Supporting Information

A dual organelle-targeting photosensitizer based on

curcumin for enhanced photodynamic therapy

Yanping Wang,^{†,a,b} Xuewei Li,^{†,a,b} Weimin Liu,^{*,a,b,c} Jie Sha,^{a,b} Zhe Yu,^{a,b} Shuai Wang,^{a,b} Haohui Ren,^{a,c} Wenjun Zhang,^d Chun-Sing Lee,^d and Pengfei Wang^{*,a,b} ^a Key Laboratory of Photochemical Conversion and Optoelectronic Materials & CityU-CAS Joint Laboratory of Functional Materials and Devices, Technical Institute of Physics and Chemistry, Chinese Academy of Sciences, Beijing 100190, P. R. China. ^b School of Future Technology, University of Chinese Academy of Sciences, Beijing, 100049, P. R. China.

^c Qingdao Casfuture Research Institute CO., LTD, P. R. China.

^d Department of Materials Science and Engineering & Center of Super-Diamond and Advanced Films, City University of Hong Kong, Hong Kong, P. R. China.

* E-mail: <u>wmliu@mail.ipc.ac.cn; wangpf@mail.ipc.ac.cn</u>

† These authors contributed equally.



Fig. S1. Synthetic routes to CN.



Fig. S2. ¹H NMR (400 MHz, CDCl₃) spectrum of CN.



Fig. S3. ¹³C NMR (151 MHz, CDCl₃) spectrum of CN.



Fig. S4. High resolution mass spectrum of CN.



Fig. S5. HPLC chromatogram of CN.

Solvent	ET (30)	$\lambda_{abs}{}^a$	$\lambda_{em}{}^{b}$	stoke shift	3	$\Phi_{\rm F}{}^{\rm c}$
	(kcal/mol)	(nm)	(nm)	(nm)	M ⁻¹ cm ⁻¹	(%)
Toluene	33.9	469	527	58	5.8×10 ⁴	36.3
THF	37.4	477	550	73	7.2×10 ⁴	50.2
DCM	40.7	498	580	82	7.7×10 ⁴	64.3
DMF	43.2	504	587	83	7.8×10 ⁴	38.3
DMSO	45.1	511	606	95	9.6×10 ⁴	38.1

Table S1. The photophysical properties of CN.

a: absorption maximum. b: fluorescence maximum. c: Absolute fluorescence quantum yield determined using a calibrated integrating sphere. Concentration = 10μ M. ET (30) of each solvent were collected from reference.



Fig. S6. PL spectra of DCFH-DA in the presence of (A) pure DCFH-DA and (B) CN+ DCFH-DA under 532 nm laser irradiation (10 mW cm⁻²). Concentration = 10 μ M; λ ex = 488 nm.



Fig. S7. (A) $O_2^{-\bullet}$ and (B) •OH generation of CN under 532nm laser irradiation (10 mW cm⁻², 10 min).



Fig. S8. UV-Vis spectra of DPBF (20 μ M) in DMF solutions under 532nm laser irradiation (10 mW cm⁻²) in the presence of (A) RB and (C) CN. The absorbance decay of the DPBF at 415 nm under 532 nm laser irradiation (10 mW cm⁻²) in the presence of (B) RB and (D) CN.



Fig. S9. (A) Absorption spectra and (B) Photostability (A/A_0) of CN under laser irradiation (532 nm, 0.1 W cm⁻²).



Fig. S10. Fluorescent images of HeLa cells stained with 1 μ M CN in (A) bright field, (B) green channel (λ ex =488 nm, λ em = 500-550 nm), (C) orange channel (λ ex =561 nm, λ em = 570-620 nm), and (D) merged image for image B and C. Scale bar = 10 μ m.



Fig. S11. Fluorescent images of (A, B) HepG-2 cells and (C, D) A549 cells stained with CN (1 μ M) in green channel (λ ex =488 nm, λ em = 500-550 nm), orange channel (λ ex =561 nm, λ em = 570-620 nm), LDDR (0.2 μ m) (λ ex =638 nm, λ em = 663-738 nm) and ERB (0.5 μ m) (λ ex =405 nm, λ em = 425-475 nm); (a-d) The profile plot of two channels along the arrow in merge channel. Scale bar = 10 μ m.



Fig. S12. Fluorescent images of HeLa cells stained with CN (1 μ M) in green channel (λ ex = 488 nm, λ em = 500-550 nm), orange channel (λ ex = 561 nm, λ em = 570-620 nm), (A, B) LTDR (0.2 μ m) (λ ex = 638 nm, λ em = 663-738 nm) and (C, D) MTDR (0.2 μ m) (λ ex =638 nm, λ em = 663-738 nm); (a-d) profile plot of two channels along the arrow in merge channel. Scale bar = 10 μ m.



Fig. S13. (A) Absorption spectra and (B) FL spectra of CN (15 μ M) in a THF/water mixed solution with different water fractions ($\lambda ex = 480$ nm).



Fig. S14. (A) Fluorescence intensity of HeLa cells after being incubated with CN (1 μ M) and loaded with DCFH-DA (10 μ M) under laser irradiation (532 nm, 20 mW cm⁻²); Fluorescence intensity of (B) HeLa cells and (C) MCSs with different treatments (L: laser irradiation with 532 nm, 0.1 W cm⁻²).



Fig. S15. Cell viability of HeLa cells after being incubated with different concentrations of CN and CUR after 72h.

 Table S2
 The calculated IC50 of CUR and CCN for HeLa cells.

	532 nm laser (µM)	dark (µM)
CUR	/	29.66
CN	0.45	26.68