

## Electronic Supplementary Information

### **AIE fluorophore with enhanced cellular uptake for tracking esterase-activated release of taurine and ROS scavenging**

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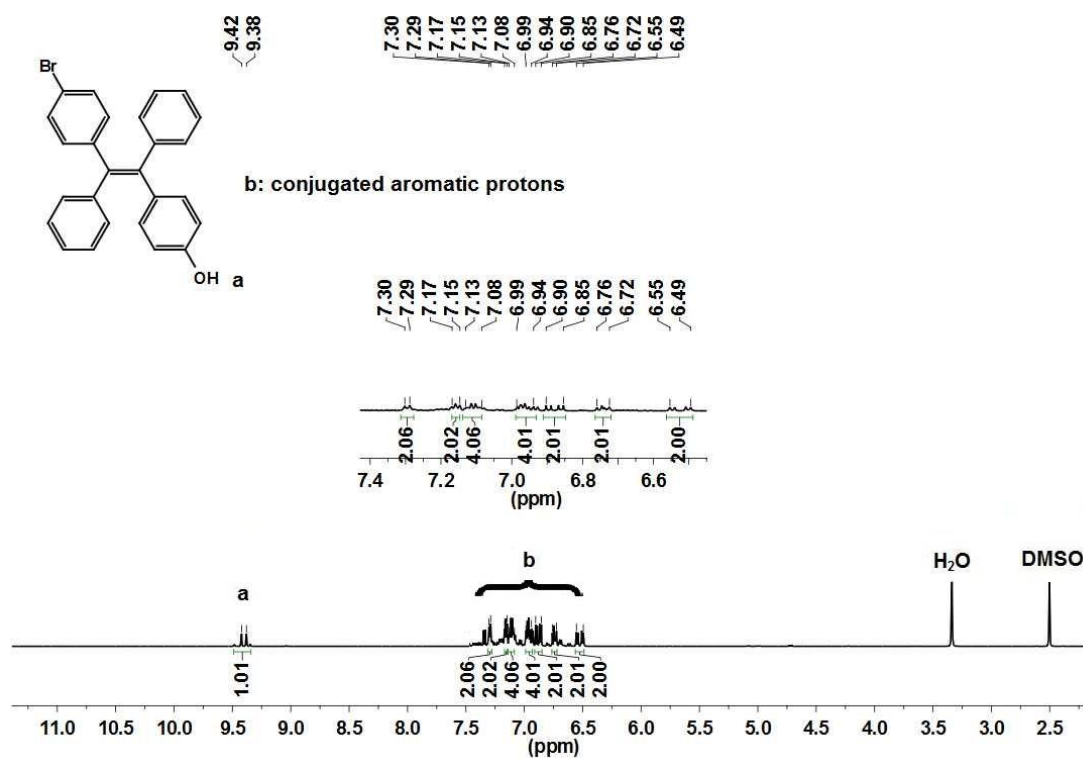


Fig. S1 <sup>1</sup>H NMR spectrum of Compound 3 in DMSO.

