Supplemental Material

Dynamic PET and Optical Imaging and Compartment Modeling using a Dual-labeled Cyclic RGD Peptide Probe

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MATERIAL AND METHODS

Stability test

1 mL of RPMI1640 supplemented with 25% (v/v) of mouse serum was allocated into a 1.5 Eppendorf tube and temperature-equilibrated at 37˚C for 15 min before adding of c(RGDyK)-C(DOTA)-ZW-1. Thereafter, 100 µL of the reaction solution was removed immediately and added into 200 µL of 96% ethanol for precipitation of serum proteins. The cloudy reaction sample is cooled at 4˚C for 15 min and centrifuged at 14, 000 rmp for 2 min to pellet the precipitated serum proteins. The reaction supernatant is then analyzed by RP-HPLC on C18 column (5 µm, 120Å, 250 × 4.6 mm) using 5% to 65% acetonitrile containing 0.1% TFA versus distilled water containing 0.1% TFA over 30 minutes at a flow rate of 1 mL/min. Sample after 60 minutes incubation with serum was taken out for HPLC test under the same condition as above.

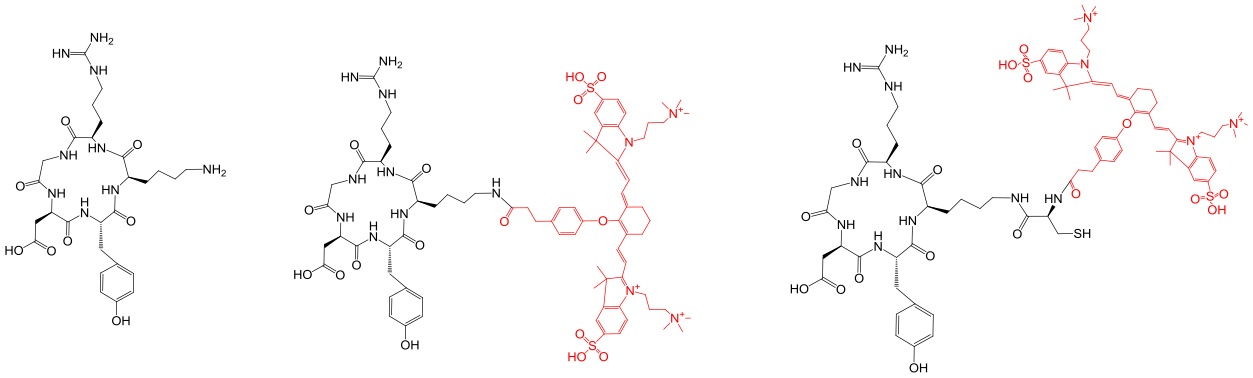


Figure S1. Chemical structures of compounds involved in the synthesis of c(RGDyK)-C (DOTA)-ZW-1.

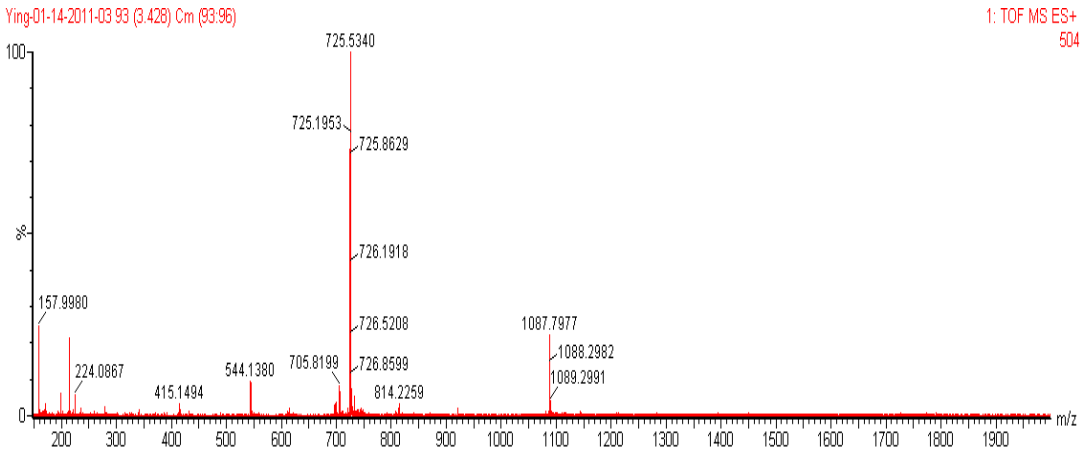
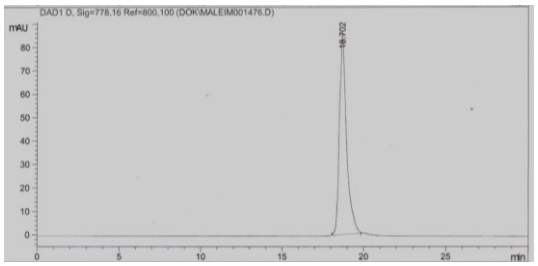
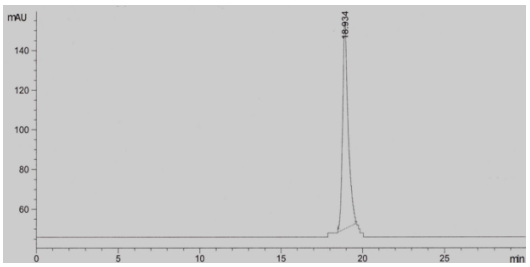


Figure S2. Mass spectrum of c(RGDyK)-C(DOTA)-ZW-1. m/z calculated/found: 724.33/725.534 $[M + H]^{3+}$) .

