Supporting Information

Riboflavin-Based Carbon Dots with High Singlet Oxygen Generation for Photodynamic Therapy†

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1. Solubility comparison between VB2 and CDs

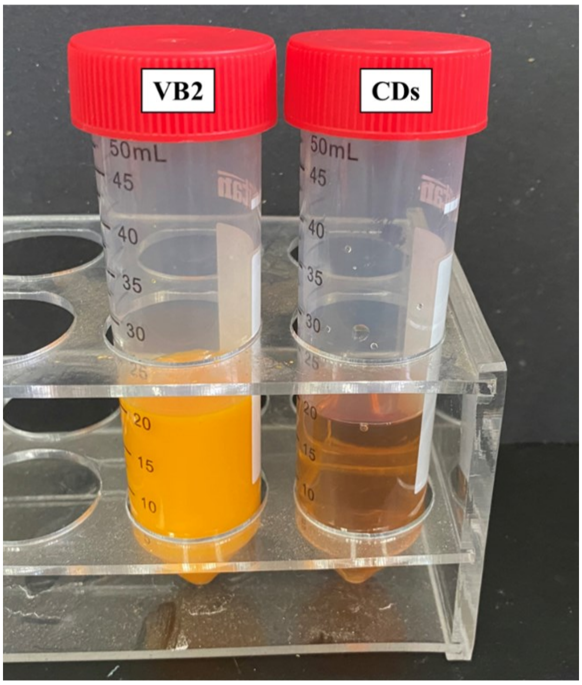

Fig. S1 Solubility comparison between VB2 and CDs; Left: before the reaction, 300 mg VB2 in 20 mL water.; Right: after the reaction, the prepared CDs in water.

2. FT-IR spectrum

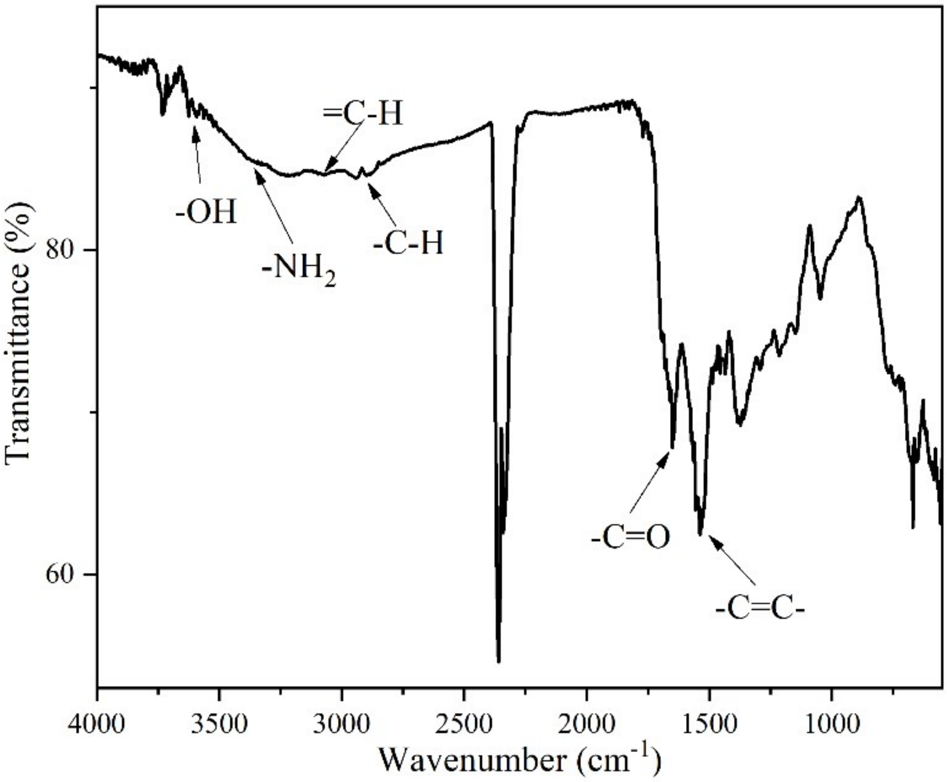

Fig. S2 FT-IR spectrum of carbon dots.

