Electronic Supplementary Information

Insight on the Solvatochromic Effect in N-Doped Yellow-orange Emissive Carbon dots

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Cdots synthesized from trimesic acid (TMA) and *para* Benzoquinone (*p*-BQ): 27 mg of TMA and 27mg of *p*-BQ were dissolved in 4mL formamide followed by microwave treatment of the resultant reaction mixture under 600W for 4 min.

Cdots from TMA: Cdots from TMA is not getting synthesized under the same reaction conditions.

Cdots from *Ortho* phenylenediamine (*o*-PD): 27 mg of ***o*-PD** was dissolved in 4mL formamide and followed by microwave treatment (600W) for 8 minutes. Final product was dissolved in 10mL water.

Cdots from *p*-BQ: 27mg of ***p*-BQ** was dissolved in 4mL formamide and followed by microwave treatment (600W) for 8 minutes.

Cdots from TMA and *o*-PD Cdot: Reaction was carried out with same amount/molar ratio of the starting materials with identical reaction conditions, described in main manuscript. But the reaction time was 8 min.

Cdots from *p*-BQ and *o*-PD: Similar procedure along with a reaction time of 8 min was followed as mentioned in main manuscript.

Quantum Yield Calculation

We have calculated quantum yield with respect to quinine sulphate (QS) in 0.1 M H_2SO_4, using the following formula.[1,2]

$$Q_S = Q_R \times (I_s/I_R) \times (A_R/A_S) \times (\eta_{S/}\, \eta_R)^2 \qquad \text{Equation S1}$$

Where, Q_S= quantum yield of sample; Q_R= quantum yield of reference; I_S= area under PL curve of sample; I_R= area under PL curve of reference; A_R= absorbance of the reference; A_S= absorbance of the sample; η_S= refractive index of sample; η_R= refractive index of reference.

QY of quinine sulphate = 0.54; Refractive index of water = 1.33

(The concentration of all samples and the reference quinine sulphate were adjusted so that the optical densities of all samples were 0.020 ± 0.003 at the excitation wavelength (380 nm).

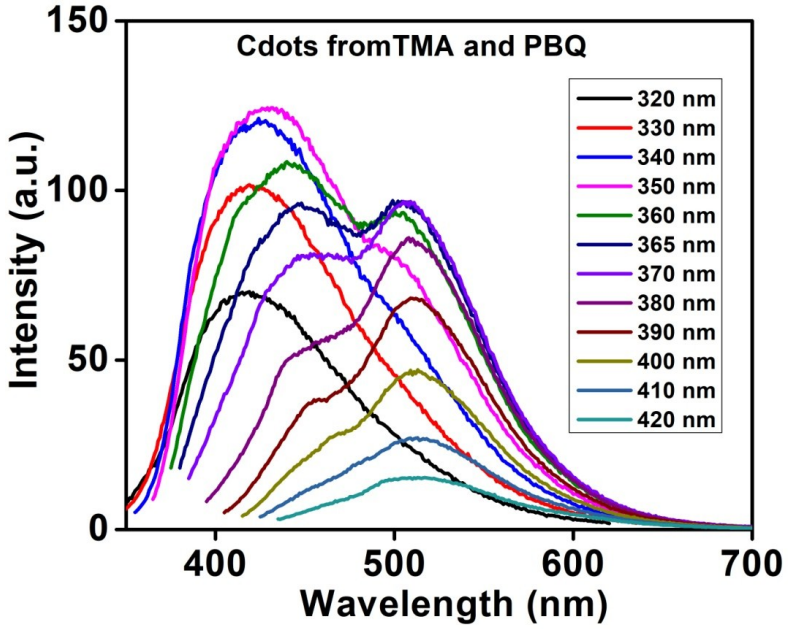

Fig S1: Photoluminescence (PL) spectra of the Cdots (in water) synthesized from TMA and *p*-BQ.

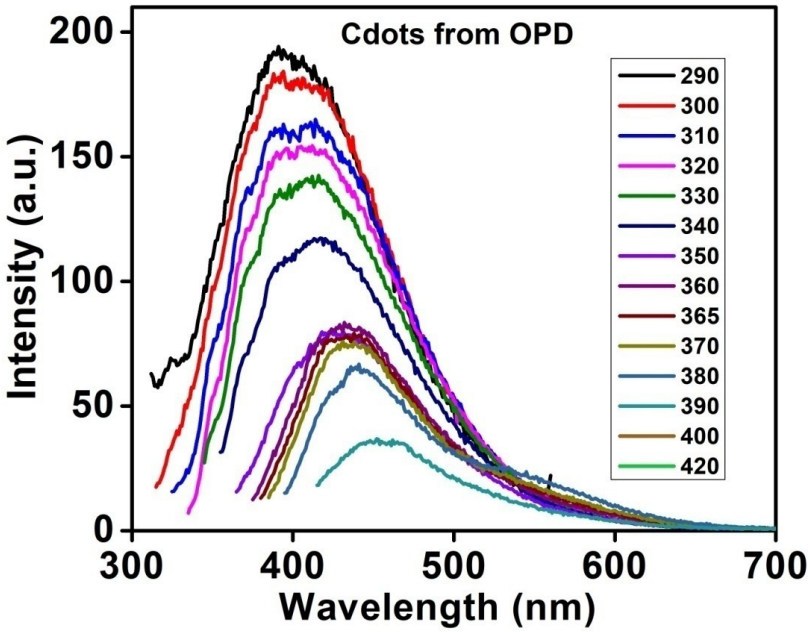

Fig S2: PL spectra of the Cdots (in water) synthesized from *o*-PD.

