Supplementary Information

Biogenic Synthesis of Dual-emission Chlorophyll-rich Carbon Quantum Dots for Detection of Heavy Toxic Metal Ions – Hg (II) and As (III) in Water and Mouse Fibroblast Cell Line NIH-3T3

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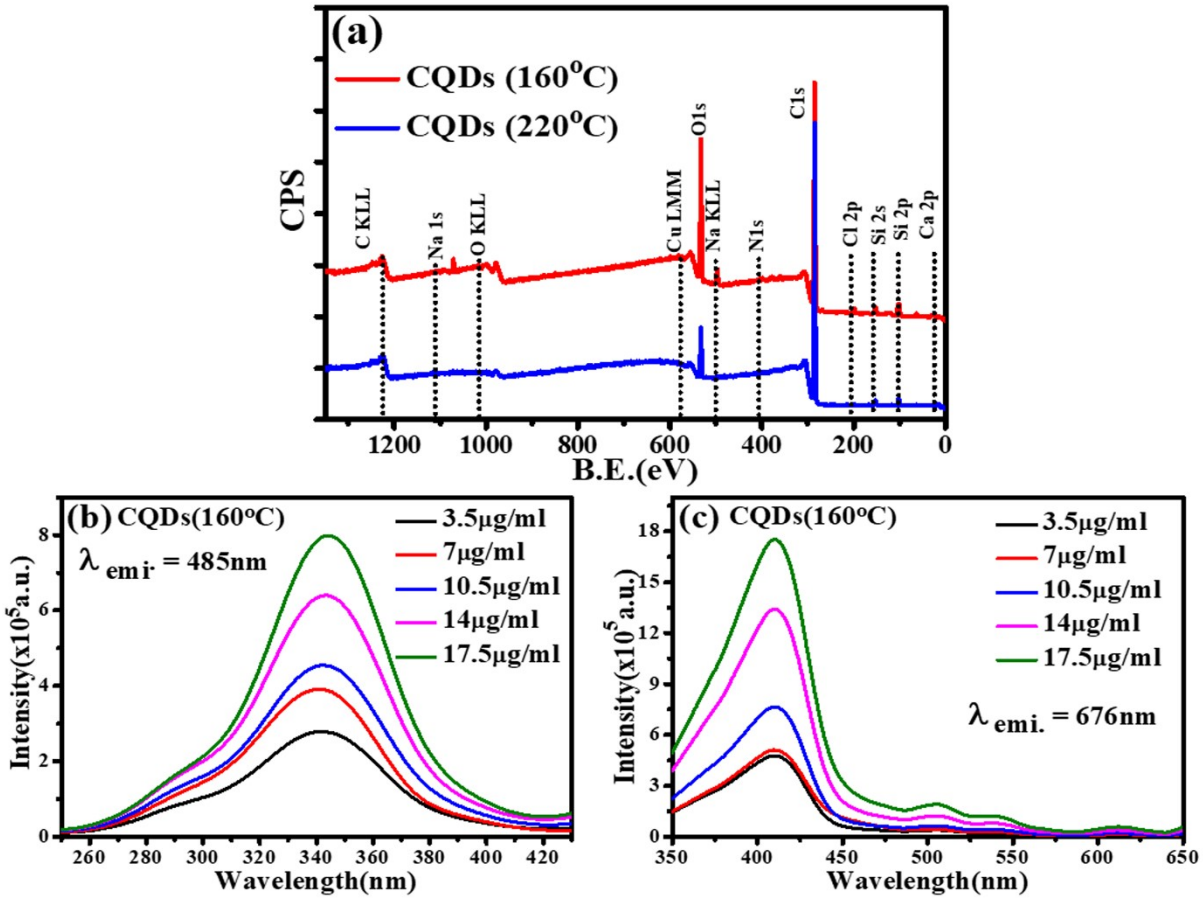

Fig.S1. (a) XPS survey spectra of CQDs as synthesized temperature at 160°C and 220°C. (b), and (c) Shows the concentration dependent excitation spectra of CQDs160 corresponding emission wavelength as 485nm and 676nm.

