Electronic Supplementary Information

RNA-mediated fluorescent colloidal CdSe nanostructures in aqueous medium - analysis of Cd^{2+} induced folding of RNA associated with morphological transformation (0D to 1D), change in photophysics and selective Hg^{2+} sensing

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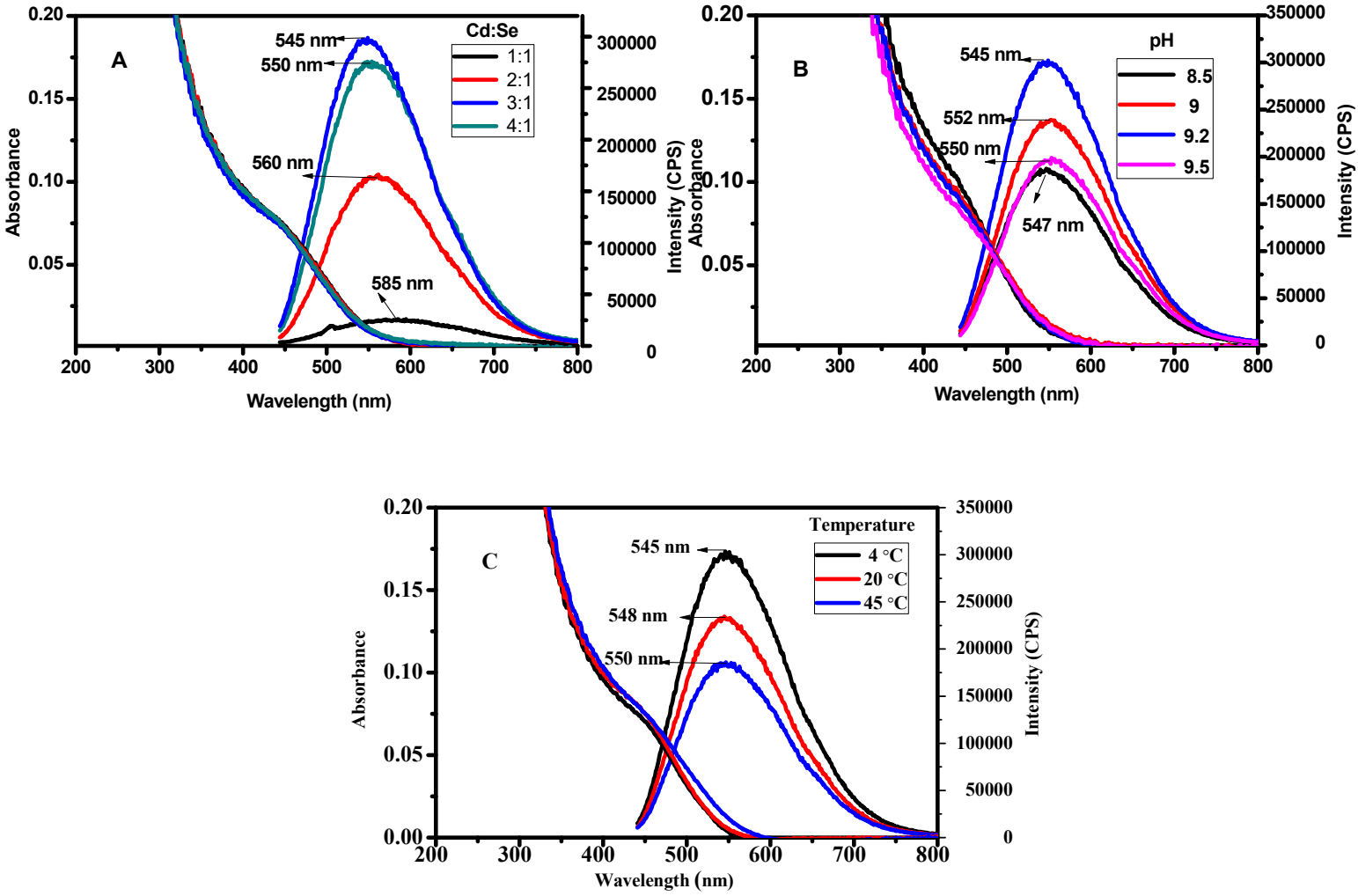


Fig. S1 Effect on absorbance and fluorescence behaviour of CdSe NPs for: different stoichiometric ratio of Cd/Se from 1:1-4:1 (A), variation in pH from 8.5-9.5 (B), variation in temperature (C).

