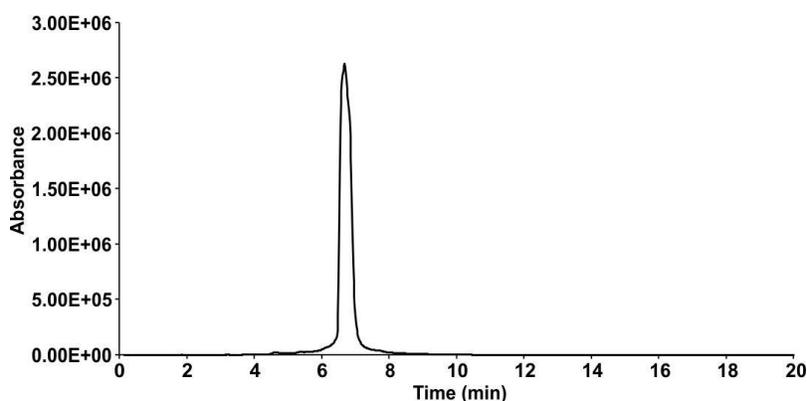
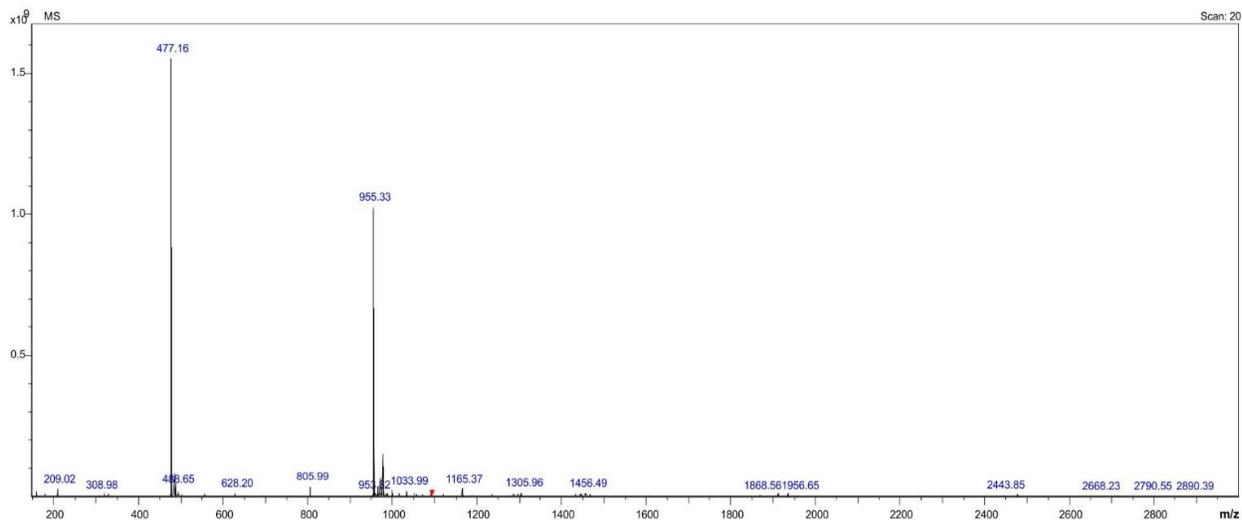


## Supporting Information: Highly-Soluble Cyanine J-aggregates Entrapped by Liposomes for In Vivo Optical Imaging around 930 nm

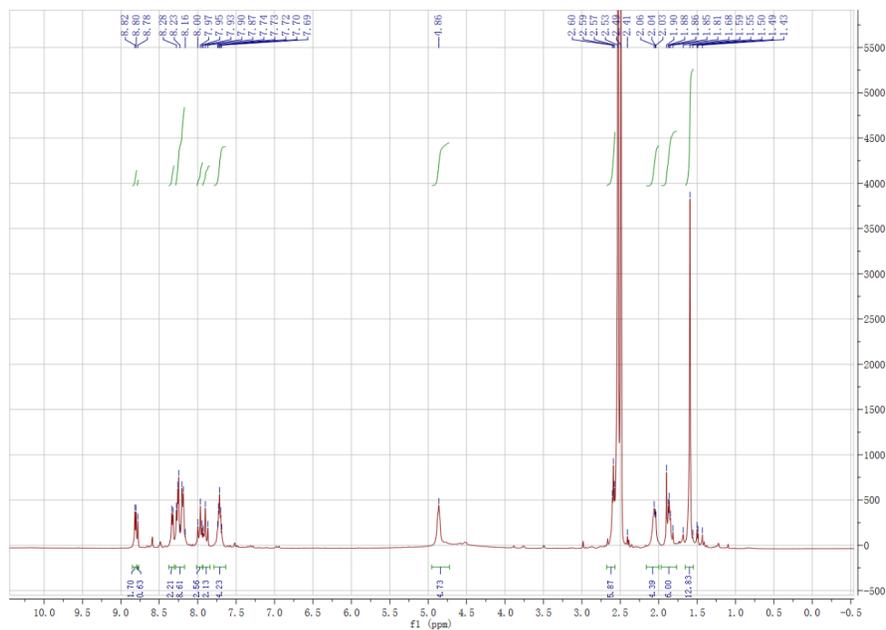
*Dyego Miranda, Haoyuan Huang, Homan Kang, Ye Zhan, Depeng Wang, Yang Zhou, Jumin Geng, Hailey I. Kilian, Wesley Stiles, Aida Razi, Joaquin Ortega, Jun Xia, Hak Soo Choi, Jonathan F. Lovell\**



