

**Comparative study on the interaction of gold nanoparticles with
trypsin and pepsin: Thermodynamical perspectives**

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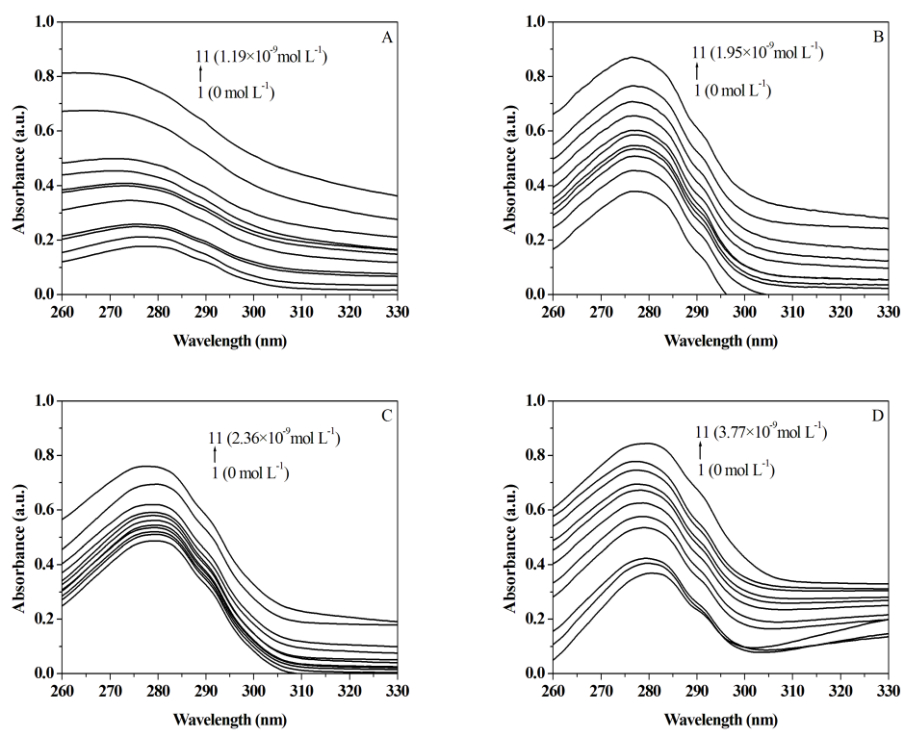


Figure S1. UV-vis absorption spectra of trypsin (A, C) and pepsin (B, D) in the presence of different concentrations of 17 nm and 30 nm AuNPs at 298 K, respectively. c (trypsin) = $5.0 \times 10^{-6} \text{ mol L}^{-1}$ (A) or $2.0 \times 10^{-5} \text{ mol L}^{-1}$ (C), c (pepsin) = $1.0 \times 10^{-5} \text{ mol L}^{-1}$ (B, D).

