Supporting information

Lysosome-targeted triazole near-infrared cyanine fluorescent probe for in vivo long-term cell tracking

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Experimental section:

Synthesis of IR780-PO-NH_2

IR780-PO-NH_2 was synthesized mainly according to the literature.[13] Briefly, Boc-tyramine (113 mg, 0.476 mmol) was added into anhydrous DMF solution, and the solution was dropped into NaH (16.7 mg, 0.417 mmol) anhydrous DMF solution. This mixture solution was stirred in an ice bath for 30 min in a flask to completely dissolve. IR780 (100 mg, 0.150 mmol) was dissolved in anhydrous DMF solution and dropped into the flask under the ice water for 30 min and at room temperature for 90 min sequentially. When the reaction finished, the solution was dissolved in saturated NH_4Cl solution, extracted with CH_2Cl_2 (3×100 mL), and dried by Na_2SO_4. Through filtering and evaporating under reduced pressure, the crude was purified by normal-phase chromatography (CH_2Cl_2: MeOH = 40: 1) to yield IR780-PO-NH_2-BOC as a green solid.

The above products were dissolved in 1 mL CH_2Cl_2 and bathed in ice water for 10 min. Then, 1 mL of trifluoroacetic acid (TFA) was dropped in the CH_2Cl_2 and stirred at room temperature for 3 h. After evaporating under reduced pressure, IR780-PO-NH_2 was obtained as a green solid and stored at -20℃ away from light. ^{1}H NMR (600 MH_Z, DMSO-d_6): δ 1.15-1.35(m, 16H), 1.65-1.75(m, 4H), 2.71(m, 4H), 2.78(m, 4H), 4.11(t, 4H), 6.22-6.24(d, 2H), 7.02-7.06(d, 2H), 7.10-7.15(m, 2H), 7.18-7.23(t, 2H), 7.26-7.28(d, 2H), 7.47-7.52(m, 2H), 7.76-7.86(m, 6H). HR-MS: calculate for $C_{44}H_{54}N_3O^+$ m/z 640.4261, found 640.4260.