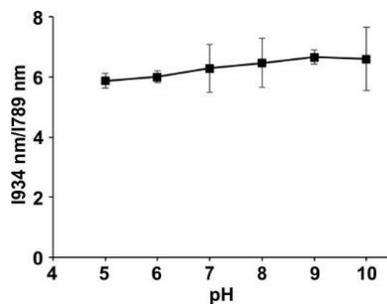
**Figure S1.** HPLC chromatogram (at 789 nm) demonstrating DCP-Cy purity (>99%).



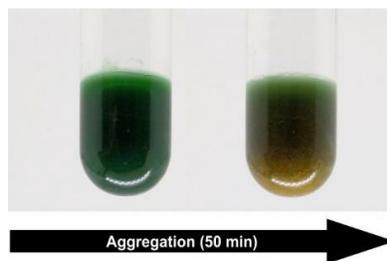
**Figure S2.** Maldi-TOF mass spectrum of DCP-Cy dye, 477.16 pointed to the product with two charges, and 955.33 indicated the intact compound.



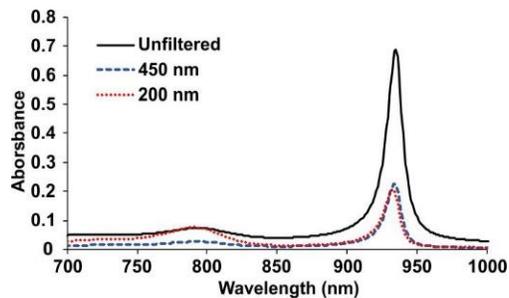
**Figure S3.** DCP-Cy  $^1\text{H}$  NMR:  $\delta$  1.59 (s, 12H), 1.86 (m, 6H), 2.06 (m, 4H), 2.59 (m, 6H), 4.86 (m, 4H), 7.72 (m, 4H), 7.90 (t,  $J = 15$  Hz, 2H), 7.97 (t,  $J = 15$  Hz, 2H), 8.23 (m, 8H), 8.34 (d,  $J = 10$  Hz, 2H), 8.82 (d,  $J = 10$  Hz, 2H).



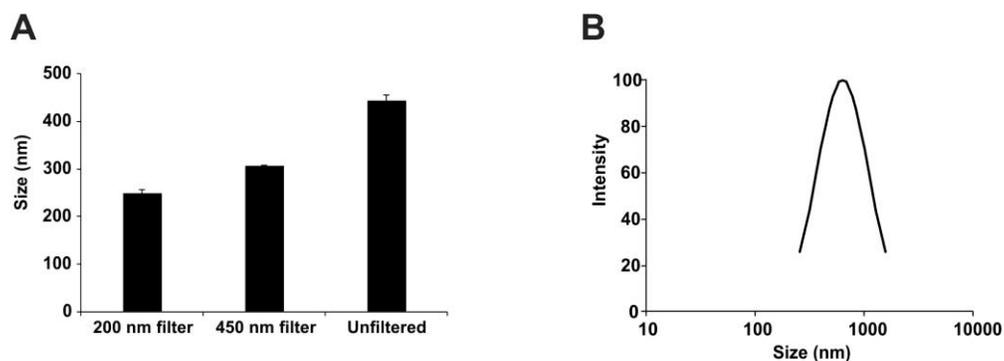
**Figure S4.** Effect of pH on the 934 to 789 nm absorption ratio of DCP-Cy.



