# One-step Synthesis of Orange-red Emissive Carbon Dots: Photophysical Insight into Their Excitation Wavelength-Independent and Dependent Luminescence

*Swayam Prakash[a*], Bamadeb Patra,[b] Saugata Sahu,[a] and Ashok Kumar Mishra[a]*

[a]Department of Chemistry, Indian Institute of Technology Madras, Chennai-600036, India.

[b]Department of Biotechnology, Indian Institute of Technology Madras, Chennai-600036, India.

*Email: swayamprakash.in@gmail.com, swayamprakash@alumni.iitm.ac.in*

## Supplementary information

**Figure S11** EEMF graph of yellow and orange emissive CDs in dichloromethane

**Figure S12** Steady-state absorbance and emission of CDs with the increase in the concentration of TEA

**Instrumentation:** The absorbance and fluorescence spectra were obtained by Horiba Aqualog Jobin-Yvon spectrophotometer with 150 W xenon lamp. The solid-state steady-state measurements of CDs-PMMA were carried out with the optical fiber setup of the Aqualog Horiba Jobin-Yvon spectrophotometer. The absorbance of the solid sample was measured using the UV-visible spectrophotometer's integrating sphere attachment (SHIMADZU UV-2600). The time-resolved studies were carried out using the Horiba Jobin-Yvon FluoroCube TCSPC lifetime instrument. The IBH (DAS-6) was used for time resolved analysis. The goodness of decay fit or "$\chi^2$" value was within the acceptable range ($0.9 \leq \chi^2 \leq 1.4$). The average fluorescence lifetime ($\tau_{avg}$) was measured by equation 1.

$$\tau_{avg} = \frac{\sum_i B_i \tau_i^2}{\sum_i B_i \tau_i} \qquad \text{(Eq. 1)}$$

where "$B_i$" is the pre-exponential factor of the fluorescence of the i$^{th}$ species, and "$\tau_i$" is the fluorescence lifetime of the i$^{th}$ species.

The relative photoluminescence quantum yield ($\Phi_f$) for the orange-red CDs in various solvents was calculated using the equation 2.

$$\Phi_u = \Phi_r \frac{F_u A_r \eta_u^2 I_r}{F_r A_u \eta_r^2 I_u} \qquad \text{(Eq. 2)}$$

Where *"$\Phi$"* represent the quantum yield of the test samples, *"F"* indicates the emission peak area, "*A*" is the absorption value at the excitation wavelength, *"I"* is the excitation intensity and *"$\eta$"* is the refractive index of the solvent. Subscripts *"r"* and *"u"* refer to the reference and the unknown samples. The absorption value of testing samples and reference were kept at ~ 0.05 to avoid the inner filter effect. Standard quantum yield reference was used as perylene ($\Phi_f$ = 0.94 in cyclohexane) with $\lambda_{ex}$ = 440 nm for $\Phi_f$ calculations.[32] FTIR spectras for these CDs were recorded with JASCO FT/IR-4100 spectrometer. The dynamic light scattering (DLS) analysis was measured by Malvern Zetasizer Nano series. A high-resolution transmission electron microscope (HRTEM) was used at an accelerating voltage of 200KV on a JEOL 3010 instrument equipped with energy-dispersive X-ray spectroscopy (EDX). XRD analysis was carried out using Bruker D8 advance powder X-ray diffractometer using Cu Kα as the X-ray source (λ= 1.54 Å). The ESI-MS spectra were obtained from Agilent 6545A Q-TOF mass spectrometer in ESI ionization mode.

