

*Supporting Information for*

**An Ultrasensitive Lipid Droplet-Targeted NIR Emission Fluorescent Probe for  
Polarity Detection and Its Application in Liver Disease Diagnosis**

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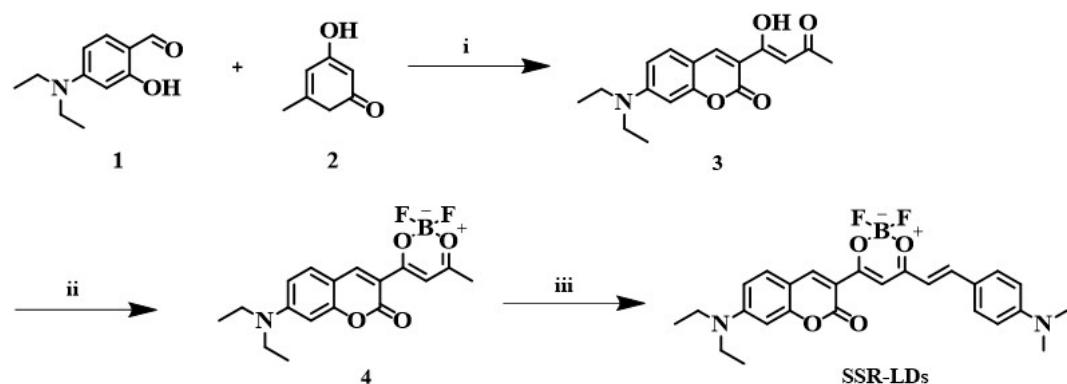
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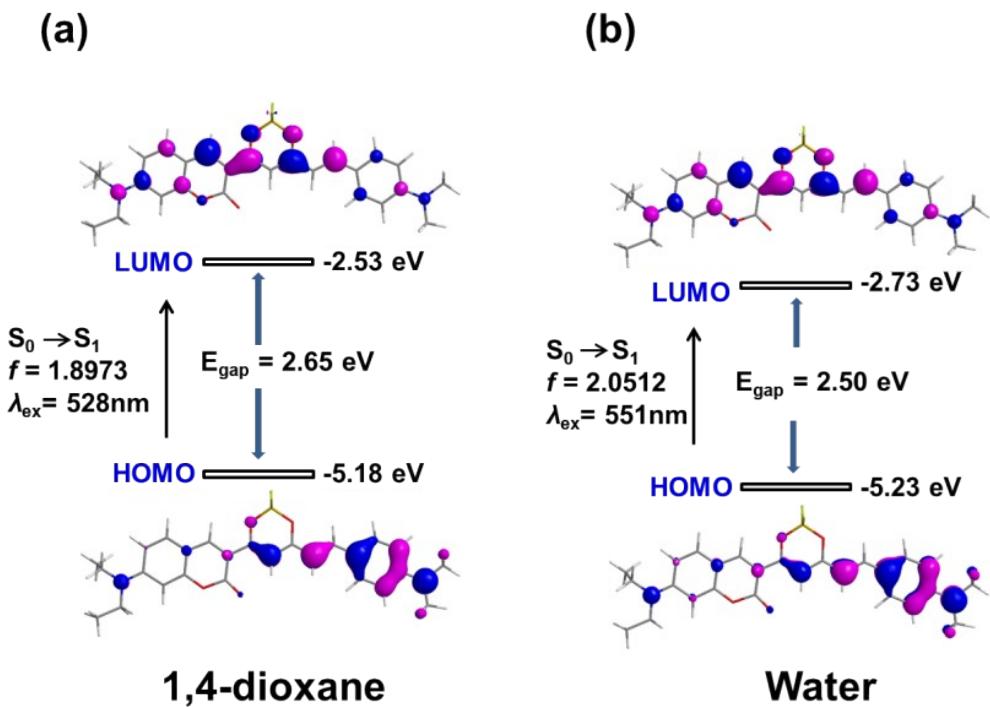
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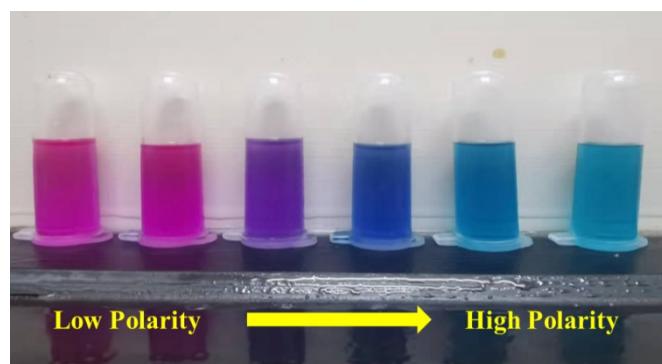
**Scheme S1.** Synthesis process of probe SSR-LDs.



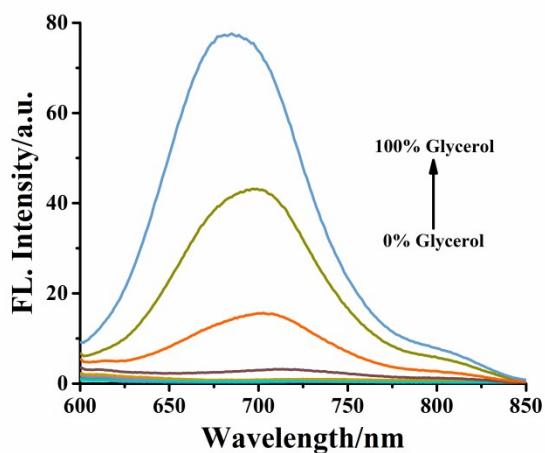
Reagents and conditions: (i) Absolute ethanol, 85 °C, 4 h; (ii) anhydrous dichloride, 0 °C, under the protection of nitrogen, 8 h; (iii) 4-(dimethylamino)-benzaldehyde, toluene, room temperature, 24 h.



