Multifunctional CdSNPs@ZIF-8: Potential Antibacterial Agent against GFP-expressing *Escherichia coli* and *Staphylococcus aureus* and Efficient Photocatalyst for Degradation of Methylene Blue

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Keywords: Multi-core-shell composites, Photodegradation, Methylene Blue, *E. coli, S. aureus*

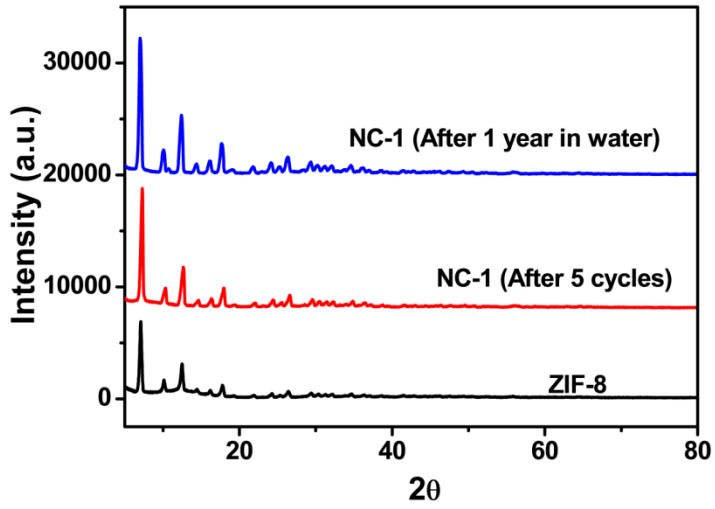


Figure S1. PXRD patterns of ZIF-8, NC-1 after 5 cycles of photocatalysis and NC-1 after keeping it in water for 1 year.

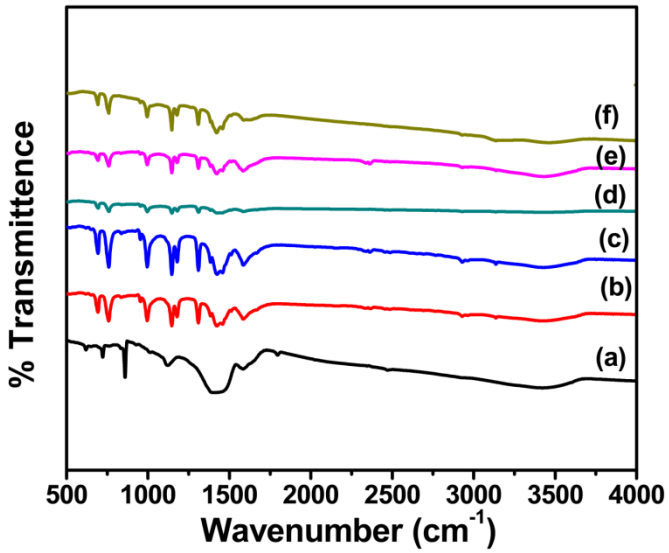


Figure S-2 FTIR spectra of CdSNPs (a), ZIF-8 (b), NC-1 (c), NC-2 (d), NC-3 (e) and NC-1 after photocatalysis (f).

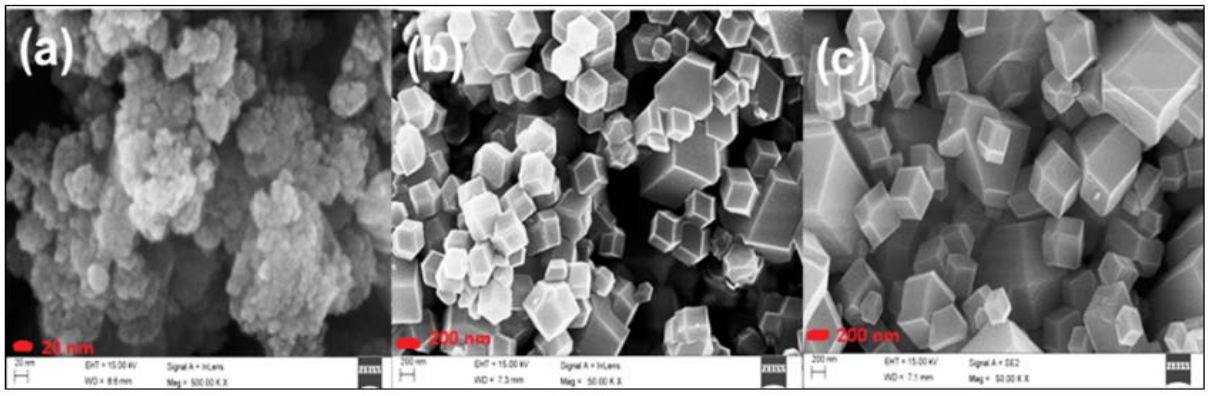


Figure S3. FE-SEM images of (a) CdSNPs; (b) ZIF-8 and (c) NC-1.

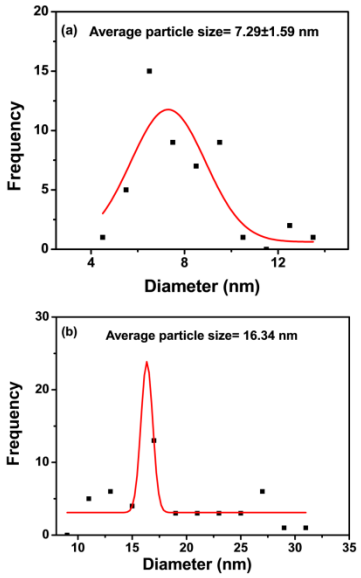


Figure S4: Particle size distribution plot of (a) CdSNPs and (b) CdSNPs encapsulated into NC-1 composite (by HRTEM).

