

Article

Carbon Dots from Coffee Grounds: Synthesis, Characterization, and Detection of Noxious Nitroanilines

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Table S1. Organic composition of CGs and CBs.

Parameter	Coffee Grounds			Coffee Beans		
	CGsSV	CGsCQ	CGsNP	CBsSV	CBsCQ	CBsNP
Total phenols¹						
(Equiv. gallic acid)	9.87	9.87	6.05	12.89	10.21	9.14
(Equiv. tannic acid)	12.82	12.88	7.91	16.79	13.10	11.83
(Equiv. vanilin)	18.70	18.78	11.53	24.48	19.12	17.26
Flavonoids¹						
(Equiv. quercetin)	3.24	2.43	2.01	2.81	2.10	1.62
Total sugars¹						
(Equiv. β -D-glucose)	27.62	25.77	22.04	16.26	12.22	10.87
Proteins¹						
(Equiv. BSA)	3.22	1.67	2.53	3.89	0.51	1.03
Lipids²	11.62	10.29	10.72	8.49	7.91	9.61

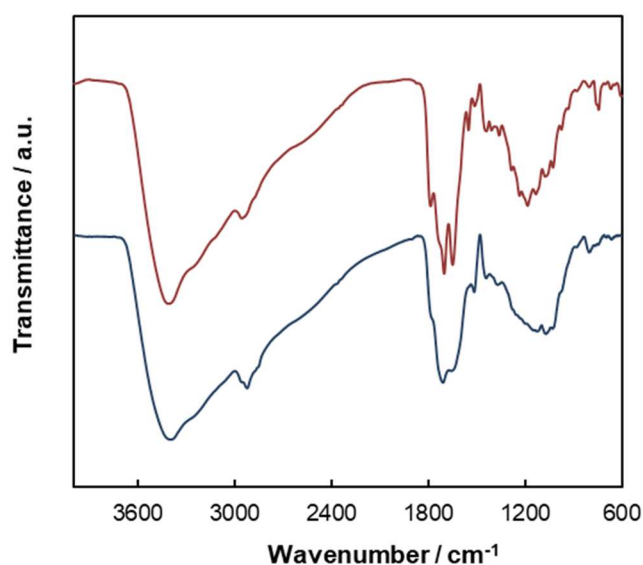
¹Values determined from the water extracts and expressed as percentages of TS-WE (see Experimental).

²Values obtained from extraction of CGs/CBs with *n*-hexane, expressed as percentages (see Experimental).

Table S2. Dipole moments and hyperpolarizabilities of NAs [1].

Analyte	μ/D	$\beta/10^{-30}$ esu
<i>p</i> -NA ¹	6.2	34.5
<i>o</i> -NA ²	4.3	10.2
<i>m</i> -NA ²	4.9	6.0

Solvent: ¹ Methanol; ² Acetone.