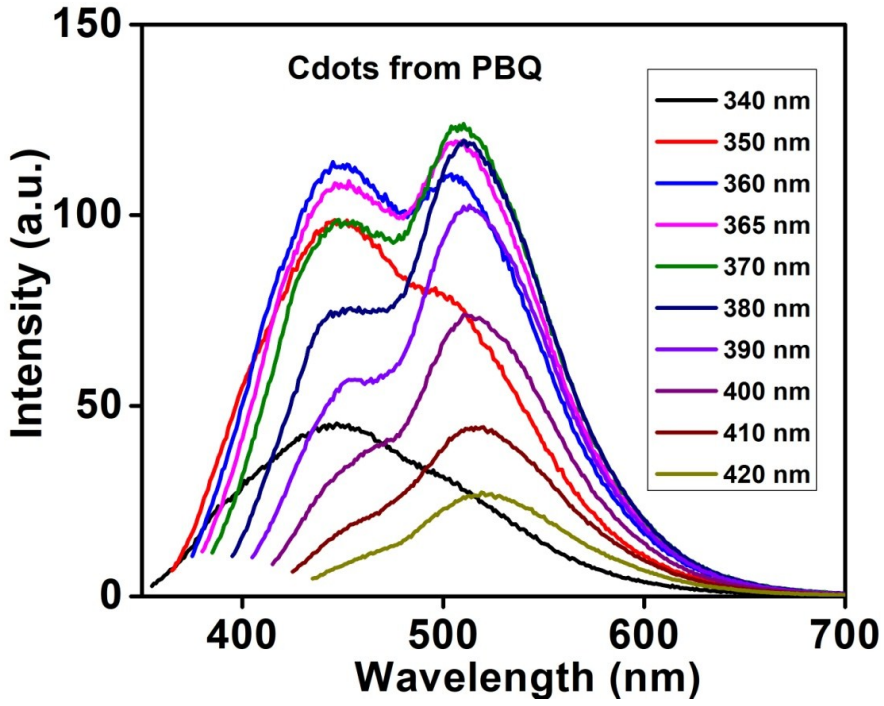

Fig S3: PL spectra of Cdots (in water) synthesized from *p*-BQ.

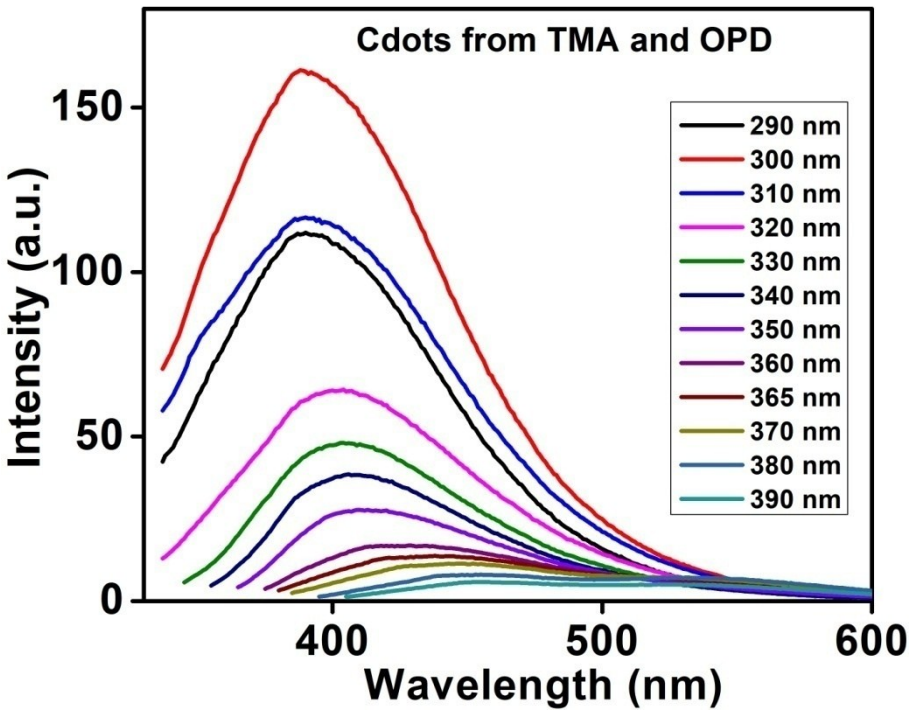

Fig S4: PL spectra of Cdots (in water) synthesized from TMA and *o*-PD.

