# Supporting Information

**Seeking values from biomass materials: preparation of coffee bean shells-derived fluorescent carbon dots via molecular aggregation for anti-oxidation and bioimaging applications**

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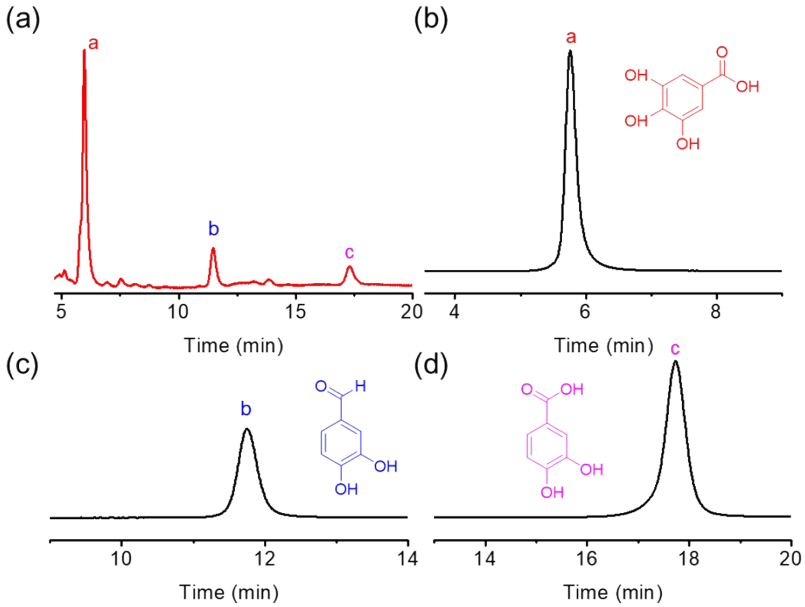


**Figure S1.** HPLC spectra of a) CS-CDs, b) 3,4,5-trihydroxybenzoic acid, c) 3,4-dihydroxybenzaldehyde and d) 3,4-dihydroxybenzoic acid. (Mobile phase was methanol: water: acetic acid = 90:10:0.1, flow rate = 1.0 mL/min, detected temperature = 25 ℃, wavelength = 274 nm).

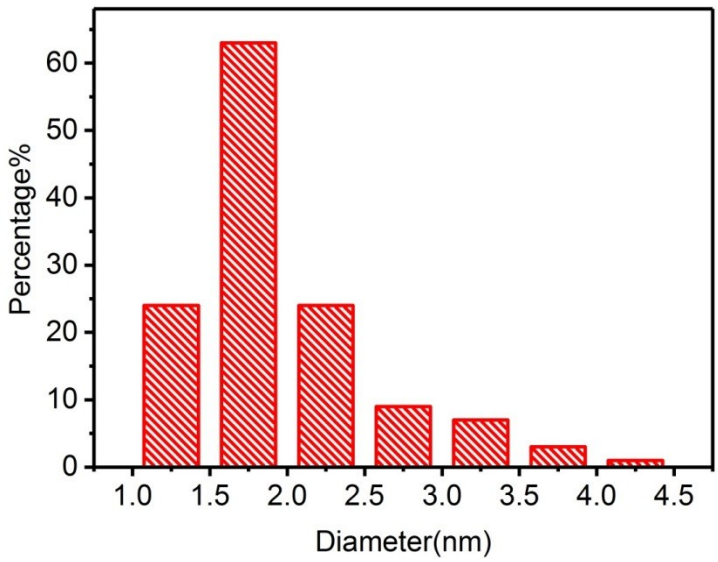


**Figure S2.** Diameter distribution histogram. The diameters of CS-CDs were in the range of 1.0-4.5 nm. Most of the CS-CDs had diameters in the range of 1.5-2.0 nm.

