Electronic Supplementary Material

All-in-one functional supramolecular nanoparticles based on pillar[5]arene for controlled generation, storage and release of singlet oxygen

Bing Lu **(✉)**, Zhecheng Zhang, Meiyu Qi, Yuehua Zhang, Hualing Yang, Jin Wang, Yue Ding, Yang Wang, Yong Yao **(✉)**

College of Chemistry and Chemical Engineering, Nantong University, Nantong 226019, China
E-mails: 2020028lubing@ntu.edu.cn (Lu B); yaoyong1986@ntu.edu.cn (Yao Y)

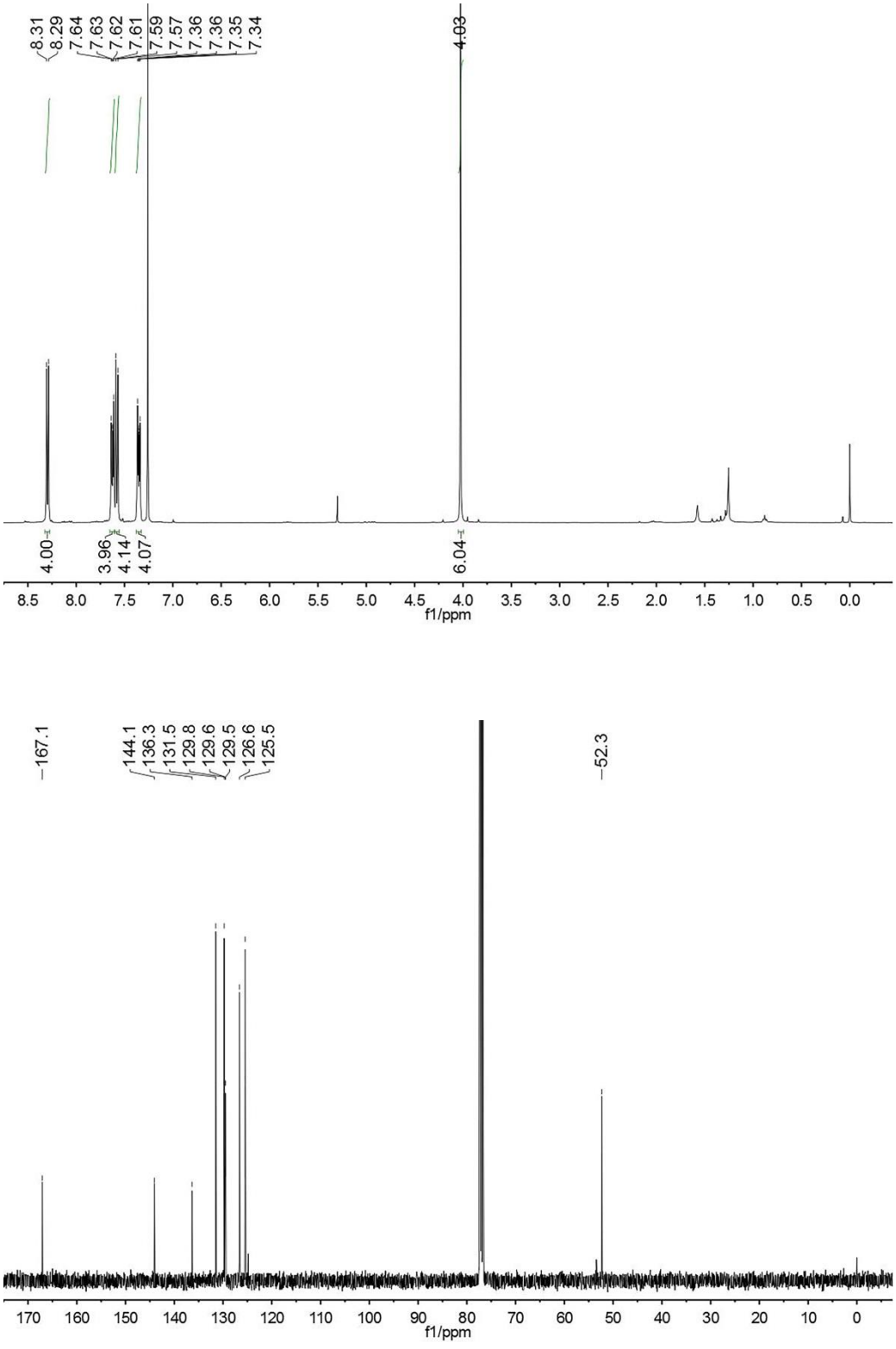

Fig. S1 ^{1}H NMR and ^{13}C NMR spectra ($CDCl_3$, 298 K) of compound **1**

