Supporting Information:

Design and Mechanistic Study of a Novel Gold Nanocluster-Based Drug Delivery System

Qinzhen Li,[a] Yiting Pan,[a] Tiankai Chen,[b] Yuanxin Du, [a] Honghua Ge,[c] Buchang Zhang,[c] Jianping Xie,[b] Haizhu Yu,*[a] and Manzhou Zhu*[a]

[a] Department of Chemistry and Centre for Atomic Engineering of Advanced Materials, Institute of Physical Science and Information Technology, Anhui Province Key Laboratory of Chemistry for Inorganic/Organic Hybrid Functionalized Materials, Anhui University, Hefei, Anhui, 230601, China.

[b] Department of Chemical and Biomolecular Engineering, National University of Singapore, 4 Engineering Drive 4, Singapore 117585, Singapore.

[c] Institute of Physical Science and Information Technology, Anhui University, Heifei, Anhui, 230601, China

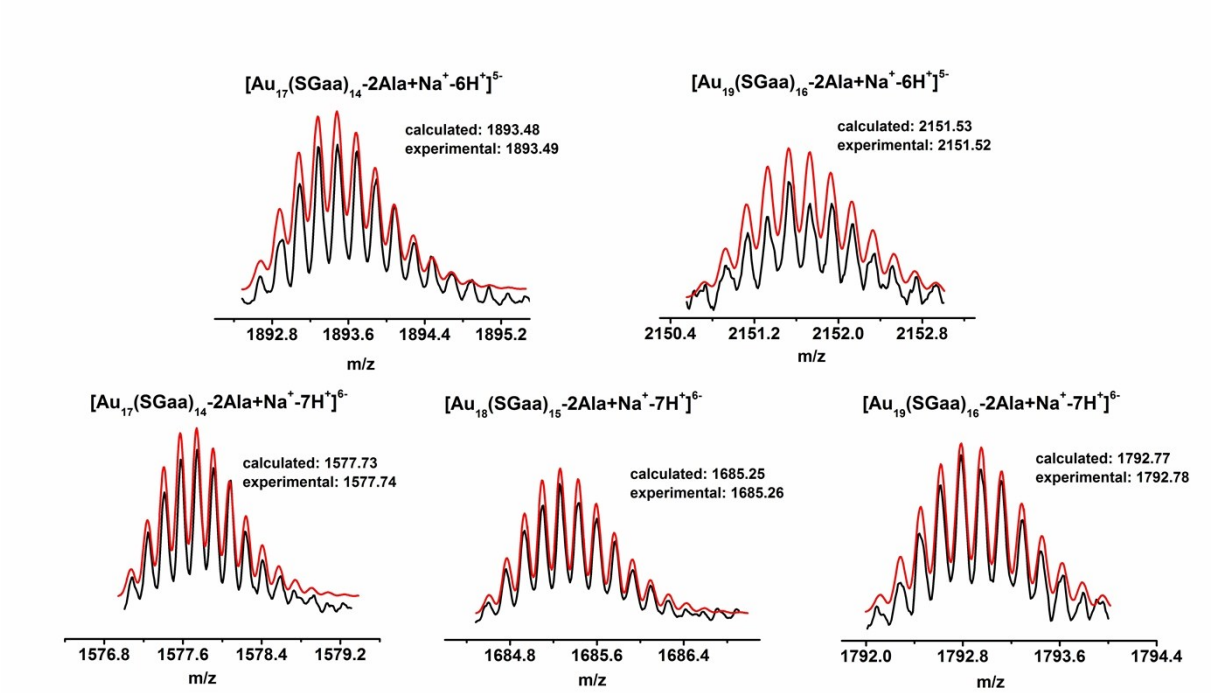

Fig. S1. Experimental (black line) and simulated (red line) isotope patterns of the other five peaks below m/z 2400.

