

*Electronic Supplementary Information (ESI) for:*

**Multifunctional AIEgen with high cell-penetrating ability for intracellular fluorescent assay, imaging and drug delivery**

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Supporting figures.

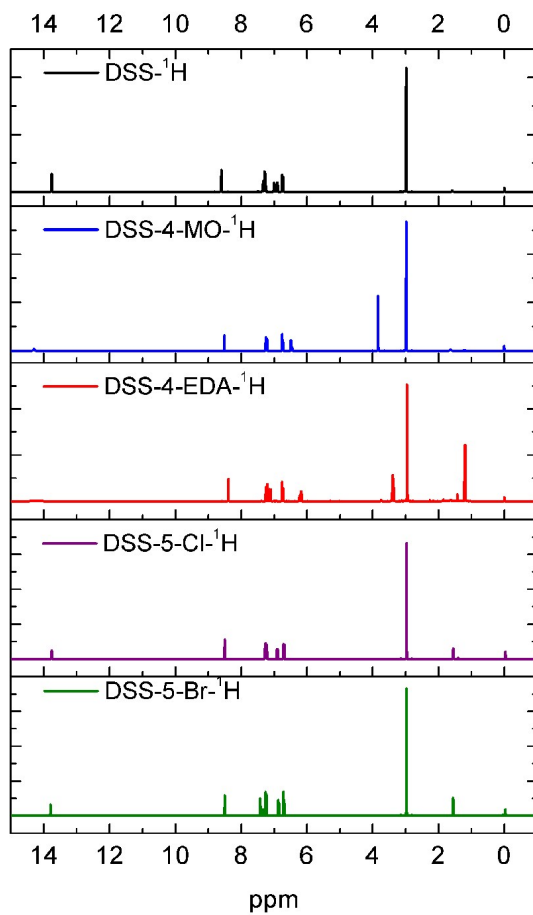
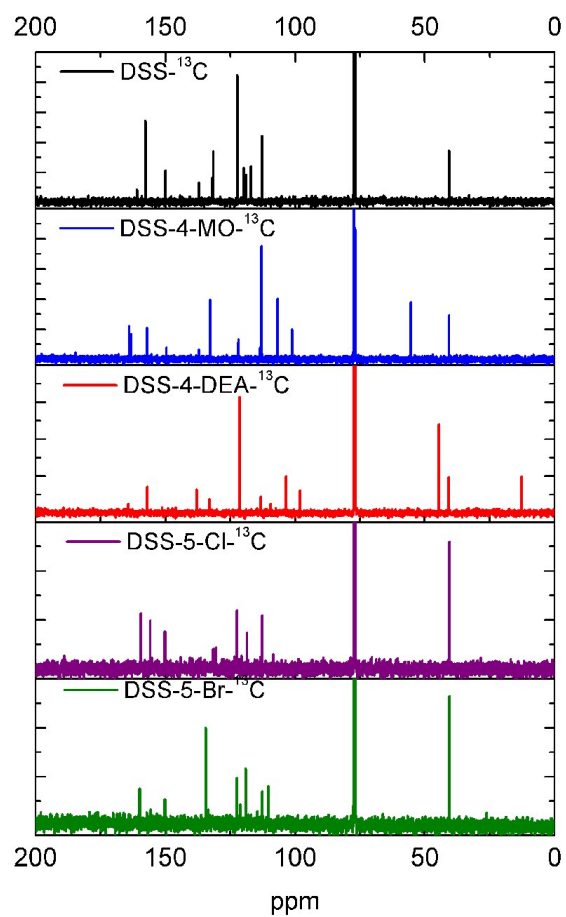
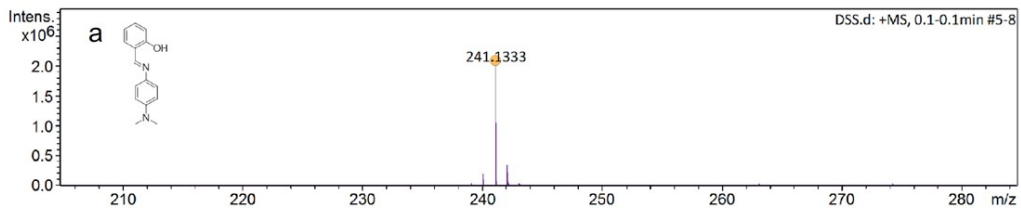


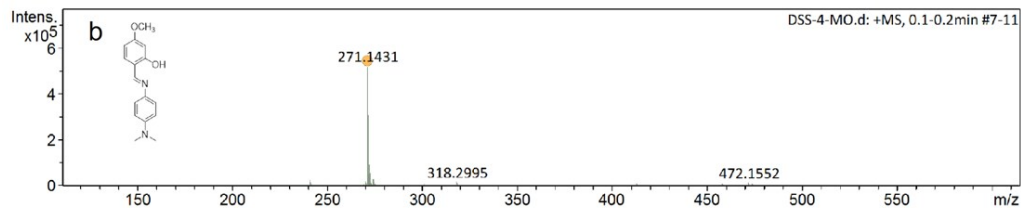
Figure S1 <sup>1</sup>H-NMR spectra of the DSS and the four derivatives.



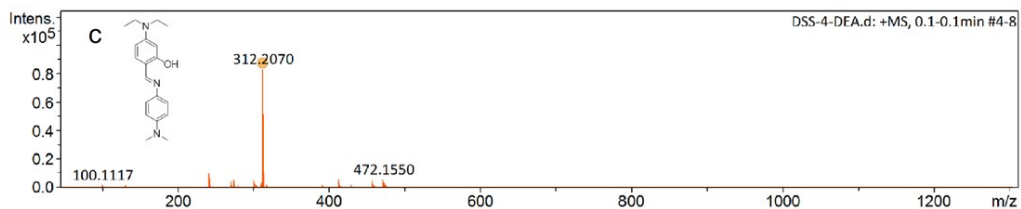
**Figure S2**  $^{13}\text{C}$ -NMR spectra of the DSS and the four derivatives.



