Electronic Supplementary Material (ESI) for Chemical Science.

Supporting information

An endogenous stimulus detonated nanoclusters-bomb for contrast enhanced cell imaging and combination therapy

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Table S1. The names and properties of peptides used in this work.

Name	Sequence (from N' to C')	PI	Net charge (pH=7.0)
P_{T1}	CCYRRRRRRRRRGD *(provide the positive charge)*	12.3	8.9
P_{T2}	CCYGGGGRGRK(TAMRA)RGD *(signal unit)*	~ 10.5	~ 3.9
P_{L1}	CCYAANRRRRRRRRGD *(provide the positive charge)*	12.3	6.9
P_{L2}	CCYGGGGAANRK(TAMRA)RRGD *(signal unit)*	~ 10.5	~ 3.9
P_3	CCYGGGGRGRKRGD *(improve the S/N of NSET)*	10.5	3.9

Table S2. The comparison of S/N corresponded to AuNCs probes synthesized in different concentration of P_{T1}, P_{T3} (collectively named as P_0) and P_2.

P_0 (P_{T1}+P_3):P_{T2}	**P_{T1}:P_3:P_{T2}**	**S/N**
0:1	0:0:1	6.59
1:1	0.5:0.5:1	8.7
10:1	5:5:1	2.16
30:1	15:15:1	7.17
60:1	30:30:1	20

Table S3. The comparison of S/N corresponded to AuNCs probes synthesized with different concentration of NaOH at the peptide ratio of P_0:P_3=30:1, 60:1.

Name	P_{T1}:P_3:P_{T2}	0.5 M NaOH	1 M NaOH
30:1	30:0:1	sediment	6.18
	20:10:1	sediment	6.54
	15:15:1	7.17	sediment
60:1	60:0:1	sediment	3.71
	40:20:1	sediment	6.54
	30:30:1	20	sediment

Table S4: The names and properties of nucleic acid used in this work.

Name	Sequence (from 5′ to 3′)	Length
Dz	CCGCGGCCAGGCTAGCTACAACGACCTGGACGA	33
mDz	CCGCGGCCAGGCTA**C**CTACAACGACCTGGACGA	33
Dz4	CCGCGGCCAGGCTAGCTACAACGACCTGGACGA TTTCGCTGCTGCTGCTGC	51
mDz4	CCGCGGCCAGGCTA**C**CTACAACGACCTGGACGA TTTCGCTGCTGCTGCTGC	51
S1-Bhq1	Bhq1-CCGCGGCCAGGCTAGCTACAACGACCTGGA CGATTTCGCTGCTGCTGCTGC	51
S1	TCGTCCAGGrArUGGCCGCGG	19
S2	TCGTCCAGGrArUGGCCGCGGT$_{11}$	30
S3	TCGTCCAGGATGGCCGCGGT$_{11}$	30
S4	GCAGCAGCAGCAGCG	15
S4-FAM	GCAGCAGCAGCAGCGTT-FAM	17
S4-Cy7	GCAGCAGCAGCAGCGTT-Cy7	17
S5	T$_{15}$GCAGCAGCAGCAGCG	30

[a] The underlined letters in mD$_Z$ represent the mutant base.

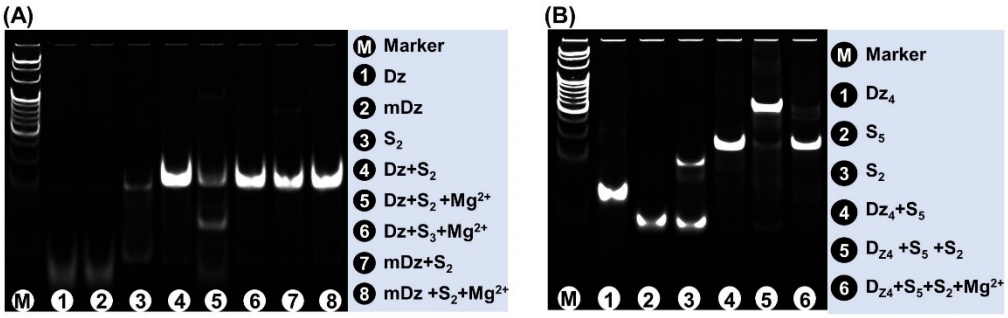

Fig. S1. 12% PAGE electrophoresis analysis of (A) the specific cleavage activity to EGR-1 of DNAzyme, (B) assemble and cleavage ability of functional nucleic acids.

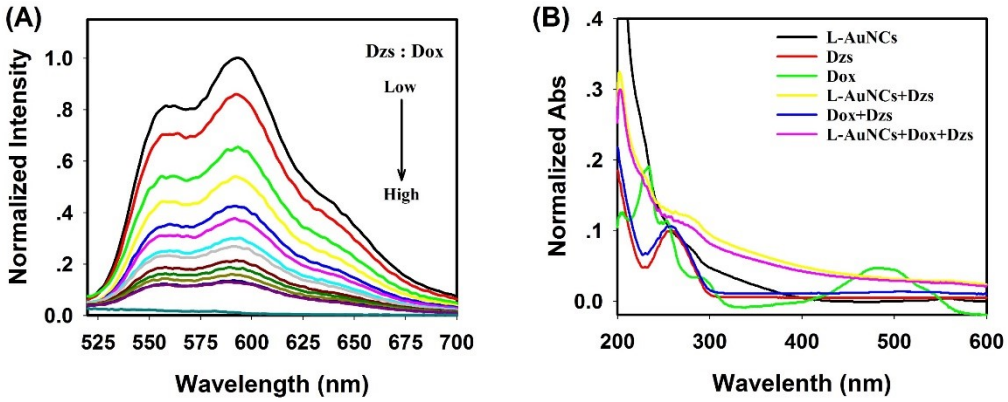

Fig. S2. (A) Drug loading capacity of Dzs. (B) Drug loading capacity analysis of L-AuNCs by UV-Vis absorption spectra.

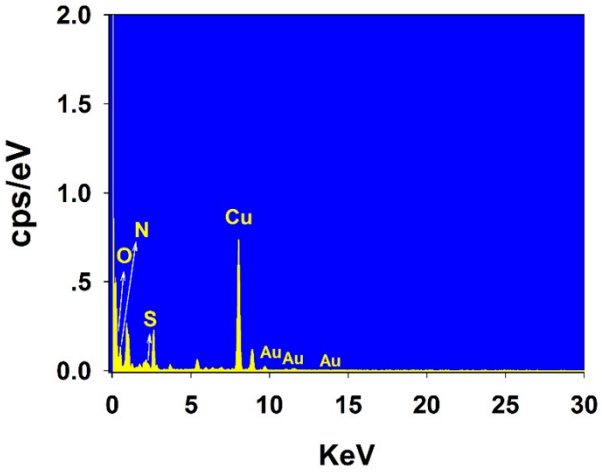

Fig. S3. EDS spectrum of T-AuNCs.

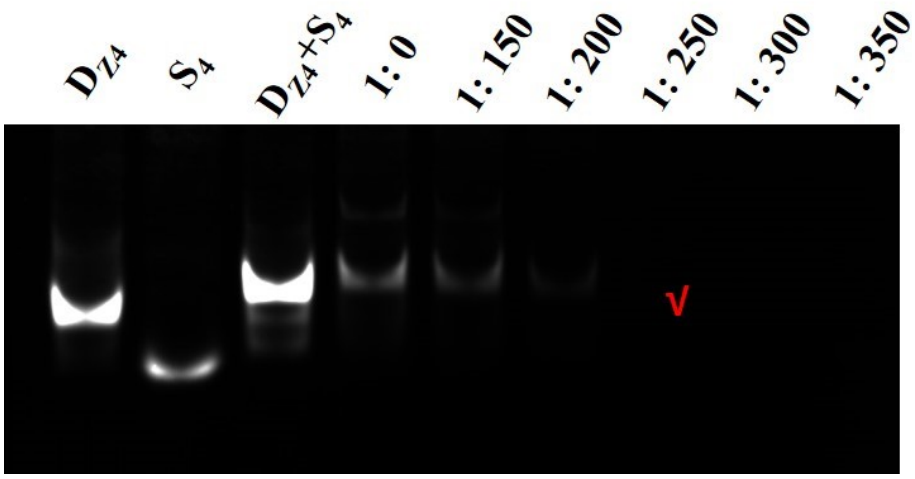

Fig. S4. Gel electrophoresis patterns of the T-AuNCs/Dzs nanoparticles.

