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 °C, 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=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/cm²) in aqueous solution, excitation wavelength = 365 nm. I is fluorescence intensity after UV irradiation, and I₀ is fluorescence intensity without UV irradiation.