Supporting Information

Detection of Nanomolar Level of Total Cr [(III) and (VI)] by Functionalized Gold Nanoparticles and a Smartphone with the Assistance of Theoretical Calculation Models

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Table S1. ΔG of the interactions between the DMSA-Au NPs and various metal ions (1 nm Au NPs as the simplified model).

Metal ions	Gibbs free energy (kcal mol^{-1})
$Cr_2O_7^{2-}$	-234.21
Cr^{3+}	-229.90
Al^{3+}	-209.44
Fe^{3+}	-202.69
Ba^{2+}	-91.25
Ca^{2+}	-89.35
Cd^{2+}	-100.45
Co^{2+}	-117.81
Cu^{2+}	-141.30
Fe^{2+}	-99.03
Mg^{2+}	-90.81
Mn^{2+}	-105.27
Ni^{2+}	-125.40
Pb^{2+}	-110.68
Zn^{2+}	-96.71
Hg^{2+}	-152.34

Table S2. Comparison of the performance of different sensors published for Cr detection.

Probe	Targets	Readout	LOD	Pertreatment	Time required for the assay (min)	Rely on large Instrument	ref
Glutathione-CdTe QDs	Cr(VI)	Fluoresence	~ 150 nM	---	>40	YES	1
Terbium NPs	Cr(VI)	Fluoresence	~ 15 nM	---	5	YES	2
AuNPs-SPE	Cr(VI)	Voltammetric	~ 96 nM	---	1	YES	3
Ag@Au NPs	Cr(VI)	Colorimetric/UV	100 nM	---	30	NO	4
Ag NPs	Cr(VI)	Colorimetric/UV	100 nM	---	5	NO	5
DTT-Au NPs	Cr(VI)	Colorimetric/UV	20 nM	---	5	NO	6
Tripolyphosphate-Au NPs	Cr(III)	Colorimetric/UV	100 nM	---	5	NO	7
BP-DTC-Au NPs	Cr(III)	Colorimetric/UV	~ 0.6 μM	---	1	NO	8
TNBA-Au NPs	Cr(III),Cr(VI)	Colorimetric/UV	1 μM	Cr(VI) Reduction	>10	NO	9
Citrate-capped Au NPs	Cr(III),Cr(VI)	Colorimetric/UV	4 μM	Cr(VI) Reduction	>30	NO	10
DMSA-Au NPs	Cr(III),Cr(VI)	Colorimetric/UV	10 nM	---	5	NO	This work

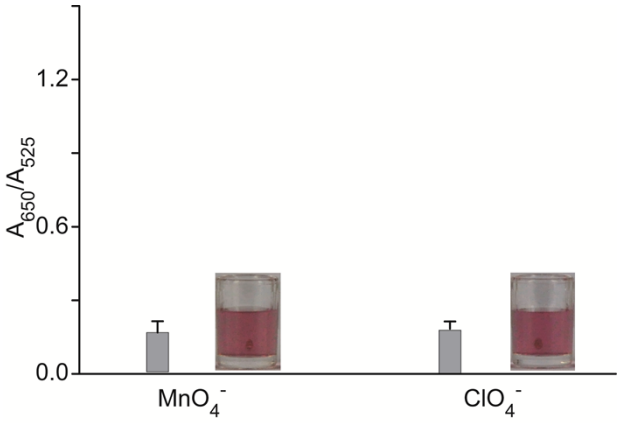


Fig. S1. The response of DMSA-Au NPs to the other ions containing O atom (MnO_4^- and ClO_4^-).

