

## Supporting Information

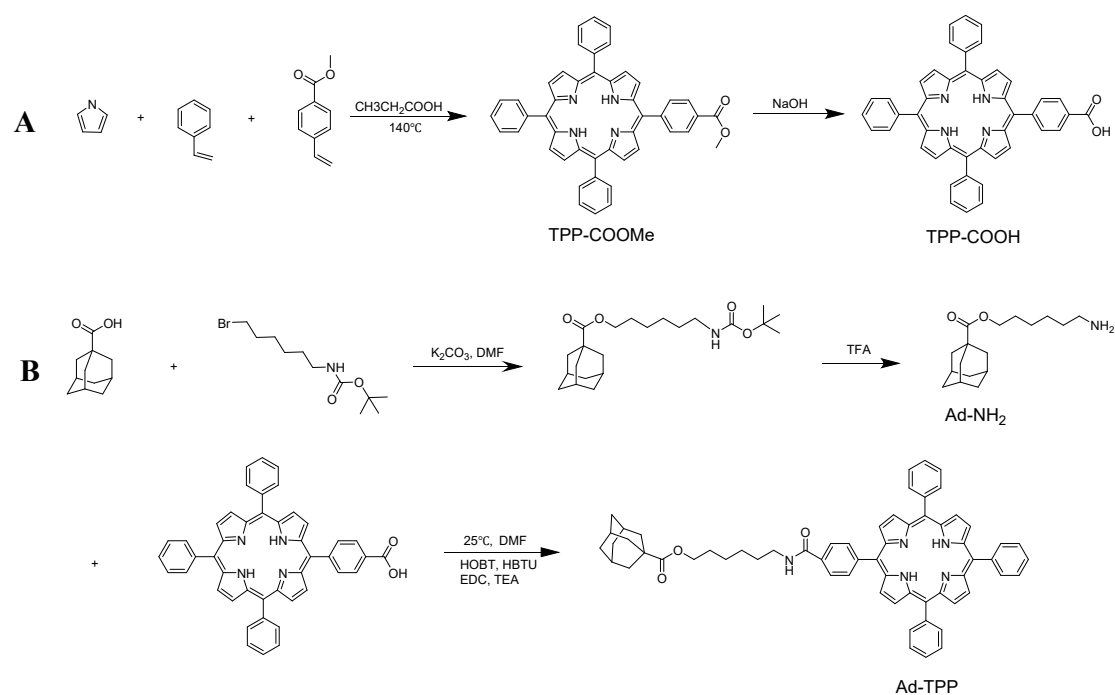
### A Cucurbit[7]uril-Based Upconversion Nanoplatfor for Targeted Photodynamic Drug Delivery