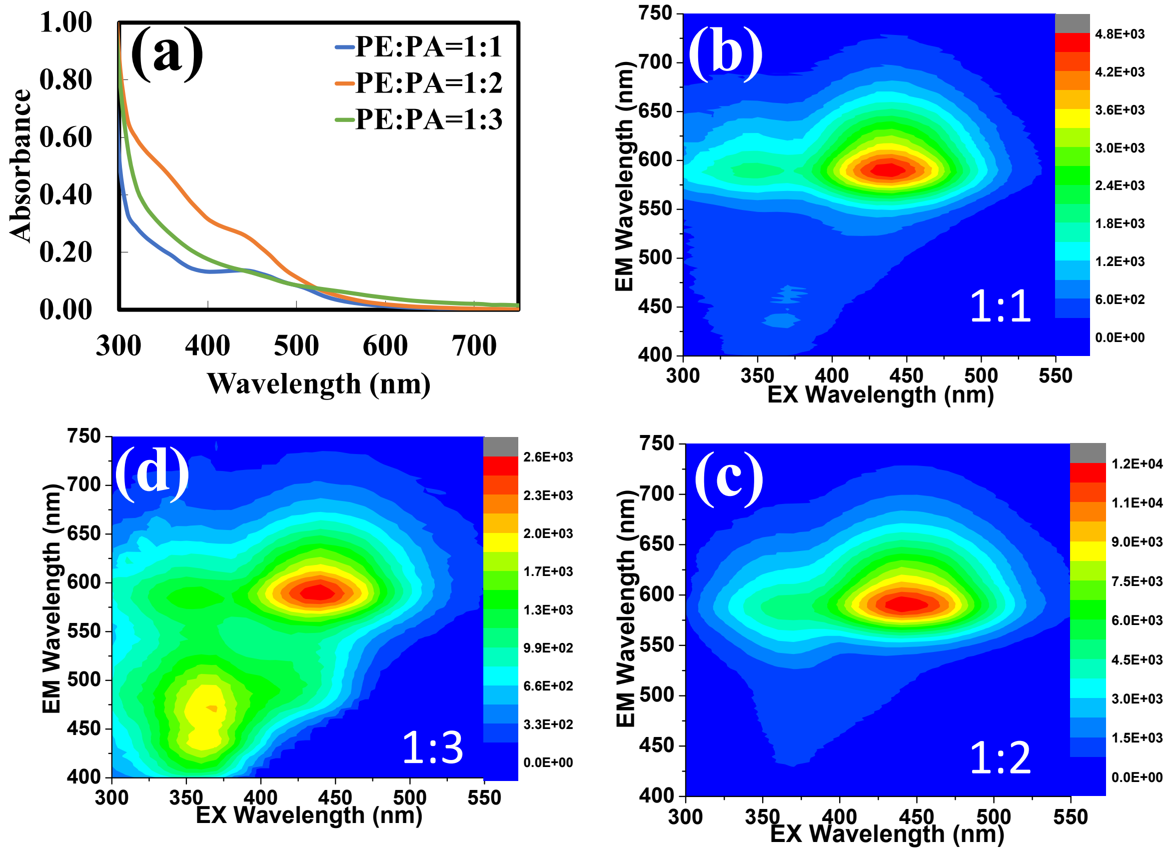


**Figure S1** (a) Absorbance of banana peel extract/acetone (PE) and phosphoric acid (PA) with different proportions, (b) EEMF of PE:PA= 1:1, (c) EEMF of PE:PA= 1:2 and (c) EEMF of PE:PA= 1:3

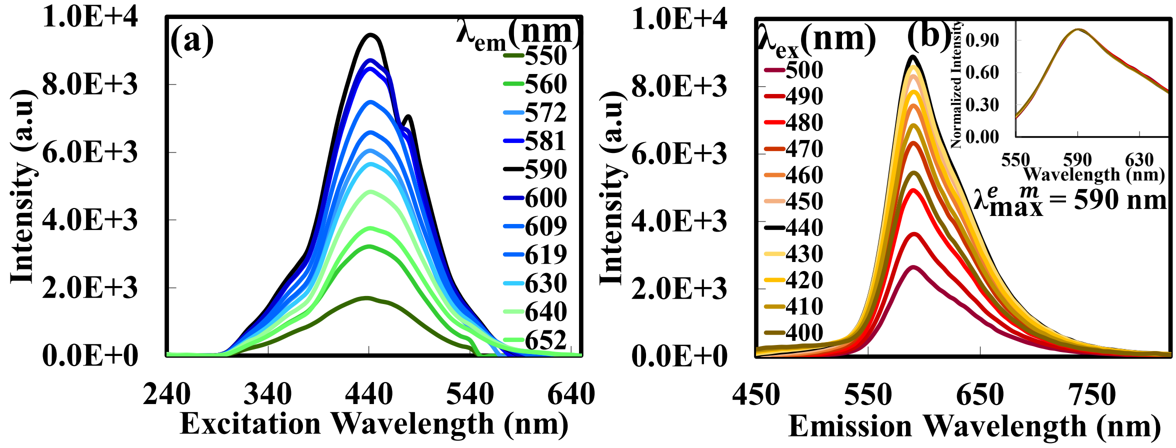


**Figure S2** (a) Excitation spectra of orange emissive CDs with variation in $\lambda_{em}$ = 550 to 652 nm and (b) Emission spectra of orange emissive CDs with variation in $\lambda_{ex}$ = 400 to 500 nm

