

Supporting Information

Metal-Free Nanoassemblies of Water-Soluble Photosensitizer and Adenosine Triphosphate for Efficient and Precise Photodynamic Cancer Therapy

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1. Loading capacity of 1-ATP

The loading capacity is the ratio of (mass of the porphyrin encapsulated in assemblies)/(mass of the assemblies)×100%. As the pKa values for ATP are 0.9, 1.5, 2.3, and 7.7, at a pH close to 7, one ATP molecule bears 3 negative charges. To ensure the charge neutrality in the assemblies, the ratio of porphyrin/ATP has to be close to 3/4. So, we calculated the loading capacity which is $(1014 \times 3 / (1014 \times 3 + 505 \times 4)) \times 100\% = 60.1\%$.

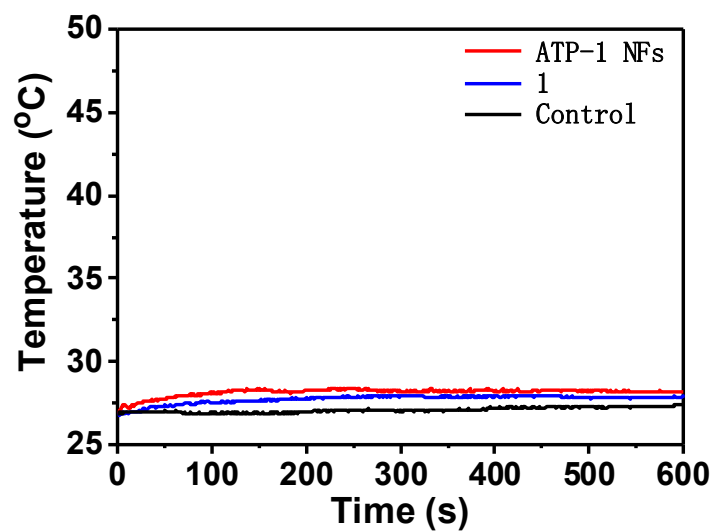


Figure S1. Temperatures of water, aqueous solutions of porphyrin **1** and **1**-ATP nanofibers, recorded during 10 min under laser irradiation. [**1**] = [**1**+ATP] = 20 μ M, laser power: 0.3 W cm^{-2} at 635 nm for 10 min.

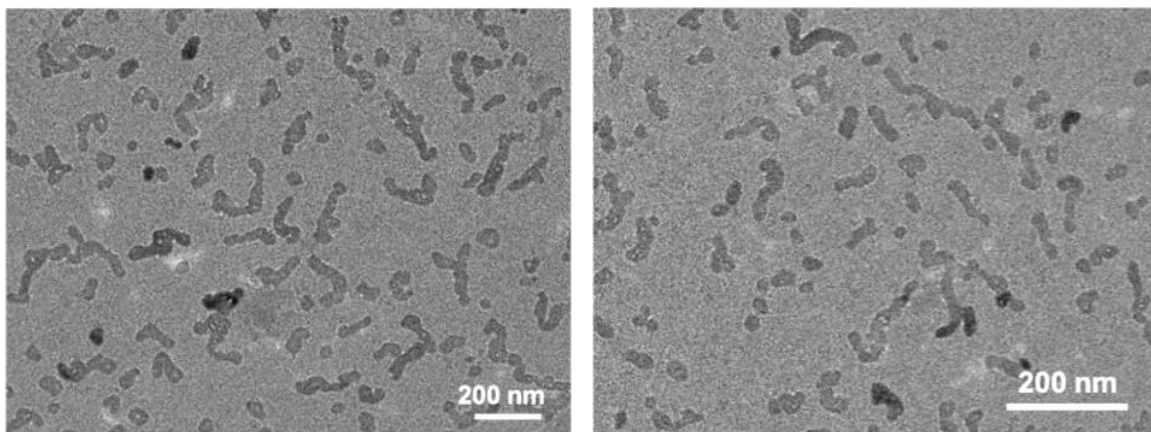


Figure S2. TEM images of the **1**-ATP nanofibers incubated in cell culture media for 24h.

