

## **Electronic Supplementary Material (ESI) for New Journal of Chemistry.**

### **Electronic Supplementary Information (ESI)**

#### **A novel ratiometric fluorescence probe with AIE-based for specific detection of Hcy/Cys and imaging of living cells in vivo**

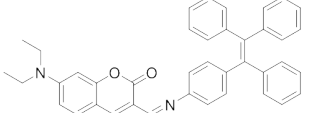
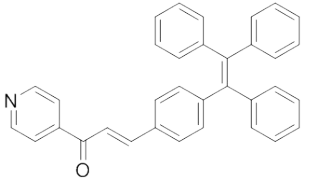
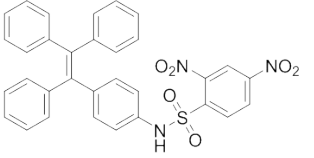
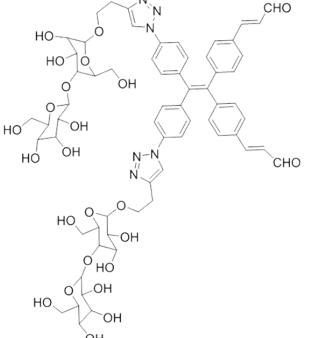
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Table S1 Fluorescent probes based on TPE ligands for the selective detection of biothiols (individually or in pairs)

Probe	Selectivity	Type	detection limit	Biological system	Ref.
	Cys+Hcy	Turn-on	5 $\mu$ m	No study	[16g]
	Hcy	Ratiometric	0.346 $\mu$ m	No study	[16b]
	Cys	turn-on	0.18 $\mu$ m	HeLa cells	[16f]
	Cys	Ratiometric	25 $\mu$ m	HepG2 cells	Ref.16h

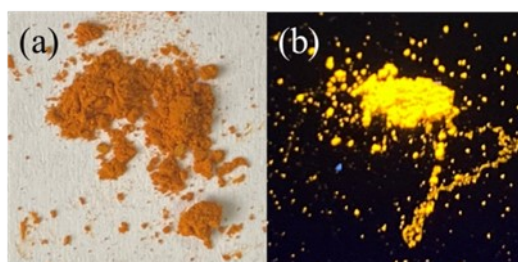


Fig.S1 Color of the probe powder under visible light (a) and UV light (b).

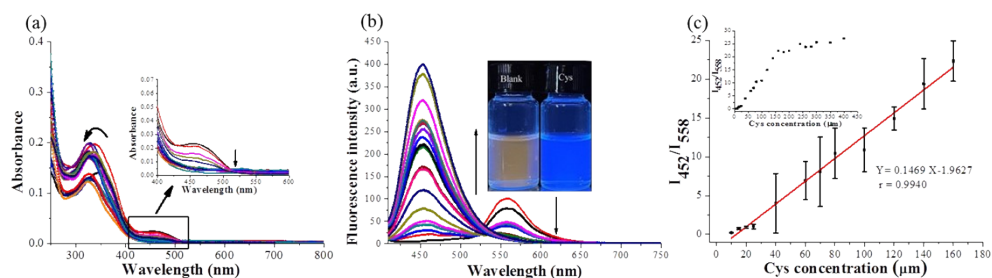


Fig.S2 (a) Absorption spectra of probe (10  $\mu$ M) upon addition of increasing concentrations of Cys (0–400  $\mu$ M) in  $\text{CH}_3\text{CN}$ /phosphate buffer (3:7 v/v, 20 mM, pH 7.4) for 35 min. (b) Fluorescence spectra of probe (10  $\mu$ M) upon addition of increasing concentrations of Cys (0–400  $\mu$ M) in

acetonitrile/phosphate buffer (3:7 v/v, 20mM, pH 7.4) for 35min. The inset shows fluorescence changes of 1 in the absence and presence of Cys under UV light at 365 nm.(c)Linear plot of the emission ratio ( $I_{452}/I_{558}$ ) against Cys concentration (10–160  $\mu\text{M}$ ) when using probe(10  $\mu\text{M}$ ). The inset shows the emission ratio ( $I_{452}/I_{558}$ ) as a function of Cys concentration.