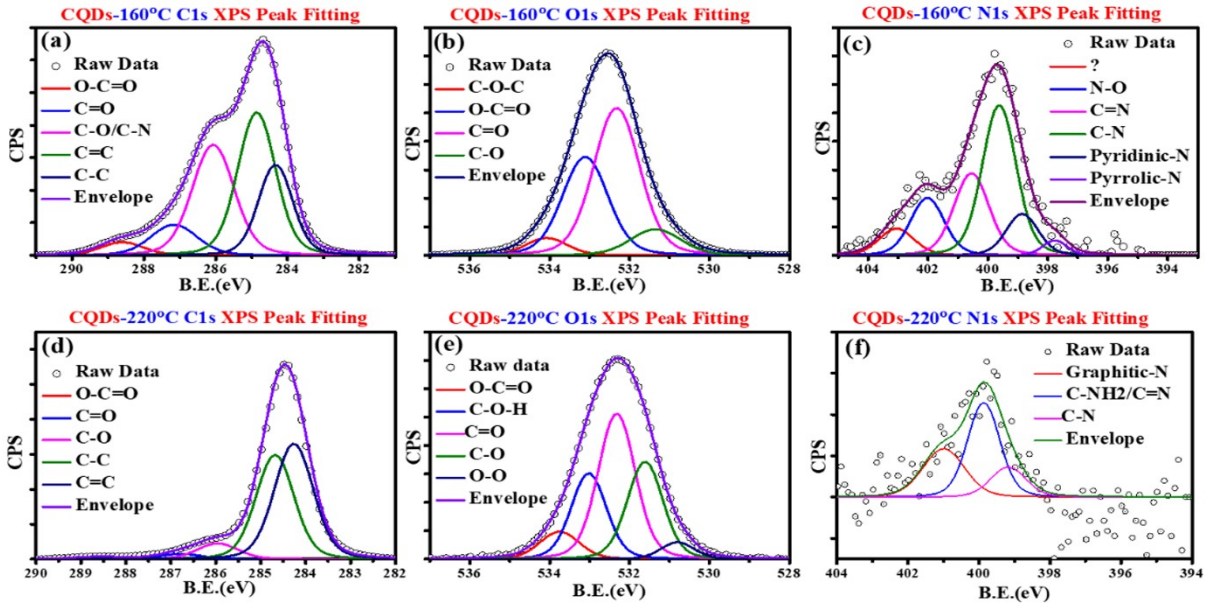

Fig.S2. Deconvolution of photoelectron XPS peaks with different synthesized temperature. (a), (b), and (c) shows the deconvolution of C1s, O1s, and N1s photoelectron spectra of as synthesized CQDs at 160°C. (d), (e), and (f) shows the deconvolution of C1s, O1s, and N1s photoelectron spectra of as synthesized CQDs at 220°C.

(a)

C1s	CQDs-160°C		CQDs-220°C	
	Position (eV)	% Area	Position (eV)	% Area
O-C=O	288.6	3.7	288.6	1.0
C=O	287.1	9.3	286.8	2.3
C-O/C-N	286.0	30.7	286.0	6.9
C=C	284.6	30.8	284.7	42.9
C-C	284.3	20.4	284.3	47.9

(b)

O1s	CQDs-160°C		CQDs-220°C	
	Position (eV)	% Area	Position (eV)	% Area
C-O-C	534.15	5.8	-	-
O-C=O	533.55	9.9	533.78	7.9
C-O-H	532.9	32.8	532.98	22.3
C=O	532.2	44.5	532.2	39.9
C-O	531.2	7.5	531.58	25.6
O-O	-	-	530.78	4.1

Table S1: (a), and (b) The C1s, O1s peak positions obtained after peak fitting. The error ± 0.2 eV for peak C1s and O1s peak of CQDs at different synthesis temperature.