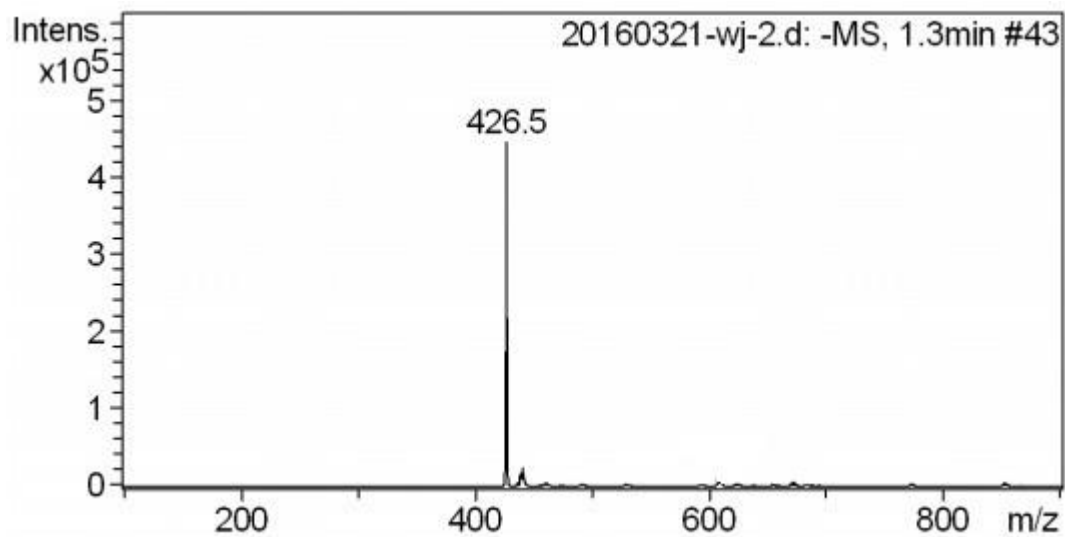


Fig. S2 Mass spectrum of Compound 3. MS (ESI):  $m/z$  426.5 [M].

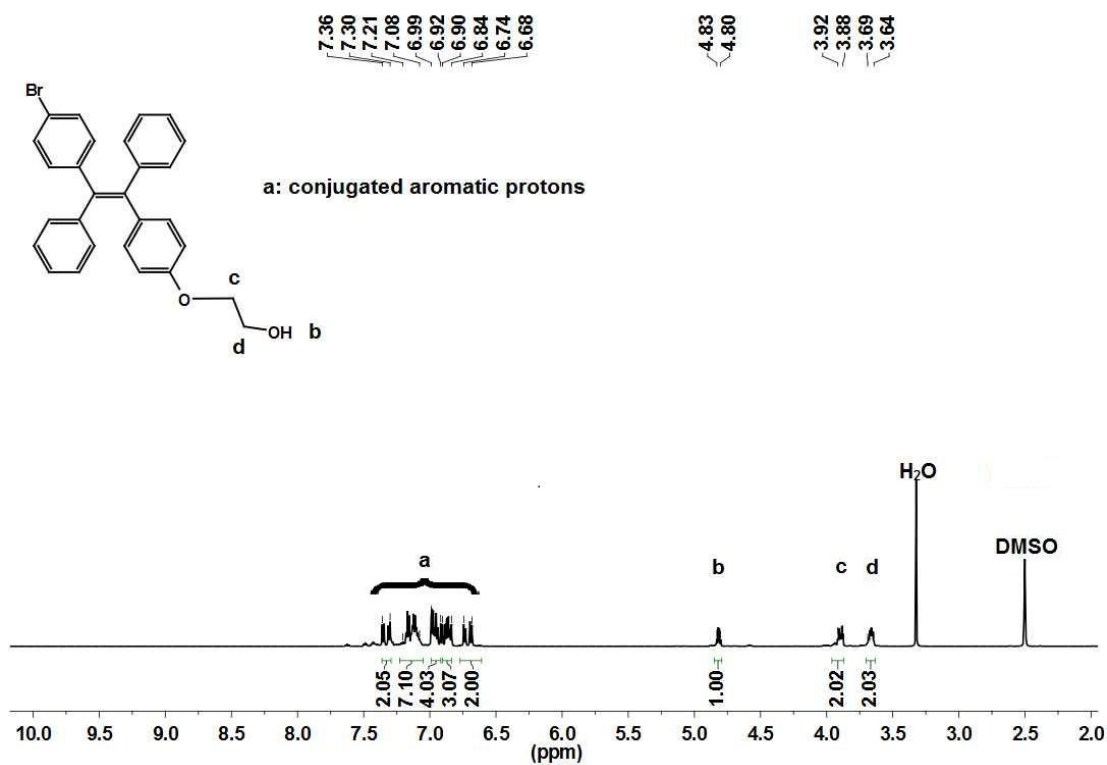


Fig. S3 <sup>1</sup>H NMR spectrum of Compound 5 in DMSO.