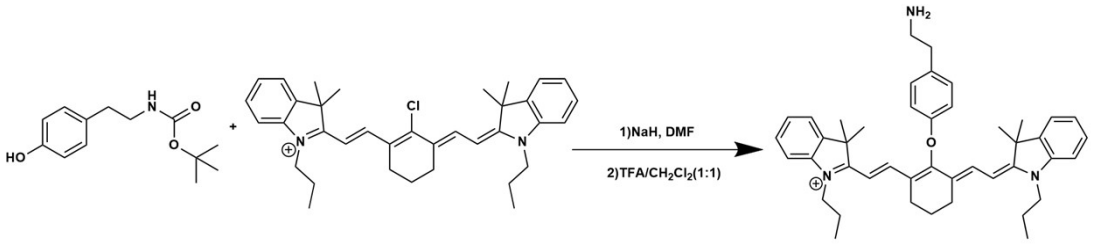

Figure S1. Synthesis route of IR780-PO-NH_2

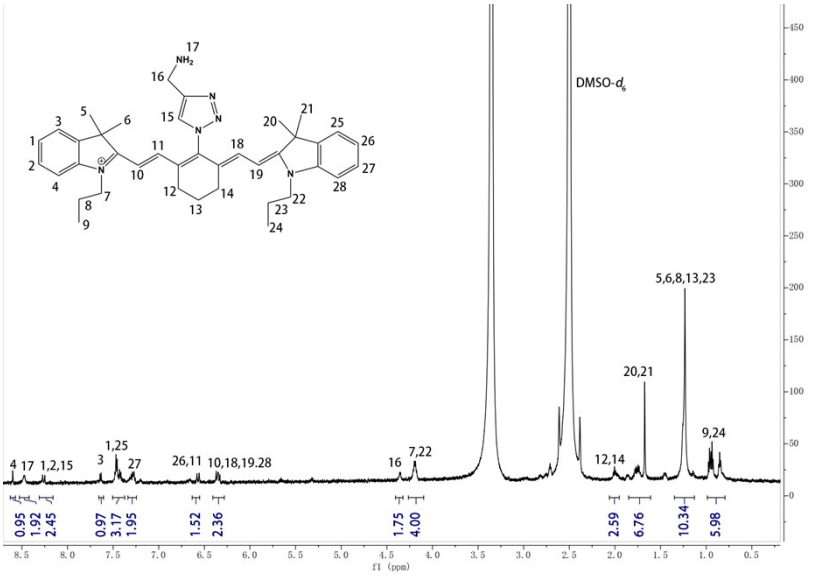

Figure S2. ^{1}H NMR of IR780-NT-NH_2

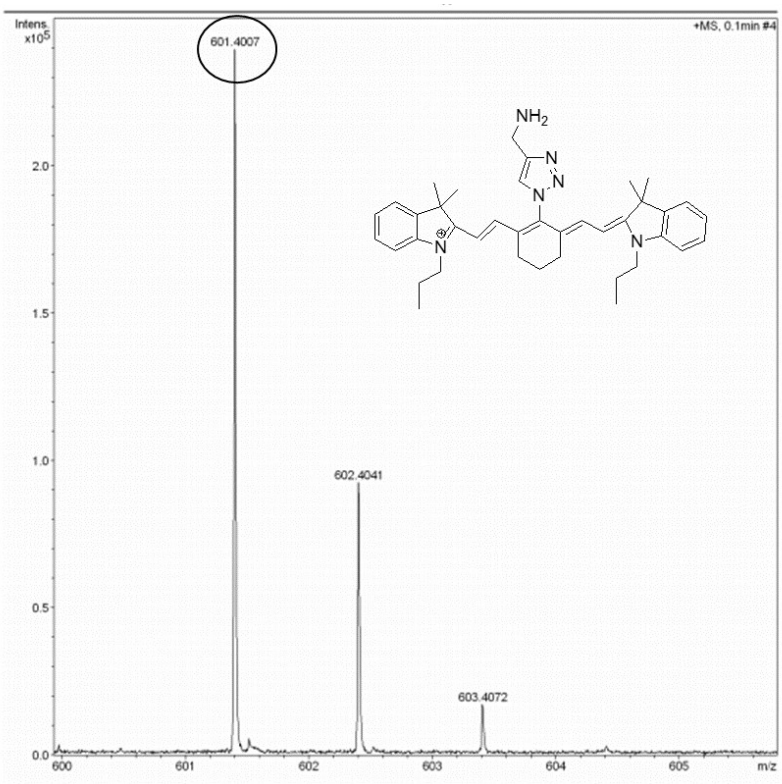

Figure S3. HR-MS of IR780-NT-NH_2

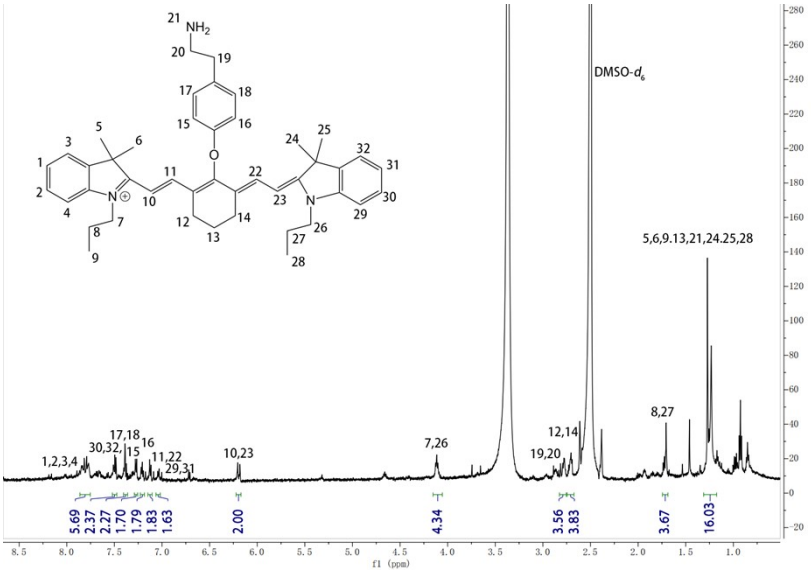