**Figure S1.** FTIR spectra (KBr) of CGsSV (blue line) and CBsSV (brown line).

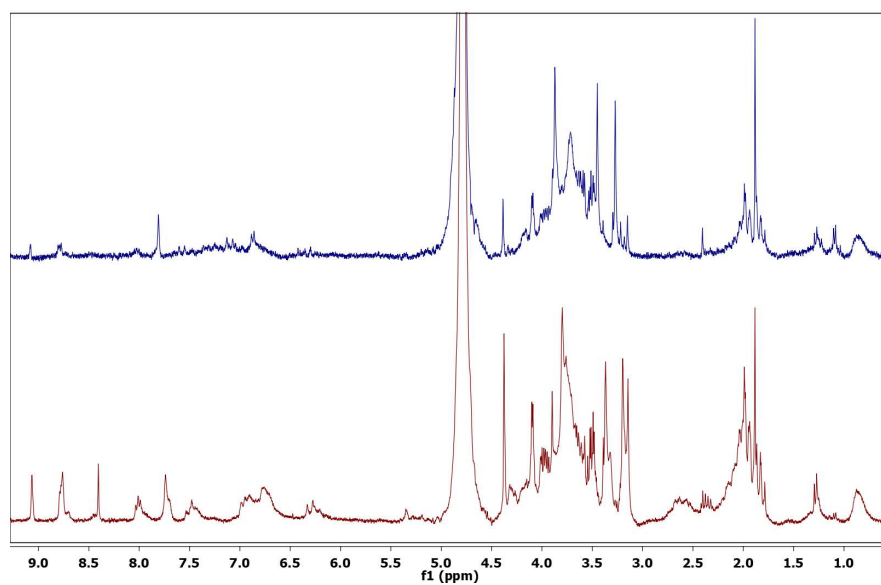


Figure S2. ^1H NMR spectra of CGsSV (blue line) and CBsSV (brown line) (300 MHz, D_2O , 25 $^\circ\text{C}$).

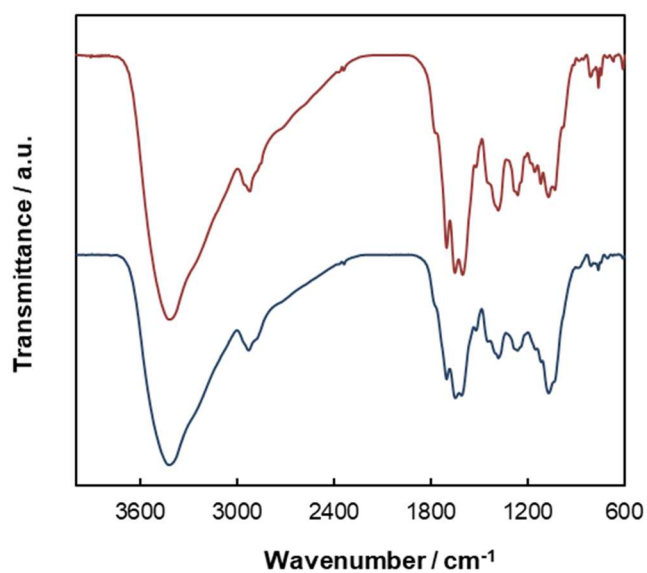


Figure S3. FTIR spectra (KBr) of CGsNP (blue line) and CBsNP (brown line).

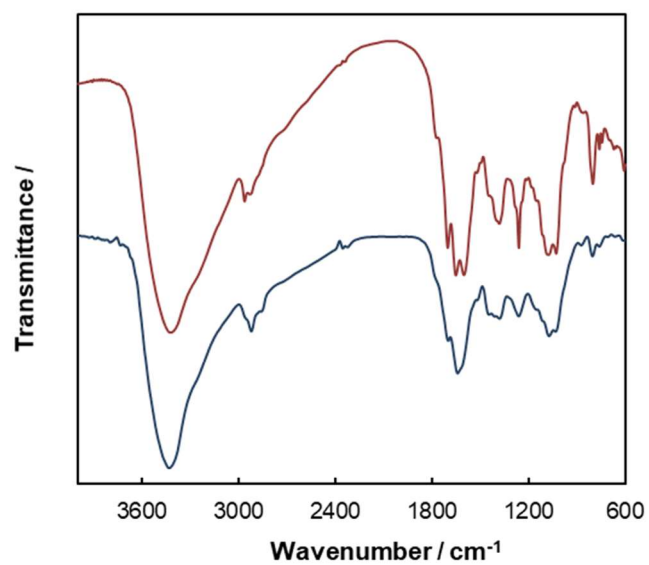


Figure S4. FTIR spectra (KBr) of CGsCQ (blue line) and CBsCQ (brown line).

