

Supporting Information

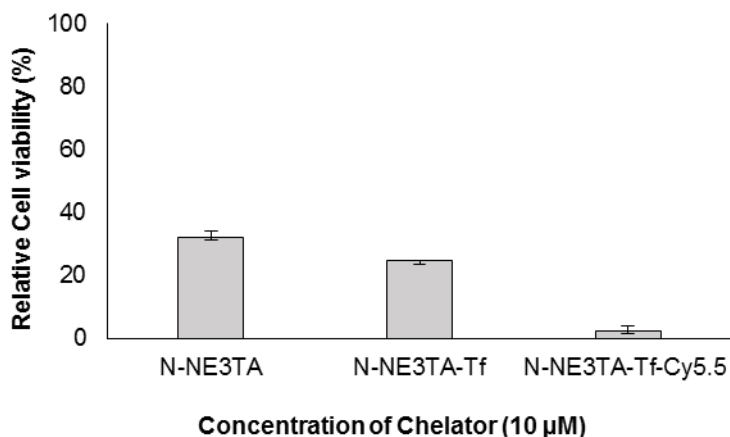
Theranostic Polyaminocarboxylate-Cyanine-Transferrin Conjugate for Anti-Cancer Therapy and Near IR Optical Imaging

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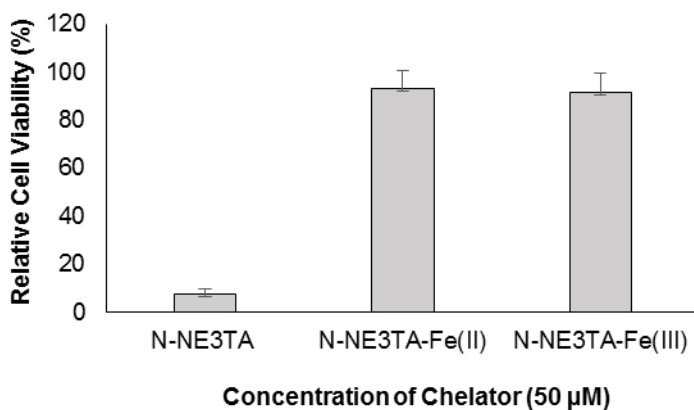
I. Effect of *N*-NE3TA, *N*-NE3TA-Tf, and *N*-NE3TA-Tf-Cy5.5 on viability of PC3 cells.

The PC3 cells were incubated with the anti-tumor agent (10 μ M, based on concentration of chelator) for 72 h, and the cell viability was determined using MTS assay. The cytotoxicity data of the conjugates were compared to that of the parent chelator *N*-NE3TA.¹⁰