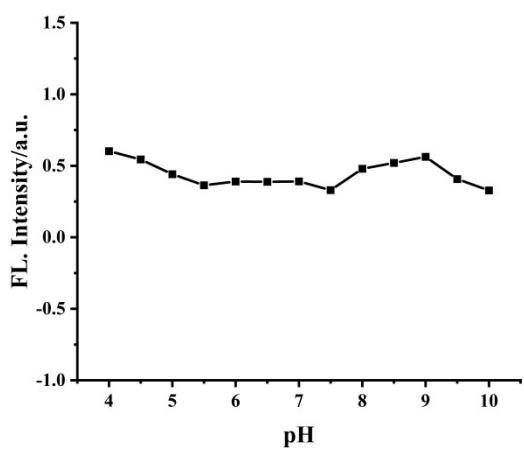
**Fig. S1.** Calculated orbital energy levels and electron density contours of HOMOs and LUMOs for S<sub>0</sub>-optimized geometry and S<sub>1</sub>-optimized geometry of **SSR-LDs** in 1,4-dioxane (a) and water (b), respectively. Transition properties (the energy gap E<sub>gap</sub>, wavelength  $\lambda$ , and oscillator strength  $f$ ) for absorption and emission were also given.



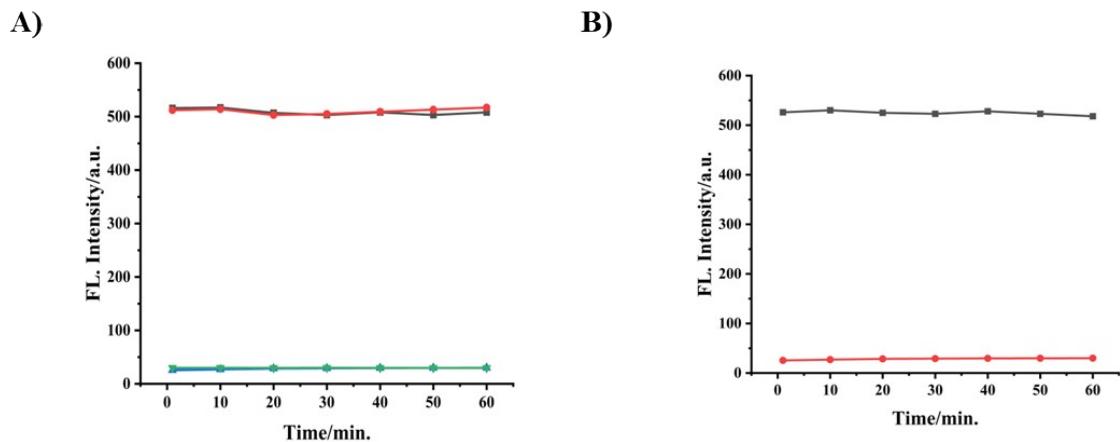
**Fig. S2.** The visual change of solution color of SSR-LDs in different solvents (10 μM). The solvents in sequence: toluene, 1,4-dioxane, tetrahydrofuran (THF), ethanol (ETOH), N,N-dimethylformamide (DMF), dimethyl sulfoxide (DMSO).



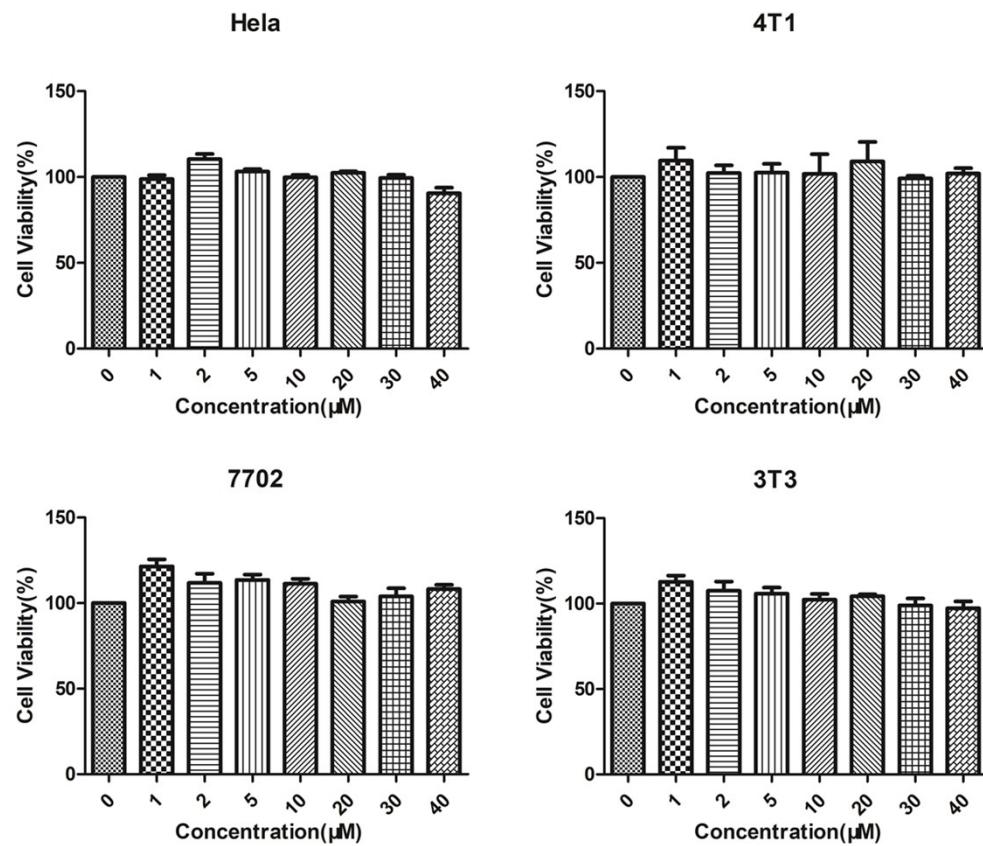
**Fig. S3.** Fluorescence emission spectra of **SSR-LDs** (10  $\mu\text{M}$ ) in different ratios of mixed solvents of PBS and Glycerol.