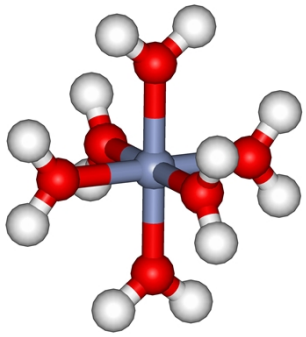
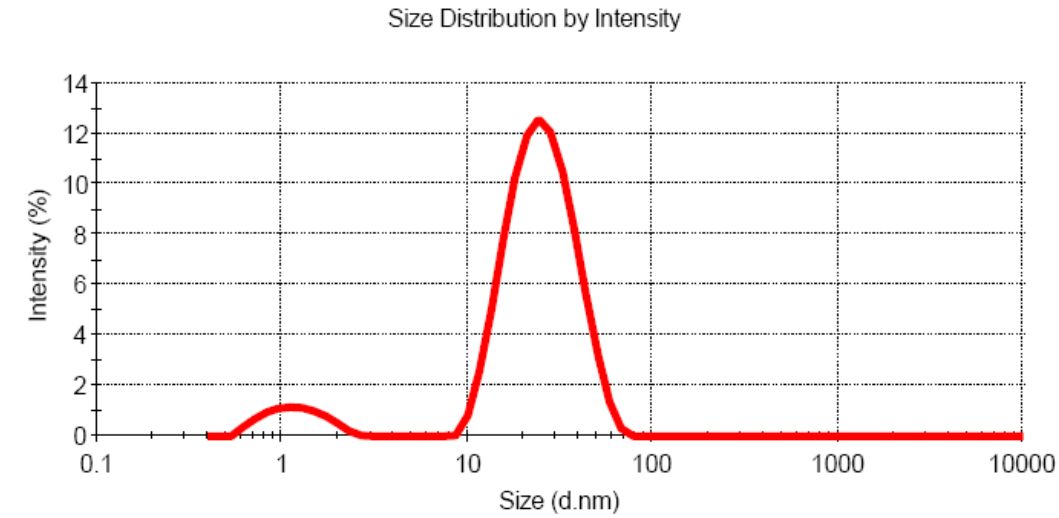


Fig. S2. Models of the metal ions (M^{n+}) and six water molecules coordinated in the $[M(H_2O)_6]^{n+}$ form.

(a)


Size Distribution by Intensity
Intensity (%)
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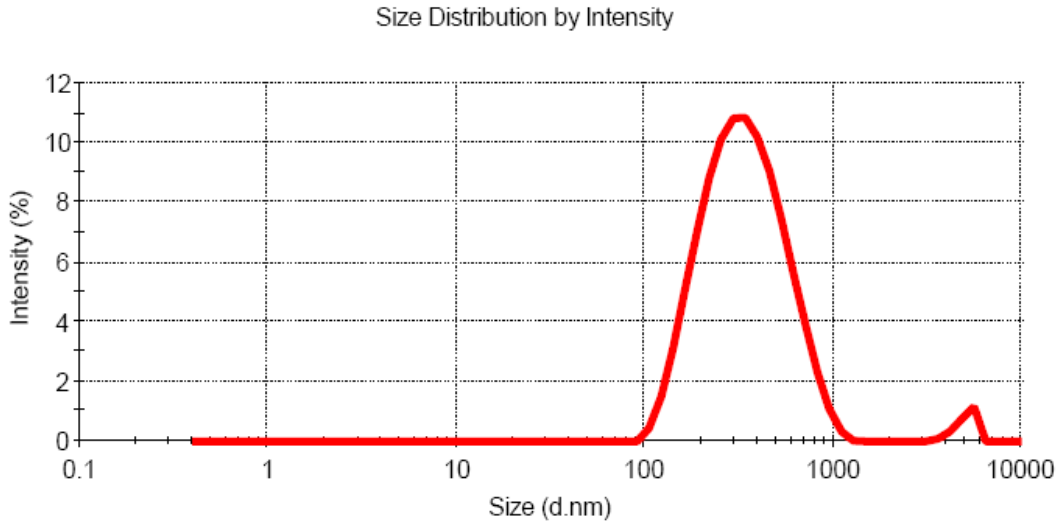
10
8
6
4
2
0
0.1
1
10
100
1000
10000
Size (d.nm)