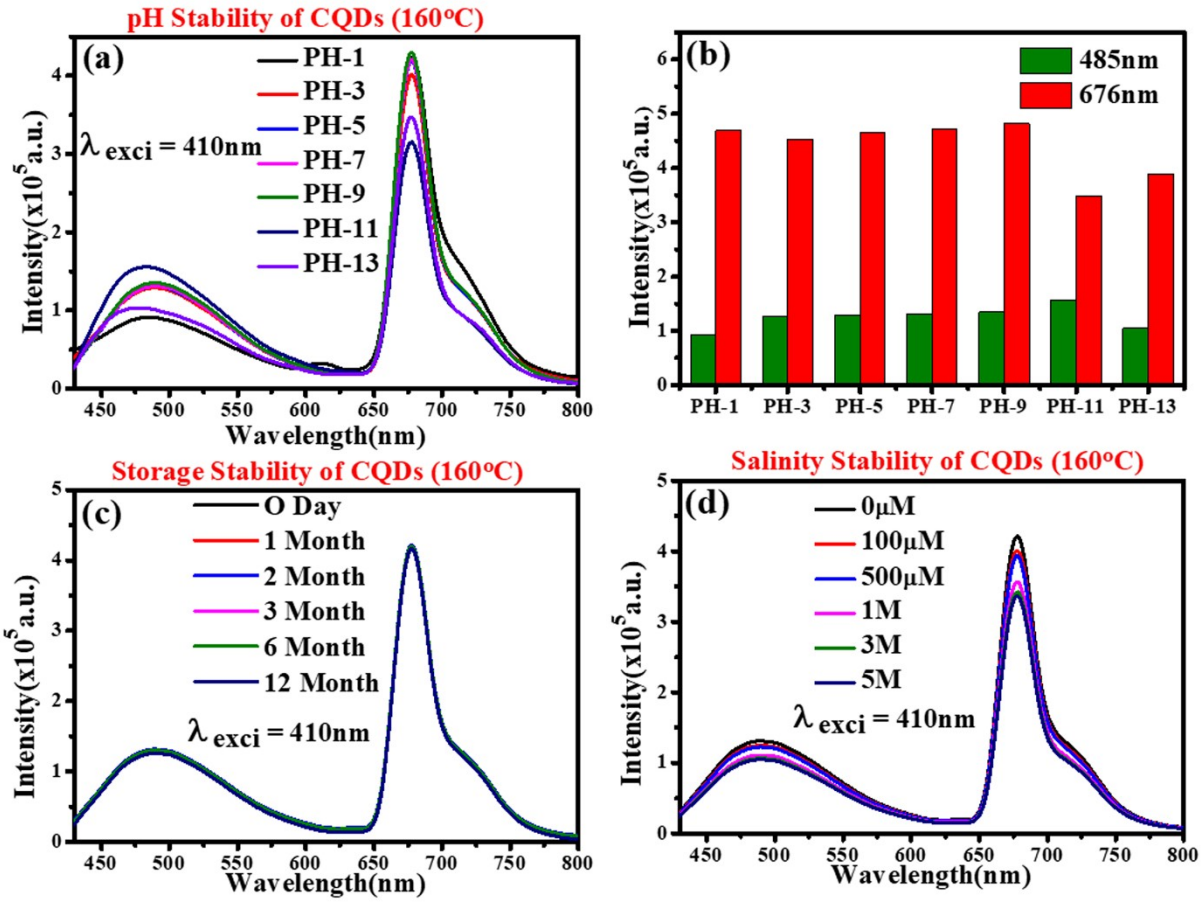

Fig.S3. Stability measurement of CQDs160. (a) measurement of PL emission at different pH value, (b) Bar diagram of pH stability of CQDs160 corresponding 485nm and 676nm. (c) PL emission stability of CQDs160 with respect to storage time. (d) Salinity stability of CQDs160 at different molarity value.