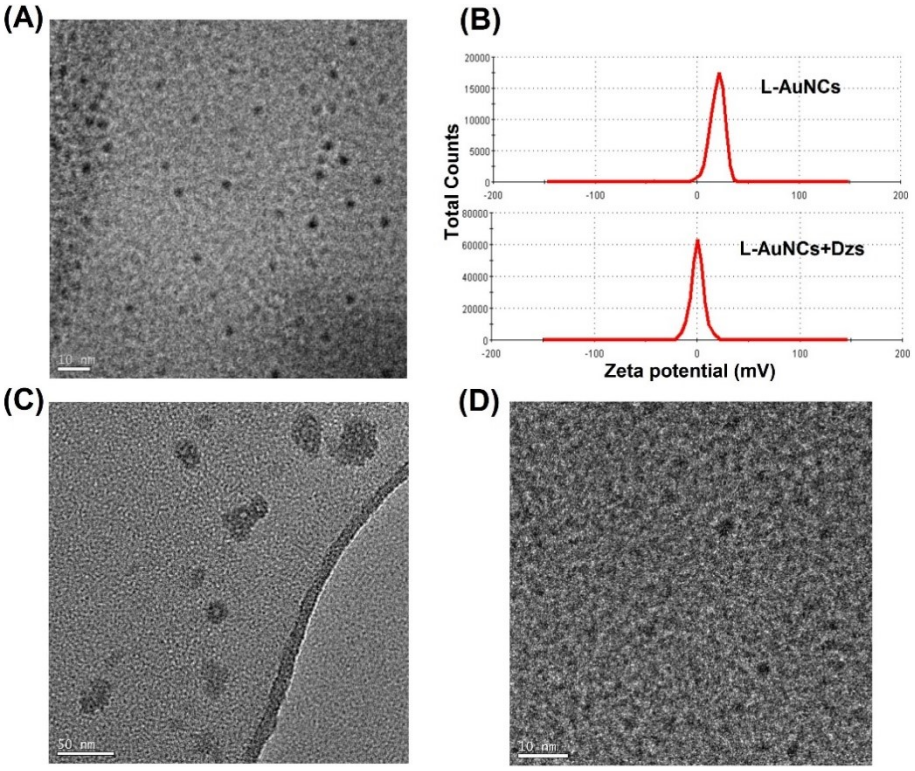

Fig. S5. (A) TEM image of L-AuNCs. (B) Zeta potential of L-Au NCs and L-AuNCs/Dzs nanoparticles. (C) TEM image of L-AuNCs/Dzs nanoparticles. (D) L-AuNCs/Dzs+legumain.

