Electronic Supplementary Information

Green synthesis of fluorescent nitrogen/sulfur-doped carbon dots and investigation of their properties by HPLC coupled with mass spectrometry

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Table S1. Elemental analysis of the as-synthesised C-dots: **(A)** Elemental content and **(B)** relative number of atom in C-dots

(A)

Type of C-dots	Elemental content (%)				
	C	H	O (Calculated)	N	S
Undoped C-dots	41.12	6.35	52.05	0.39	0.092
N,*S*-C-dots	40.93	5.90	38.71	6.23	8.23

(B)

Type of C-dots	Relative number of atom				
	C	H	O	N	S
Undoped C-dots	12	22	12	0.1	0.01
N,*S*-C-dots	13	23	9	2	1

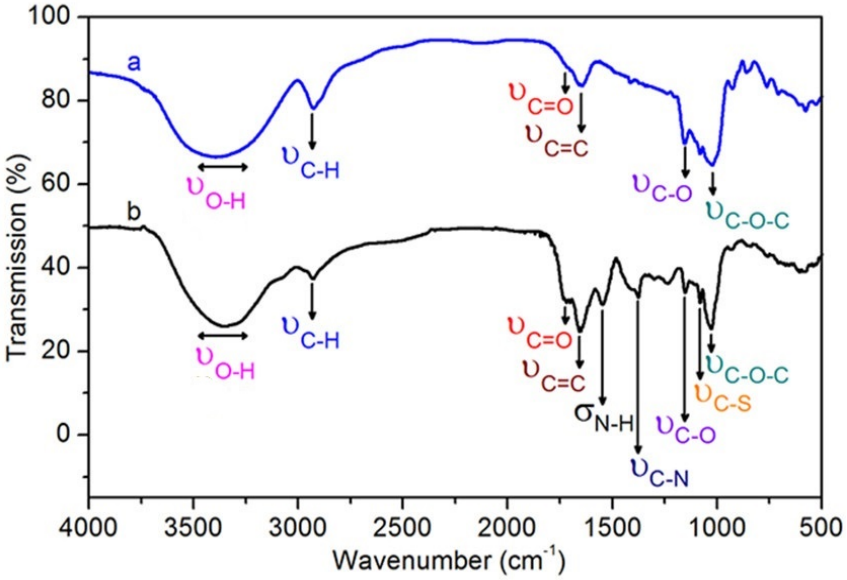


Fig. S1. FTIR spectra of (a) undoped C-dots and (b) *N*,*S*-C-dots.