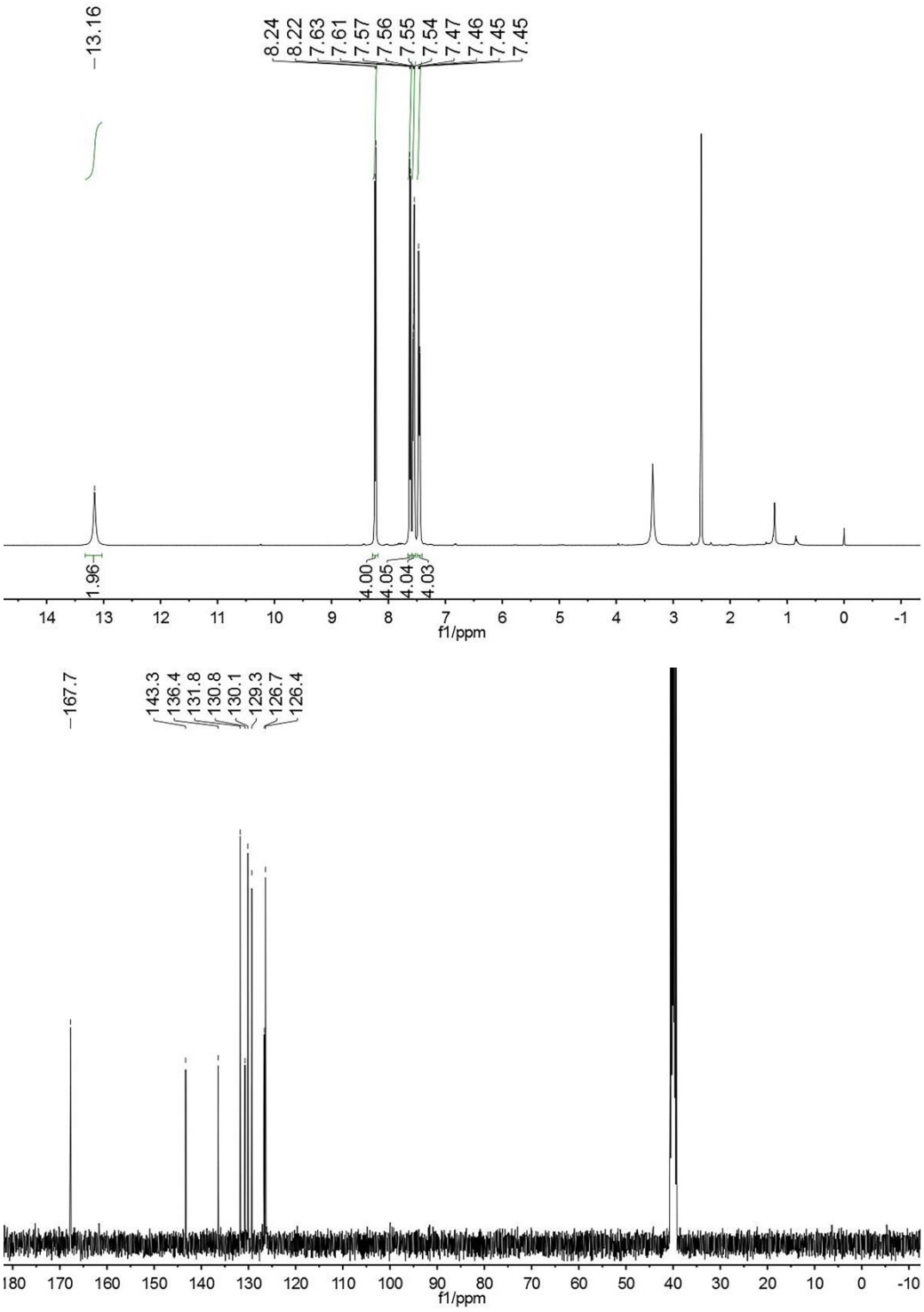

Fig. S2 ^{1}H NMR and ^{13}C NMR spectra (DMSO-d6, 298 K) of compound **2**

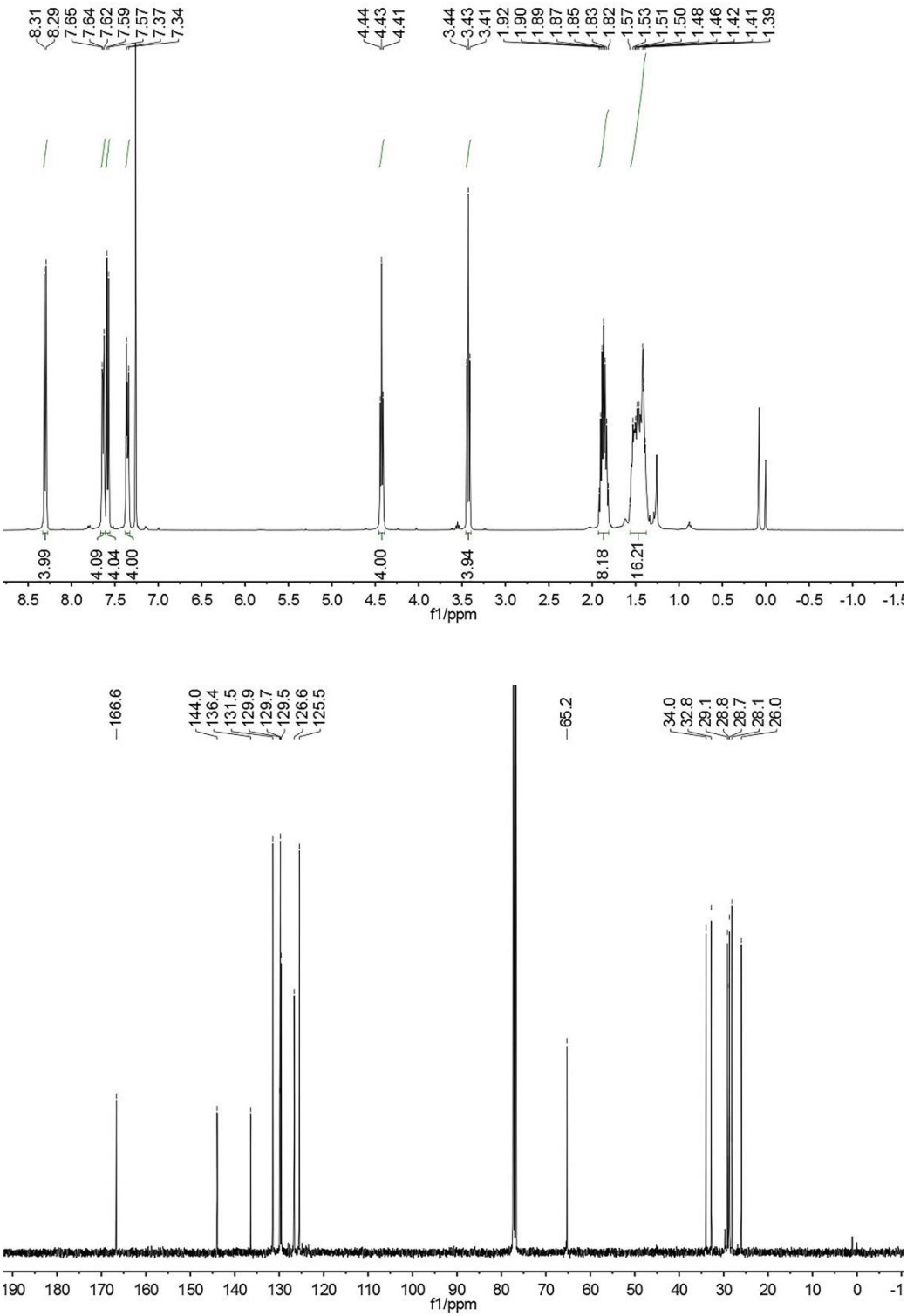

Fig. S3 ^{1}H NMR and ^{13}C NMR spectra ($CDCl_3$, 298 K) of compound **3**

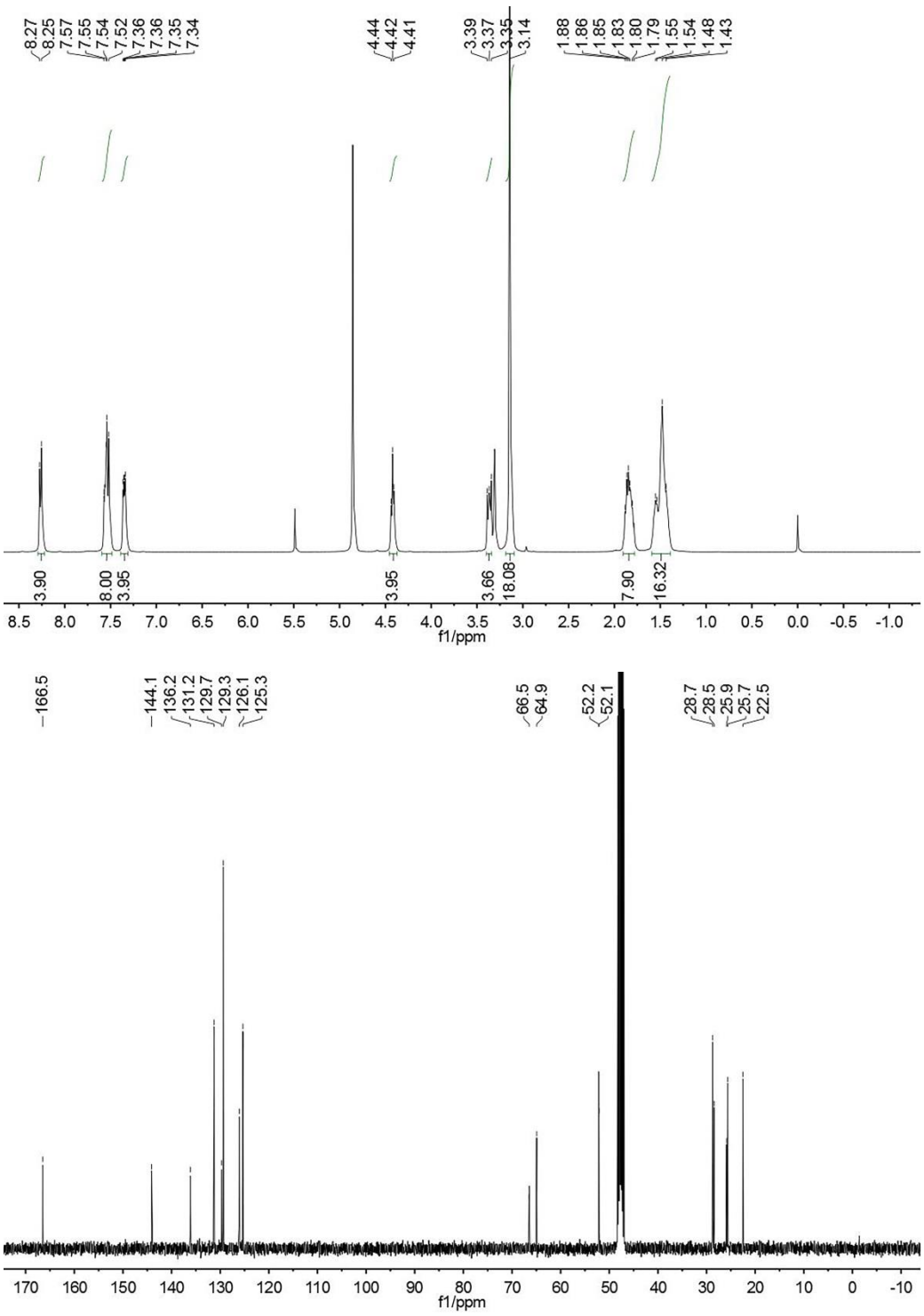