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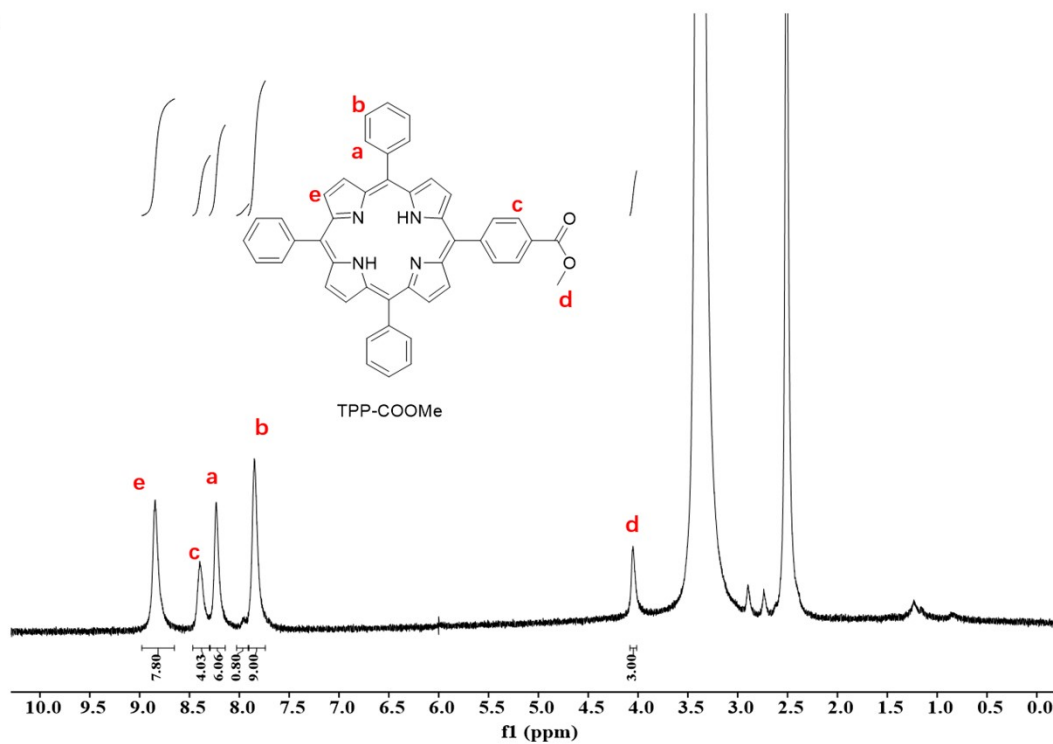
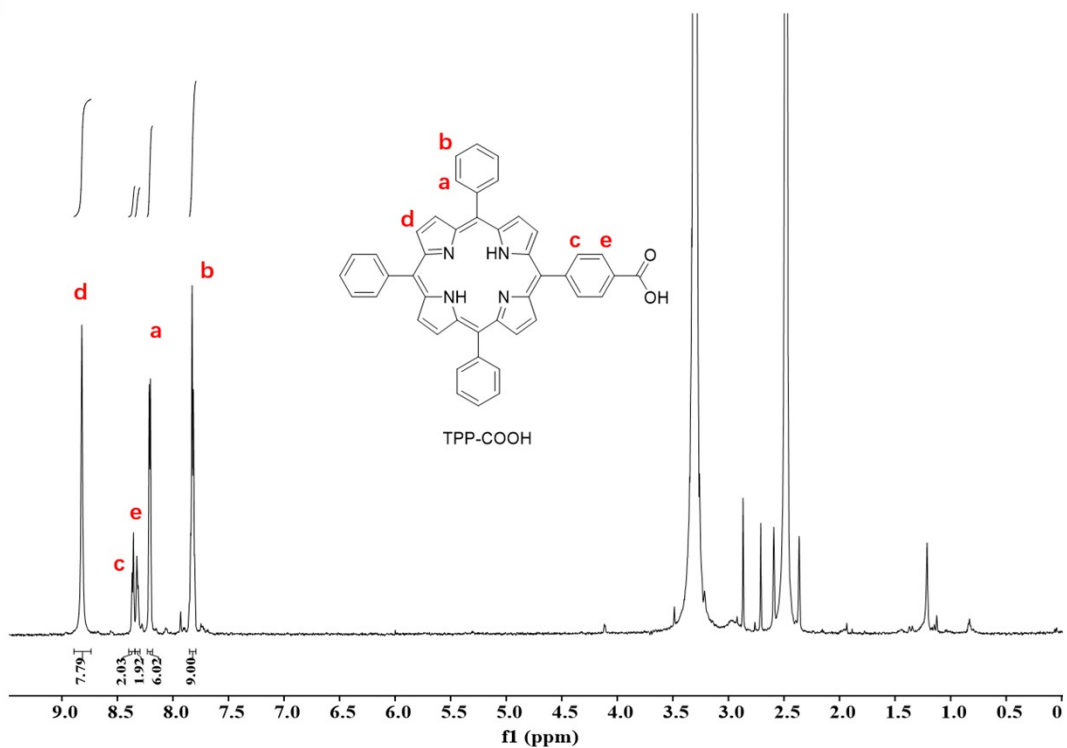
