

## Supporting information

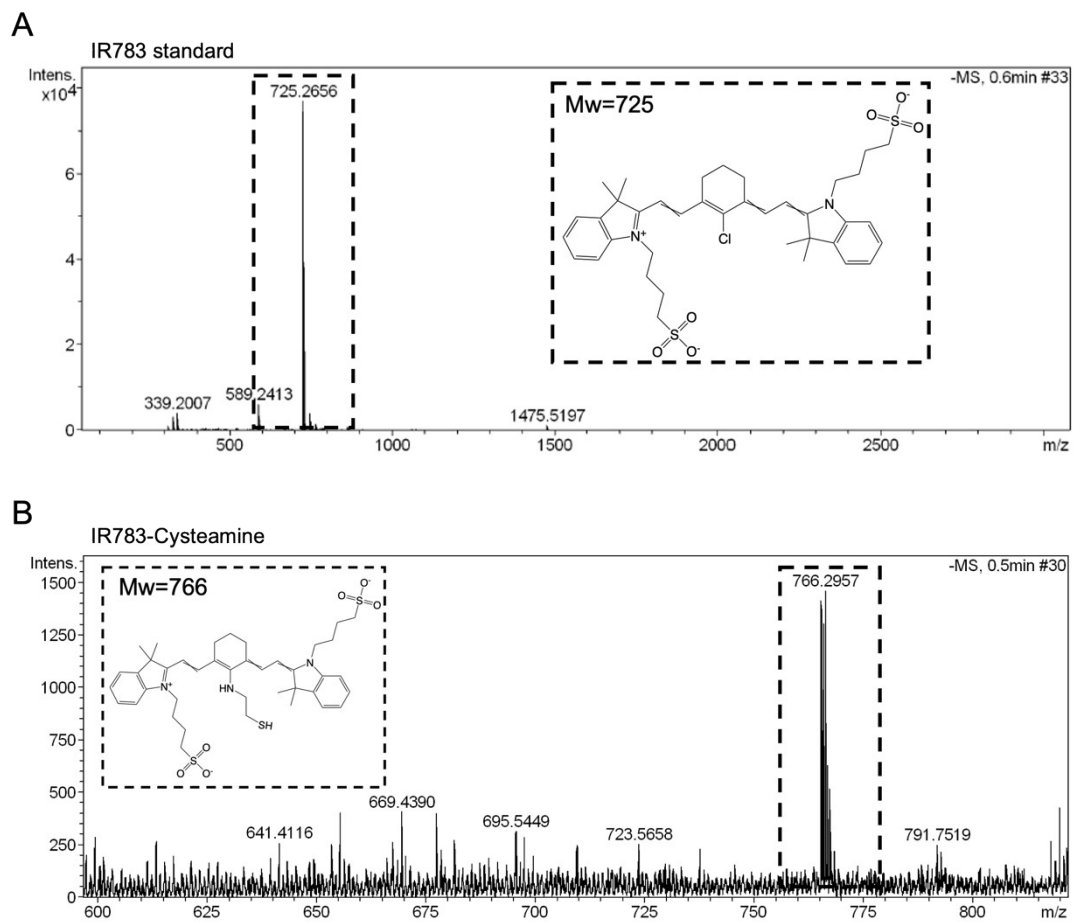
### **Nanoassemblies of Heptamethine Cyanine Dye-Initiated Poly(Amino Acid) Enhance ROS Generation for Effective Antitumour Phototherapy**