Fig. S4 ^{1}H NMR and ^{13}C NMR spectra (CD_3OD, 298 K) of compound **G**

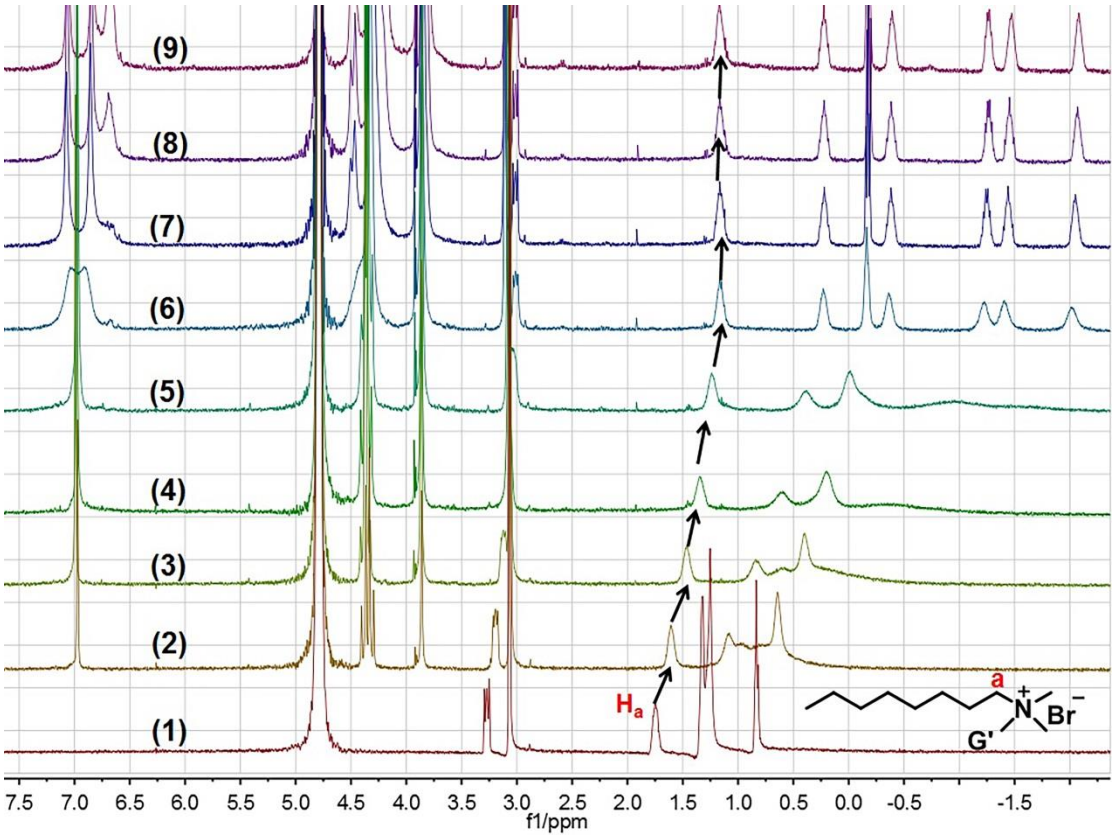

Fig. S5 ^{1}H NMR spectra (400 MHz, D_2O, 298 K) of **G′** at the concentration of 3.0 mM with different concentrations (mM) of **WP5**: (1) 0.0, (2) 0.75, (3) 1.5, (4) 