A.



B.



C.

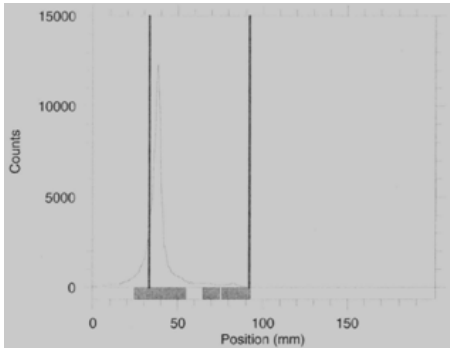


Figure S3. HPLC analyze of ^{64}Cu labeled c(RGDyK)-C(DOTA)-ZW-1. A. Radiologic signal from ^{64}Cu labeled c(RGDyK)-C(DOTA)-ZW-1. B. Fluorescent signal from ^{64}Cu labeled c(RGDyK)-C(DOTA)-ZW-1. C. TLC analyze of Copper labeled c(RGDyK)-C(DOTA)-ZW-1.

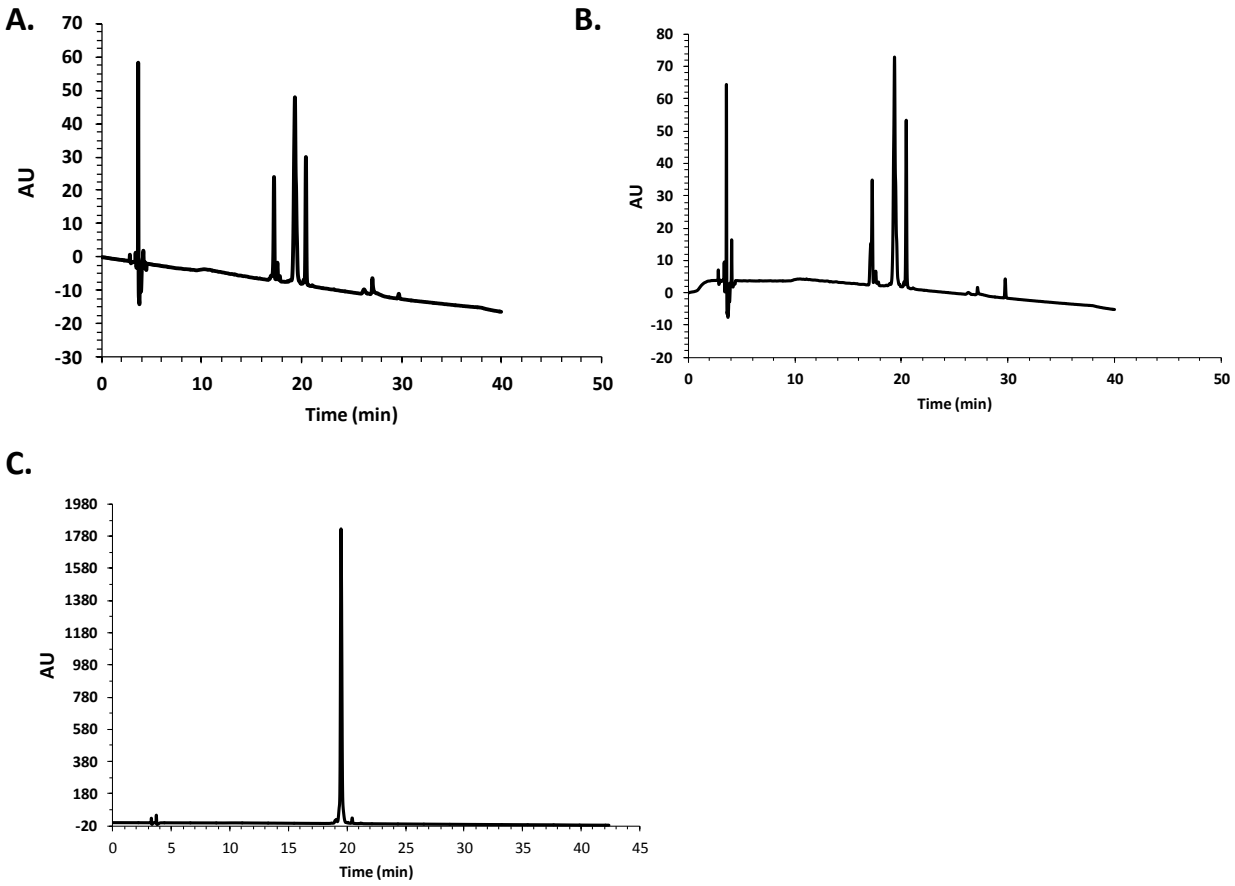


Figure S4. RP-HPLC analysis of c(RGDyK)-C(DOTA)-ZW-1 stability in mouse serum after 60 min of incubation. A. HPLC of c(RGDyK)-C(DOTA)-ZW-1 at starting time point. B. HPLC of c(RGDyK)-C(DOTA)-ZW-1 at 60 min after incubation with mouse serum. C. HPLC of c(RGDyK)-C(DOTA)-ZW-1 dissolved in H_2O. Retention time of c(RGDyK)-C(DOTA)-ZW-1 is 19.4 min.