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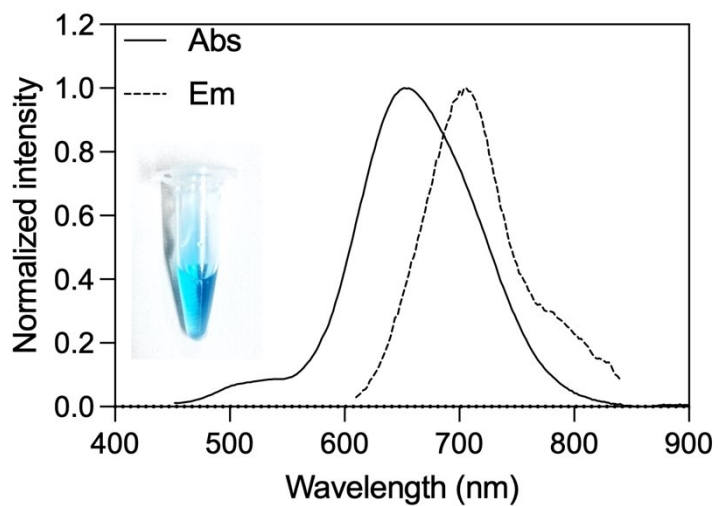
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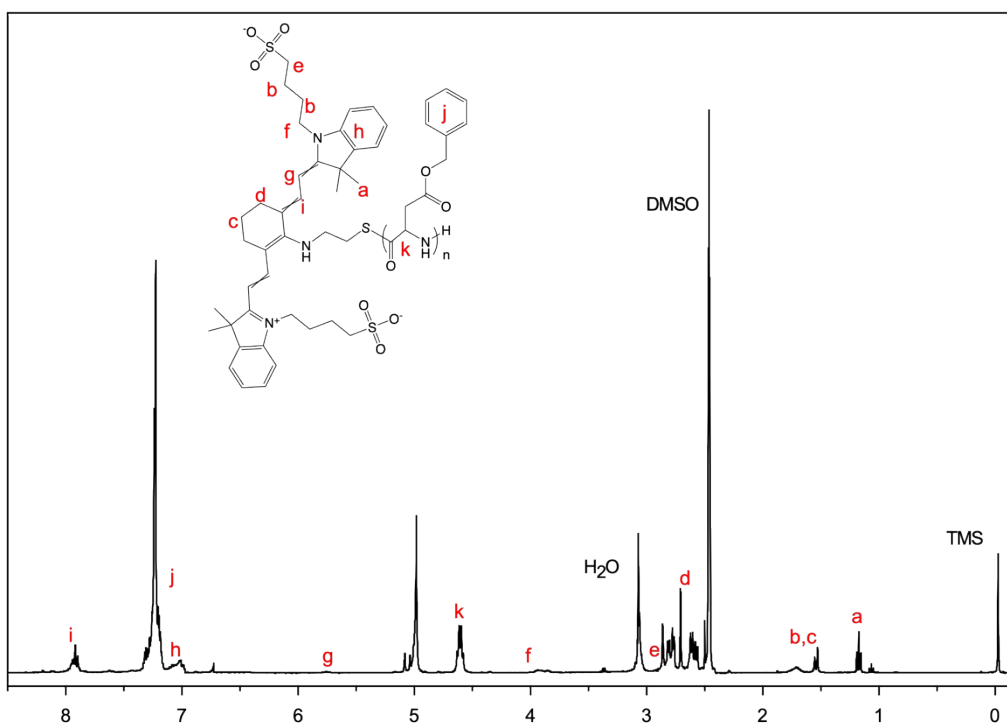
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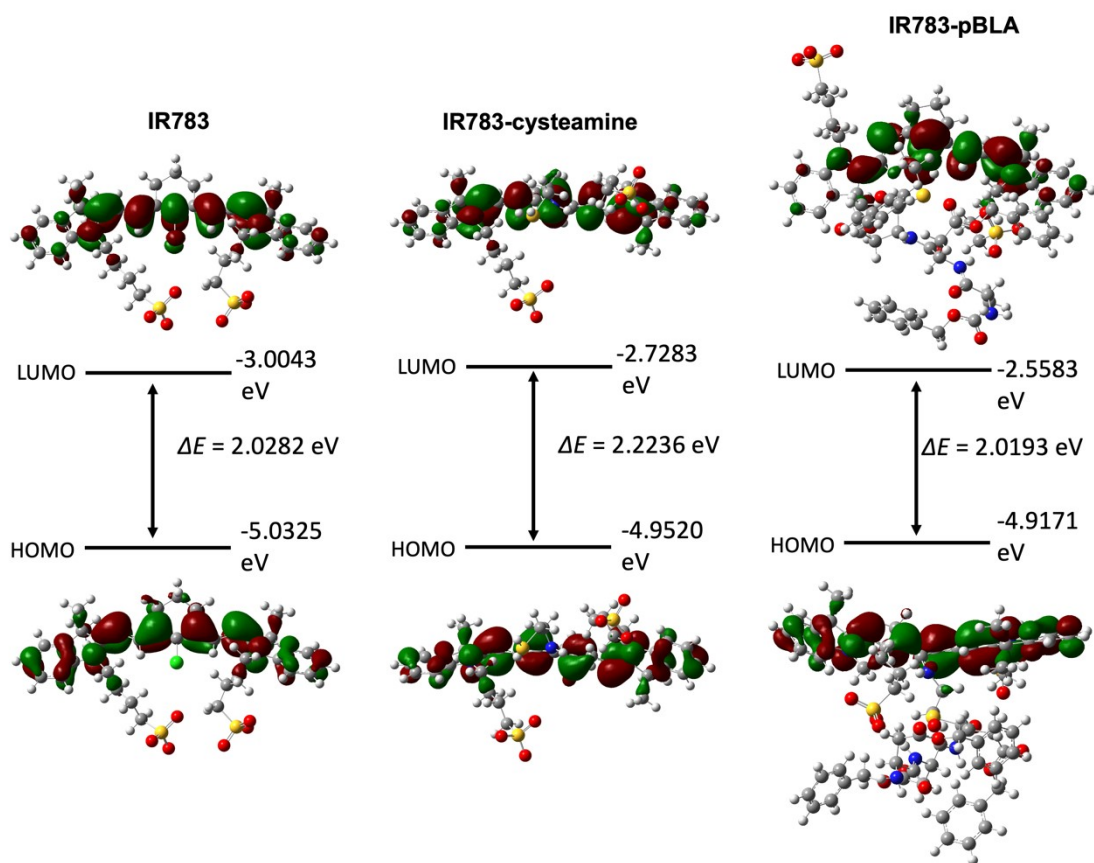
**Figure S1.** Mass spectra of IR783 (A) and IR783-cysteamine (B)