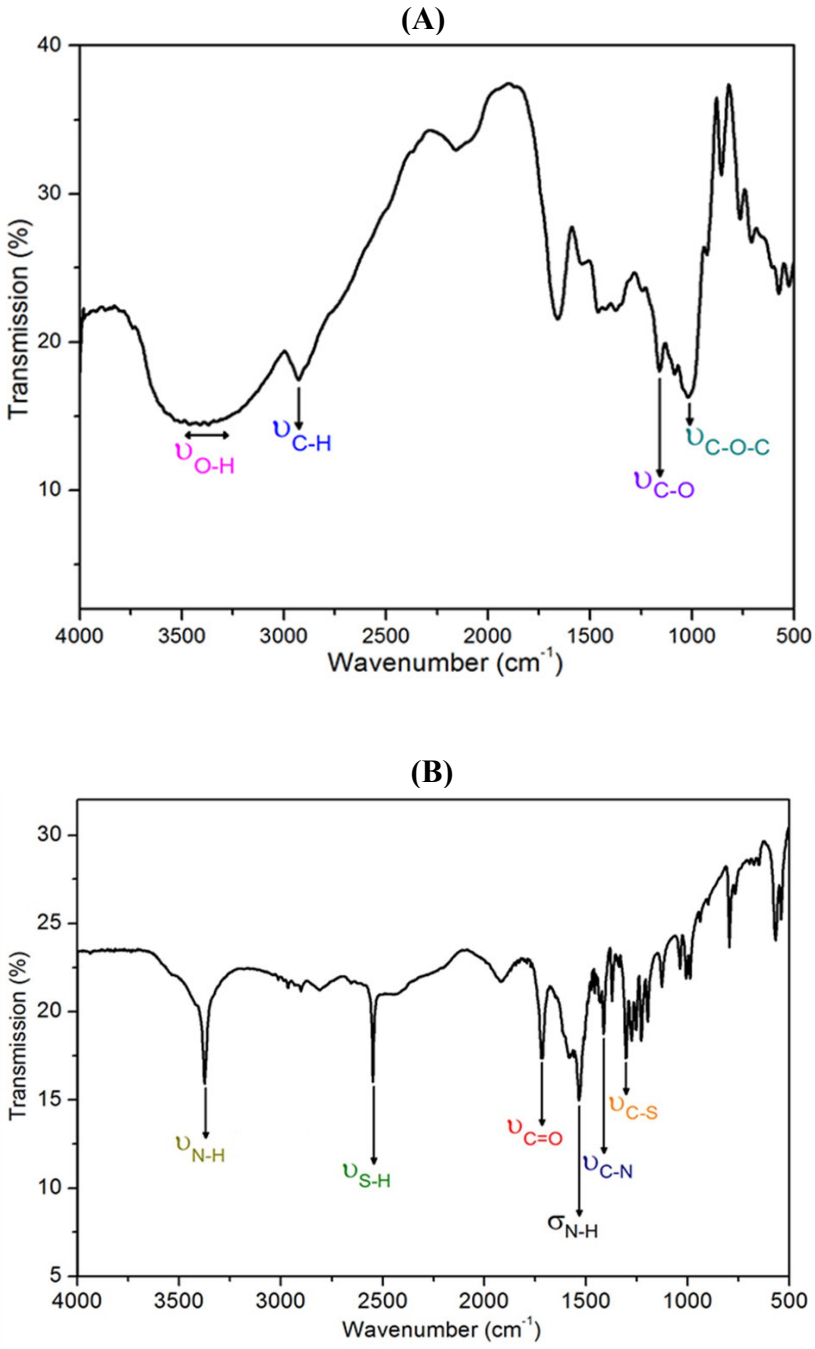


Fig. S2. FTIR spectra of (A) rice and (B) NAC.

Measurement of quantum yield

Quantum yield (Φ_S) of the C-dots sample was determined by a comparative method. Quinine sulfate (Φ_R = 0.54) in 0.10 M H_2SO_4 (refractive index, η = 1.33) was selected as the reference to determine the Φ_S of the C-dots sample in distilled water (η = 1.33) at different concentrations. All the absorbances of the solutions at the excitation wavelength (λ_{ex}) were recorded by a UV-vis absorption spectrophotometer (Varian, Palo Alto, CA, USA). PL spectra of C-dots were measured by a Photon Technology International QM4 spectrofluorometer (Birmingham, NJ, USA). The λ_{ex}/integrated PL intensity area under the PL curve in the wavelength range were 340/360–650 nm for undoped C-dots sample, 340/360–650 and 390/410–650 nm for *N*,*S*-C-dots sample, and 390/410–650 nm for *N*,*S*-C-dots HPLC fractions. Graphs of integrated PL intensity against absorbance were plotted. The Φ_S of the C-dot sample was calculated as follows:

$$\Phi_S = \Phi_R \, (Grad_S / Grad_R) \, (\eta^2_S / \eta^2_R)$$

where the subscripts *S* and *R* denote the sample and reference, respectively. *Grad* is the gradient from the plot of integrated PL intensity against absorbance, and η is the refractive index of the solvent. In order to minimise the self-absorption effect, the absorbances in the 10-mm pathlength fluorescence cuvette should never exceed 0.050 at the excitation wavelength.[1,2]

