Supporting Information

Structure-Activity Relationships for Biodistribution, Pharmacokinetics and Excretion of Atomically Precise Nanoclusters in a Murine Model

O. Andrea Wong[1], Ryan J. Hansen[2], Thomas W. Ni[1], Christine Heinecke[1], W. Scott Compel[1], Daniel L. Gustafson[2] and Christopher J. Ackerson[1*]

1. Department of Chemistry, Colorado State University, Fort Collins, CO 80523

2. Department of Clinical Sciences, Colorado State University, Fort Collins, CO, 80523

Phone: 970-491-0521
Fax: 970-491-1801
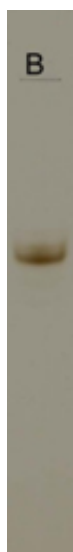Email: ackerson@mail.colostate.edu

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Fig. S1 Polyacrylamide gel electrophoresis of $Au_{102}(pMBA)_{44}$ that shows the purity of the compound.
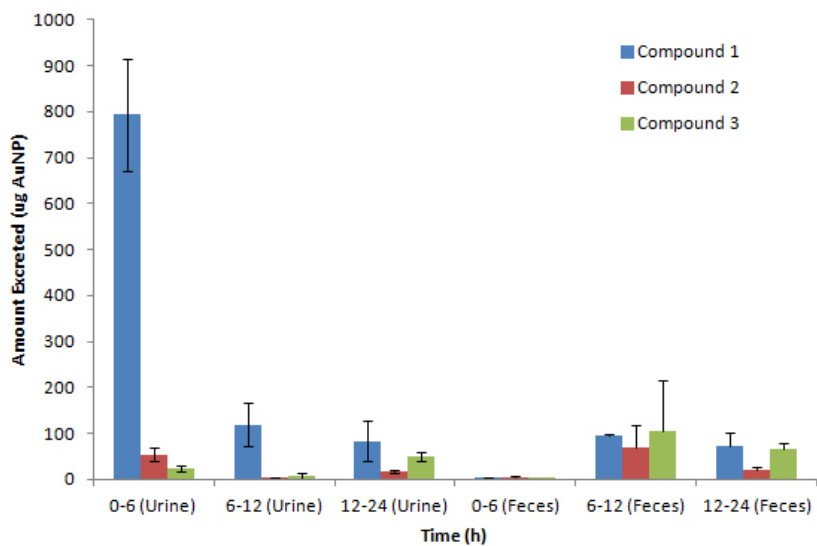

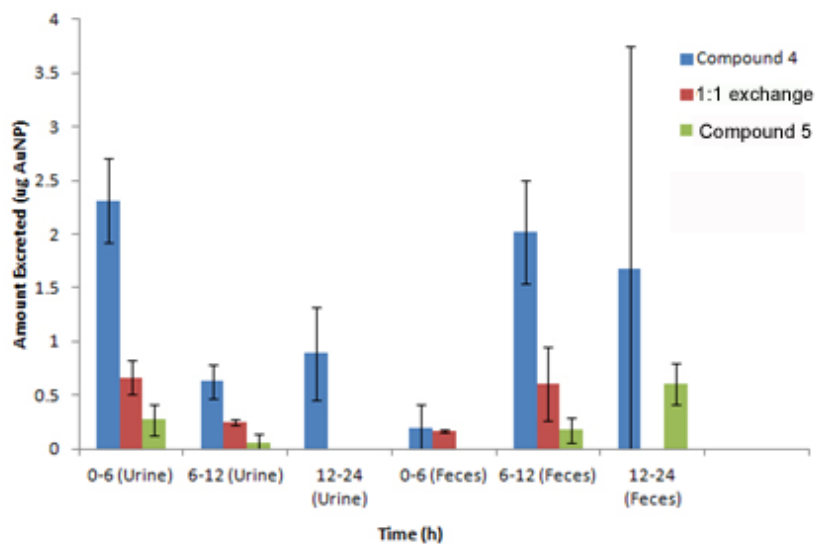**Fig. S2** Relative amounts of compounds **1**-**3** in urine and feces at 6, 12, and 24 hours post injection time.