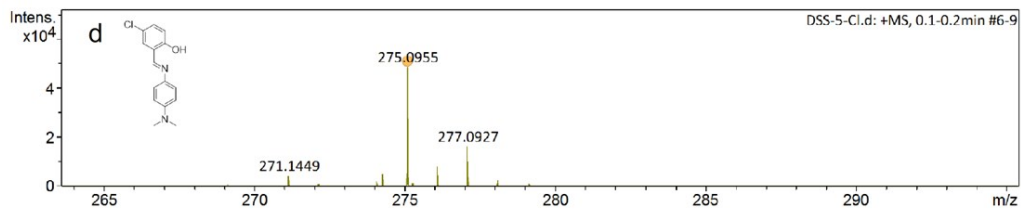
Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# mSigma	Score	rdb	e <sup>-</sup> Conf	N-Rule
241.1333	1	C <sub>15</sub> H <sub>17</sub> N <sub>2</sub> O	241.1335	0.9	1.0	1	100.00	9.0	even	ok



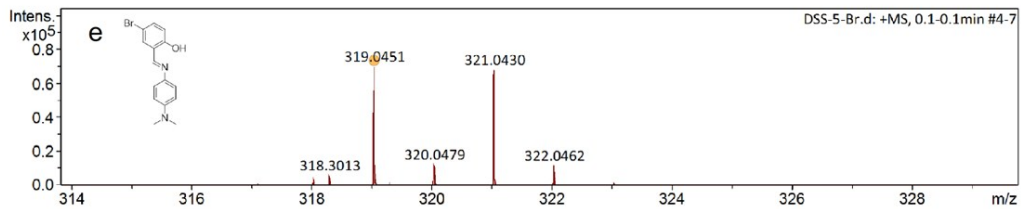
Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# mSigma	Score	rdb	e <sup>-</sup> Conf	N-Rule
271.1431	1	C <sub>16</sub> H <sub>19</sub> N <sub>2</sub> O <sub>2</sub>	271.1441	3.8	4.2	1	100.00	9.0	even	ok



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# mSigma	Score	rdb	e <sup>-</sup> Conf	N-Rule
312.2070	1	C <sub>19</sub> H <sub>26</sub> N <sub>3</sub> O	312.2070	0.2	2.2	1	100.00	9.0	even	ok

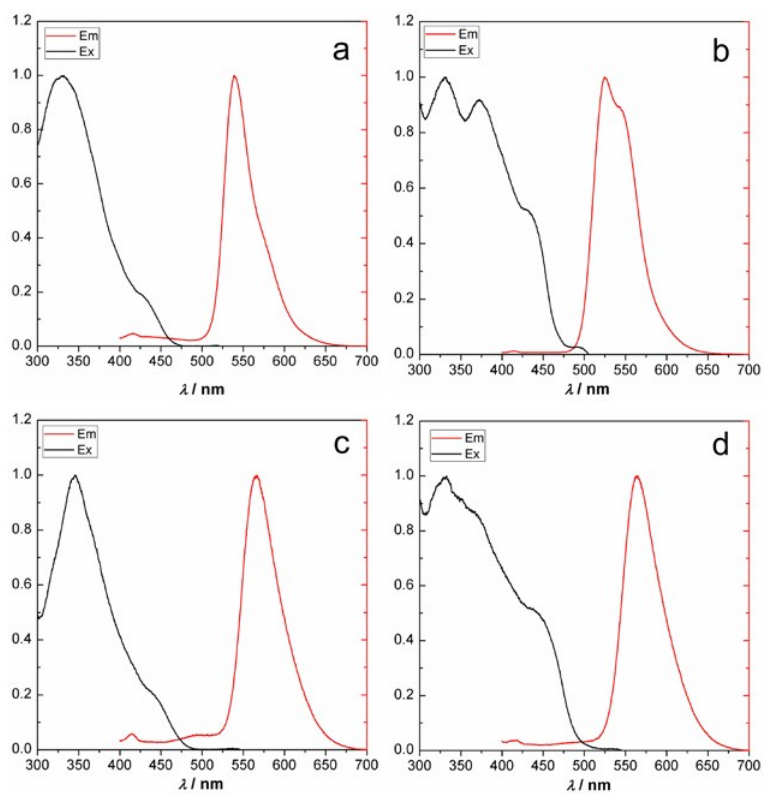


Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# mSigma	Score	rdb	e <sup>-</sup> Conf	N-Rule
275.0955	1	C <sub>15</sub> H <sub>16</sub> ClN <sub>2</sub> O	275.0946	-3.5	3.8	1	100.00	9.0	even	ok

