Electronic Supplementary Information (ESI) of

Synergistic molecular assembly of aptamer and surfactant on gold nanoparticles for colorimetric detection of trace level As^{3+} ion in real samples

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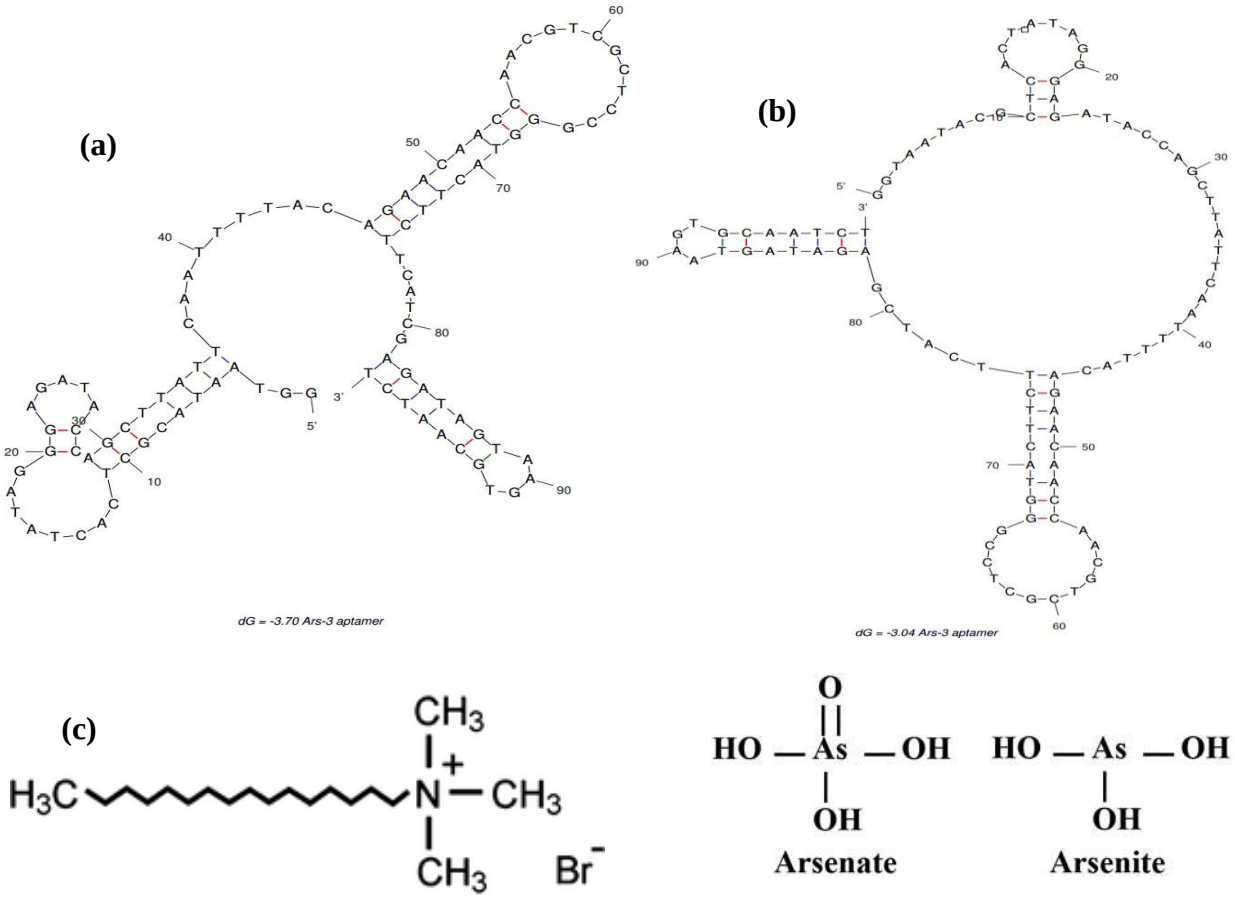

Fig. S1. Chemical structures of used compounds in As^{3+} ion detection using aptamer-CTAB-AuNPs-based aptasensor. (a) Secondary structures of the selected DNA aptamers predicted using Zuker algorithm, m-fold. (5'-GGTAATACGACTCACTATAGGGAGAATACCAGCTTATTCAATTTTACAGAACAACCAAC GTCGCTCCGGGTACTTCTTCATCGAGATAGTAAGTGCATCT-3'), (b) structures of CTAB, (c) arsenate (As^{5+}) and arsenite (As^{3+}) ions.