Fig. S3 Relative amounts of compounds **4,5**, and the 1:1 exchange Au_{102}-based compound ($Au_{102}pMBA_{44}$ exchanged with $HS\text{-}(CH_2)_{11}\text{-}EG_4\text{-}OH$) in urine and feces at 6, 12, and 24 hours post injection time.

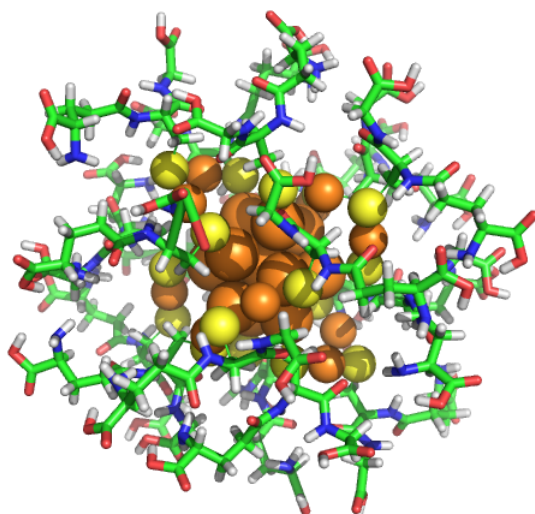**Fig. S4** $Au_{25}(GSH)_{18}$, Compound **1**