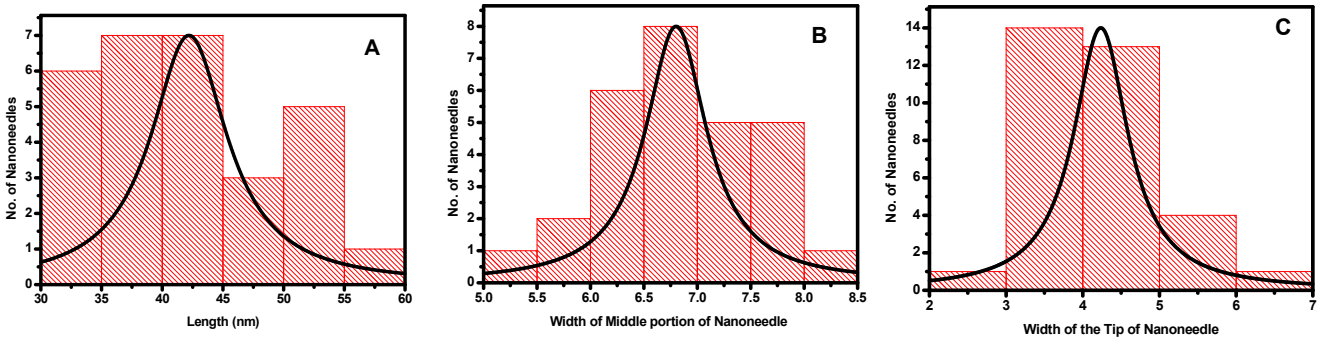


Fig. S2 Histograms for the average dimensions of nanoneedles (nm): length (A), middle portion (B) and tip (C)