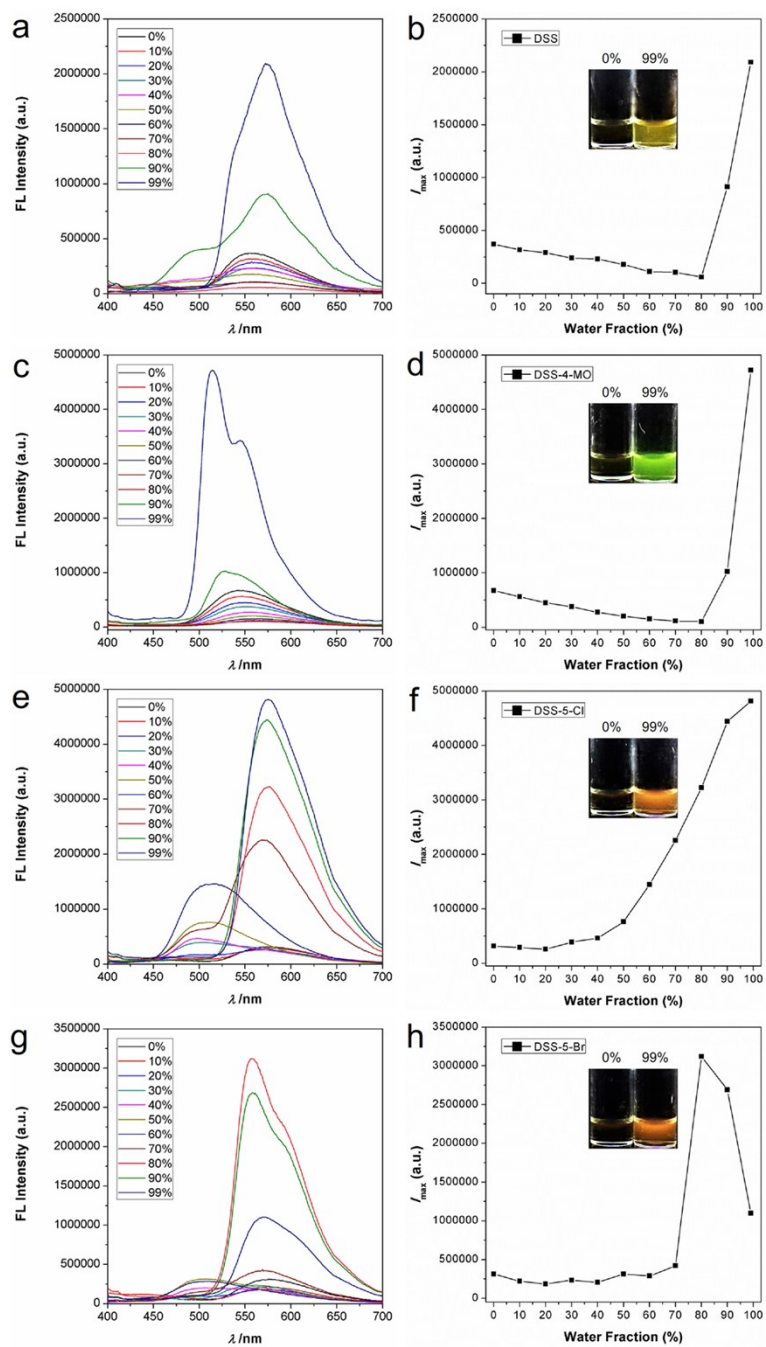


Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# mSigma	Score	rdb	e <sup>-</sup> Conf	N-Rule
319.0451	1	C <sub>15</sub> H <sub>16</sub> BrN <sub>2</sub> O	319.0441	-3.2	7.0	1	100.00	9.0	even	ok

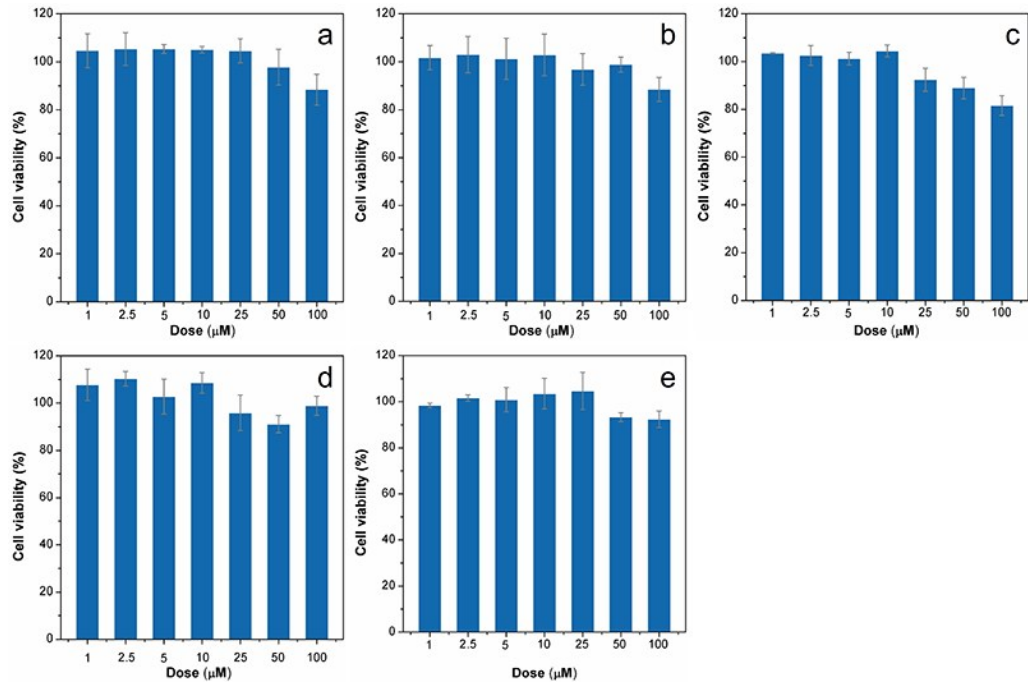
**Figure S3** High resolution mass spectra of the DSS and the four derivatives.