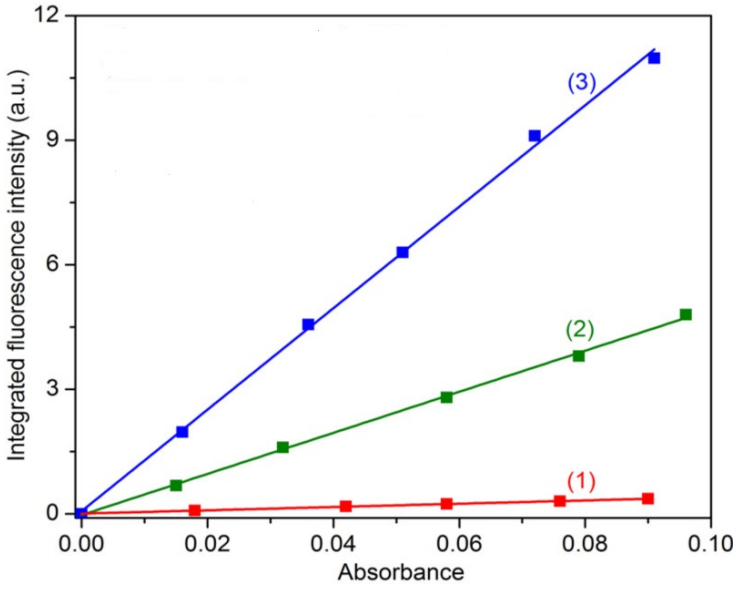
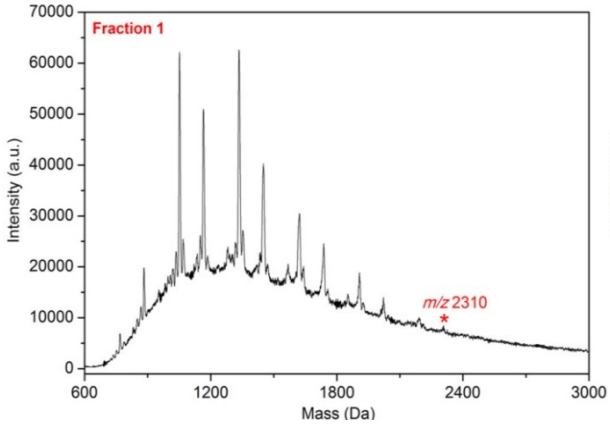


Fig. S3. Plots of integrated PL intensity against absorbance of C-dots: (1) undoped C-dots at λ_{ex} 340 nm. (2) *N*,*S*-C-dots at λ_{ex} 340 nm, and (3) *N*,*S*-C-dots at λ_{ex} 390 nm. The gradients of quinine sulfate are 2298.5 and 2801.36 at λ_{ex} 340 and 390 nm, respectively.

References

1 S. Sahu, B. Behera, T.K. Maiti and S. Mohapatra, *Chem. Commun.*, 2012, **48**, 8835.
2 C. Liu, P. Zhang, F. Tian, W. Li, F. Li and W. Liu, *J. Mater. Chem.*, 2011, **21**, 13163.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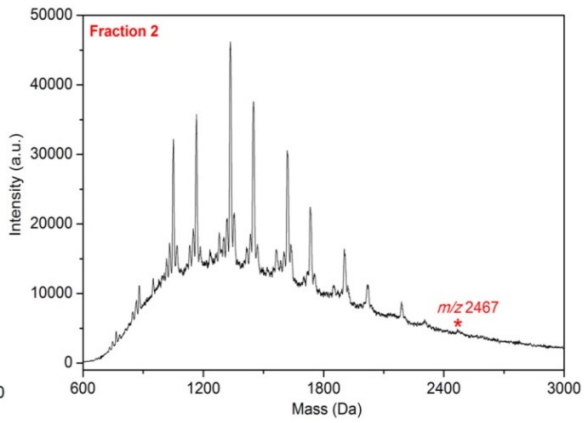
m/z 2310
Intensity (a.u.)
Mass (Da)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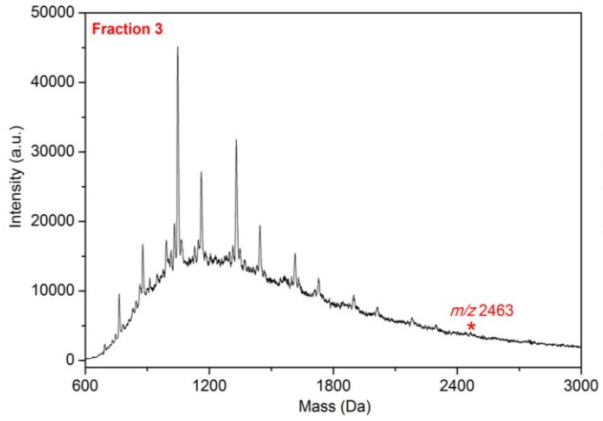
Mass (Da)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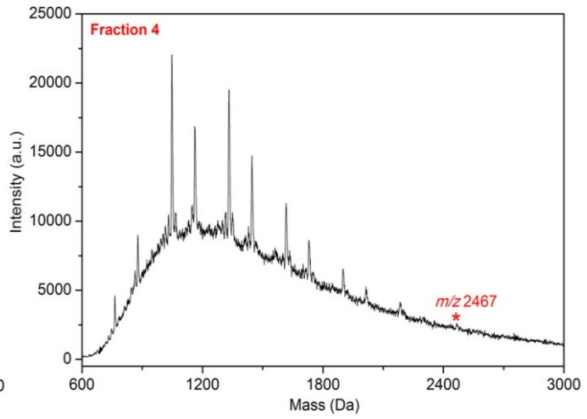
Mass (Da)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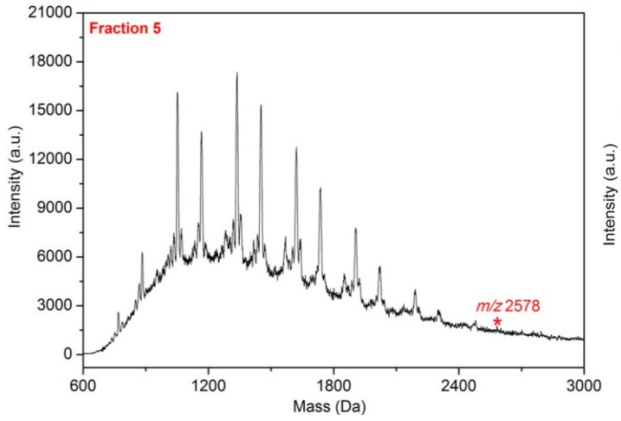
Intensity (a.u.)
Mass (Da)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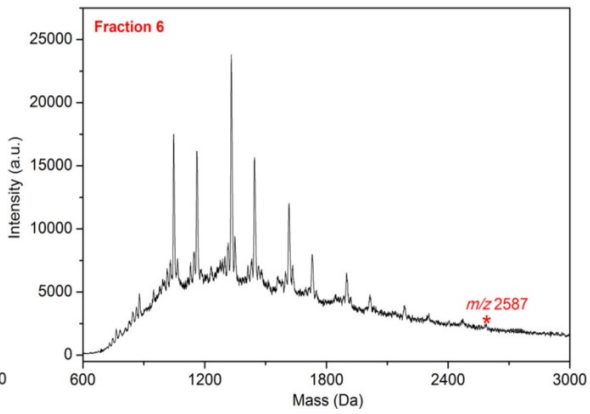
Intensity (a.u.)
Mass (Da)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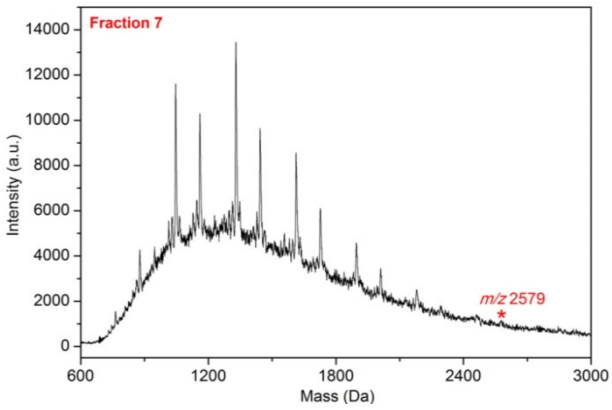
Intensity (a.u.)
Mass (Da)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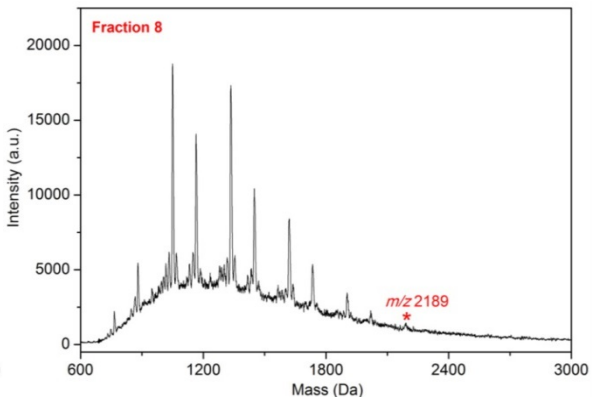
Intensity (a.u.)
Mass (Da)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Intensity (a.u.)
Mass (Da)