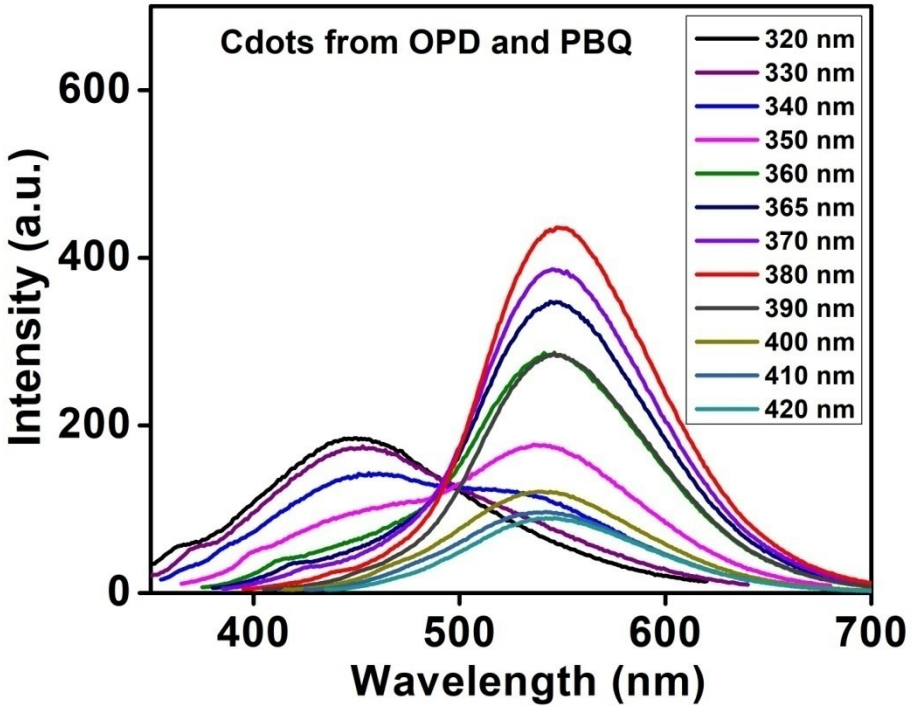

Fig S5: PL spectra of Cdots (in water) synthesized from *o*-PD and *p*-BQ.

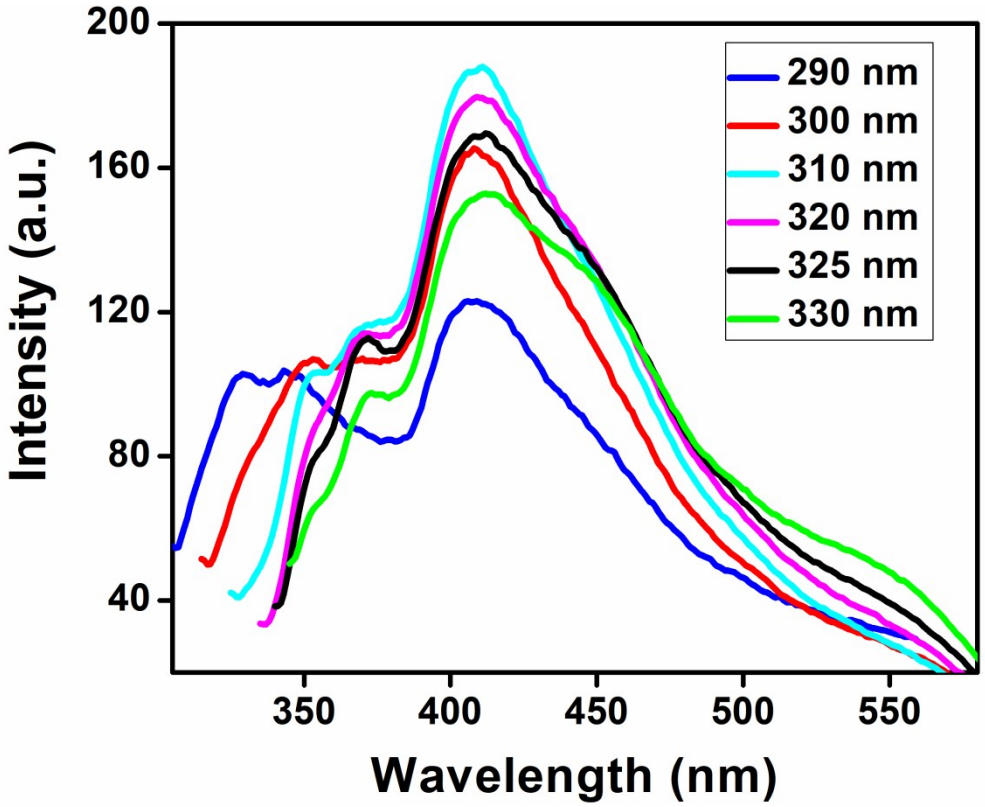

Fig S6: Emission spectra of Cdots in the range 2 (290 nm to 330 nm).

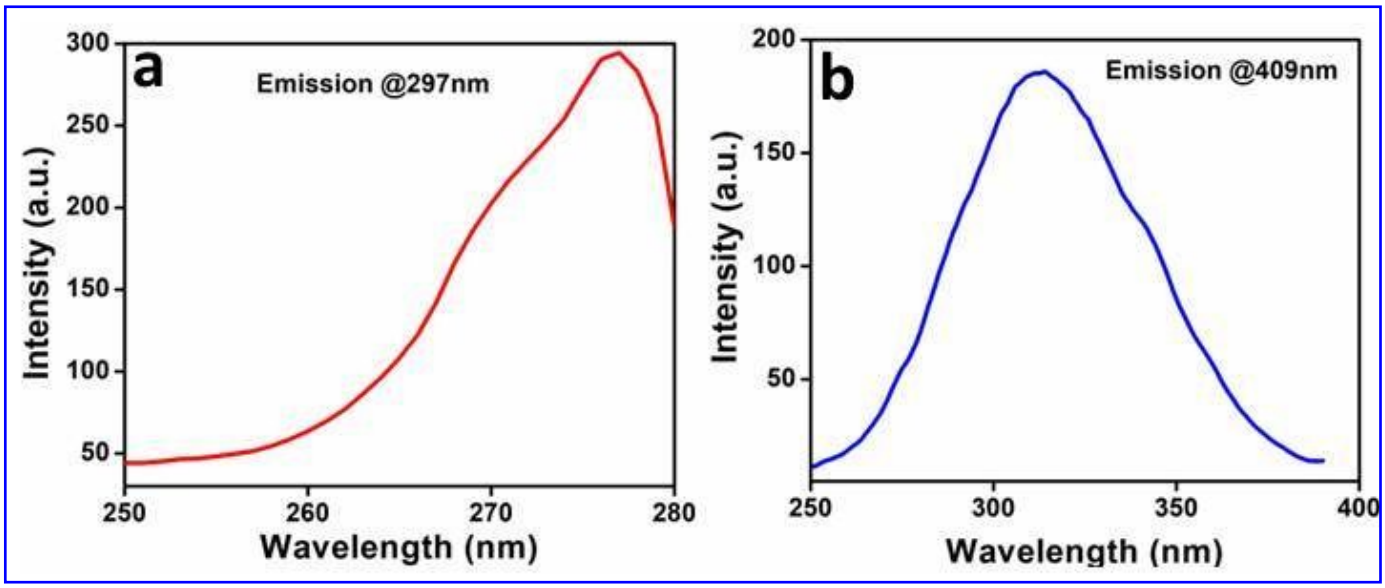

Fig S7: Excitation spectra for the emission peaks centred at a) 297 nm and b) 409 nm.