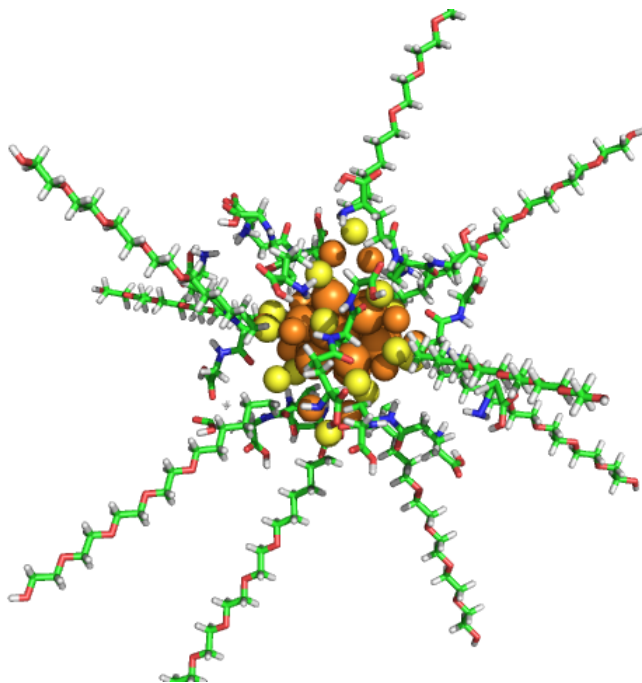**Fig. S5** $Au_{25}(GSH)_9(OEG)_9$, (OEG = HS-$(CH_2)_6$-EG-OH), Compound **2**
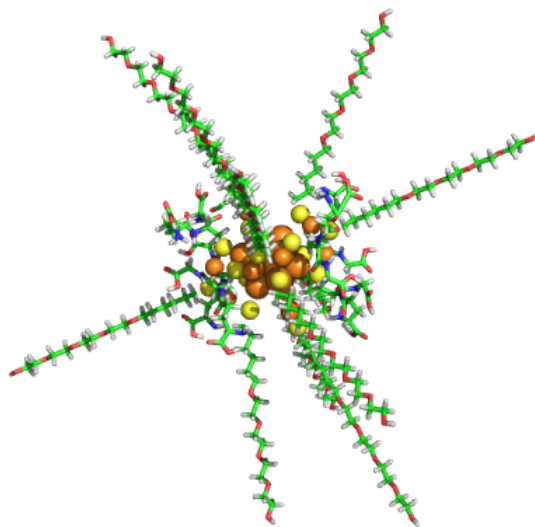
Fig. S6 $Au_{25}(GSH)_6(OEG)_{12}$, (OEG = HS-$(CH_2)_6$-EG-OH), Compound **3**
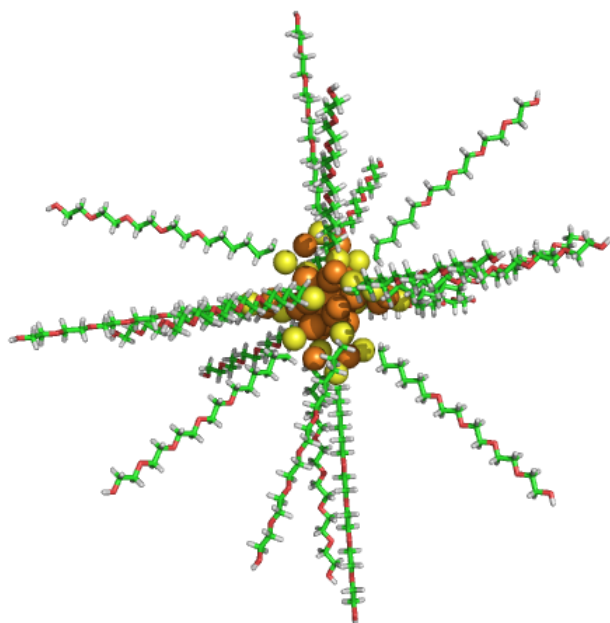
Fig. S7 $Au_{25}(OEG)_{18}$, (OEG = HS-$(CH_2)_6$-EG-OH)
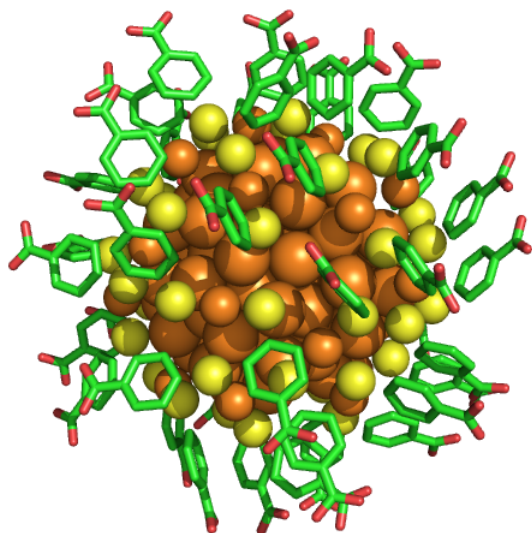
Fig. S8 $Au_{102}(pMBA)_{44}$, Compound **4**
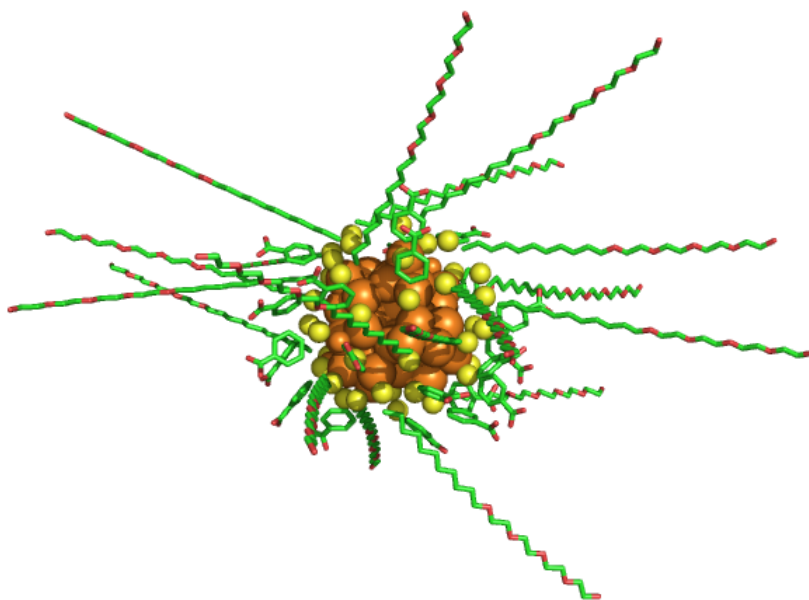
Fig. S9 $Au_{102}(pMBA)_{25}(OEG)_{19}$, (OEG = HS-$(CH_2)_{11}$-EG-OH), Compound **5**
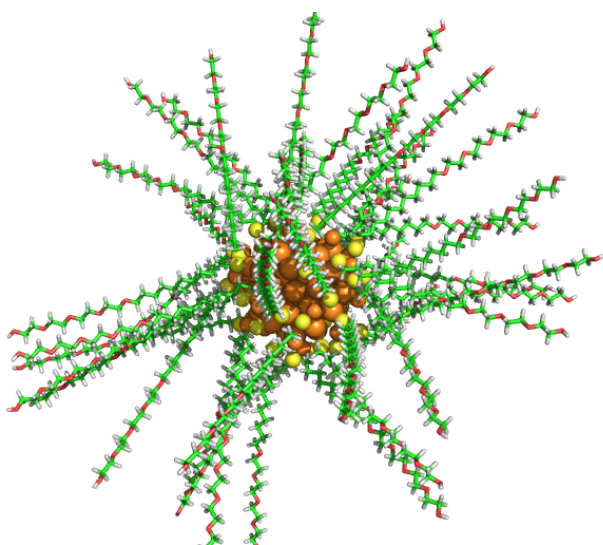
Fig. S10 $Au_{102}(OEG)_{44}$, (OEG = HS-$(CH_2)_{11}$-EG-OH)

