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Electronic Supplementary Information

Dual fluorogenic and ¹⁹F NMR probe for detection of the esterase activity



Figure S1. MS spectra of FlE (A, the blue part), the product of FlE reacted with esterase (B, the yellow part) and Fl (C, the gray part).

Table S1 The fluorescence quantum yield of FIE, the product of FIE reacted with esterase and FI.

sample	FIE	FlE+esterase	Fl
${\it P}_{ m F}(\%)$	0.20	5.21	18.10



Figure S2. The plot of the fluorescence intensity at 510 nm versus the concentration of esterase. The linear fitting between fluorescence intensity and esterase concentration (0.05-0.30 U mL⁻¹) with R²=0.99. The slope is 3779.3. The standard deviation was calculated to be 1.408 according to 20 blank samples. And the detection limit was calculated to be 0.001 U mL⁻¹ (3 δ / slope).



Figure S3. (A) Michaelis-Menten plot. (B) Lineweaver-Burk plot of FIE hydrolysis catalyzed by esterase with the fluorometric method. According to the equation $(V=V_{max}[S]/(K_m+[S]))$, where V is the reaction rate, [S] is the concentration of FIE and Km is the Michaelis constant.), the K_m and V_{max} values were calculated to be 27.0609 μ M and 14.4928 μ M s⁻¹ for FIE. The concentration of esterase is 0.5 U mL⁻¹.



Figure S4. Curve of time-dependent integral area ratio of FIE $(1.0 \times 10^{-4} \text{ mol } \text{L}^{-1})$ with esterase (0.4 U mL⁻¹).



Figure S5. Confocal fluorescence images of MCF-7 cells incubated with different concentration of FIE.



Figure S6. (A) ¹⁹F NMR spectra of probe FIE mixed with Hela cells, MCF-7 cells, and Hela cells with eletroporation. (B) ¹⁹F NMR spectra of Hela cells.



Figure S7. ¹H NMR spectrum of Compound 3 in CDCl_{3.}



Figure S8. ¹³C NMR spectrum of Compound 3 in CDCl_{3.}



Figure S9. ¹H NMR spectrum of **Fl** in CDCl_{3.}



175 165 155 145 135 125 115 105 95 90 85 80 75 70 65 60 55 50 45 40 35 30 25 20 15 10 5 0 f1 (ppm)

Figure S10. ¹³C NMR spectrum of Fl in CDCl_{3.}



^{8.4} 7.8 7.2 6.6 6.0 5.4 4.8 4.2 3.6 3.0 2.4 1.8 1.2 0.6 0.0 **Figure S11.** ¹H NMR spectrum of **FIE** in CDCl_{3.}



Figure S12. ¹³C NMR spectrum of FIE in CDCl_{3.}



Figure S13. The MS spectrum of Compound 3.



Figure S14. The HRMS spectrum of Compound 3.



Figure S15. The MS spectrum of Fl.



Figure S16. The HRMS spectrum of Compound Fl.



Figure S17. The MS spectrum of FIE.



Figure S18. The HRMS spectrum of FIE.



Figure S19. The IR spectrum of FIE.