Nitrogen-Doped Carbon Quantum Dots as Fluorescent Sensor for Doxorubicin and Chlortetracycline: Experimental and DFT Insights

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Supplementary Information

3.1.2. XRD analysis

Table S1

Diffraction peak details of the NEDA-CQDs sensor.

2θ (°)	Height [cts]	d value (Å)	Relative Intensity (%)
17.7553	201.68	4.99141	11.21
19.1134	1798.78	4.63971	100.00
25.7035	1176.41	3.46313	65.40
25.7845	978.92	3.45242	54.42
29.5880	305.35	3.01671	16.98
30.6888	269.9	2.91096	15.00
30.9303	281.85	2.88878	15.67
33.2457	411.4	2.69269	22.87
33.6214	804.92	2.66345	44.75
35.7184	950.67	2.51175	52.85
40.7760	220.89	2.21112	12.28
42.7702	517.61	2.11252	28.78

3.1.2. DLS and Zeta Potential analysis

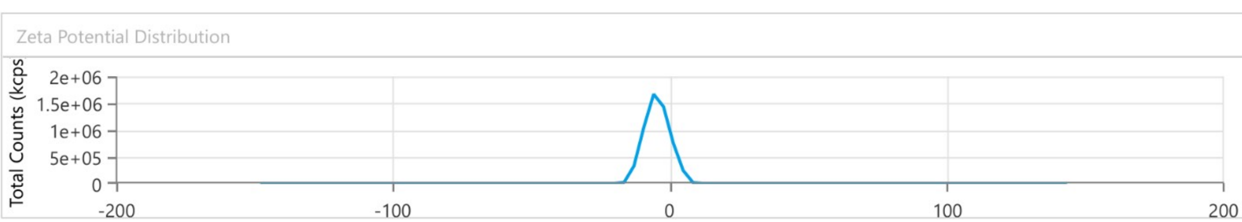

Fig. S1. The Zeta Potential analysis of the NEDA-CQDs sensor.

3.2. Optical properties of the NEDA-CQDs

To investigate the excitation-dependent emission behavior of the NEDA-CQDs, fluorescence emission spectra were recorded at excitation wavelengths of 300, 350, and 405 nm (Figure S2). The emission maximum remained nearly constant at approximately 490 nm, with only variations in fluorescence intensity observed. The absence of noticeable peak shifting indicates excitation-independent emission behavior, suggesting that the luminescence originates predominantly from uniform surface states rather than multiple energy trap levels. This observation supports the structural consistency and electronic stability of the synthesized carbon quantum dots.

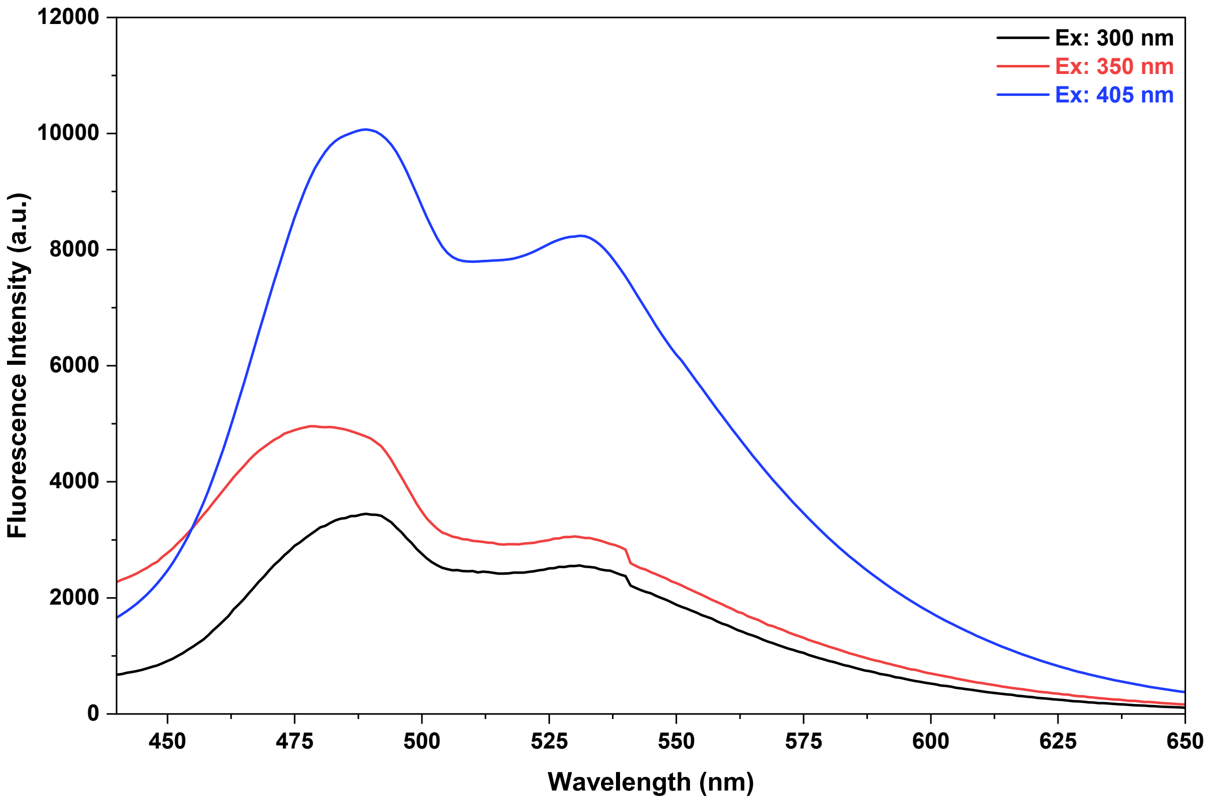

Fig. S2. Fluorescence emission spectra of NEDA-CQDs recorded at different excitation wavelengths: 300 nm, 350 nm, and 405 nm, demonstrating excitation-independent emission behavior.