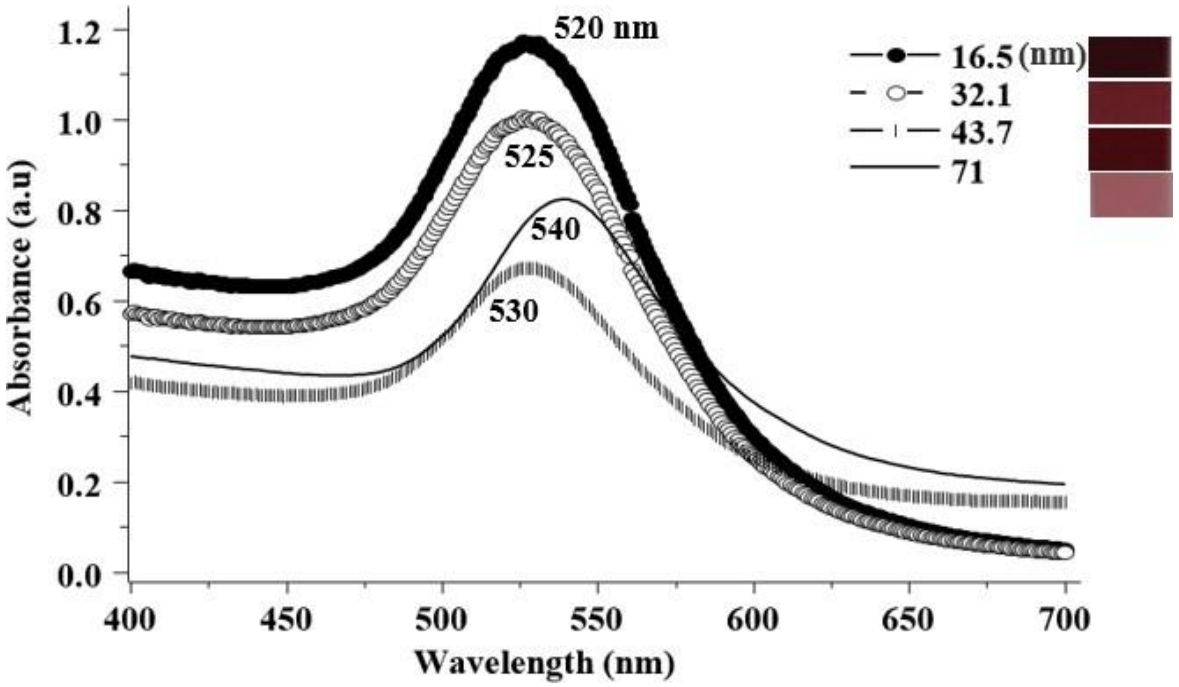

Fig. S2 UV-visible absorption of AuNPs using different volumes (300, 240, 180, and 120 mL) of citrate with different sizes (16.5, 32.1, 43.7 and 71.0 nm) and the corresponding color of the AuNPs solutions.

