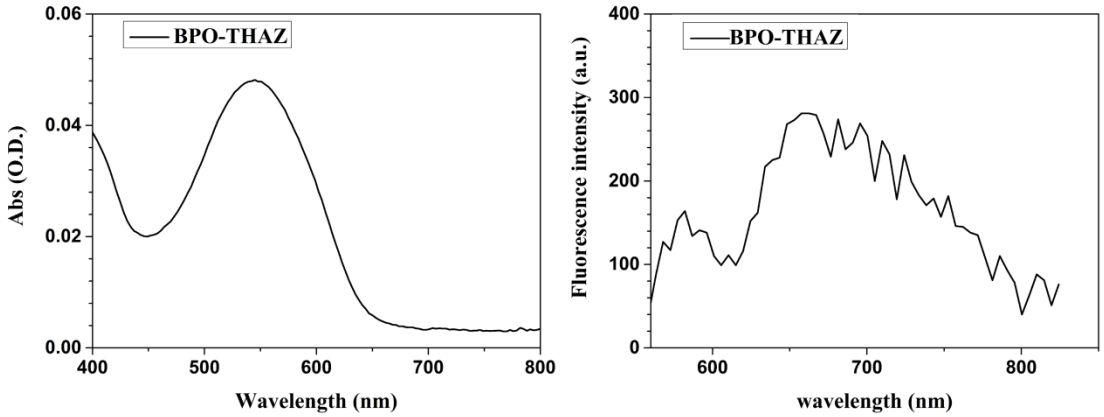


Fig. S11 The absorption and emission spectrum of **BPO-THAZ** for quantum yields testing.

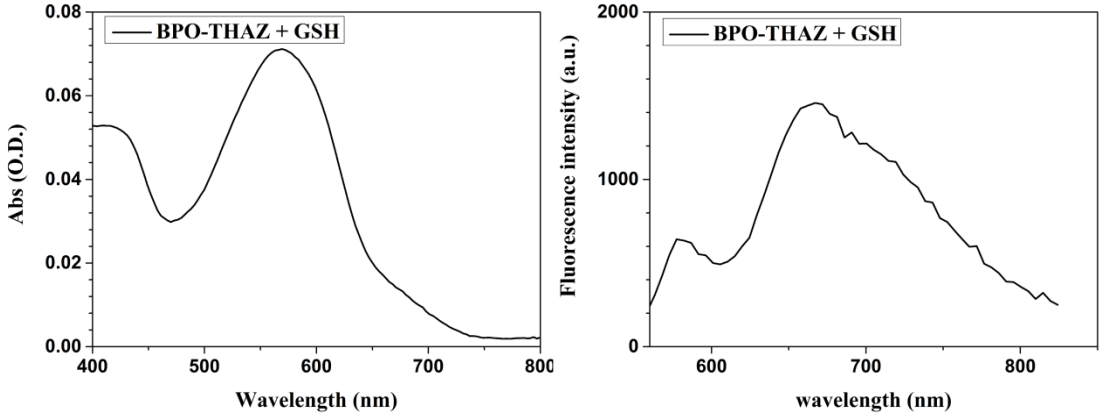
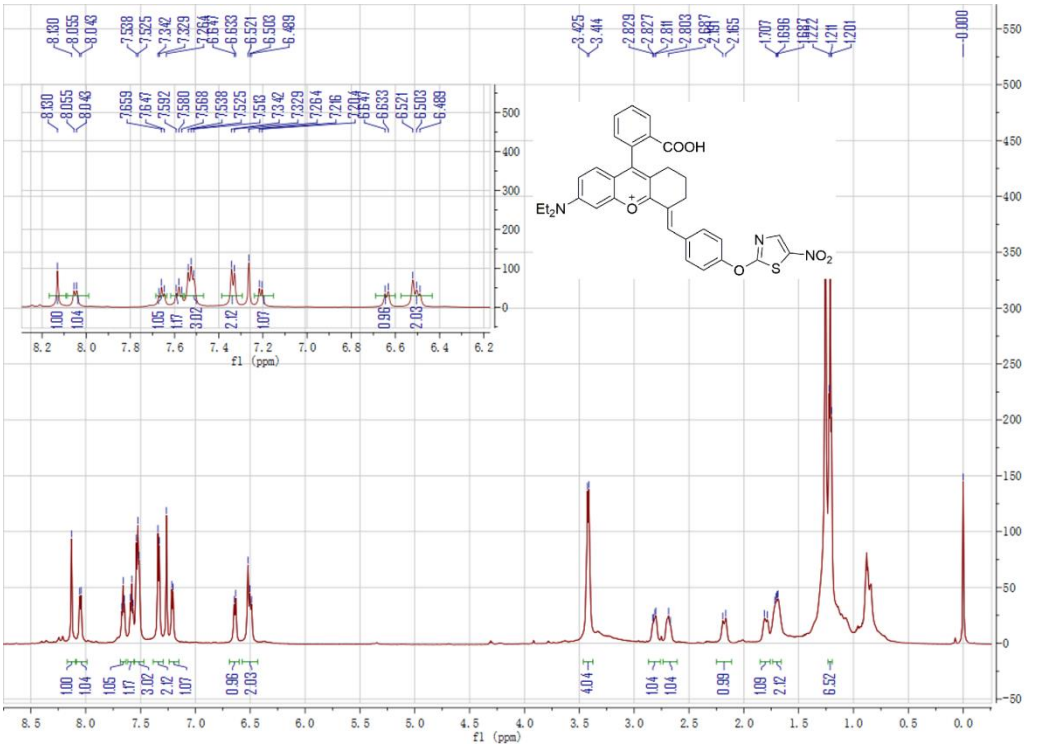