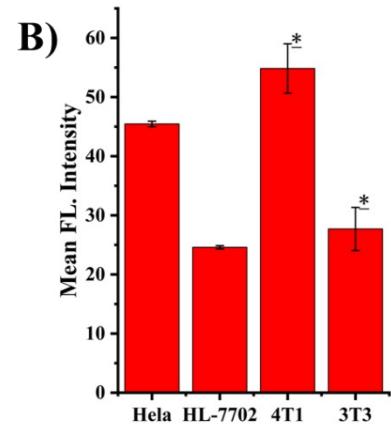
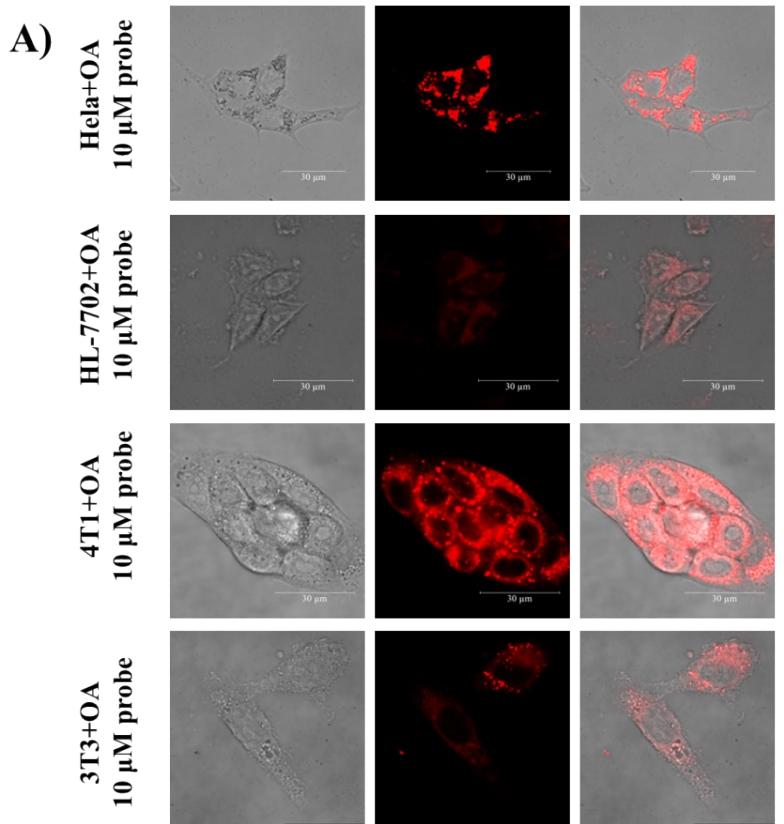
**Fig. S4.** The pH adaptability tests of **SSR-LDs** (10  $\mu\text{M}$ ) at  $\lambda_{\text{ex}}=580$  nm



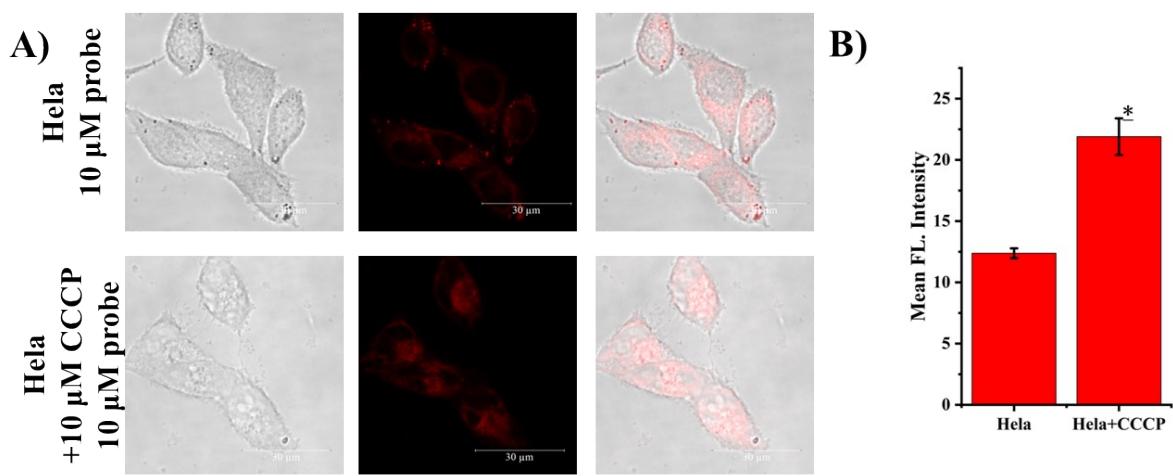
**Fig. S5.** The photo-stability performance test curves of the probe **SSR-LDs** ( $10 \mu\text{M}$ ) in two different polarities solutions (the PBS buffer (red and black), and the mixed solution (1,4-dioxane: PBS = 9:1, v: v) (blue and green)) with different wavelengths (580 nm and 365 nm) of light radiation. A) The photo-stability tests of **SSR-LDs** in the PBS buffer ( $10 \text{ mM}$ , pH 7.4) and the mixed solution (1,4-dioxane: PBS = 9:1, v: v) under light irradiation of 580 nm. B) The photo-stability tests of **SSR-LDs** in the PBS buffer ( $10 \text{ mM}$ , pH 7.4) (red) and the mixed solution (1,4-dioxane: PBS = 9:1, v: v) (black) under light irradiation of 365 nm.