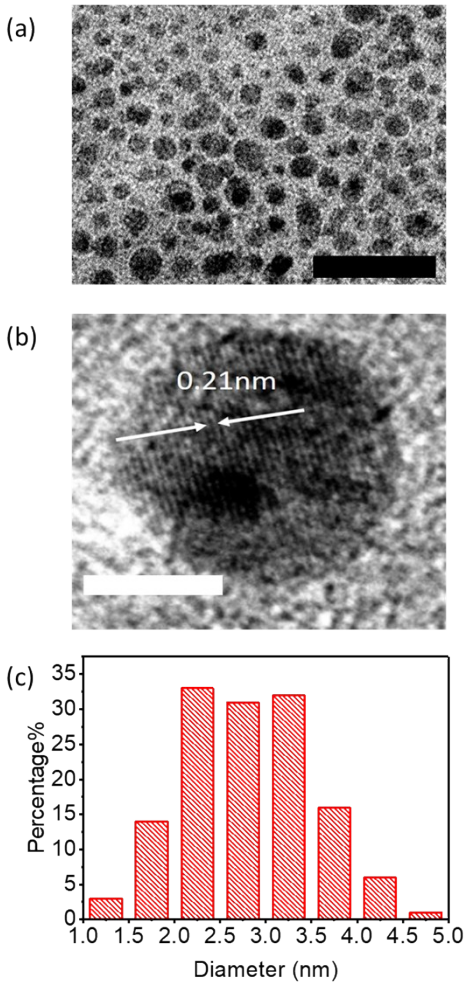


**Figure S3.** a) TEM image of CS-CDs in PBS buffer, scale bar: 20 nm; b) High resolution TEM image of CS-CDs in PBS buffer (pH = 7.4), scale bar: 2 nm; c) Diameter distribution histogram. The diameter of CS-CDs was in the range of 1.0-5.0 nm. Most of the CS-CDs had diameters in the range of 2.0-3.5 nm.

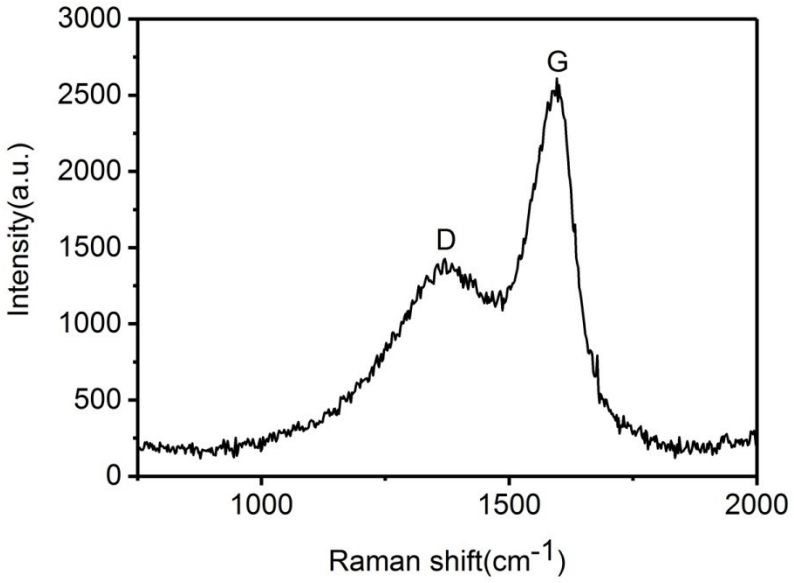


**Figure S4.** Raman spectrum of CS-CDs. Peaks centered at 1366 $cm^{-1}$ (D band) and 1592 $cm^{-1}$ (G band) correspond to $sp^3$ and $sp^2$ carbon atoms, respectively.

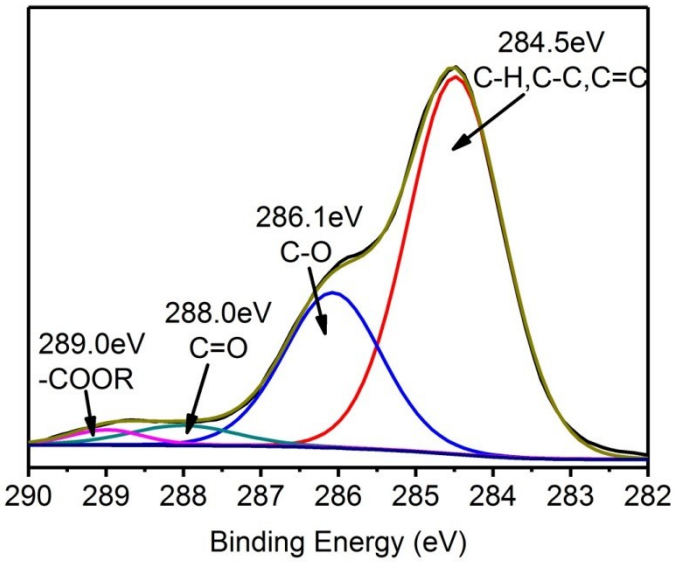


**Figure S5.** XPS $C_{1S}$ spectrum of CS-CDs was fitted to four curves and assigned to groups C-C, C-H, C=C (284.5 eV), C-O (286.1 eV), C=O (288.0 eV) and –COOR (289.0 eV).