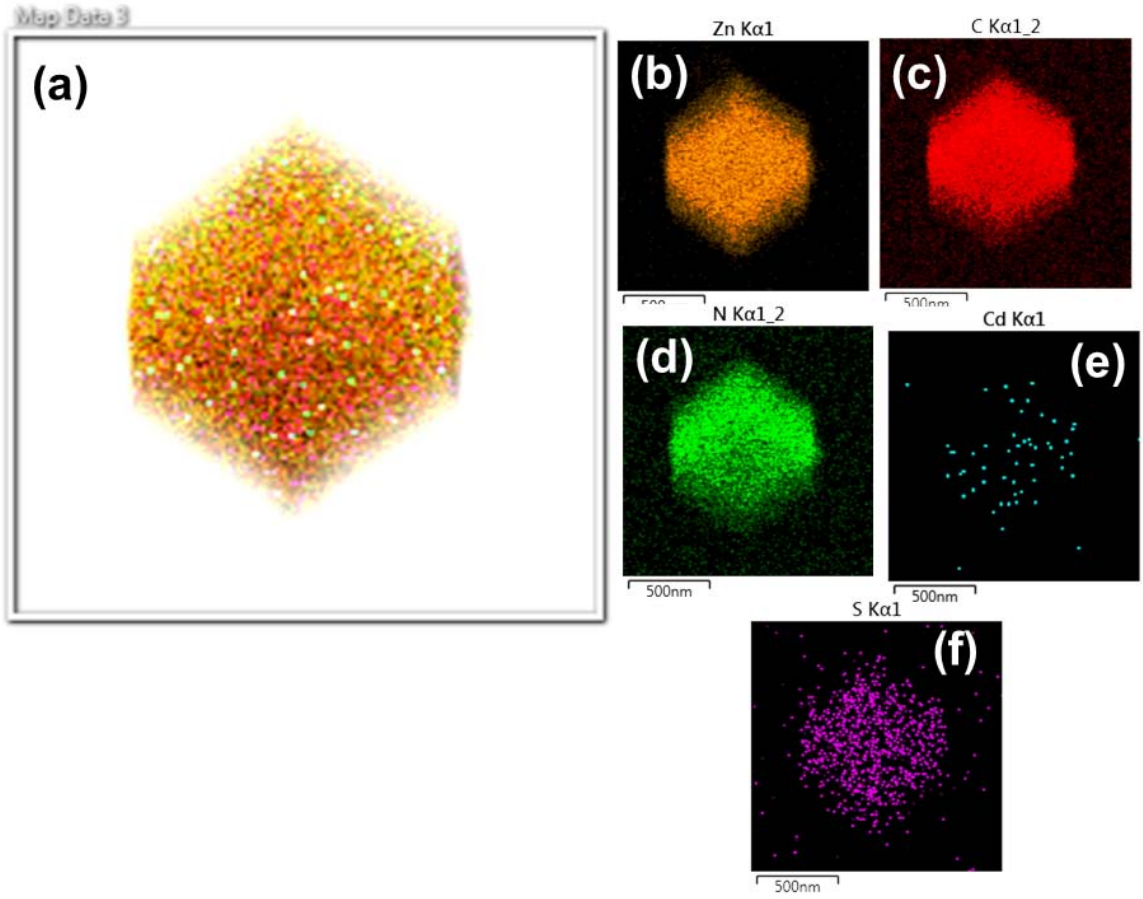


Figure S5. Elemental mapping of NC-1 (a) Layered Map, (b) Zn Kα1, (c) C Kα_1, (d) N Kα_1, (e) Cd Kα1 and (f) S Kα1.

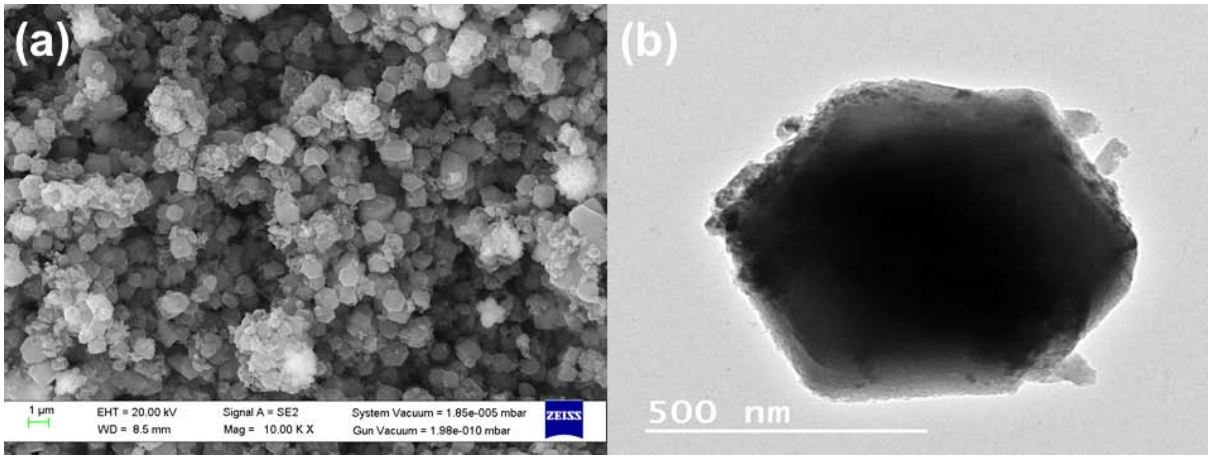


Figure S6. (a) FESEM images and (b) TEM images of NC-1 after photocatalytic degradation of MB..

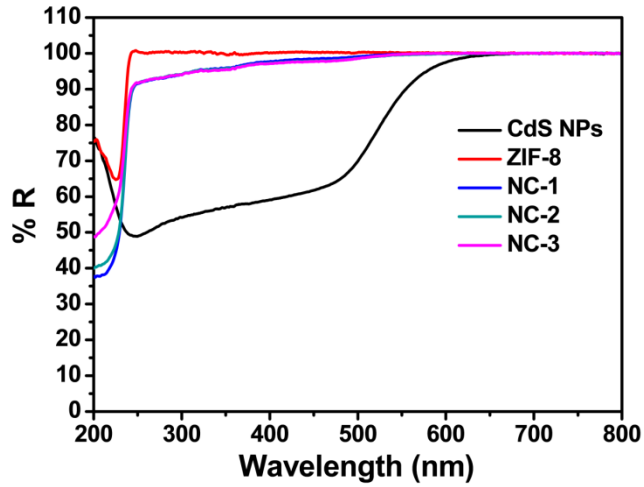


Figure S7. Reflectance spectra of CdSNPs, ZIF-8, NC-1, NC-2 and NC-3.

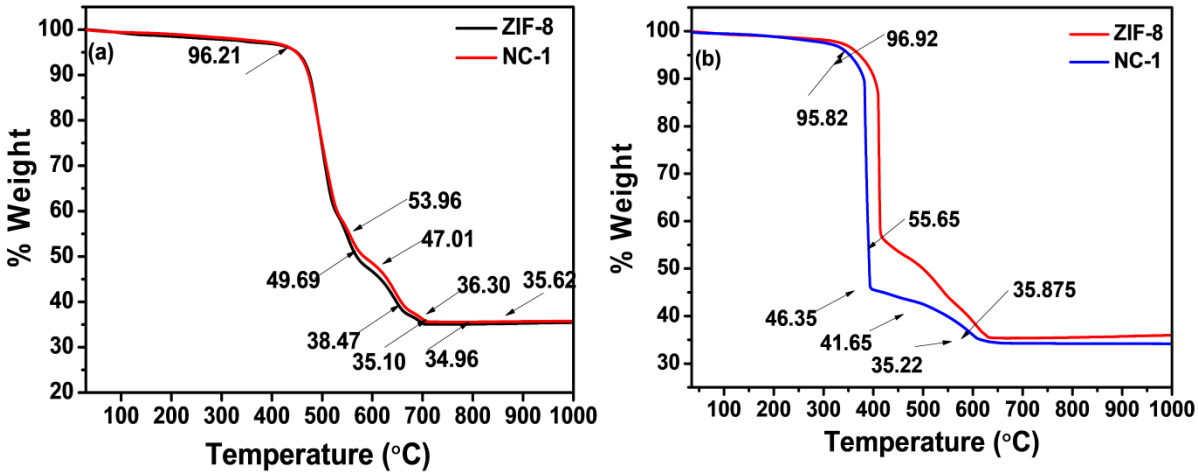


Figure S8. TGA plots of ZIF-8 and NC-1 (a) under nitrogen; (b) under air.

