

Electronic Supplementary Information

## Exploration of Biocompatible AIEgens from Natural Resources

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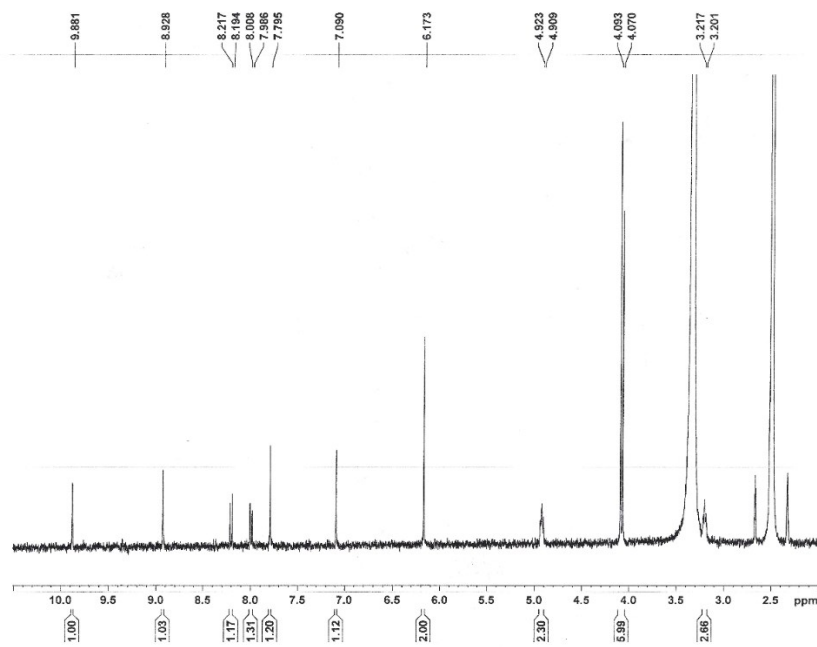
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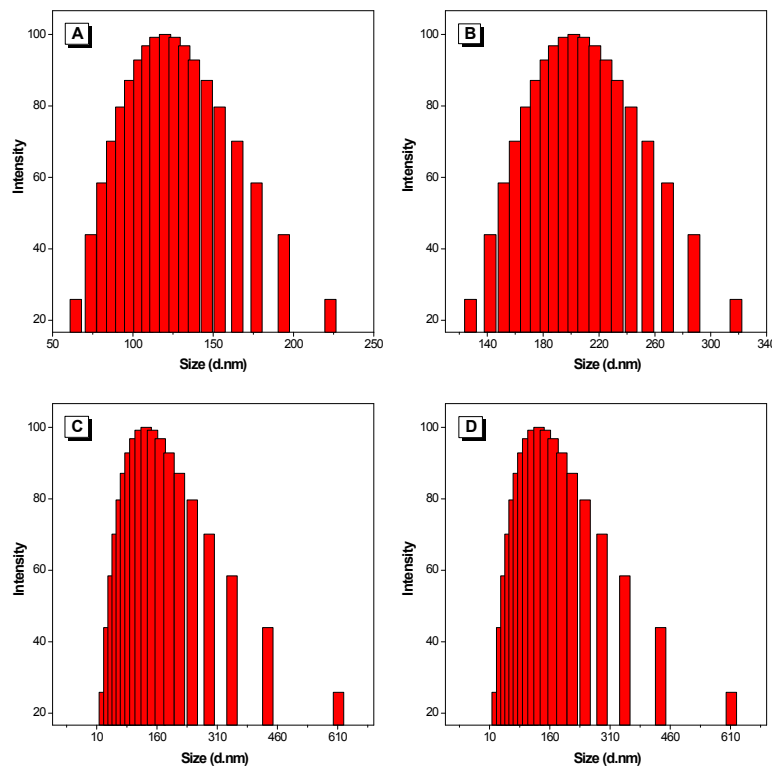
<sup>#.</sup> Y. Gu, Z. Zhao contributed equally to this work.