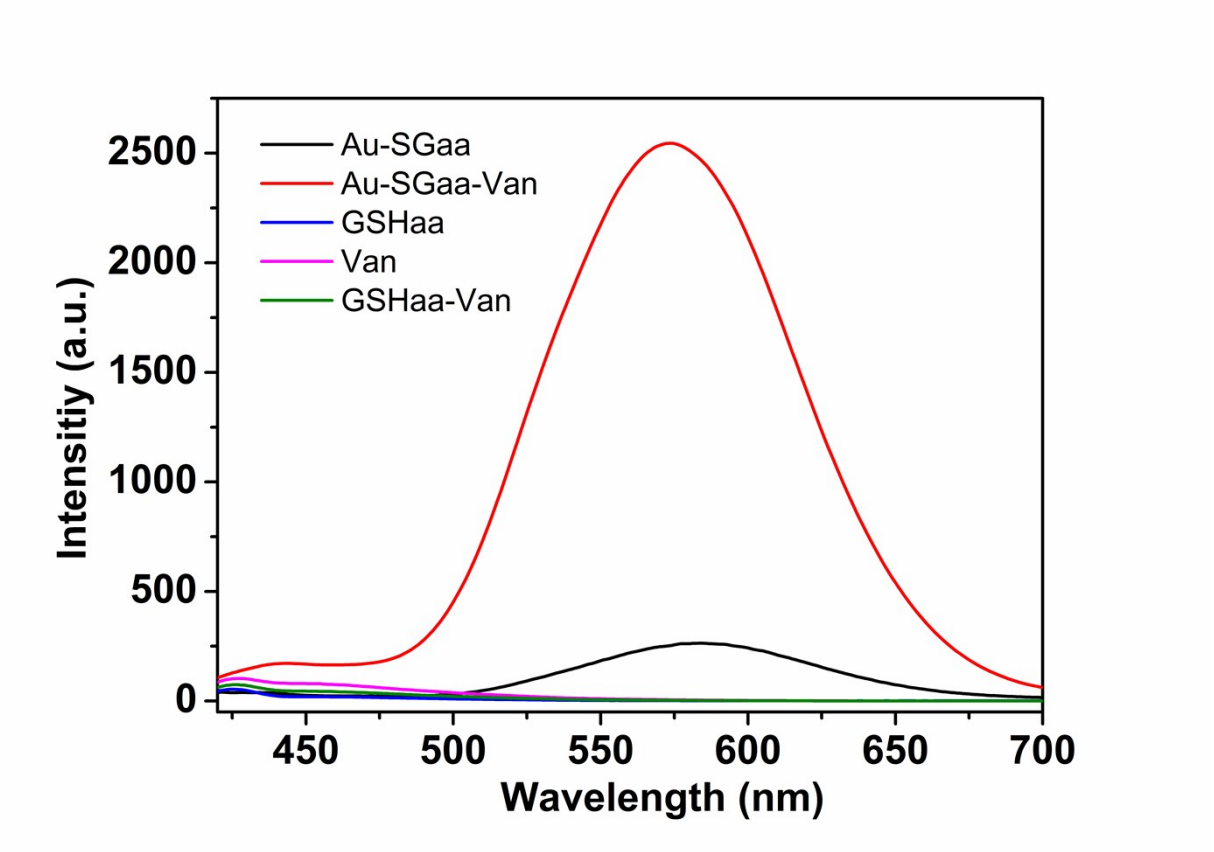

Fig. S2. Fluorescence spectra of Au-SGaa, Au-SGaa-Van, GSHaa, Van, mixture of GSHaa and Van (λ_{ex}= 380 nm).