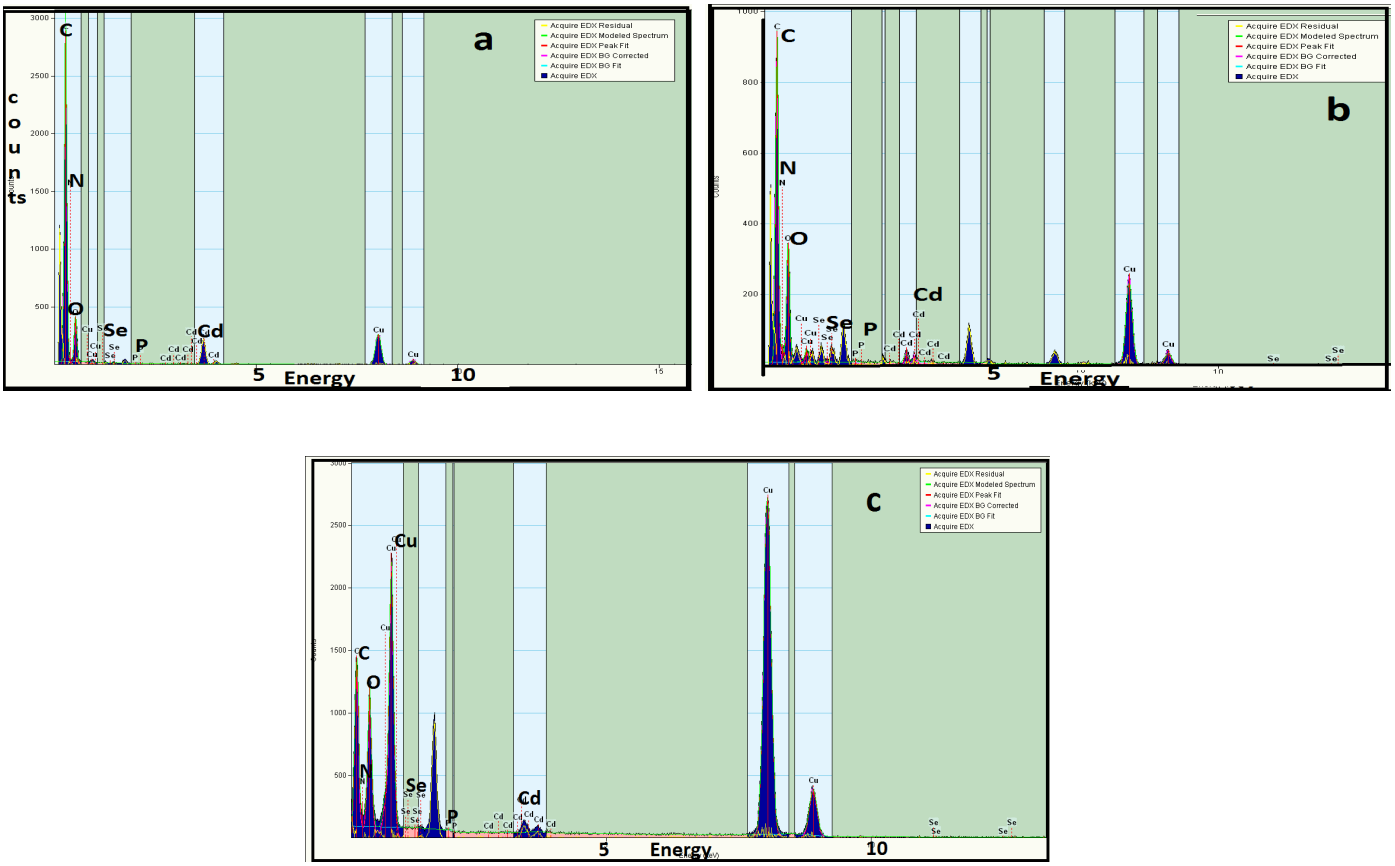
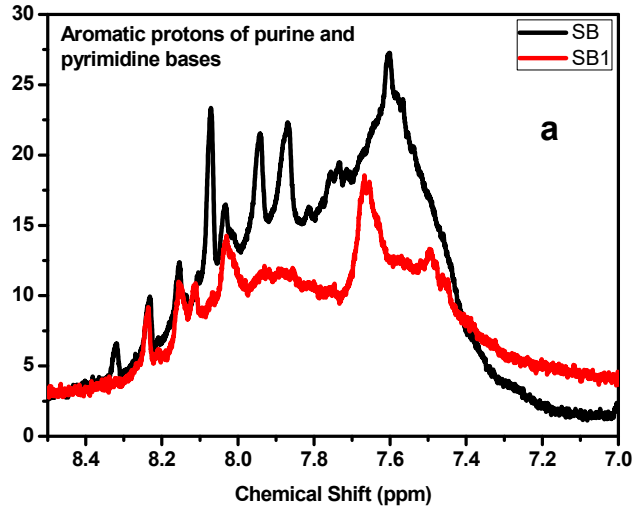
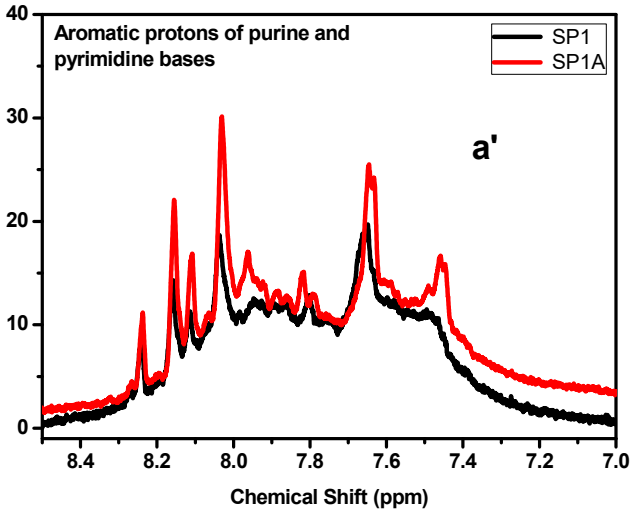
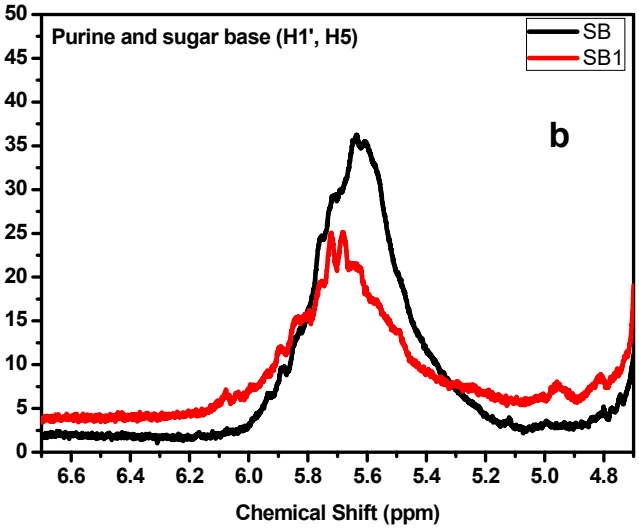
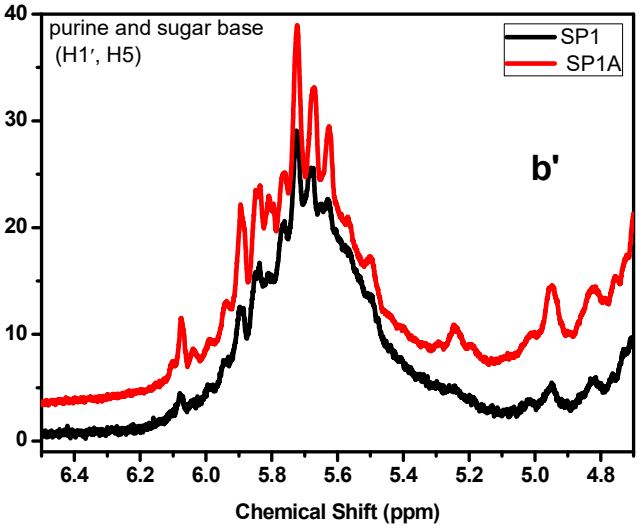