<sup>1</sup>H NMR of BBR Chloride

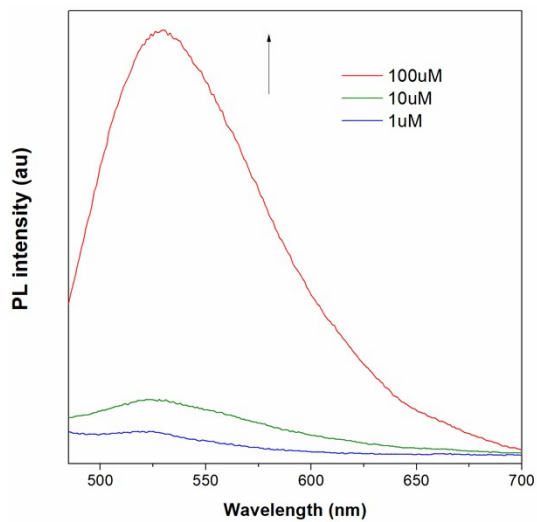
<sup>1</sup>H NMR (400 MHz, DMSO, 25 °C),  $\delta$  (ppm): 9.88 (s, 1H), 8.93 (s, 1H), 8.21–8.19 (d,  $J = 8.0$  Hz, 1H), 8.01–7.99 (d,  $J = 8.0$  Hz, 1H), 7.80 (s, 1H), 7.09 (s, 1H), 6.17 (s, 2H), 4.92–4.91 (d,  $J = 5.6$  Hz, 2H), 4.09–4.07 (d,  $J = 8.0$  Hz, 6H), 3.22–3.20 (m, 2H).



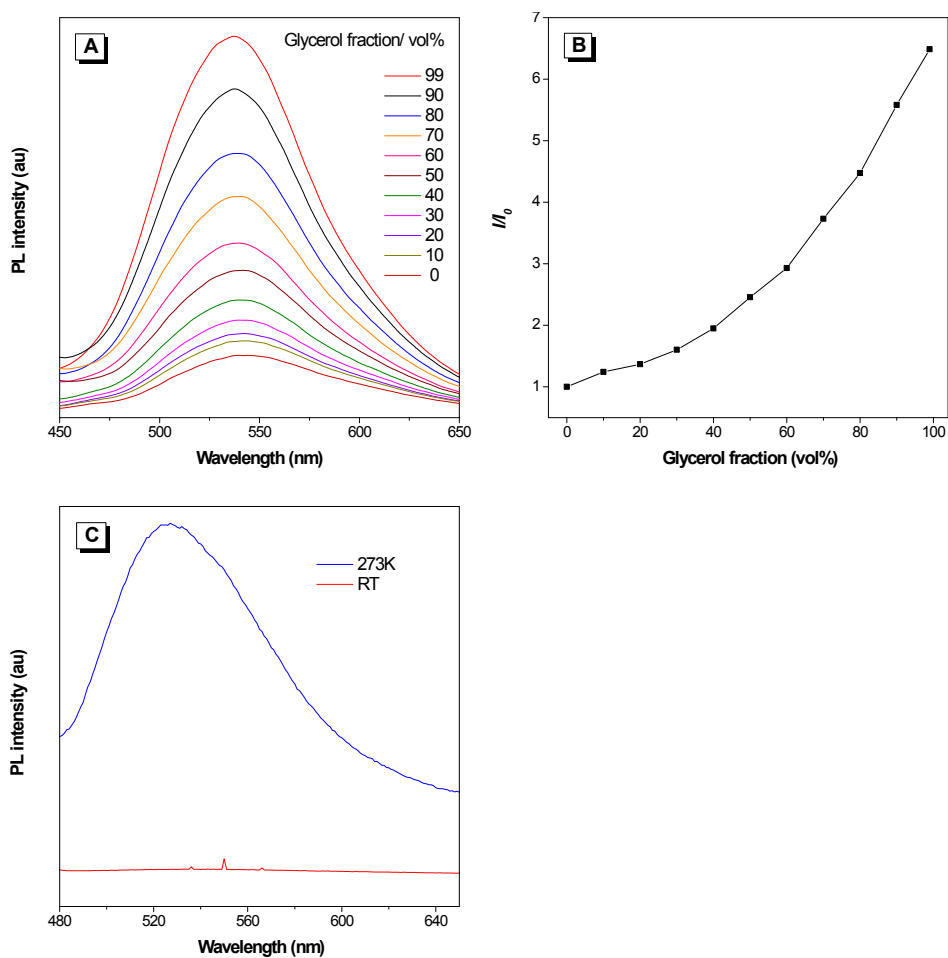
**Fig. S1** <sup>1</sup>H NMR of BBR Chloride



