Radioactive ¹⁹⁸Au-Doped Nanostructures with Different Shapes for *in vivo* Analyses of Their Biodistribution, Tumor Uptake, and Intratumoral Distribution

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Figure S1. UV-vis-NIR extinction spectra of the four different types of Au nanostructures: (a) nanospheres, (b) nanodisks, (c) nanorods, (d) cubic nanocages.



Figure S2. Biodistribution of the different types of ¹⁹⁸Au-incorporated Au nanostructures at (a) 1 h, (b) 6 h, and (c) 24 h post injection. The data was presented as %ID/organ.



Figure S3. A quantitative comparison of the intensities of Cerenkov luminescence integrated from the whole tumor regions after the injection of ¹⁹⁸Au-incorporated Au nanospheres, nanodisks, nanorods, and cubic nanocages.



Figure S4. Cerenkov luminescence images of the organs that were harvested 24 h post injection of the ¹⁹⁸Au-incorporated (a) nanospheres, (b) nanodisks, (c) nanorods, and (d) cubic nanocages. The luminescence images were merged with photographs taken using an ordinary camera.



Figure S5. Histology of the EMT6 tumor after staining with hematoxylin and eosin (H&E). The samples show blood vessels (BVs), individual red blood cells (RBCs) from the leaky vasculature, inflammatory cells (ICs), and necrotic regions.



Figure S6. PET/CT image of a mouse bearing a EMT6 tumor (marked by the elliptic circle) after the injection of ⁶⁴Cu-ATSM.



Figure S7. Plots of the hydrodynamic diameter of PEGylated nanostructures as a function of the incubation time. The PEGylated nanostructures were incubated with 10% Fetal Bovine Serum (FBS) in PBS at 37 °C for different periods of time. The hydrodynamic diameter was measured using dynamic light scattering.

Nanostructures	Size (nm)	Surface area (nm ²)	¹⁹⁸ Au radiolabeling specific activity (mCi/mg)
Nanosphere	diameter $= 56.8$	10130	1.6
Nanodisk	diameter = 92 thickness = 7	13577	0.18
Nanorod	length = 39.2 diameter = 9.1	1975	2.1
Nanocage	edge length = 49.6 wall thickness = 4.5	14760	0.34

Table S1. A summary of physical parameters for the Au nanostructures used in this study.