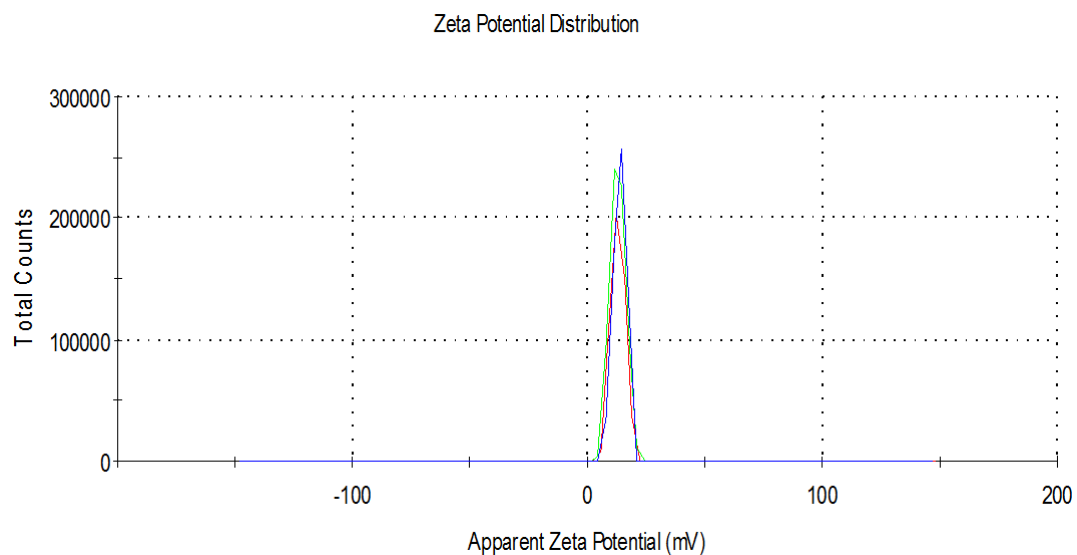


Figure S3. The Zeta potential distribution of 1-ATP in aqueous solution.

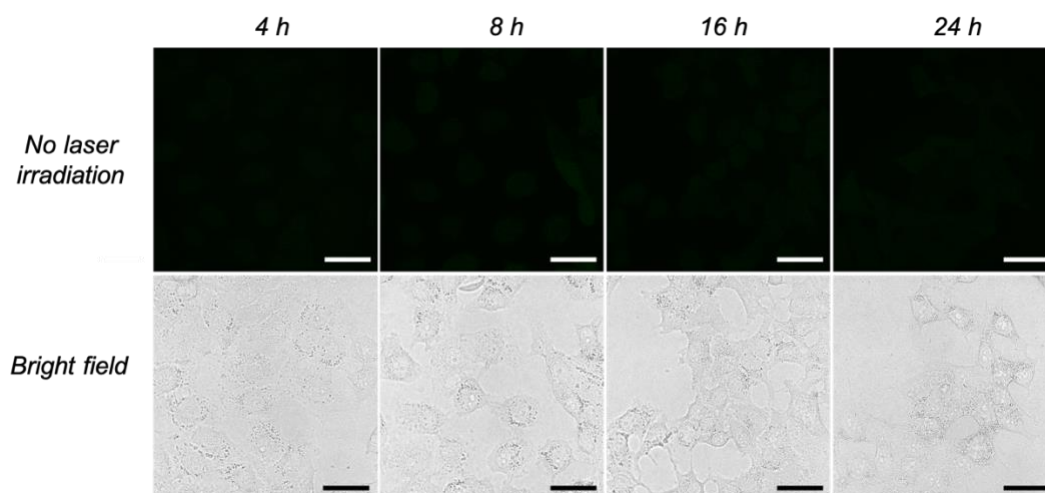


Figure S4. Images of MCF7 cells taken during the *in vitro* ROS generation test for nanofibers without irradiation. The MCF7 cells were incubated with the 1-ATP nanofibers for different periods of time as indicated and then with 10 μ M DCFH-DA for 0.5 h. (The concentration of 1-ATP nanofibers is 20.0 μ M in concentration of porphyrin. Scale bar: 50 μ m)