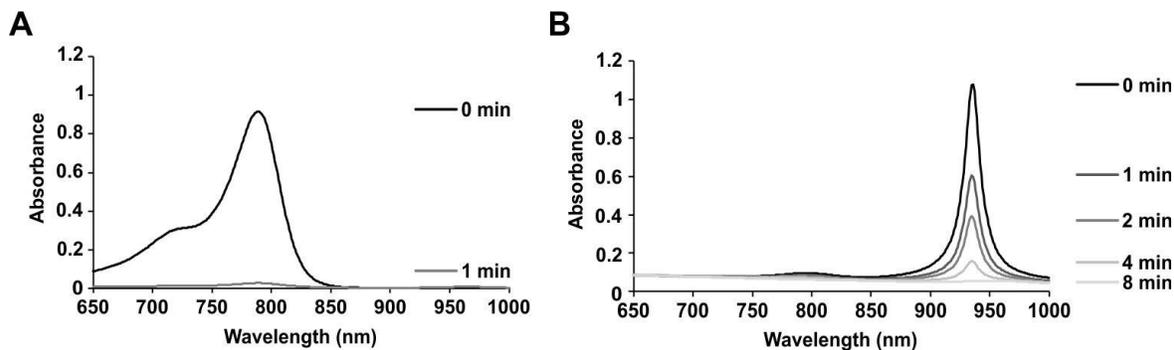
**Figure S5.** Appearance of DCP-Cy dye right after EtOH injection of dissolved lipids to dissolved dicarboxylic IR-820 at 60 °C. The appearance of a copper metallic color in the solution is noted.



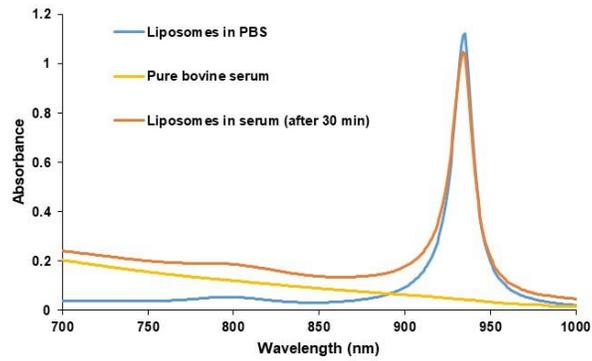
**Figure S6.** Absorbance in PBS with no filtration, 450 nm filtration and 200 nm filtration.



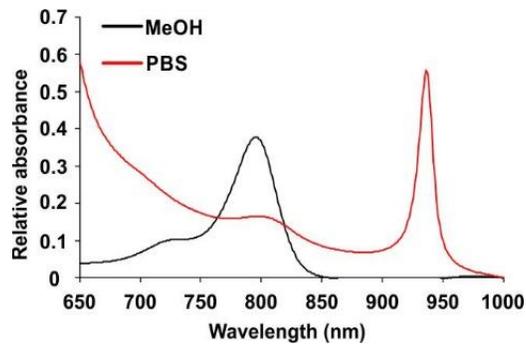
**Figure S7. A)** Particle size of liposomal DCP-Cy with no filtration, 0.4  $\mu\text{m}$  filtration, or 0.2  $\mu\text{m}$  filtration. **B)** Size distribution of unfiltered liposomal DCP-Cy. Samples were measured in PBS using dynamic light scattering.



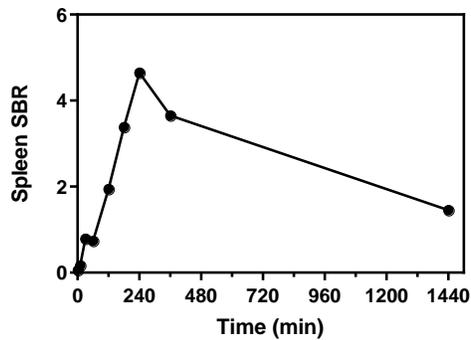
**Figure S8.** Photobleaching effect on **(A)** DCP-Cy free dye in Di-water and **(B)** its liposomal counterpart in PBS (150 mM NaCl, pH 10) under an 808 nm laser,  $1000 \text{ mW/cm}^2$ .



**Figure S9.** Absorbance of liposomal DCP-Cy after 30 min incubation in serum.



**Figure S10.** Absorbance scans from samples in the spleen 24 h after IV injection and obtained by either MeOH or PBS extraction methods.



**Figure S11.** Kinetics of spleen fluorescence following intravenous injection of liposomal DCY-Cy.

**Table S1 Quantification of photoacoustic (PA) images in Fig 2F and 3E (arbitrary units)**

<b>DCP-Cy measurement condition</b>	<b>789 nm PA signal</b>	<b>934 nm PA signal</b>
0 mM NaCl	17800	1780
120 mM NaCl	10324	8010
150 mM NaCl	3916	15130
Liposome - det.	20700	45000
Liposomes + det.	33750	26100