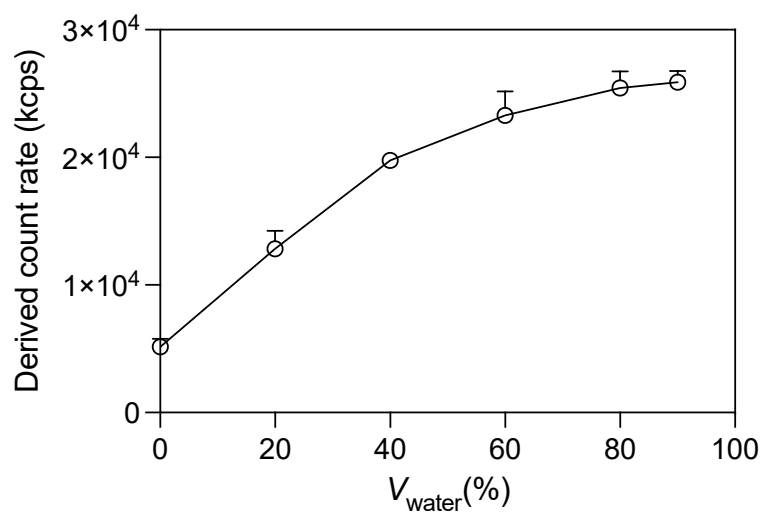
**Figure S2.** Absorbance and emission (Ex = 650 nm) spectra of IR783-cysteamine in water.