Table S1. Fluorescent lifetime of Au-SGaa and Au-SGaa-Van

	τ_1	τ_2	τ_3	$\tau_{average}$
Au-SGaa	32 ns (0.09)	234 ns (0.23)	1854 ns (0.68)	1317 ns
Au-SGaa-Van	44 ns (0.05)	277 ns (0.20)	2417 ns (0.75)	1870 ns

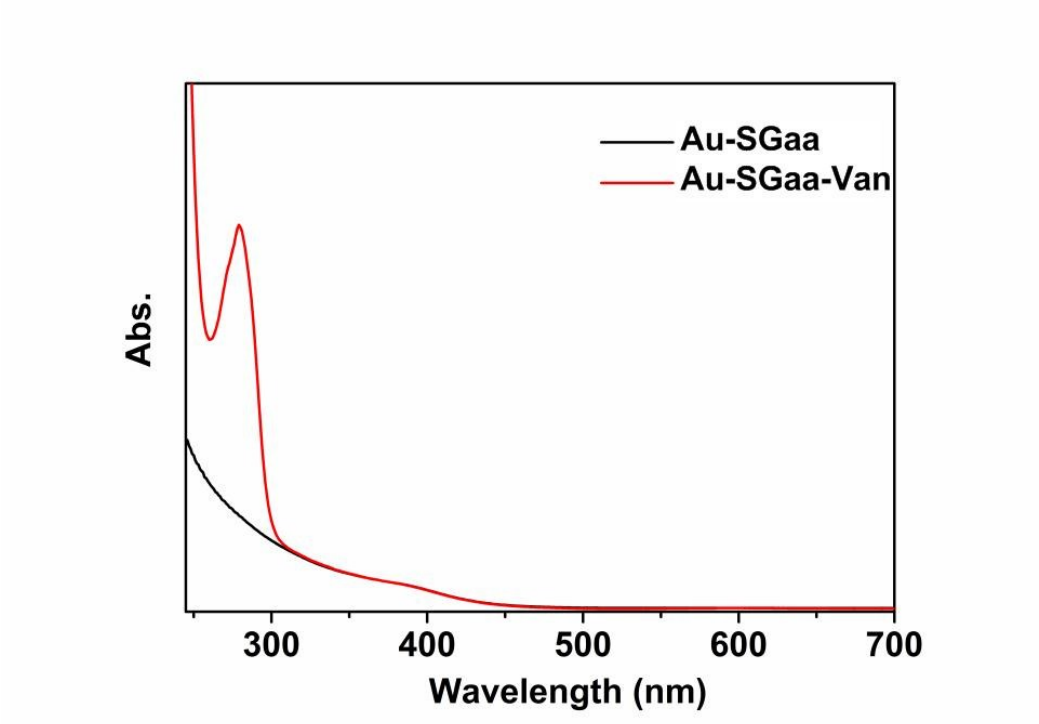

Fig. S3. UV-vis spectra of Au-SGaa and Au-SGaa-Van

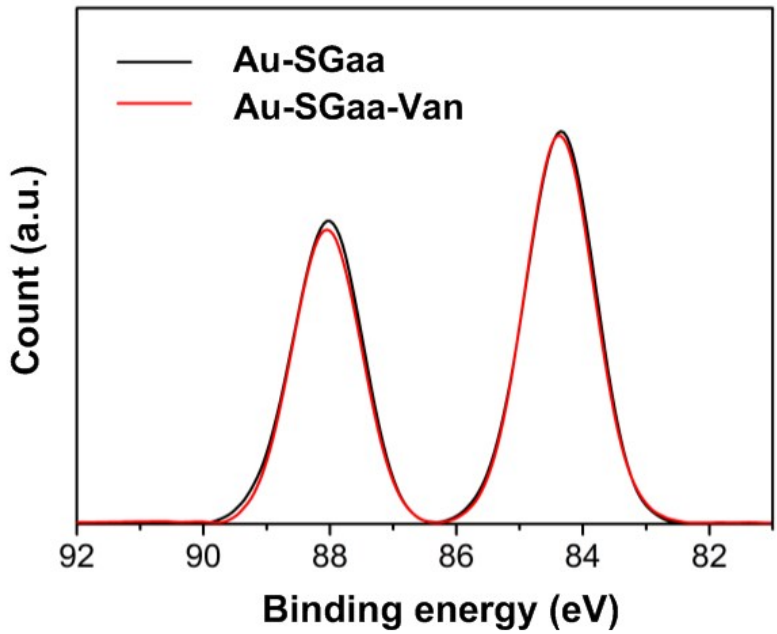