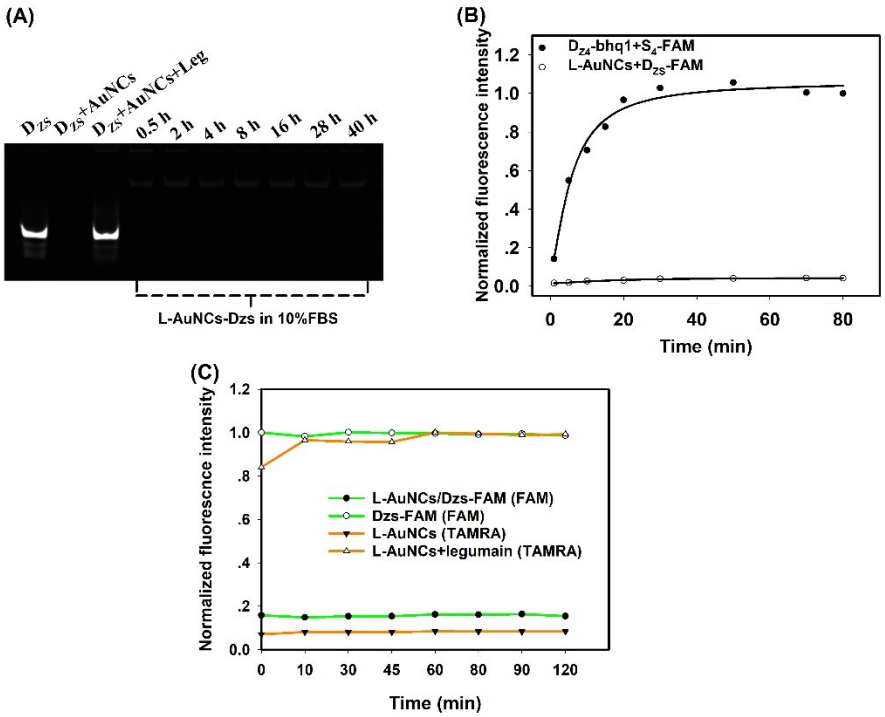

Fig. S6. Stability investigation of AuNCs/Dzs. (A) PAGE analysis of L-AuNCs/Dzs after incubating with 10% FBS. (B) Digestion resistant ability of L-AuNCs/Dzs to DNase I (1.5 U/mL). (C) Fluorescence analysis of the AuNCs/Dzs against 100% FBS.

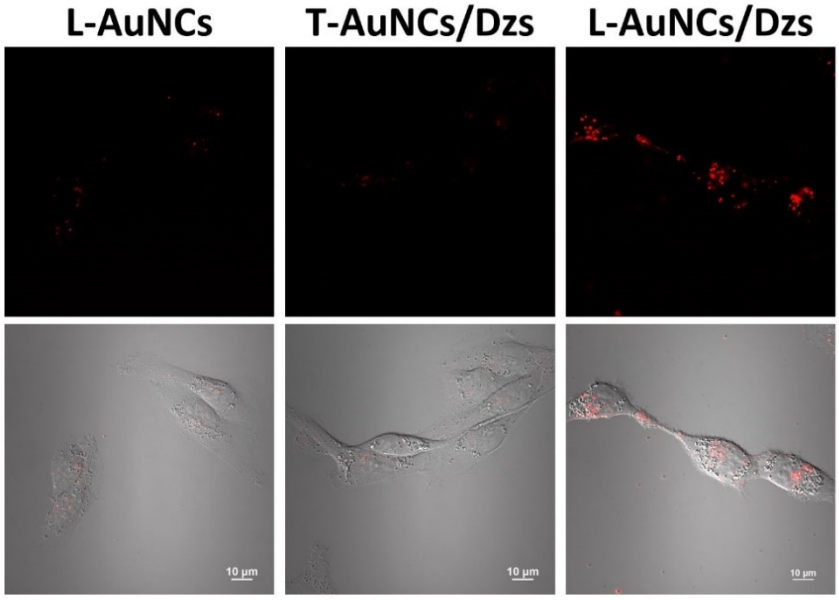

Fig. S7. Fluorescence imaging treated with L-AuNCs, T-AuNCs/Dzs, L-AuNCs/Dzs of MDA-MB-231 cells. Scale bar = 10 μm.