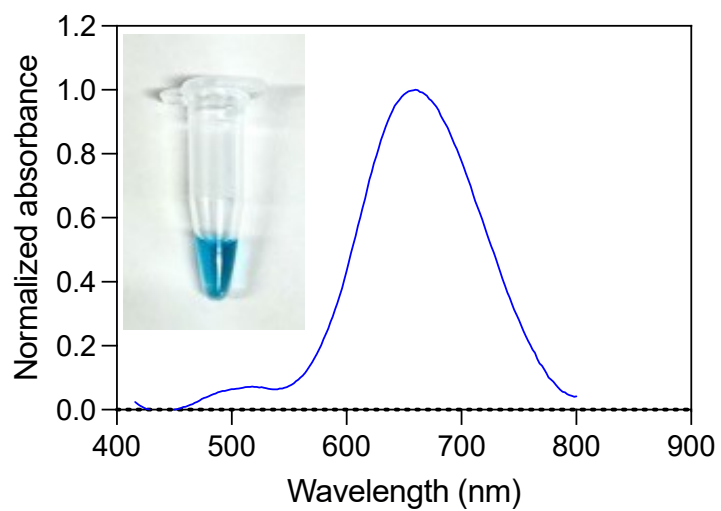
**Figure S3.** <sup>1</sup>H-NMR spectrum of IR-pBLA. The successful polymerization of BLA groups was confirmed by the appearance of the peak corresponding to the -CH- on the backbone of pBLA block ( $\delta \approx 4.6$  ppm, peak k). The number of BLA groups on one molecule was determined by comparing the peaks corresponding to -CH- on IR783 moiety ( $\delta \approx 7.9$  ppm, peak i) with peak k and calculated to be 17.



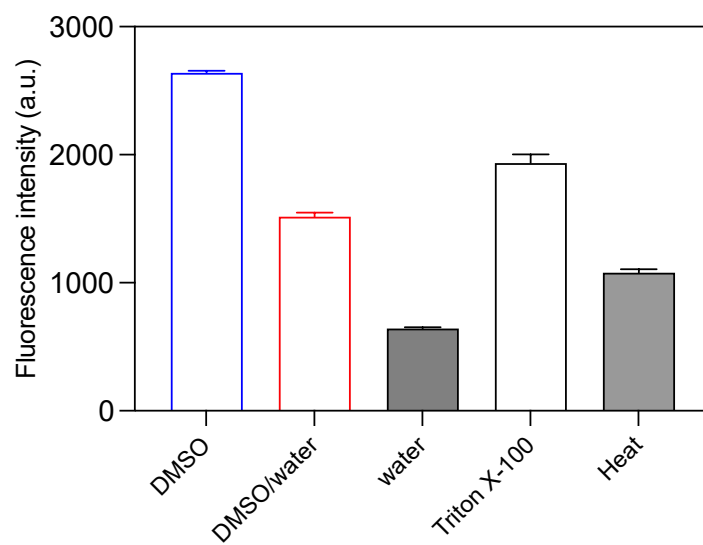
**Figure S4.** Theoretically predicted LUMO and HOMO distributions of the IR783 derivatives. The energy levels and band gaps were marked.



**Figure S5.** Light scattering intensity (measured by DLS) of IR783-pBLA dispersed in DMSO-water mixture with different water fraction. Data shown as mean  $\pm$  S.D.,  $n = 3$ .



**Figure S6.** Representative absorbance spectrum and photography of IR-PA dispersed in water.

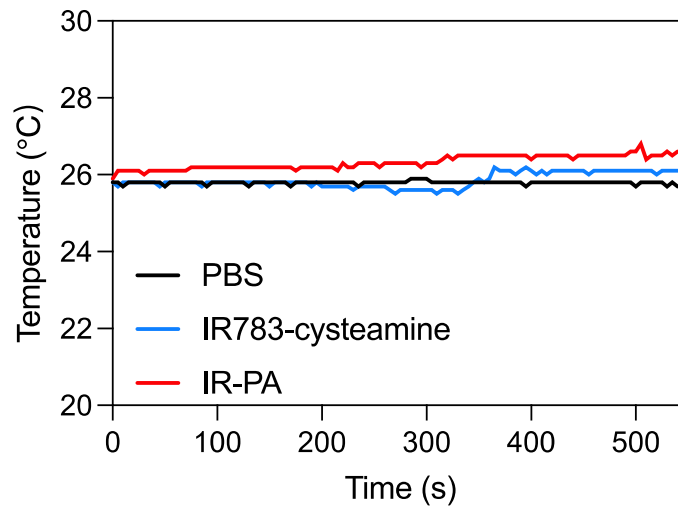


**Figure S7.** Fluorescence emission intensity (Ex 650/Em 770 nm) of IR-PA under different condition. Data shown as the mean  $\pm$  S.D.;  $n = 3$ .