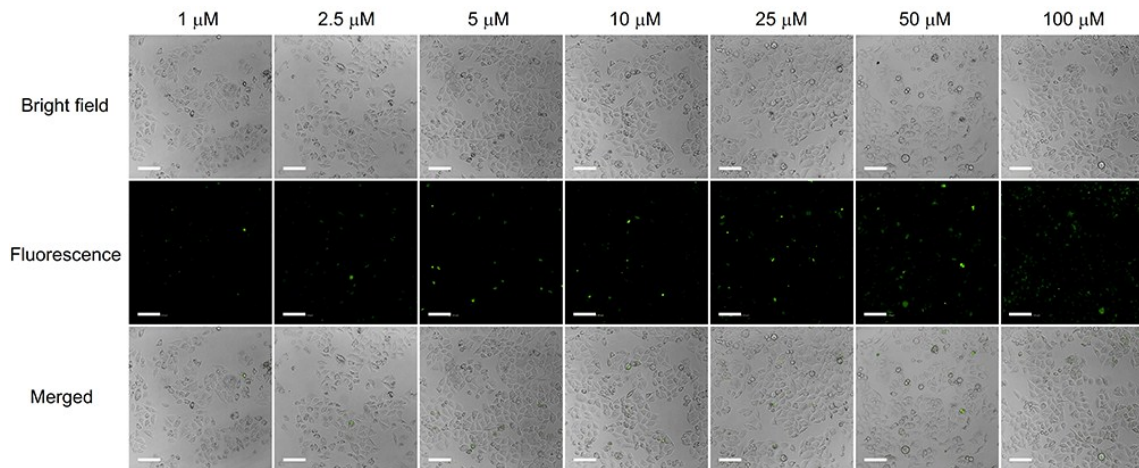
**Figure S4** Excitation and emission spectra of the DSS and the four derivatives (DMSO/water, water fraction 99%).



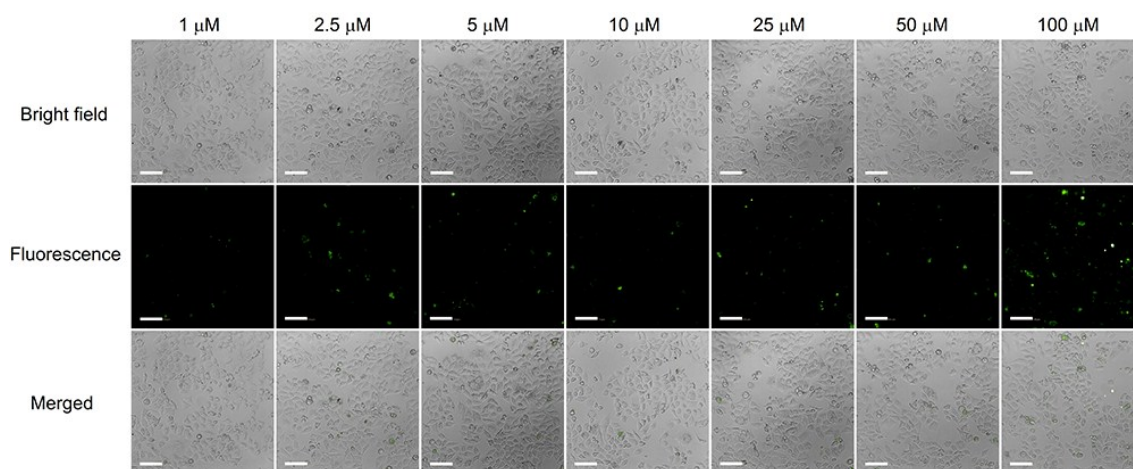
**Figure S5** Photoluminescence (PL) spectra (a-e) and AIE curves (f-j) of DSS and four derivatives in DMSO/water mixtures with different water fractions.



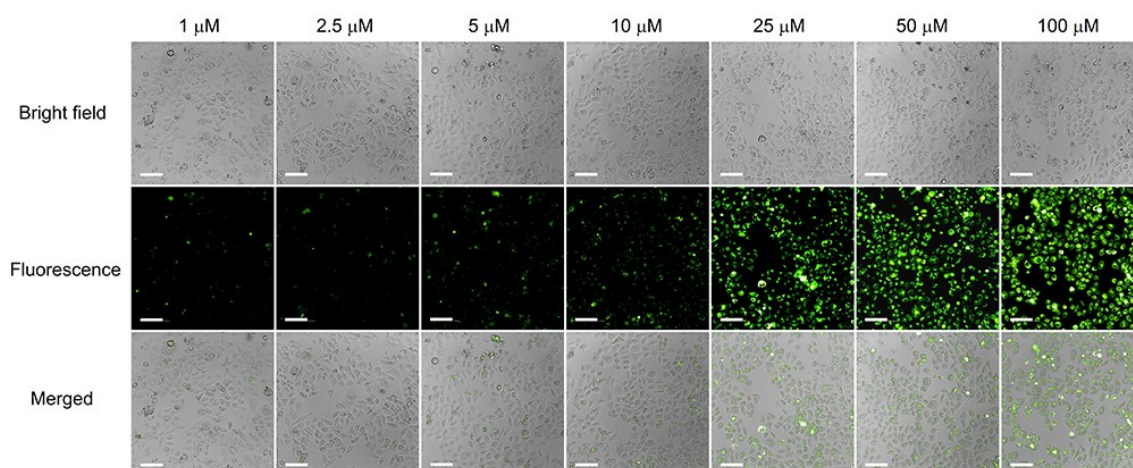
**Figure S6** The cytotoxicity of DSS and four derivatives on HeLa cells.



**Figure S7** Fluorescence images of HeLa cells stained with different concentrations of DSS in 30 min. Scale bar 100  $\mu\text{m}$ .