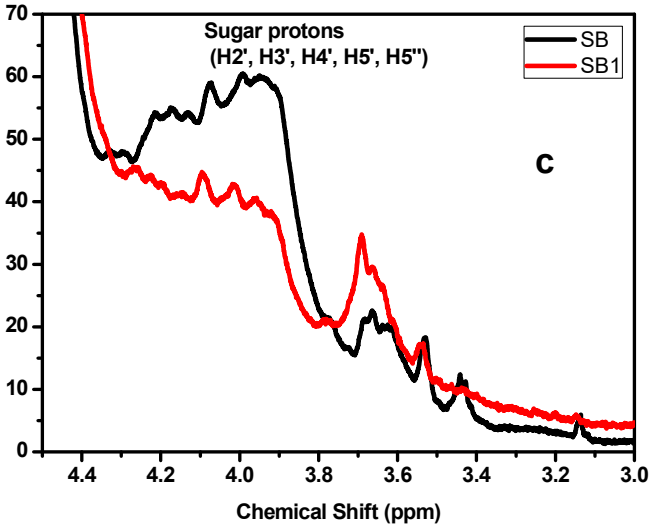
Fig. S3 EDS analysis of SP1 recorded after different day(s) of aging: (a) 0, (b) 10, (c) 30.

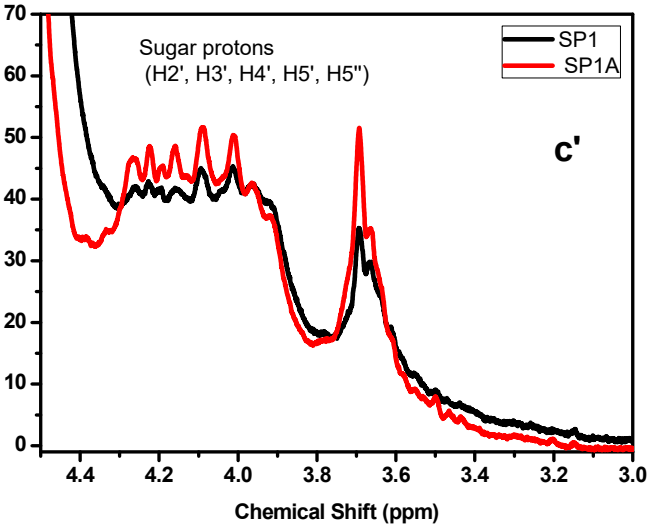

Aromatic protons of purine and pyrimidine bases
SB
SB1
a
Chemical Shift (ppm)


Aromatic protons of purine and pyrimidine bases
SP1
SP1A
a'
Chemical Shift (ppm)


Purine and sugar base (H1', H5)
SB
SB1
b
Chemical Shift (ppm)


purine and sugar base (H1′, H5)
SP1
SP1A
b'
Chemical Shift (ppm)


Sugar protons (H2', H3', H4', H5', H5'')
SB
SB1
c
Chemical Shift (ppm)


Sugar protons (H2', H3', H4', H5', H5'')
SP1
SP1A
c'
Chemical Shift (ppm)

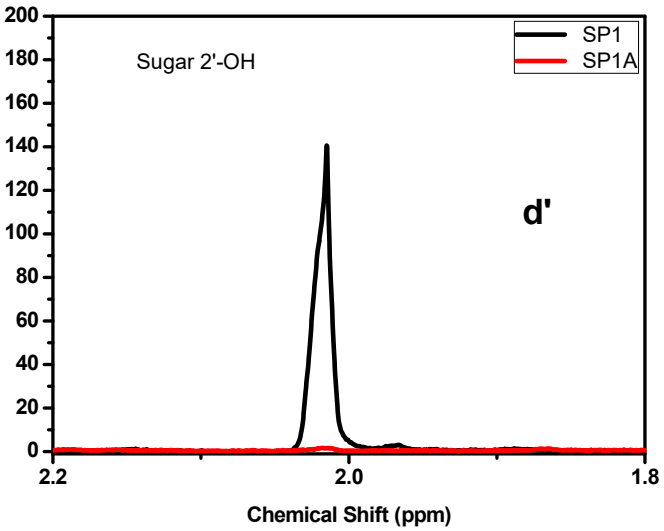


Fig. S4 Spectral changes in ^{1}H NMR spectra of SB with SB1 (a-c) and SP1 with SP1A (a'-d') for different chemical shift regions**.**

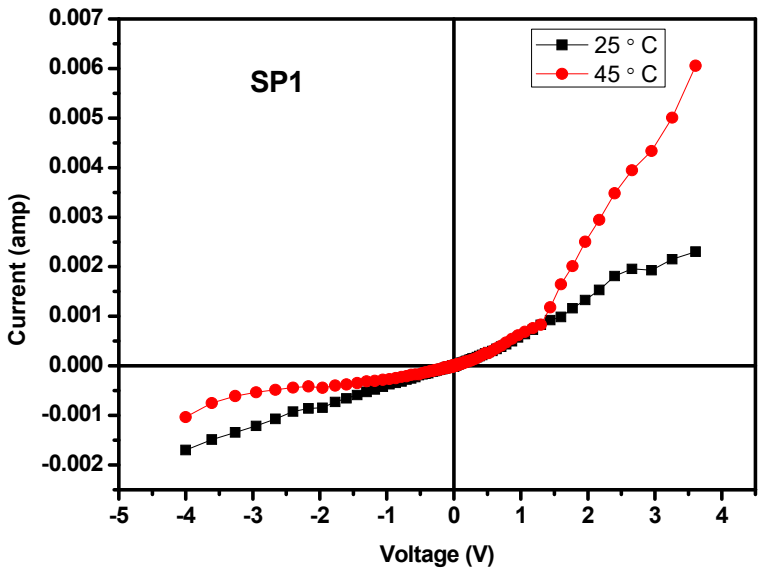


Fig. S5 I-V measurements of SP1 at different temperatures.