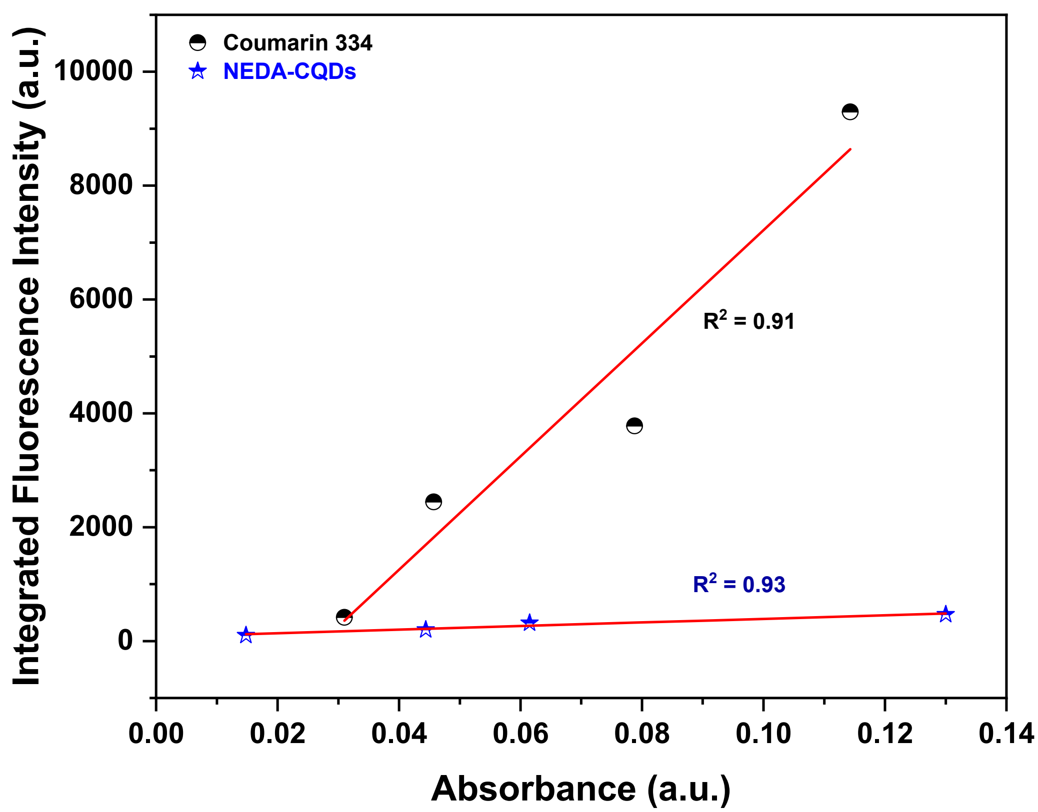

Fig. S3. Quantum yield determination of NEDA-CQDs using the relative method with Coumarin 334 as a reference standard. The integrated fluorescence intensity (area) was plotted against the absorbance at the excitation wavelength (λ_{Ex} = 405 nm) for both the reference and NEDA-CQDs. The emission maximum of NEDA-CQDs was observed at λ_{Em} = 492 nm. The slopes obtained from the linear fitting (R^2 = 0.91–0.93) were used for quantum yield calculation according to the standard comparative method.

3.9.1. The structural and electronic characteristics of the NEDA-CQDs nanosheet and the DOX and CTC drug molecules

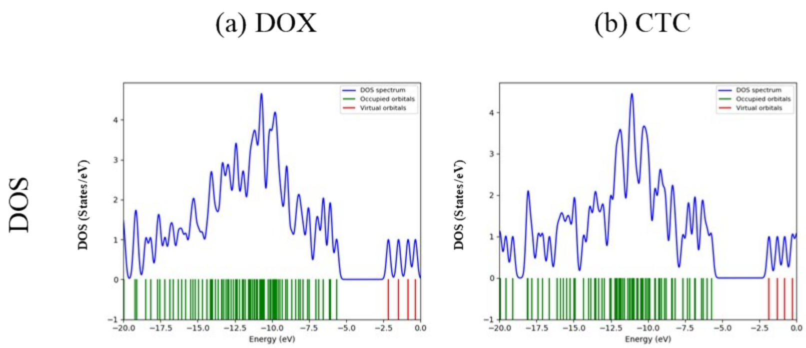

Fig. S4. The DOS spectra diagrams for (a) DOX and (b) CTC drug molecules, respectively.