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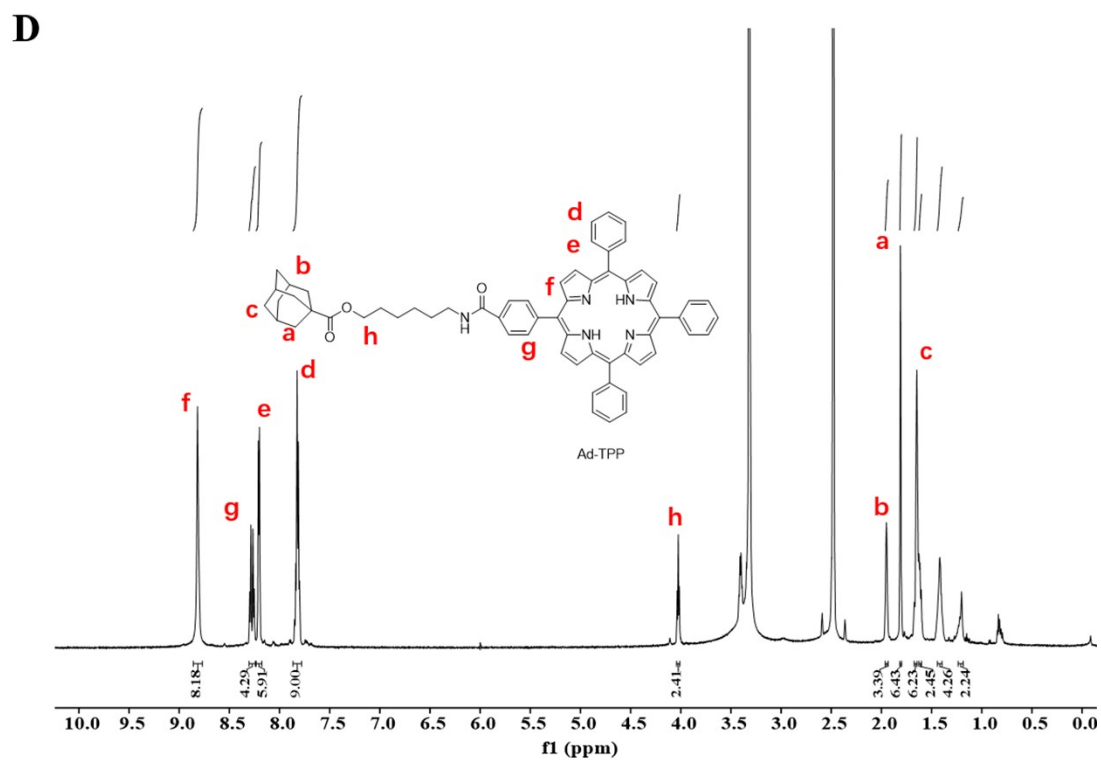
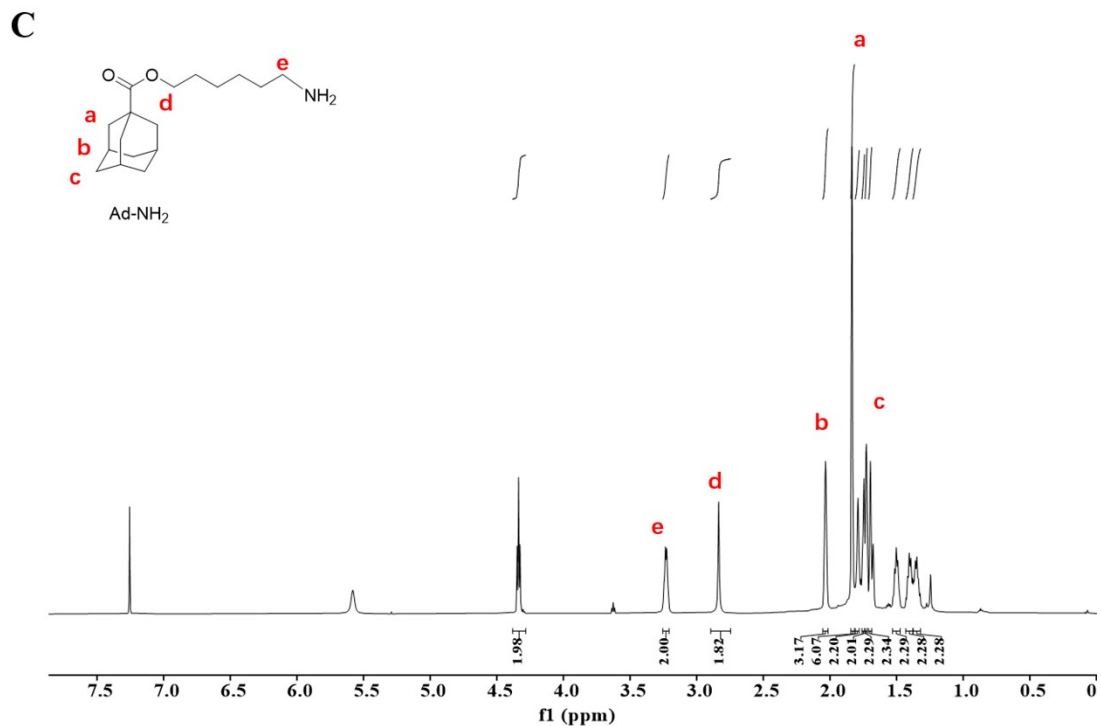