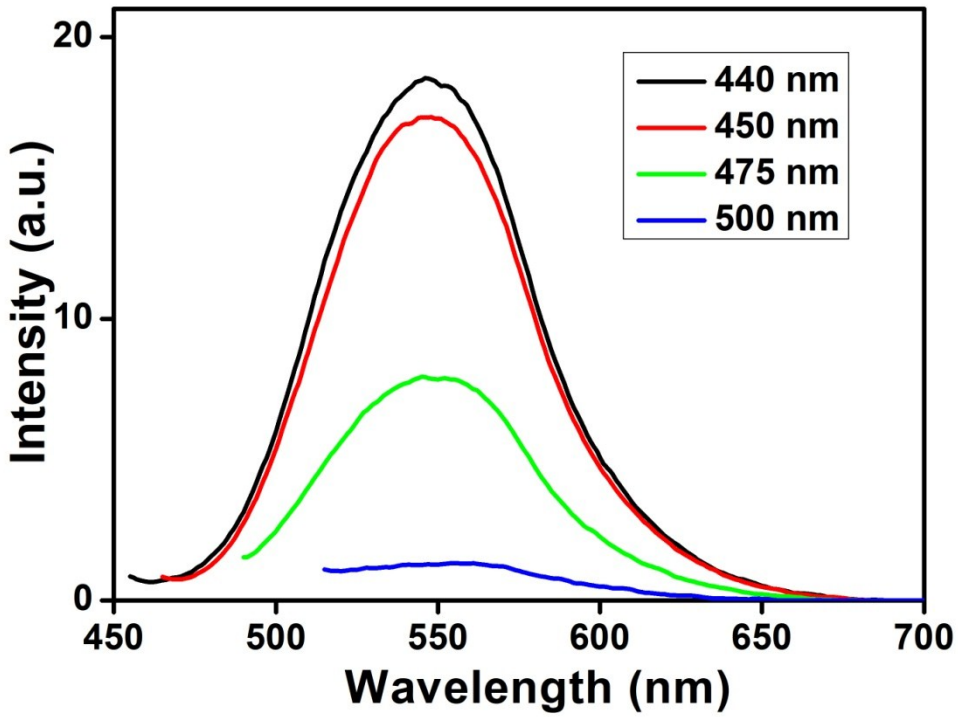

Fig S8: Emission Spectra of Cdots in water, excited in the range between 440 to 500 nm (surface states).

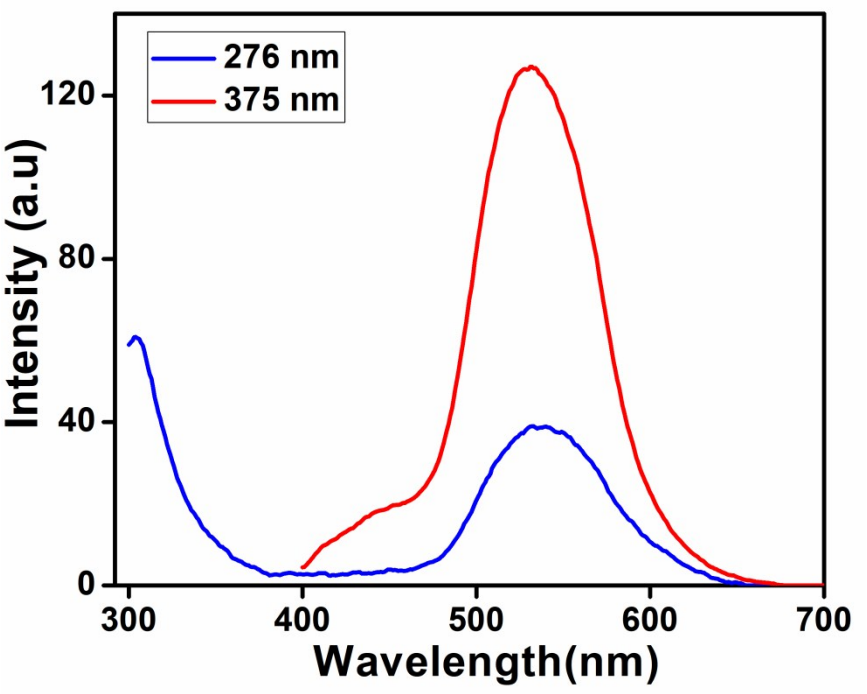

Fig S9: Emission spectra Cdots (in DMSO) excited at 276 nm and 375 nm.