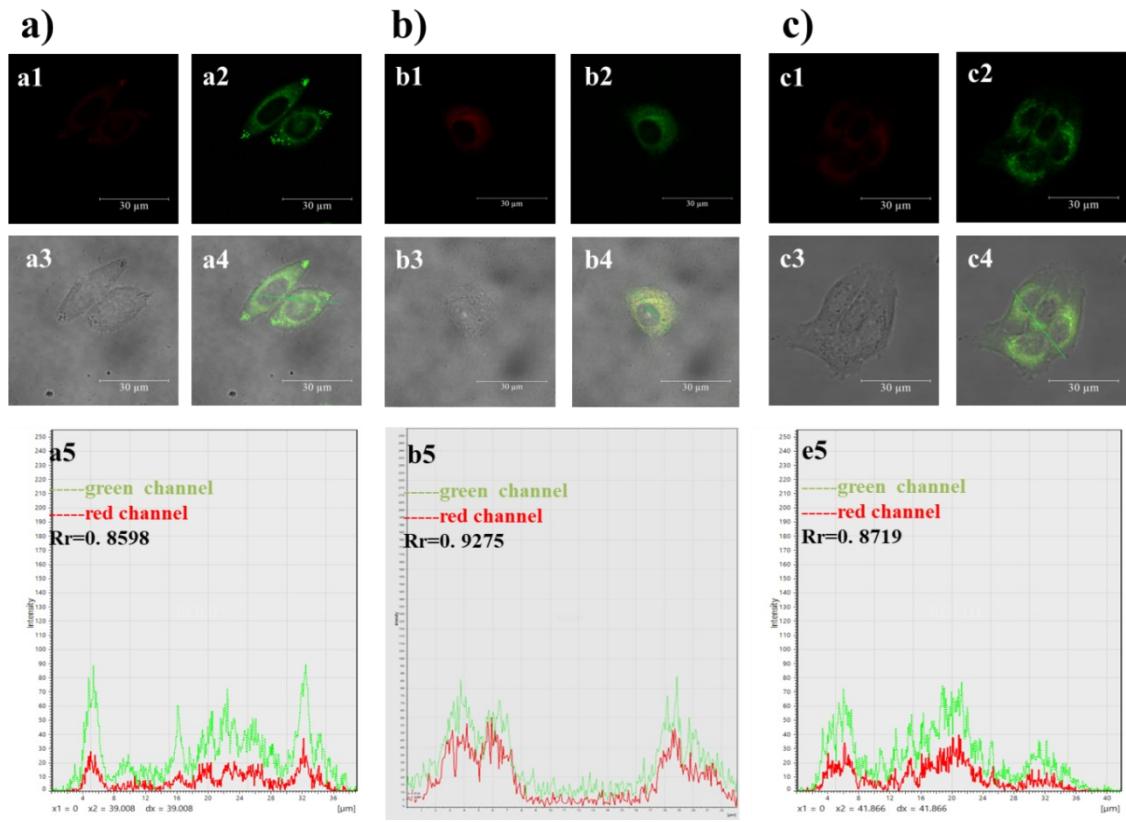
**Fig. S6.** Cytotoxicity tests of four kinds of cell lines (HeLa cells, HL7702 cells, 4T1 cells, and 3T3 cells).



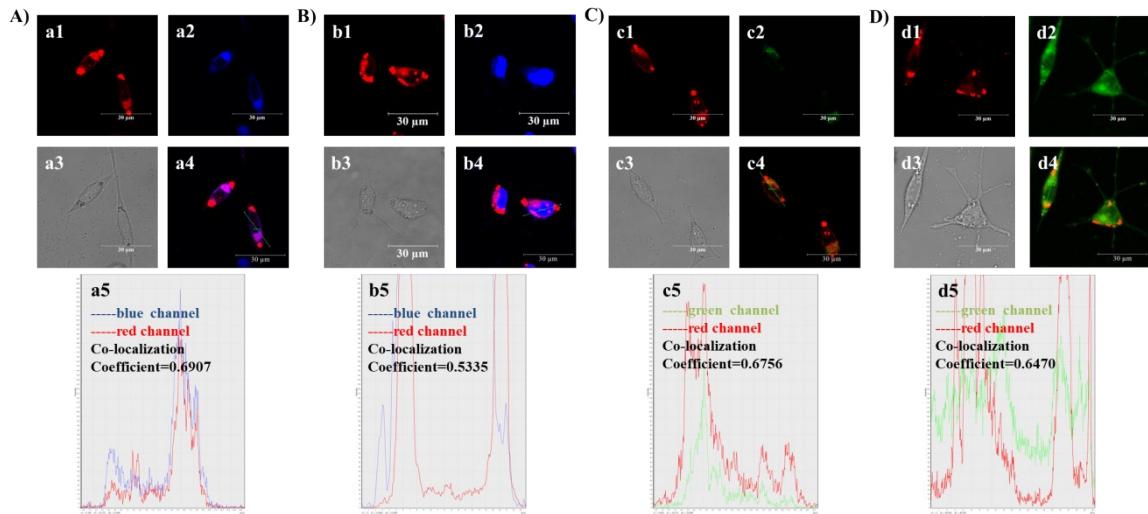
**Fig. S7.** A) Confocal imaging of four different cell lines treated with SSR-LDs (10  $\mu$ M) and OA (400  $\mu$ M). ( $\lambda_{\text{ex}} = 580$ ,  $\lambda_{\text{em}} = 610-750$ ), Scale bar = 30  $\mu$ m; B) The relative fluorescence intensities of the red channels of A). (\*p<0.05).



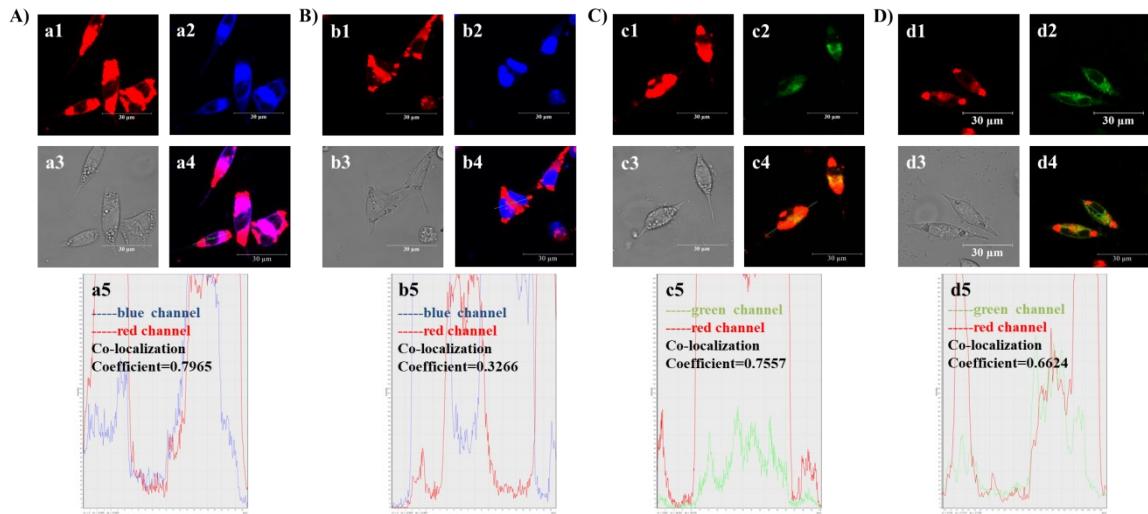
**Fig. S8.** A) The confocal fluorescence imaging of probe **SSR-LDs** (10  $\mu$ M) in living HeLa cells stimulated by CCCP ( $\lambda_{\text{ex}} = 580$ ,  $\lambda_{\text{em}} = 610\text{-}750$ ), Scale bar = 30  $\mu$ m; B) The relative fluorescence intensities of the red channels of A) (\* $p < 0.05$ ).