Fig. S12 The absorption and emission spectrum of **BPO-THAZ** after reacting with GSH for quantum yields testing.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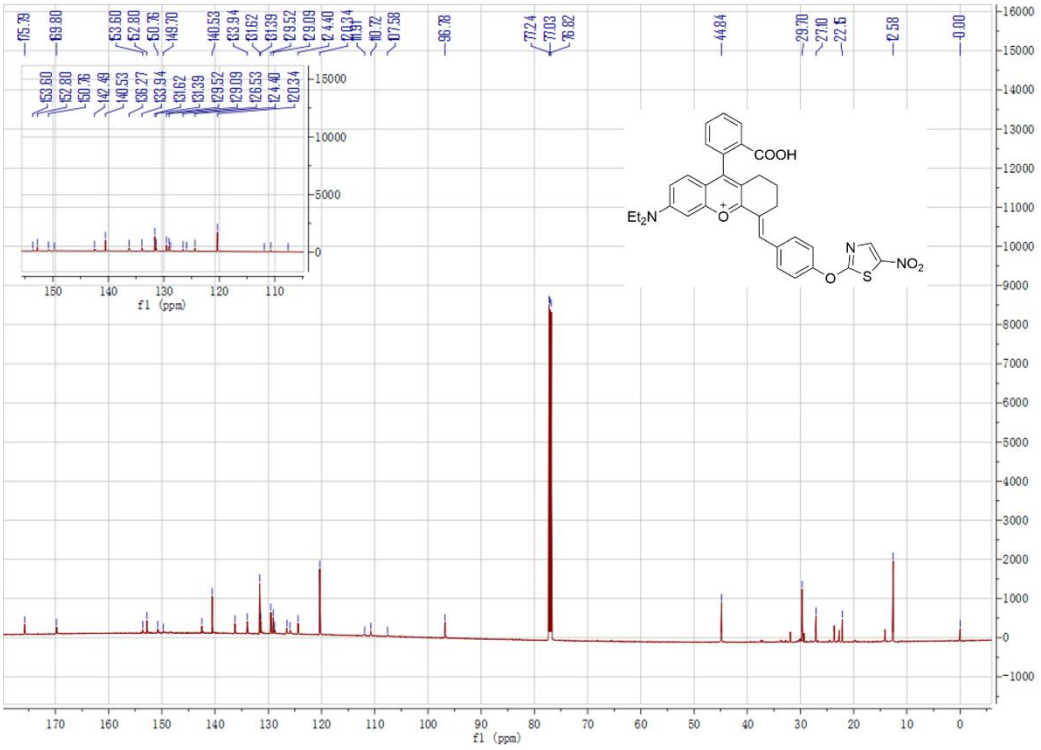
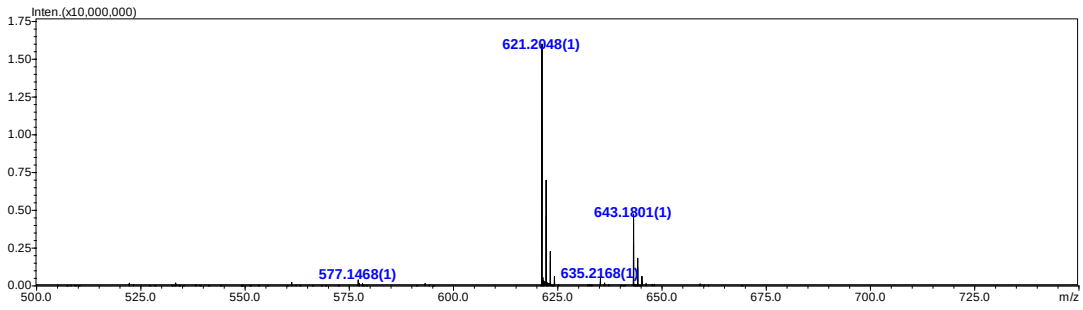
Et2N
N
S
NO2
O
f1 (ppm)