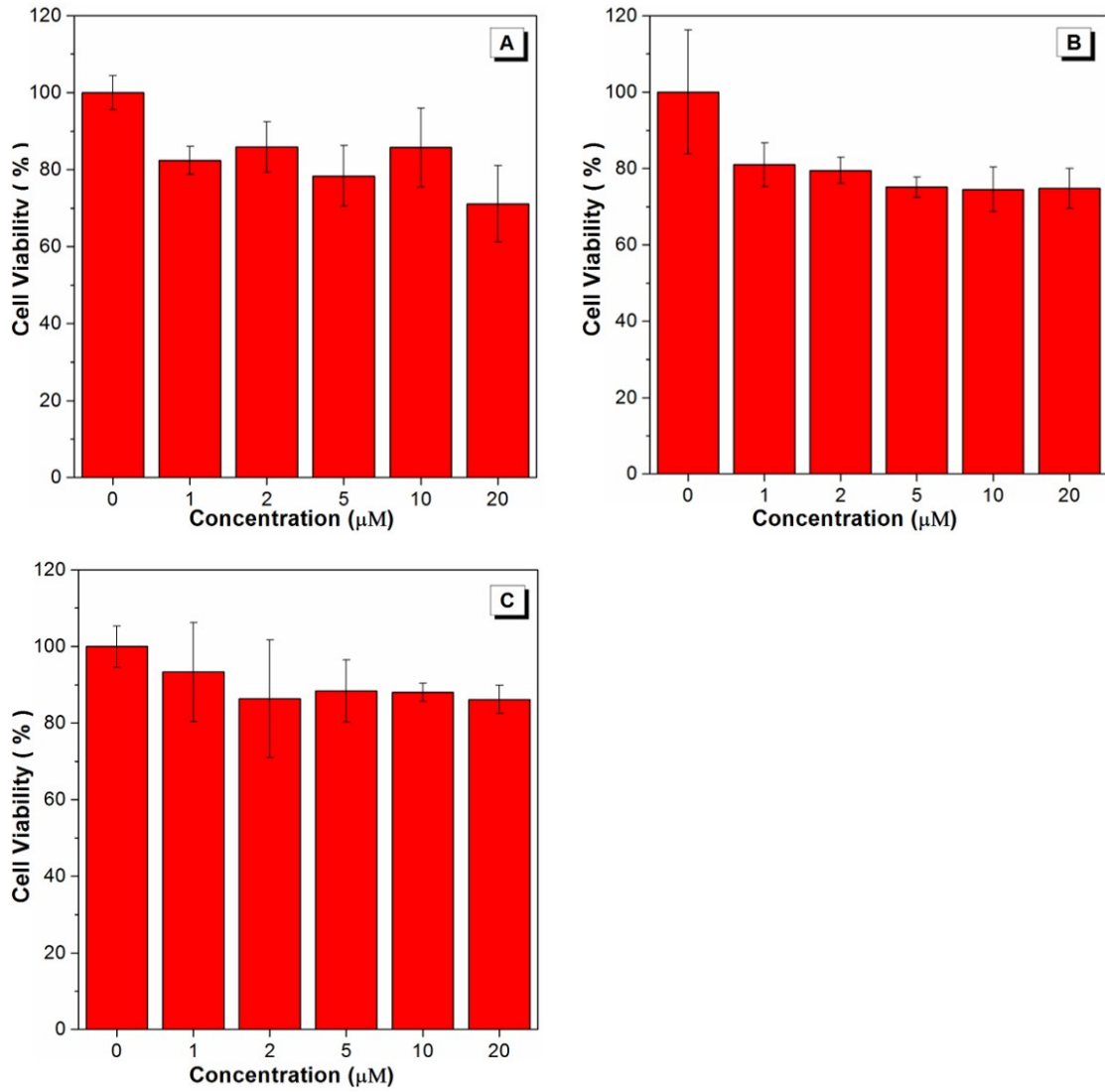
**Fig. S2** DLS results of BBR Chloride in different THF/water mixtures:  $f_{\text{THF}} = 10\%$  (A);  $f_{\text{THF}} = 50\%$  (B);  $f_{\text{THF}} = 80\%$  (C);  $f_{\text{THF}} = 99\%$  (D). Concentration:  $10\mu\text{M}$ .