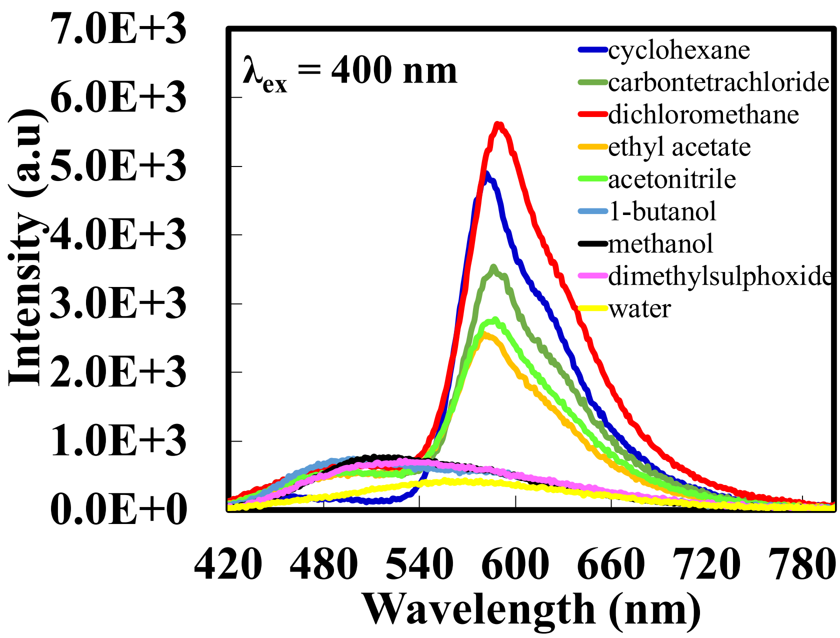


**Figure S3** Emission spectrum of CDs in different solvents with $\lambda_{ex}$ = 400 nm

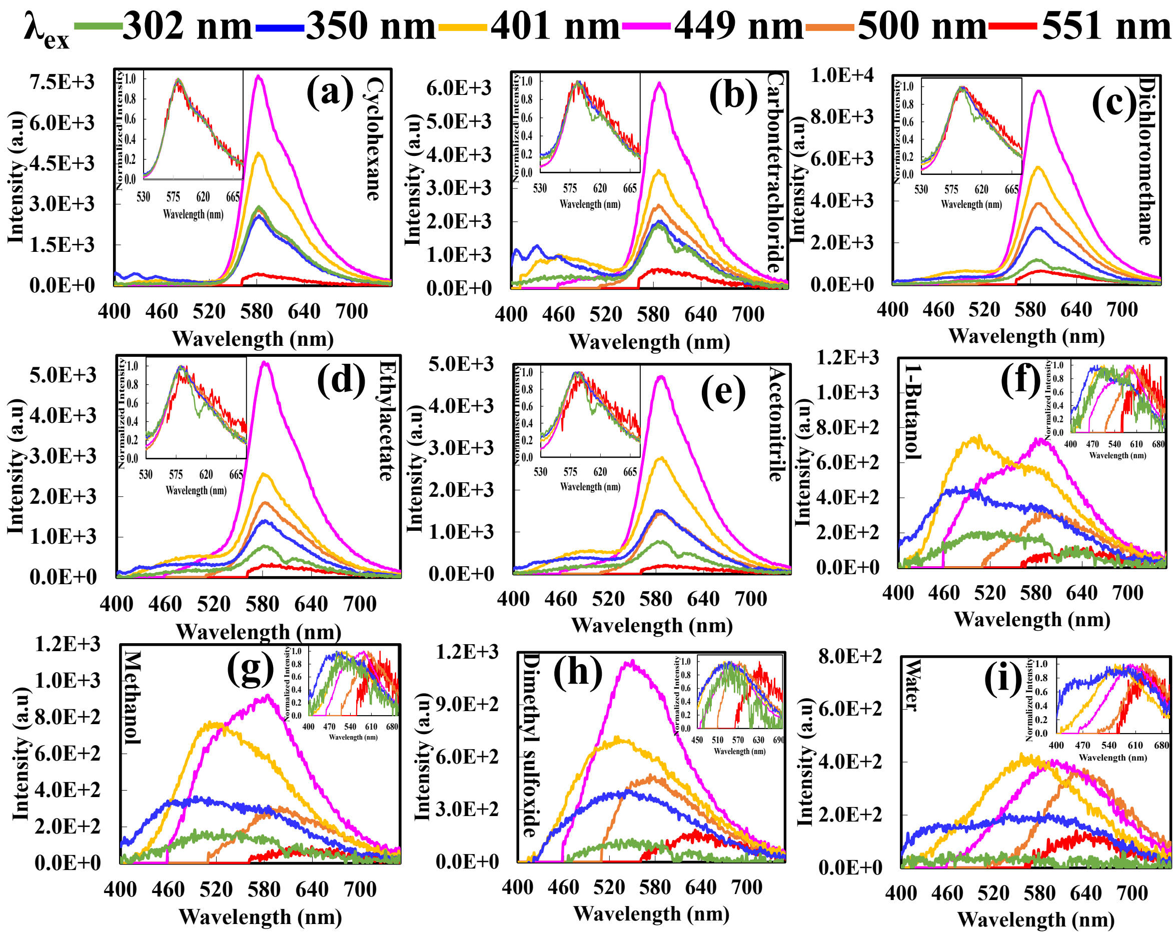

**Figure S4** Emission spectra of CDs in various solvents with vary in $\lambda_{ex}$ =300 to 550 nm (a) cyclohexane, (b) tetrachloromethane, (c) dichloromethane, (d) ethyl acetate, (e) acetonitrile, (f) dimethyl sulfoxide, (g) 1-butanol, (h) methanol and (i) water