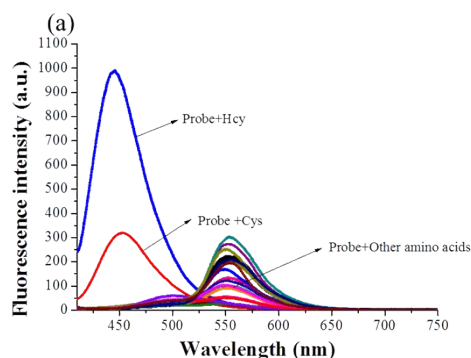


Fig.S3 Fluorescence responses of Probe (10 $\mu\text{M}$ ) to 300  $\mu\text{M}$  of different amino acids in  $\text{CH}_3\text{CN}$ /phosphate buffer (3:7 v/v, 20mM, pH 7.4)

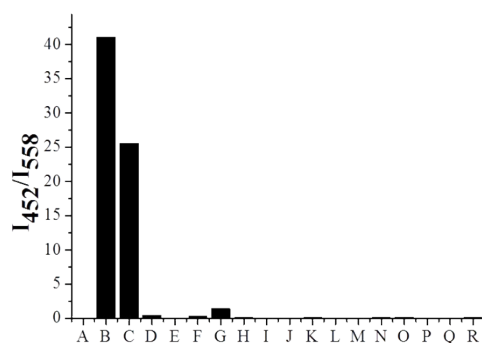


Fig.S4 The emission ratio  $I_{452}/I_{558}$  of Probe (10  $\mu\text{M}$ ) in the presence of other analytes. (A) Blank, (B) Hcy, (C) cys, (D) Cystine, (E) 3-Mercaptopropionic acid, (F)  $\text{SO}_3^{2-}$ , (G)  $\text{HS}^-$ , (H)  $\text{Al}^{3+}$ , (I)  $\text{Br}^-$ , (J)  $\text{C}_2\text{O}_4^{2-}$ , (K)  $\text{Ca}^{2+}$ , (L)  $\text{F}^-$ , (M)  $\text{K}^+$ , (N)  $\text{Mg}^{2+}$ , (O)  $\text{S}_2\text{O}_3^{2-}$ , (P)  $\text{SO}_4^{2-}$ , (Q) ascorbic acid, (R)  $\text{Zn}^{2+}$

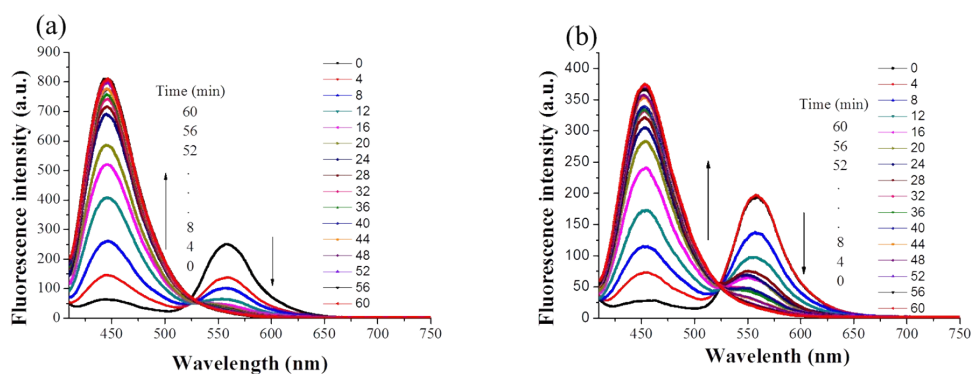


Fig.S5 Time-dependent fluorescence spectra of probe (10  $\mu\text{M}$ ) with 30 equiv. of Hcy (a) and Cys (b)

Spectrum from 20210411-POS-ZJ-5.wiff (sample ... iment 1, +TOF MS (100 - 1500) from 0.164 min