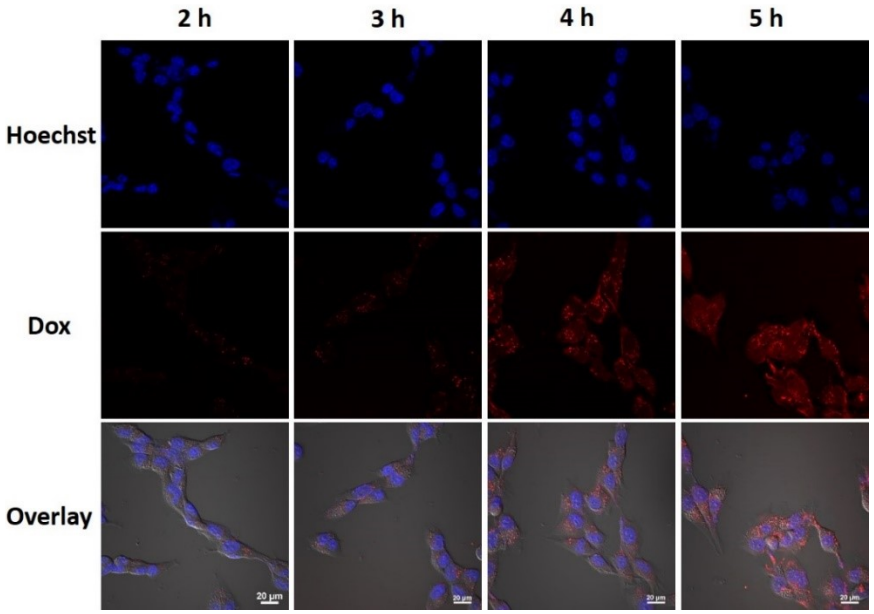

Fig. S8. Real-time fluorescence imaging treated with L-AuNCs/Dzs-Dox of MDA-MB-231 cells, blue and red color indicated Hoechst and Dox respectively. Scale bar = 20 μm.

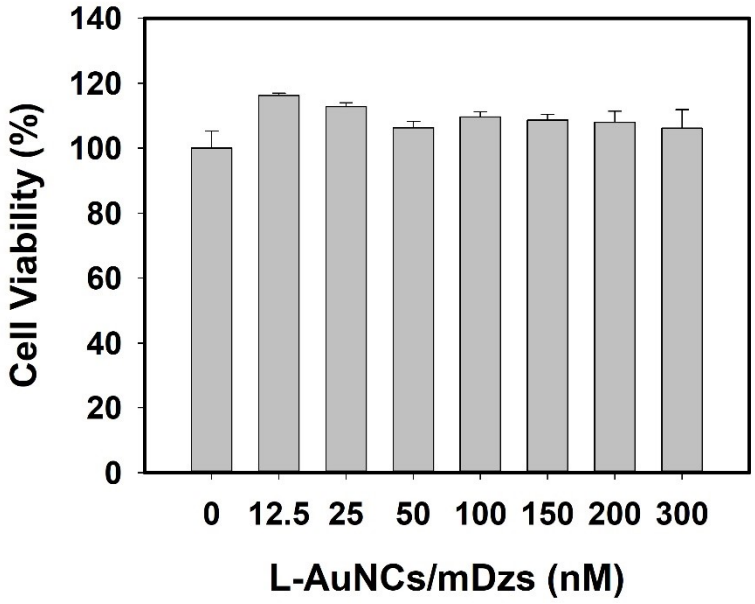

Fig. S9. Viability of MDA-MB-231 cells incubated for 48 h with different concentrations of L-AuNCs/mD_{ZS} (L-AuNCs: 0-90 μM, mDzs: 0-300 nM).

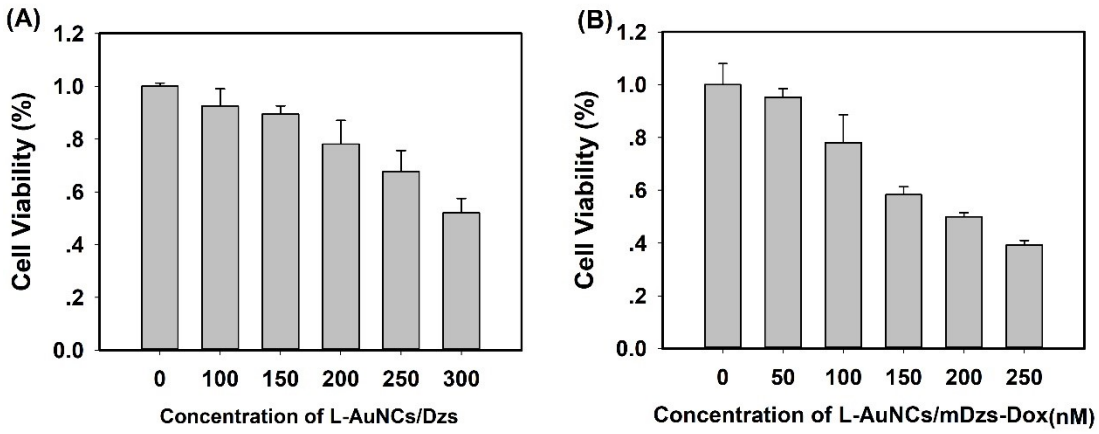

Fig. S10. Cytotoxicity evaluation of MDA-MB-231 cells (A) different concentrations of L-AuNCs-Dzs, (B) treated with different concentrations of L-AuNCs-mDzs-Dox.