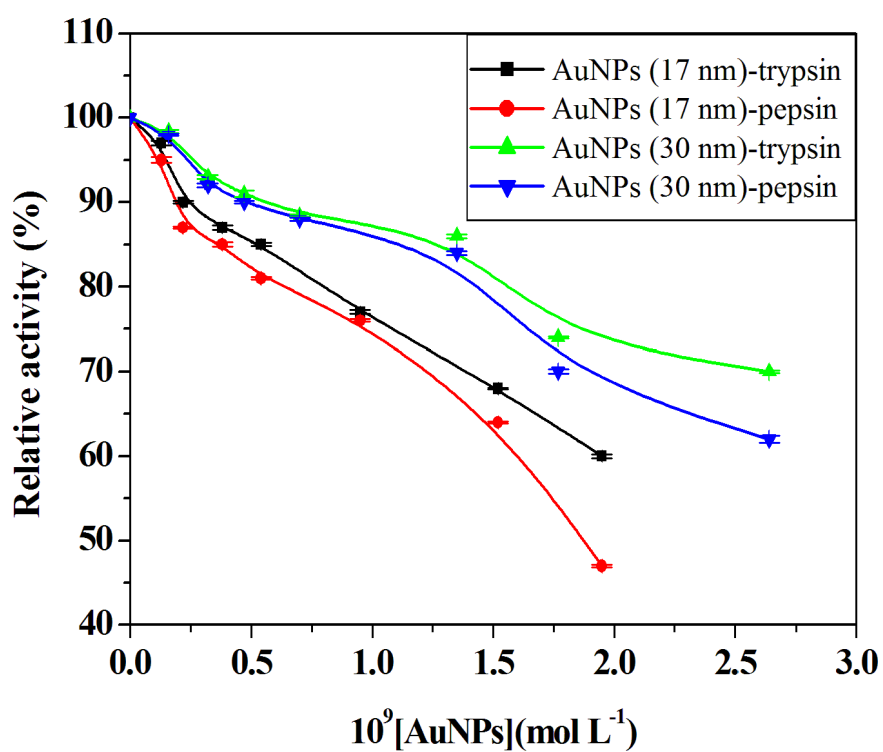


Figure S2. Effect of AuNPs concentration on the trypsin/pepsin activity. $c(\text{trypsin}) = c(\text{pepsin}) = 4.0 \times 10^{-5} \text{ mol L}^{-1}$,
 $c(17 \text{ nm AuNPs}) / (10^{-9} \text{ mol L}^{-1}) = 0.13, 0.22, 0.38, 0.54, 0.95, 1.52 \text{ and } 1.95$. $c(30 \text{ nm AuNPs}) / (10^{-9} \text{ mol L}^{-1}) =$
 $0.16, 0.32, 0.47, 0.70, 1.35, 1.77 \text{ and } 2.64$.

Table S1. All time-resolved parameters of trypsin/pepsin in the absence and presence of AuNPs.

System	$c(\text{AuNPs})$	τ_1 (ns)	τ_2 (ns)	a_1	a_2	τ_{avg} (ns)	χ^2
Native trypsin	/	2.316	5.948	0.936	0.064	2.858	1.000
AuNPs (17 nm)-trypsin	1.19×10^{-9}	2.012	4.112	0.854	0.146	2.557	1.000
AuNPs (30 nm)-trypsin	2.36×10^{-9}	2.464	5.364	0.879	0.121	3.130	1.000
Native pepsin	/	3.565	5.489	0.229	0.771	5.178	1.000
AuNPs (17 nm)-pepsin	1.95×10^{-9}	3.280	5.786	0.189	0.811	5.495	1.007
AuNPs (30 nm)-pepsin	3.77×10^{-9}	3.473	5.355	0.007	0.993	5.346	1.000

Table S2. Secondary structure analysis from native trypsin/pepsin and AuNPs-trypsin/pepsin system at 298 K using CDNN program.

System	$c(\text{AuNPs})$	CDNN (program)				
		α -Helix (%)	Antiparallel (%)	Parallel (%)	β -Turn (%)	Rndm. coil (%)
Native trypsin	/	6.8	41.3	5.6	17.0	29.3
AuNPs (17 nm)-trypsin	0.49×10^{-9}	6.9	41.4	5.6	16.8	29.3
	1.19×10^{-9}	6.8	41.4	5.6	16.9	29.3
AuNPs (30 nm)-trypsin	0.70×10^{-9}	6.6	41.3	5.6	17.0	29.5
	2.36×10^{-9}	6.6	41.4	5.6	17.1	29.4
Native pepsin	/	7.4	39.8	5.6	17.4	29.8
AuNPs (17 nm)-pepsin	0.70×10^{-9}	7.6	39.7	5.6	17.3	29.8
	1.95×10^{-9}	7.7	39.2	5.6	17.3	30.2
AuNPs (30 nm)-pepsin	1.68×10^{-9}	7.5	39.3	5.6	17.3	30.3
	3.77×10^{-9}	7.6	39.1	5.6	17.3	30.4