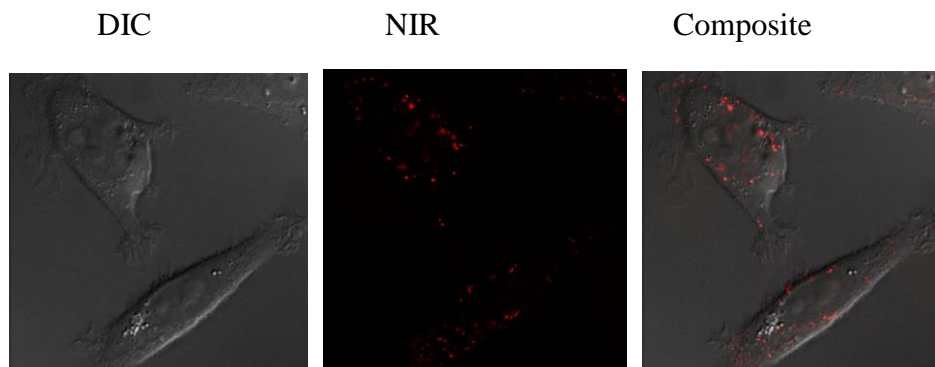


II. Effects of iron saturation and chelator on growth of HeLa cells.

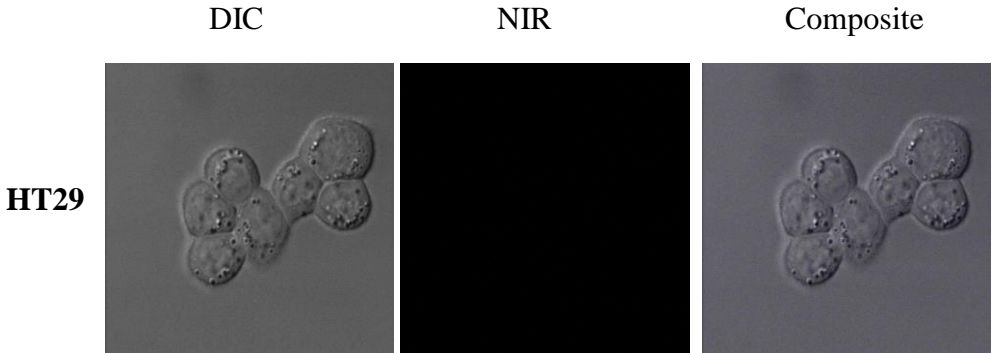
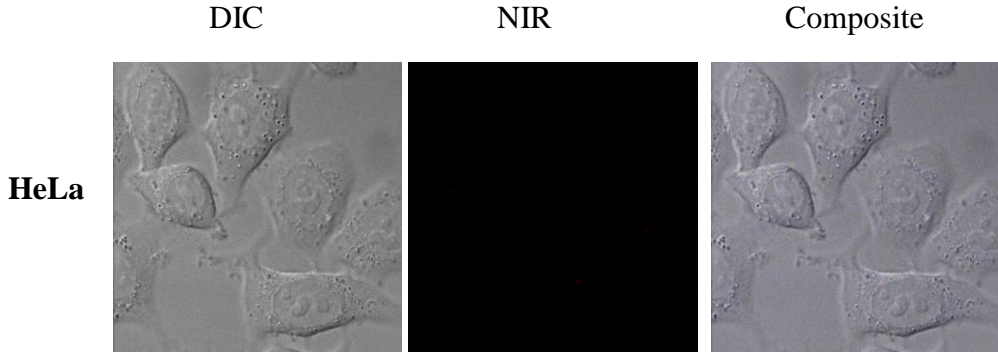
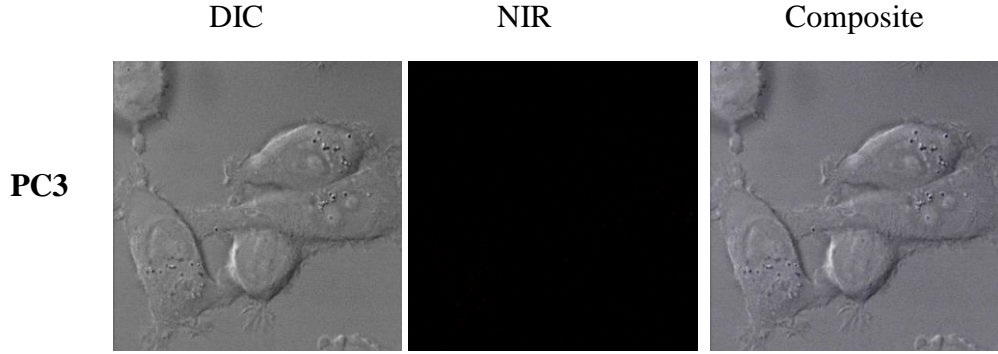
The chelator *N*-NE3TA (50 μ M) was mixed with the stoichiometric amount of an aqueous solution (50 μ M) of ferric citrate or ferrous chloride in complete medium, and the resulting co-mixture of *N*-NE3TA-Fe(II) or *N*-NE3TA-Fe(III) was then added into the triplicate plates containing HeLa cells and incubated at 37 $^{\circ}$ C for 72 h, and the cell viability was determined using MTS assay.¹⁰



III. Phase contrast, near IR fluorescent, and composite images of live PC3 cells incubated with both *N*-NE3TA-Tf conjugate (1.5 μ M) and Tf (2 mg) for 3 hr at 37 $^{\circ}$ C (Blocking experiment).



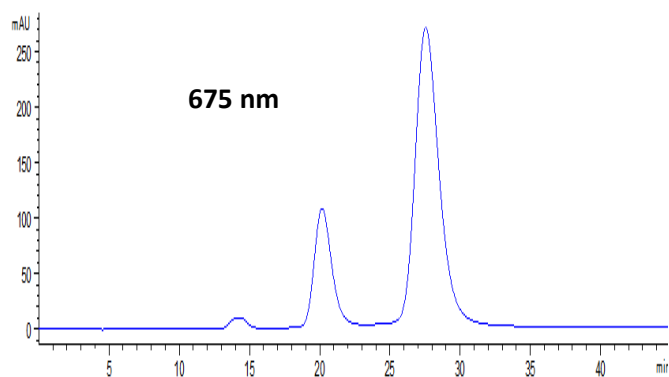
IV. DIC, near IR fluorescence, and composite images of live cancer cells incubated without fluorescent Cy5.5 conjugate for 3 hr at 37 °C.



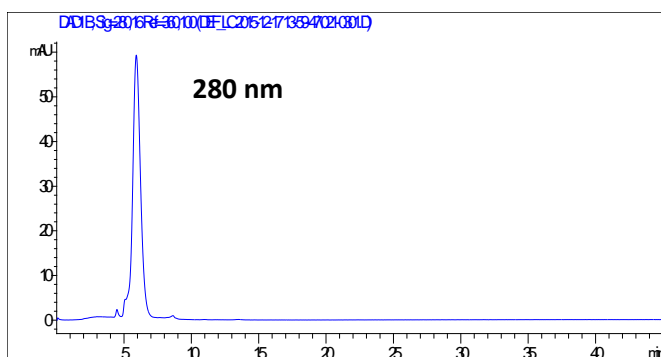
V. HPLC chromatograms of N-NE3TA-Tf and N-NE3TA-Tf-Cy5.5 conjugates and Cy5.5

Analytical SE-HPLC (TSKgel G3000PW column, Tosoh Biosep) using the isocratic mobile phase (PBS, pH 7.4, 45 min, flow rate of 1 mL/min, $\lambda = 280$ and 675 nm).

Cy5.5



N-NE3TA-Tf Conjugate



N-NE3TA-Tf-Cy5.5 Conjugate