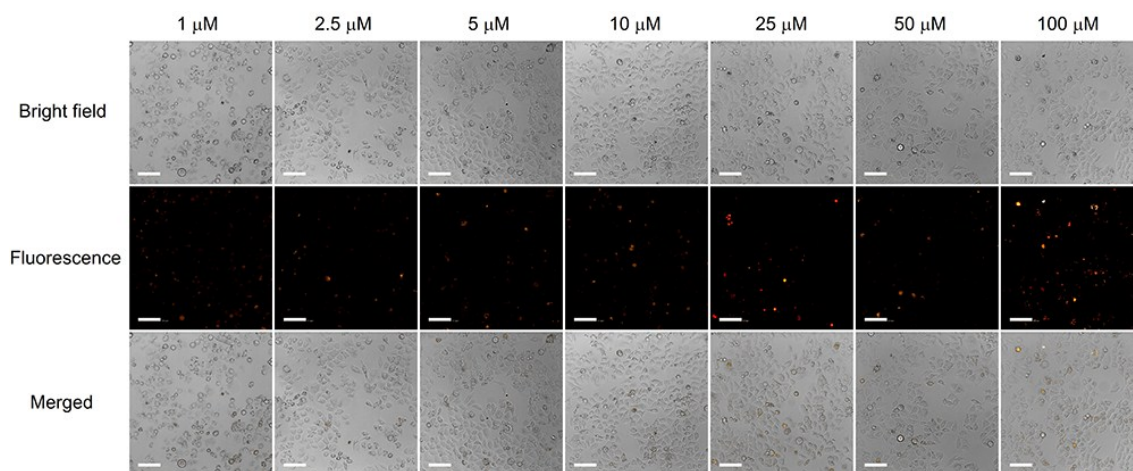


**Figure S8** Fluorescence images of HeLa cells stained with different concentrations of DSS-4-MO in 30 min. Scale bar 100  $\mu$ m.

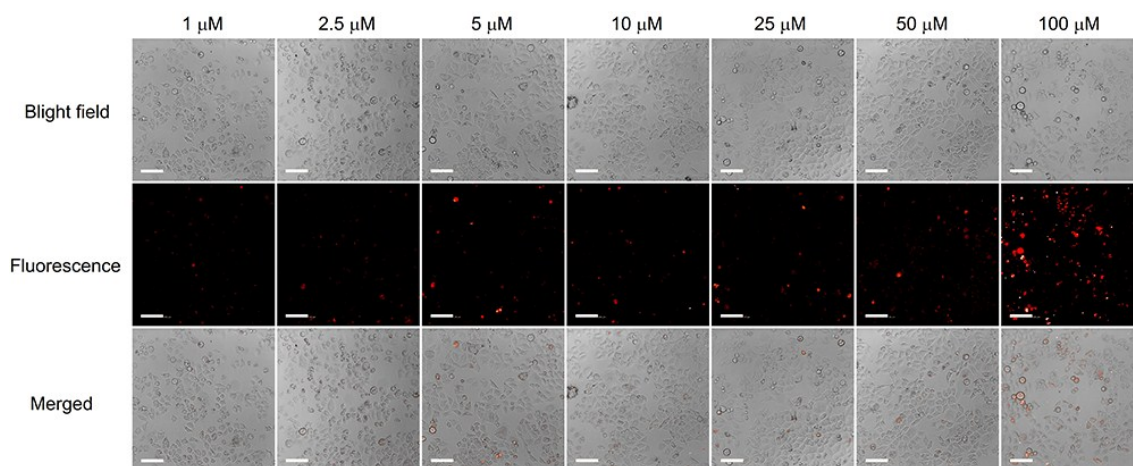


**Figure S9** Fluorescence images of HeLa cells stained with different concentrations of DSS-4-DEA in 30 min. Scale bar 100  $\mu$ m.