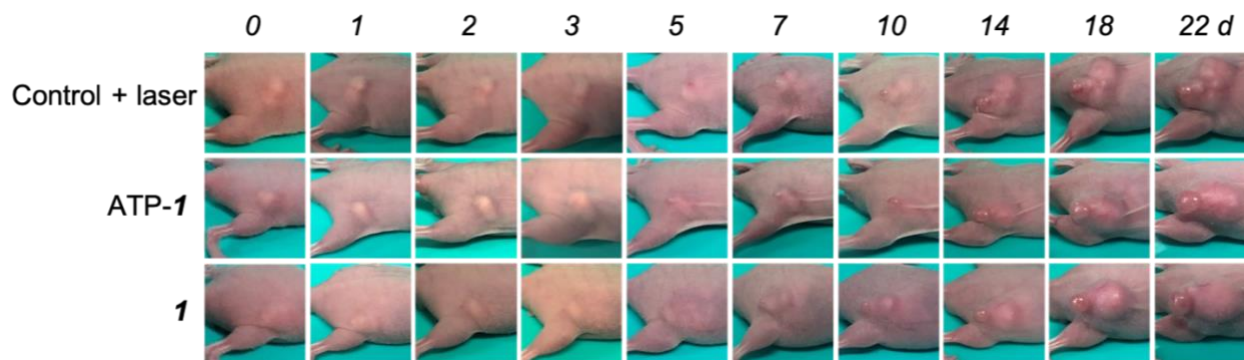


Figure S5. Representative photos of tumor-bearing mice at various time points of observation period. The mice were injected with aqueous solutions of **1**-ATP nanofibers, unencapsulated porphyrin **1**, or 5% glucose for the control group. At 4 h post injection, only the tumor sites in the group of “control” were irradiated by a 635 nm laser for 10 min (0.3 W cm^{-2}).

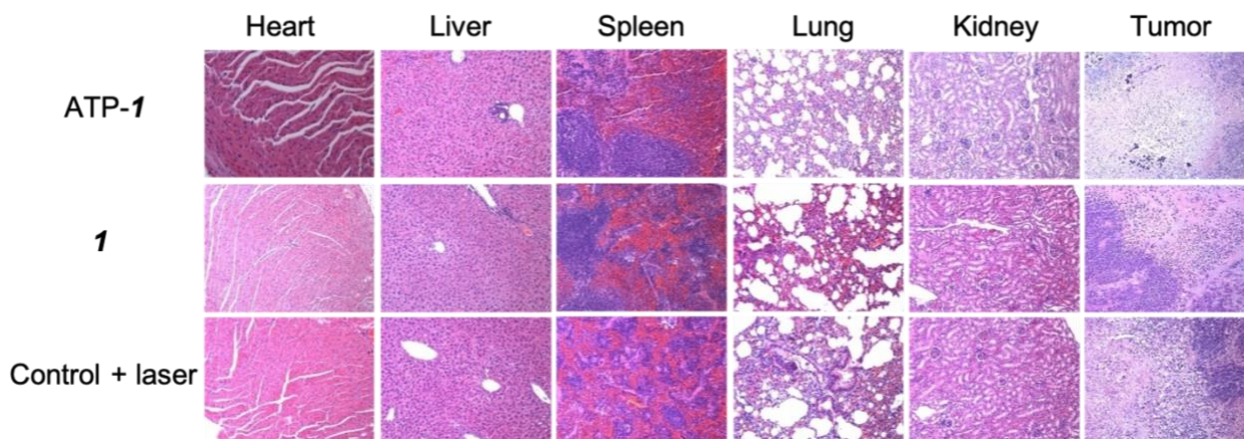


Figure S6. Hematoxylin and eosin (H&E)-stained histological section of heart, spleen, kidney, liver, lung and tumor tissues obtained from mice of the control groups.