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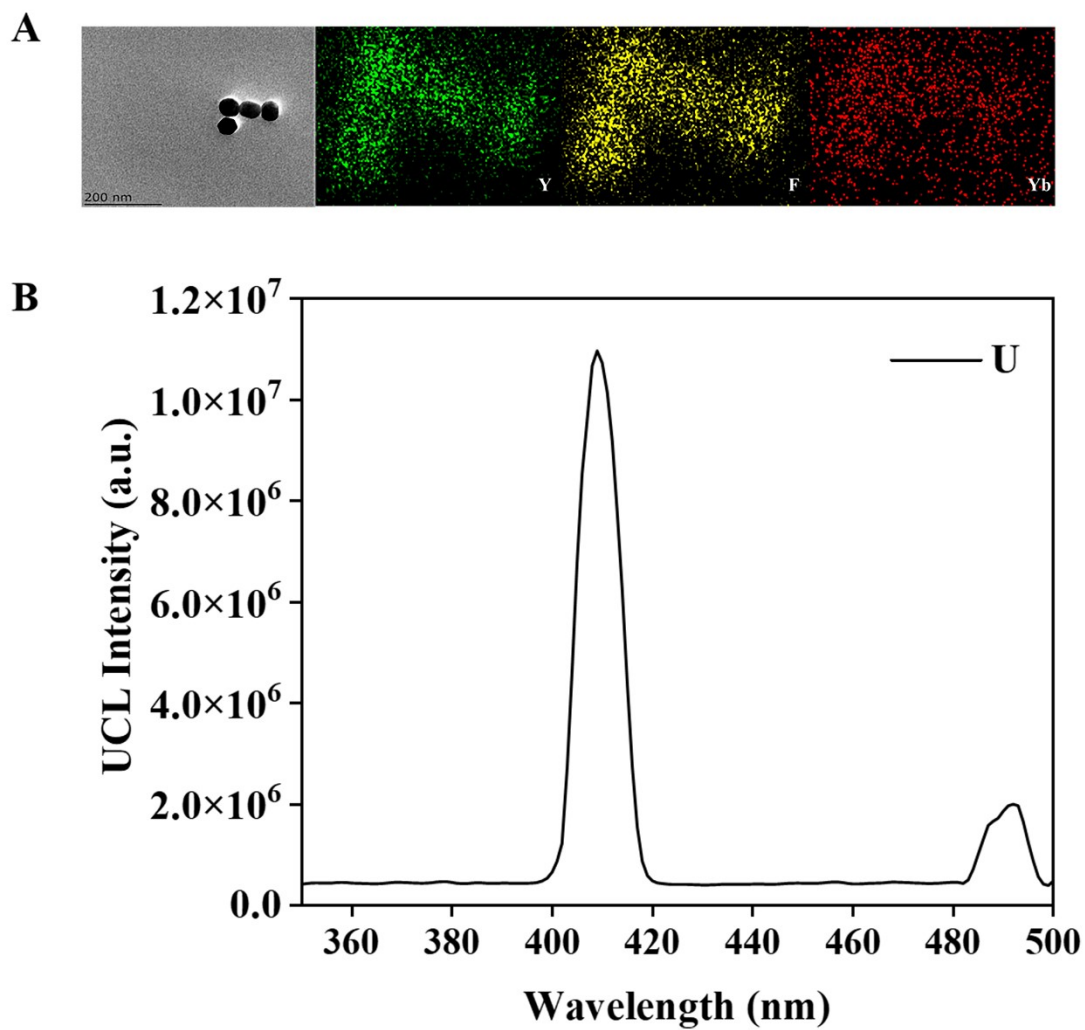
**Scheme S1.** Synthetic route of Ad-TPP conjugates