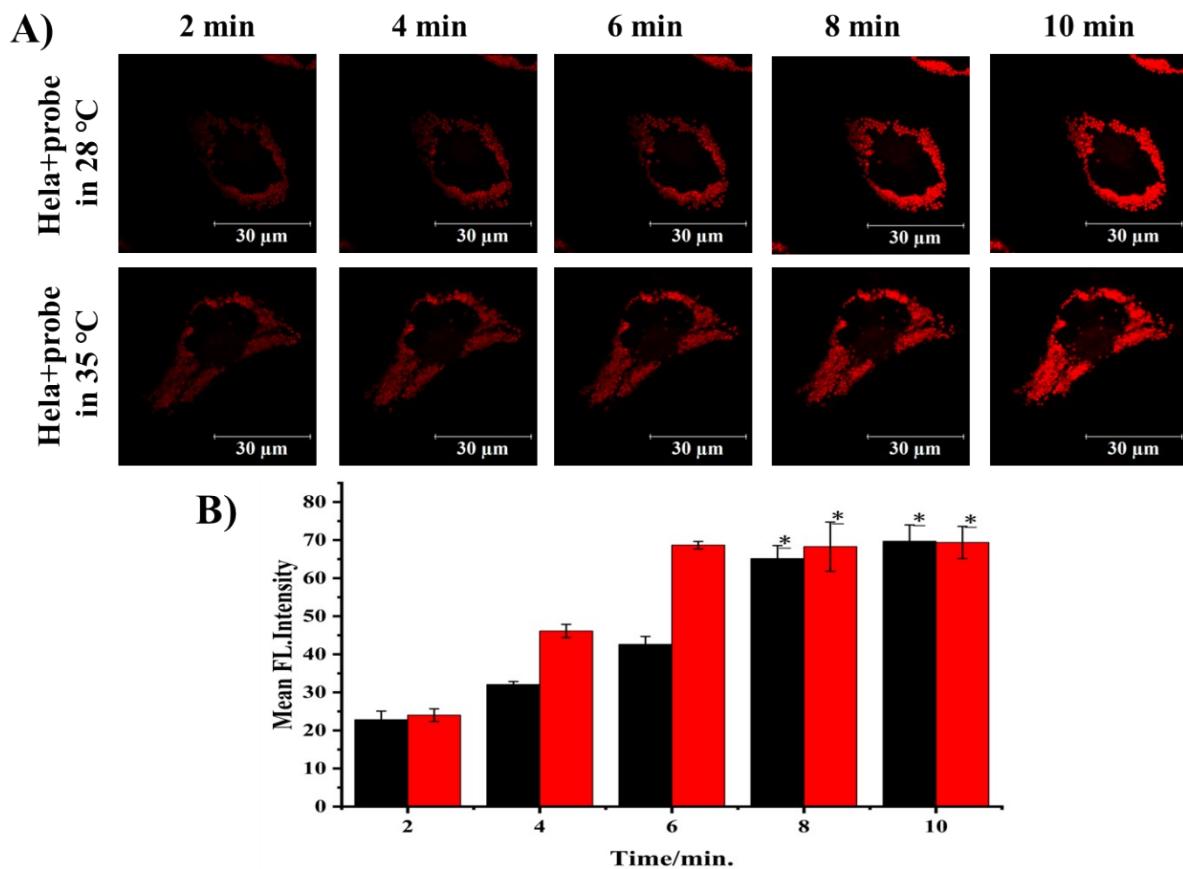
**Fig. S9.** Co-localization imaging of **SSR-LDs** (10  $\mu$ M) and bodipy (200 nM) for imaging three cell lines (HeLa cells, 3T3 cells, and 4T1 cells) pre-treated, Scale bar: 30  $\mu$ M. A) The co-localization imaging of HeLa cells treated with **SSR-LDs** (10  $\mu$ M) and bodipy (200 nM); B) The co-localization imaging of 3T3 cells treated with **SSR-LDs** (10  $\mu$ M) and bodipy (200 nM); C) The co-localization imaging of 4T1 cells treated with **SSR-LDs** (10  $\mu$ M) and bodipy (200 nM). 1) The red channel of **SSR-LDs**; 2) the green channel of bodipy; 3) the bright field channel; 4) the merge of 1-3); 5) Intensity profile of **SSR-LDs** in the red channel and bodipy in green channel. Green channel:  $\lambda_{ex}$ : 580 nm, collected 610 nm-750 nm.