3. XPS spectra

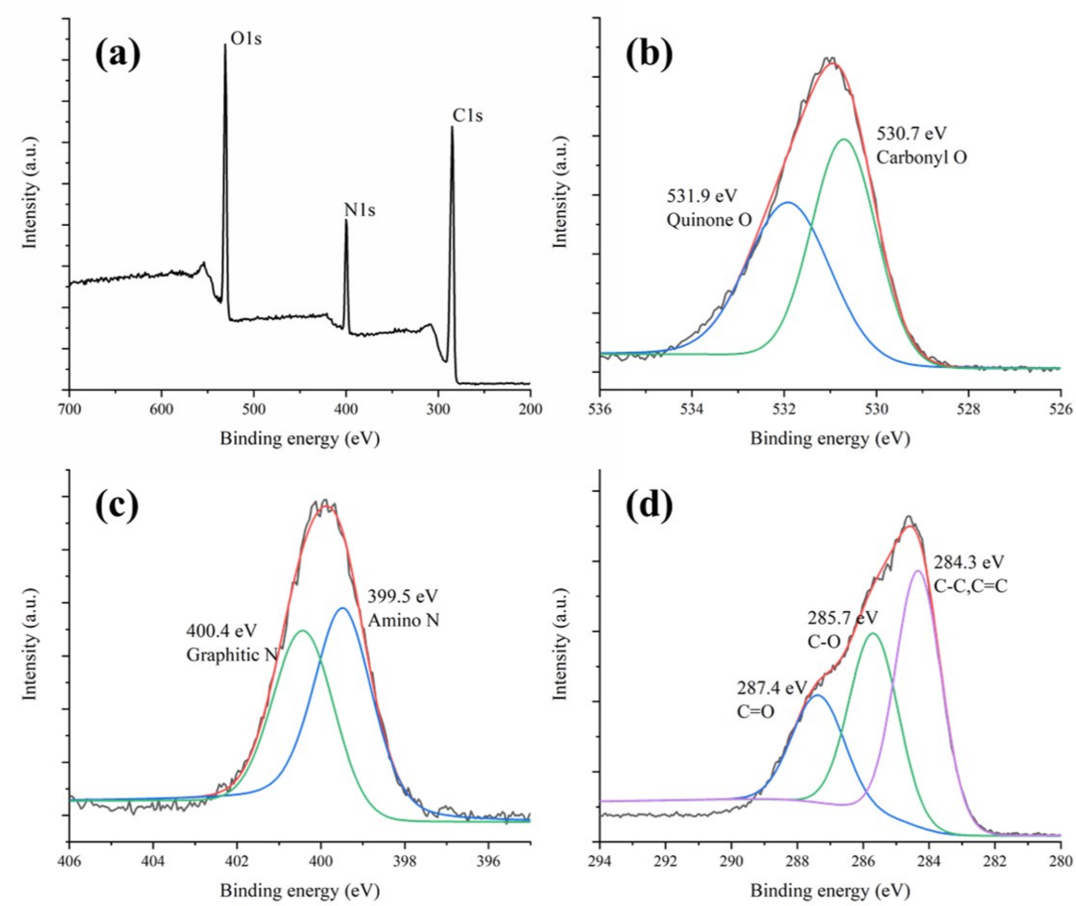

Fig. S3 XPS spectra of the CDs. Full-scan spectrum (a) and high-resolution spectrum of O 1s (b), N 1s (c), and C 1s (d).