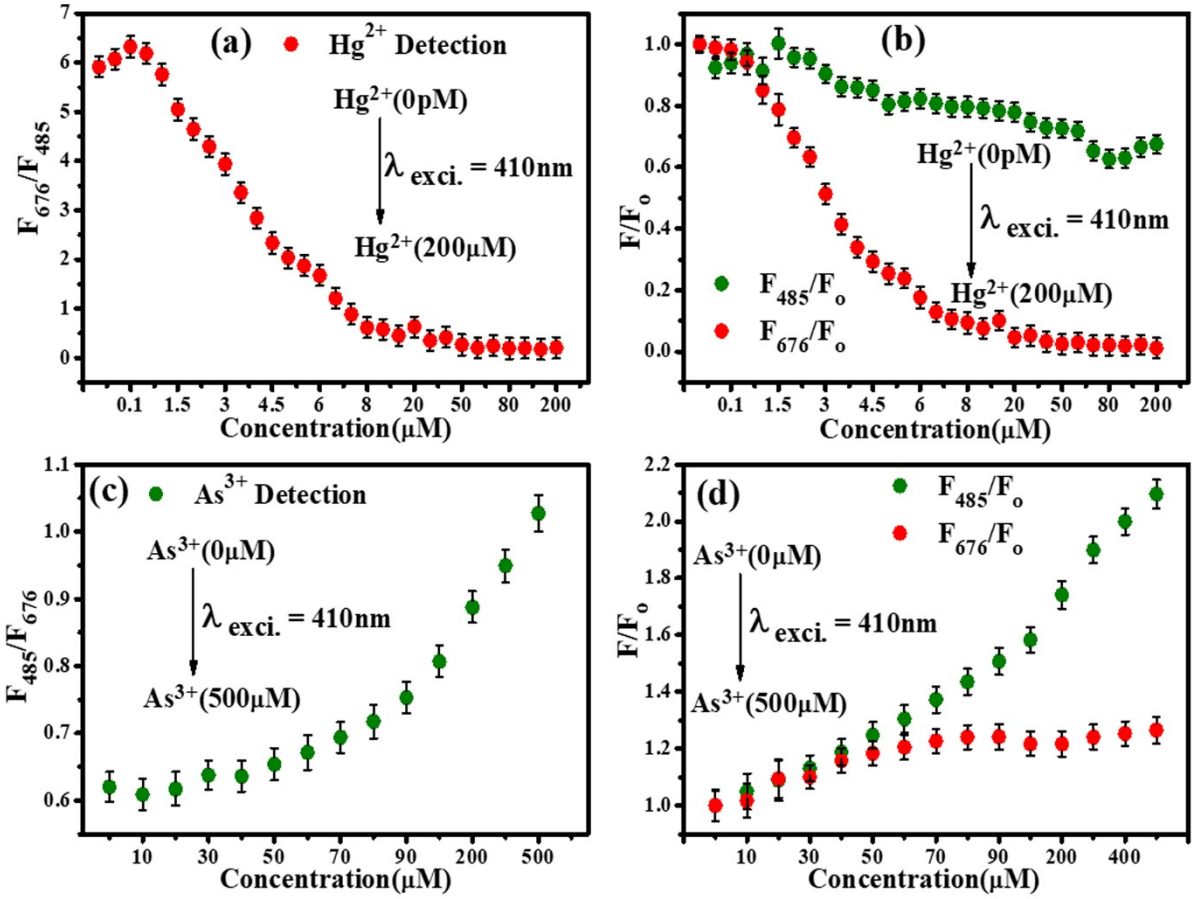

Fig.S4. Intensity ratio plot of CQD160. (a) F_{676}/F_{485} vs Concentration plot of Hg^{2+} detection. (b) shows the F/F_0 vs concentration graph corresponding 485 nm and 676 nm peaks with addition of Hg^{2+} ions. (c) F_{485}/F_{676} vs Concentration plot of As^{3+}detection. (d) shows the F/F_0 vs concentration graph corresponding 485 nm and 676 nm peaks with addition of As^{3+} ions.