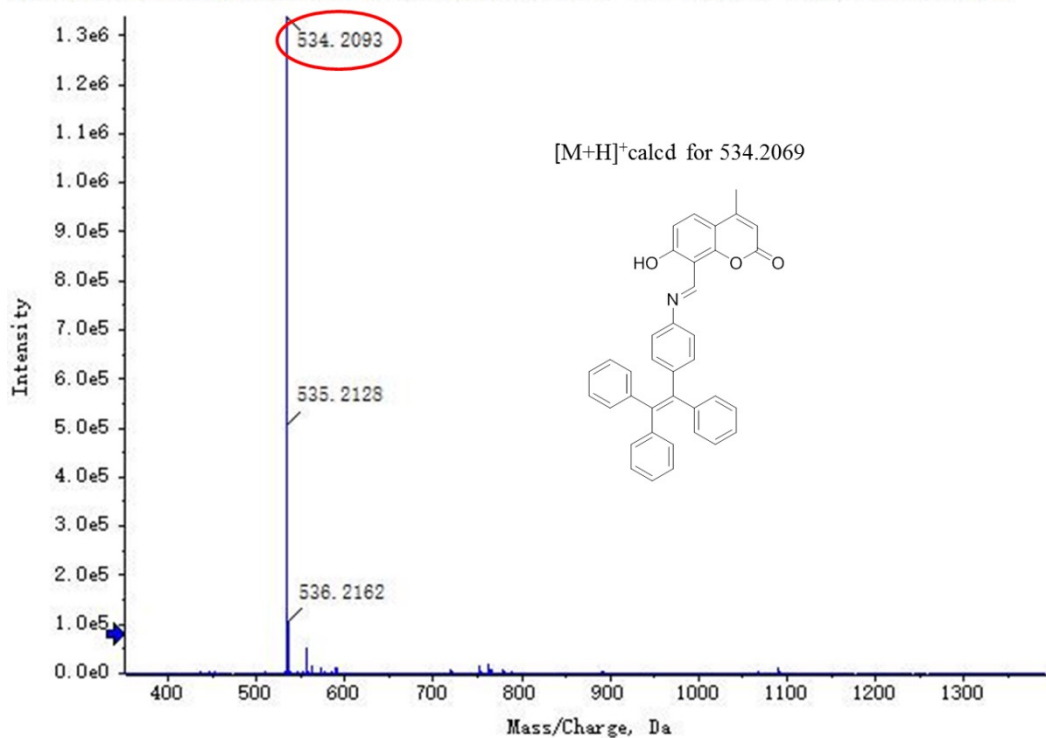


Fig.S6 HRMS spectrum of probe in CH<sub>3</sub>OH

20210407-0406-M-1-HNMR  
HNMR

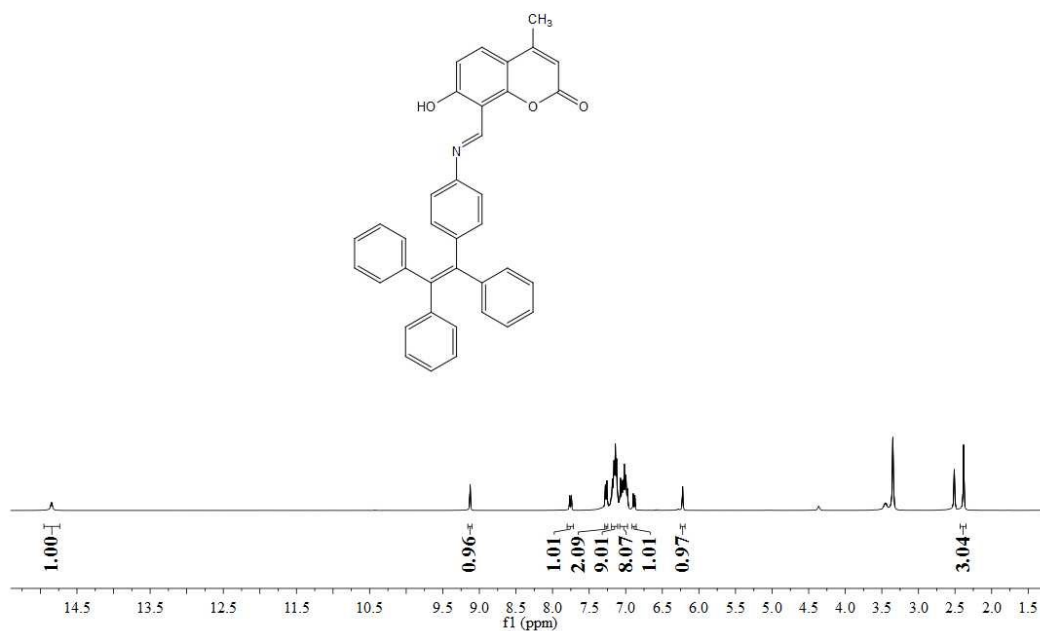


Fig.S7 <sup>1</sup>H-NMR spectrum of probe in DMSO-d<sub>6</sub>

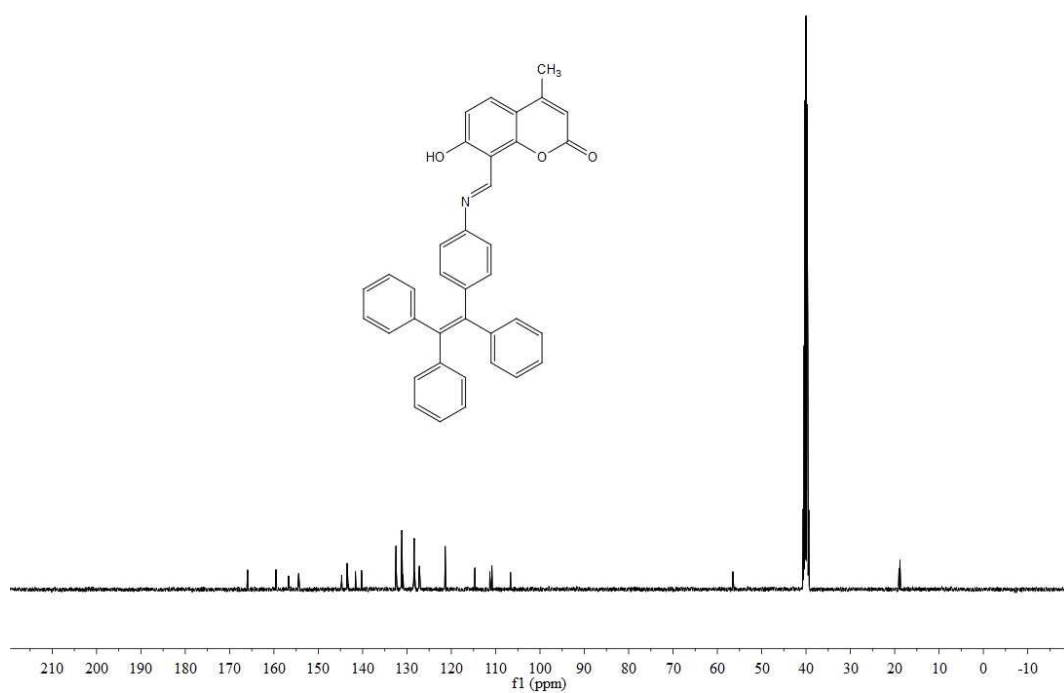