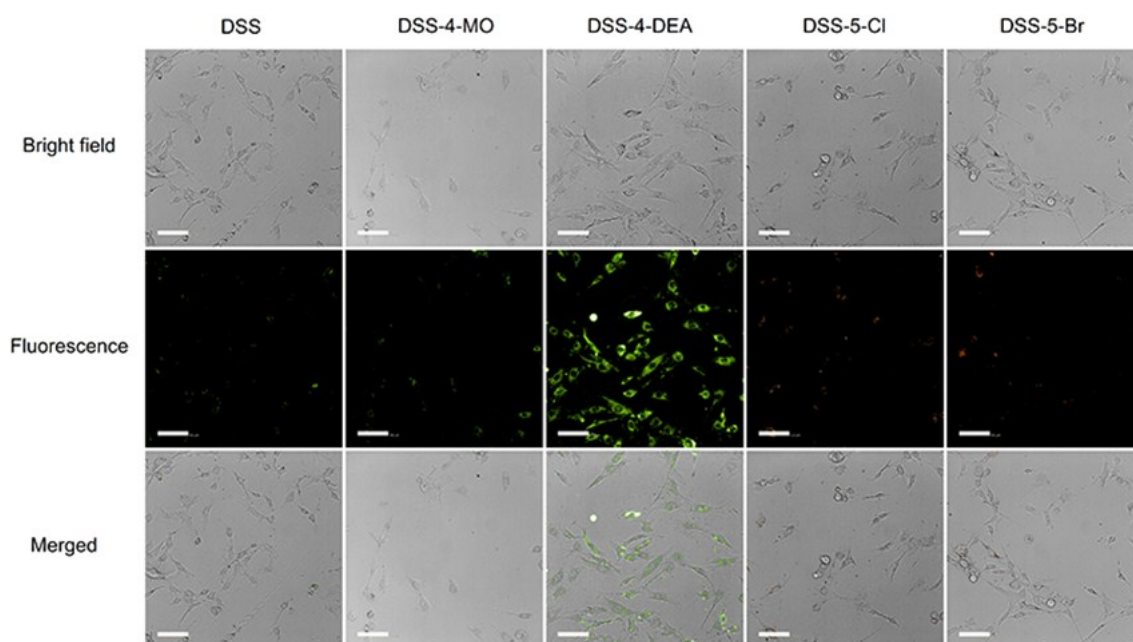




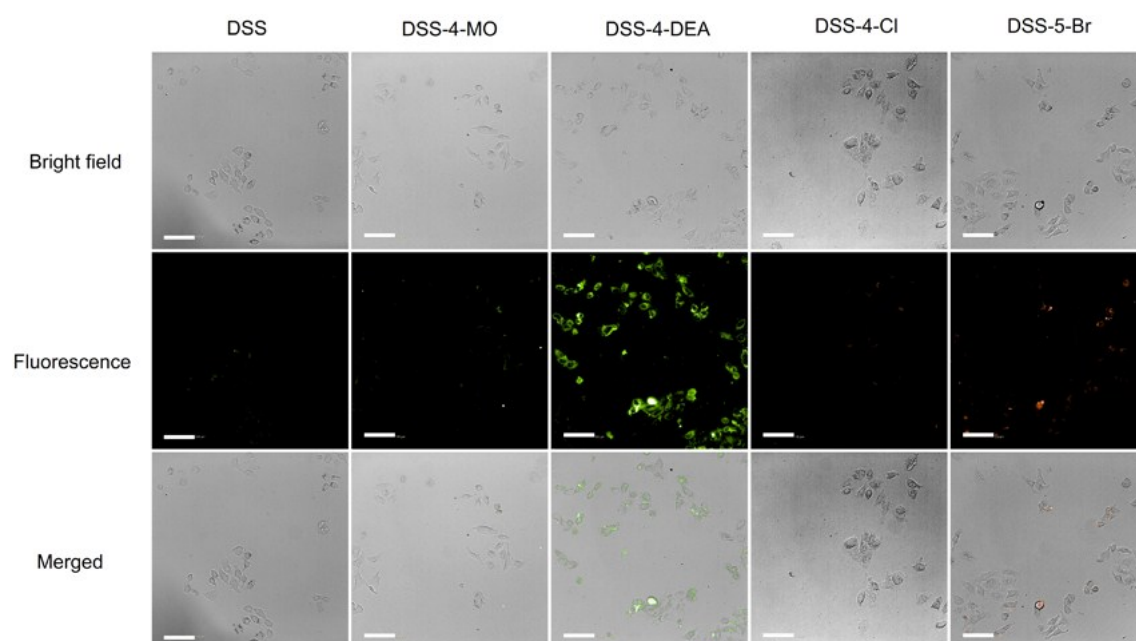
**Figure S10** Fluorescence images of HeLa cells stained with different concentrations of DSS-5-Cl in 30 min. Scale bar 100  $\mu$ m.



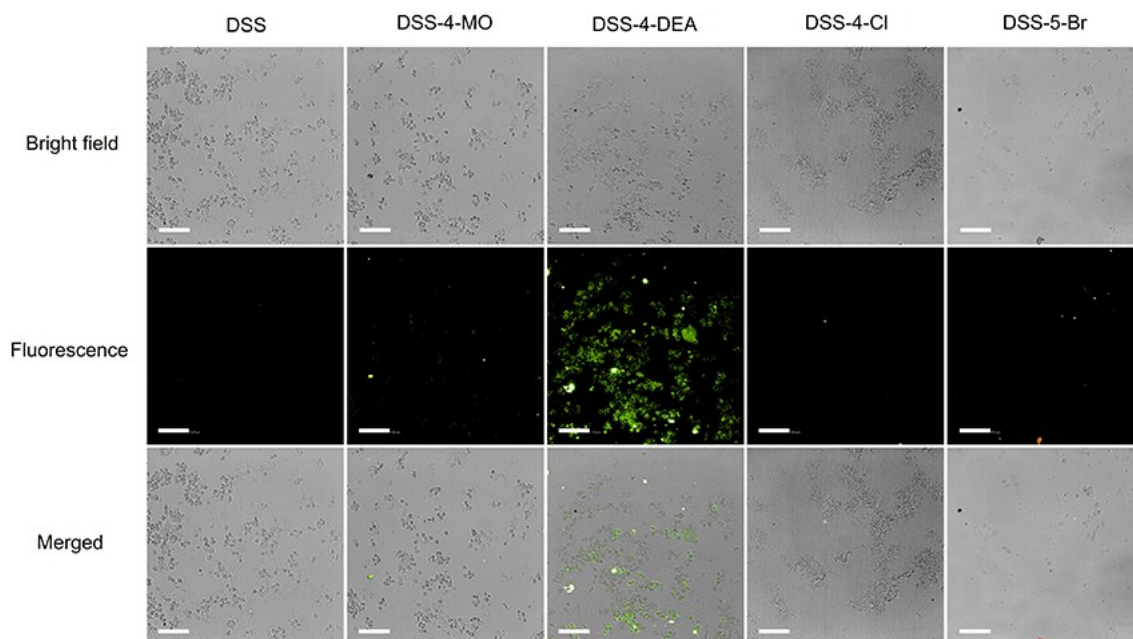
**Figure S11** Fluorescence images of HeLa cells stained with different concentrations of DSS-5-Br in 30 min. Scale bar 100  $\mu$ m.



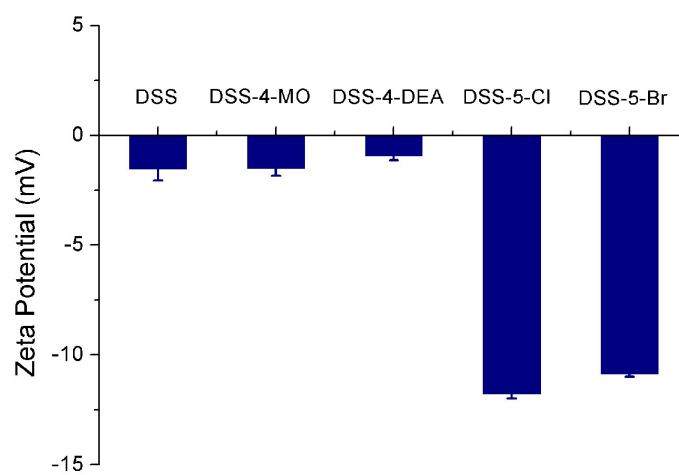
**Figure S12** Fluorescence images of C3H10 T1/2 cells stained 25  $\mu$ M of DSS and four derivatives in 30 min. Scale bar 100  $\mu$ m.