4. Stability of the CDs

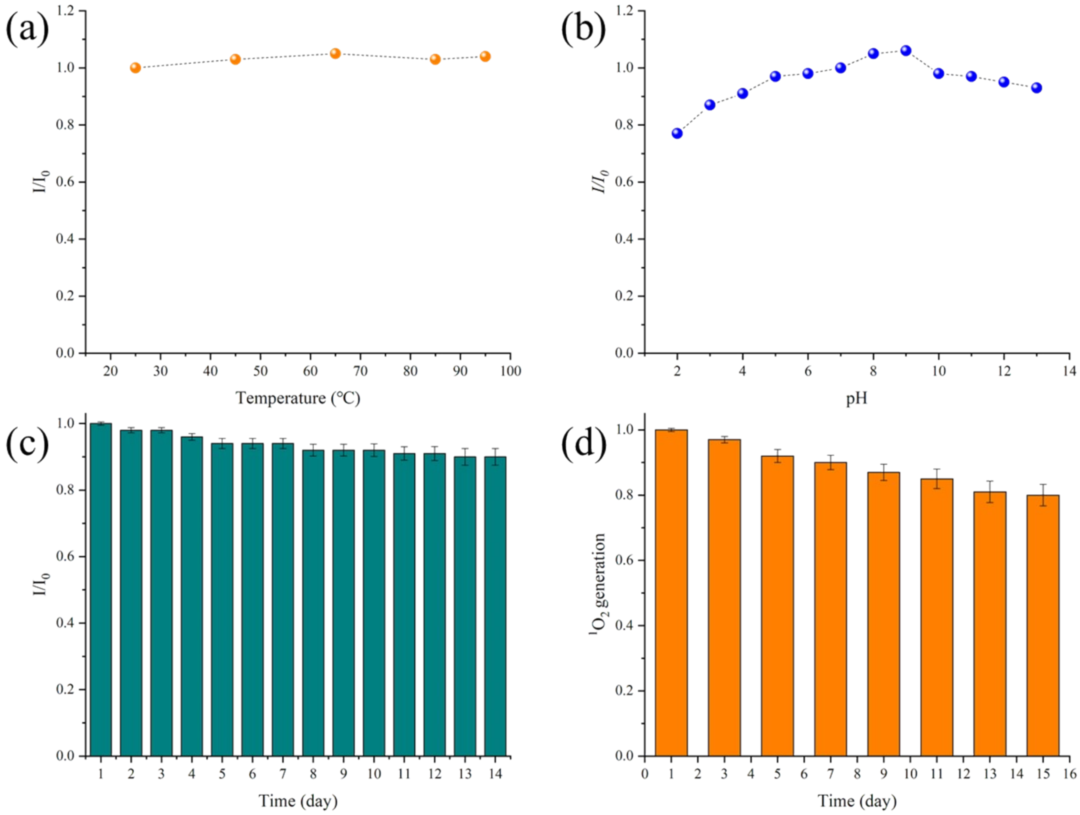

Fig. S4 (a) The integrated PL intensity of CDs at different temperatures; (b) Influence of the pH on the PL intensity of CDs; (c) The integrated PL intensity of CDs after different storage time; (d) Singlet oxygen generation ability of CDs with time (measured by SOSG).