Fig.S8  $^{13}\text{C}$ -NMR spectrum of probe in DMSO-d<sub>6</sub>

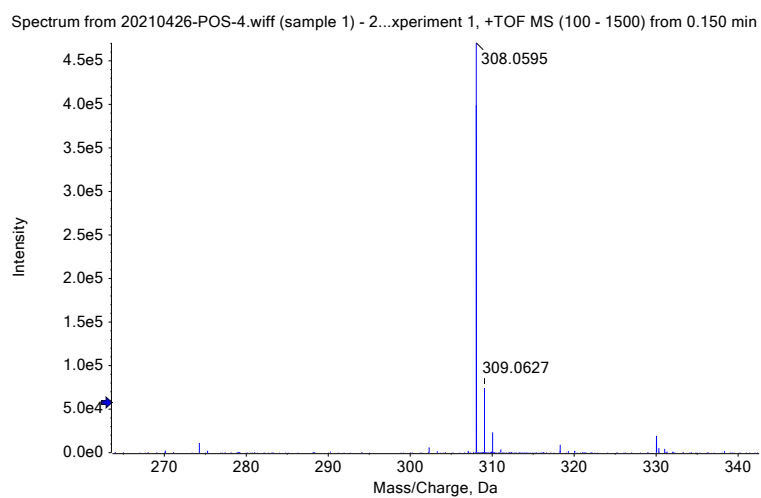


Fig.S9 HRMS spectrum of condensation product of **1** with Cys

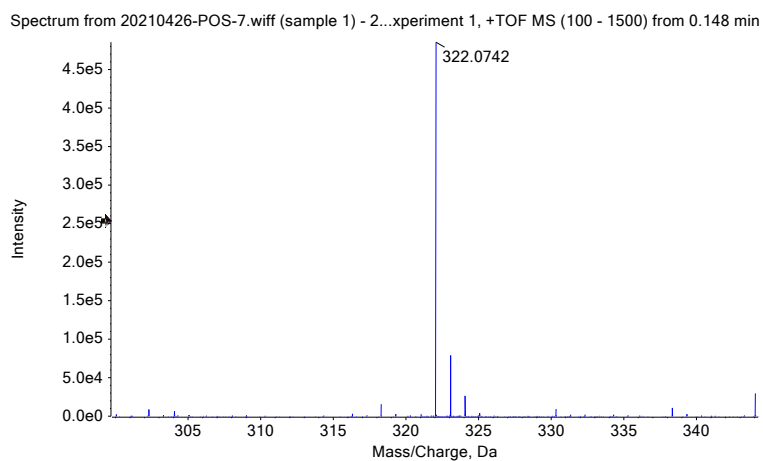


Fig.S10 HRMS spectrum of condensation product of 1 with HCy

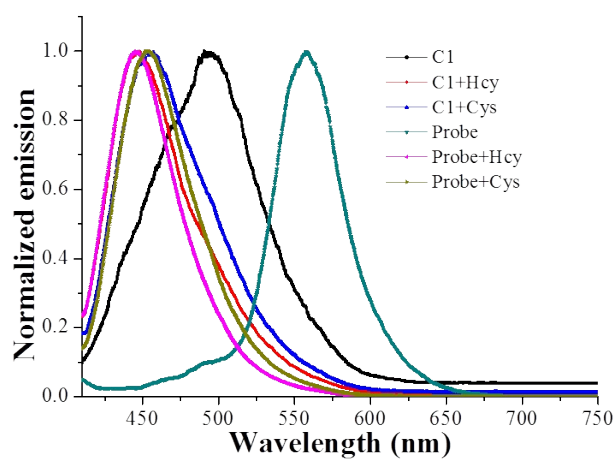


Fig.S11 Normalized fluorescence spectra of Probe and C1 (10  $\mu$ M) in absence and presence of Hcy/Cys (300  $\mu$ M) in acetonitrile/phosphate buffer (3:7 v/v, 20mM, pH 7.4)

