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PSMA-targeted dendrimer as an efficient anticancer drug delivery vehicle for prostate cancer

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## **Supplementary Figures: -**

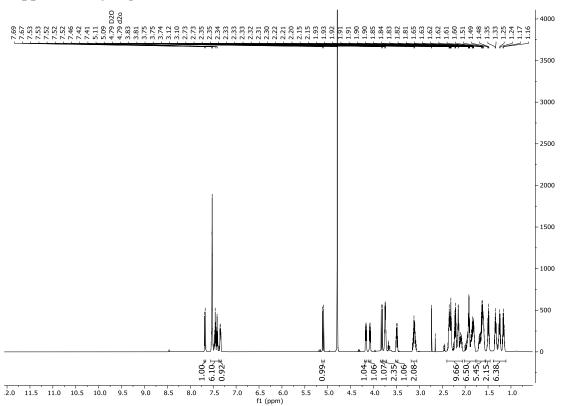


Figure S1. <sup>1</sup>H NMR of compound 3 in D<sub>2</sub>O (600 MHz).

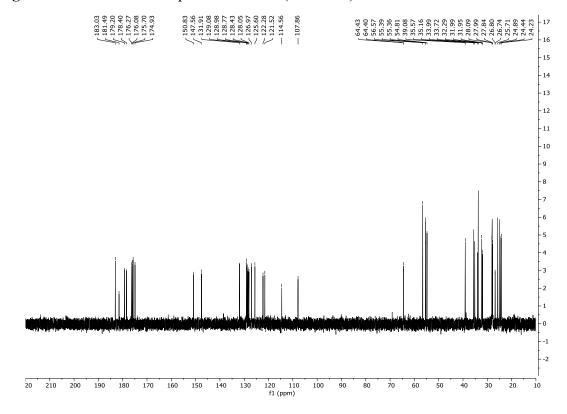


Figure S2. <sup>13</sup>C NMR of compound 3 in D<sub>2</sub>O (101 MHz).

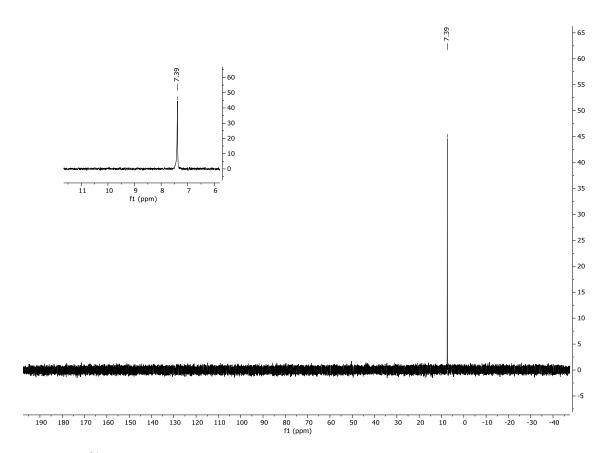


Figure S3. <sup>31</sup>P NMR of compound 3 in D<sub>2</sub>O (162 MHz).

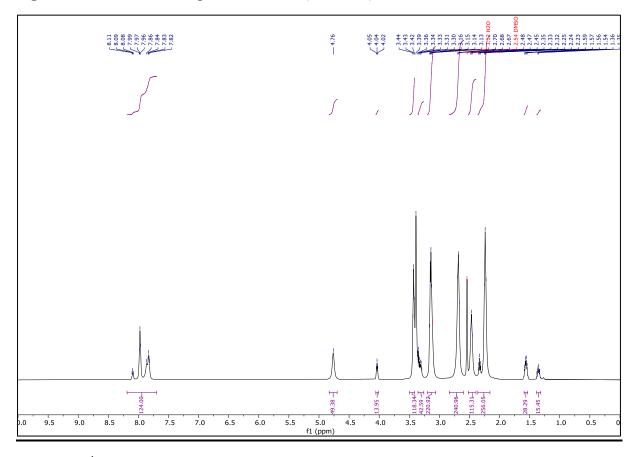


Figure S4. <sup>1</sup>H NMR of compound 5 in DMSO-d<sub>6</sub> (500 MHz).