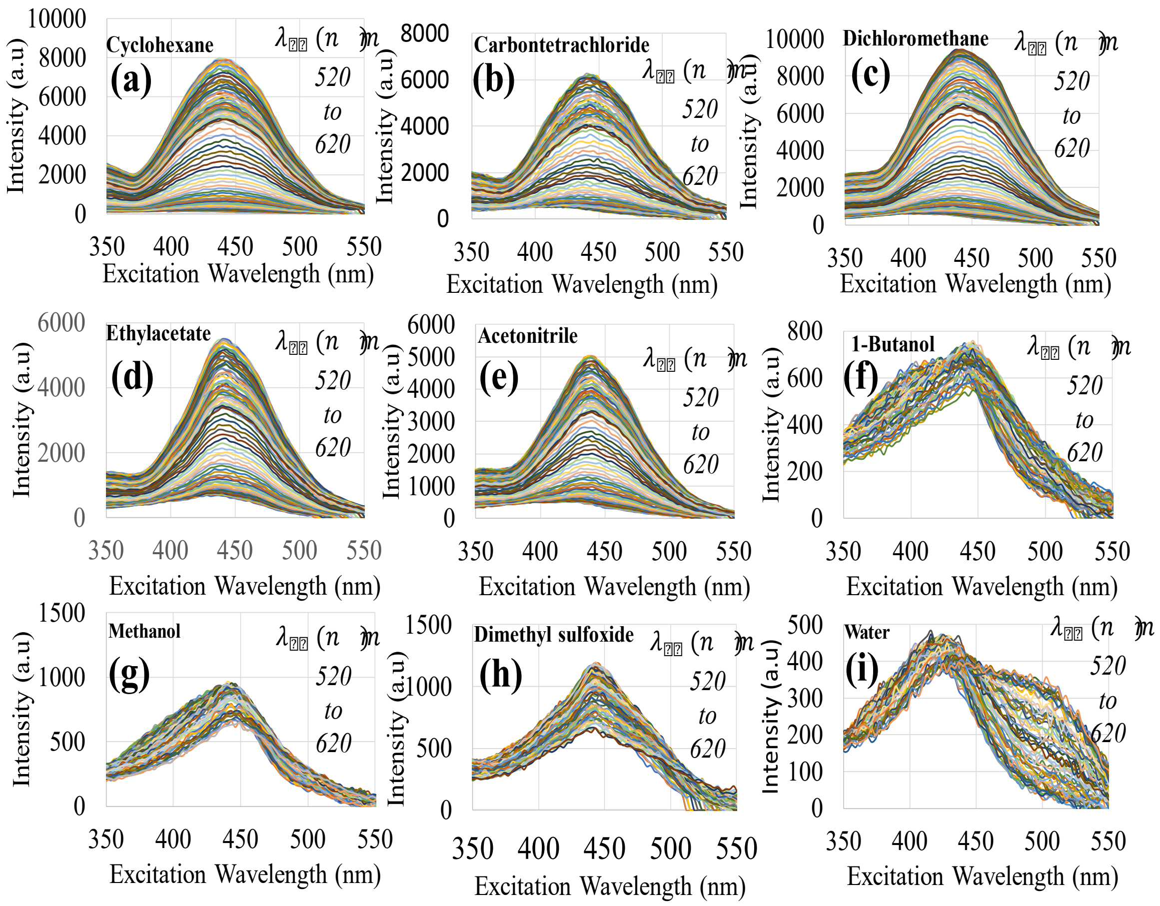


**Figure S5** Excitation spectra of CDs in various solvents with vary in $\lambda_{em}$ =520 to 620 nm (a) cyclohexane, (b) tetrachloromethane, (c) dichloromethane, (d) ethyl acetate, (e) acetonitrile, (f) dimethyl sulfoxide, (g) 