COOH
Et2N
N
S
NO2
O
f1 (ppm)

ESI+


Inten.(x10,000,000)
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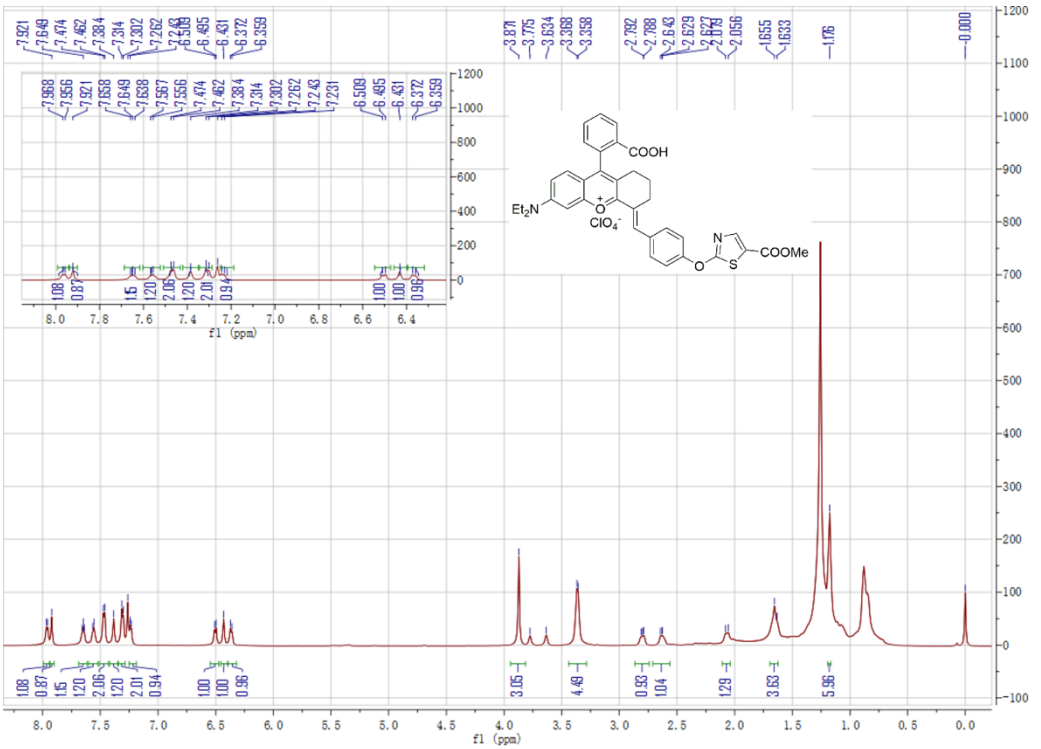
643.1801(1)
577.1468(1)
635.2168(1)
m/z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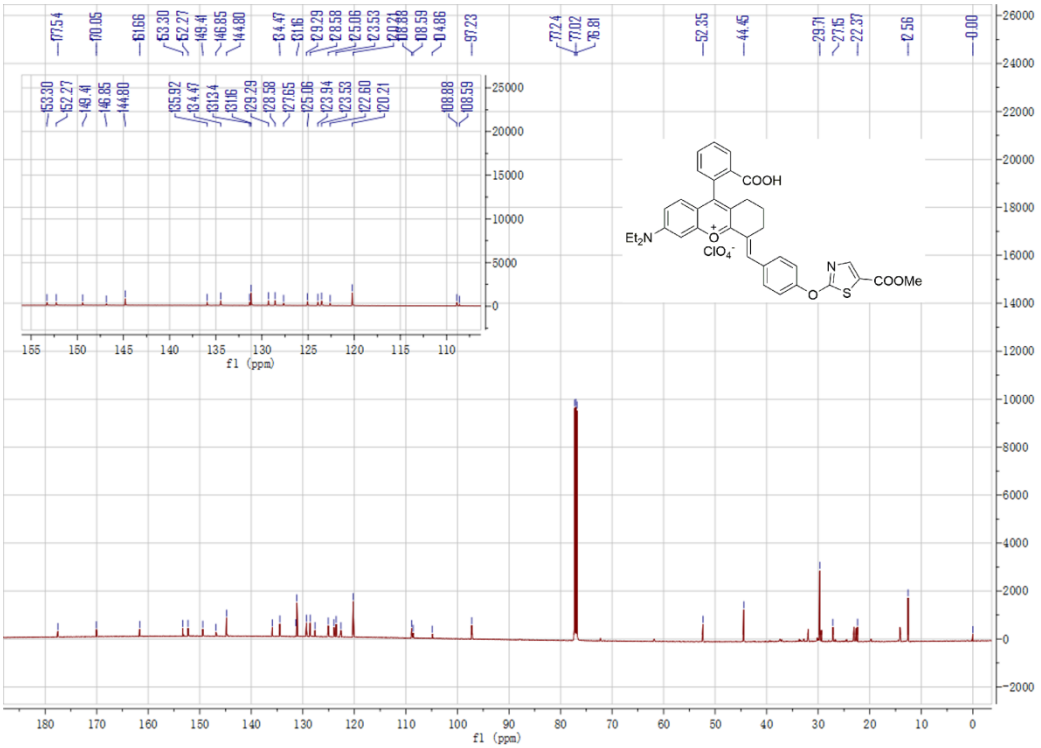
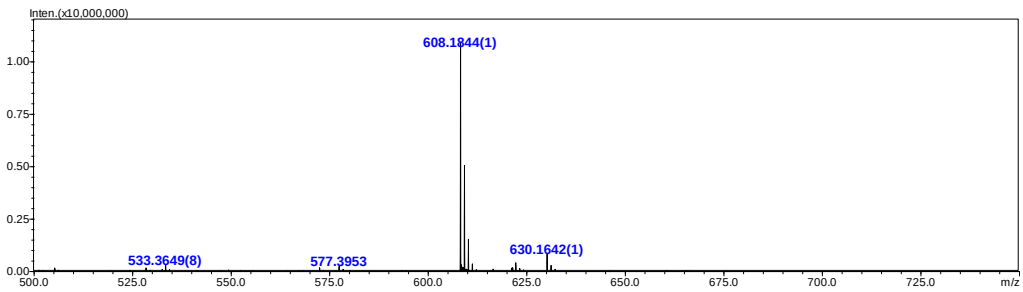
Et2N
ClO4-
COOMe
f1 (ppm)


COOH
Et2N
ClO4-
COOMe
f1 (ppm)

ESI+


Inten.(x10,000,000)
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533.3649(8)
577.3953
630.1642(1)
m/z