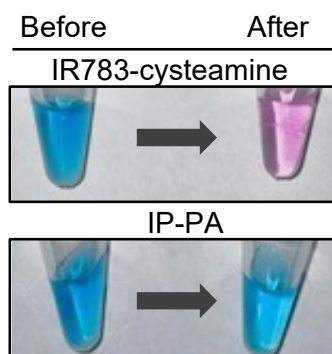


**Table S1.** Optical properties of IR783-cysteamine and IR-PA in water

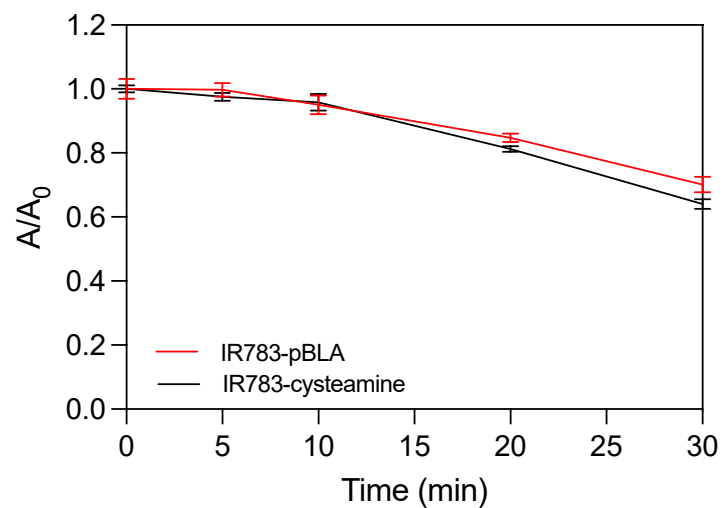
Sample	absorption $\lambda_{ab}$ (nm)	emission $\lambda_{em}$ (nm)	Stokes Shift (nm)	$\epsilon$ ( $\times 10^5$ )	$\Phi$
Cy5	651	670	19	2.3	0.27
IR783- cysteamine	652	706	54	1.55	0.11
IR-PA	660	770	110	1.89	0.05



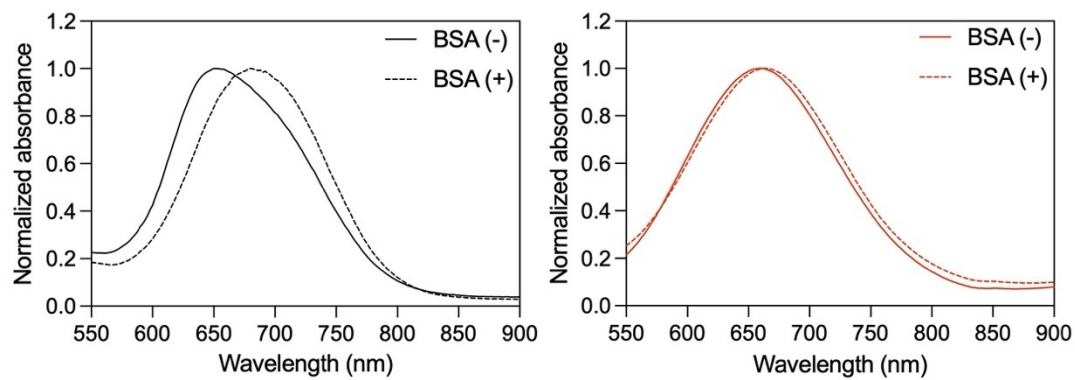
**Figure S8.** Temperature change of IR783-cysteamine and IR-PA water solution during irradiation with 633 nm laser.