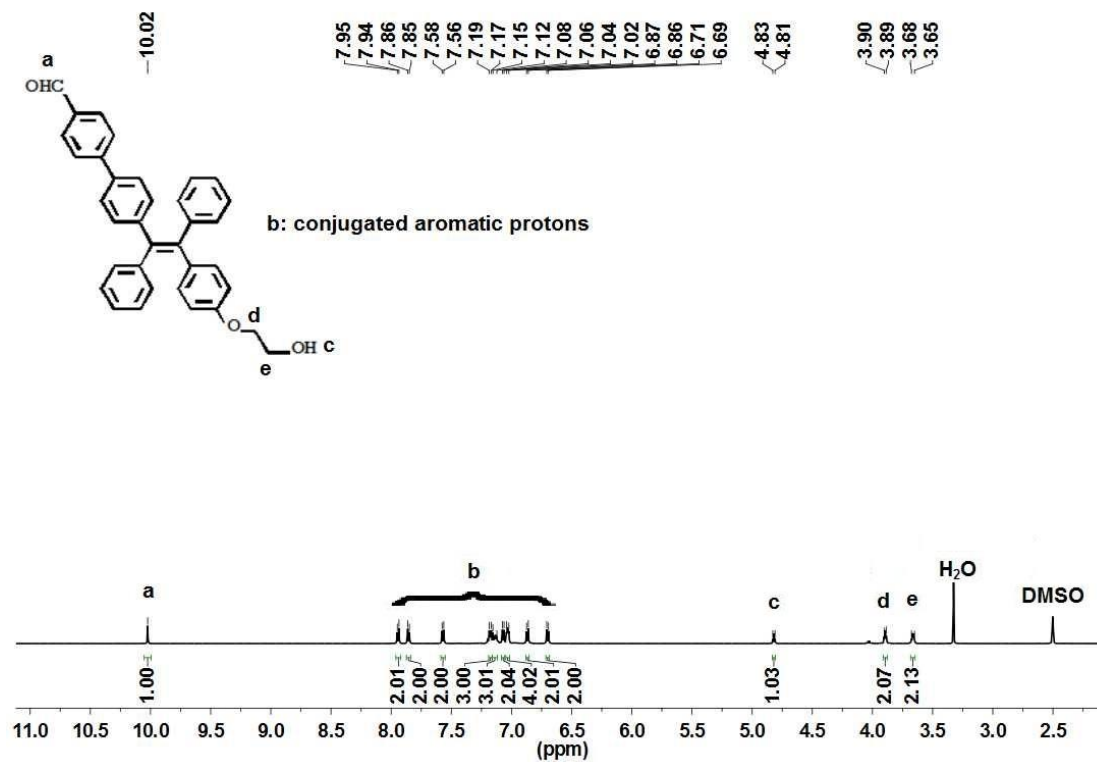


Fig. S4 <sup>1</sup>H NMR spectrum of Compound 7 in DMSO.

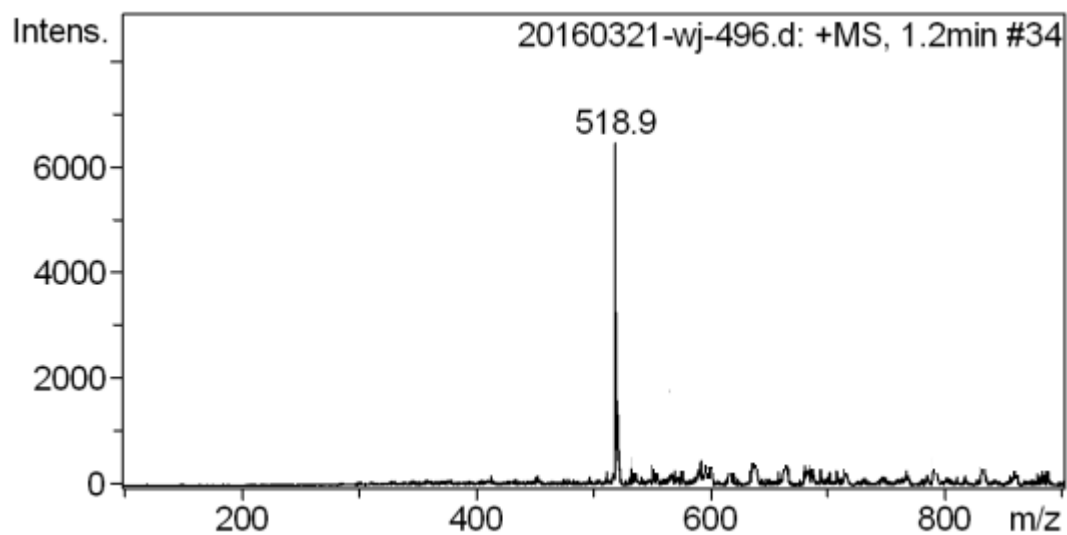


Fig. S5 Mass spectrum of Compound 7. MS (ESI):  $m/z$  518.9  $[M]^+$ .