Figure S4. ^{1}H NMR of IR780-PO-NH_2

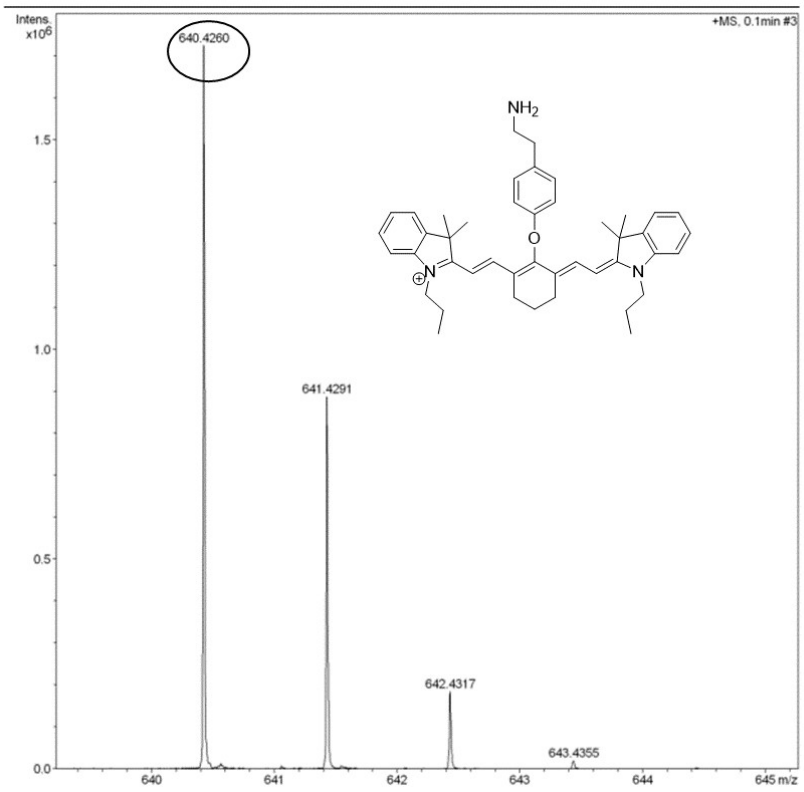

Figure S5. HR-MS of IR780-PO-NH_2

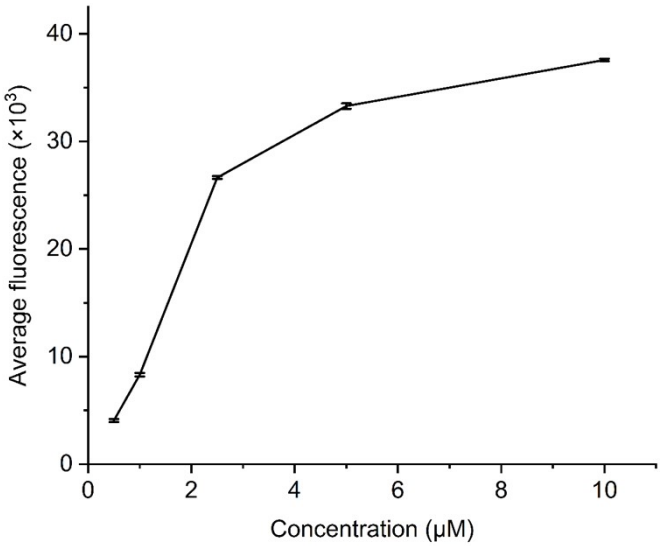

Figure S6. In vitro cellular uptake of IR780-NT-NH_2 in PC-3 cells with various concentrations (0.5, 1, 2.5, 5 and 10 μM).