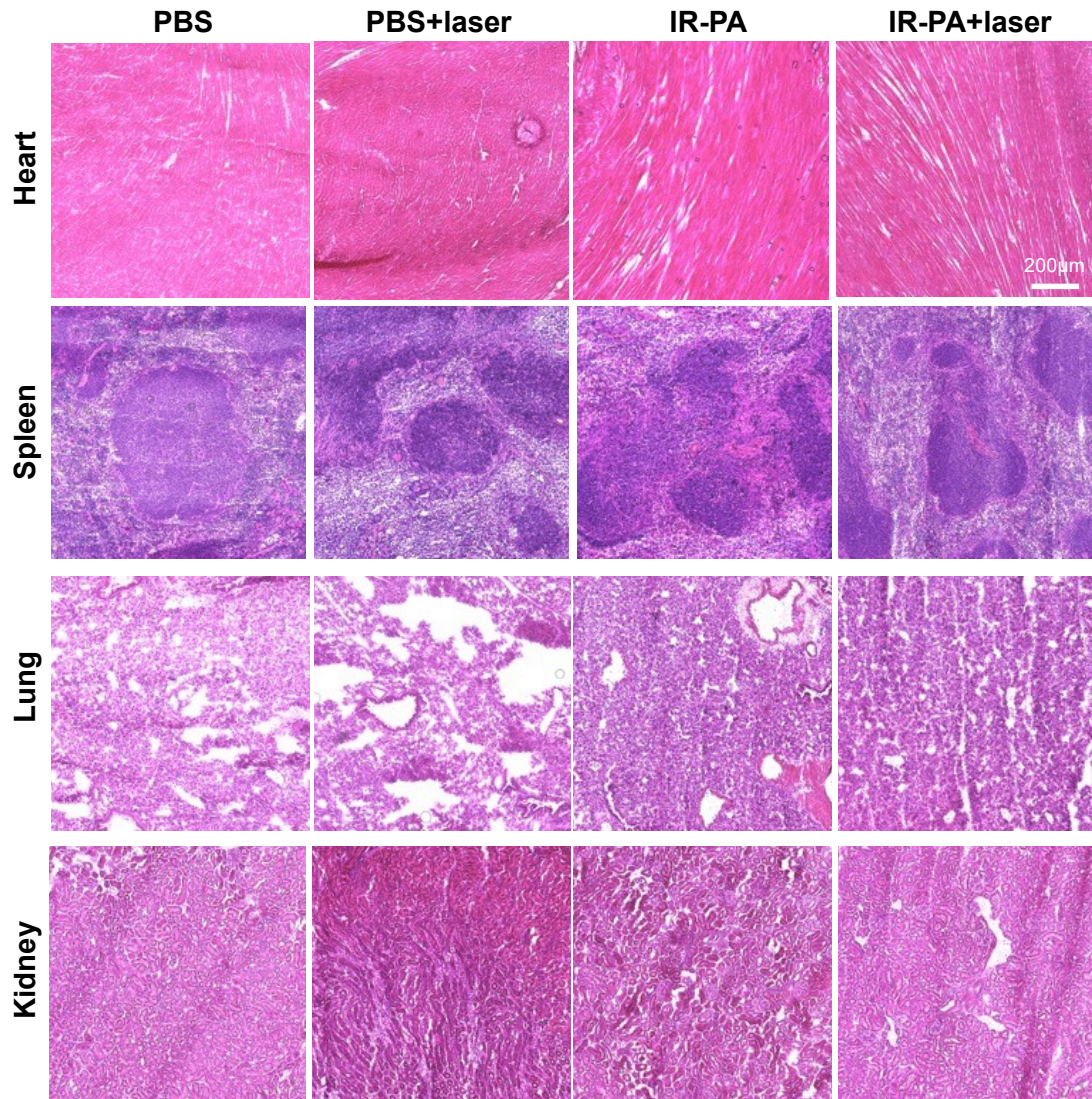
**Figure S9.** Colour change of IR783-cysteamine and IR-PA water solution after irradiation by 633 nm laser for 30 min.



**Figure S10.** Photostability of IR783-pBLA and IR783-cysteamine in DMSO after irradiation by 633 nm laser. Data shown as mean  $\pm$  S.D.,  $n = 3$ .



**Figure S11.** UV-vis absorbance spectra of IR783-cysteamine (left panel) and IR-PA (right panel) in aqueous buffer with or without BSA.



**Figure S12.** Representative H&E staining of organ sections after treatment. Scale bar = 200  $\mu$ m.