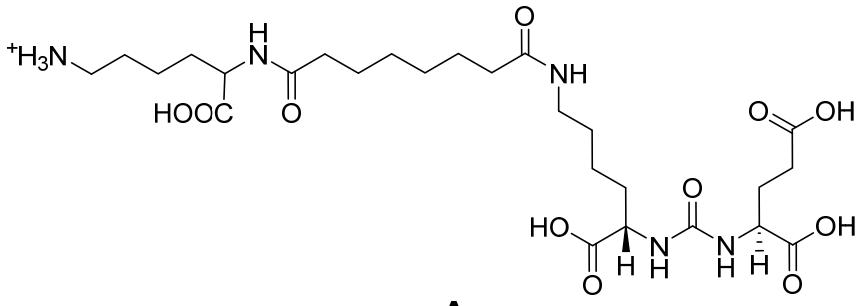
SUPPLEMENTAL MATERIALS AND METHODS

Synthesis of compound **YC-36:**



A

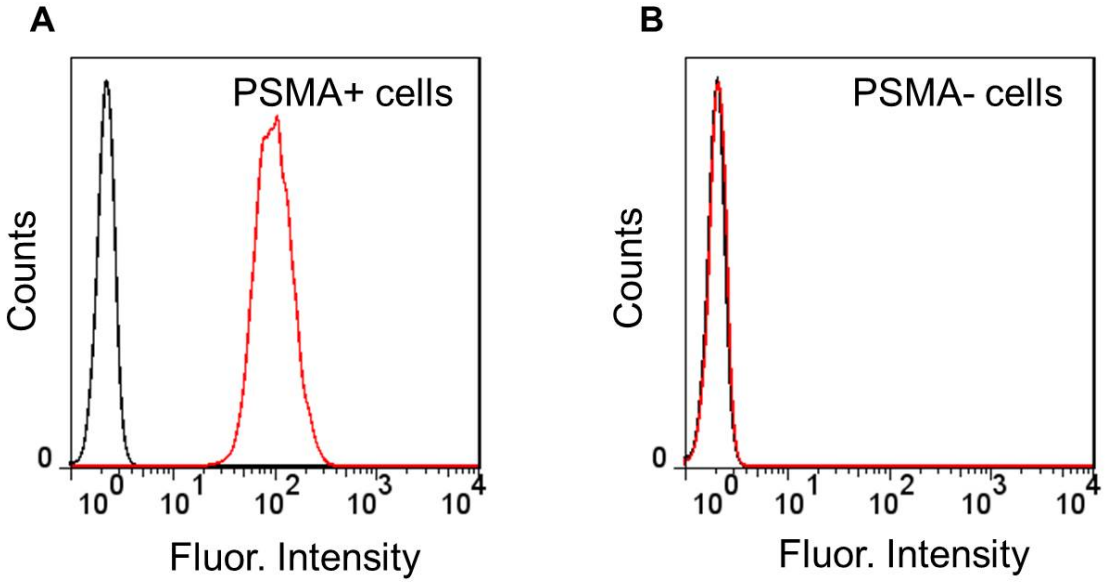
To a solution of compound **A**[1] (1.5 mg, 2.10 μmol) in dimethylformamide (1 mL) was added triethylamine (0.005 mL, 35.9 μmol), followed by fluorescein isothiocyanate isomer 1 (1 mg, 2.57 μmol). After 2 hour at room temperature, the reaction mixture was purified by high performance liquid chromatography (column, Econosphere C18 5μ, 150 × 4.6 mm; retention time, 15 min; mobile phase, $H_2O/CH_3CN/TFA$ = 75/25/0.1; flow rate, 1 mL/min) to afford 1.5 mg (72%) of compound **YC-36**. ESI-Mass calcd for $C_{47}H_{57}N_6O_{16}S$ $[M+H]^+$ 993.4, found 992.8.

Fluorescence-Activated Cell Sorting:

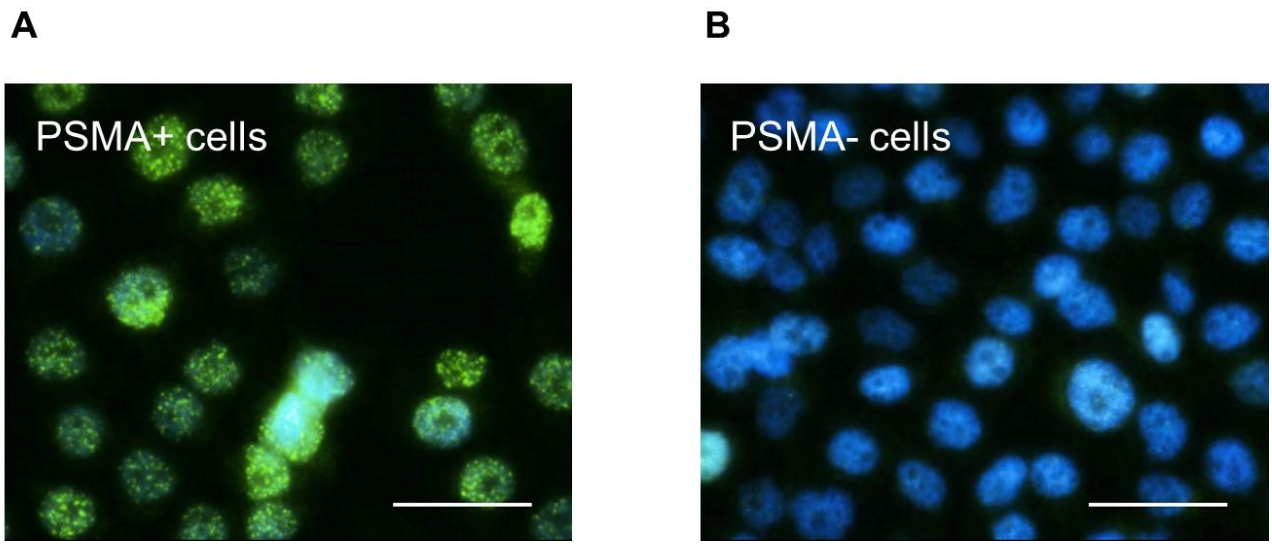
PC3 PIP and PC3 flu cells were prepared in RPMI supplemented with 1% FBS at 1 million cells per mL density. Cells were stained with 100nM YC-36 for 1 h at room temperature and washed twice with the same media. Cells were analyzed using the FACSCalibur (BD Biosciences) and FlowJo software (FLOWJO, LLC).