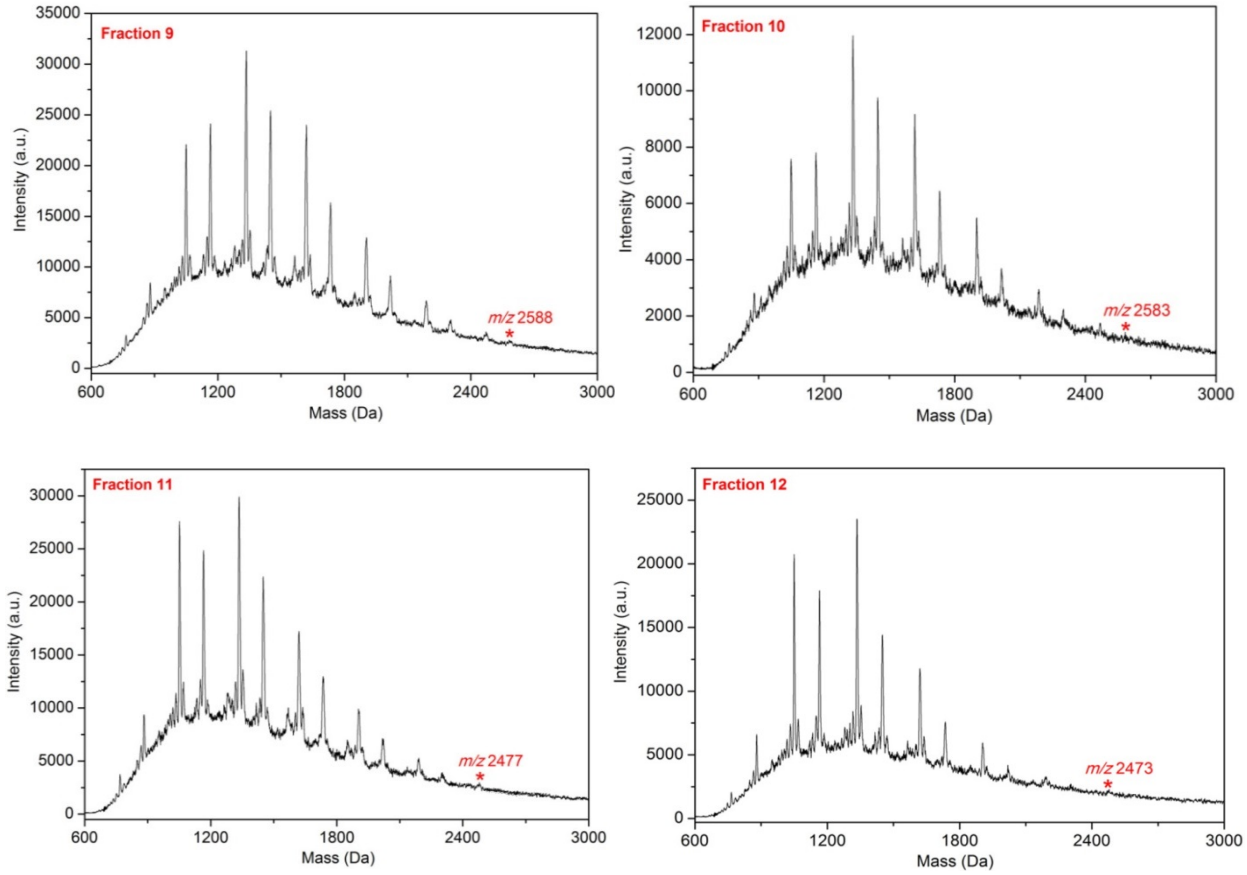

Fig. S4. MALDI-TOF MS of fractions 1–12 in *N*,*S*-C-dots.