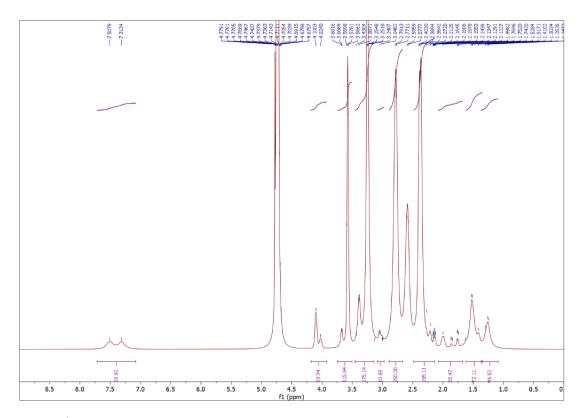


Figure S5. <sup>1</sup>H NMR of compound 6 in D<sub>2</sub>O (500 MHz).

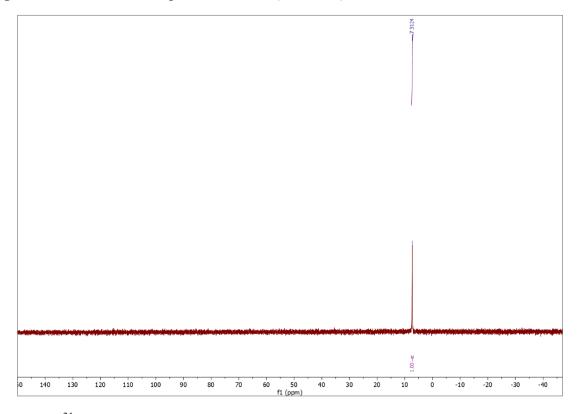


Figure S6.  $^{31}P$  NMR of compound 6 in  $D_2O$  (202 MHz).

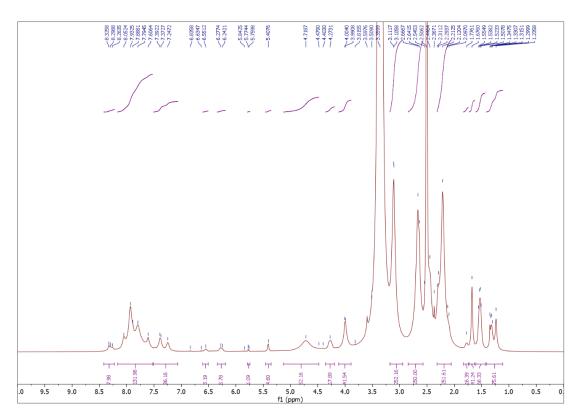
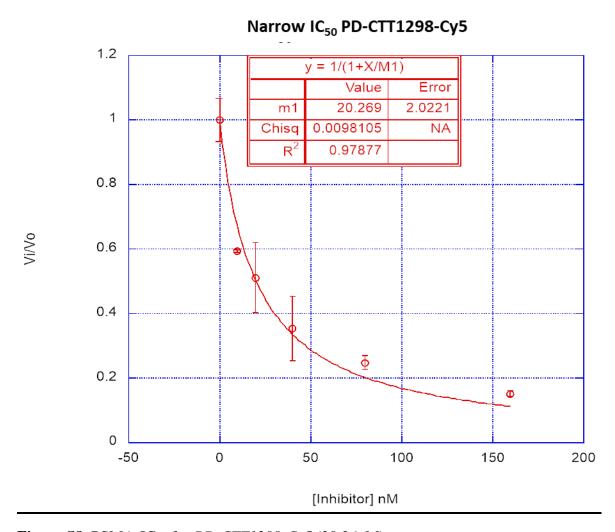
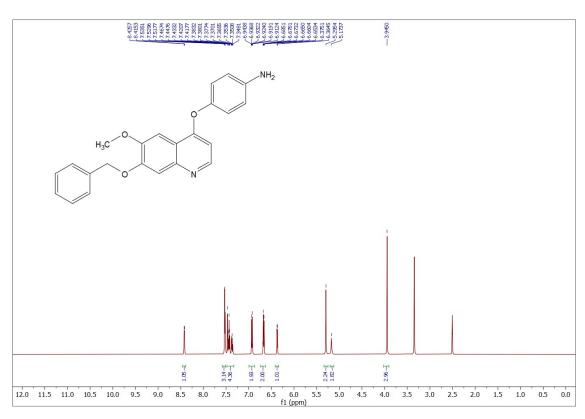


Figure S7.  $^{1}$ H NMR of compound 7 in DMSO-d<sub>6</sub> (500 MHz).

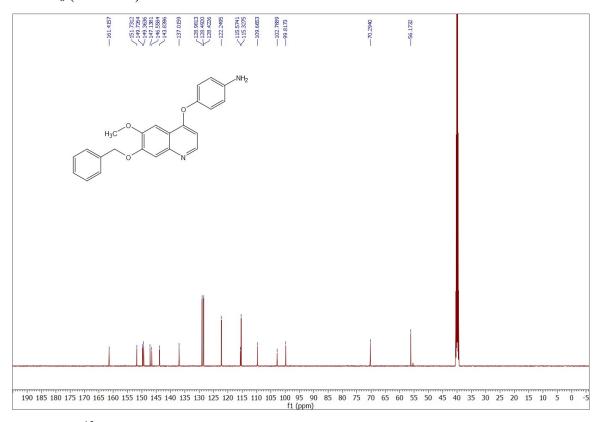




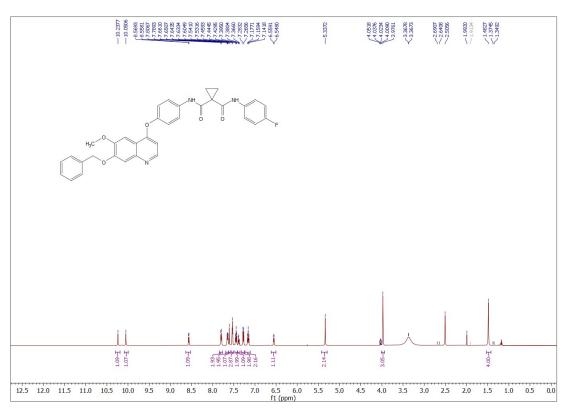
**Figure S8.** PSMA-IC<sub>50</sub> for *PD-CTT1298-Cy5* (20.26nM).



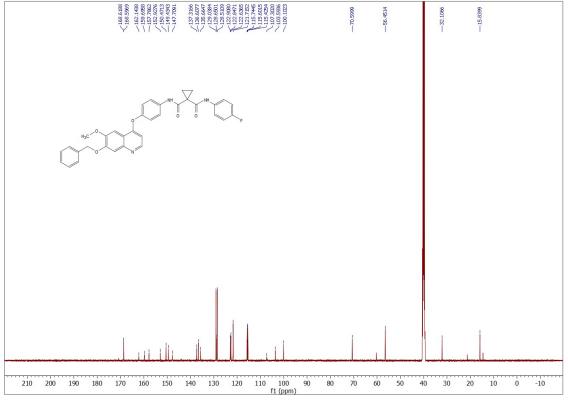
**Figure S9.** <sup>1</sup>H NMR spectra of 4-((7-(benzyloxy)-6-methoxyquinolin-4-yl)oxy)aniline (**10**) in DMSO-d<sub>6</sub> (500 MHz).



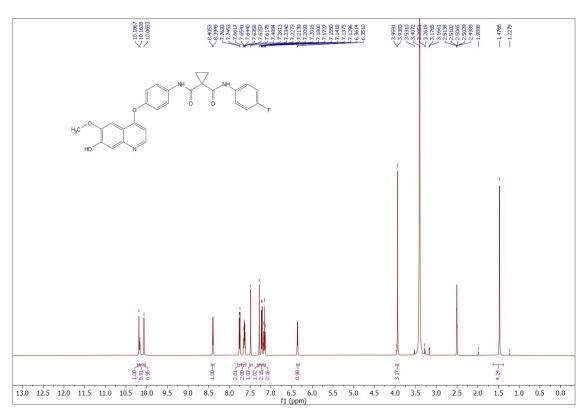
**Figure S10.** <sup>13</sup>C NMR spectra of 4-((7-(benzyloxy)-6-methoxyquinolin-4-yl)oxy)aniline (**10**) in DMSO-d<sub>6</sub> (125 MHz).