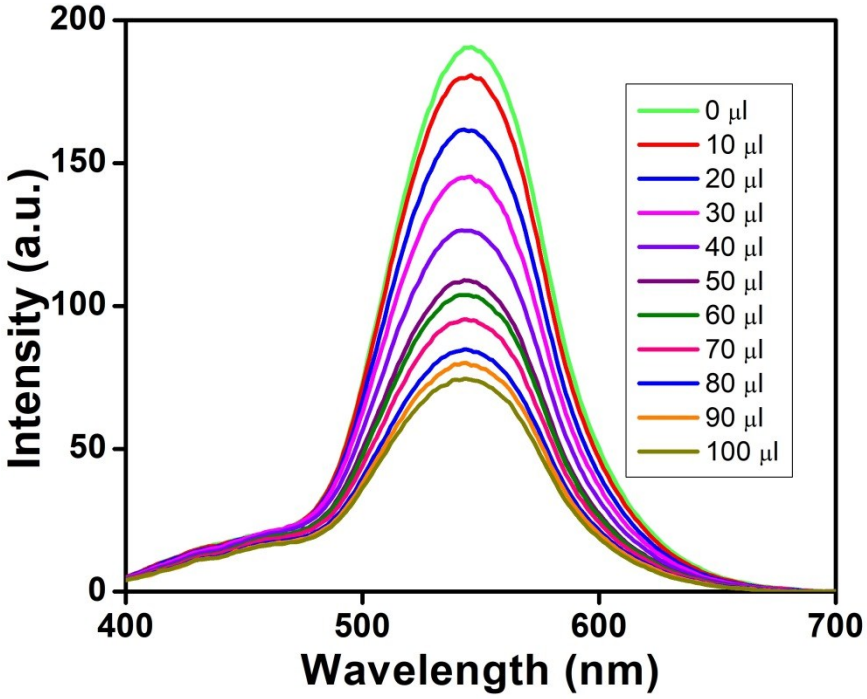

Fig S10: Emission spectra of Cdots (in water) excited at 375 nm with different conc. of 0.01N HCl.

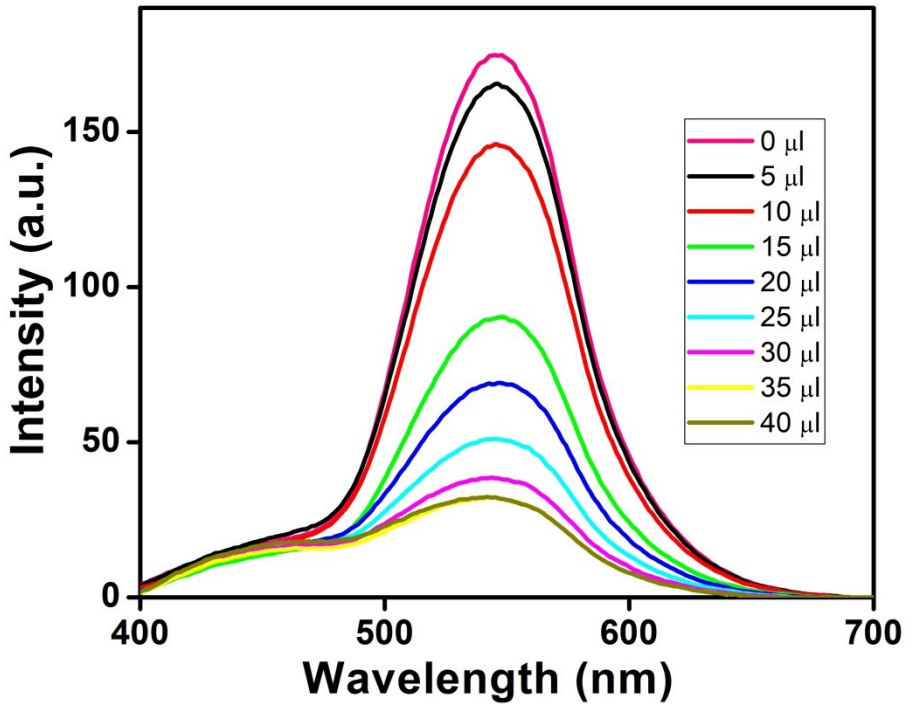

Fig S11: Emission spectra of Cdots (in water) excited at 375 nm with different conc. of 0.01N NaOH.