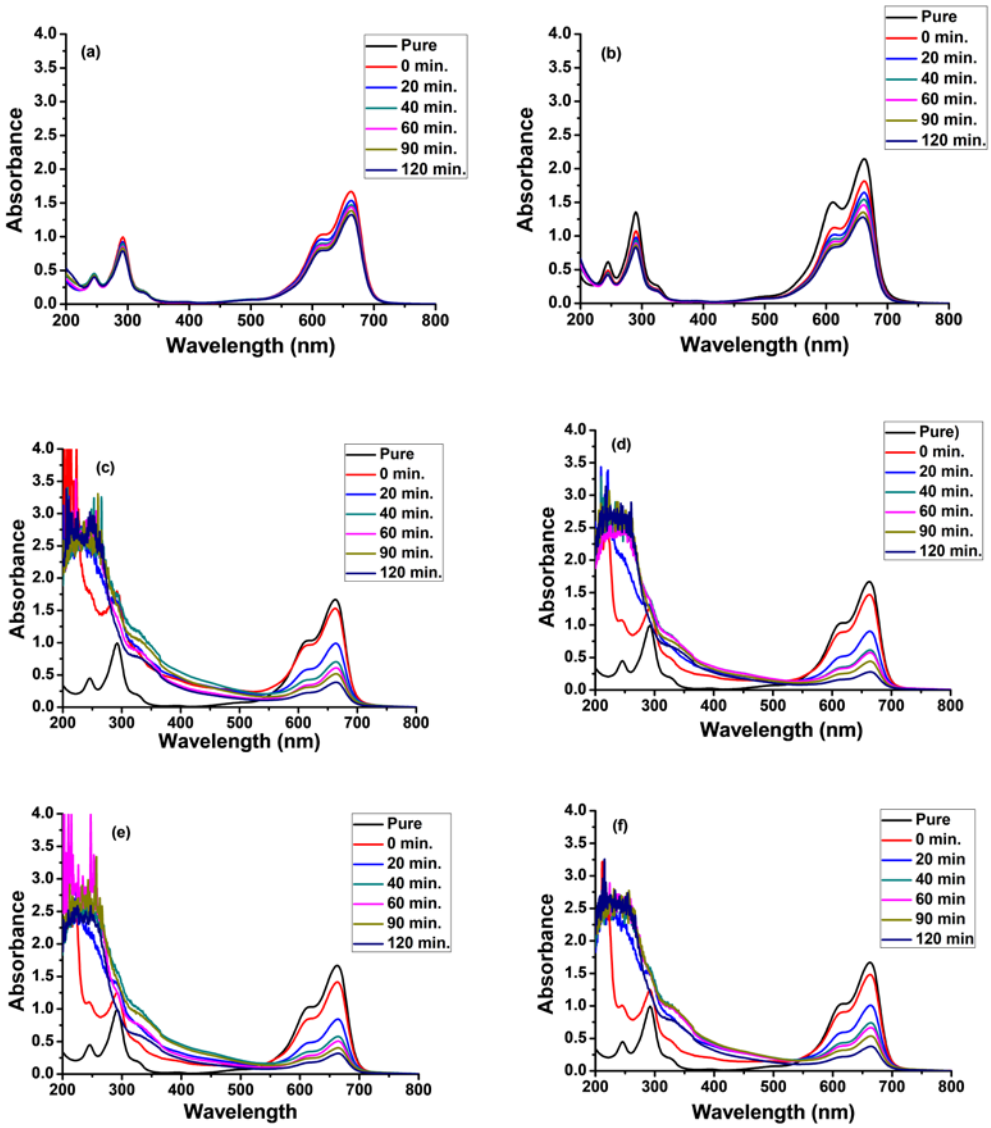


Figure S9.1. UV-Visible spectra for photodegradation study of methylene blue (a) pure 10 ppm MB, (b) CdSNPS, (c) ZIF-8, (d) NC-1, (e) NC-2 and (f) NC-3 at pH 6.85.

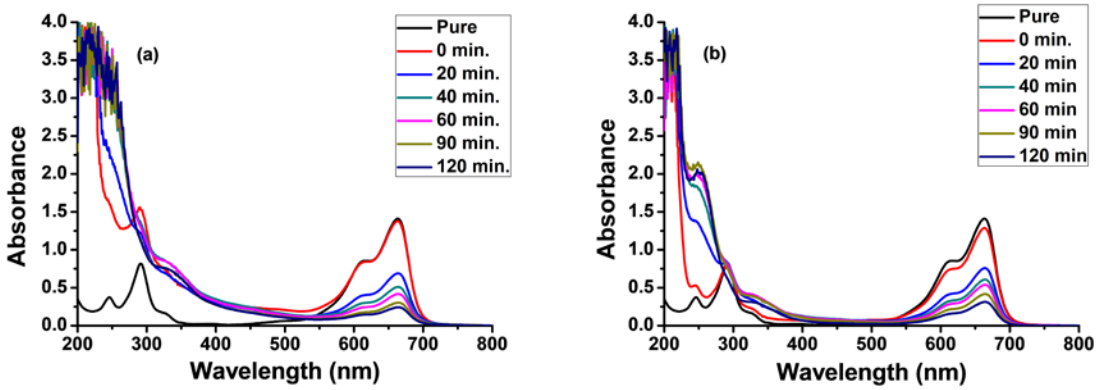


Figure S9.2. UV-Visible spectra for photodegradation study of methylene blue under UV-Visible by NC-1 with varying amount of catalyst (a) 5 mg, and (b) 15 mg.

