Supporting Information

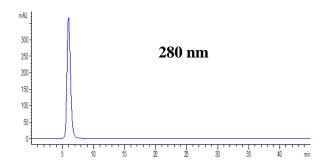
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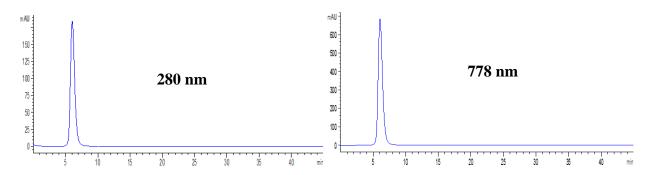
I. HPLC chromatograms of the purified antibody conjugates (CAB-NE3TA-PAN and CAB-NE3TA-PAN-IR800) and IR800 CW.

The antibody conjugates were purified and characterized by 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, λ = 280 and 778 nm). CAB-NE3TA-Pan-IR800 conjugate ($t_R = \sim 6$ min) was eluted earlier than unbound IR800 ($t_R = \sim 13$, 17 min) at 778 nm.

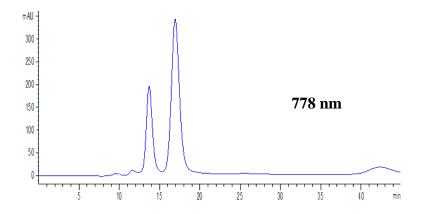
CAB-NE3TA-Pan



CAB-NE3TA-Pan-IR800

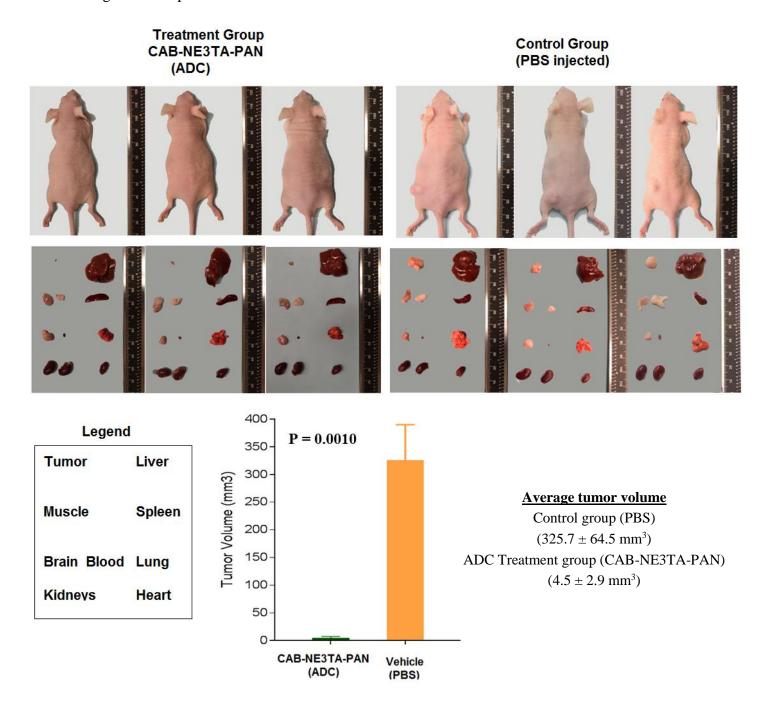


IR800CW



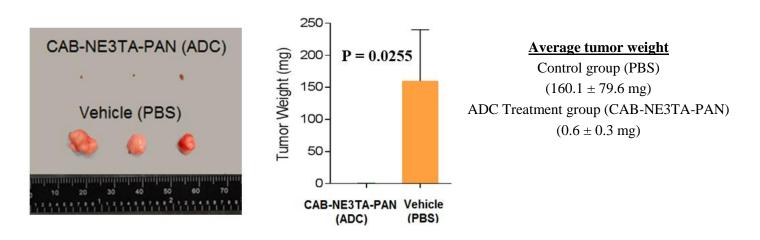
II. Images of the treated and untreated mice before dissection and tumors and normal organs removed from the mice.

The treated mice (N = 3) were dissected at 21 days post-treatment. The control PBS group (N = 3) were dissected at 11, 16, and 20 days post-treatment). The tumors were measured with the digital caliper, and the volumes of tumors were calculated based on the formula (V = $0.5 \times a \times b^2$) and expressed as mean \pm standard deviation mm³ (SD). The data of tumor volume were analyzed by two-sided Student's t test. Difference was considered significant if p values are less than 0.05.



III. Images of tumors removed from the mice and dehydrated and measurement of tumor weight

The treated mice (N = 3) were dissected at 21 days post-treatment. The control PBS group (N = 3) were dissected at 11, 16, and 20 days post-treatment. The tumors removed from the mice were frozen and dehydrated and dried under vacuum and weighed. The data of tumor weight were analyzed by two-sided Student's t test. Difference was considered significant if p values are less than 0.05.



IV. *In vivo* NIR fluorescence images of A431-bearing male nude mice intraperitoneally (IP) injected with the theranostic conjugate (CAB-NE3TA-PAN-IR800, N=3).

Mouse 1 Dorsal 0.09 0.08 0.07 0.06 Pre-Inj Post-Inj day 1 day 2 day3 day 4 day 5 day 7 day 10 Ventral 0.1 0.09 0.08 0.07 0.06 Pre-Inj Post-Inj day 1 day 2 day3 day 4 day 10 day 7 day 5

Mouse 2