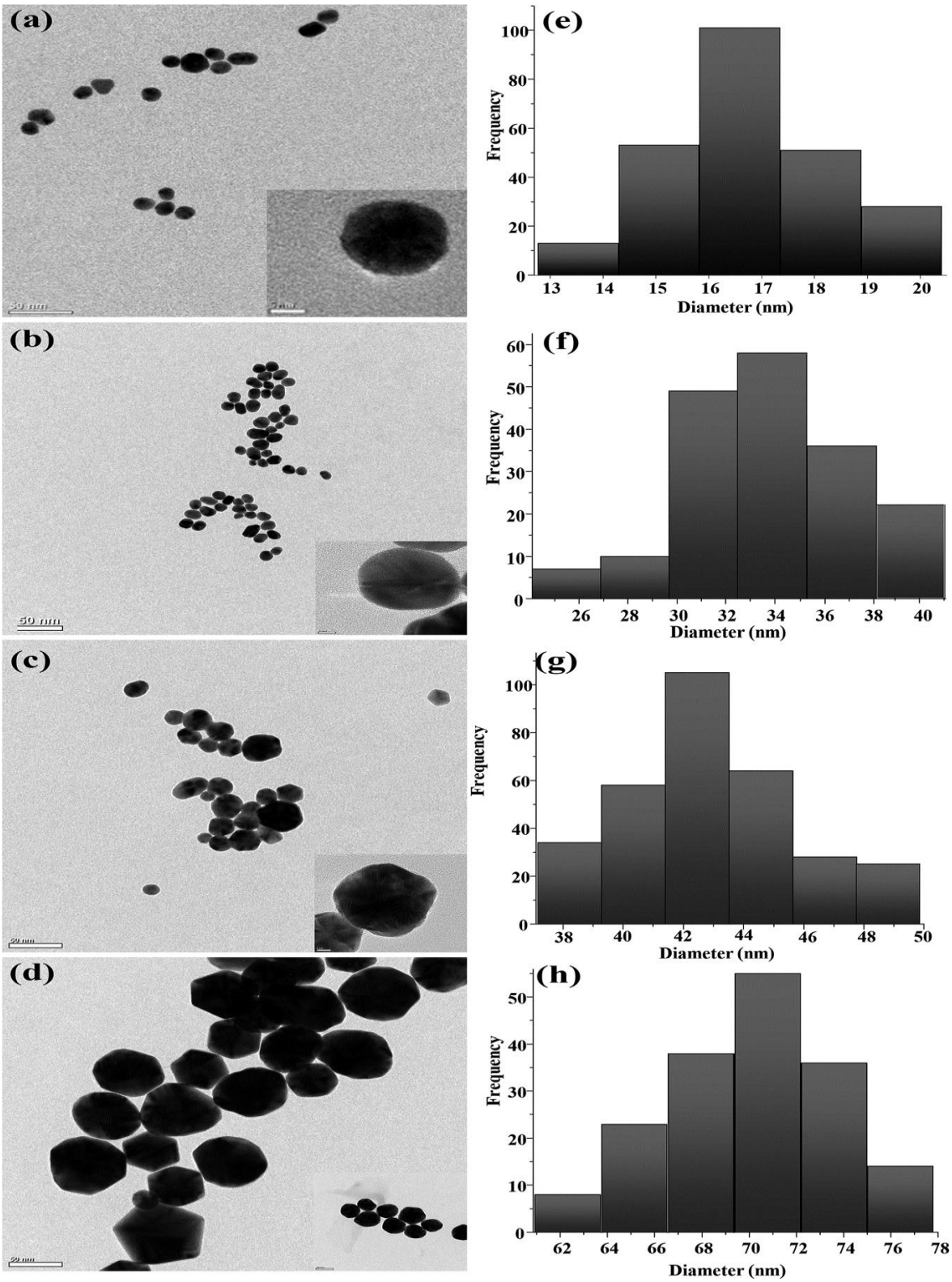

Fig. S3. TEM images and the corresponding histograms of AuNPs using (a, e) 300, (b, f) 240, (c, g) 180, and (d. h) 120 mL of citrate.

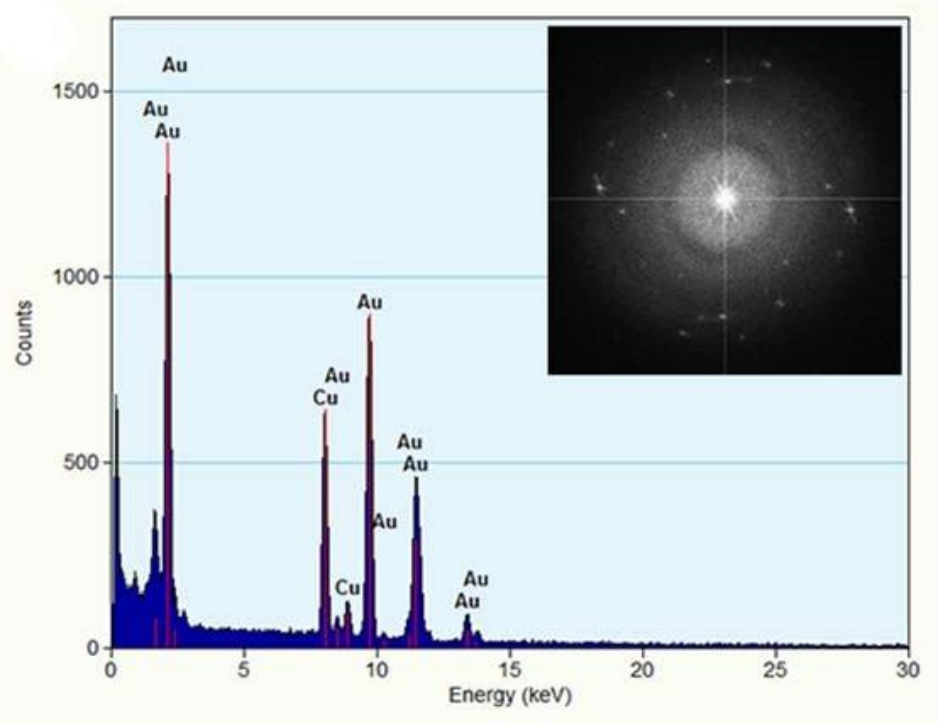

Fig. S4. Energy-dispersive X-ray spectrum of AuNPs.