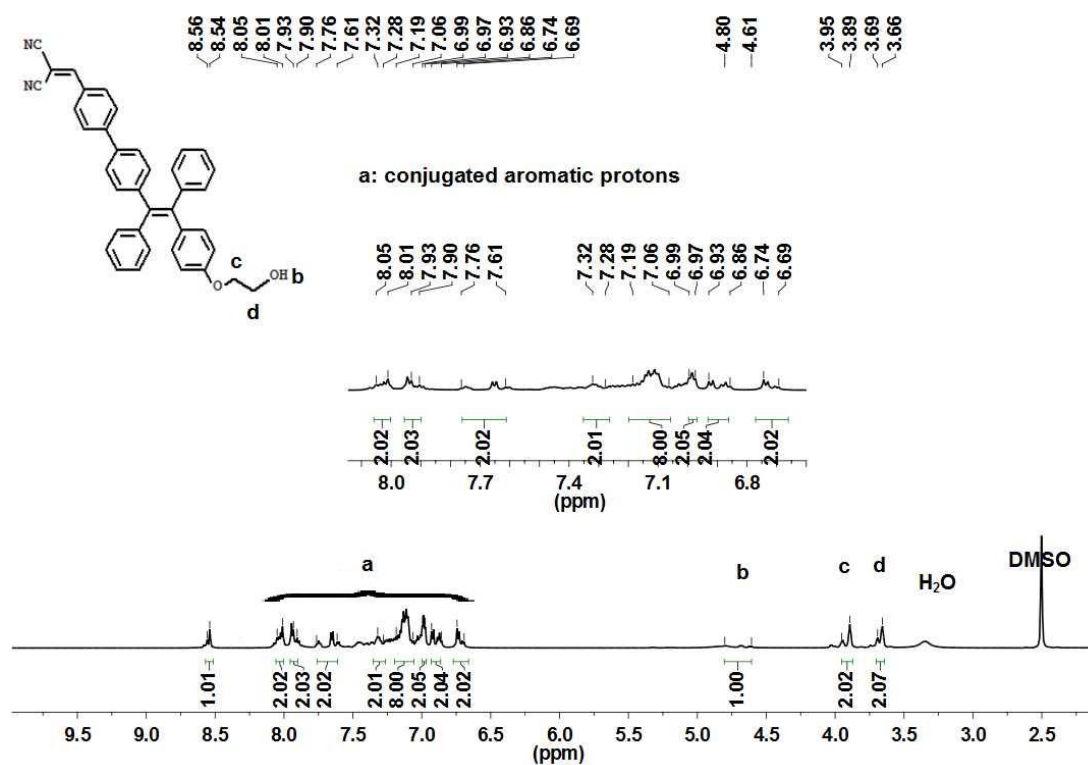


Fig. S6  $^1\text{H}$  NMR spectrum of Compound 9 in DMSO.

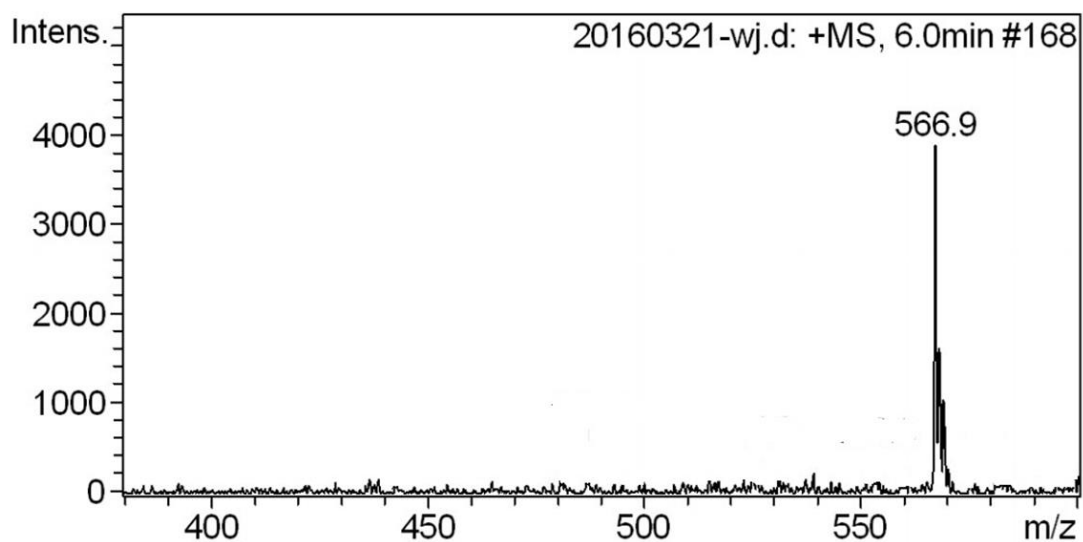


Fig. S7 Mass spectrum of Compound 9. MS (ESI):  $m/z$  566.9  $[M]^+$ .