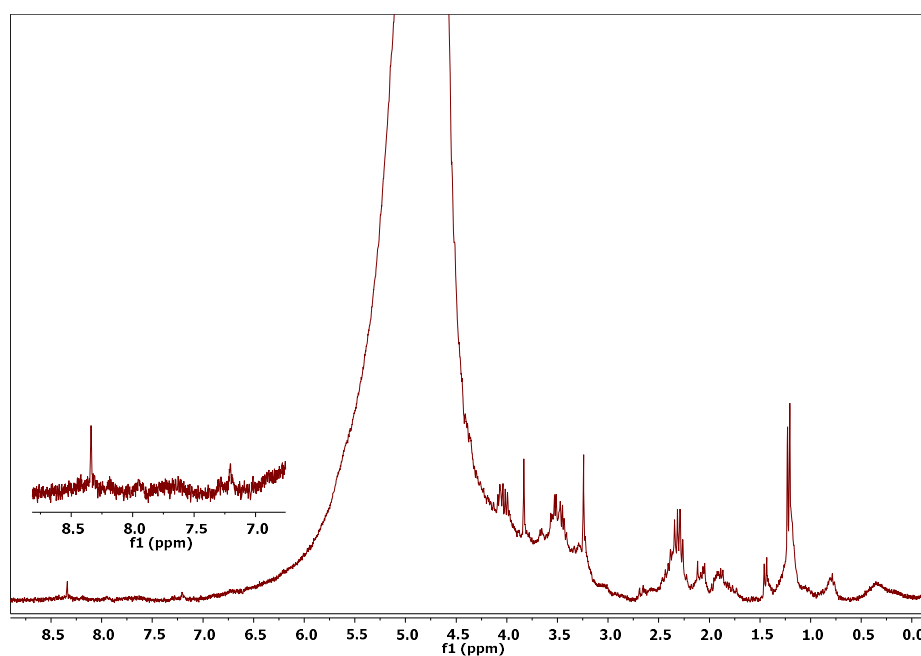


Figure S5. ¹H NMR spectrum (300 MHz, D₂O, 25 °C) of C-dots from CGsSV by HTC method.

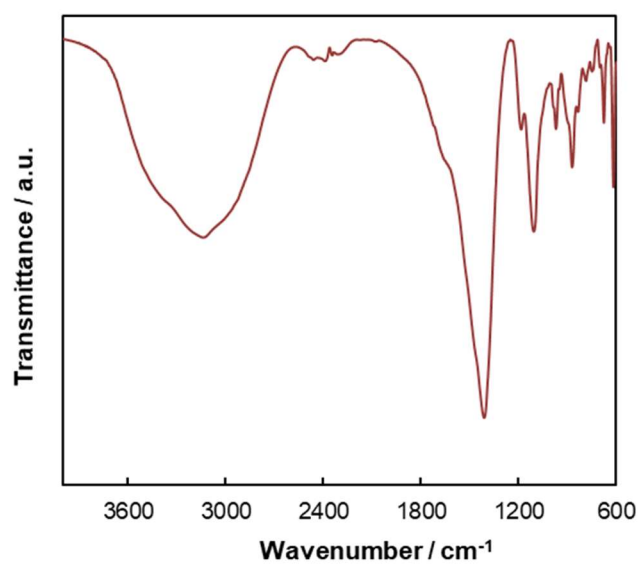


Figure S6. FTIR spectrum (KBr) of C-dots' ashes from HTC method.