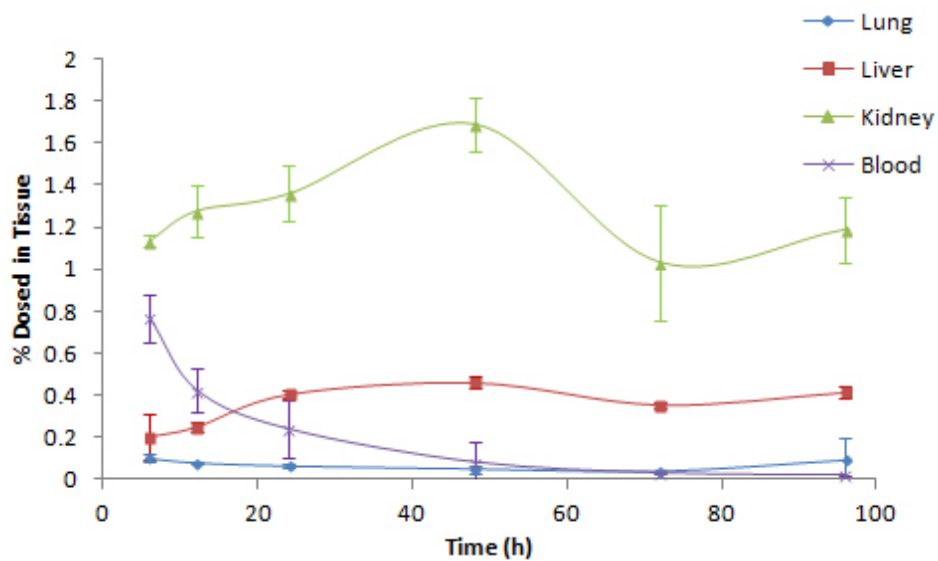**Fig. S11** Percent dosed in tissue for compound **1** at noted post-injection time points.

Fig. S12 Percent dosed in tissue for compound **2** at noted post-injection time points.