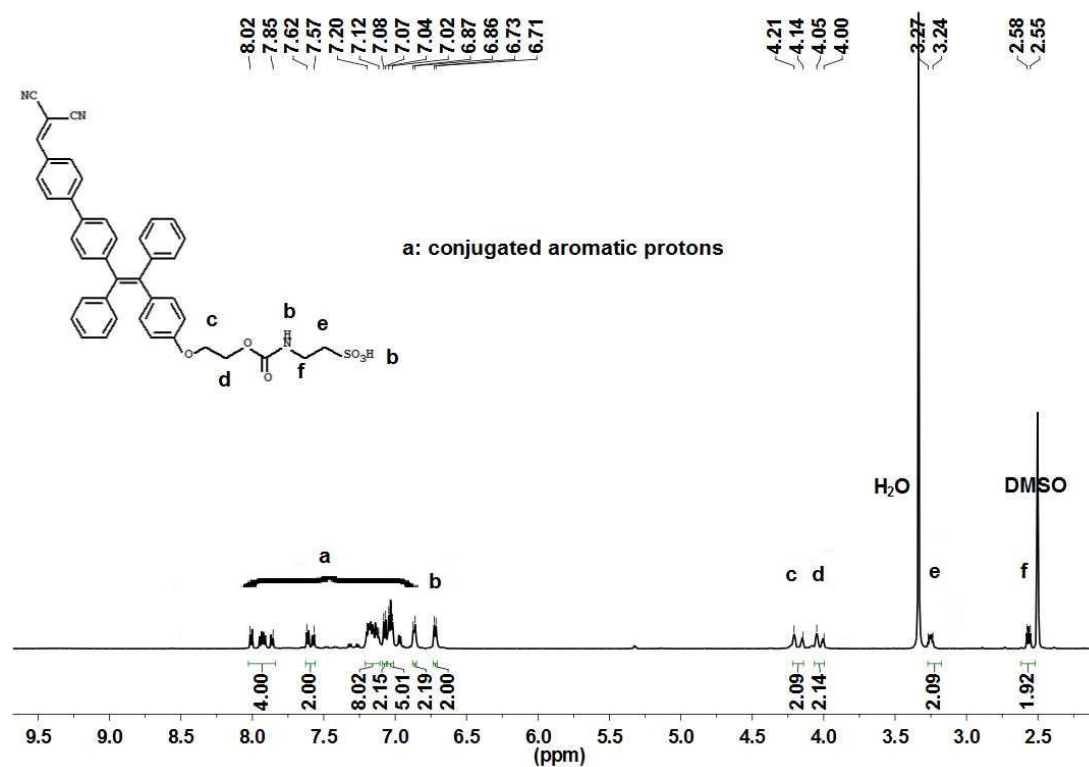
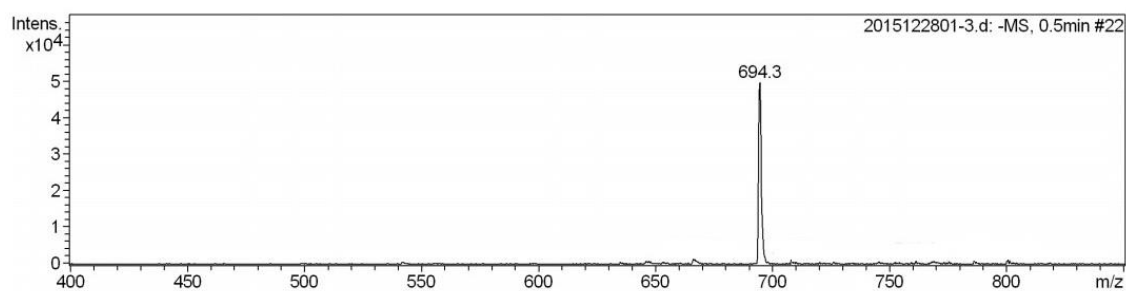