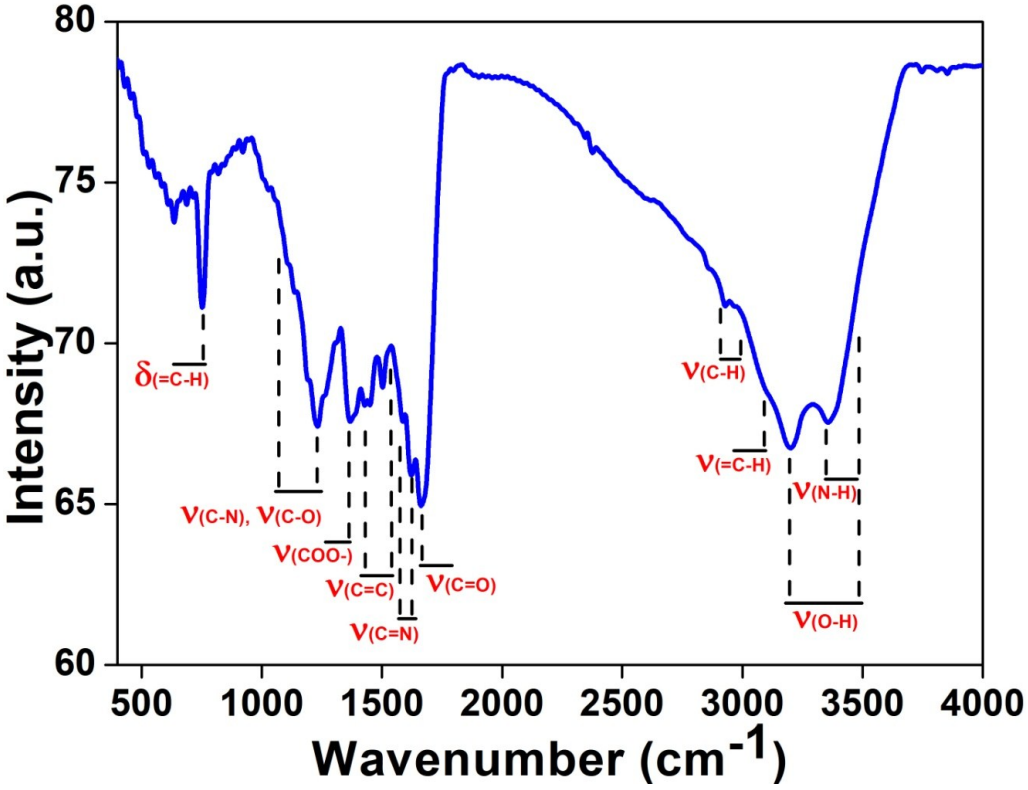

Fig S12: IR Spectrum of powdered Cdots.

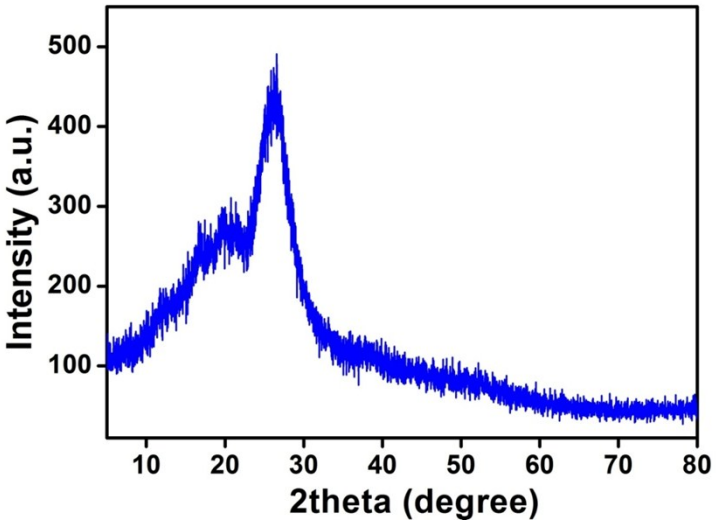

Fig S13: Powder X-ray diffraction (PXRD) pattern of the Cdot sample.

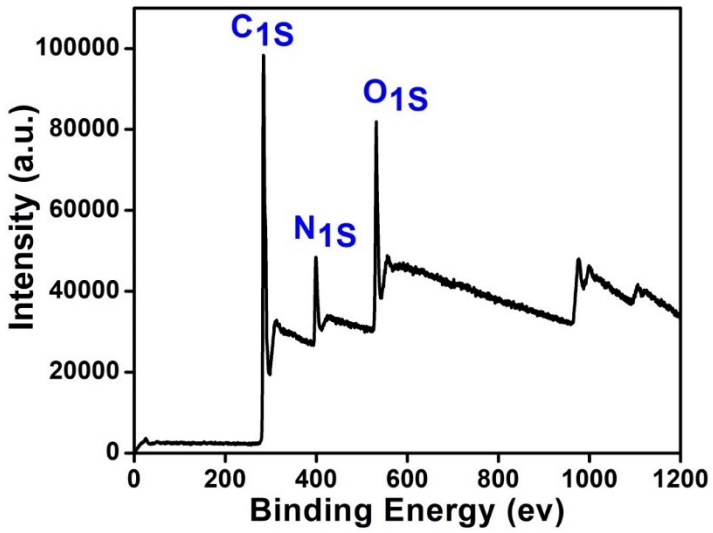

Fig S14: XPS full-survey spectrum of Cdots.

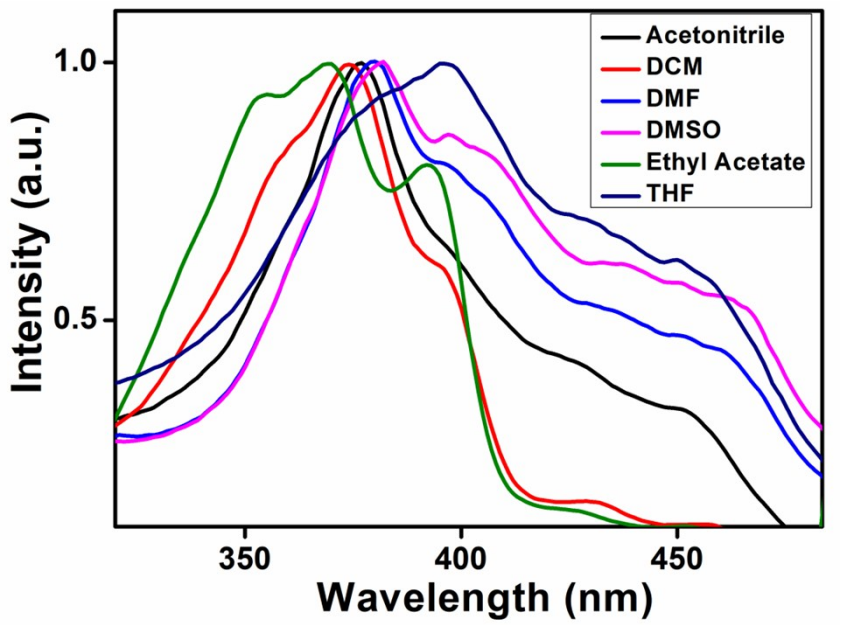

Fig. S15: Excitation spectra of the Cdots in different solvents corresponding to 550 nm emission wavelength.