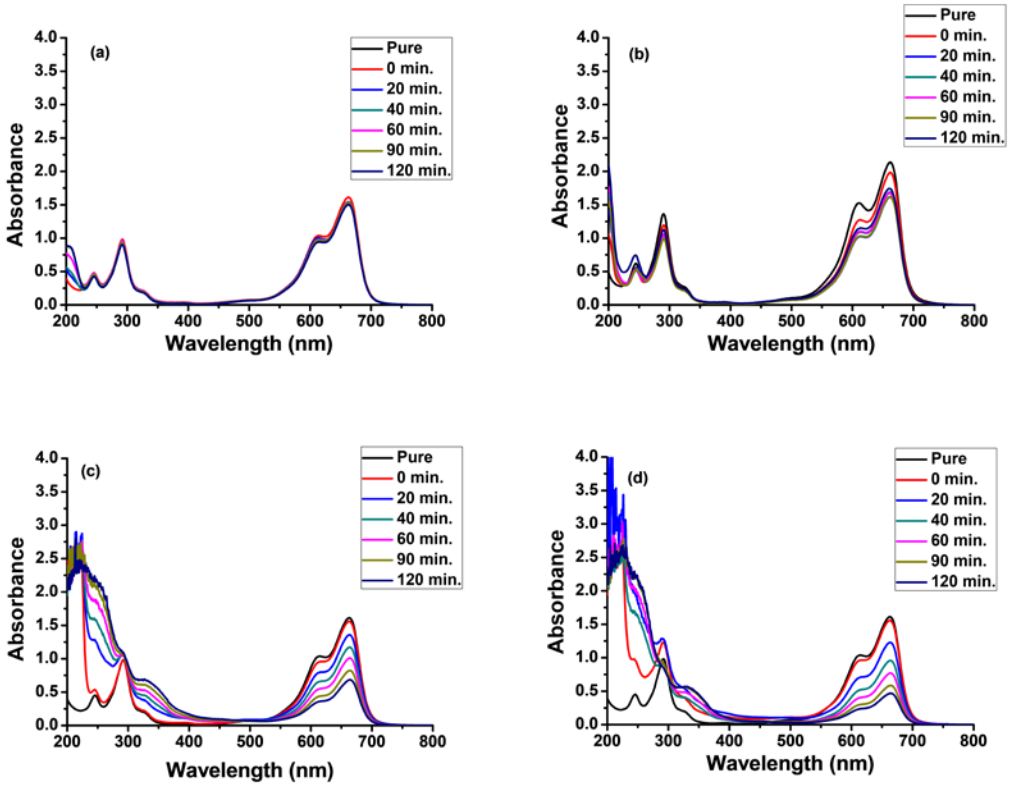


Figure S9.3. UV-Visible spectra for photodegradation study of methylene blue under UV-Visible at initial dye pH 3, (a) 10 ppm Pure MB, (b) CdSNPs (c) ZIF-8 and (d) NC-1.

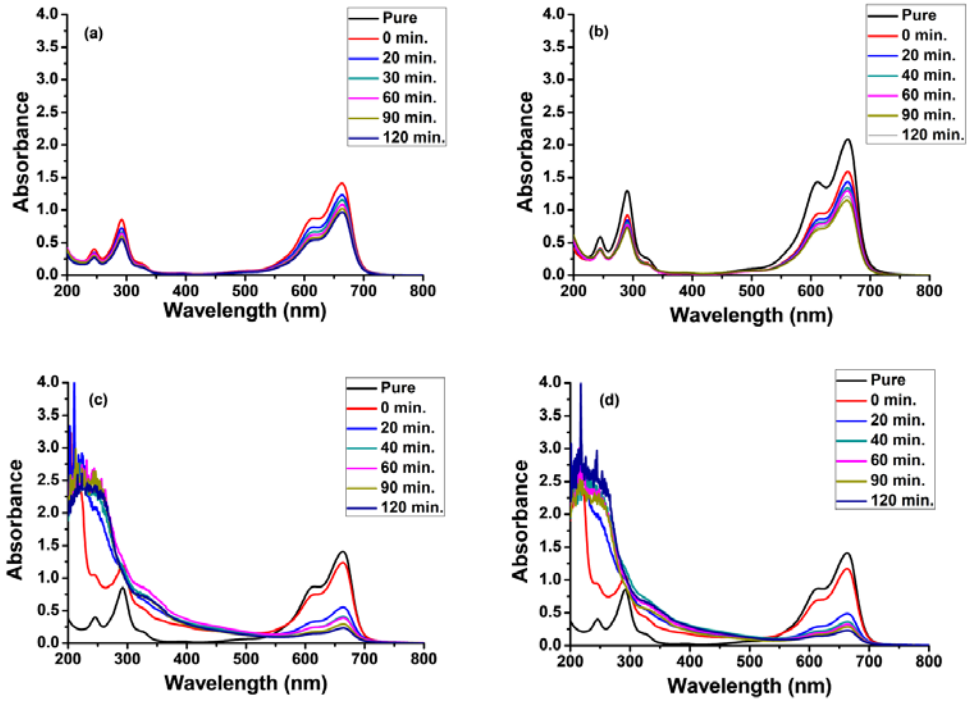


Figure S9.4. UV-Visible spectra for photodegradation study of methylene blue under UV-Visible at initial dye pH = 11 (a) 10 ppm Pure MB, (b) CdSNPs (c)ZIF-8 and (d) NC-1, respectively.

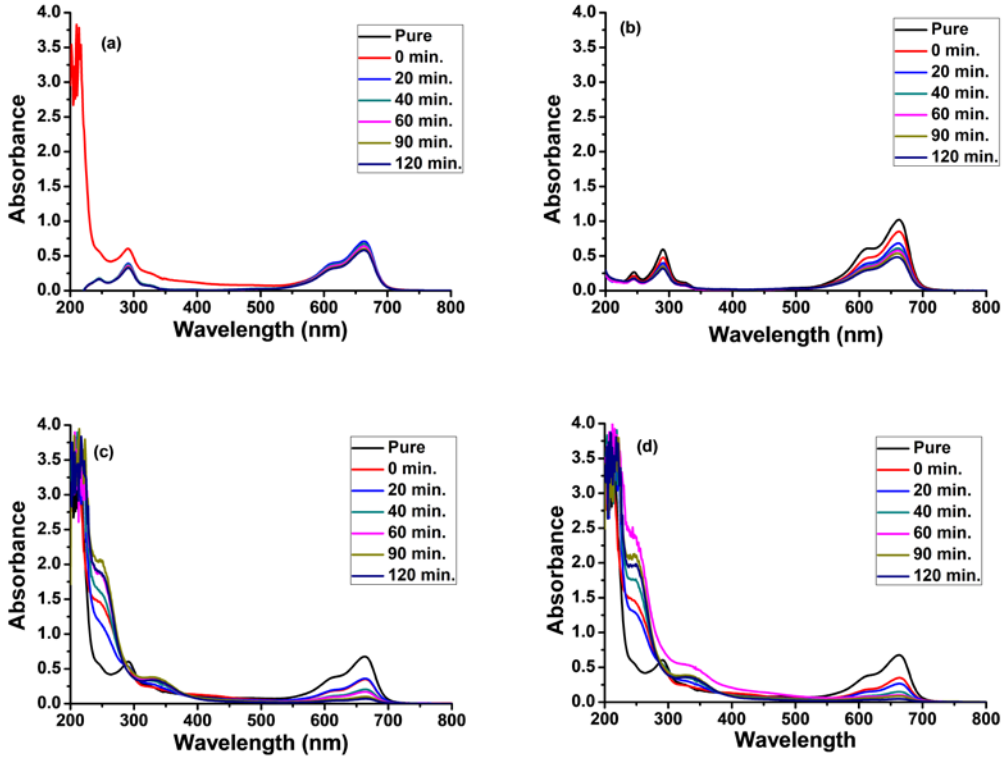


Figure S9.5. UV-Visible spectra for photodegradation study of methylene blue under UV-Visible at initial dye concentration = 5 ppm (a) 5 ppm Pure MB, (b) CdSNPs (c)ZIF-8 and (d) NC-1, respectively.