SPECT/CT Imaging (single photon emission computed tomography):

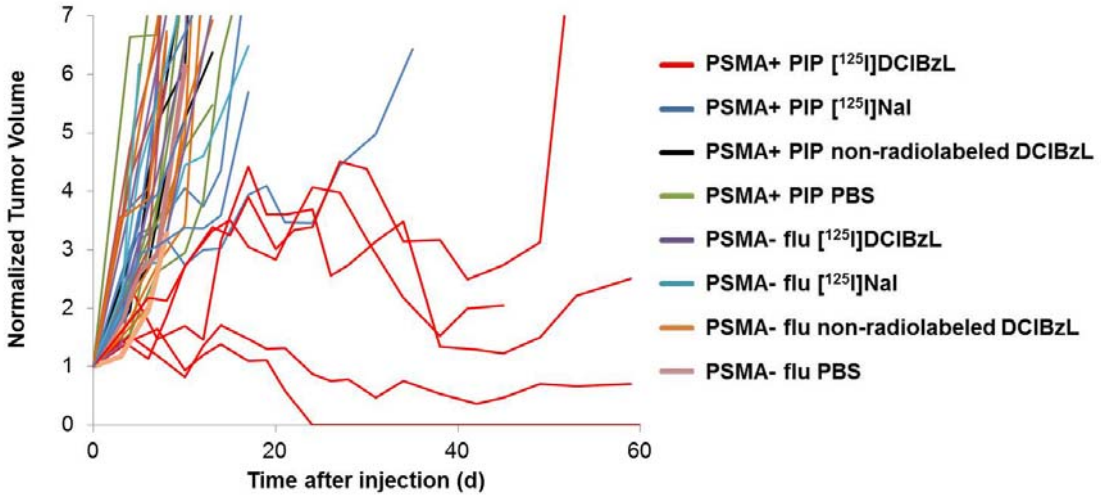
At 24 h post injection, the mice were anesthetized with isoflurane and maintained under 1% isoflurane in oxygen. The mice were positioned on the X-SPECT (Gamma Medica) gantry and scanned using two low energy, high-resolution pinhole collimators. All gamma images were reconstructed using LumaGEMsoftware (GammaMedica). Immediately following SPECT acquisition, the mice were then scanned by CT (X-SPECT) over a 4.6 cm field-of-view using a 600 μA, 50 kV beam. The SPECT and CT data were then coregistered using the supplier's software (Gamma Medica) and displayed as maximum intensity projection image.



Supplemental Figure 1. Fluorescence-activated cell sorting of live cells of PSMA+ PC3 PIP (A) and PSMA- PC3 flu (B) after staining with 100nM of YC-36. Black line indicates non-stained cells, and red line indicates cells stained with YC-36.



Supplemental Figure 2. Images of γH2AX staining (green) in PSMA+ PC3 PIP (A) and PSMA- PC3 flu (B) cells after treatment for 18 hours with 10 μCi/ml ^{125}I-DCIBzL. Hoechst dye (blue) stains all DNA. Scale bars indicate 50 μm. Quantification of γH2AX foci per cell is shown in Figure 3B.



Supplemental Figure 3. Tumor growth delay in nude mice bearing PSMA+ PC3 PIP or PSMA- PC3 flu flank xenografts after treatment with 3 mCi (111 MBq) ^{125}I-DCIBzL or equal amount of control compounds (n = 5 mice per group; p = 0.002 by log rank test). This plot shows the normalized tumor size of individual animals, and the corresponding Kaplan-Meier plot is shown in Figure 5A. Please note that one animal treated with ^{125}I-DCIBzL died at 45 days after treatment due to unrelated infection with no prior weight loss or evidence of metastatic spread.

REFERENCES

1. Chen, Y.; Dhara, S.; Banerjee, S. R.; Byun, Y.; Pullambhatla, M.; Mease, R. C.; Pomper, M. G., A low molecular weight PSMA-based fluorescent imaging agent for cancer. *Biochem Biophys Res Commun* **2009,** *390* (3), 624-9.