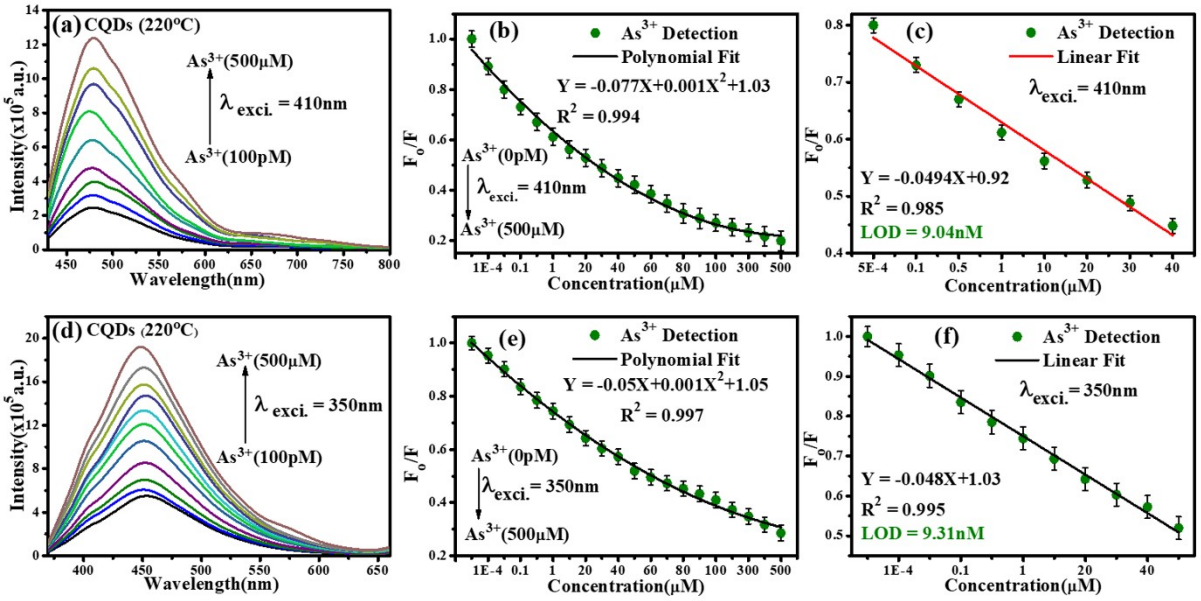

Fig.S5. (a) PL emission spectra of CQD220 derived by As^{3+} by using excitation wavelength as 410nm, (b) showing the polynomial fitting between F_o/F vs concentration, (c) plotting the linear range of As^{3+} detection and find the LOD value as 9.04nM, (d) PL emission spectra of CQD220 derived by As^{3+} by using excitation wavelength as 350nm, (e) showing the polynomial fitting graph between F_o/F vs concentration, (f) plotting the linear range of As^{3+} detection and find the LOD value as 9.31nM.

(a)

Concentration Hg^{2+}(μM)	τ_1(ns)	τ_2(ns)	τ_{av}(ns)	τ_o/τ_{av}
0	1.127	4.803	2.12	1
1	1.059	4.685	1.98	1.070
3	0.961	4.429	1.70	1.247
5	0.848	4.258	1.65	1.284

(b)

Concentration As^{3+}(μM)	τ_1(ns)	τ_2(ns)	τ_{av}(ns)	τ_o/τ_{av}
0	0.436	3.529	1.55	1
10	0.482	3.82	1.81	0.854
30	0.679	4.25	2.37	0.653
50	0.961	4.826	3.68	0.421

Table S2. (a), and (b) Decay time of CQDs160 with and without addition of Hg^{2+} and As^{3+} ions.