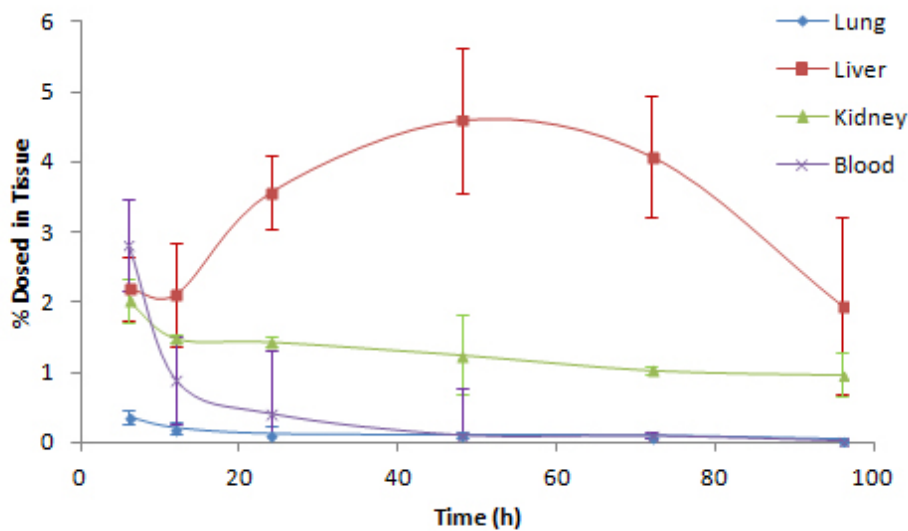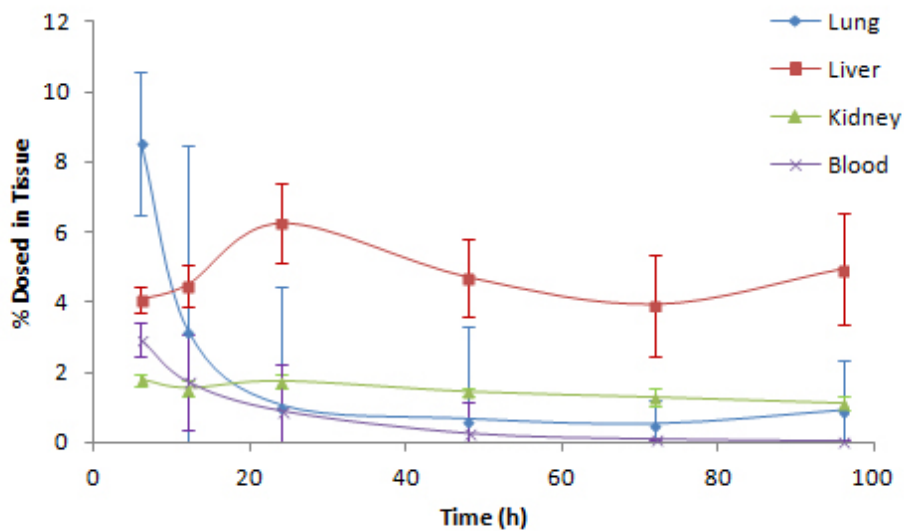**Fig. S13** Percent dosed in tissue for compound **3** at noted post-injection time points.
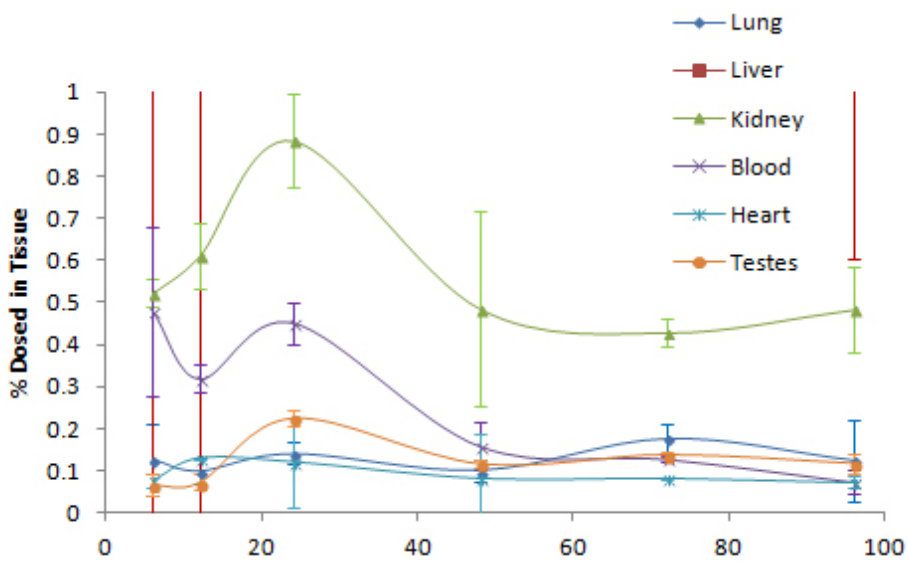