**A****B**

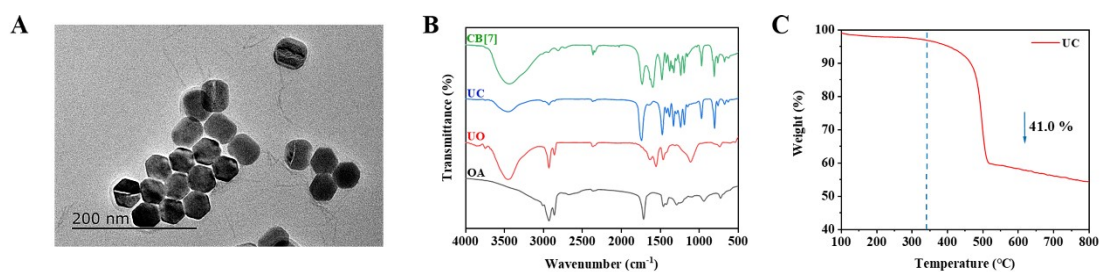


**Figure S1.** (A) <sup>1</sup>H NMR spectrum (600 MHz, DMSO-d<sub>6</sub>, 298 K) of TPP-COOMe. (B) <sup>1</sup>H NMR spectrum (600 MHz, DMSO-d<sub>6</sub>, 298 K) of TPP-COOH. (C) <sup>1</sup>H NMR spectrum (600 MHz, CDCl<sub>3</sub>, 298 K) of Ad-NH<sub>2</sub>. (D) <sup>1</sup>H NMR spectrum (600 MHz, DMSO-d<sub>6</sub>, 298 K) of Ad-D18.