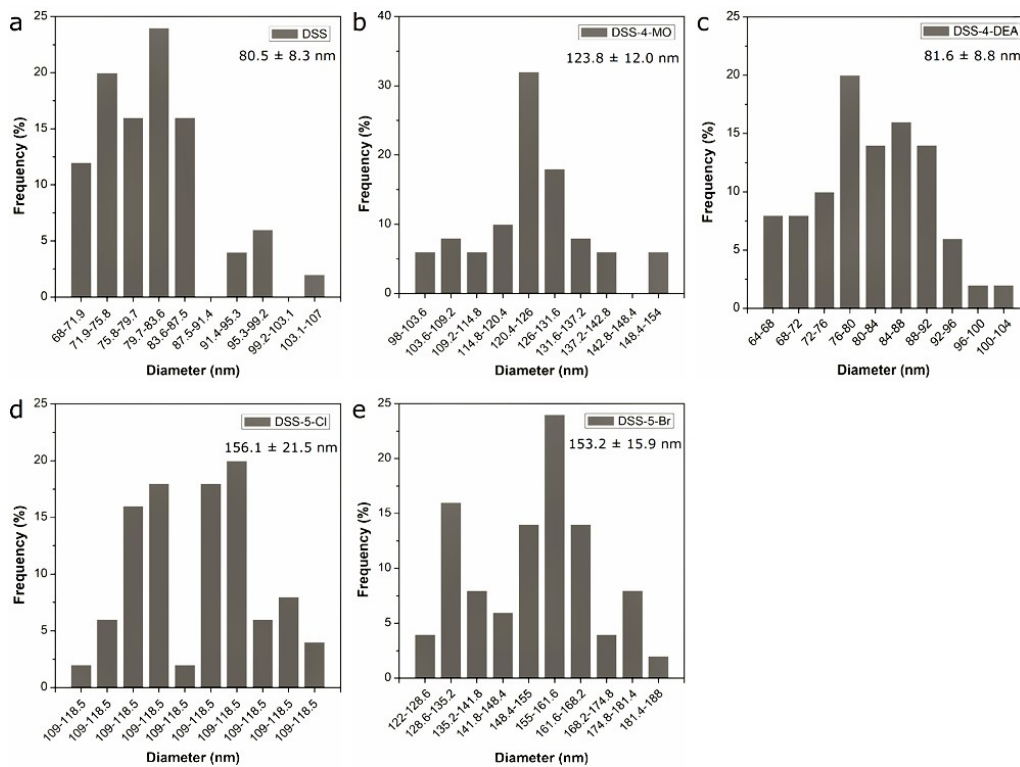
**Figure S13** Fluorescence images of LO2 cells stained 25  $\mu$ M of DSS and four derivatives in 30 min. Scale bar 100  $\mu$ m.



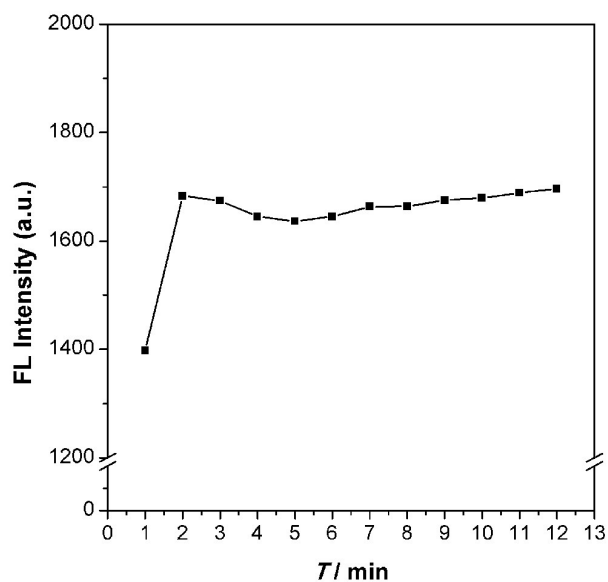
**Figure S14** Fluorescence images of RAW 246.7 cells stained 25  $\mu$ M of DSS and four derivatives in 30 min. Scale bar 100  $\mu$ m.