Fig. S4. XPS survey spectrum of the Au-SGaa and Au-SGaa-Van. The slight shift of the binding energy (~0.05 eV) of Au-SGaa-Van compared to Au-SGaa was in the range of the systematic error of the equipment.

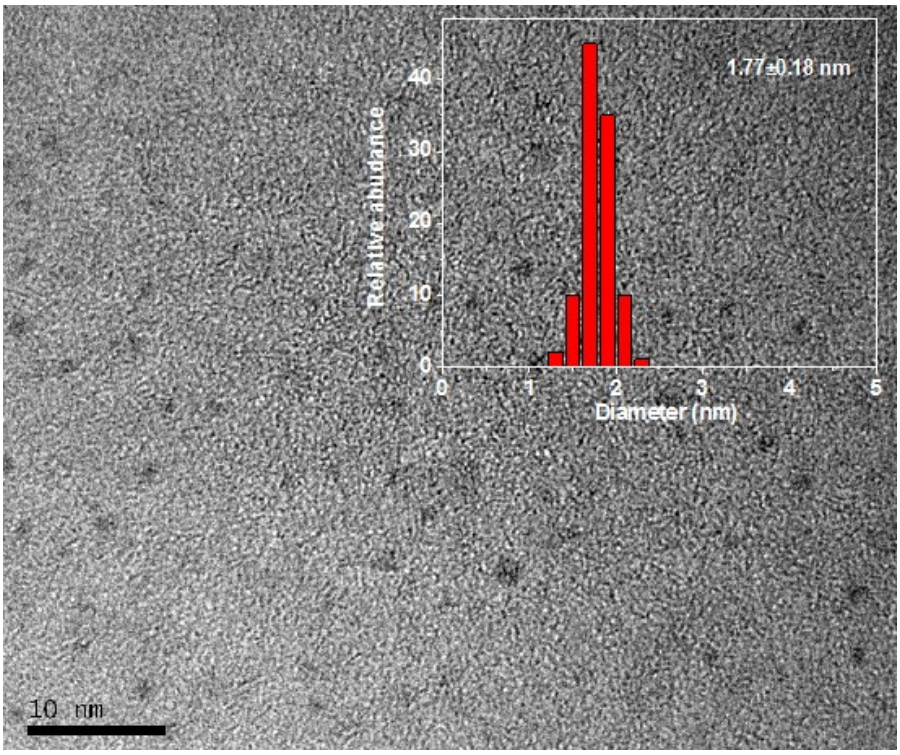

Fig. S5. TEM image of Au-SGaa-Van. Inset shows the histograms of core sizes.