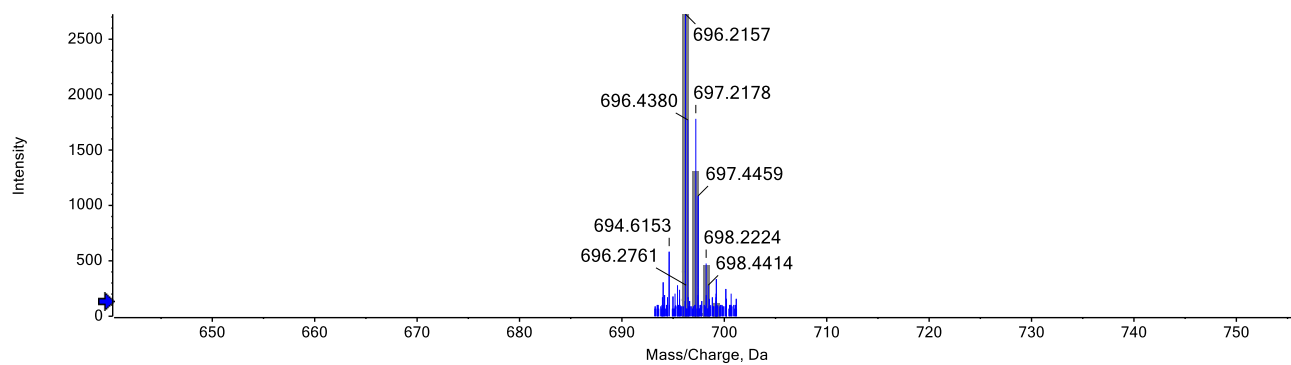
Fig. S8  $^1\text{H}$  NMR spectra of Compound 13 in DMSO.



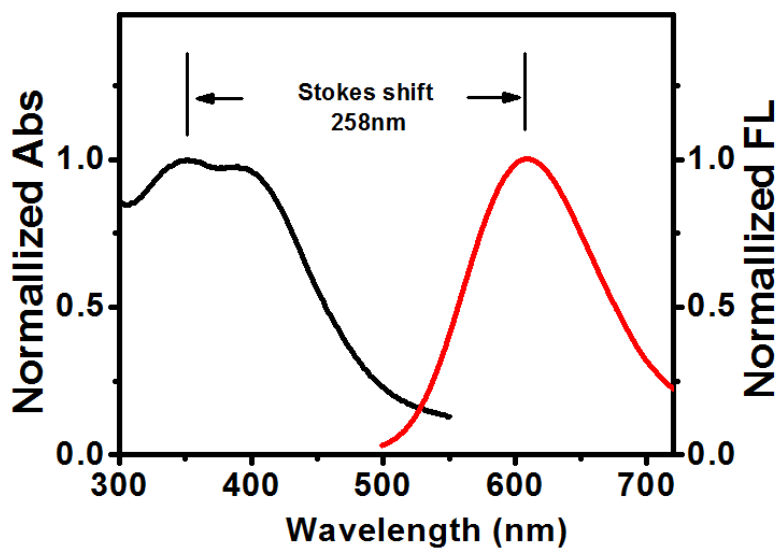
**Fig. S9** Mass spectrum of Compound **13**. MS (ESI):  $m/z$  694.3 [M].

<small>Match</small> <small>RT</small> <small>Intensity</small> <small>Library</small> <small>Formula</small>	Compound Name (Library Hit)	Formula	Intensity	Threshold	Expected $m/z$	Found at $m/z$	Error (ppm)
✓ ✓ ✓ ✓ ✓	695.209007984 (No Acquired MSMS)	C <sub>41</sub> H <sub>33</sub> N <sub>3</sub> O 6S	21281	50	696.2163	696.2157	-0.9

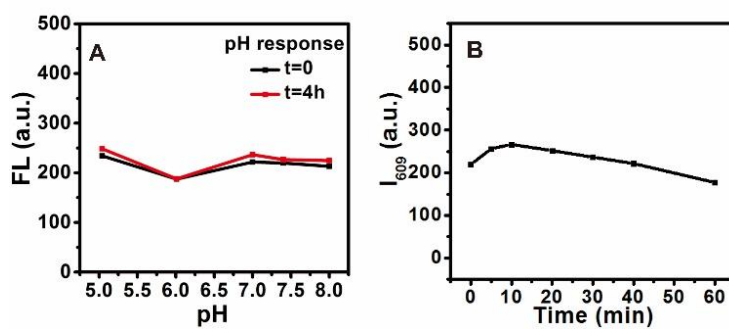
● Spectrum from sample D.wiff (sample 1) - Sample005, Experiment 1, +TOF MS (100 - 1000) from 0.134 to 0.166 min  
 ● C<sub>41</sub>H<sub>33</sub>N<sub>3</sub>O<sub>6</sub>S +H