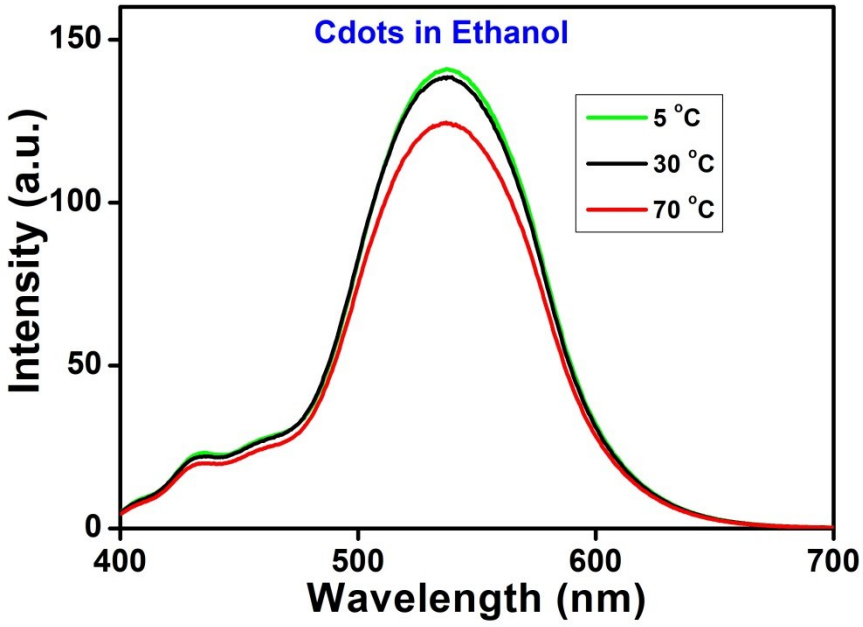

Fig S16: Temperature dependent fluorescence of Cdots in ethanol, excited at 375 nm.

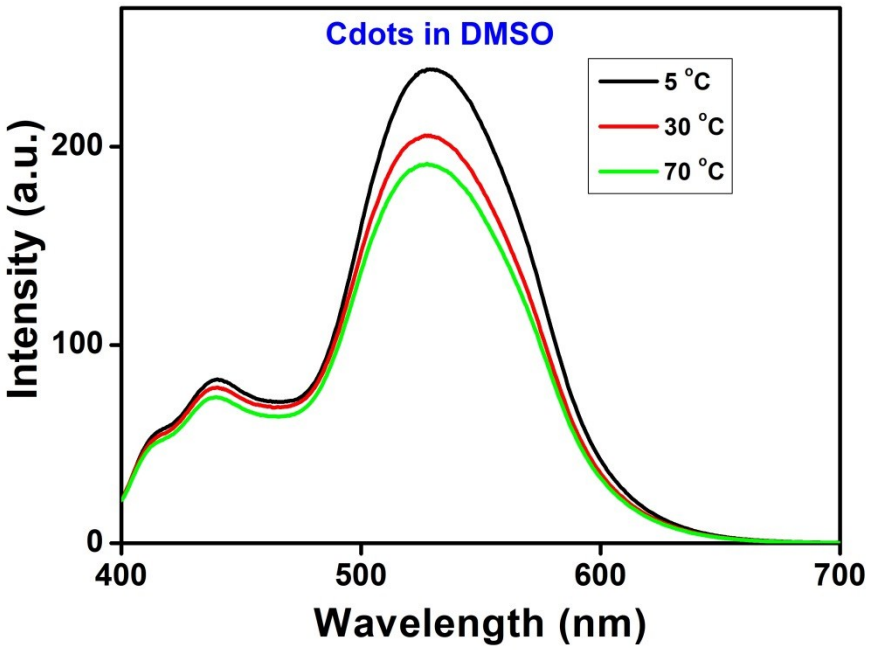

Fig S17: Temperature dependent fluorescence of Cdots in DMSO, excited at 375 nm.

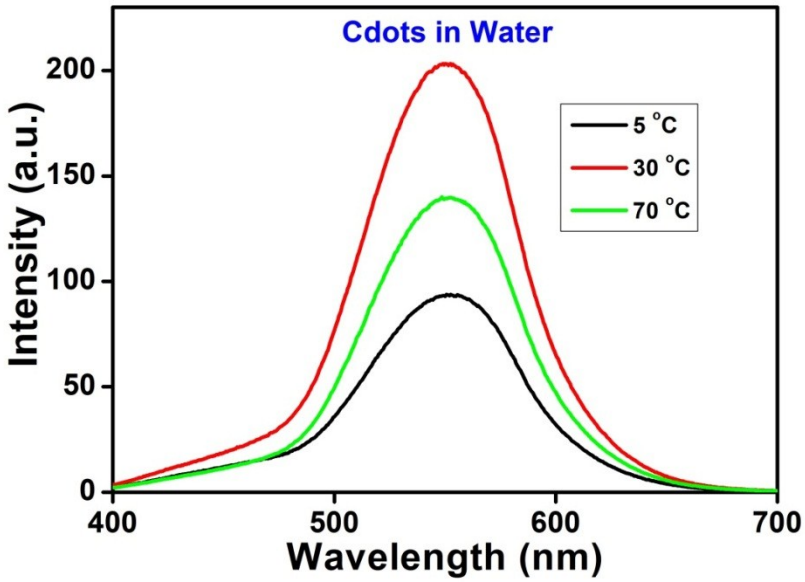

Fig S18: Temperature dependent fluorescence of Cdots in water excited at 375 nm.

Table S1: Dielectric constant, E_T^N polarity parameter, and Kamlet-Taft polarity parameters of the solvents.