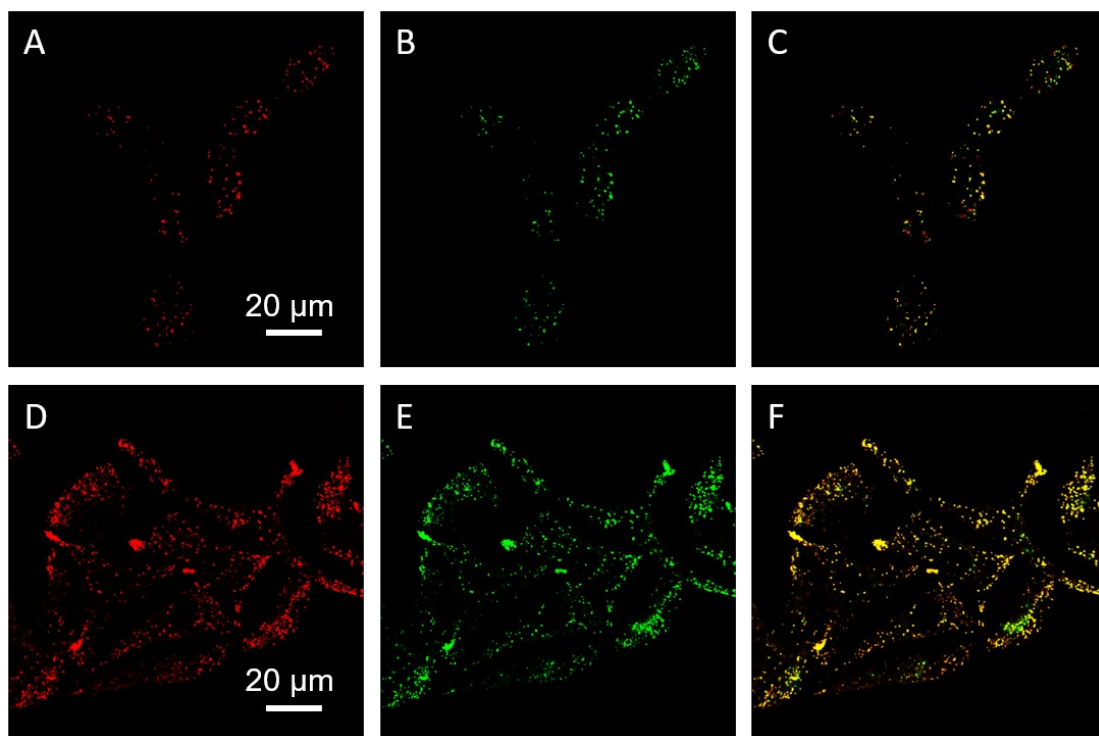
**Fig. S3** Concentration dependence of the PL spectra of BBR Chloride in aqueous solution. Excitation wavelength: 405 nm. Slit width: 5 nm.