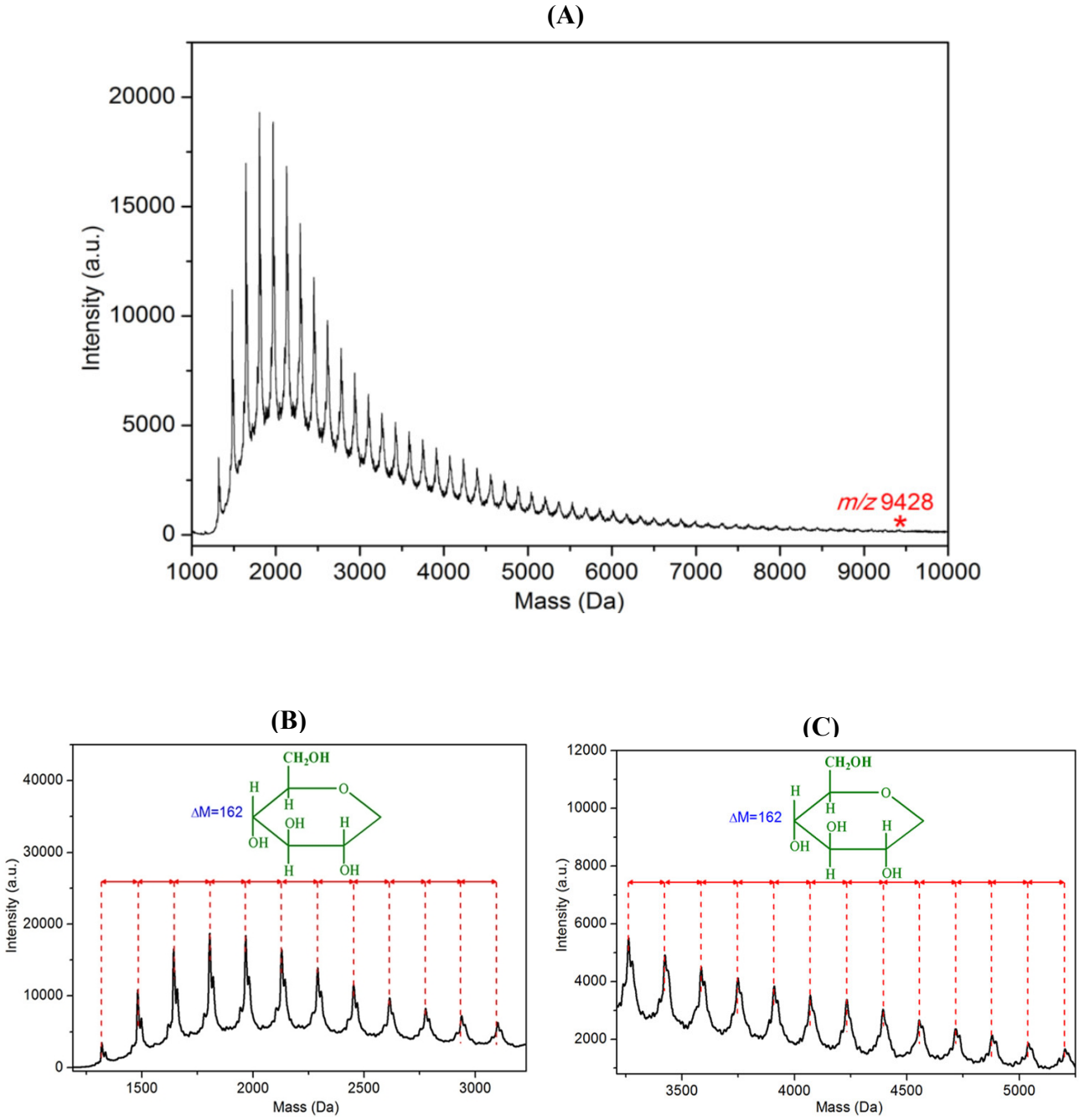

Fig. S5. (A) MALDI-TOF MS of rice. (B) Expanded MS in the mass range 1190–3230 Da. (C) Expanded MS in the mass range 3210–5250 Da.

