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 $^1$O$_2$ quantum yield

![Graphs](image-url)

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).

$^1$O$_2$ quantum yield calculation

To assess the ability of CDs to generate $^1$O$_2$, the $^1$O$_2$ quantum yield was measured by a fluorescence enhancement method (SOSG as the trapping agent) with VB2 as the standard photosensitizer ($^1$O$_2$ quantum yield $\Phi_{VB2} = 0.51^{1,2}$).

The $^1$O$_2$ 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 $^1$O$_2$ 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, $\frac{I_c}{I_s} = 3.632$, $\frac{A_s}{A_c} = 0.387$, $Q_s=0.51$, 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:
