Supporting Information

Perylene Diimide Oligomer Nanoparticles with Ultra-high Photothermal Conversion Efficiency for Cancer Theranostics

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Scheme S1. Preparation of dibromo perylene diimide (PDI-2Br).

Figure S1. ¹H NMR spectrum of PDI-2Br.







Figure S3. HR-MS spectrum of PDI-2Br.



Scheme S2. Preparation of diamino perylene diimide (PDI-2NH₂, MPDI).

Figure S4. ¹H NMR spectrum of PDI-2NO₂.



Figure S5. ¹³C NMR spectrum of PDI-2NO₂.



Figure S6. HR-MS spectrum of PDI-2NO₂.



Figure S7. ¹H NMR spectrum of PDI-2NH₂.



Figure S8. ¹³C NMR spectrum of PDI-2NH₂.



Figure S9. HR-MS spectrum of PDI-2NH₂.

Scheme S3. Preparation of OPDI, here just selecting the product resulted from the reaction of a and b (n = 0, dimer; n = 1/2, trimer; n = 1, tetramer; n = 3/2, pentamer; n = 2, hexamer). The structures of the three main product (trimer, tetramer and pentamer, analyzed from MALDI-TOF MS results) will be detailed below.



OPDI



Figure S10. a) The photos of fluorescence of corresponding PDI materials in this study $(\lambda_{ex}: 365 \text{ nm})$. b) The fluorescence emission of above PDI materials.



Figure S11. a) Thermal images of **OPDI** NPs in PBS solutions (200 μ g mL⁻¹, after self-assembly of 5 months) after laser irradiation. b) The representative TEM image of **OPDI** NPs after self-assembly of 5 months.



Figure S12. Thermal photographs of **OPDI** NPs with different concentrations (0, 25, 50, 100, 150, 300 µg mL⁻¹) under a fixed near-infrared light irradiation (808 nm, 1.5 W cm⁻²).



Figure S13. Thermal photographs of **OPDI** NPs (200 μ g mL⁻¹) under different near-infrared light irradiations (808 nm, 0.6, 0.9, 1.2, 1.8 and 2.1 W cm⁻²).



Figure S14. a) The photothermal cycle performance of OPDI NPs (200 μ g mL⁻¹) under laser irradiation (808 nm, 1.5 W cm⁻²). b) The temperature response of OPDI NPs (200 μ g mL⁻¹) to NIR (808 nm, 1.5 W cm⁻²) laser on and off in period of 1800 s. The inset shows the linear time data versus -ln (θ) obtained from the cooling period of NIR laser off.



Figure S15. The effect of concentrations of OPDI NPs on the cell viability.



Figure S16. Photos of tumor-bearing mice with the growth time after the laser irradiation.



Figure S17. Histological analysis of main organs from the mice injected with 50 μ L of PBS or **OPDI** NPs (50 μ L of 0.5 mg mL⁻¹) for 14 days.

References

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