2.25, (5) 3.0, (6) 3.75, (7) 4.5, (8) 5.25, (9) 6.0.

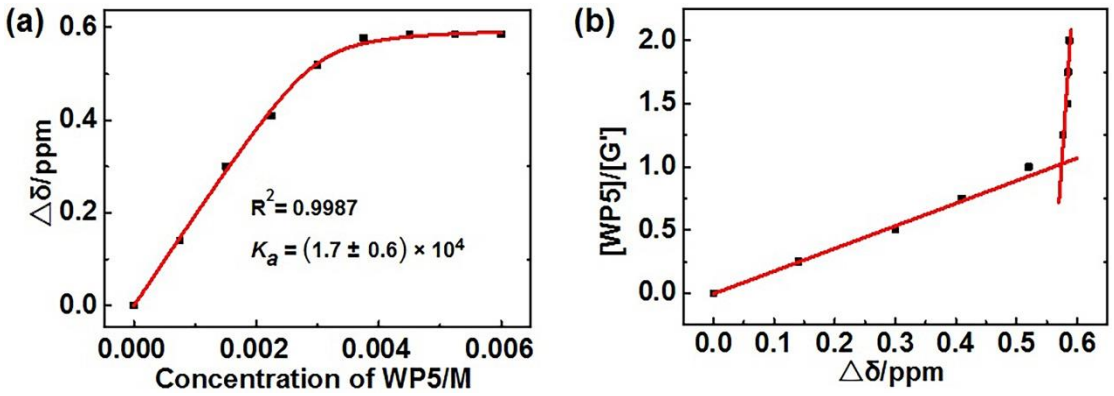

Fig. S6 (a) The fitting curves of Δδ versus concentration of **WP5**. (b) The stoichiometry of host and guest complex. Δδ is the chemical shift change of H_a on **G′** upon addition of **WP5**.