Fig. S14 Percent dosed in tissue for compound **4** at noted post-injection time points. Data points of liver are not included.
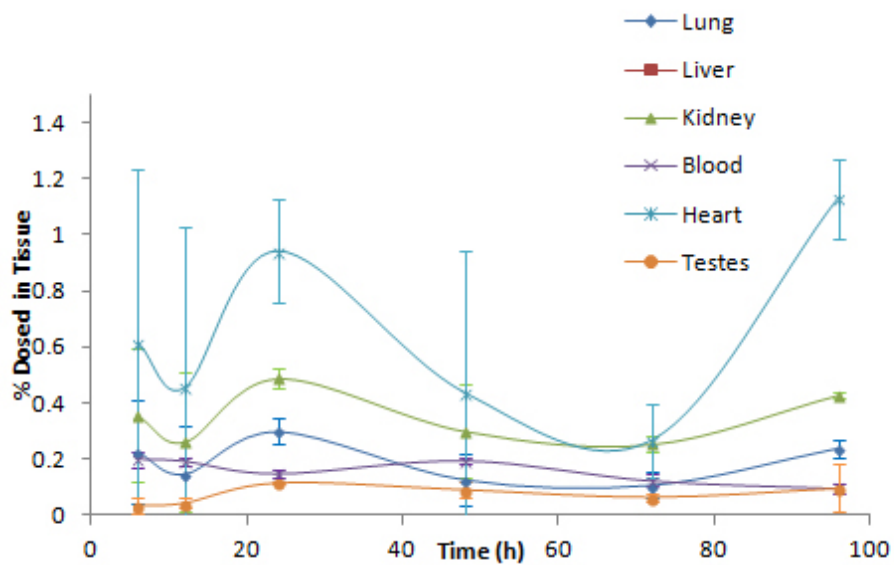
Fig. S15 Percent dosed in tissue for compound **5** at noted post-injection time points. Data points of liver are not included.
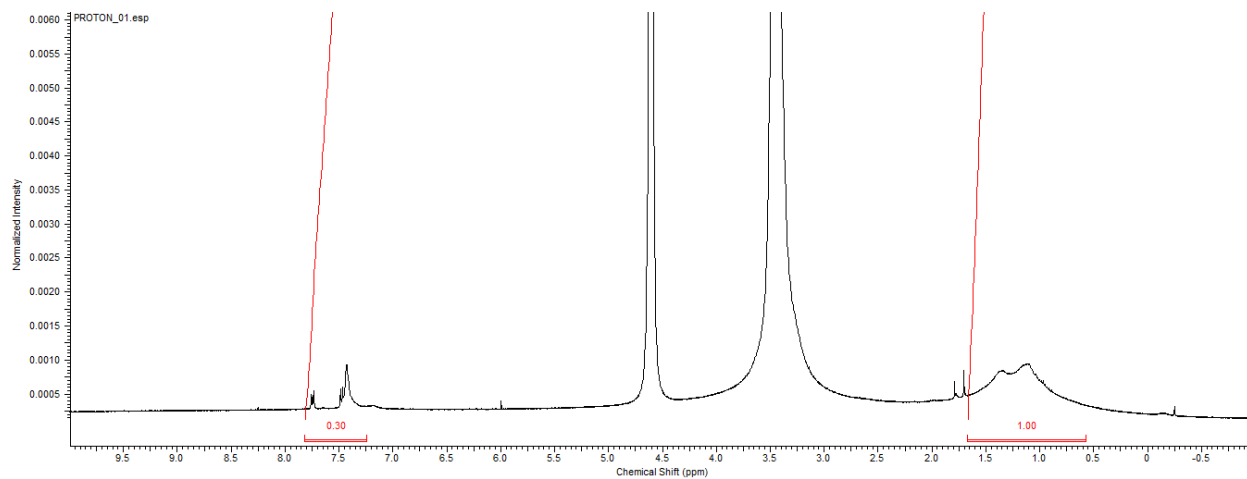