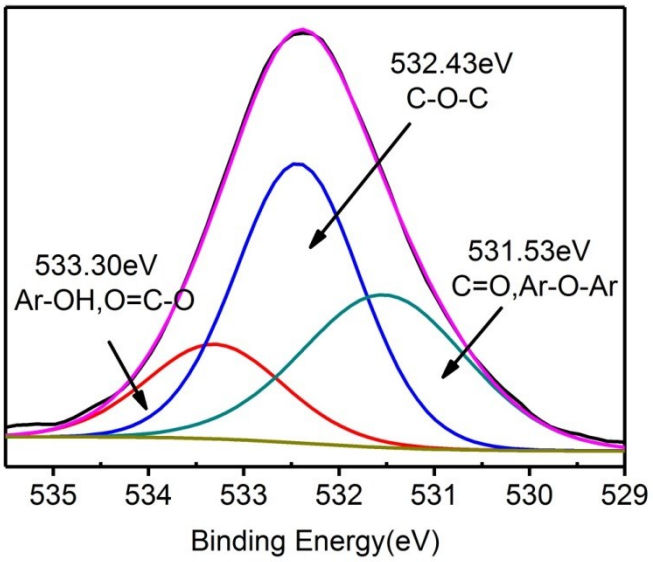


**Figure S6.** XPS $O_{1S}$ spectrum of CS-CDs could be divided into three peaks at 531.53 eV, 532.43 eV, 533.30 eV, corresponding to C=O/Ar-O-Ar, C-O-C and Ar-OH/O=C-O, respectively.

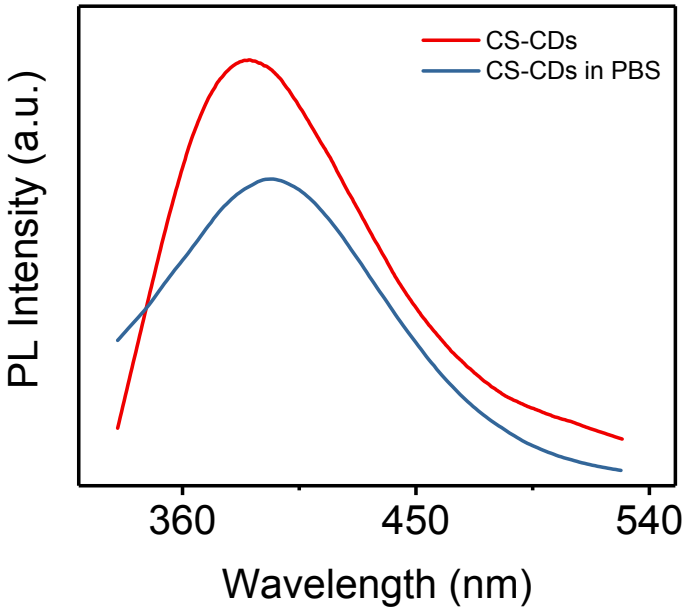


**Figure S7.** Intensity of fluorescence spectra of CS-CDs in aqueous solution and PBS buffer (pH = 7.4).

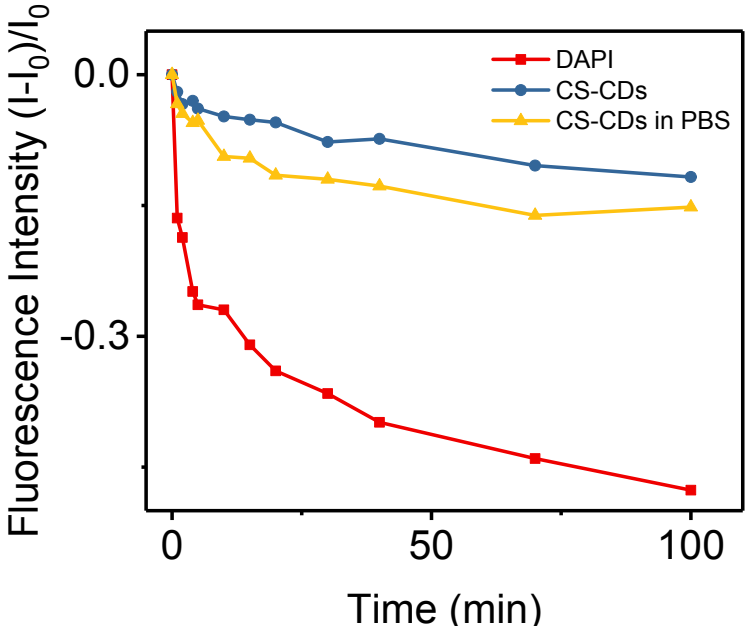


**Figure S8.** Fluorescence intensity of CS-CDs (in aqueous solution and PBS buffer) at 410 nm and DAPI at 455 nm upon irradiation with UV light at 365 nm (0.1 mw/cm$^2$) in aqueous solution, excitation wavelength = 365 nm. I is fluorescence intensity after UV irradiation, and $I_0$ is fluorescence intensity without UV irradiation.