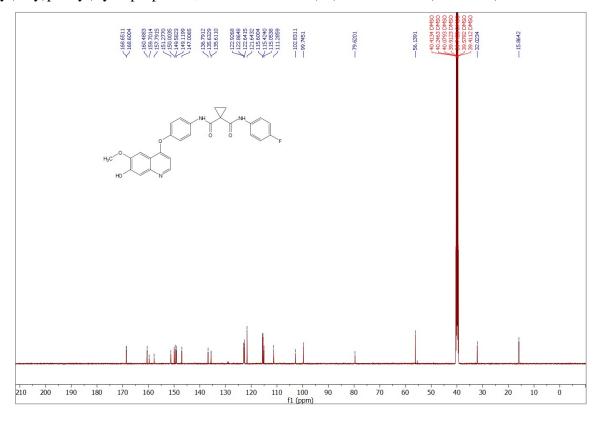
**Figure S11.** <sup>1</sup>H NMR spectra of N-(4-((7-(benzyloxy)-6-methoxyquinolin-4-yl)oxy)phenyl)-N-(4-fluorophenyl)cyclopropane-1,1-dicarboxamide (**12**) in DMSO-d<sub>6</sub> (500 MHz).



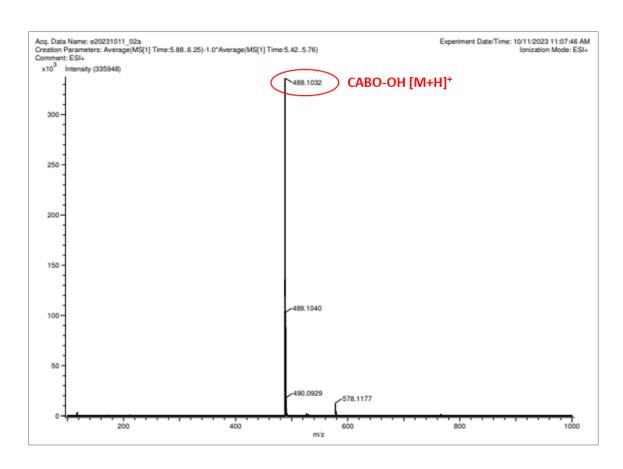
**Figure S12.** <sup>13</sup>C NMR spectra of N-(4-((7-(benzyloxy)-6-methoxyquinolin-4-yl)oxy)phenyl)-N-(4-fluorophenyl)cyclopropane-1,1-dicarboxamide (**12**) in DMSO-d<sub>6</sub> (125 MHz).



**Figure S13.** <sup>1</sup>H NMR spectra of *N*-(4-fluorophenyl)-*N*-(4-((7-hydroxy-6-methoxyquinolin-4-yl)oxy)phenyl)cyclopropane-1,1-dicarboxamide (**13**) in DMSO-d<sub>6</sub> (500 MHz).



**Figure S14.** <sup>13</sup>C NMR spectra of *N*-(4-fluorophenyl)-*N*-(4-((7-hydroxy-6-methoxyquinolin-4-yl)oxy)phenyl)cyclopropane-1,1-dicarboxamide (**13**) in DMSO-d<sub>6</sub> (125 MHz).



**Figure S15.** Mass spectra of N-(4-fluorophenyl)-N-(4-((7-hydroxy-6-methoxyquinolin-4-yl)oxy)phenyl)cyclopropane-1,1-dicarboxamide (13).

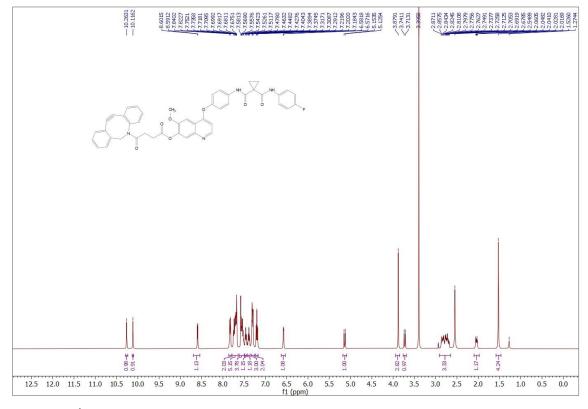


Figure S16. <sup>1</sup>H NMR spectra of *Cabo-DBCO* (15) in DMSO-d<sub>6</sub> (500 MHz).