Fig. S16 ¹H NMR of compound **5**

Table S1 Information on Au_{102}-based 1:1 exchanged compound

Calculated Stokes Diameter (nm)[a]	Net Surface Charge (e⁻)	Surface Charge Density (Charge/Å²)	Hydrophobic Surface Area (%)	Expected Clearance Mechanism % Renal / % RES
5.92	22⁻	1.8×10^{-4} (-)	74%	40 / 60

Ligand exchange reaction of $Au_{102}(pMBA)_{44}$ with 23-mercapto-3,6,9,12-tetraoxatricosan-1-ol [HS-$(CH_2)_{11}$-EG_4-OH]

A 500 µM solution of $Au_{102}pMBA_{44}$ (6.6 µmol, 178 mg in 13.37 mL H_2O) and a 0.1 M solution of HS-$(CH_2)_{11}$-EG_4-OH (0.79 mmol, 304 mg in 7.90 mL THF) were prepared.   For the 1:1 incoming ligand:outgoing ligand reaction: 3 mL of $Au_{102}pMBA_{44}$ solution and 0.66 mL of HS-$(CH_2)_{11}$-EG_4-OH solution were mixed and diluted with H_2O to a final volume of 15 mL.   Then the reaction was shaken at rt for 1 h, then the crude product was purified by ultrafiltration spin columns (5000 Da cutoff) and was washed with 3 x 10 mL 1:1 H_2O:MeOH.   The remaining orange liquid was placed into a 15 mL conical and lyophilized until dry.

The Au_{102}-based 1:1 exchanged compound was dissolved in 5% DMSO, 5% Tween-80 in 90% D5W solution. The particle solutions were filtered through a 0.45 micron filter, and the dosage concentrations were determined after the filtration step. Approximate dosage concentration for this compound was 3.14 x 10^{-5} M.
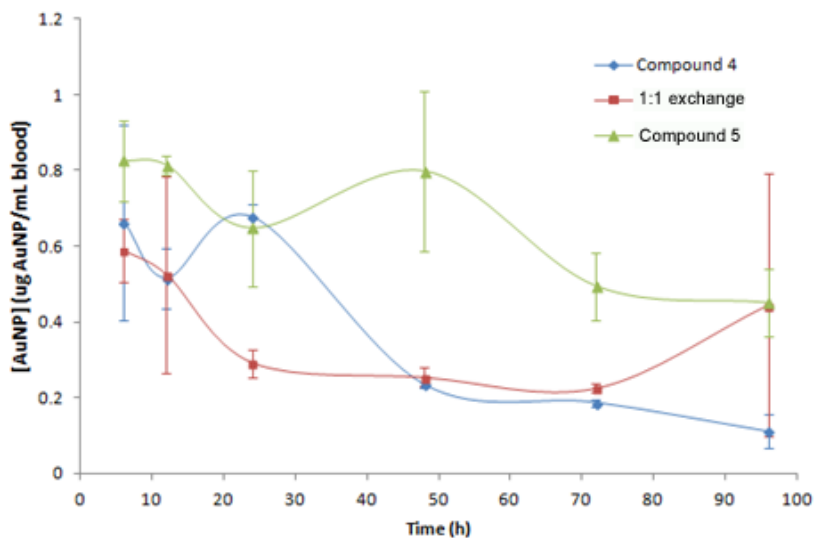

Fig. S17 Blood drug concentration vs. time curves of Au_{102}-based compounds