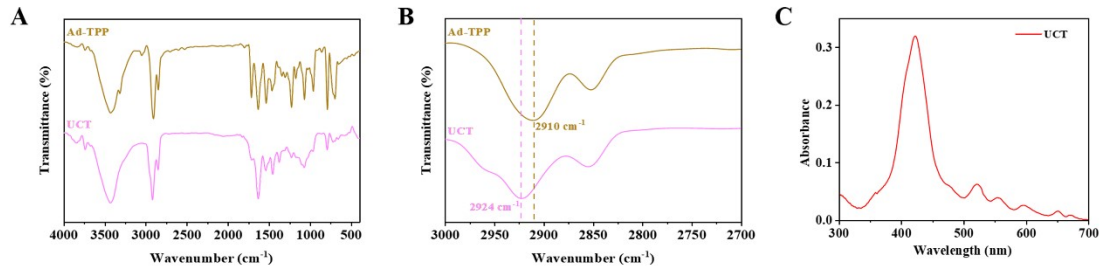




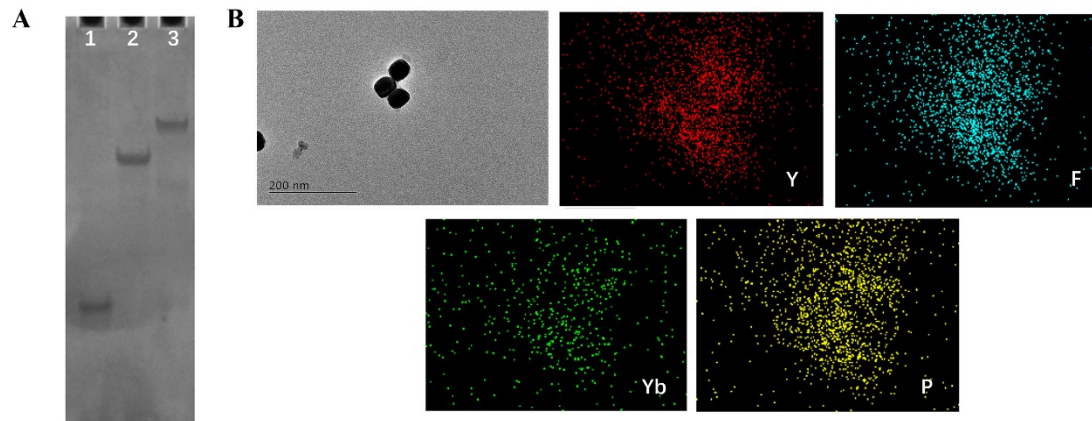
**Figure S3.** (A) TEM image and EDS spectrum of U. (B) Upconversion fluorescence spectrum of U.



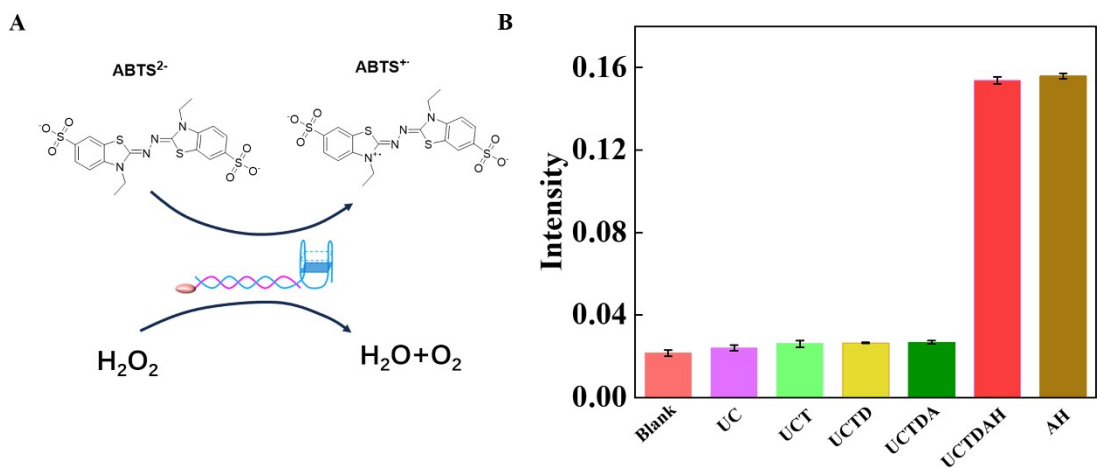
**Figure S4.** (A) TEM image of UC. (B) FTIR spectra of CB[7], free OA, UO, and UC. (C) TGA curve of UC.