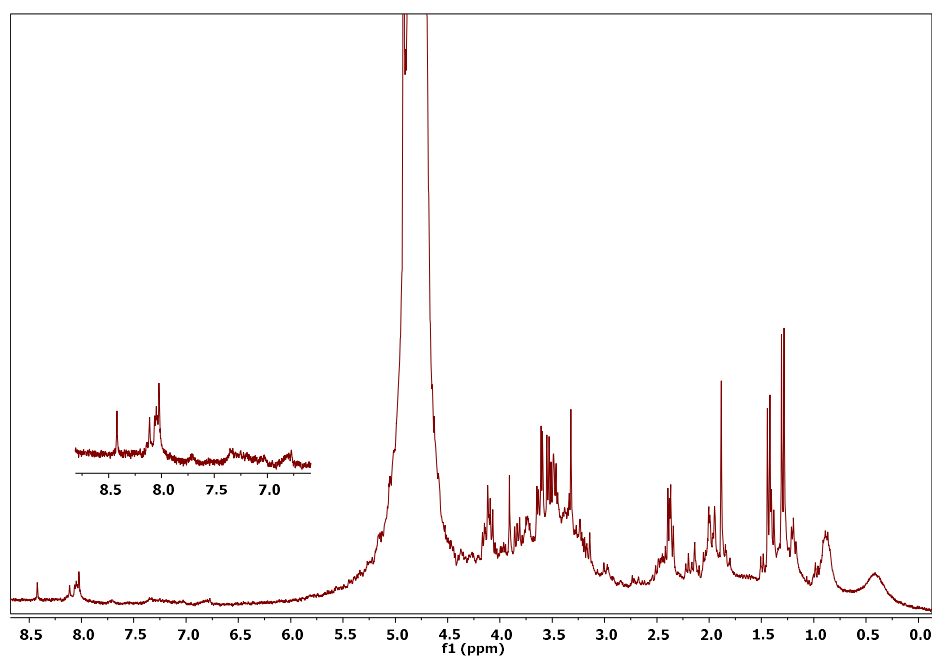


Figure S7. ¹H NMR spectrum (300 MHz, D₂O, 25 °C) of C-dots from CGsSV by Mw-HTC method.

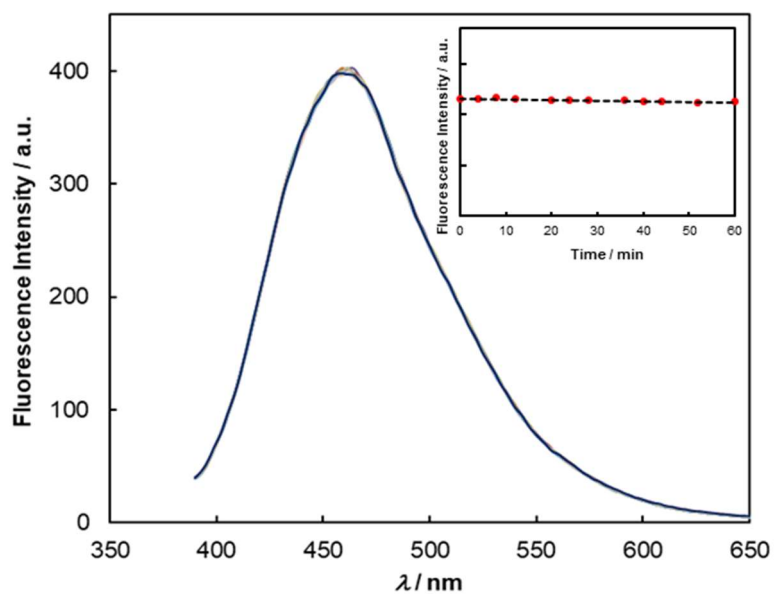


Figure S8. Emission spectra of aqueous dispersions (0.1 mg/mL) of C-dots ($\lambda_{\text{em}} = 461$ nm) obtained by HTC in the presence of ED upon continuous irradiation ($\lambda_{\text{exc}} = 380$ nm) for 1h.

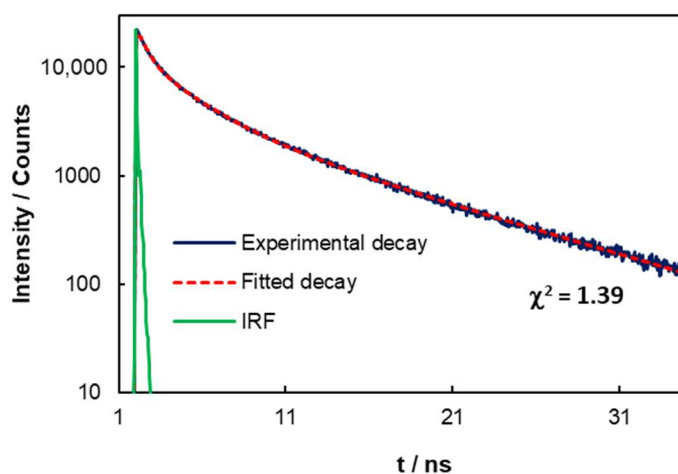


Figure S9. Intensity decay of aqueous dispersions of C-dots (Mw-HTC) excited at 340 nm and observed at 447 nm.