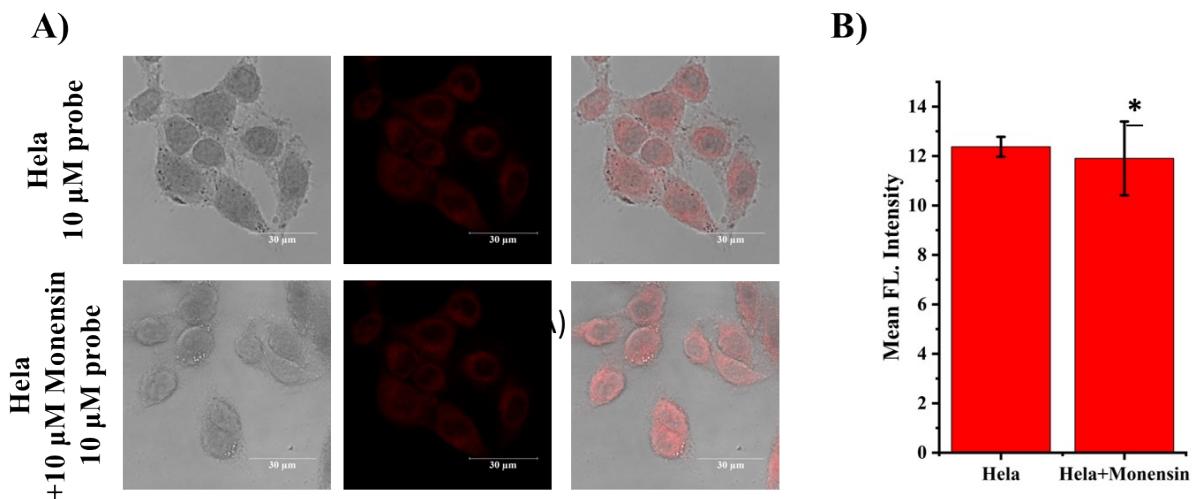
**Fig. S10.** Co-localization imaging of **SSR-LDs** (10  $\mu$ M) and different organelle localization dyes in HeLa cells, Scale bar: 30  $\mu$ M. A) The co-localization imaging of HeLa cells treated with **SSR-LDs** (10  $\mu$ M) and ER tracker blue (200 nM). B) The co-localization imaging of HeLa cells treated with **SSR-LDs** (10  $\mu$ M) and Hoechst 33342 (200 nM). C) The co-localization imaging of HeLa cells treated with **SSR-LDs** (10  $\mu$ M) and Lyso Tracker green (200 nM). D) The co-localization imaging of HeLa cells treated with **SSR-LDs** (10  $\mu$ M) and Mito Tracker green (200 nM).



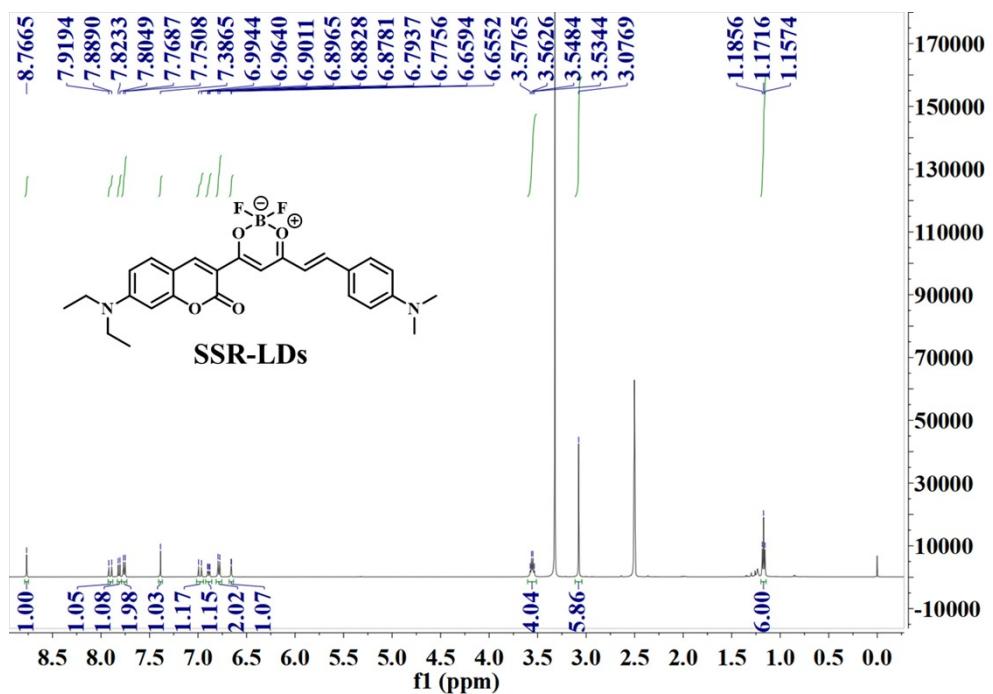
**Fig. S11.** Co-localization imaging of **SSR-LDs** (10  $\mu\text{M}$ ) and different organelle localization dyes in HeLa cells pre-treated with OA (400  $\mu\text{M}$ ). Scale bar: 30  $\mu\text{M}$ . A) The co-localization imaging of HeLa cells pre-treated with OA (400  $\mu\text{M}$ ), then treated with **SSR-LDs** (10  $\mu\text{M}$ ) and ER tracker blue (200 nM). B) The co-localization imaging of HeLa cells pre-treated with OA (400  $\mu\text{M}$ ), then treated with **SSR-LDs** (10  $\mu\text{M}$ ) and Hoechst 33342 (200 nM). C) The co-localization imaging of HeLa cells pre-treated with OA (400  $\mu\text{M}$ ), then treated with **SSR-LDs** (10  $\mu\text{M}$ ) and Lyso Tracker green (200 nM). D) The co-localization imaging of HeLa cells pre-treated with OA (400  $\mu\text{M}$ ), then treated with **SSR-LDs** (10  $\mu\text{M}$ ) and Mito Tracker green (200 nM).