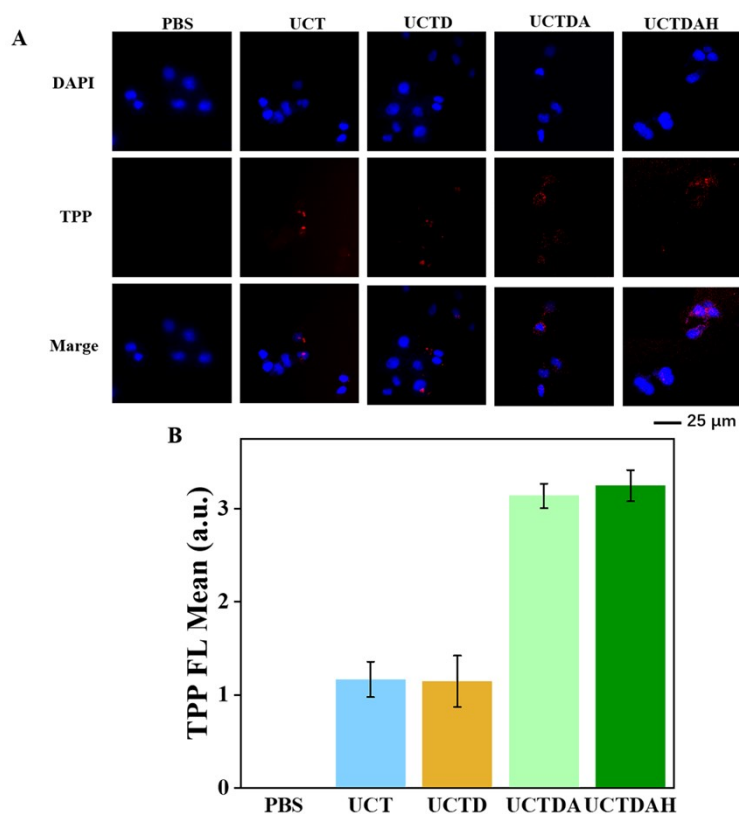
**Figure S5.** (A) FTIR spectra of Ad-TTP and UCT. (B) Magnified FTIR spectra of Ad-TTP and UCT in the range of 2700–3000  $\text{cm}^{-1}$ . (C) UV–Vis spectra of UCT assemblies



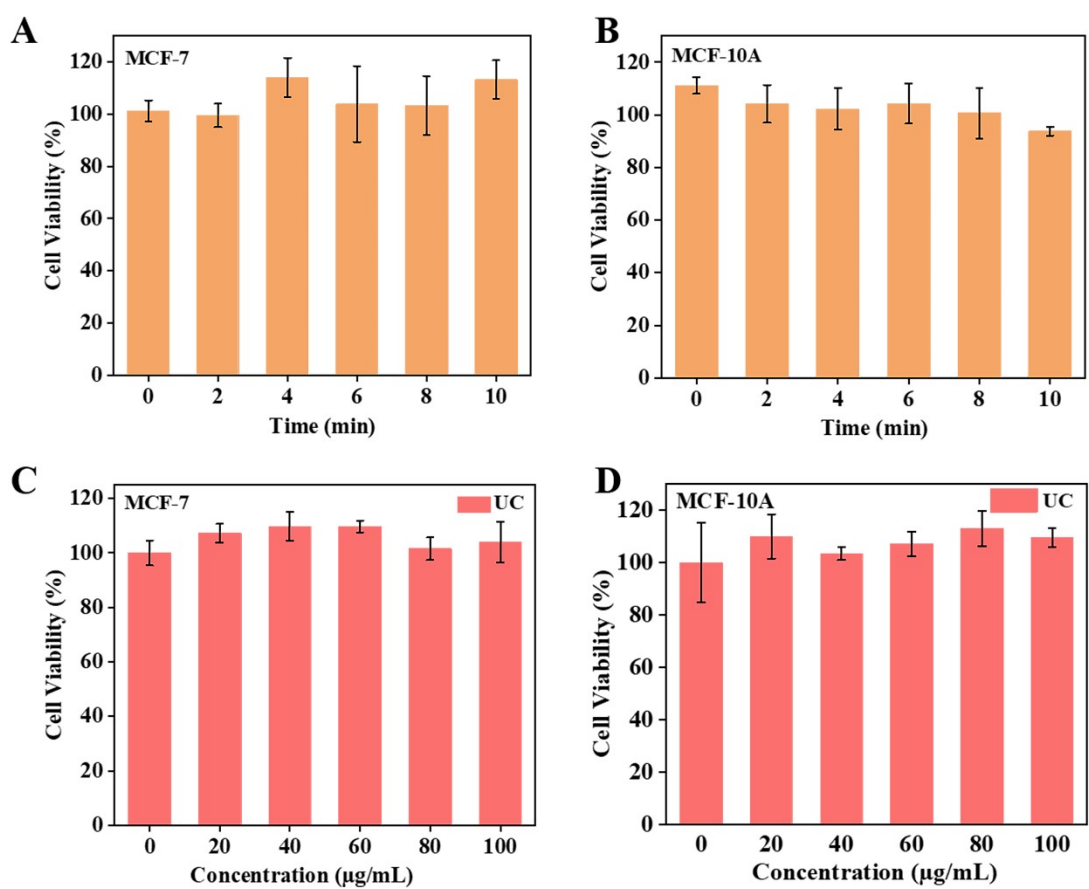
**Figure S6.** (A) 20 % Native PAGE (150 V at room temperature). Line 1 was Ad-D18, line 2 was AS1411-C15 and line 3 was the product of the complementary pairing of Ad-D18 and AS1411-C15. (B) EDS spectrum of UCTDAH.