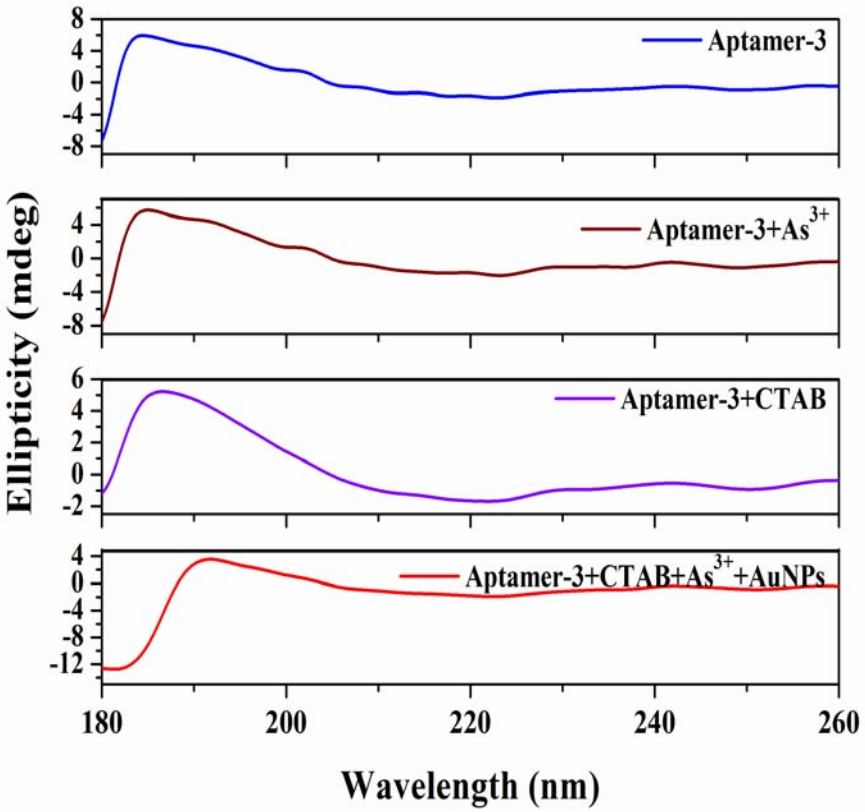

Fig. S5. CD spectra of aptamer-3, aptamer-3 + As^{3+} ion, aptamer-3 + CTAB and aptermer-3 + CTAB + As^{3+} ion + AuNPs.

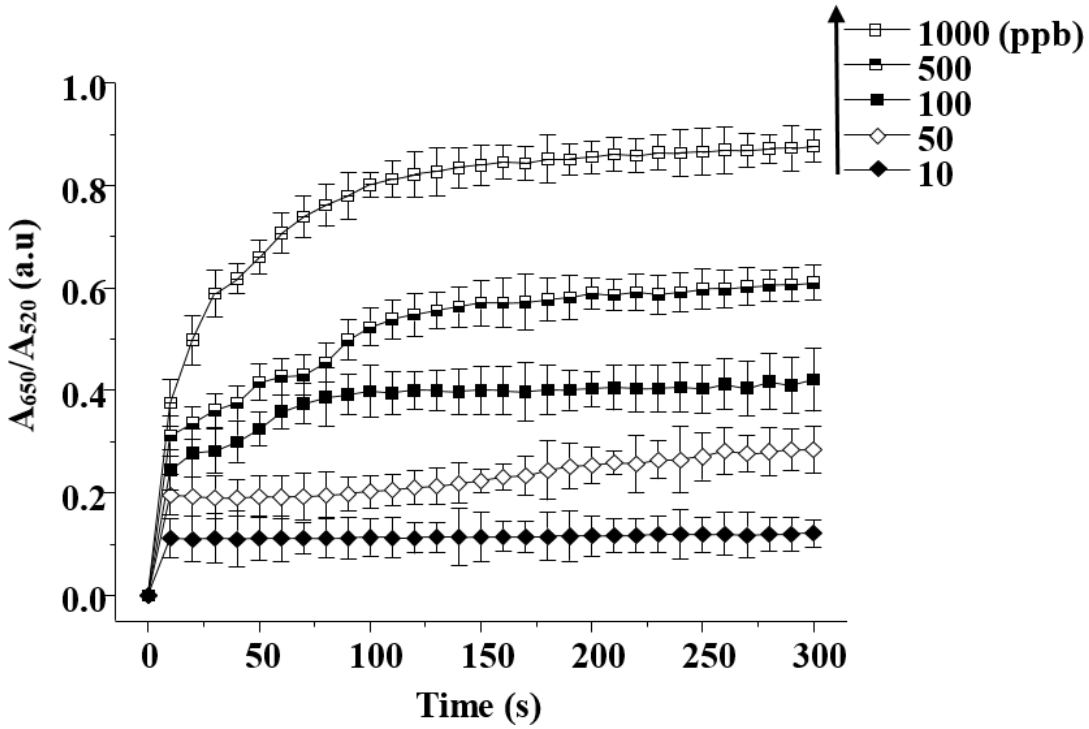

Fig. S6. Aggregation kinetics of AuNPs upon the addition of aptamer, CTAB and different concentrations of As^{3+} ion (10, 50, 100, and 1000 ppb) (n=3).