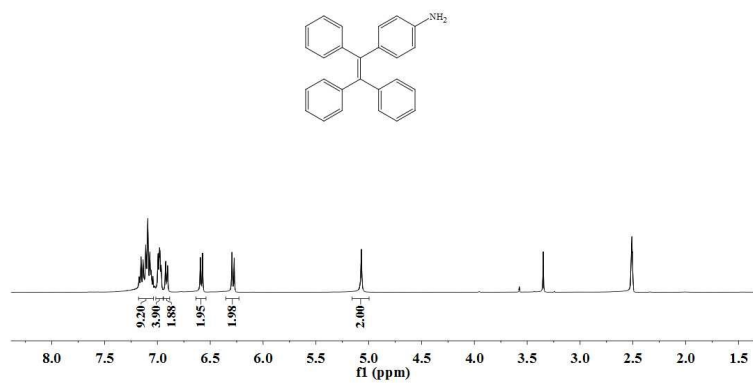


Fig.S12 <sup>1</sup>H-NMR spectrum of TPE-NH<sub>2</sub> in DMSO-d<sub>6</sub>

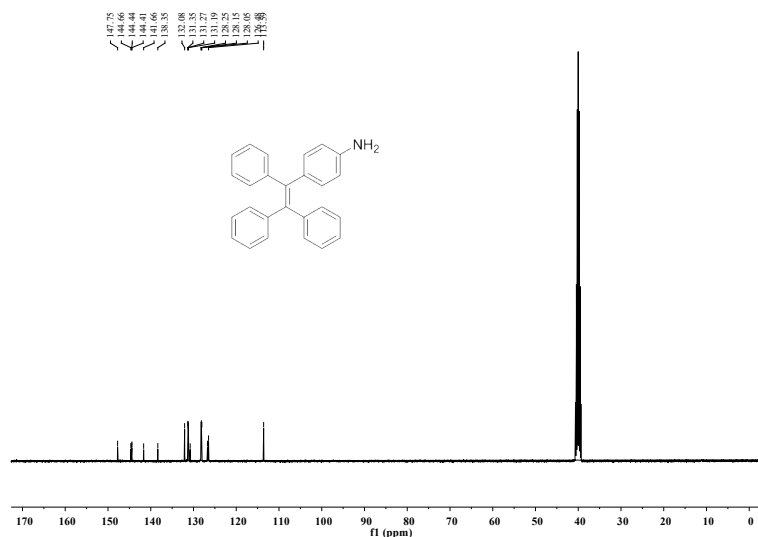


Fig.S13 <sup>13</sup>C-NMR spectrum of TPE-NH<sub>2</sub> in DMSO-d<sub>6</sub>  
 Spectrum from 20210411-POS-ZJ-5.wiff (sample 1...riment 1, +TOF MS (100 - 1500) from 0.134 min

