Supporting Information

Supramolecular Nanomedicine Derived from Cucurbit[7]uril-Conjugated Nano-Graphene Oxide for Multi-modality Cancer Therapy

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Figure S1. AFM image of NGO (A). ICP standard curve of oxaliplatin (B). ¹H NMR spectrum of ADA-HA in D₂O with ADA substituted rate of 18.86% (C). DLS size distribution of NGO-CB[7] before and after ADA-HA coating (D). FT-IR spectrum (E) and solvent stability (F) in water, PBS and DMEM of NGH.



Figure S2. UV-Vis-NIR spectrum of NG, CNG and ACNG (A), standard curve of Ce6 (B) and AQ4N (C). UV-Vis spectrum of DPA mixture with NG (D), CNG (E) and Ce6 (F) after 660 nm laser irradiation for 10 min.



Figure S3. Biocompatibility evaluation for NGH in B16 cell line (A) and L0-2 cell line (B). Cellular uptake of free Ce6 by B16 cell line for 0, 1.5, 3, 6, and 12 h (C). Cellular uptake of free Ce6, CNGH

and CNGH with HA pretreated B16 cells (D). CLSM of B16 cell lines stained with anti-HIF- α protein after normoxia, hypoxia and normoxia with PDT treatment (E, scale bar: 20 μ m).



Figure S4. *In vivo* imaging of mice treated with free Ce6 (A) and CNGH (B) for 6, 12 and 24h circulation. Semiquantitative analysis of relative FL intensity in tumor site within different time point (C). *In vivo* thermal imaging of mice with treatment of saline and ACNGH after an 808 nm laser irradiation for 5 min (D), and corresponding temperature curve in tumor site (E).



Figure S5. Immunofluorescent staining of tumor tissues before and after PDT process (A) and corresponding semiquantitative analysis of hypoxia-positive signals in those tumor slices (B), HE staining assay of different organs after different treatment (C).