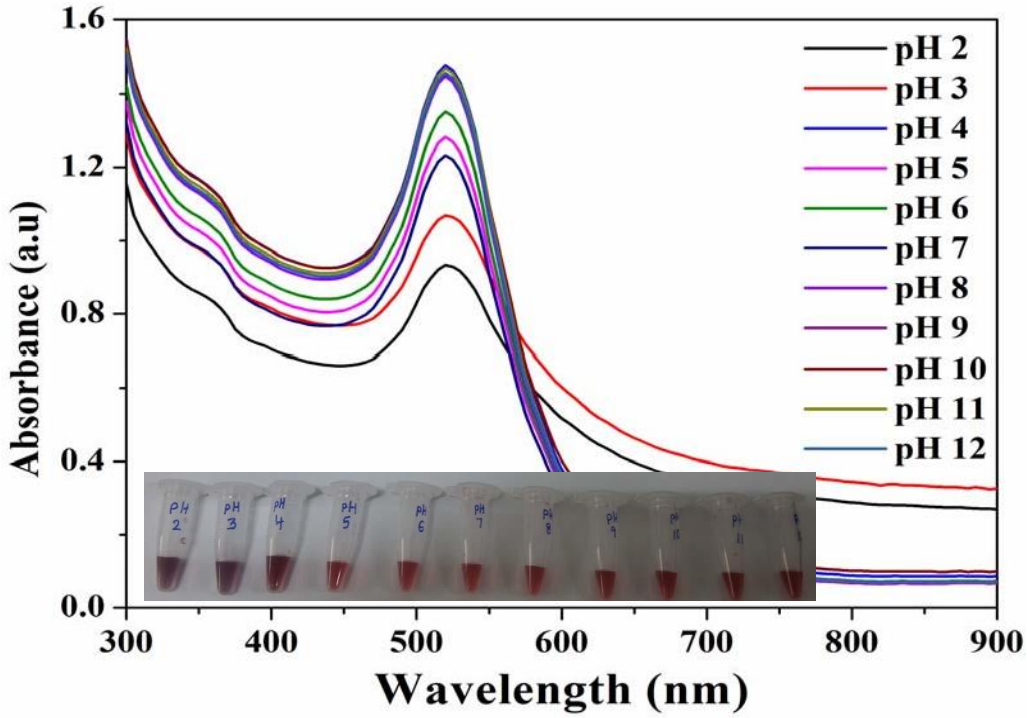

Fig. S7. Absorption spectra of AuNPs at different pHs from 2.0 – 12.0 without addition of aptamer-3, CTAB and As^{3+} ion. Inset: photographic image of corresponding solutions.

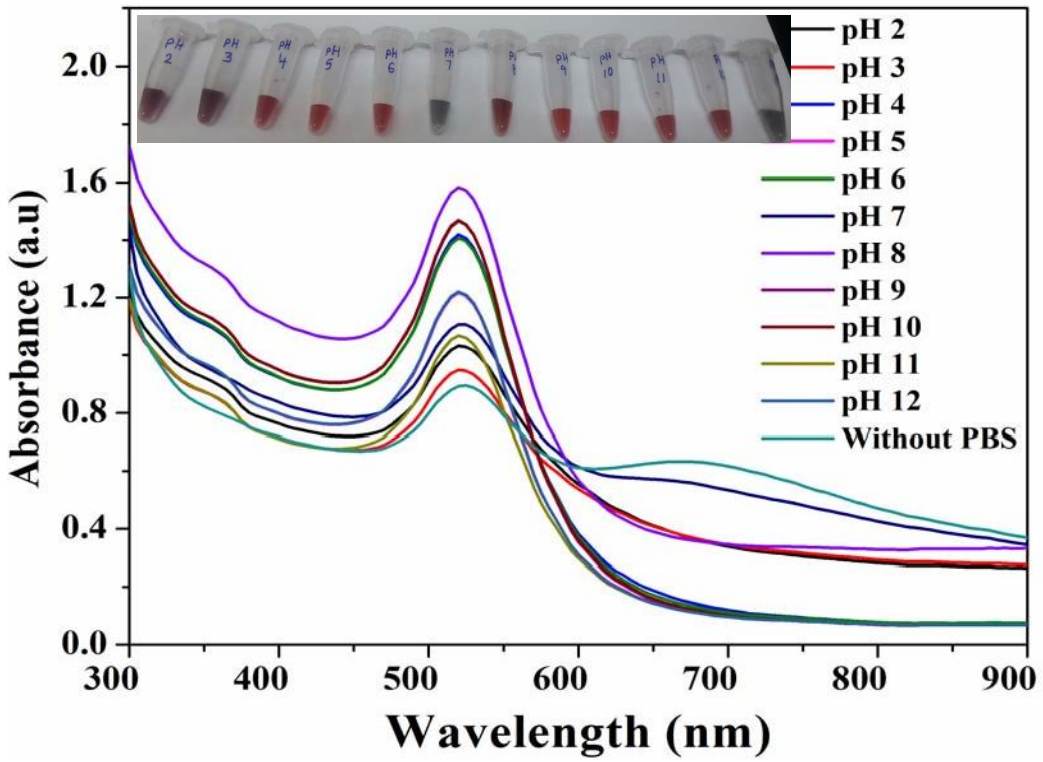

Fig. S8. Absorption spectra of AuNPs at different pHs from 2.0 – 12.0 with addition of aptamer-3, CTAB and As^{3+} ion and without addition of PBS buffer. Inset: photographic image of corresponding solutions.