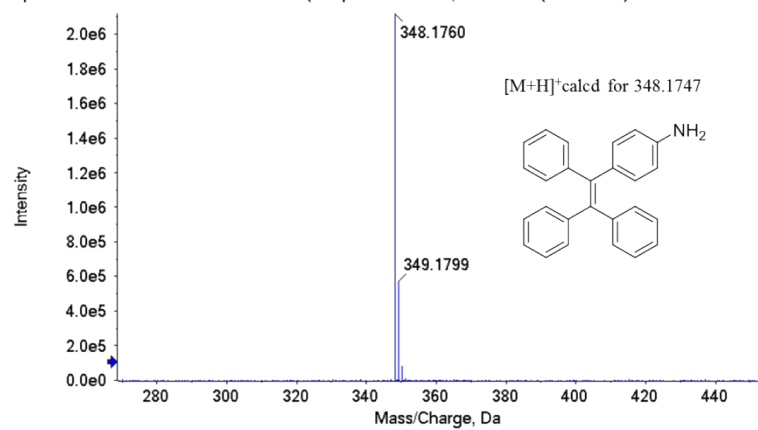


Fig.S14 HRMS spectrum of TPE-NH<sub>2</sub> in CH<sub>3</sub>OH

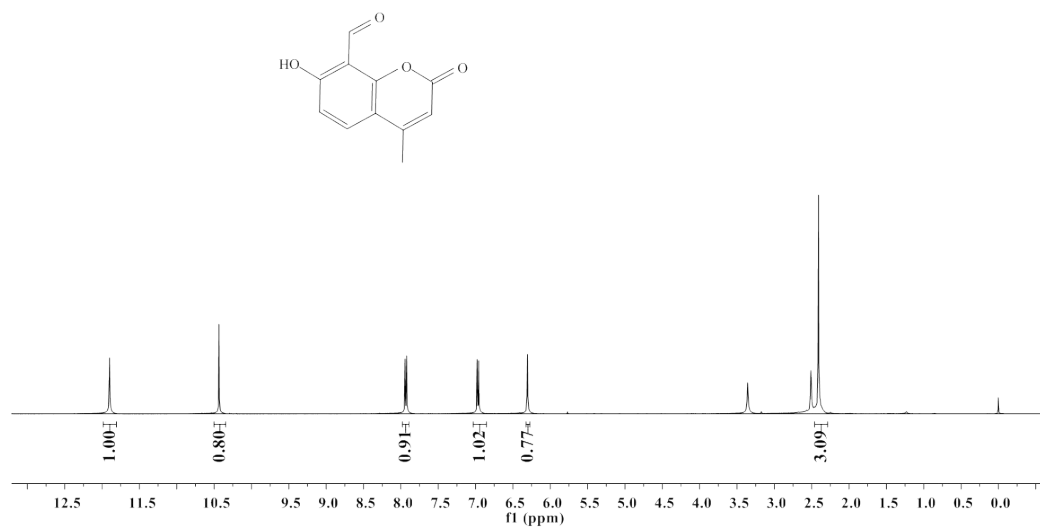


Fig.S15 <sup>1</sup>H-NMR spectrum of C1 in DMSO-d6

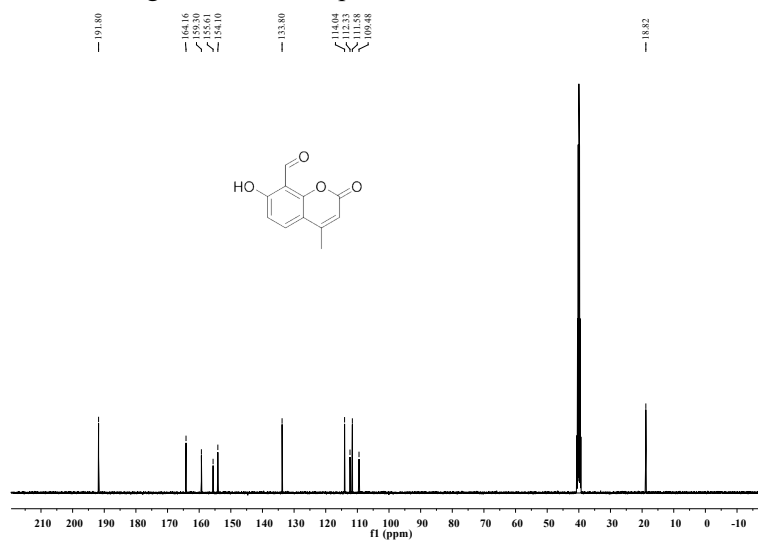


Fig.S16 <sup>13</sup>C-NMR spectrum of C1 in DMSO-d6

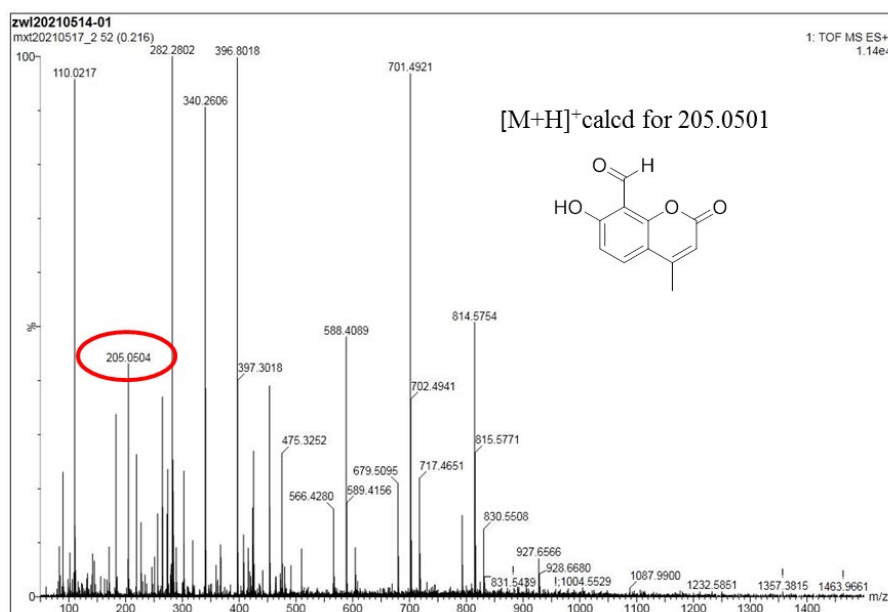


Fig.S17 HRMS spectrum of C1 in CH<sub>3</sub>OH