5. Calculation of $^1O_2$ quantum yield

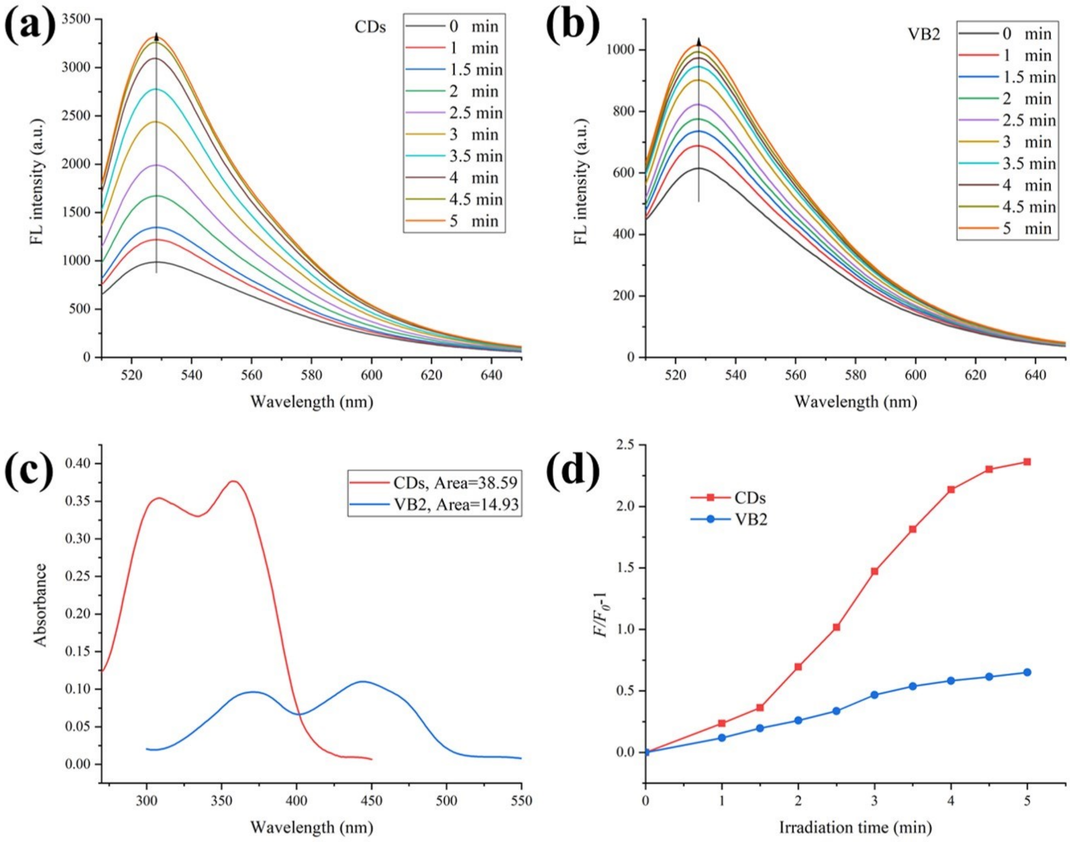

Fig. S5 (a) Fluorescence increase of SOSG with CDs at different irradiation times; (b) Fluorescence increase of SOSG with VB2 after different irradiation time; (c) The absorption peak area of CDs and VB2; (d) Rate of fluorescence increase of SOSG with CDs and VB2 after different irradiation times (F_0 and F are the fluorescence intensity of SOSG with CDs or VB2 before and after irradiation, respectively).

$^1O_2$ quantum yield calculation

To assess the ability of CDs to generate $^1O_2$, the $^1O_2$ quantum yield was measured by a fluorescence enhancement method (SOSG as the trapping agent) with VB2 as the standard photosensitizer ($^1O_2$ quantum yield $\Phi_{VB2} = 0.51$ [1, 2]).

The $^1O_2$ quantum yield of the CDs was calculated using the equation below,

$$Q_c = Q_s \cdot \frac{I_c}{I_s} \cdot \frac{A_s}{A_c}$$

where 'Q' means the $^1O_2$ quantum yield; 'I' represents the intensity of relative fluorescence enhancement (F/F_0-1) and 'A' signifies the absorbance. The subscript 'C' and 'S' stand for the CDs and the reference VB2, respectively.

Here, after 5 minutes of irradiation, $I_c/I_s = 3.632$, $A_s/A_c = 0.387$, Q_s=0.51, thus, the Q_c is calculated as 0.716.