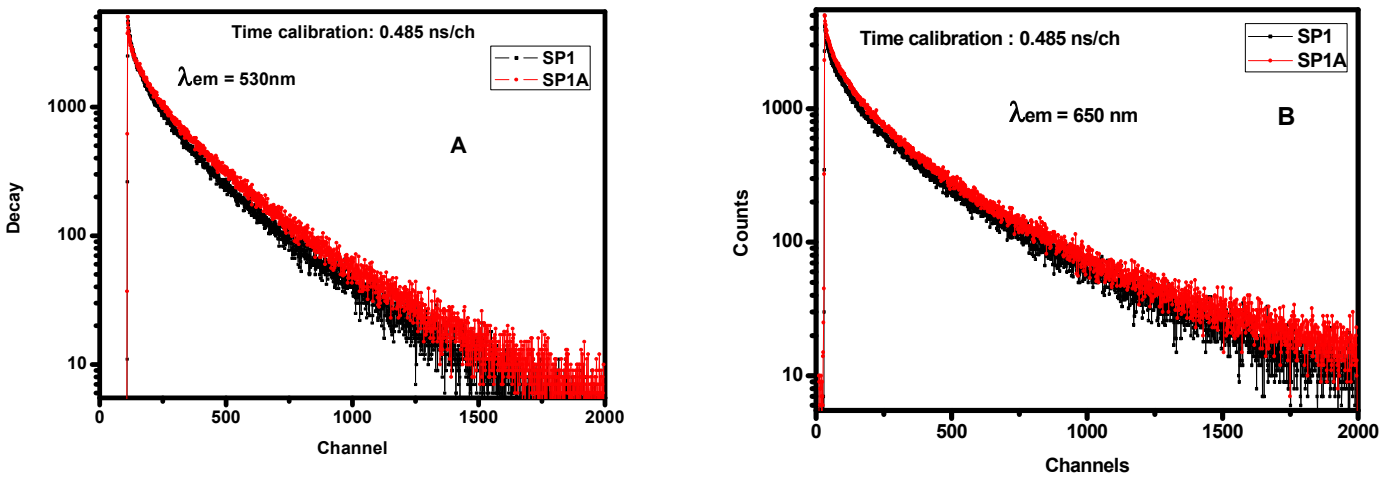


Fig. S6 Fluorescence lifetime decay of SP1 and SP1A at λ_{em} = 530 nm (A) and 650 nm (B) (λ_{ex}= 440nm).

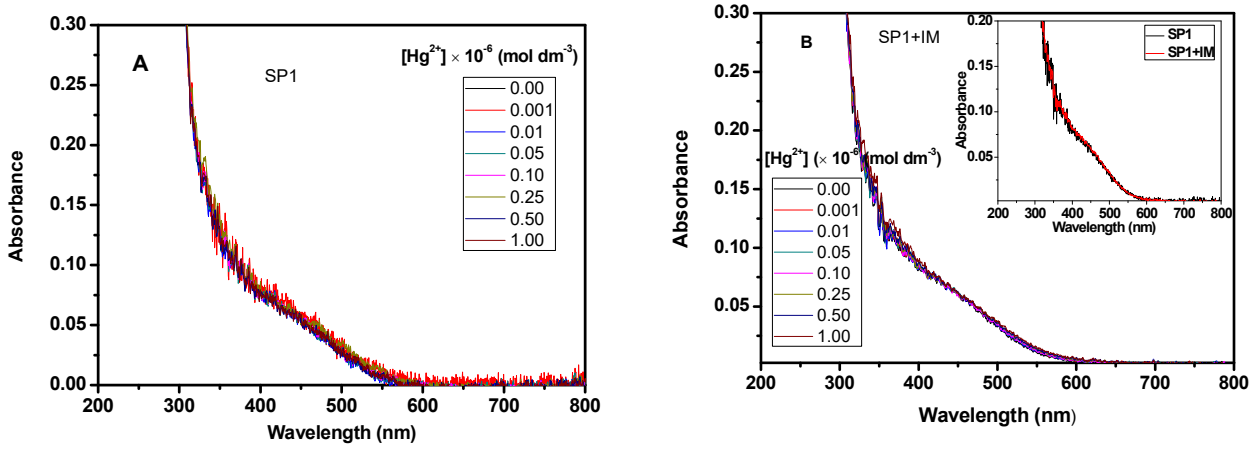


Fig. S7 A: Absorption spectra of SP1 in the presence of varied amount of $[Hg^{2+}]$(0-5 × 10^{-6} mol dm^{-3}), (B) Absorption spectra of SP1 containing mixture of other metals (IM) with varied concentration of $[Hg^{2+}]$(0-5 × 10^{-6} mol dm^{-3});), Inset: Absorption spectra of SP1 and SP1 containing IM.