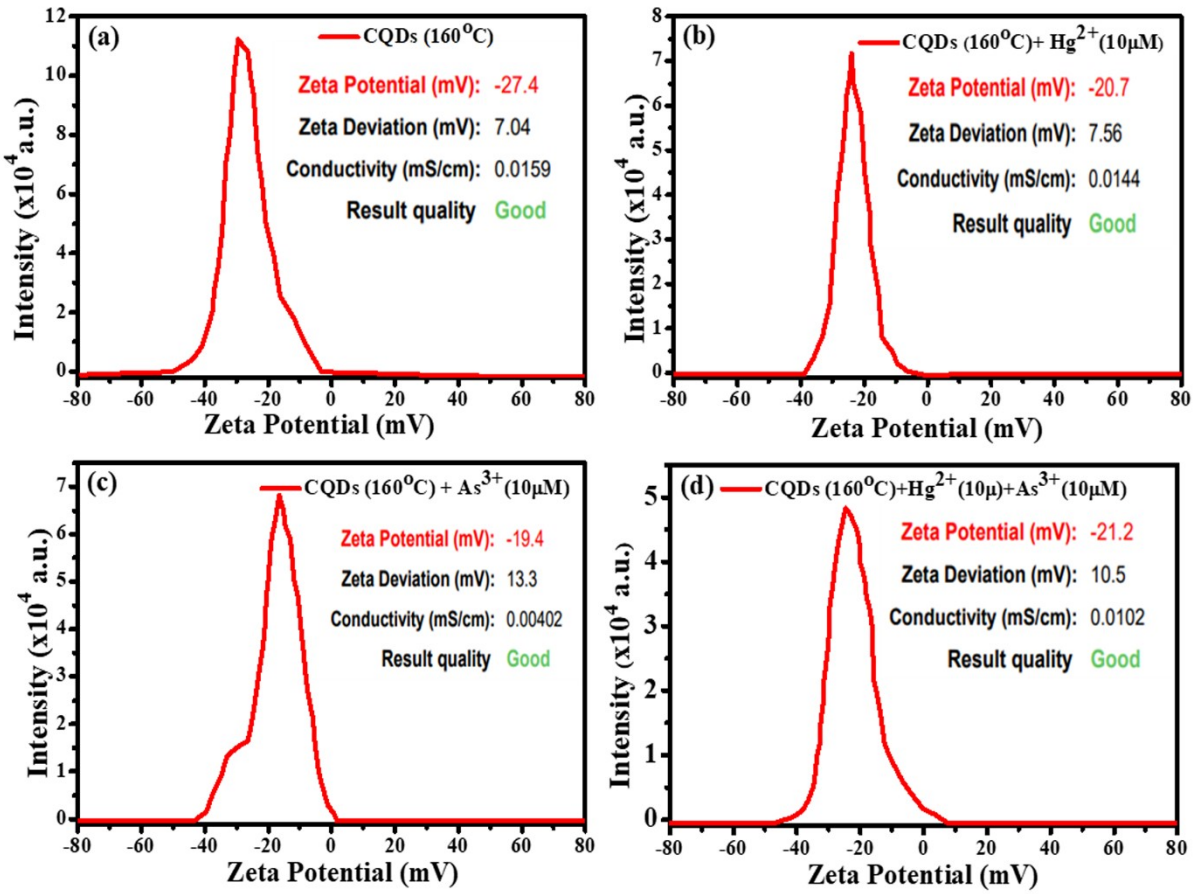

Fig. S6. Zeta potential behaviour with metal ions. (a) Zeta potential of synthesized CQDs160 in aqueous medium. (b), and (c) shows the zeta potential of CQDs160 with Hg^{2+}(10μM) and As^{3+}(10μM). (d) zeta potential of CQDs160 with mixed Hg^{2+}(10μM) and As^{3+}(10μM).