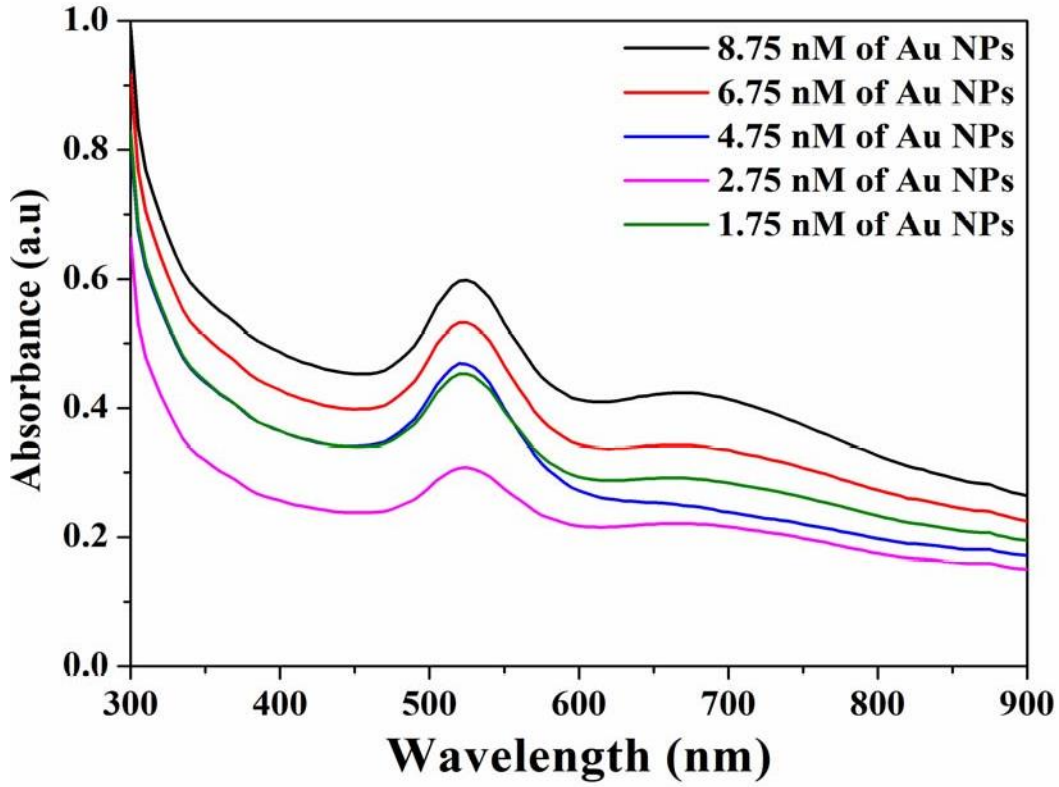

Fig. S9. Absorption spectra of different concentrations of AuNPs (8.75, 6.75, 4.75, 2.75 and 1.75 nM) with aptamer-3+CTAB+As^{3+} ion.

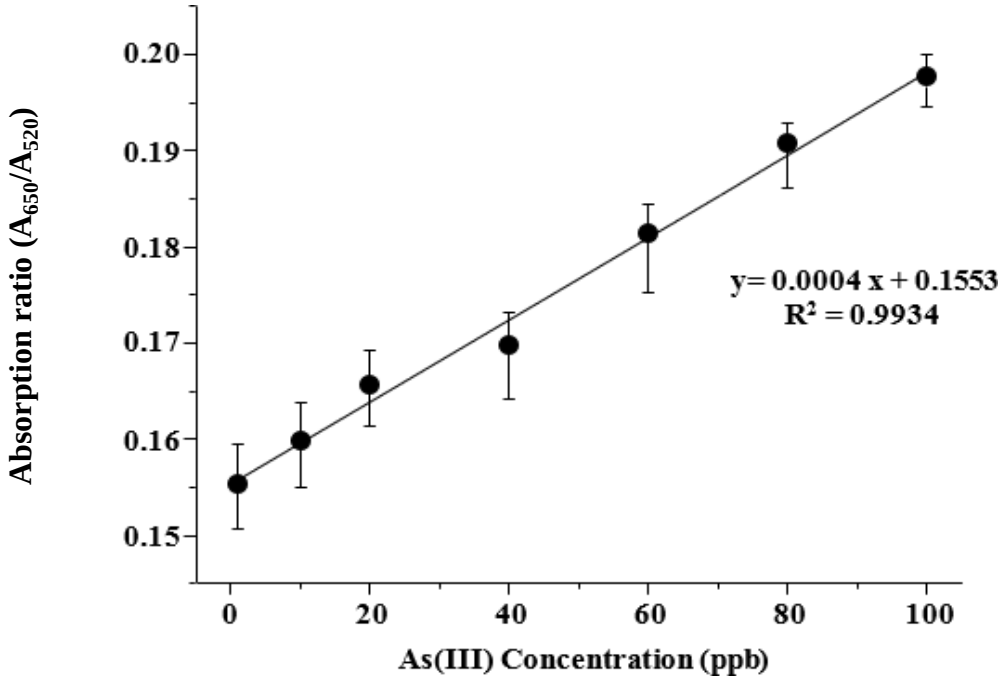

Fig. S10. The calibration curve plotted between the values of absorption ratio at A_{650}/A_{520} and concentration of As^{3+} ion in the range of 1.0 – 100 ppb.