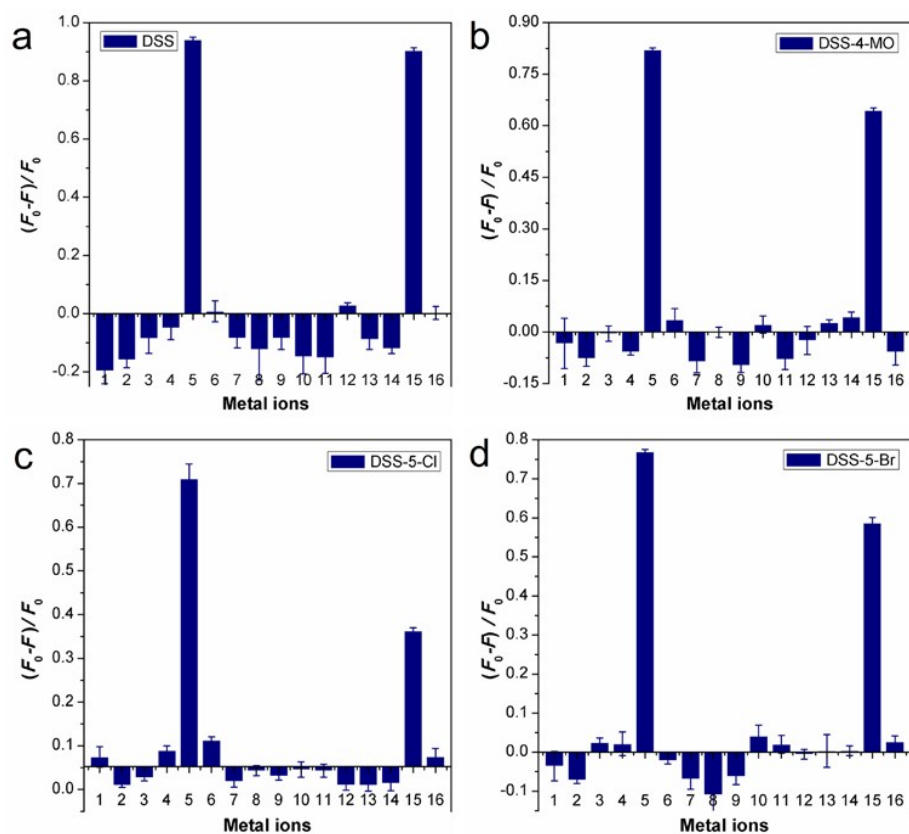
**Figure S15** Zeta potential of the DSS and the four derivatives (DMSO/water, water fraction 99%).



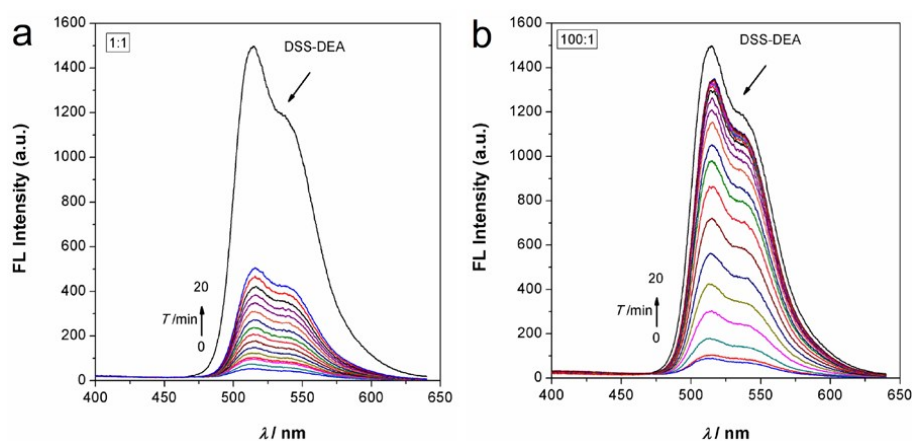
**Figure S16** The average size and statistically size distribution ( $n = 50$ ) of DSS and the four derivatives (DMSO/Imaging medium, water fraction 99%). (a-e) DSS, DSS-4-MO, DSS-4-DEA, DSS-5-Cl, DSS-5-Br.



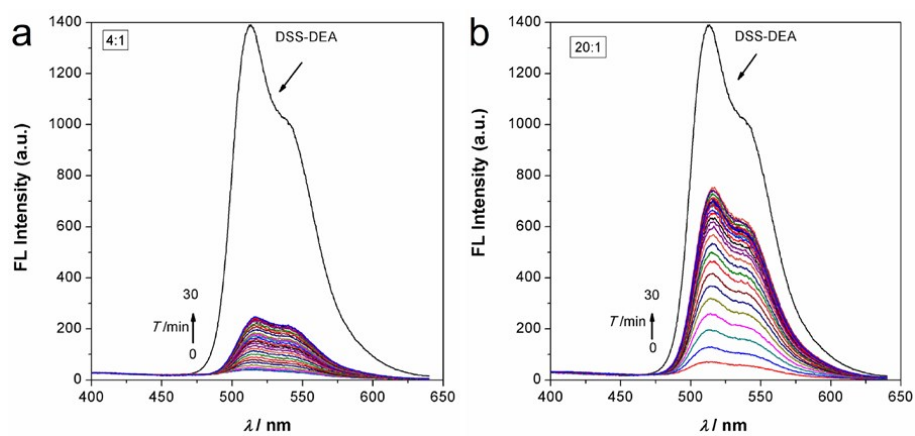
**Figure S17** The stability of the fluorescence of DSS-4-DEA in the DMSO/water solutions (water fraction 99%).



**Figure S18** Metal ions induced fluorescence quench of the (a) DSS, (b) DSS-4-MO, (c) DSS-5-Cl, (d) DSS-5-Br (1-16: 1  $\text{Ca}^{2+}$ , 2  $\text{Cd}^{2+}$ , 3  $\text{Co}^{2+}$ , 4  $\text{Cr}^{3+}$ , 5  $\text{Cu}^{2+}$ , 6  $\text{Fe}^{2+}$ , 7  $\text{Fe}^{3+}$ , 8  $\text{K}^+$ , 9  $\text{Mg}^{2+}$ , 10  $\text{Mn}^{2+}$ , 11  $\text{Na}^+$ , 12  $\text{Ni}^{2+}$ , 13  $\text{Pb}^{2+}$ , 14  $\text{Zn}^{2+}$ , 15 all metal ions 1-14, 16 all metal ions 1-14 except  $\text{Cu}^{2+}$ ).



**Figure S19** EDTA-2Na induced fluorescence recovery in 20 min. (a) EDTA-2Na: $\text{Cu}^{2+}$  1:1, (b) EDTA-2Na: $\text{Cu}^{2+}$  100:1.



**Figure S20** PPI induced fluorescence recovery in 30 min. (a) PPI:Cu<sup>2+</sup> 4:1, (b) PPI:Cu<sup>2+</sup> 20:1.