(b)


Size Distribution by Intensity
Intensity (%)
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10
8
6
4
2
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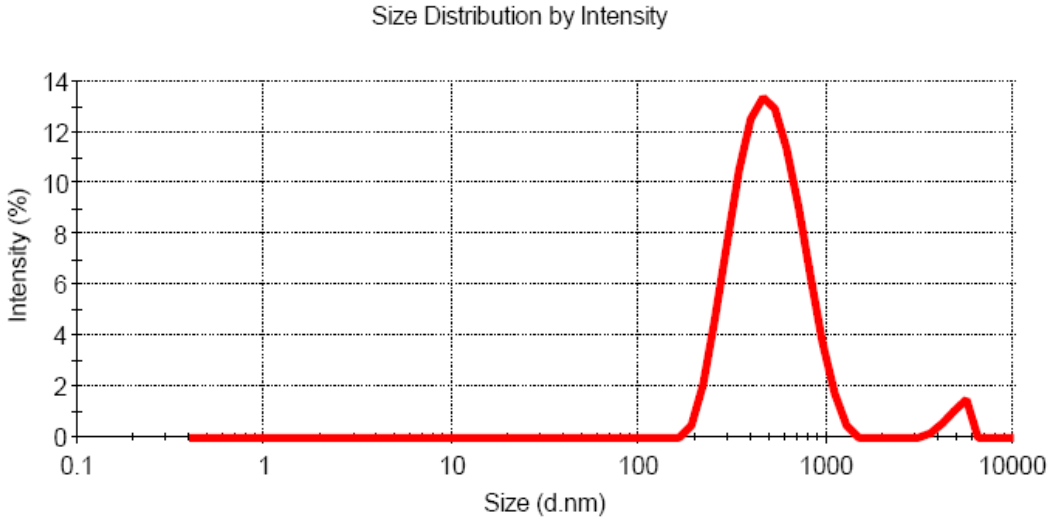
0.1
1
10
100
1000
10000
Size (d.nm)

(c)


Size Distribution by Intensity
Intensity (%)
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8
6
4
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0.1
1
10
100
1000
10000
Size (d.nm)

(d)

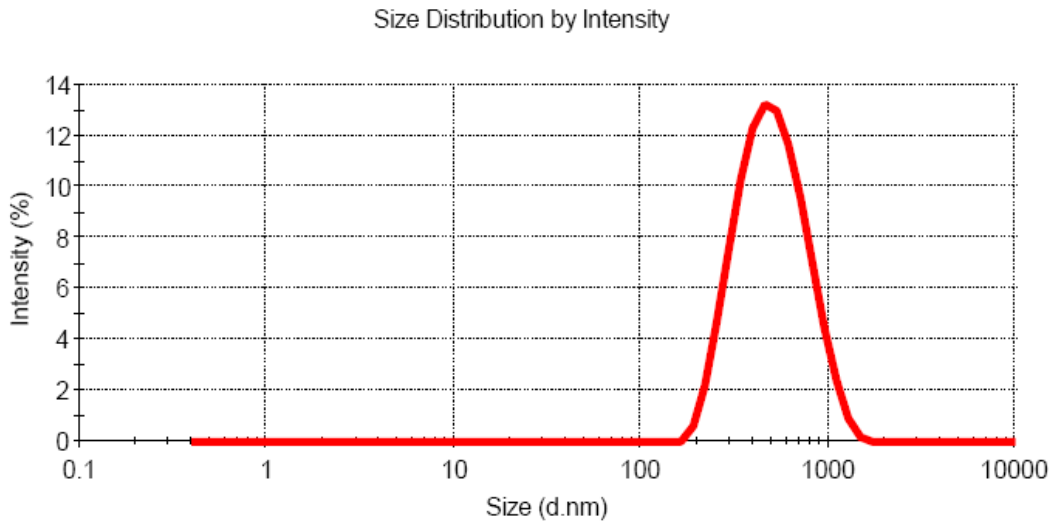

Fig. S3. DLS measurements for DMSA-Au NPs before (a) and after adding Cr^{3+} (b), $Cr_2O_7^{2-}$ (c), Cr^{3+} and $Cr_2O_7^{2-}$ mixtures (d), the concentration of DMSA-Au NPs is 2.5 nM.