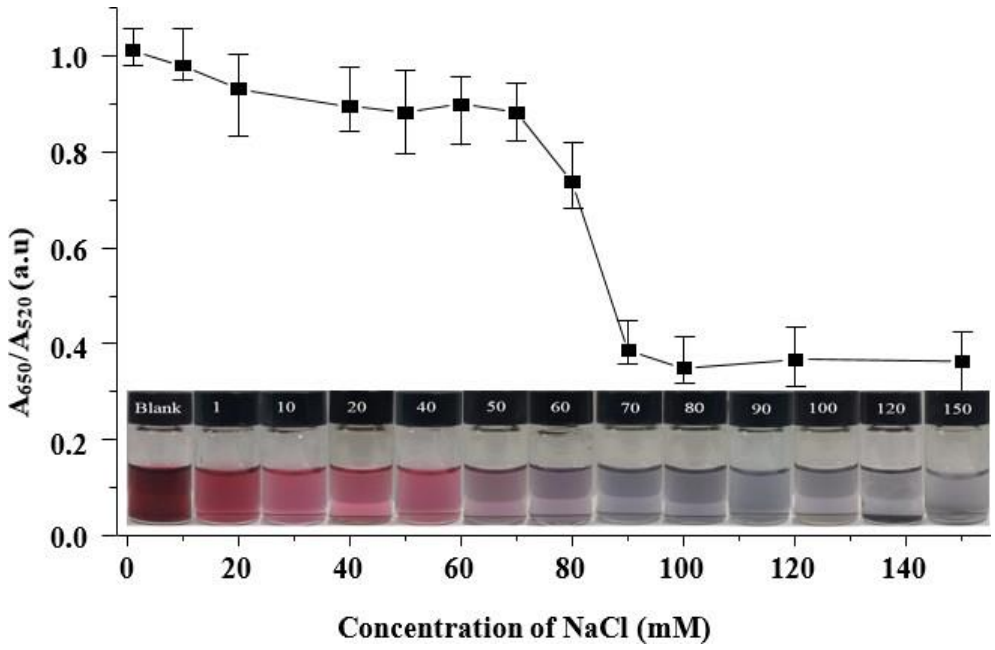

Fig. S11. Effect of NaCl concentration on the aggregation of AuNPs. The insert photograph shows the color change of AuNPs upon the addition of different concentrations of NaCl.

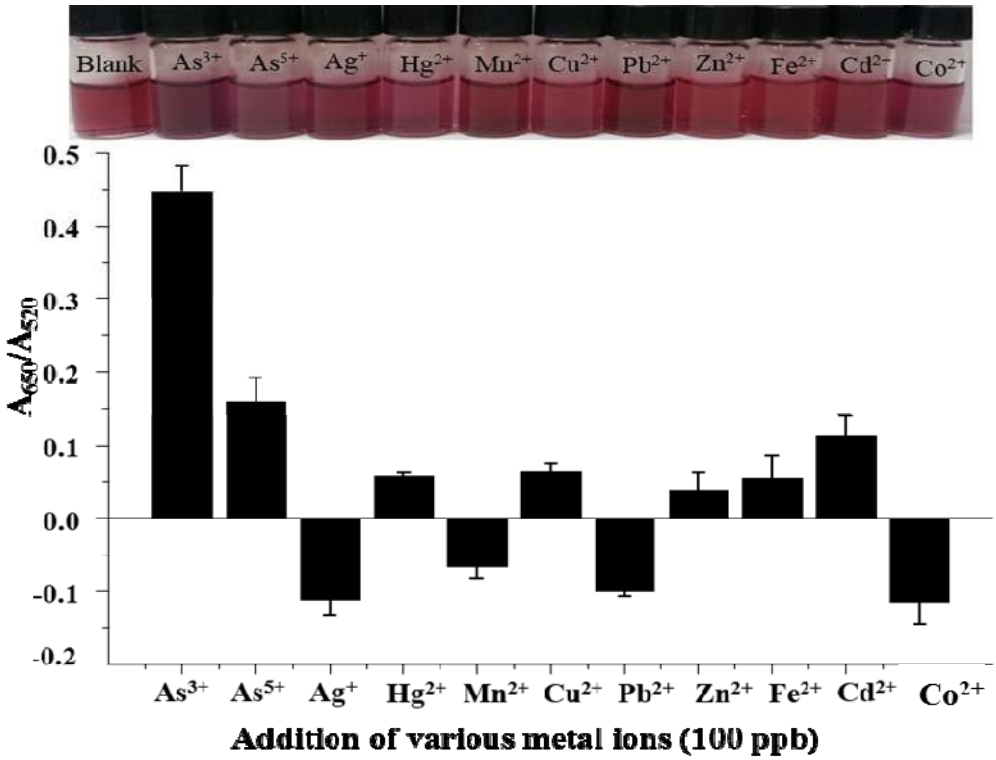

Fig. S12. Absorption ratio of AuNPs at A_{650}/A_{520} upon the addition of various metal ions including As^{3+} ion (Ag^{+}, Cd^{2+}, Hg^{2+}, Mn^{2+}, Cu^{2+}, Mg^{2+}, Fe^{2+}, Co^{2+}, As^{3+} and As^{5+} ion, 1000 ppb) in the presence of aptamer and CTAB.