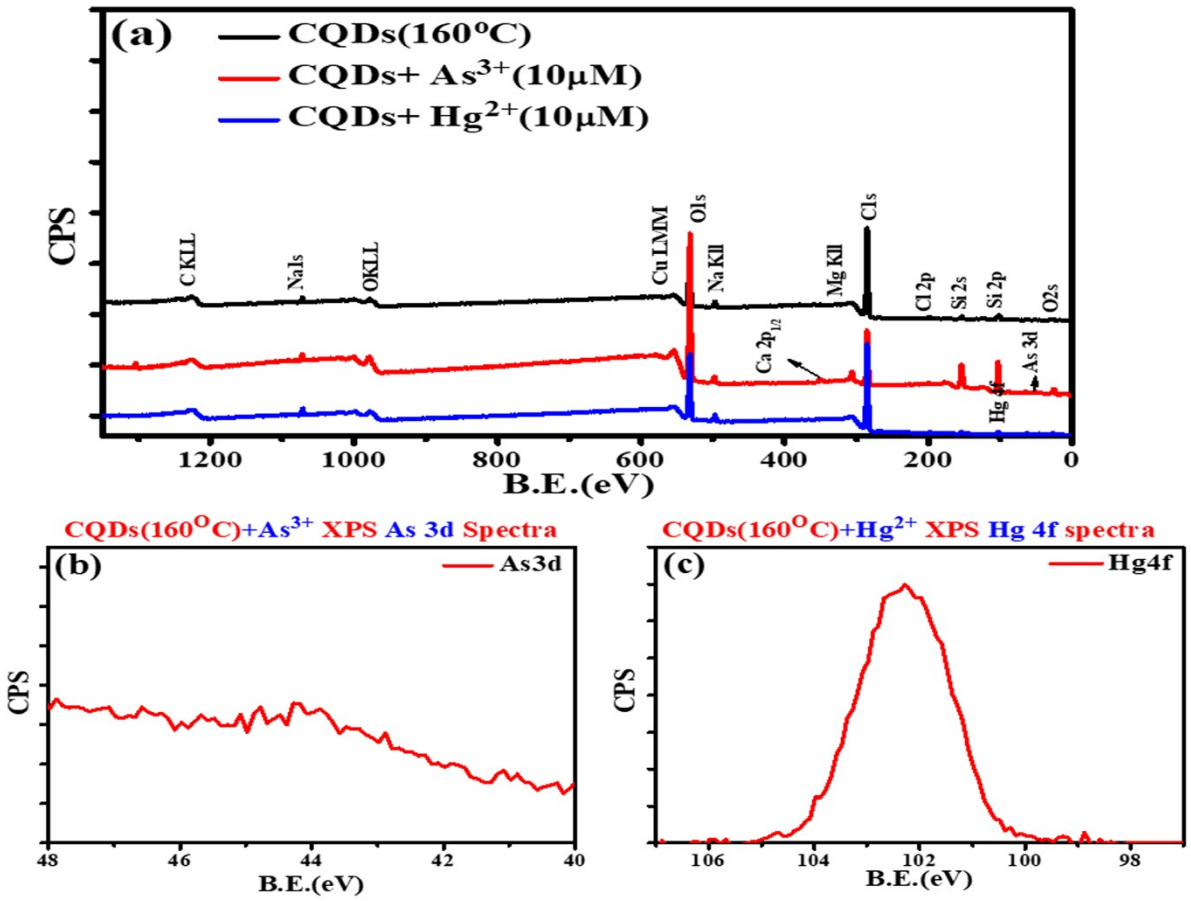

Fig. S7. (a) XPS survey spectrum of CQDs160 synthesized with metal ions (As^{3+} and Hg^{2+})in range 0 to 1350eV. (b) High resolution XPS spectra of As3d. (c) High resolution XPS spectra of Hg 4f.