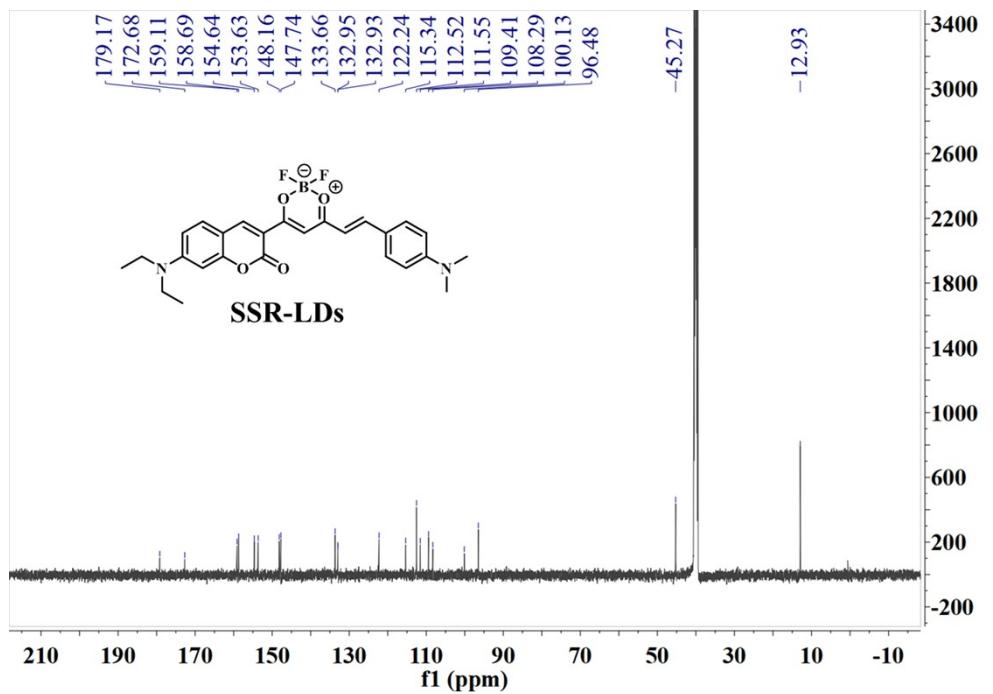
**Fig. S12.** A) Time-dependent confocal fluorescence imaging of the probe SSR-LDs (10  $\mu\text{M}$ ) at different temperatures in living Hela cells treated with OA (28 °C and 35 °C) ( $\lambda_{\text{ex}} = 580$ ,  $\lambda_{\text{em}} = 610\text{-}750$ ), Scale bar = 30  $\mu\text{m}$ . B) The relative fluorescence intensities of the red channels of A). (black represents 28 °C and red represents 35 °C) (\*p<0.05).



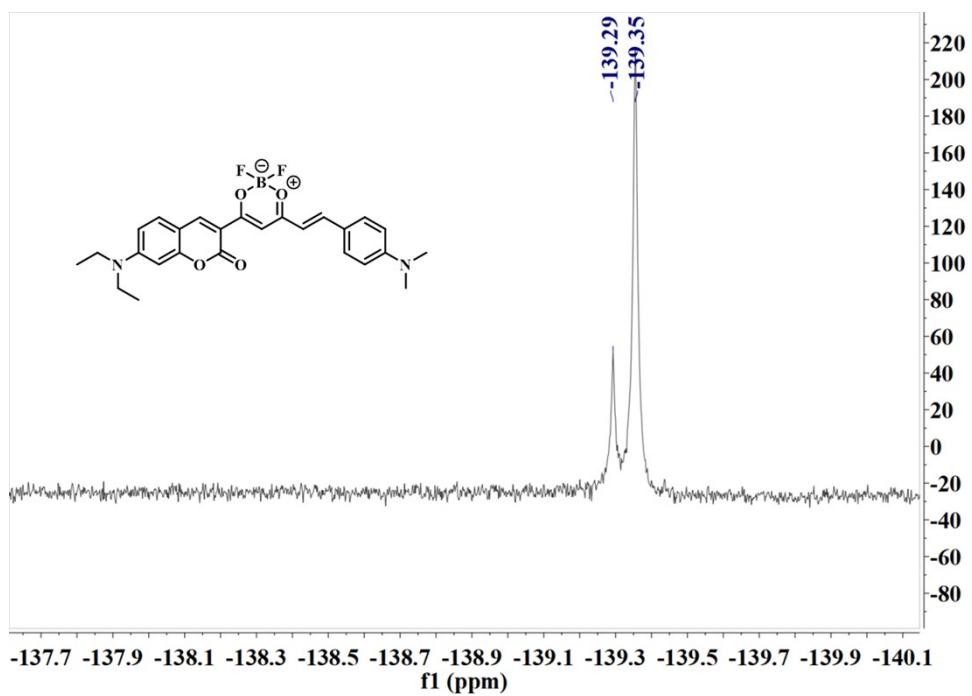
**Fig. S13.** A) The confocal fluorescence imaging of probe **SSR-LDs** (10  $\mu$ M) in living HeLa cells stimulated by monensin ( $\lambda_{\text{ex}} = 580$ ,  $\lambda_{\text{em}} = 610\text{-}750$ ), Scale bar = 30  $\mu$ m; B) The relative fluorescence intensities of the red channels of A) (\* $p < 0.05$ ).



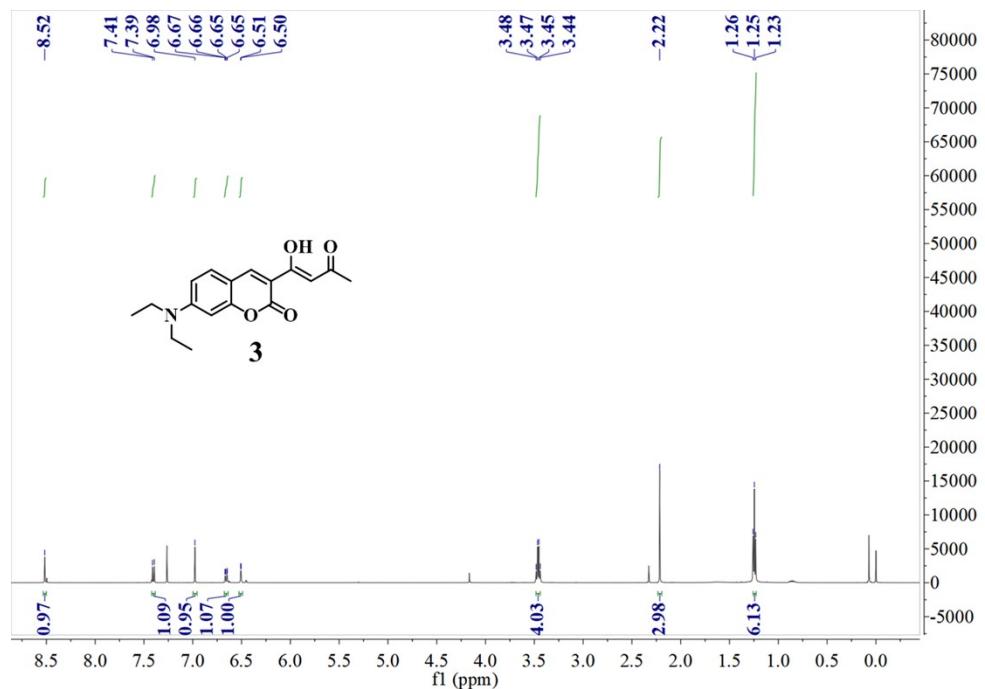
**Fig. S14.** <sup>1</sup>H NMR (DMSO-*d*<sub>6</sub>) spectrum of SSR-LDs.