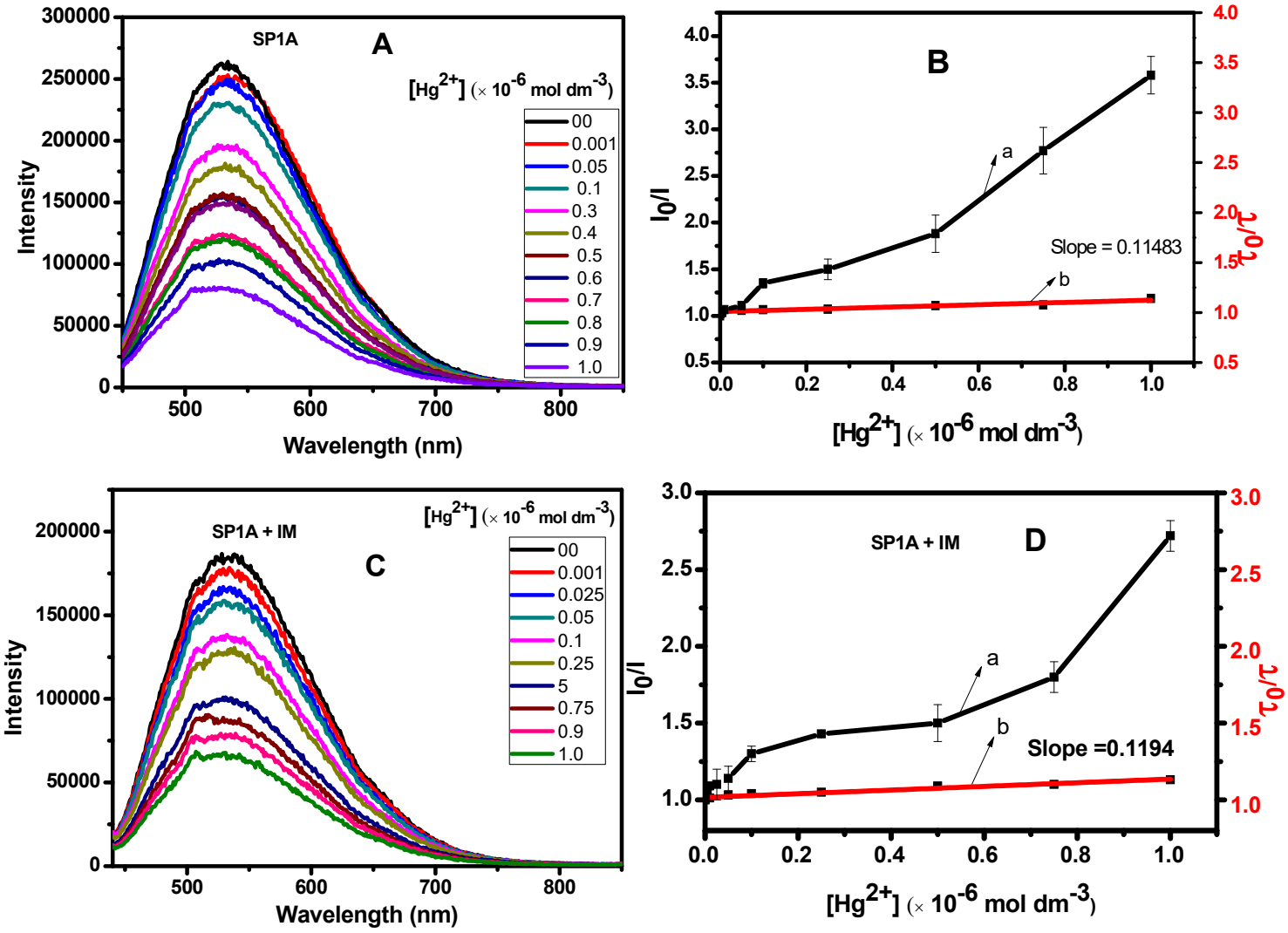


Fig. S8: A - Fluorescence spectra of SP1A with varied concentration of $[Hg^{2+}]$ (mol dm^{-3}) (0 – 1 × 10^{-6}); **B-** Stern Volmer plots: I_0/I vs $[Hg^{2+}]$ (Curve a); τ_0/τ vs $[Hg^{2+}]$ (curve b)**. C**- Fluorescence spectra of SP1A with varied concentration of $[Hg^{2+}]$ (mol dm^{-3}) (0 – 1 × 10^{-6}) in the presence of ionic mixture; **D-** Stern Volmer plots: I_0/I vs $[Hg^{2+}]$ (Curve a); τ_0/τ vs $[Hg^{2+}]$ (curve b)**.**