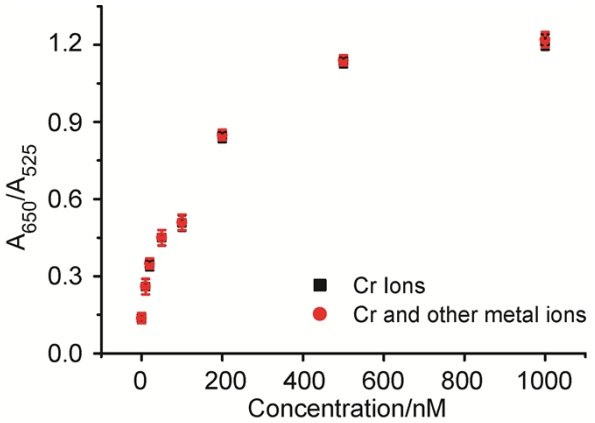

Fig. S4. A dose response curve for Cr ions (Cr^{3+} and $Cr_2O_7^{2-}$ mixtures) detection with and without other metal ions. The concentration of Cr^{3+} and $Cr_2O_7^{2-}$ mixtures are from 0 nM to 1 μM (mole ratio is 1:1) and the final concentration of other metal ions is 1 μM.

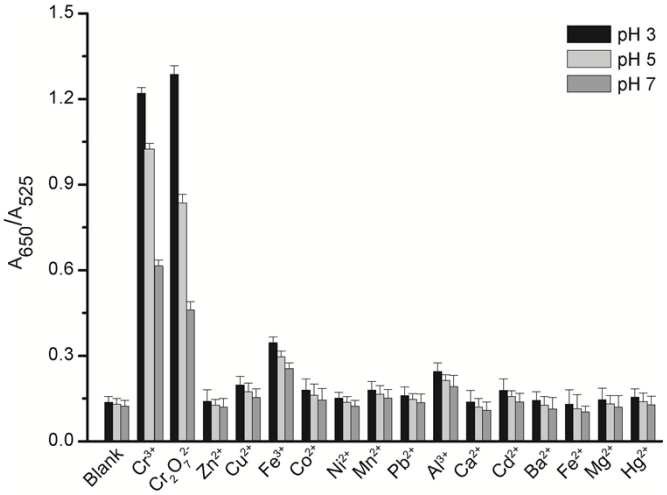

Fig. S5. The plot of A_{650}/A_{525} of AuNPs versus different metal ions at different pH values (pH 3, 5 and 7). The concentrations of various metallic ions are 10 μM and that of Cr^{3+} and $Cr_2O_7^{2-}$ are 1 μM.

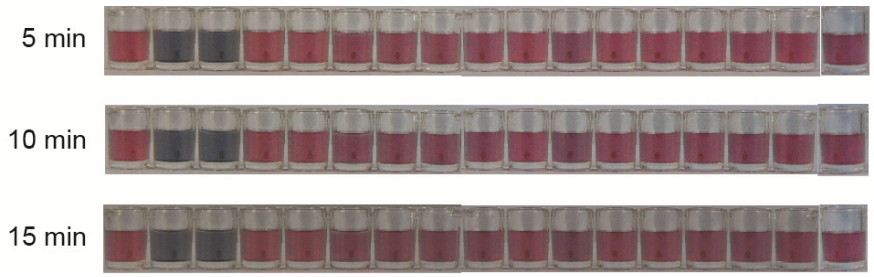

Fig. S6. The pictures of DMSA-Au NPs solution with adding different metal ions taken at different time point (5 min, 10 min, 15 min respectively).

References

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