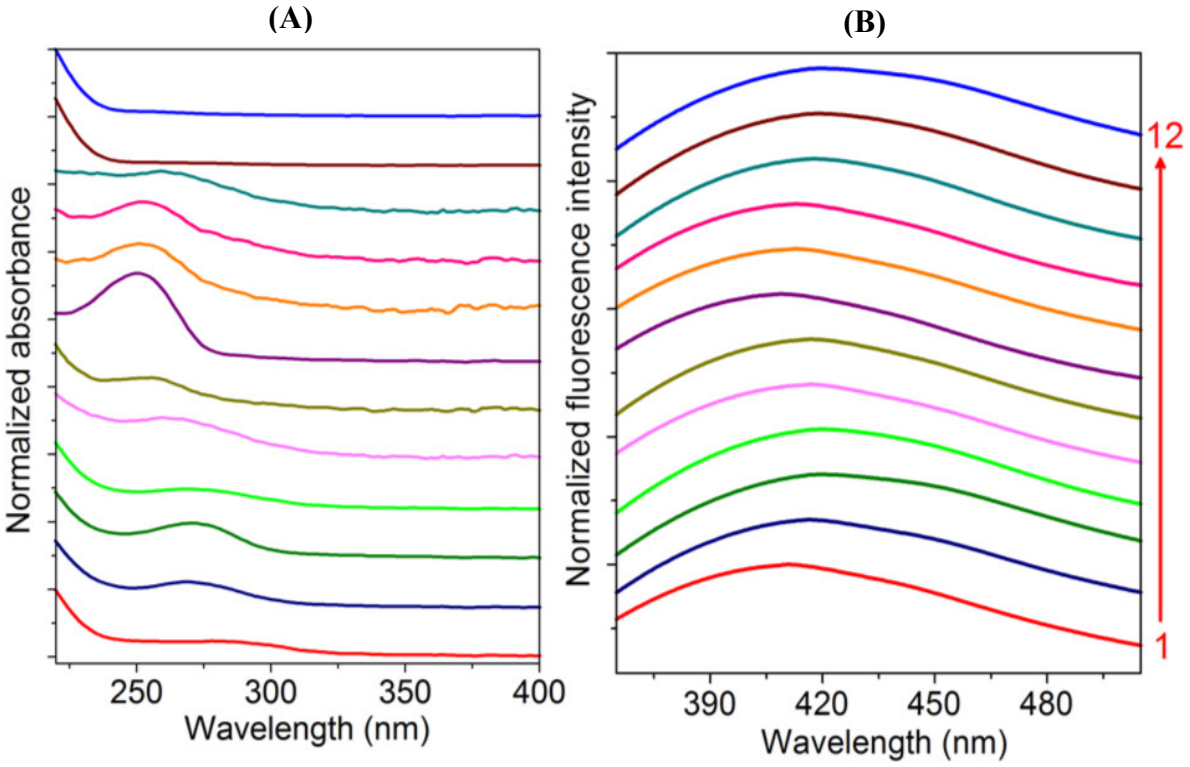

Fig. S6. (A) Absorption and (B) PL spectra at λ_{ex} 340 nm of fractions 1–12 (from bottom to top) in the undoped C-dots in Fig. 5B.