The total weight of nanoparticles was obtained through freeze-drying. The

nanoparticles were then dissolved into DMF. The weight of TPP in nanoparticles was determined using a UV spectrophotometer according to the calibration curves of TPP. The weight of WP5 and G was obtained through the subtraction the weight of TPP and their weight ratio was estimated to be 2 :1 based on the stoichiometry.

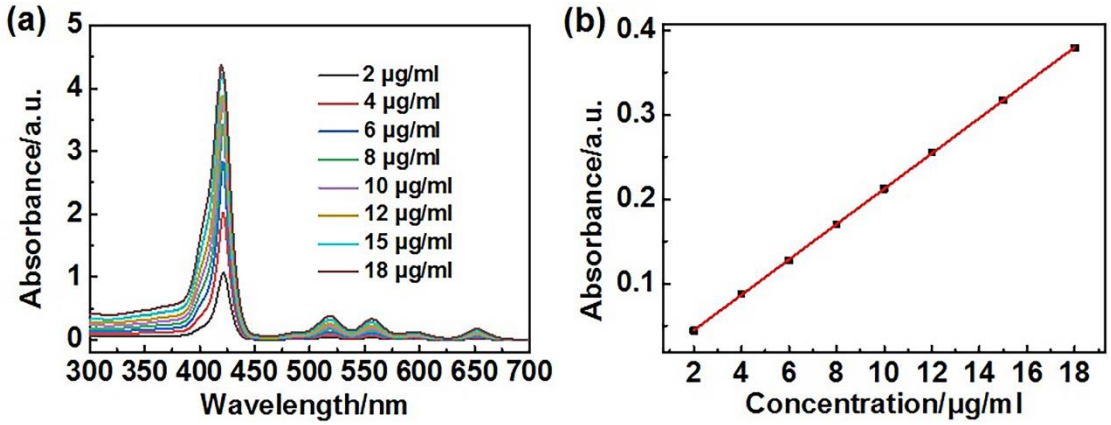

Fig. 7 (a) The UV-Vis spectra of TPP in DMF, (b) the calibration curve of the absorbance of TPP.

TPP in DMF (0.1 μM) aqueous solution with different concentrations in quartz cuvettes were mixed with DPBF (50.0 μM), which was then irradiated by lasers (660 nm, 1W) for a period of 240 s.

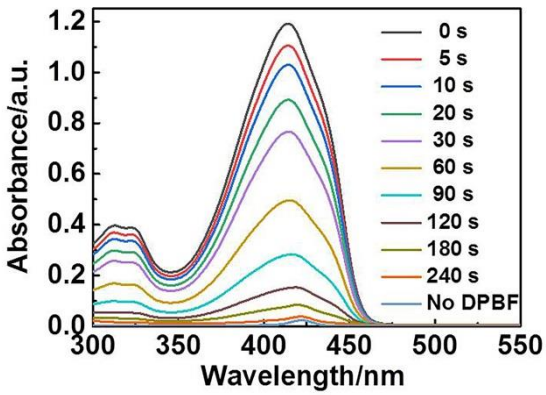

Fig. S8 The absorption spectra of the mixture of **TPP** and DPBF under laser irradiation for different time.