SN	Cdots in Solvent	E_T (eV)	Dielectric Constant	E_T^N	α	β	Π*
1	Water	2.25	80	1	1.17	0.47	1.09
2	Formamide	2.26	111	0.77	0.71	0.48	0.97
3	Methanol	2.32	33	0.76	0.98	0.66	0.60
4	Ethanol	2.33	24	0.65	0.86	0.75	0.54
5	DMSO	2.35	47	0.76	0.00	0.76	1.00
6	DMF	2.37	36.7	0.38	0.00	0.69	0.88
7	Acetone	2.41	38	0.47	0.08	0.43	0.71
8	THF	2.43	7.58	0.20	0.00	0.55	0.58
9	Acetonitrile	2.45	38	0.47	0.19	0.40	0.75
10	DCM	2.47	9.1	0.32	0.13	0.10	0.82
11	Acetic Acid	2.48	6.15	0.64	1.12	0.45	0.64
12	Ethyl acetate	2.51	6.02	0.22	0.00	0.45	0.55

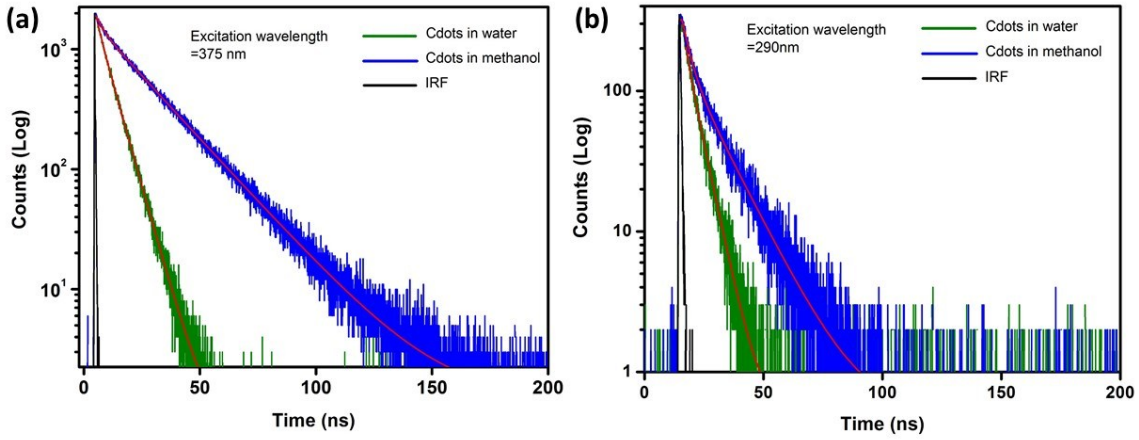

Fig S19: Time resolved photoluminescence (TRPL) plots of the Cdots in water and methanol, excited using a (a) 375 nm and (b) 290 nm wavelength source.

Decay pattern fitting and average lifetime calculation

The decay patterns of the as-synthesized Cdots were recorded using a 375 nm and 290 nm excitation sources. Obtained profiles were fitted bi-exponentially using following equations.

$$I(t) = \sum_i \alpha_i \exp\left(-t/\tau_i\right) \quad \text{Equation S2}$$

$$\tau_{av} = \frac{\sum_i \alpha_i \tau_i^2}{\sum_i \alpha_i \tau_i} \quad \text{Equation S3}$$

Here, α corresponds to pre-exponential factor and τ correspond to excited-state life time of the components. Also, τ_{av} corresponds to the calculated average lifetime.

$$K_r = \frac{\phi_D}{\tau_{av}} \quad \text{Equation S4}$$

$$K_{nr} = \frac{1 - \phi_D}{\tau_{av}} \quad \text{Equation S5}$$

ϕ_D is measured quantum yield of the Cdot samples. Besides, K_r is the radiative rate constant and K_{nr} is the non-radiative recombination rate constant.

Table S2: Calculated parameters, obtained during time resolved photoluminescence (TRPL) analysis of the Cdots in different dispersion medium (using a 375 nm pulsed diode laser sources).

Cdot Medium	λ^2	Fraction of the first component (α_1) (%)	First component lifetime (τ_1) (ns)	Fraction of the second component (α_2) (%)	Second component lifetime (τ_2) (ns)	Average lifetime (τ_{av}) (ns)
Cdots in water	1.016	6.3	2.1	93.6	6.3	6.2
Cdots in methanol	1.024	3.8	3.0	96.1	20.6	20.5

Table S3: Calculated quantum yield and corresponding radiative and non-radiative decay rate constants of the Cdots.

Cdot Medium	Measured quantum yield (QY) (%)	Radiative decay rate constant (K_r) (sec^{-1})	Non radiative decay rate constant (K_{nr}) (sec^{-1})
Cdots in water	2.3	3.7×10^6	1.6×10^8
Cdots in methanol	14.0	6.8×10^6	4.2×10^7

Table S4: TRPL result of the Cdots, dispersed in water and methanol under a 290 nm excitation source.

Cdot Medium	λ^2	Fraction of the first component (α_1) (%)	First component lifetime (τ_1) (ns)	Fraction of the second component (α_2) (%)	Second component lifetime (τ_2) (ns)	Average lifetime (τ_{av}) (ns)

Cdots in water	1.034	15.5	1.8	84.5	5.4	5.2
Cdots in methanol	1.044	24.6	3.1	75.4	12.9	12.2

References:

1. J. E. Murphy, M. C. Beard, A. G. Norman, S. P. Ahrenkiel, J. C. Johnson, P. Yu, O. I. Micic, R. J. Ellingson, A. J. Nozik, *J. Am. Chem. Soc*, 2006,**128**, 3241.

2. M. P. Sk and A. Chattopadhyay, *RSC Adv.*, 2014, **4**, 31994-31999.