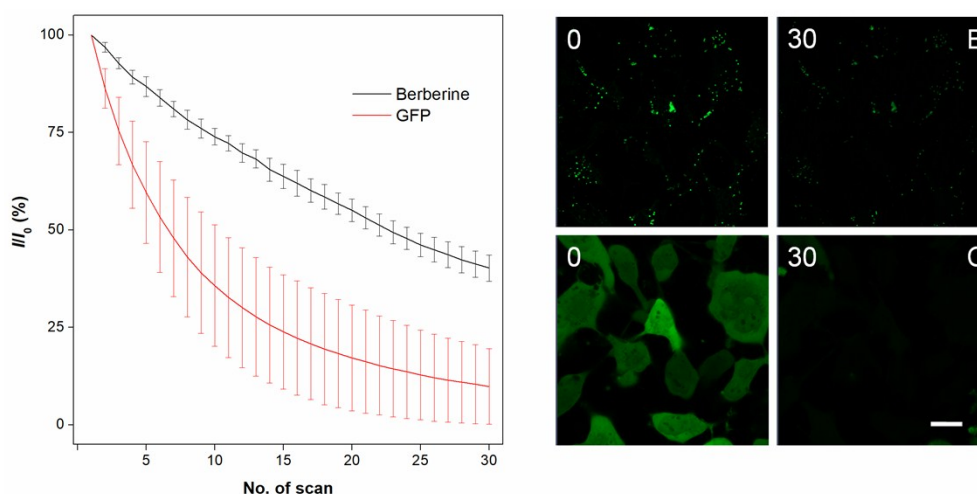
**Fig. S4** (A) PL spectra of BBR Chloride in ethylene glycol/glycerol mixtures with different fractions of glycerol. Slit width: 15 nm. (B) Plot of the  $I/I_0$  value of BBR Chloride versus the fractions of glycerol in the ethylene glycol/glycerol mixture.  $I_0$  is the PL intensity of BBR Chloride in ethylene glycol. (C) Temperature dependence of the PL spectra of BBR Chloride in water solution. Slit width: 5 nm. Solution concentration: 10  $\mu$ M; Excitation wavelength: 405 nm.



**Fig. S5** Viability of HeLa cells (A), A549 cells (B), and MCF-10A cells (C) in the presence of different concentrations of BBR Chloride for 24 h. Data are expressed as mean value of six separate trials.



**Fig. S6** (A–C) Confocal fluorescence images of A549 cells stained with MeOTTMN (A) and BBR Chloride (B), and the merged image of panel A and B (C). (D–F) Confocal fluorescence images of MCF-10A cells stained with MeOTTMN (D), BBR Chloride (E) and the merged image of panel D and E (F).  $\lambda_{\text{ex}}$ : 488 nm; scale bar = 20  $\mu\text{m}$ .



**Fig. S7** (A) Photostability of BBR Chloride and green fluorescent protein (GFP) under continuous scanning at 488 nm (2.3  $\mu\text{W}$ ).  $I_0$  is the initial PL intensity, while  $I$  is that of the corresponding sample after a designated No. of scan. (B and C) Confocal images of (B) HeLa cells stained with BBR Chloride (10  $\mu\text{M}$ ) and (C) 786-O cells containing GFP gene before and after 30 scans of light irradiation.  $\lambda_{\text{ex}}$  : 488 nm; All the images share the same scale bar: 20  $\mu\text{m}$ . Error bars are  $\pm$  relative standard deviations (RSD),  $n = 6$ .

**Table S1.** Average Fluorescence Lifetimes and Radiative and Non-radiative Decay Rates for BBR Chloride in aqueous solution (10  $\mu\text{M}$ ), powder, and crystal.

Berberine Chloride	$\langle\tau\rangle$ (ns)			$k_r$ ( $\times 10^8 \text{ s}^{-1}$ )			$k_{nr}$ ( $\times 10^8 \text{ s}^{-1}$ )		
	soln	crystal	powder	soln	crystal	powder	soln	crystal	powder
	0.68	7.93	4.86	0.022	0.19	0.24	14.69	1.08	1.82