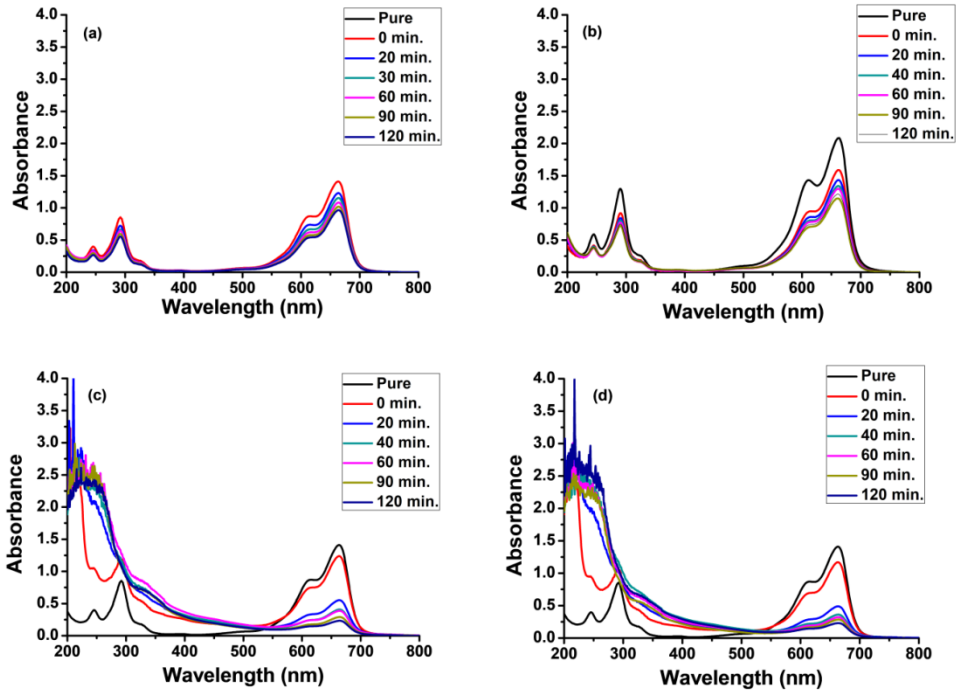


Figure S9.6. UV-Visible spectra for photodegradation study of methylene blue under UV-Visible at initial dye concentration = 15 ppm (a) 15 ppm Pure MB, (b) CdSNPs (c) ZIF-8 and (d) NC-1, respectively.

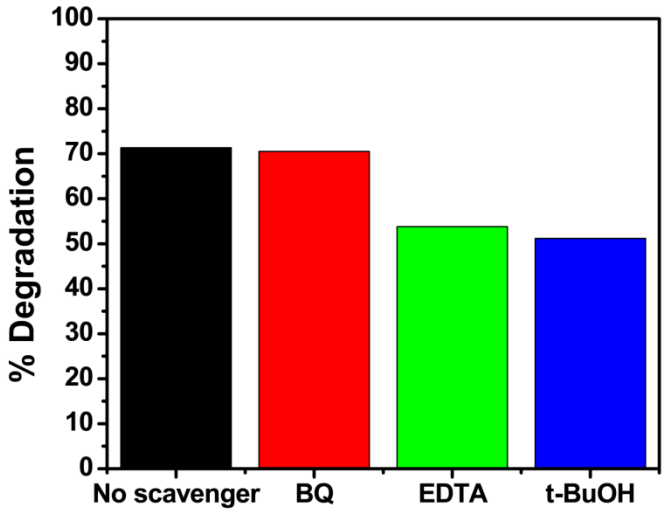


Figure S10. Photodegradation of MB using NC-1 as photocatalyst in presence of scavengers at pH = 7, [MB] = 10 ppm and amount of NC-1 = 5 mg; BQ = benzoquinone, EDTA= ethylenediaminetetraacetic acid, t-BuOH= t-butanol.

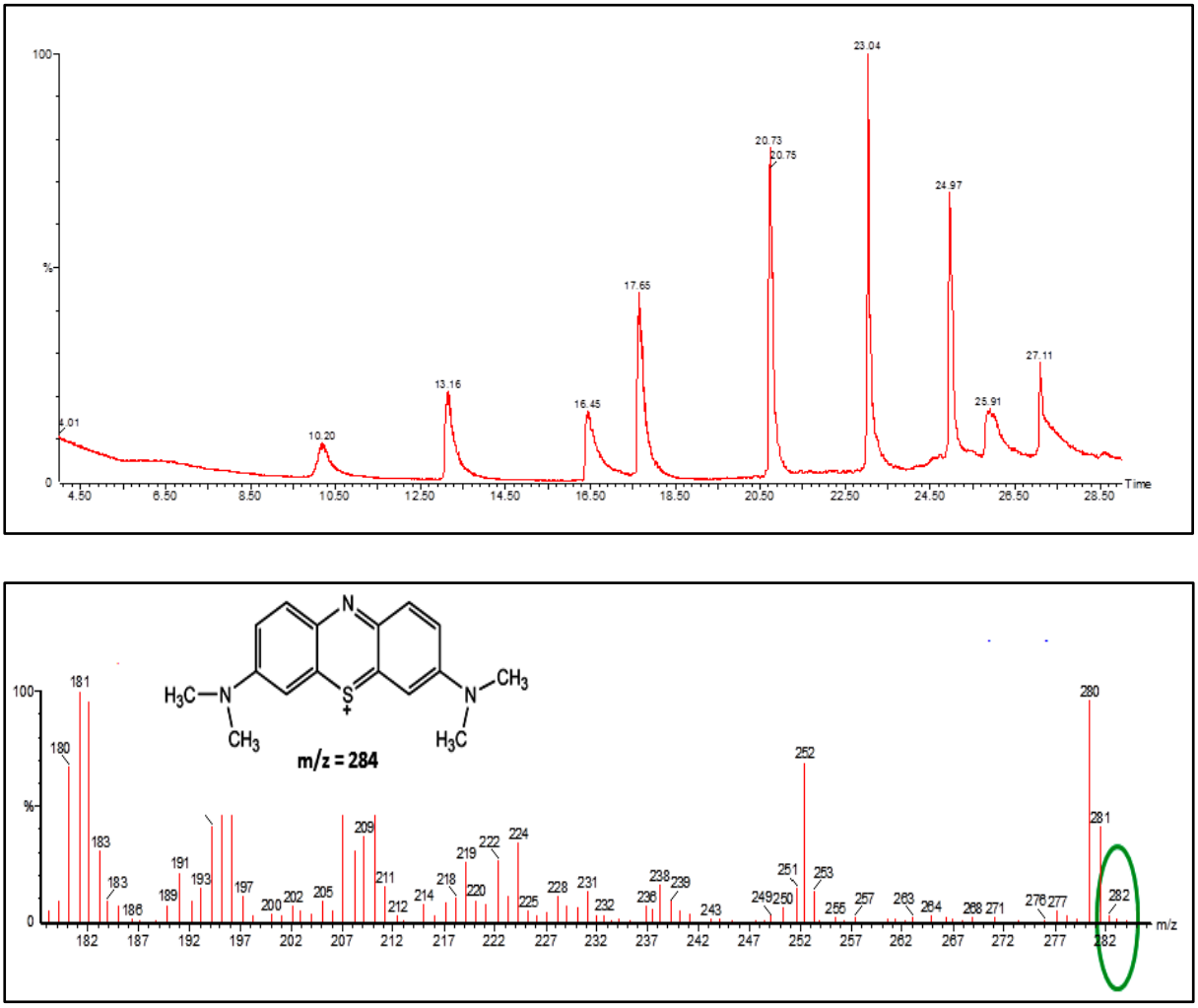


Figure S11.1. GC-MS spectra of intermediates and its fragments after photodegradation of MB.