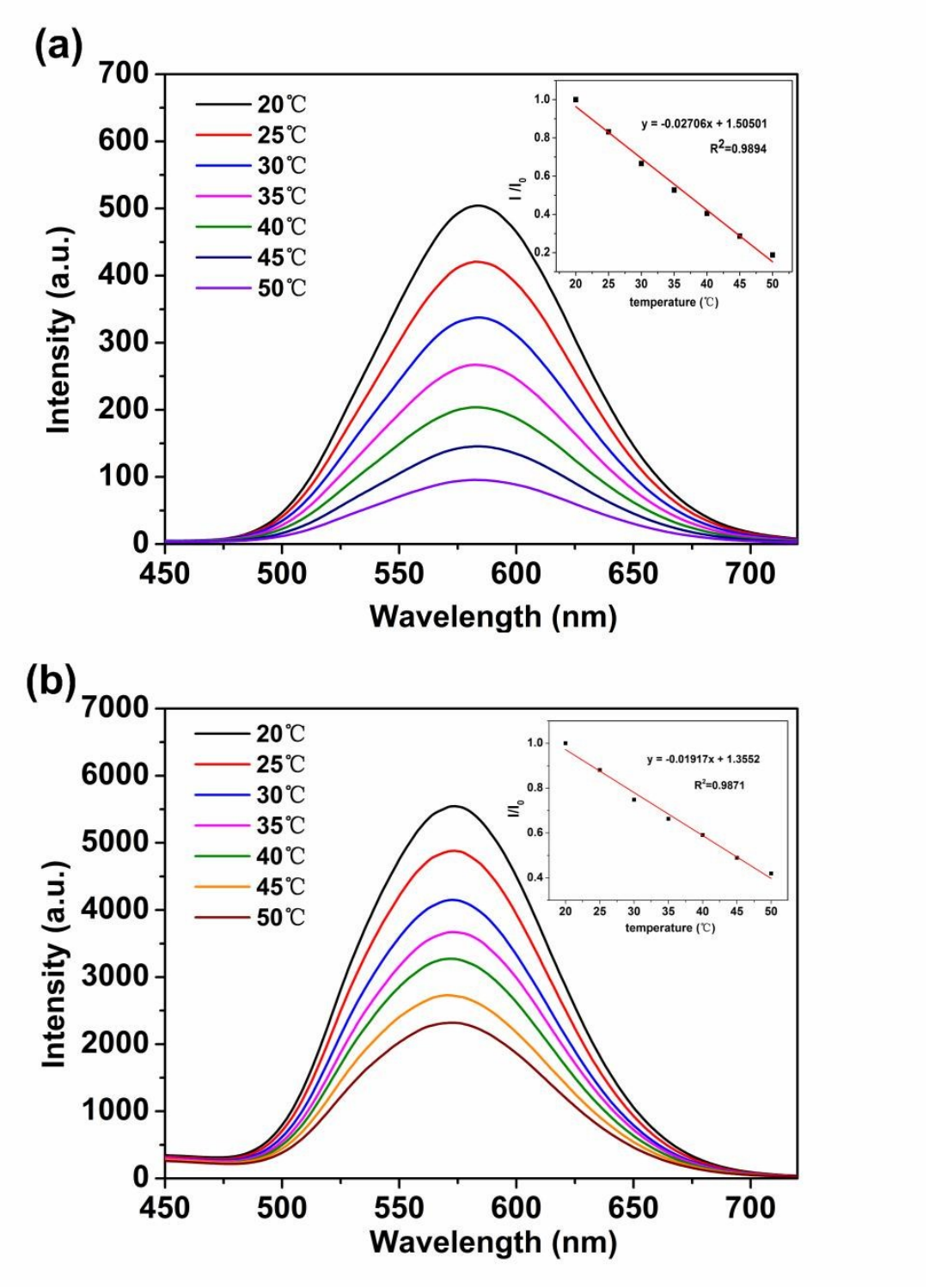

Fig. S6. Fluorescence spectra of Au-SGaa (a) and Au-SGaa-Van (b) at different temperature (from 20 to 50 °C). Insets show the corresponding fluorescence intensity at λ_{max} (580 nm for Au-SGaa and 570 nm for Au-SGaa-Van) vs temperature in range of 20-50 °C.