1-butanol, (h) methanol and (i) water

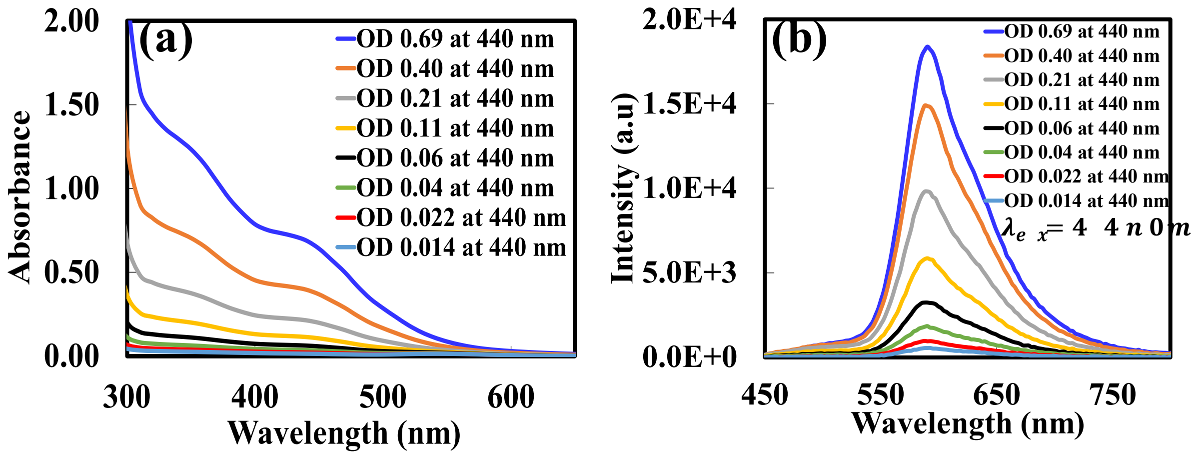

**Figure S6** (a) Steady-state absorbance of CDs with concentration variation in tetrachloromethane ($CCL_4$) and (b) Steady-state emission of CDs with concentration variation in $CCL_4$ at $\lambda_{ex}$ 440 nm.