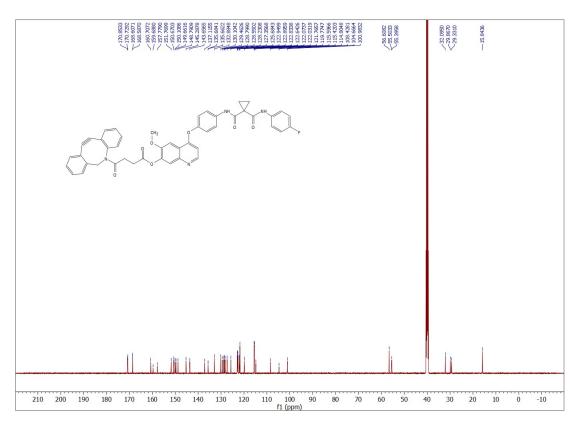


Figure S17. <sup>13</sup>C NMR spectra of *Cabo-DBCO* (15) in DMSO-d<sub>6</sub> (125 MHz).

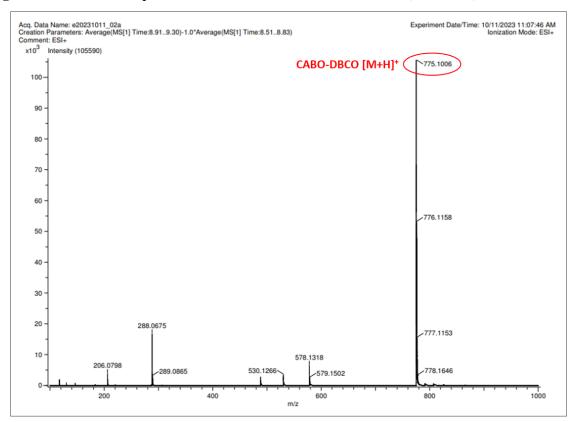


Figure S18. Mass spectra of Cabo-DBCO (15).

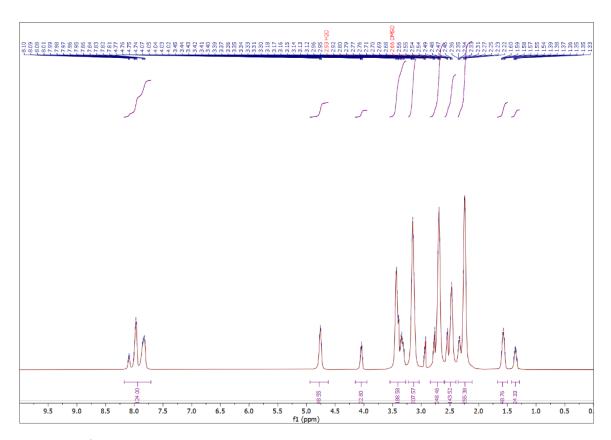


Figure S19. <sup>1</sup>H NMR of compound 16 in DMSO-d<sub>6</sub> (500 MHz).

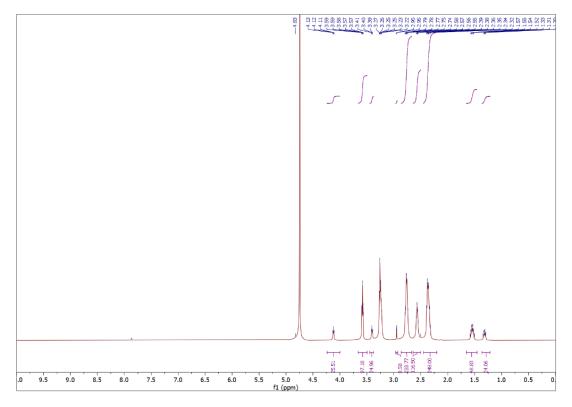


Figure S20.  $^{1}$ H NMR of compound 16 in  $D_{2}O$  (500 MHz).