Fluorescence microscopic images

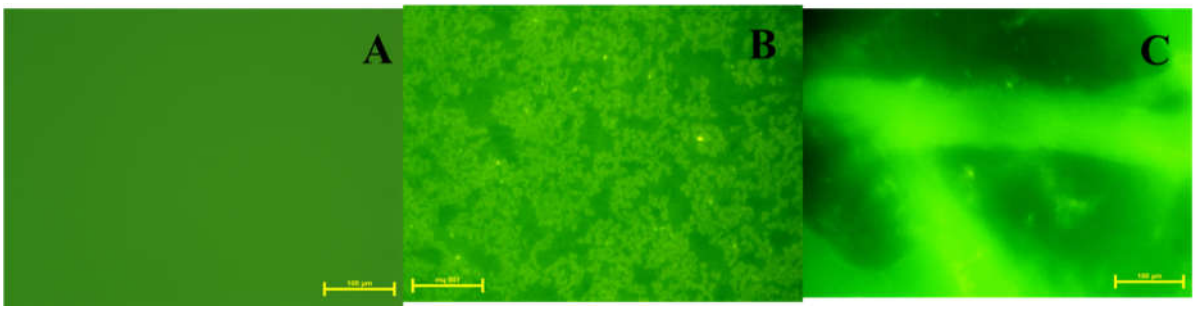


Fig. S9 Fluorescence microscopic images: (A) Blank slide, (B) 3 days aged SP1, (C) 30 days aged SP1

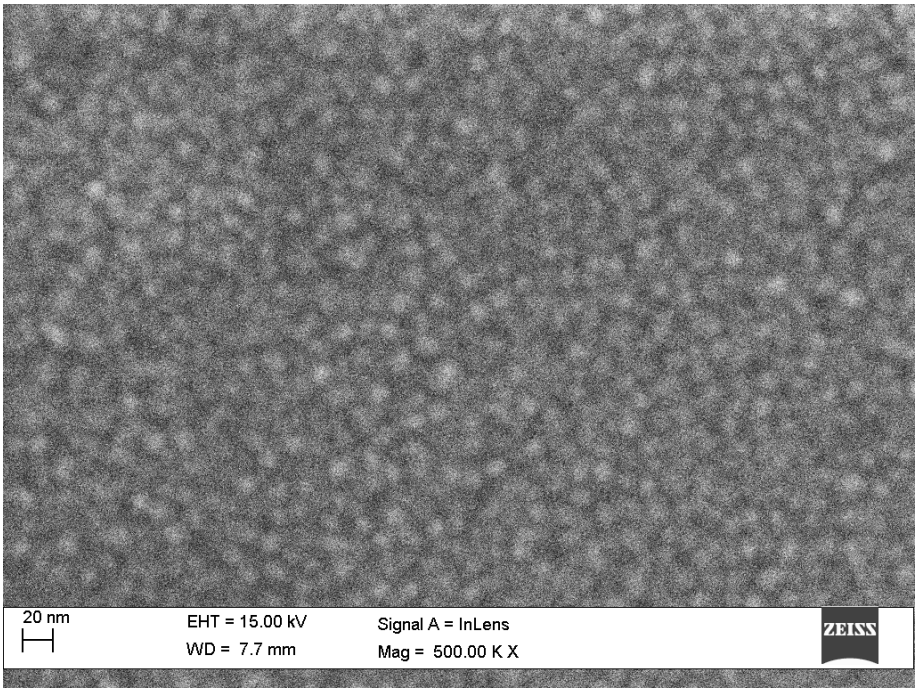


Fig. S10 FESEM image of CdSe with Cd:Se =1:1

Table S1. Circular dichroism spectral data of SB1, SP1 and SP1A.

Sample	Peak 1	Peak 2	Peak 3
SB1	X= 209.3 Y= -5.27	X= 237.2 Y= -1.26	X = 274.8 Y= 3.41
SP1	X= 209.9 Y= -4.74	X= 240.4 Y= -1.73	X= 273.5 Y= 3.94
SP1A	X=208.9 Y= -3.99	X= 240.0 Y= (-1.75)	X= 267.0 Y= 4.05

Table S2. Fluorescence lifetime data at different Cd/Se ratio from 1:1 to 4:1, (λ_{ex} = 440nm)

Molar Ratio	Lifetime (ns)							
	τ_1	Emission %	τ_2	Emission%	τ_3	Emission%	<τ>	χ2
1:1	1.18 (0.85)	28.95	13 (0.094)	34.87	83.6 (0.015)	36.18	35	1.4
2:1	2.62 (0.33)	12.63	29.7 (0.193)	35.89	123.0 (0.113)	51.49	71	1.6
3:1	2.86 0.34	8.64	33.4 (0.103)	30.95	137.0 (0.049)	60.43	92	1.3
4:1	3.42 (0.34)	7.53	34.9 (0.1858)	40.99	137.0 ns (0.085)	51.48	81	1.2