6. Cytotoxicity measurements

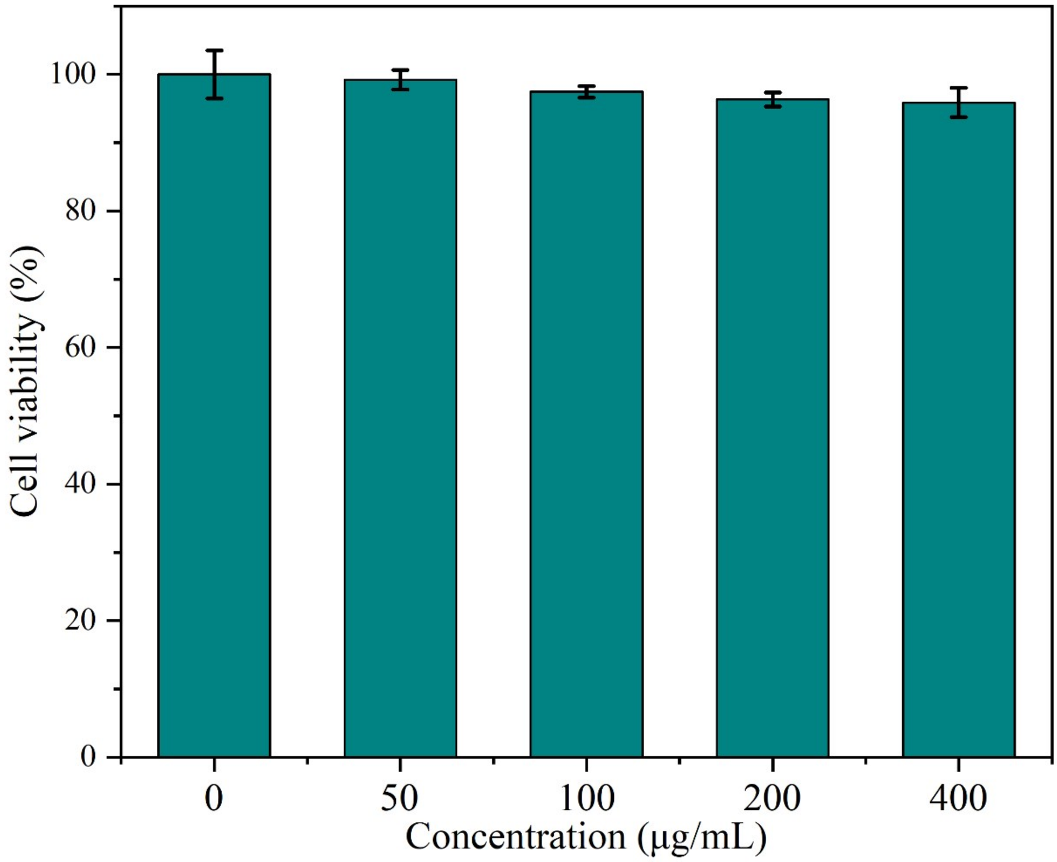

Fig. S6 CCK-8 assay results for the viability of 4T1 cells incubated with CDs (from 50 to 400 μg/mL).

7. PDT on cells

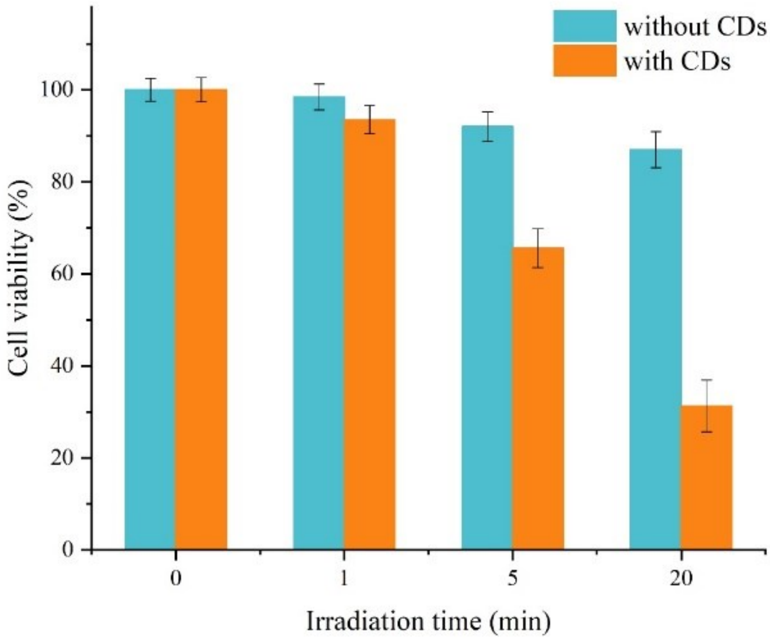

Fig. S7 Relative viabilities of 4T1 cells without and with CDs (100 μg/mL) under various irradiation times.

References:

1. M. Insińska-Rak and M. Sikorski, *Chemistry – A European Journal*, 2014, **20**, 15280-15291.
2. E. Sikorska, I. Khmelinskii, A. Komasa, J. Koput, L. F. V. Ferreira, J. R. Herance, J. L. Bourdelande, S. L. Williams, D. R. Worrall, M. Insińska-Rak and M. Sikorski, *Chem. Phys.*, 2005, **314**, 239-247.