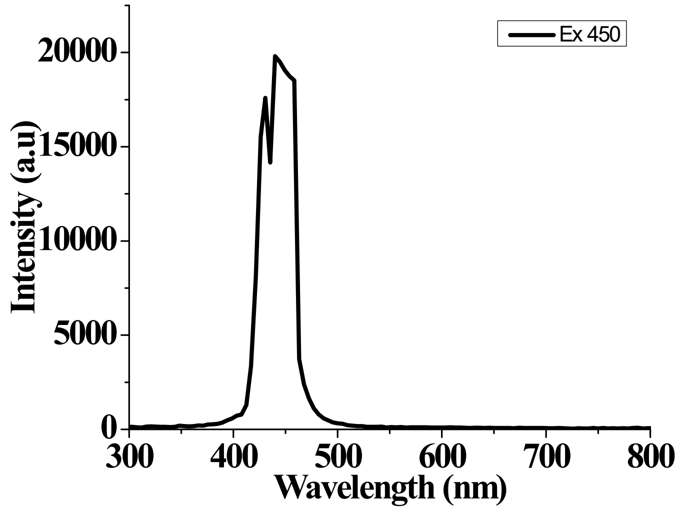


**Figure S7** Emission spectra of solid CDs with excitation at 450 nm

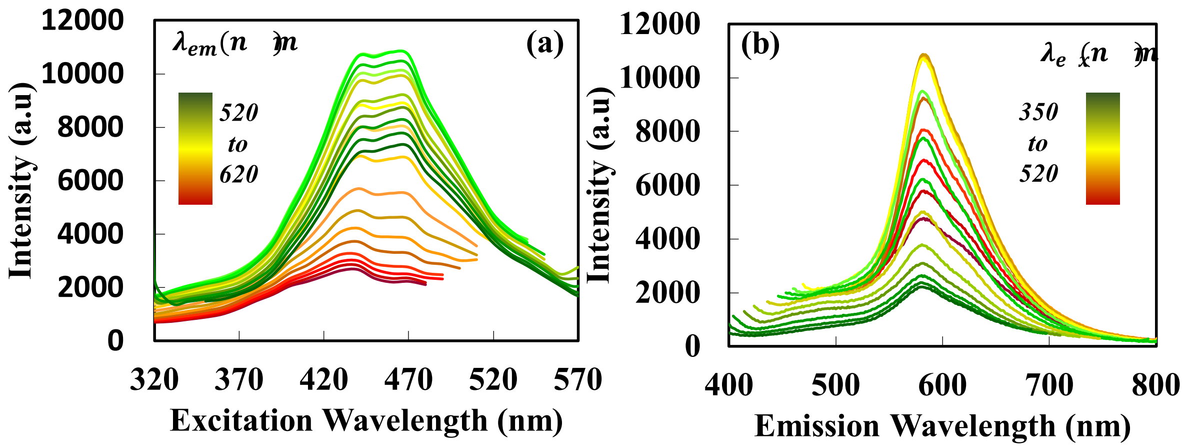


**Figure S8** (a) Excitation spectra of CDs-PMMA with vary in $\lambda_{em}$ =520 to 620 nm and (b) Emission spectra of CDs-PMMA with vary in $\lambda_{ex}$ =350 to 520 nm

### 1. 1 Preparation of CDs-PMMA composite film

Polymethyl methacrylate (PMMA) film was made by dissolving 1 g of PMMA in 10 mL of orange emissive CDs in dichloromethane solution at 50 °C for 15 minutes. Then, the sample was put into a petri dish for drying out.

**Table S1** Emission lifetime (τ, ns), average lifetime ($\tau_{avg}$, ns). The relative amplitudes are provided in parathesis. The error in the measurement = ±5%.

| **Sample name** | $\lambda_{ex} = 450\ nm, \lambda_{em} = 590\ nm$ |
|---|---|

|  | τ₁ (α₁) | τ₂ (α₂) | $\tau_{avg}$ (ns) | χ2 |
|---|---|---|---|---|
| **CD-PMMA** | 1.42 (62) | 4.41 (38) | 3.38 | 1.14 |