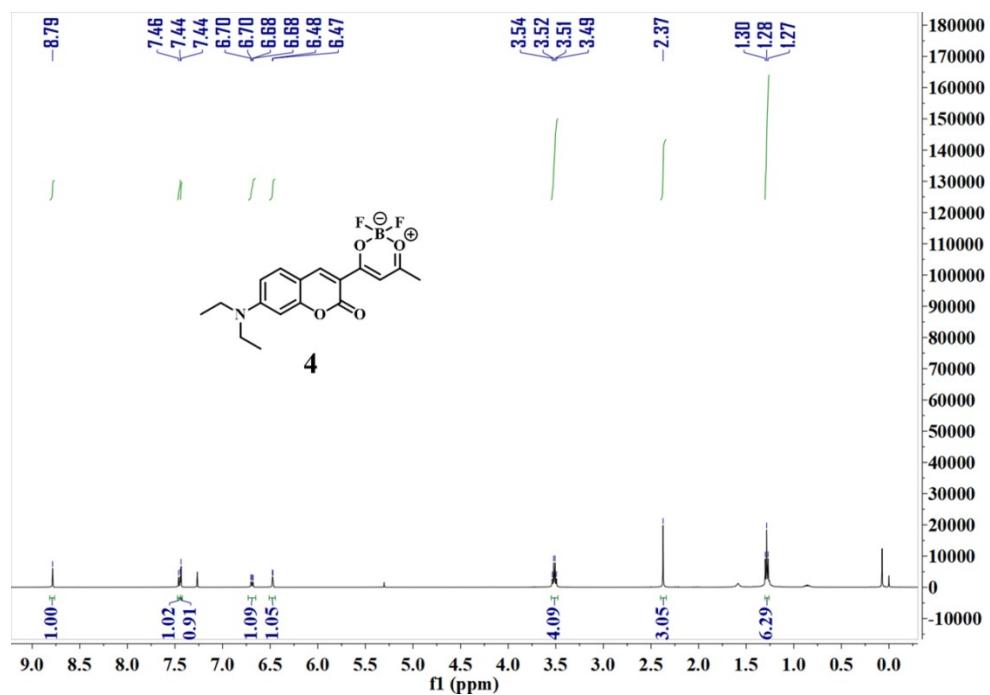
**Fig. S15.** <sup>13</sup>C NMR (DMSO-*d*<sub>6</sub>) spectrum of SSR-LDs.



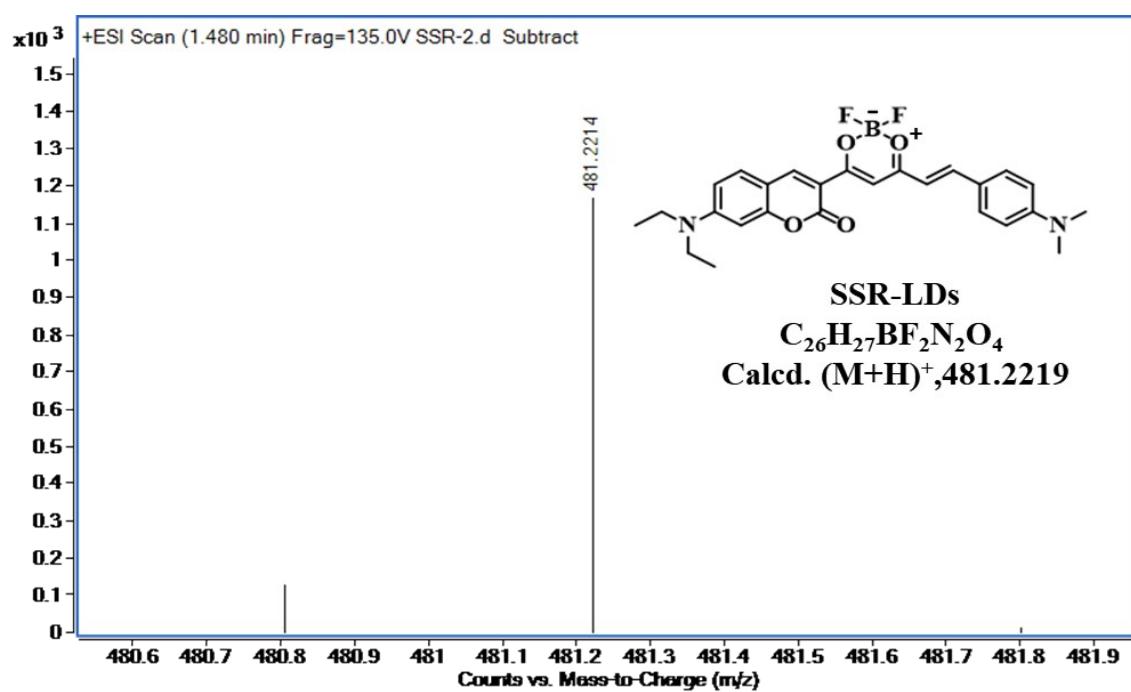
**Fig. S16.**  $^{19}\text{F}$  NMR ( $\text{DMSO}-d_6$ ) spectrum of SSR-LDs.



**Fig. S17.**  $^1\text{H}$  NMR ( $\text{CDCl}_3-d$ ) spectrum of compound 3.



**Fig. S18.**  $^1\text{H}$  NMR ( $\text{CDCl}_3\text{-}d$ ) spectrum of compound 4.



**Fig. S19.** HR-MS (ESI) spectrum of SSR-LDs,  $(\text{M}+\text{H})^+$ , 481.2219.