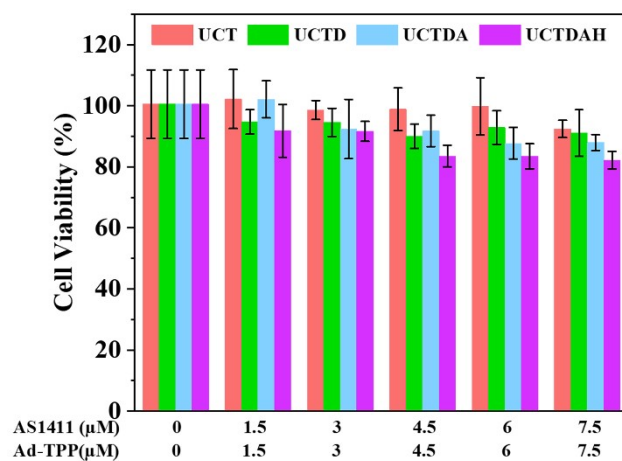
**Figure S7.** (A) Schematic diagram of using  $\text{ABTS}^{2-}$  as an indicator to investigate the generation of  $\text{O}_2$  from  $\text{H}_2\text{O}_2$  catalyzed by G4/Hemin. (B) Absorption peak intensity at 405 nm of each group in the presence of  $\text{H}_2\text{O}_2$ .



**Figure S8.** (A) Uptake of PBS, UCT, UCTDA, and UCTDAH by MCF-10A cells analyzed via CLSM. Scale bar: 25  $\mu\text{m}$ . (B) Semi-quantitative fluorescence analysis of TPP in Figure S8A.



**Figure S9.** (A) Cytotoxicity of 980 nm NIR light against MCF-7 cells under different irradiation durations. (B) Cytotoxicity of 980 nm near-NIR light against MCF-10A cells under different irradiation durations. (C) Cytotoxicity of UC at various concentrations against MCF-7 cells upon 980 nm NIR light irradiation for 10 min. (D) Cytotoxicity of UC at various concentrations against MCF-10A cells upon 980 nm NIR light irradiation for 10 min.



**Figure S10.** Cell viability of MCF-10A cells treated with different experimental groups at various concentrations after 10 min of 980 nm laser irradiation.