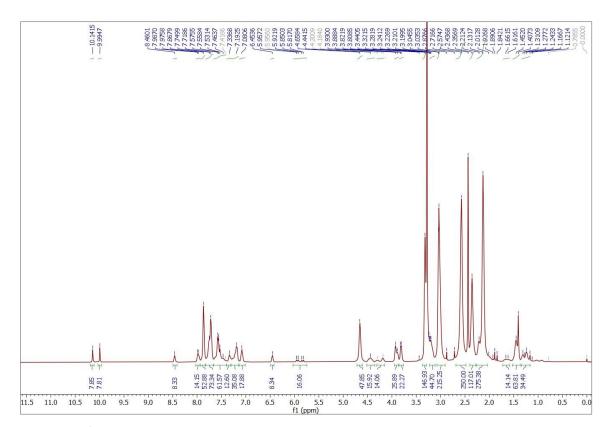
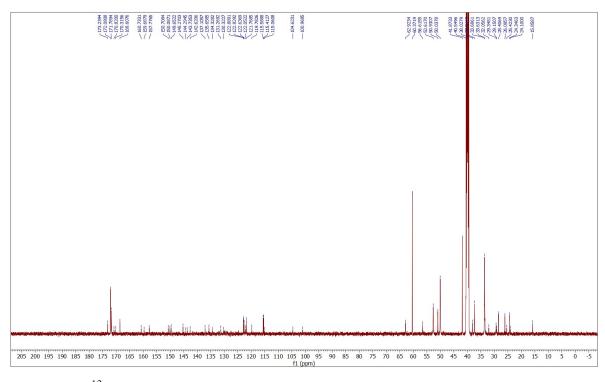
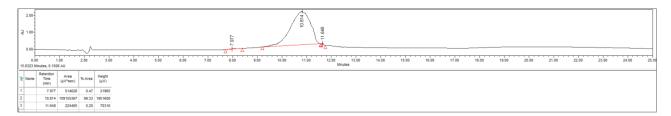


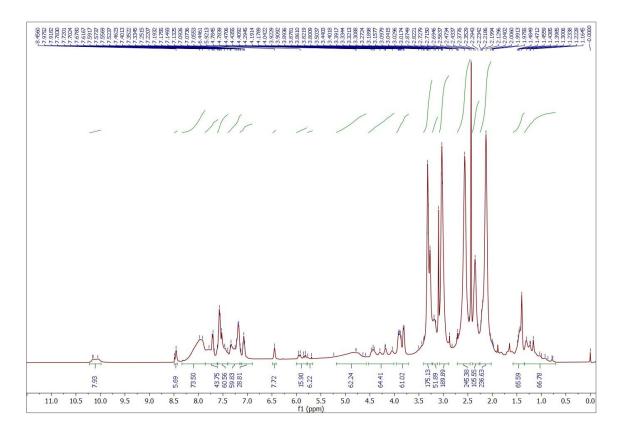
Figure S21. <sup>1</sup>H NMR spectra of *PD-Cabo* (17) in DMSO-d<sub>6</sub> (500 MHz).



**Figure S22.** <sup>13</sup>C NMR spectra of *PD-Cabo* (**17**) in DMSO-d<sub>6</sub> (125 MHz).



**Figure S23.** HPLC chromatogram *PD-Cabo* (17) (Purity >99%).



**Figure S24.** <sup>1</sup>H NMR spectra of *PD-CTT1298-Cabo* (**18**) in DMSO-d<sub>6</sub> (500 MHz).

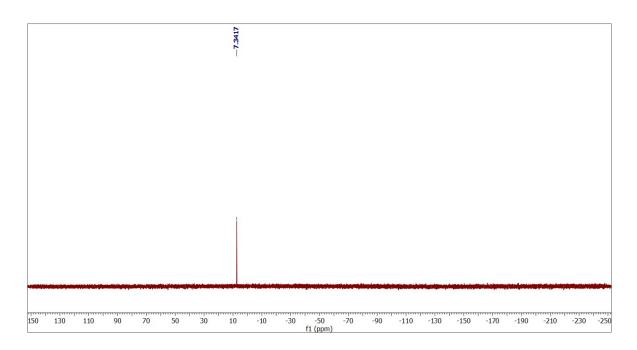


Figure S25.  $^{31}$ P NMR spectra of *PD-CTT1298-Cabo* (18) in D<sub>2</sub>O (202 MHz).