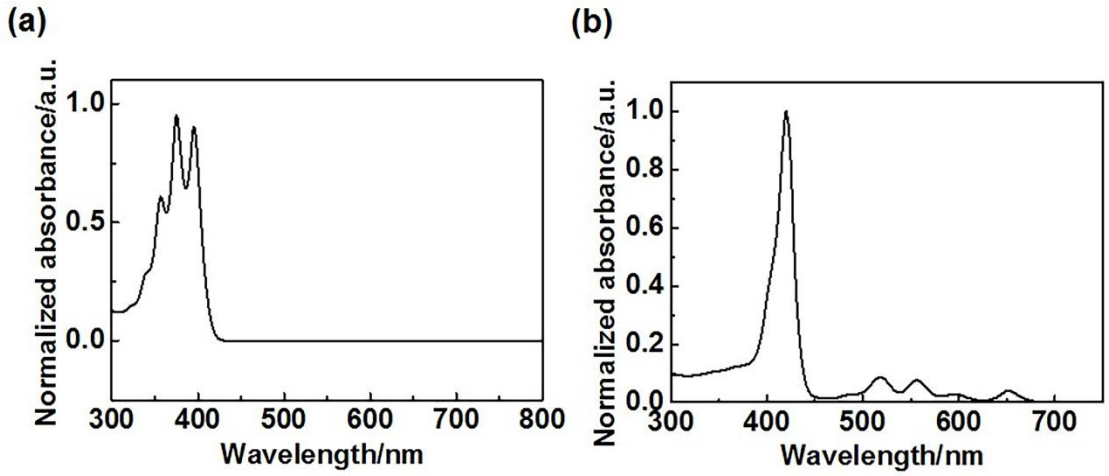

Fig. S9 The absorption curves for (a) **G** and (b) **TPP** in DMF.

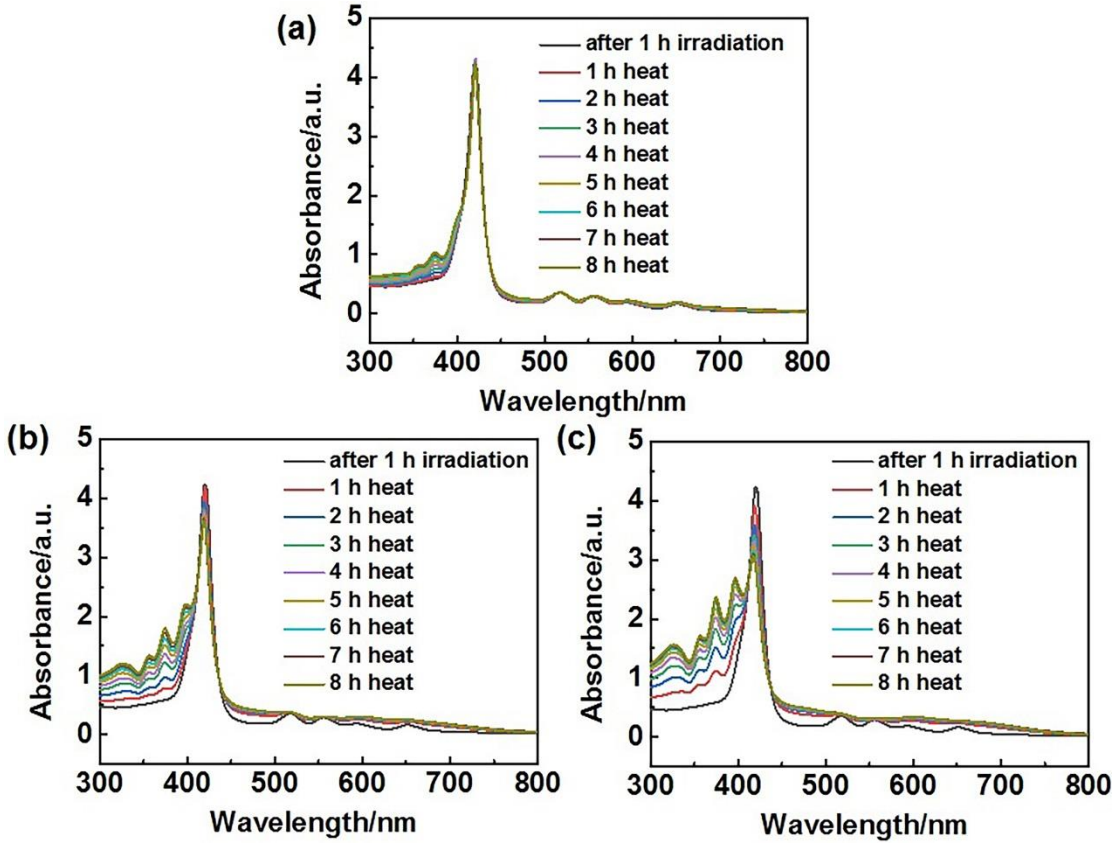

Fig. S10 The absorption spectra of the irradiated mixture (**TPP**: 25 μM, **G**: 200 μM) in DMF after heating at different temperatures: (a) 80 ºC, (b) 90 ºC, (c) 100 ºC.