(Values in bracket is pre-exponential factor corresponding to respective τ)

Table S3. Fluorescence lifetime decay data at different amount of RNA (0.005-0.025 g/100 ml), (λ_{ex} = 440 nm)

RNA (g/100 ml)	Lifetime (ns)							
	τ_1	Emission %	τ_2	Emission %	τ_3	Emission %	< τ >	χ2
0.005	4.6 (0.318)	9.02	35.8 (0.17)	38.95	136.0 (0.062)	52.03	85.1	1.44
0.01	3.76 (0.42)	8.56	36.9 (0.25)	32.42	134.0 (0.10)	59.02	88.8	1.3
0.015	2.86 (0.34)	8.64	33.4 (0.10)	30.95	137.0 (0.049)	60.43	92	1.3
0.025	4.7 (0.34)	7.35	38.06 (0.22)	39.30	135.0 (0.083)	53.35	86.8	1.20

(Values in bracket is pre-exponential factor corresponding to respective τ)

Table S4. Fluorescence lifetime decay data at different pH, (λ_{ex} = 440 nm).

pH	Emission Lifetime (ns) at 545 nm							
	τ_1	Emission %	τ_2	Emission %	τ_3	Emission %	<t>	$\chi 2$
8.5	3.4 (0.38)	5.73	32.5 (0.26)	38.10	125.0 (0.10)	56.18	82.7	1.3
9	4.97 (0.46)	7.25	37.2 (0.34)	40.15	131.0 (0.125)	52.60	84	1.2
9.2	2.86 (0.34)	8.64	33.4 (0.10)	30.95	137.0 (0.049)	60.43	92	1.3
9.5	4.2 (0.43)	8.71	33.2 (0.24)	39.30	125.0 0.081	50.50	77.3	1.20

(Values in bracket is pre-exponential factor corresponding to respective τ)

Table S5. Fluorescence lifetime decay data at different concentration of Hg^{2+}, (λ_{ex} = 440 nm).

$[Hg^{2+}]$ × 10-6 mol/dm^3	Emission Lifetime (ns) at 545 nm							
	τ_1	Emission %	τ_2	Emission %	τ_3	Emission %	<t>	$\chi 2$
0.00	5.73 (0.50)	6.63	40.2 (0.43)	40.04	141.1 (0.16)	53.33	91.3	1.3
0.001	4.37 (0.57)	6.54	37.6 (0.40)	39.33	137.0 (0.15)	54.13	89.1	1.2
0.005	4.01 (0.59)	6.57	36.5 (0.39)	39.33	136.0 (0.145)	54.1	88.5	1.3
0.01	3.97 (0.60)	6.61	35.8 (0.38)	38.01	134.0 (0.15)	55.38	88.2	1.2
0.05	3.50 (0.62)	6.64	33.2 (0.37)	37.64	129.8 (0.142)	55.72	85.4	1.2
0.1	2.99 (0.70)	7.96	29.4 (0.34)	37.7	122.8 (0.12)	54.34	78.7	1.2
0.5	2.71 (0.74)	9.23	26.5 (0.30)	37.20	117.0 (0.10)	53.58	73.2	1.2
1	1.25 (0.68)	14.54	16.8 (0.105)	30.16	106.6 0.030	55.30	64	1.3

(Values in bracket is pre-exponential factor corresponding to respective τ)

Table S6. Fluorescence lifetime decay data of SP1 containing IM (5 μM) at different concentration of Hg^{2+}, (λ_{ex} = 440 nm).

$[Hg^{2+}] \times 10^{-6}$ (mol/dm^3)	Emission Lifetime (ns) at 545 nm							
	τ_1	Emission %	τ_2	Emission %	τ_3	Emission %	<t>	$\chi 2$
00	4.37 (0.57)	6.54	37.60 (0.40)	39.33	137.2 (0.15)	54.14	89.0	1.2
0.001	4.23 (0.53)	6.68	35.8 (0.375)	39.33	138 (0.133)	54	88.2	1.3
0.005	3.40 (0.60)	6.86	33.3 (0.34)	38.15	133 (0.123)	54.99	86.2	1.3
0.01	3.83 (0.28)	8.13	33.17 (0.157)	39.18	132.8 (0.053)	52.69	83.5	1.2
0.05	3.05 (0.40)	6.64	29.75 (0.20)	36.01	124.7 (0.078)	56.84	82.5	1.3
0.1	2.11 (0.41)	7.12	25.96 (0.16)	34.94	119.8 (0.059)	57.94	79.2	1.4
0.5	1.89 (0.42)	6.56	24.3 (0.165)	33.0	114.8 (0.064)	60.44	77.6	1.31
1	1.86 (0.84)	9.52	23.4 (0.25)	36.94	114.8 (0.076)	53.54	70.7	1.3

(Values in bracket is pre-exponential factor corresponding to respective τ)