Naphthofluorescein-Based Organic Nanoparticles with Superior

Stability for Near-Infrared Photothermal Therapy

Jing An^a, Shanliang Tang^a, Erting Feng^a, Mingyu Tian^a, Wenlong Chen^a, Miaomiao Chen^a, Gaobo Hong^a, Xiaojun Peng^a and Fengling Song^{*a,b}

^aState Key Laboratory of Fine Chemicals, Dalian University of Technology, Dalian, 116024, China

^bInstitute of Molecular Sciences and Engineering, Institute of Frontier and Interdisciplinary Science, Shandong University, Qingdao, 266237, China

E-mail: songfl @dlut.edu.cn; songfl @sdu.edu.cn

Synthesis



Scheme S1. Synthesis routes of NFOM-1 and NFOM-2.



Figure S1. Chemical structure of the NFOM-2 showing how this enhances coplanarity of the fused ring system.



Figure S2. Calculated optimized geometry and molecular frontier orbital distribution of NFOM-1 and NFOM-2 (basis set DFT B3LYP/6-31G).



Figure S3. Photostability evaluation of NFOM-1 and NFOM-2 in methanol (laser: 635 nm, 600 mW/cm², interval of 4 minutes).



Figure S4. Zeta potential of NFOMNPs.



Figure S5. Absorption spectra of NFOMNPs in different media (a, H_2O ; b, PBS; c, FBS) and particle size variation of NFOMNPs in different media during 6 days. Data in (d) is presented as mean \pm s.d. (n = 2).



Figure S6. Absorption spectra of ICG NPs before and after laser irradiation (4 cycles).



Figure S7. Confocal images of Hela cells with D&N NPs at different incubation times. Scale bars :20 μ m.



Figure S8. Body weights of mice in four groups versus treatment time.



Figure S9. Histological H&E staining of main organs slices for different groups at the 14th day after treatments, scale bar 100 μm.

Mass and NMR spectra of compounds



Figure S10. HRMS of NFOM-1.



Figure S11. ¹H-NMR spectrum of NFOM-1 in (CD₃)₂SO.



Figure S12. ¹³C-NMR spectrum of NFOM-1 in (CD₃)₂SO.



Figure S13. HRMS of NF-2.



Figure S14. ¹H-NMR spectrum of NF-2 in (CD₃)₂SO.



Figure S15. ¹³C-NMR spectrum of NF-2 in (CD₃)₂SO.



Figure S16. HRMS of NFOM-2.



Figure S17. ¹H-NMR spectrum of NFOM-2 in (CD₃)₂SO.



70 165 160 155 150 145 140 135 130 125 120 115 110 105 100 95 90 85 80 75 70 65 60 55 50 45 40 35 fl (ppm)

Figure S18. ¹³C-NMR spectrum of NFOM-2 in (CD₃)₂SO.