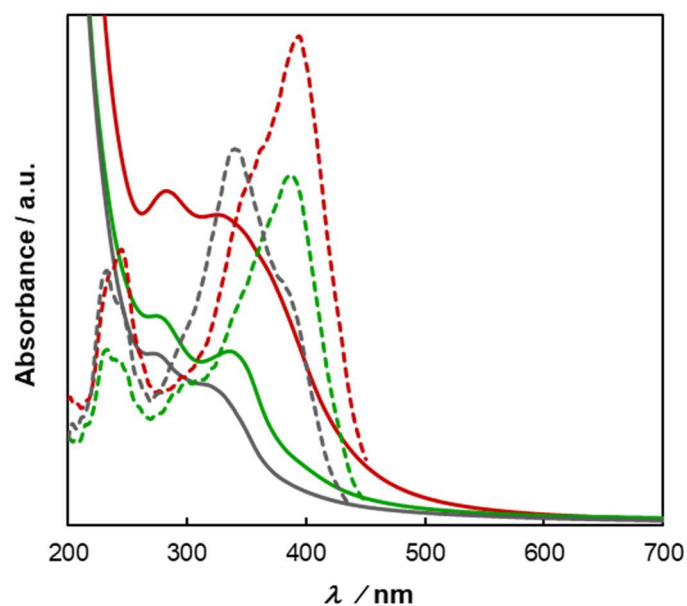


Figure S10. UV-Vis and excitation (dashed lines, monitored at the corresponding emission maximum) spectra of aqueous dispersions (0.1 mg/mL) of C-dots prepared at 200 °C (red line), 250 °C (green line) and 300 °C (grey line) under the conditions reported in Table 2.

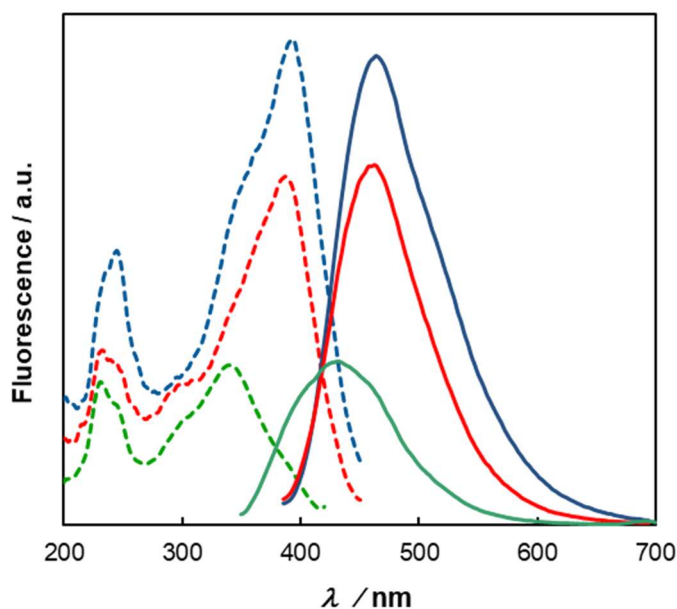


Figure S11. Emission ($\lambda_{\text{exc}} = 380$ nm; solid lines) and excitation (dashed lines, monitored at the corresponding emission maximum) spectra of aqueous dispersions (0.1 mg/mL) of C-dots prepared at 200 °C (blue lines), 250 °C (red lines) and 300 °C (green lines), under the conditions reported in Table 2.

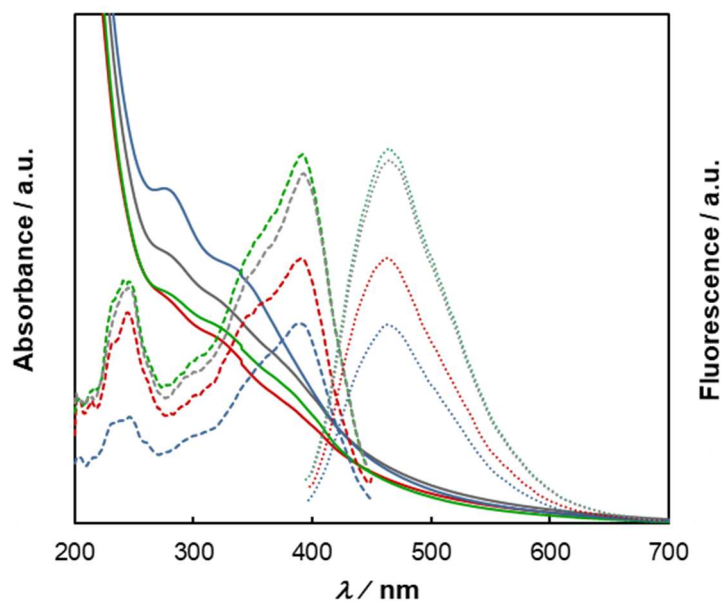


Figure S12. UV-Vis (solid lines), emission (dotted lines, $\lambda_{exc} = 380$ nm) and excitation (dashed lines, monitored at the corresponding emission maximum) spectra of aqueous dispersions (0.1 mg/mL) of C-dots prepared by Mw-HTC method with different CGs concentrations (30 mg/mL; red), (100 mg/mL; green) and (200 mg/mL; grey) at 190 °C during 15 min. For comparison, the C-dots obtained after 3h heating at the lowest CGs concentration, keeping the other reaction conditions, is also shown (blue lines).

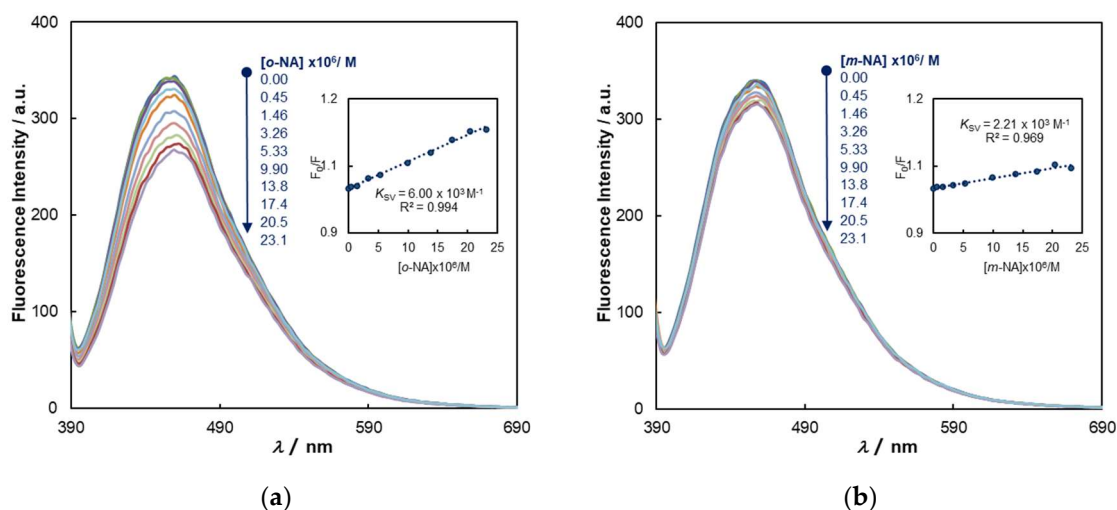


Figure S13. Emission spectra of C-dots (0.01 mg/mL) after successive additions (4.47×10^{-7} – 2.31×10^{-5} M) of *o*-NA (a) and *m*-NA (b) ($\lambda_{exc} = 380$ nm). Inset: Stern-Volmer plot after correction for *h*-IFE.

1. Oudar, J.L.; Chemla, D.S. Hyperpolarizabilities of nitroanilines. *J. Chem. Phys.* **1977**, *66*, 2664-2668. <https://doi.org/10.1063/1.434213>.