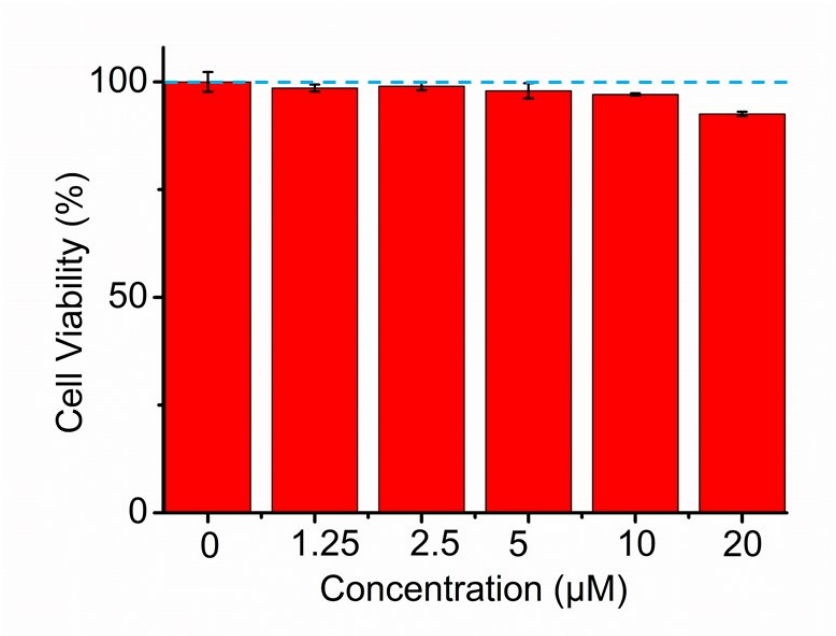

Figure S7. Cellular toxicity study of IR780-NT-NH_2 in PC-3 cells. Cells were seeded at a density of 5, 000 cells per well in a 96-well plate. After 24 h, IR780-NT-NH_2 was added to each well with gradient concentrations (0, 1.25, 2.5, 5, 10, and 20 μmol/L) and incubated for 24 h at 37°C. The cell viability was tested by MTT assay. Error bars are for n = 5.

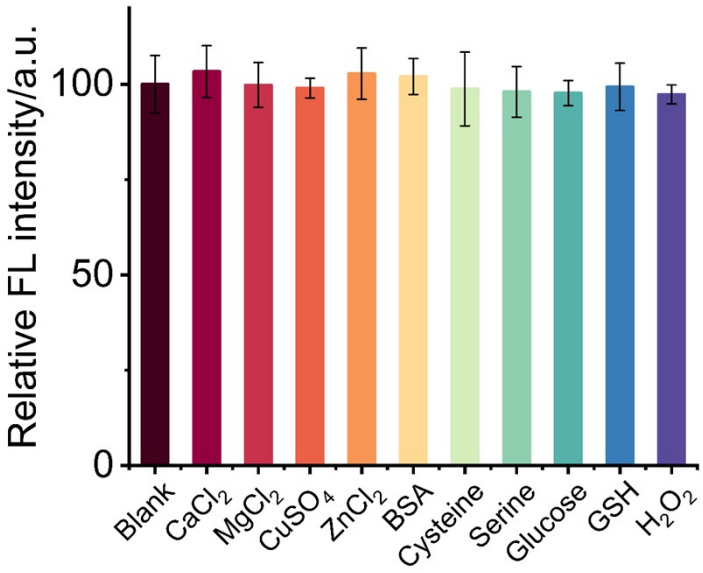

Figure S8. Relative fluorescence intensity of IR780-NT-NH_2 with various potential interfering species ($CaCl_2$ 2 mM, $MgCl_2$ 2 mM, $CuSO_4$ 50 μM, $ZnCl_2$ 100 μM, BSA 1 mg/mL, cysteine 1 mM, serine 1 mM, glucose 10 mM, GSH 100 μM, and H_2O_2 100 μM). The blank was set as no interfering species addition. The concentration of IR780-NT-NH_2 was 5 μM. Error bars represent the standard deviation (n = 3).