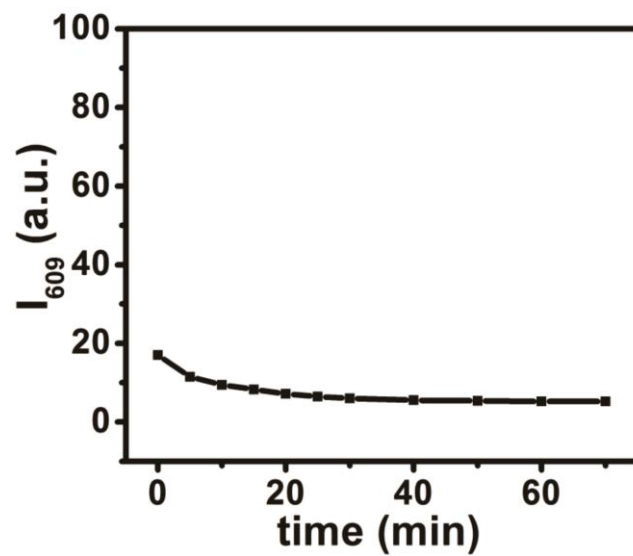
**Fig. S10** High resolution mass spectrum (HRMS) of Compound **13**.



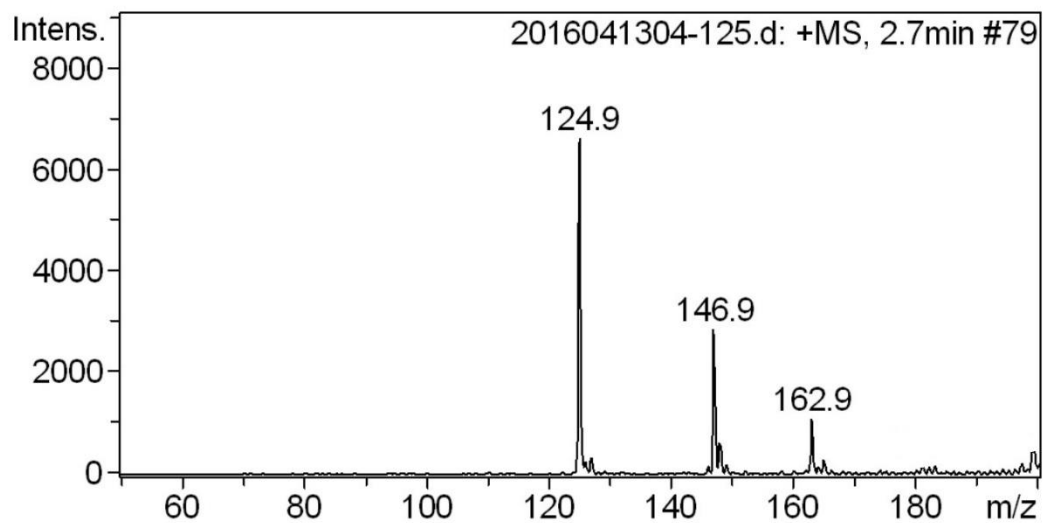
**Fig. S11** Normalized absorption spectra (black) and fluorescence spectra (red) of CTPE in 10mM PBS (pH = 7.4) containing 0.5% DMSO.



**Fig. S12** (A) Fluorescent intensity of CTPE in different PBS buffer solutions from pH=5.0 to pH=8.0 before and after 4h heating at 37°C by water bath , (B) Photo-bleaching of CTPE upon exposure to 365 nm UV.