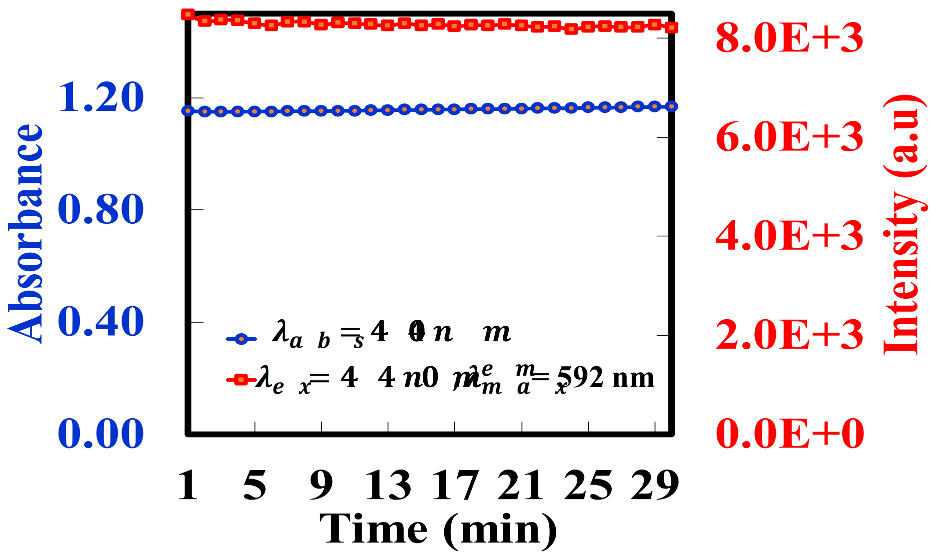


**Figure S9** Fluorescence response of CDs with time by irradiation of 440 nm light.

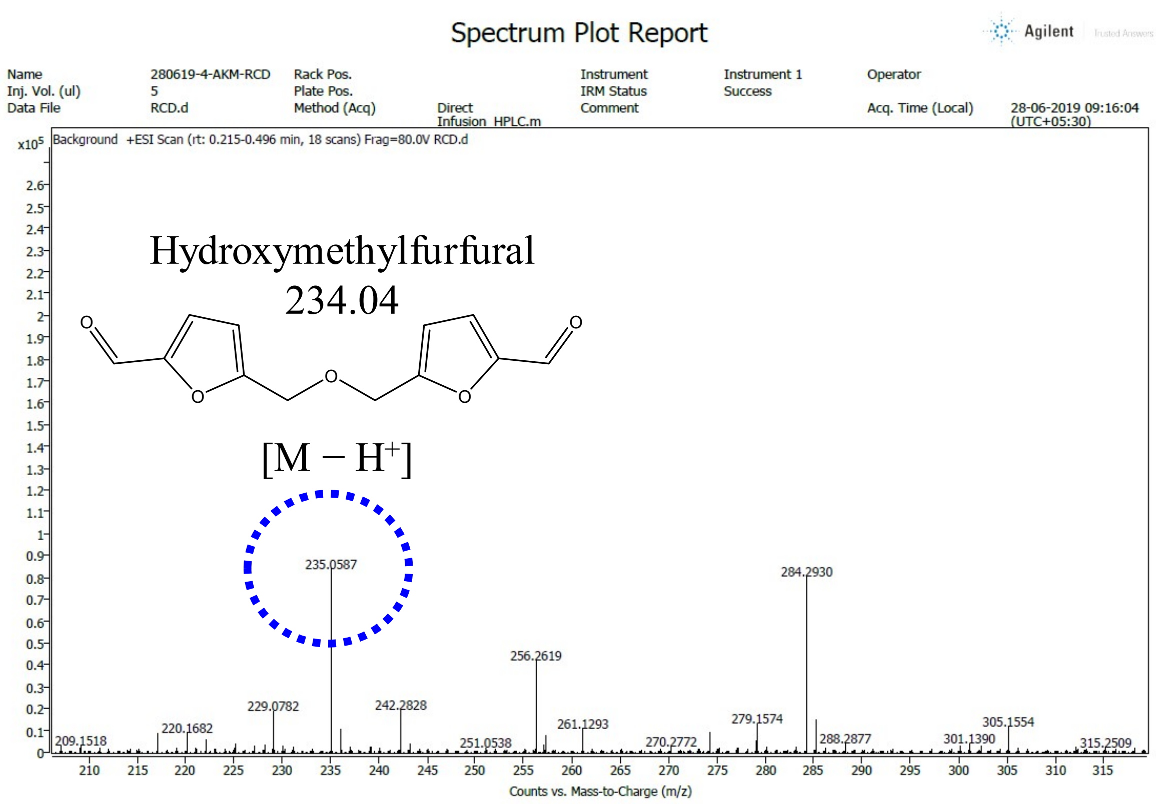


**Figure S10** ESI-MS analysis of CDs

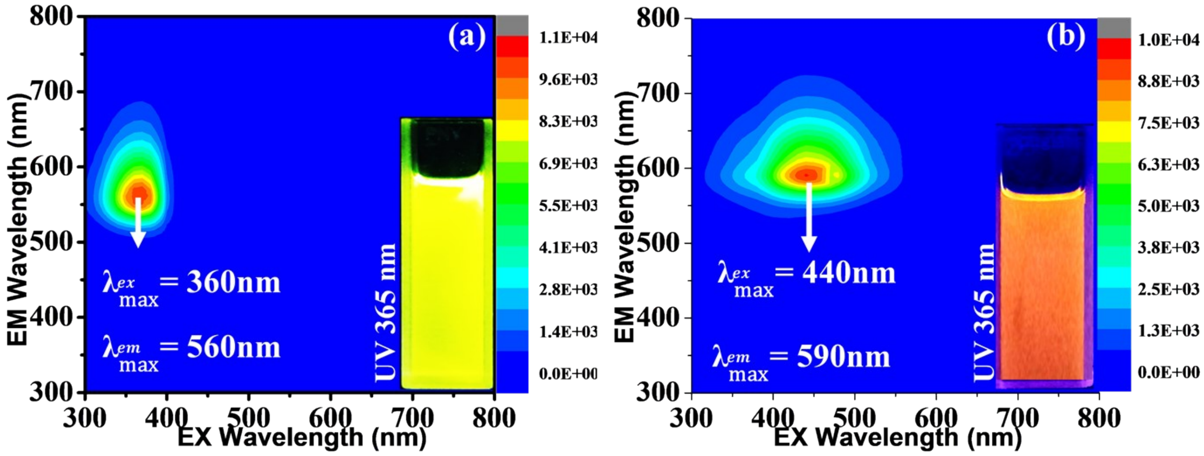


**Figure S11** EEMF graph of (a) yellow emissive