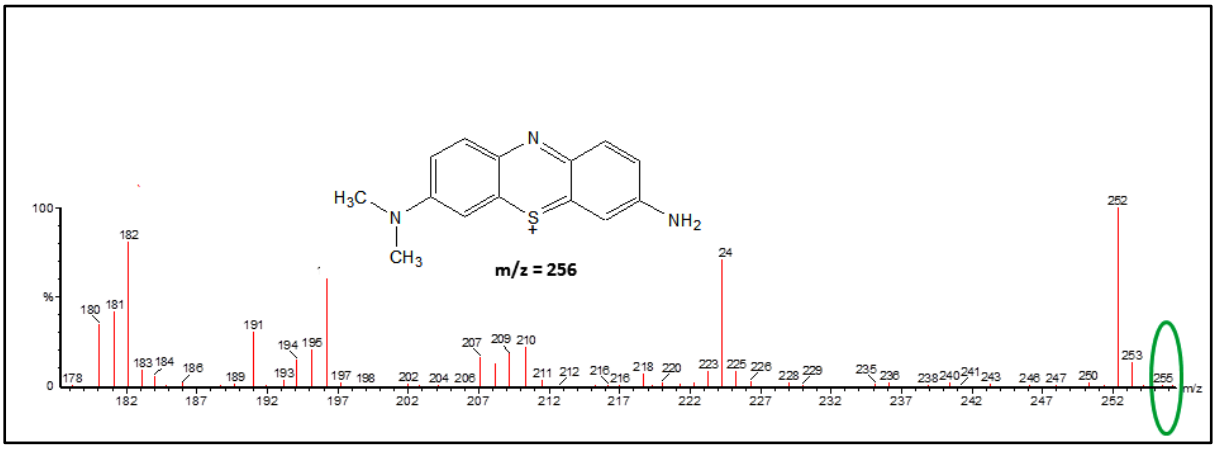
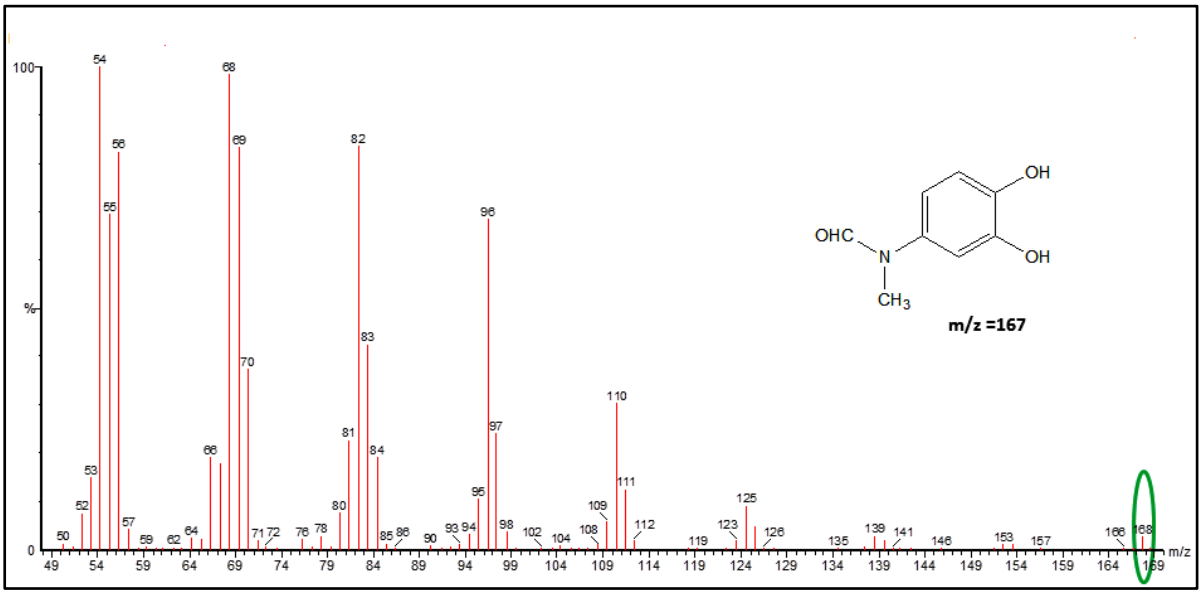


Figure S11.2. GC-MS spectra of intermediates and its fragments after photodegradation of MB.



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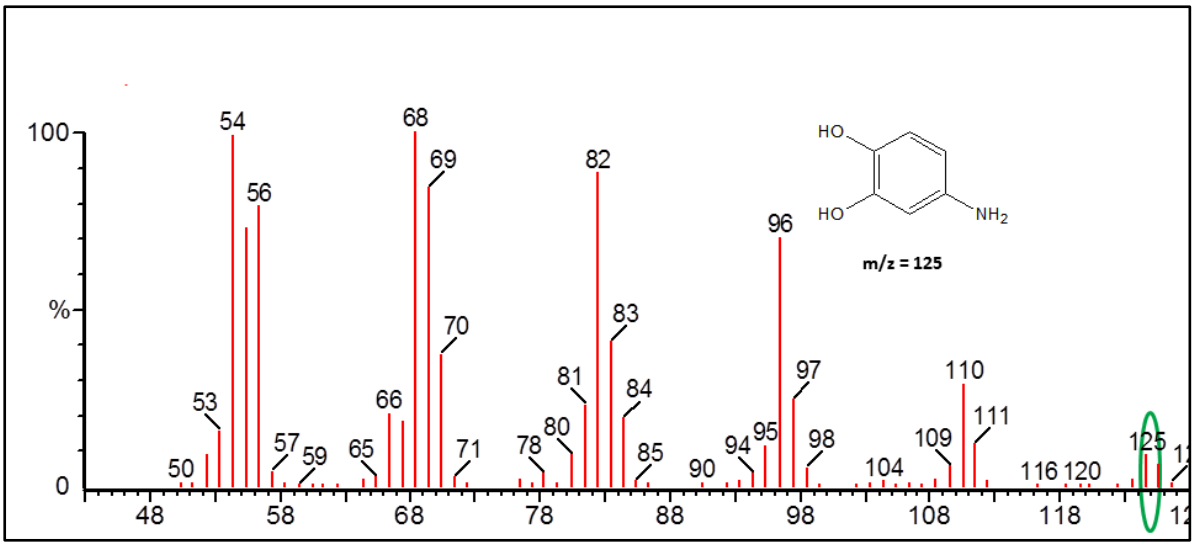


Figure S11.4. GC-MS spectra of intermediates and its fragments after photodegradation of MB.