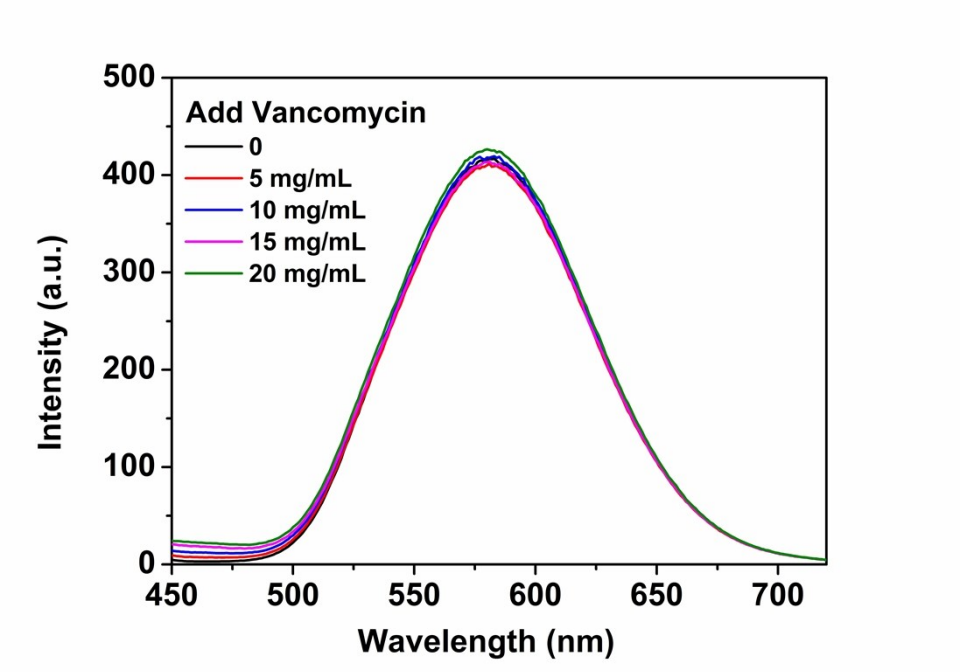

Fig. S7. Fluorescence spectra of GSH-protected Au NCs with the addition of 0, 5, 10, 15, 20 mg/mL Van. (λ_{ex}= 380 nm)

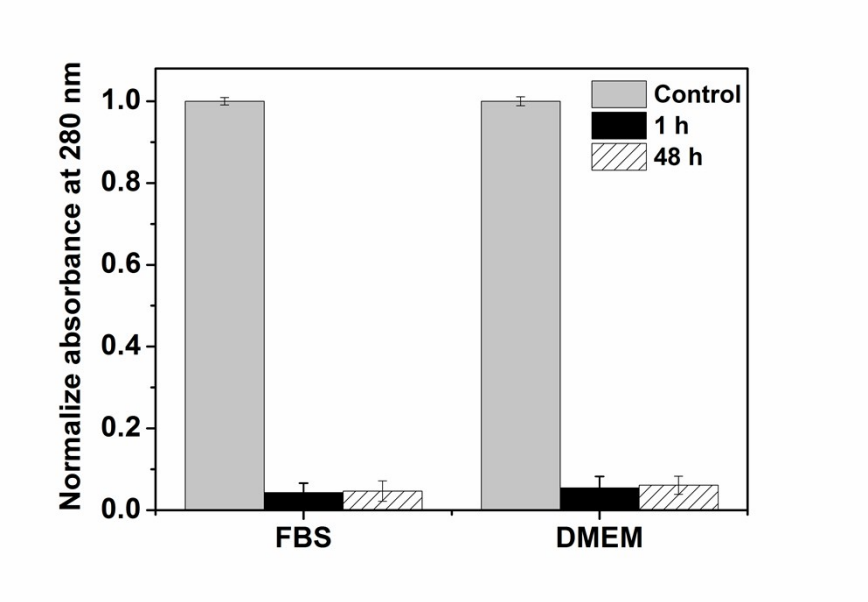

Fig. S8. Comparison of the amount of free Van (10 mg mL^{-1}) in the 10% FBS and DMEM with or without Au-SGaa. The control groups are Van in 10% FBS and DMEM for 48 h. The other groups are Au-SGaa-Van in 10% FBS and DMEM for 1 h and 48 h. The sample were centrifuged in an ultrafilter with a molecular weight cut-off (MWCO) of 3 kDa and the absorbances of filtered solution at 280 nm were recorded.