CDs (YCD) in dichloromethane and (b) orange emissive CDs (OCD) in dichloromethane

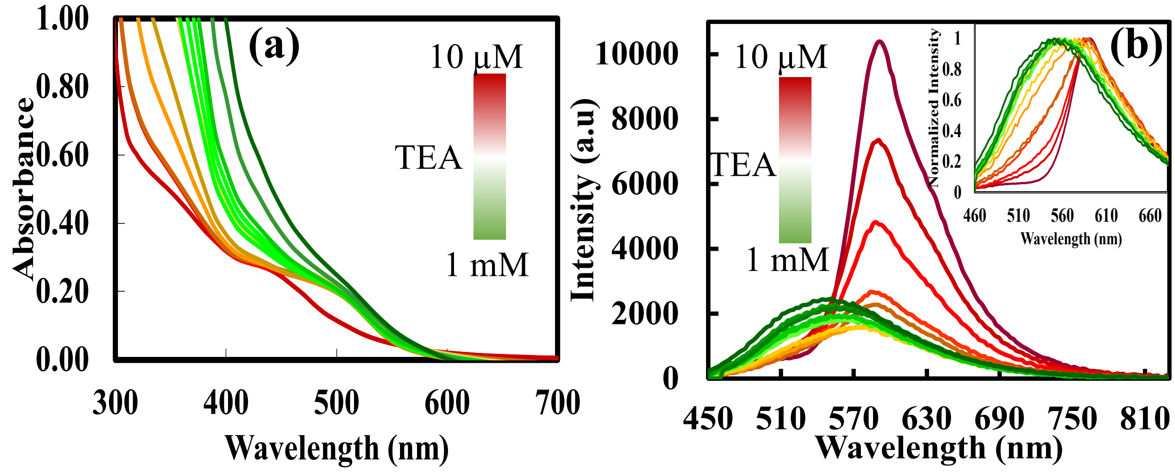


**Figure S12** (a) Steady-state absorbance of CDs with the increase in the concentration of TEA and (b) Steady-state emission of CDs with the increase in the concentration of TEA