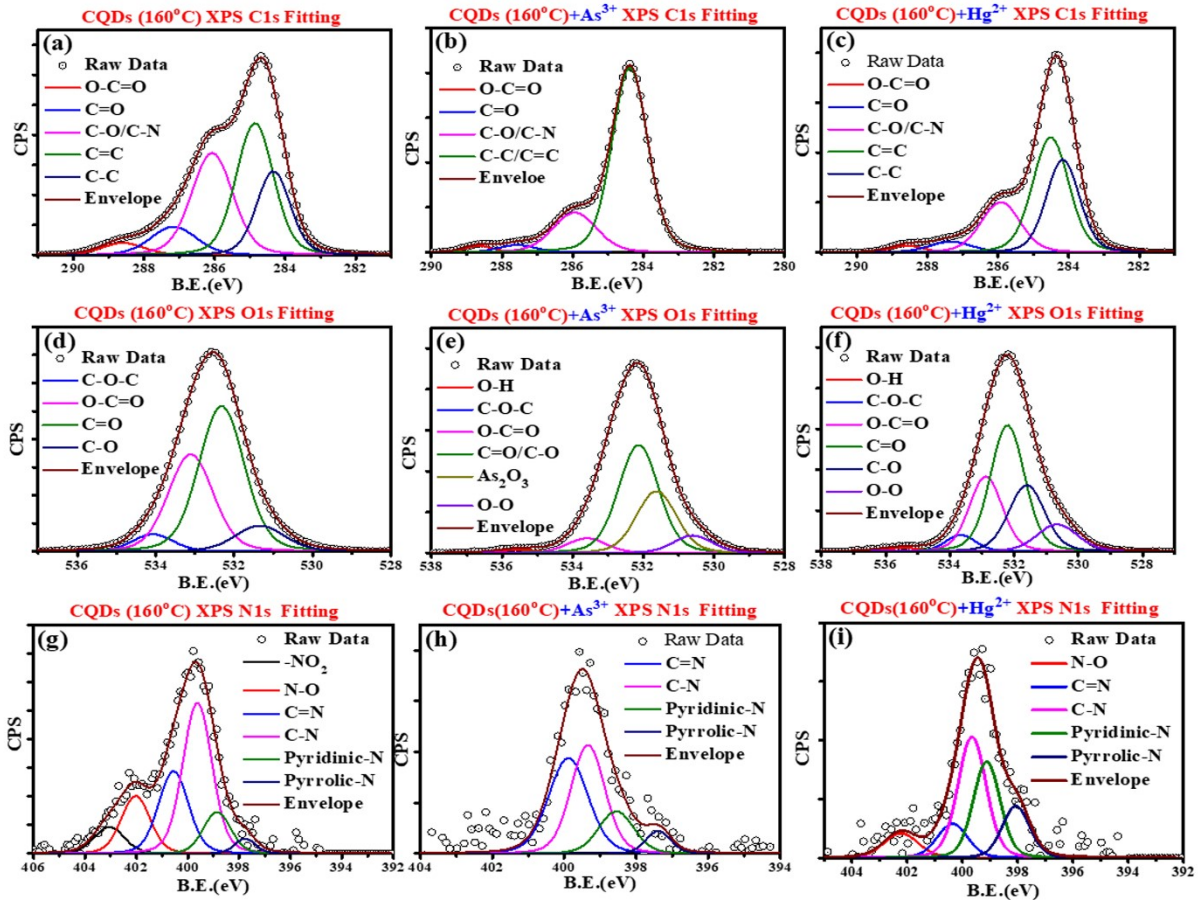

Fig. S8. Deconvolution of photoelectron XPS peaks with metal As^{3+} and Hg^{2+} ions. (a) CQDs160, (b) CQDs160 + As^{3+}(10μM), (c) CQDs160 + Hg^{2+}(10μM) shows the deconvolution of C1s photoelectron spectra. (d) CQDs160, (e) CQDs160 + As^{3+}(10μM), (f) CQDs160 + Hg^{2+}(10μM) shows the deconvolution of O1s photoelectron spectra. (g) CQDs160, (h) CQDs160 + As^{3+}(10μM), (i) CQDs160 + Hg^{2+}(10μM) shows the deconvolution of N1s photoelectron spectra.

(a)

C1s	CQDs-160°C+As3+		CQDs-160°C-Hg2+	
	Position (eV)	% Area	Position (eV)	% Area
C-O-C	--	--		
O-C=O	288.7	2.03	288.6	2.22
C-O-H	--	--		
C=O	287.6	3.08	287.4	4.56
C-O/C-N	285.9	19.90	285.9	19.98
C=C/C-C	284.4	74.99	284.5/284.2	42.14/31.09

(b)

O1s	CQDs-160°C+As3+		CQDs-160°C-Hg2+	
	Position (eV)	% Area	Position (eV)	% Area
O-H	535.5	1.11	535.5	1.24
C-O-C	533.6	5.08	533.7	4.50
O-C=O	532.8	27.68	532.9	22.69
C-O-H				
C=O/C-O	532.2	38.23	532.2	39.76
As_2O_3/ HG-O?	531.6	21.86	531.6	21.81
O-O	530.6	6.05	530.6	9.99

(c)

N1s	CQDs-160°C+As3+		CQDs-160°C-Hg2+	
	Position (eV)	% Area	Position (eV)	% Area
N-O	--	--	402.2	9.12
C=N	399.9	39.71	400.3	11.20
C-N	399.3	38.70	399.6	36.67
Pyridinic-N	398.6	15.67	399.1	27.63
Pyrrolic-N	397.4	5.92	398.0	15.38

Table S3. (a) C1s, (b) O1s, (c) N1s peak positions and area percentage obtained after peak fitting of CQD160 with Hg^{2+} and As^{3+}. The error ± 0.2 eV for peak C1s, O1s, and N1s peak of CQDs at 160°C synthesis temperature.