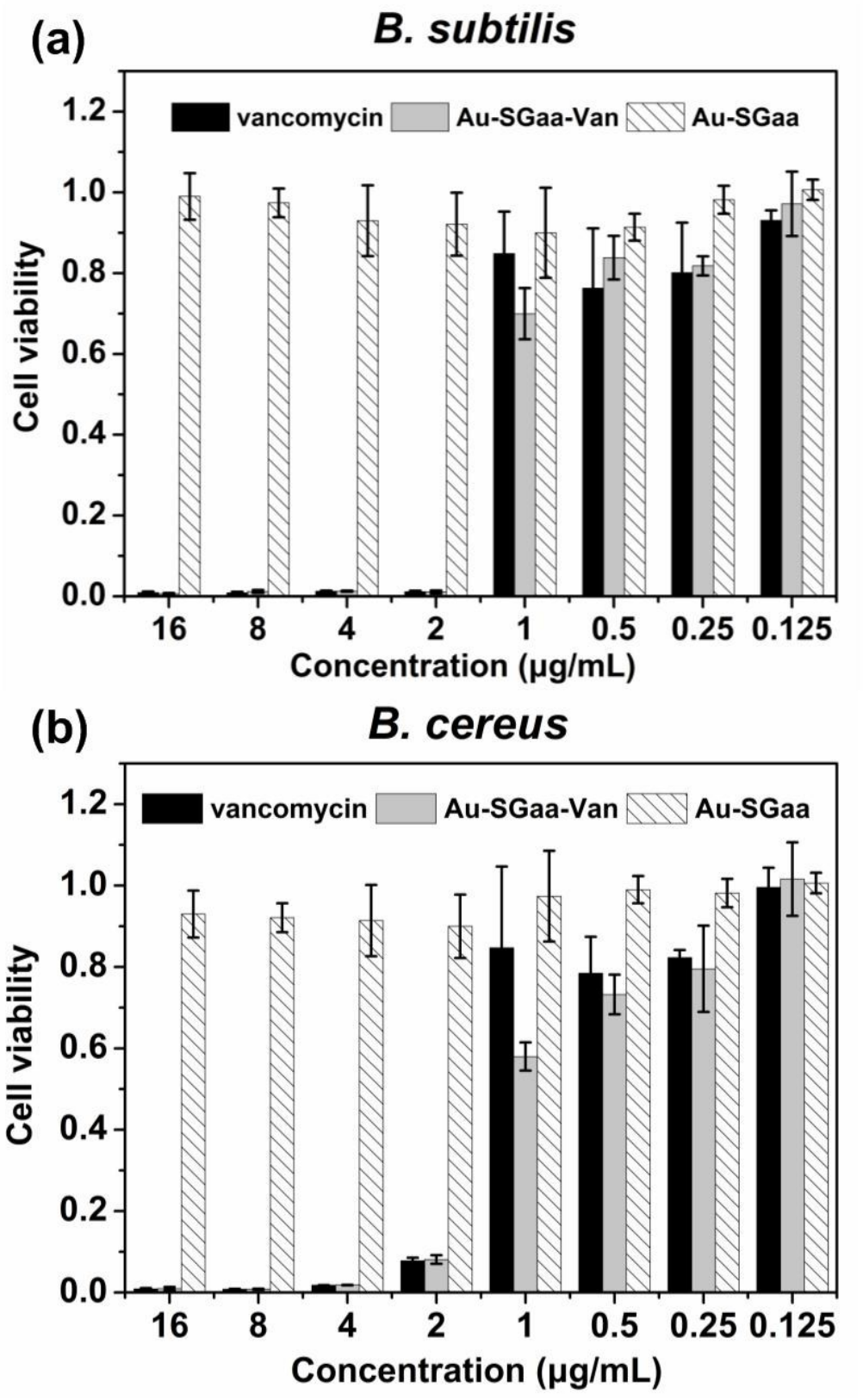

Fig. S9. Antibacterial activity of Au-SGaa-Van compared with Van and Au-SGaa against *B. Subtilis* (a) and *B. cereus* (b). Data are means ± standard deviation with n = 3.