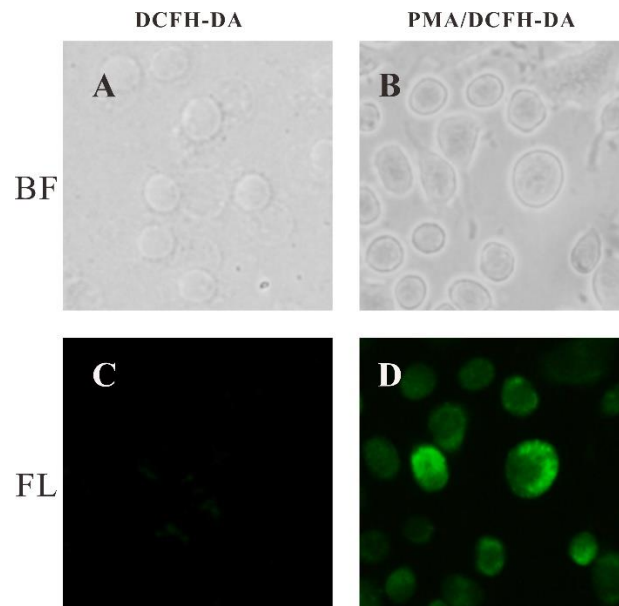


**Fig. S13** Fluorescent intensity curve of CTPe-Tau for acid response versus time in 10 mM PBS (pH = 5.0) containing 0.5% DMSO.



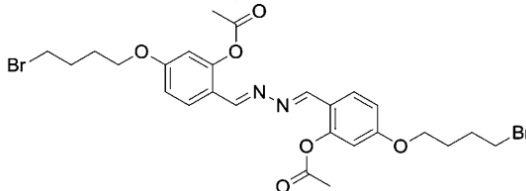
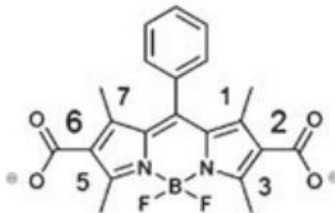
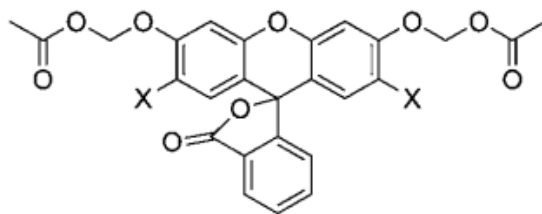
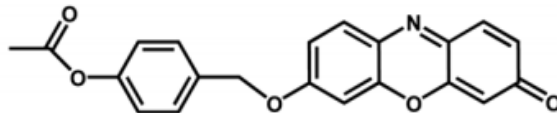
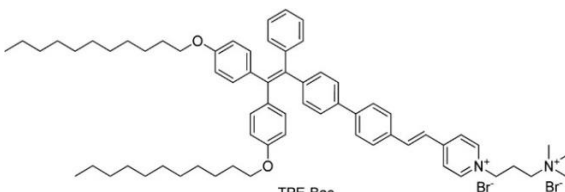
**Fig. S14** Mass spectrum of CTPe-Tau after incubation with esterase at 37°C for 1h.





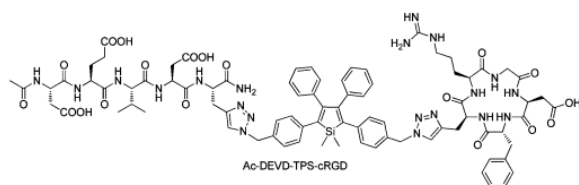
**Fig. S15** Fluorescence images of RAW 264.7 cells (A, C) incubated in culture medium without any stimulation followed by incubated with DCFH-DA 10  $\mu$ M for 30 min, (B, D) stimulated with 6 mg/mL PMA for 30 min, washed with PBS three times and then incubated in culture medium for 4h followed by DCFH-DA 10  $\mu$ M for 30 min.

**Table S1. Comparison of the system herein with other reported esterase-responsive fluorophores and AIE-active fluorophores**

Fluorophores	Stokes shift	Esterase response	Esterase-activated drug release
	176 nm	yes	no
<p><i>J. Mater. Chem. B</i>, 2014, 2, 3438</p>			
	<40 nm	yes	no
<p><i>Chem. Commun.</i>, 2009, 7015-7017</p>			
	<40 nm	yes	no
<p><i>Chem. Sci.</i>, 2011, 2, 521-530</p>			
	<40 nm	yes	no
<p><i>Analyst.</i>, 2012, 137, 716-721</p>			
 <p>TPE-Bac</p>	200 nm	no	no

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*ACS Appl. Mater. Interfaces*, 2015, 7,  
7180-7188



130  
nm      no      no

*Analyst.*, 2012, 137, 716-721

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