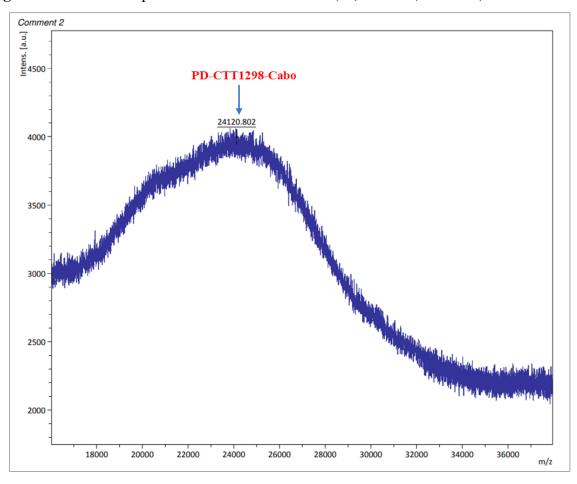
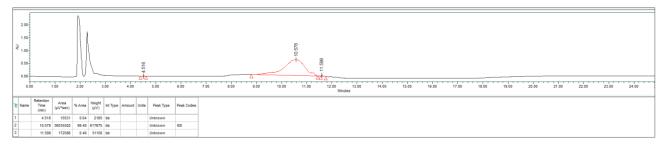
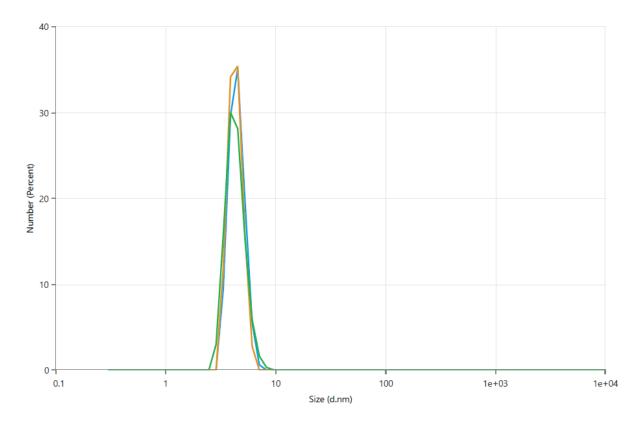


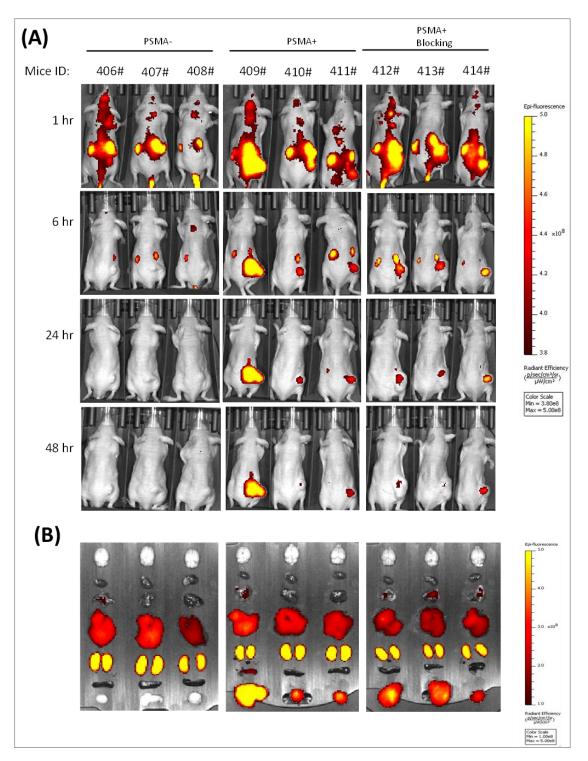
Figure S26. Mass spectra of PD-CTT1298-Cabo (18).



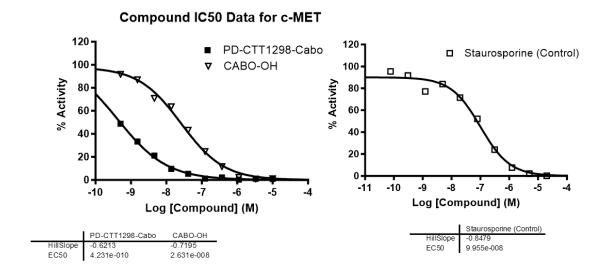
**Figure S27.** HPLC chromatogram *PD-CTT1298-Cabo* (**18**) (Purity >99%).



**Figure S28.** Hydrodyanamic radius of *PD-CTT1298-Cabo* analyzed by dynamic light scattering (4.40±0.07 nm)



**Figure S29.** (A) Fluorescent images of representative mice bearing PSMA- or PSMA+ PC-3 tumors from individual groups at 1 hr, 6 hr, 24 hr and 48 hr upon intravenously injection with Cy5.5-D-1298 in. (B) *Ex vivo* fluorescence imaging of tumors and vital organs dissected from representative mice of individual groups at 48 hr. The tissues from top to bottom are as follows: brain, heart, lungs, liver, kidneys, spleen, and tumor.



**Figure S30.** c-Met IC<sub>50</sub> for Cabo-OH and *PD-CTT1298-Cabo*.