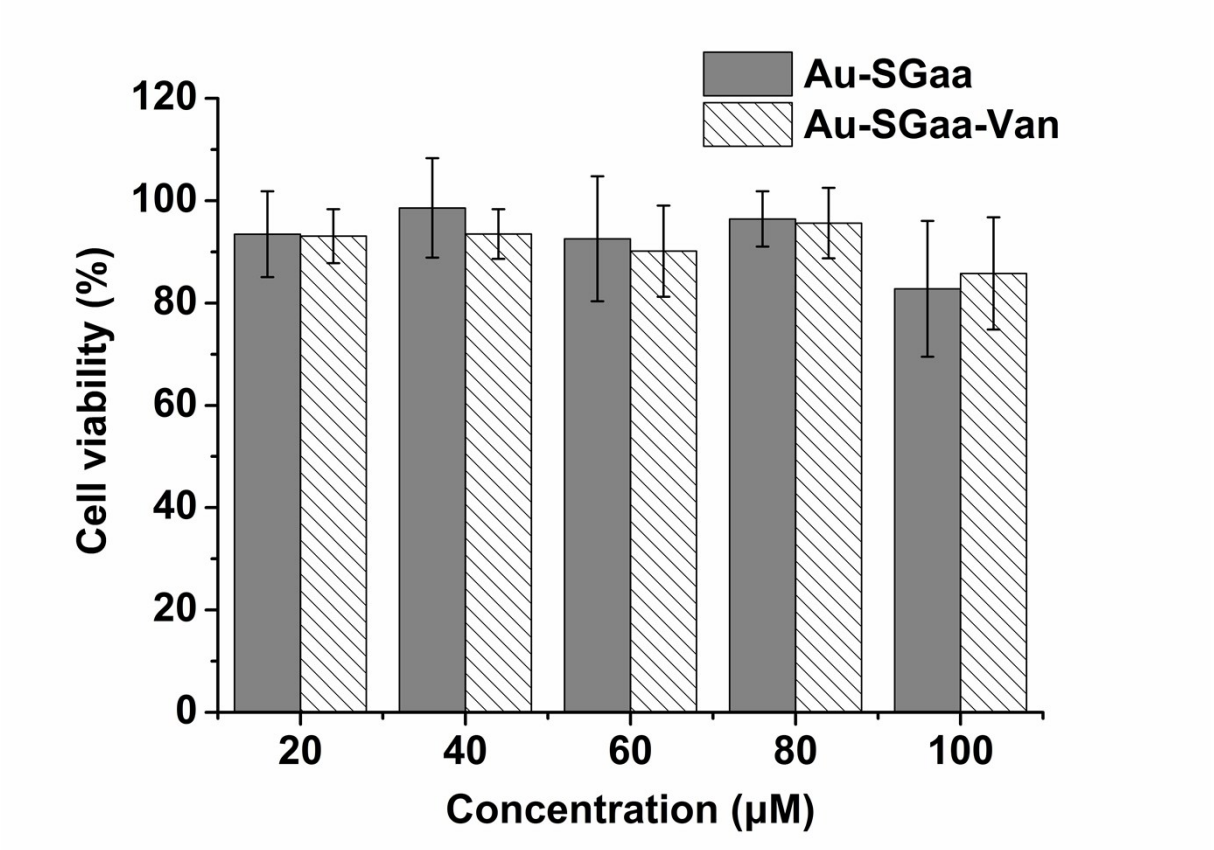

Fig. S10. The percentage viability of MCF-7 exposed to different concentrations of Au-SGaa and Au-SGaa-Van resulted from the MTT assays. The data are displayed as means ± standard deviation with n = 3.