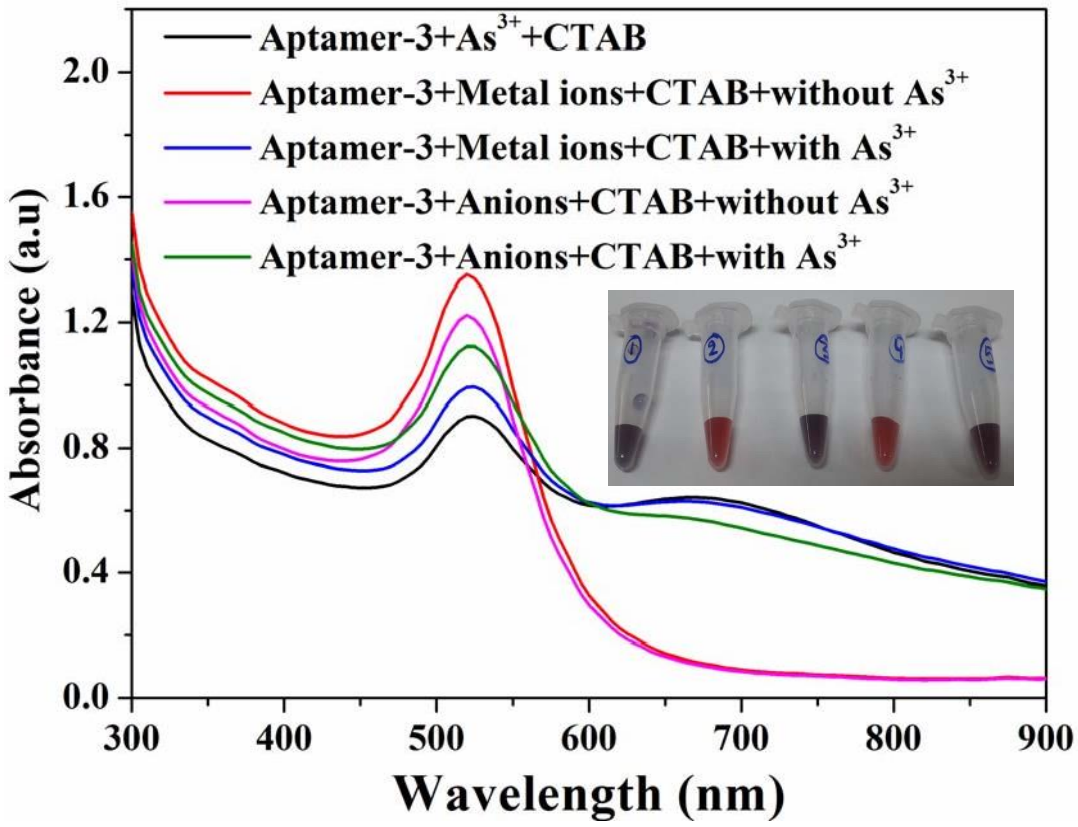

Fig. S13. Absorption spectra of AuNPs with aptamer-3+CTAB+As^{3+} ion (black line) and without As^{3+} ion in the presence of mixture of metal ions (Ba^{2+}, Ca^{2+},Cu^{2+}, Hg^{2+}, Zn^{2+}, Ni^{2+}, Fe^{2+} and Al^{3+} 100 ppb) and mixture of anions (Cl^{-}, F^{-}, Br^{-}, I^{-}, SO_4^{2-}, S^{2-}, PO_4^{3-} and $Cr_2O_7^{2-}$, 100 ppb). Inset: photographic image of corresponding solutions.

Table S1. Analytical performance of different sizes of AuNPs for detection of As^{3+} ion using aptamer as an aptasensor and CTAB as a binder (n=3)

AuNPs size (nm)	Zeta potential (mV)	Wavelength (nm)	Range (ppb)	LOD (ppb)
16.5	-41.7	520	1–100	16.9
32.1	-46.1	525	1–100	25.1
43.7	-14.5	530	1–100	31.4
71.0	-25.6	540	1–100	86.3

Table S2. Comparison of CTAB as a binder and NaCl as ionic strength for the detection of As^{3+} ion using aptamer-AuNPs-based aptasensor

Samples	CTAB	NaCl
AuNPs changes to purple (mM)	1.1	50.0
AuNPs changes to blue (mM)	1.6	70.0
Reaction time (min)	<5	<10
Concentration range	0.4–1.6 µM	1–150 mM
Temperature (°C)	24–25	Room temperature
Size (nm)	16.53	32.10
Linear range (ppb)	1–100	1–100
LOD (ppb)	16.90	22.75

Table S3. Performance of present method for the detection of As^{3+} ion in water and cosmetic samples

Added (As^{3+} ion, ppb)	**Tap water**		**Lake water**		**Cosmetic sample**	
	Found‡ (ppb)	Recovery (%)	Found‡ (ppb)	Recovery (%)	Found‡ (ppb)	Recovery (%)
1.00	0.99±0.0040	99.00	1.01±0.0005	101.00	0.96±0.0003	96.00
10.00	10.01±0.0048	100.10	10.02±0.0008	100.20	10.20±0.0002	102.00
20.00	20.02±0.0039	100.02	19.96±0.0009	99.80	20.01±0.0049	101.00
40.00	40.00±0.0056	100.00	40.04±0.0009	100.40	38.24±0.0054	95.60
60.00	60.20±0.0061	100.20	59.54±0.0008	99.20	58.80±0.0013	98.00
80.00	79.60±0.0034	99.50	79.84±0.0008	99.80	80.60±0.0028	107.30
100.00	101.20±0.0028	101.20	98.90±0.0006	98.90	100.10±0.007	100.10

‡Mean±standard deviation (n=3)