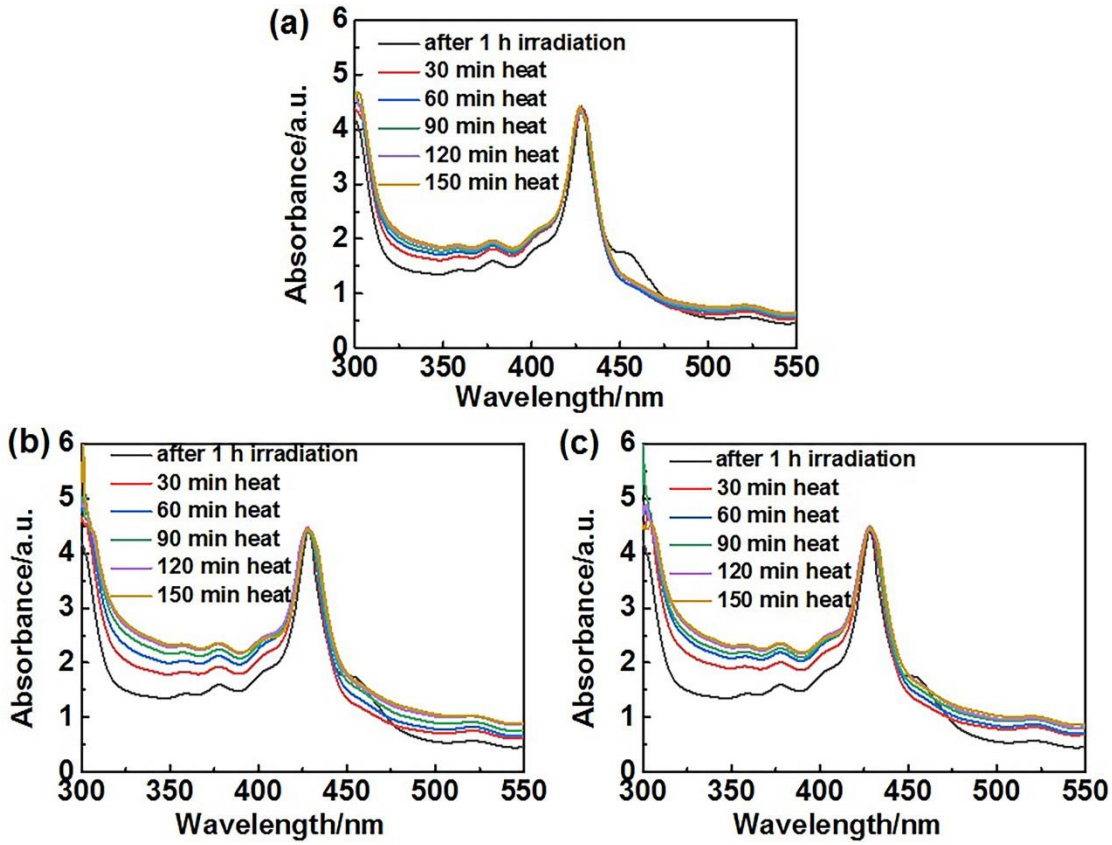

Fig. S11 The absorption spectra of the irradiated nanoparticles after heating at different temperature: (a) 80 ºC, (b) 90 ºC, (c) 100 ºC.

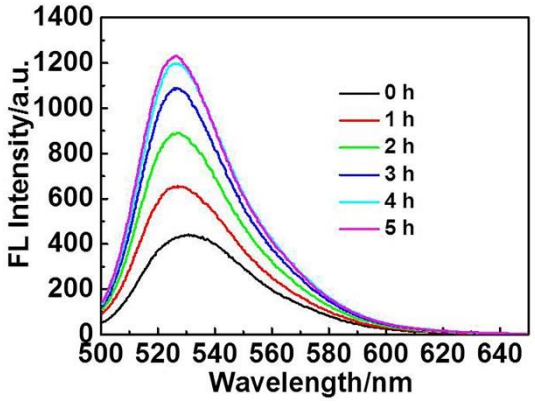

Fig. S12 The fluorescence spectra of the SOSG (10 μM) in the presence of the irradiated nanoparticles in H_2O after heating at 80 ºC for different time.