Supporting Information

Facile synthesis of multifunctional pharmaceutical carbon dots for targeted bioimaging and chemotherapy of tumors

Jiafeng Wan^a, Shiqing Xu^d, Jing Li^c, Mengliu Yu^c, Kai Zhang^c*, Gang Wei^b* and Zhiqiang Su^a*

a State Key Laboratory of Chemical Resource Engineering, Beijing Key Laboratory of Advanced Functional Polymer Composites, Beijing University of Chemical Technology, Beijing 100029, China.

b College of Chemistry and Chemical Engineering, Qingdao University, Qingdao 266071,
China. University of Bremen, Faculty of Production Engineering, D-28359 Bremen, Germany.
c Dental Medical Center, China-Japan Friendship Hospital, Beijing 100029, China.

d Institute of Clinical Medical Sciences, China-Japan Friendship Hospital, Beijing 100029, China.

*Corresponding author. Tel: 86-15066242101. E-mail: <u>weigroup@qdu.edu.cn</u> (G. Wei) E-mail: <u>suzq@mail.buct.edu.cn</u> (Z. Su).



Figure S1. The FTIR spectra of CA.

The peaks at 3496.0 cm⁻¹ and 2918.1 cm⁻¹ are the stretching vibrations of -OH and -CH₂in CA. 1750 cm⁻¹ and 1175 cm⁻¹ show two sets of parallel peaks caused by the stretching vibrations of C=O and C-O in different chemical environments.

Fluorescence lifetime:

Range				
Fitting Rang	e: 178 t	o 2047 chan	; Ove	erride low limit
$R(t) = B_1$	$e^{\left(-t/\tau_{1}\right)}+B_{2}$	$_{2}e^{(-t/\tau_{2})}+B_{3}e^{(-t/\tau_{2})}+B_{3}e^{(-t/\tau_{2})}$	$(-t/\tau_{2}) + B$	$_{4}e^{(-t/\tau_{4})}$
Fix Value / ns	Std. Dev / ns	Fix Value	Std. Dev	Rel %
C 1 0.9469	0.0187	B1 1784.7744	23.9680	12.93
7.6712	0.0234	B2 1484.0901	7.9392	87.07
L 3		B3		1
G		BA	1	
		•		
τ) 3.9998	0.0282			
τ) 6.8020	0.0282			
rint L				
		A 0.9784	1	
		x ² : 1.0526	·	
		× 1.0020		
py Results To Clipboa	rd	Results Window		
	v As Image	Add to existin	a window 🔘 Cre	ate new windo

Figure S2. Parameters related to fluorescence life.

Fluorescence life:
$$\tau = \frac{B_1 \tau_1^2 + B_2 \tau_2^2}{B_1 \tau_1 + B_2 \tau_2} \text{ or } \tau = \tau_1 * Rel_1 \% + \tau_2 * Rel_2 \%$$

Calculation method of absolute quantum yield:



Figure S3. Calculation diagram of absolute quantum yield.

As shown in **Figure S3**, Absolute quantum yield:
$$QY(\%) = \frac{S_a}{S_b}$$

Light bleaching resistant:

Natural light is simulated using Perfectligth's PCX-50 C Discover multi-channel photocatalytic system. The synthesized Met-CDs solution is placed in the above instrument and sunlight is turned on to illuminate the solution. At 0 min, 10 min, 30 min, 60 min, 100 min, 150 min, 210 min, 270 min and so on, 5 mL Met-CDs solution is taken. The fluorescence intensity of Met-CDs solution in each group is measured by fluorescence spectrophotometer LS 55.



Figure S4. The fluorescence intensity of Met-CDs changes with time at the optimal excitation wavelength, simulating natural light. (Ex=290 nm, Em= 440 nm)

Time/min	FL intensity	
0	460.58525	
10	457.46517	
30	449.07401	
60	438.72381	
100	437.18132	
150	443.0613	
210	432.62202	
270	430.22609	

Table S1. The fluorescence intensity of Met-CDs changes with time at the optimal excitation wavelength,

simulating natural light.	(Ex=290 nm, Em= 440 nm)
---------------------------	-------------------------

pH stability:

The pH of the Met-CDs solutions is first measured using a pH meter, and then the pH of the Met-CDs solutions is adjusted using concentrated HCl solution and NaOH solid particles to

obtain different pH Met-CDs solutions, and 5 mL of the Met-CDs solutions are taken separately. Finally, the fluorescence intensity of each Met-CDs solution is measured using a fluorescence spectrophotometer LS 55.



Figure S5. The fluorescence intensity of Met-CDs changes with pH at the optimal excitation wavelength. (Ex=290 nm, Em= 440 nm)

(Ex=290 nm, Em= 440 nm)		
рН	FL intensity	
0.92	65.28294	
1.32	84.49211	
2.27	131.50013	
3.06	150.87694	
3.86	201.52866	
4.19	222.87124	
5.14	310.38664	
6.28	342.17601	
7.37	392.12993	

Table S2. The fluorescence intensity of Met-CDs changes with pH at the optimal excitation wavelength.

9.00	387.35351
10.02	387.44588
11.02	377.32981
12.25	357.22826

Thermal stability:



Figure S6. The fluorescence intensity of Met-CDs changes with temperature at the optimal excitation wavelength. (Ex=290 nm, Em= 440 nm)

 Table S3. The fluorescence intensity of Met-CDs changes with temperature at the optimal excitation

 wavelength. (Ex=290 nm, Em= 440 nm)

Temperature/°C	FL intensity
25	294414.875
35	262753.75
45	220151.094
55	170878.281



Figure S7. (A) Detection of Met toxicity to A549 cells (line graph); (B) Detection of Met-CDs toxicity to A549 cells (line graph).



Figure S8. (A) Inhibitory effect of Met on the growth of A549 cells (line graph); (B) Inhibitory effect of Met-CDs on the growth of A549 cells (line graph).