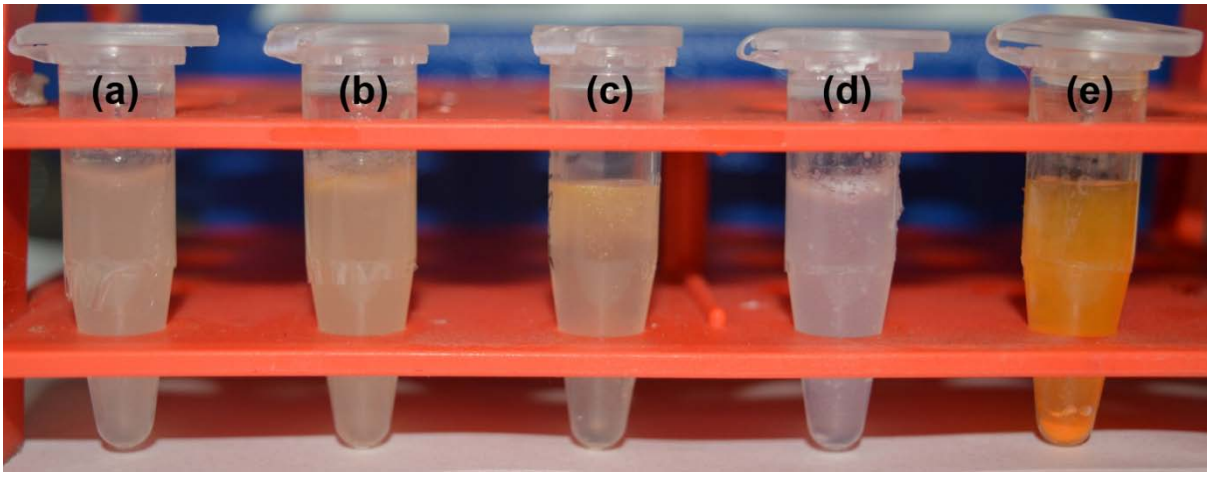


Figure S12. The aqueous dispersibilty of (a,b,c) NC-1, NC-2, NC-3, respectively, (d) ZIF-8, and (e) CdS NPs at 20 mg/mL.

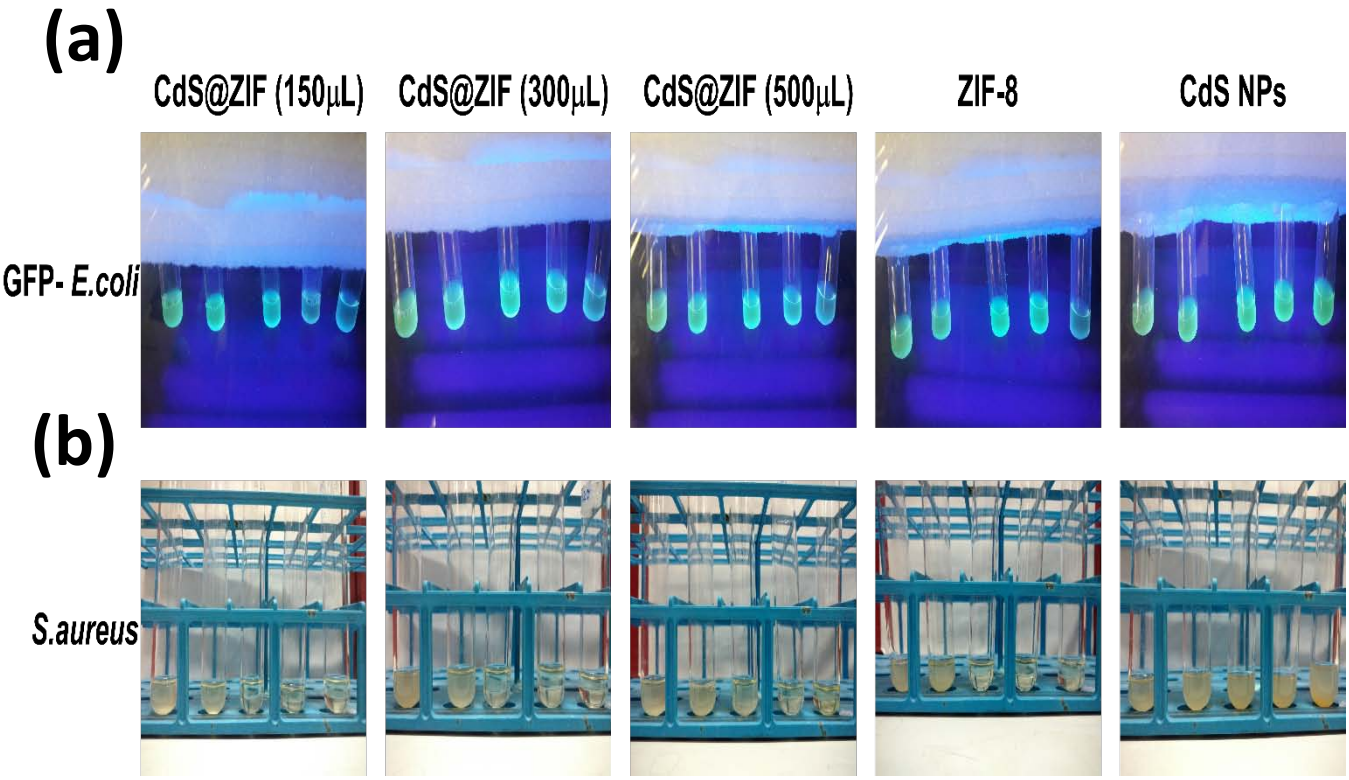


Figure S13. The UV illuminated GFP fluorescence photograph of (a) GFP *E.Coli* cells and digital photograph of (b) *S. aureus* after treatment of NC-1, NC-2, NC-3, ZIF-8, CdSNPs at various concentration.

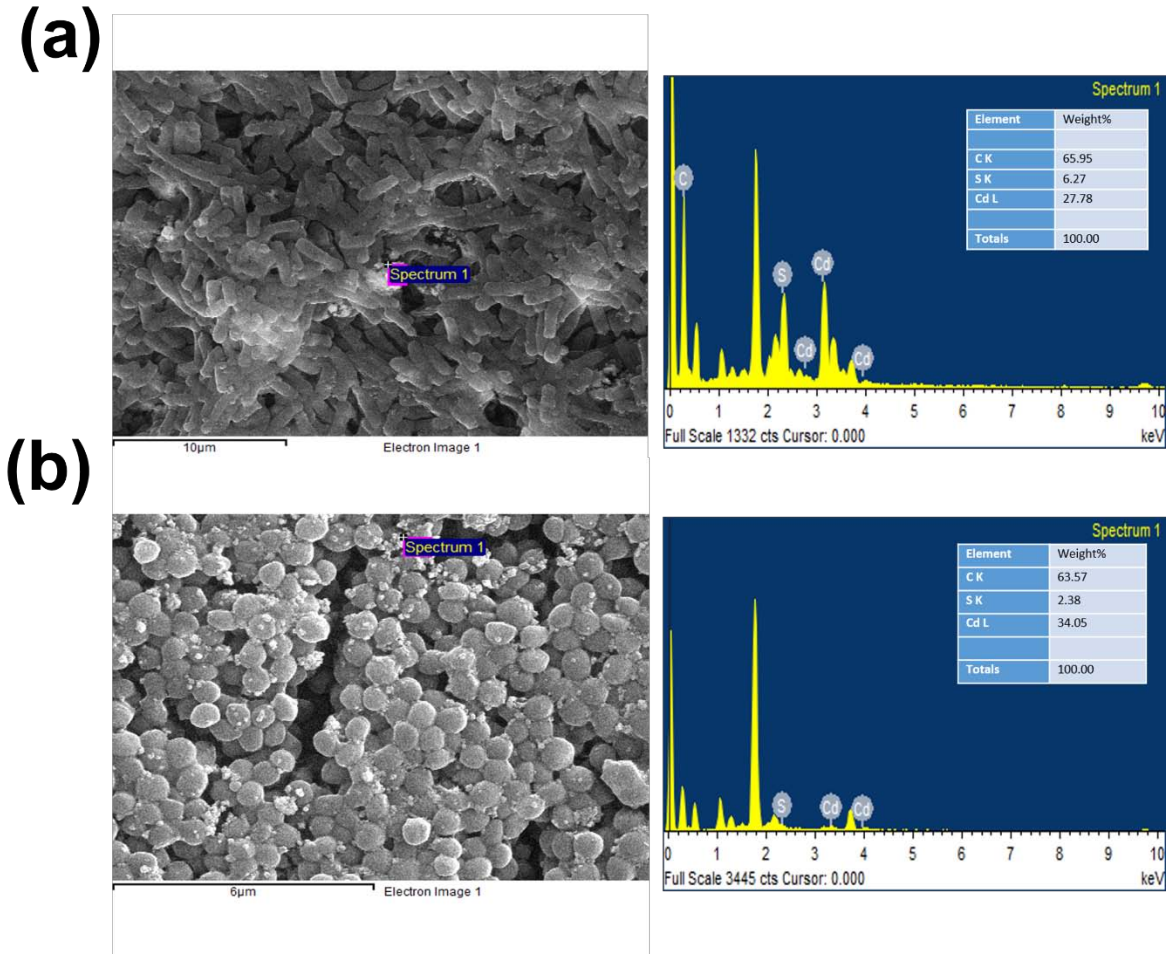


Figure S14. The Scanning Electron Micrograph of NC-1 treated (a) GFP *E.Coli*cells and (b) *S.aureus* cells along with corresponding EDAX analysis.

Table S1. Surface area, pore volume and average pore size of CdS NPs, ZIF-8 and CdS@ZIF-8 (150 µL) composite.

Sample	Surface area (m^2g^{-1})	Pore volume (cm^3g^{-1})	Average pore size (Å)
CdSNPs	34.51	0.005	29.83
ZIF-8	1296.22	0.732	36.26
NC-1	1294.15	0.753	11.64

Table S2. Effect of amount of CdSNPs encapsulated in ZIF-8 for adsorption in dark (after 60 min) and photodegradation (after 120 min) of [MB] (10 ppm); pH 6.85; 10 mg of catalyst.

S. No.	Catalyst	Adsorption (%)	Photo-degradation (%)	Total dye removal (%)
1	None	0	20.6	20.6
2	CdS	15.5	25.5	41.0
3	ZIF-8	8.2	68.4	76.6
4	NC-1	11.9	71.3	83.2
5	NC-2	11.6	69.5	81.1
6	NC-3	11.2	66.1	77.3

Table S3. Effect of pH; Experimental conditions: 10 mg of ZIF-8 or NC-1; Amount of CdSNPs equivalent to that present in its 150 µL suspension; [MB] = 10 ppm; time length: 60 min for adsorption in dark and 120 min in light.

pH	Catalyst	Adsorption (%)	Photodegradation (%)	Total dye removal (%)
3	None	0	6.8	6.8
3	CdS	7.1	17.4	24.5
3	ZIF-8	3.0	54.7	57.7
3	NC-1	2.87	68.2	71.0
11	None	0	31.6	31.6
11	CdS	24.0	21.2	45.5
11	ZIF-8	12.2	71.5	83.7
11	NC-1	17.1	66.5	83.6

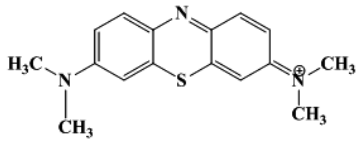
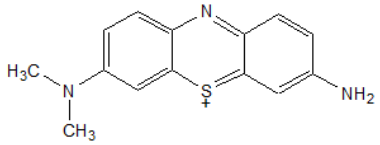
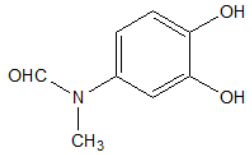
Table S4. Effect of catalyst's (NC-1) amount; Experimental conditions: [MB] = 10 ppm; pH 11; time length: 60 min for adsorption in dark and 120 min in light; Ph 11.0.

S.R.	Amount (mg)	Adsorption (%)	Photodegradation (%)	Total dye removal (%)
1	5	2.1	80.8	82.9
2	10	17.1	66.5	83.6
3	15	8.83	69.1	77.9

Table S5. Effect of initial dye concentration; Experimental conditions: 5 mg of ZIF-8 or (NC-1); Amount of CdSNPs equivalent to that present in its 150 µL suspension; pH 11.0; time length: 60 min for adsorption in dark and 120 min in light.

[MB] (ppm)	Catalyst	Adsorption (%)	Photo-degradation (%)	Total dye removal (%)
5	Pure	0	13.9	13.9
5	CdS	16.4	36.8	53.2
5	ZIF-8	0	89.6	89.6
5	NC-1	0	93.2	93.2
15	Pure	0	14.0	14.0
15	CdS	7.5	25.3	32.8
15	ZIF-8	9.3	68.3	77.6
15	NC-1	10.2	71.3	81.5

Table S6. GC-MS analysis of possible fragments of MB after its degradation

S. N.	m/z	Retention time (sec.)	Identified intermediates	Structure
1.	283	23.08	Methylene Blue	
2.	256	20.72	3-ammino-7-(dimethylammino)phenothiazin-5-ium	
3.	167	10.22	N-(3,4-dihydroxyphenyl)-N-methylformamide	
4.	125	13.16	4-aminobenzene-1,2-diol