

NIR-II imaging-guided photothermal cancer therapy combined with enhanced immunogenic death

Yukun Wang,^{a,\$} Wenjing Li,^{a,\$} Bi Lin,^a Ying Yuan,^{b,*} Pengbo Ning,^{a,*} Xiaofeng Tao,^{b,*} Ruichan Lv^{a,c,*}

^a Engineering Research Center of Molecular and Neuro Imaging, Ministry of Education, School of Life Science and Technology, Xidian University, Xi'an, Shanxi 710071, China. Email: pbning@xidian.edu.cn; rclv@xidian.edu.cn

^b Department of Medical Interdisciplinary Research, Xi'an Ninth Hospital Affiliated to Medical College of Xi'an Jiaotong University, 710054, Xi'an, Shaanxi, China. Email: yuany83@163.com; cjr.taoxiaofeng@vip.163.com

^c Interdisciplinary Research Center of Smart Sensor, Xi'an Key Laboratory of Intelligent Sensing and Regulation of trans-Scale Life Information, Xidian University, Xi'an, Shaanxi 710126, P. R. China.

Calculation of the photothermal conversion efficiency.

The photothermal conversion efficiency (η) of GdOF@PDA is calculated by the following formula.

$$\sum_i m_i C_{p,i} \frac{dT}{dt} = Q_{NC} + Q_{Dis} - Q_{Surr} \quad (1)$$

where m and C_p are the mass and heat capacity of water, respectively, T is the solution temperature, Q_{NC} is the energy inputted by NCs, Q_{Dis} is the energy inputted by the cuvette, and Q_{Surr} is the heat exchanged between the air and the system.

$$Q_{NC} = I(1 - 10^{-A_{980}})\eta \quad (2)$$

where I is laser power, η is the photothermal conversion efficiency, and A_{980} is the absorbance of the sample at wavelength of 980 nm.

$$Q_{Surr} = hS(T - T_{Surr}) \quad (3)$$

where h is heat transfer coefficient, S is the surface area of the container, and T_{Surr} is the ambient temperature.

$$Q_{NC} + Q_{Dis} = Q_{Surr-Max} = hS(T_{Max} - T_{Surr}) \quad (4)$$

Through the formulas (1), (2), (3), and (4) above, the photothermal conversion efficiency is obtained as follows:

$$\eta = \frac{hS(T_{Max} - T_{Surr}) - Q_{Dis}}{I(1 - 10^{-A_{980}})} \quad (5)$$

Observing formula (5), to get the value of light-to-heat conversion efficiency, only the value of hS needs to be calculated, while other values can be obtained during the experiment. The value of hS can be obtained through the following formulas:

$$\theta = \frac{T - T_{Surr}}{T_{Max} - T_{Surr}} \quad (6)$$

$$\tau_s = \frac{\sum_i m_i C_{p,i}}{hS} \quad (7)$$

$$\frac{d\theta}{dt} = \frac{1}{\tau_s} \left[\frac{Q_{NC} + Q_{Dis}}{hS(T_{Max} - T_{Surr})} - \theta \right] \quad (8)$$

$$dt = \tau_s \frac{d\theta}{\theta} \quad (9)$$

$$t = -\tau_s \ln \theta \quad (10)$$

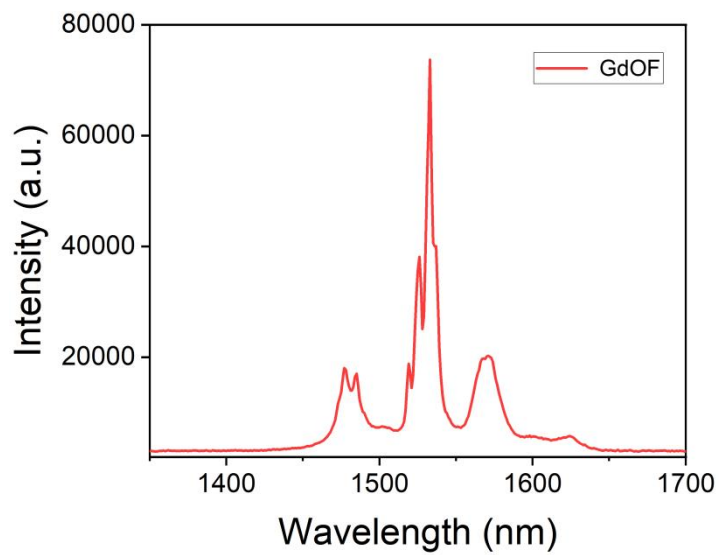


Figure S1. NIR-II spectrum of GdOF (doping with Yb,Er).

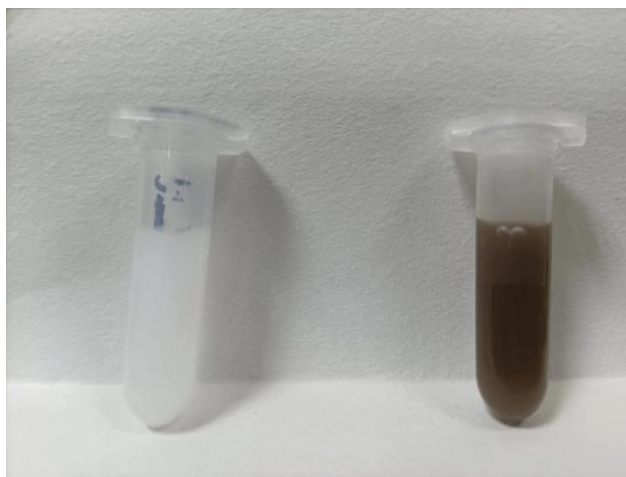


Figure S2. Solution color changes during the synthesis process of GdOF@PDA NPs.

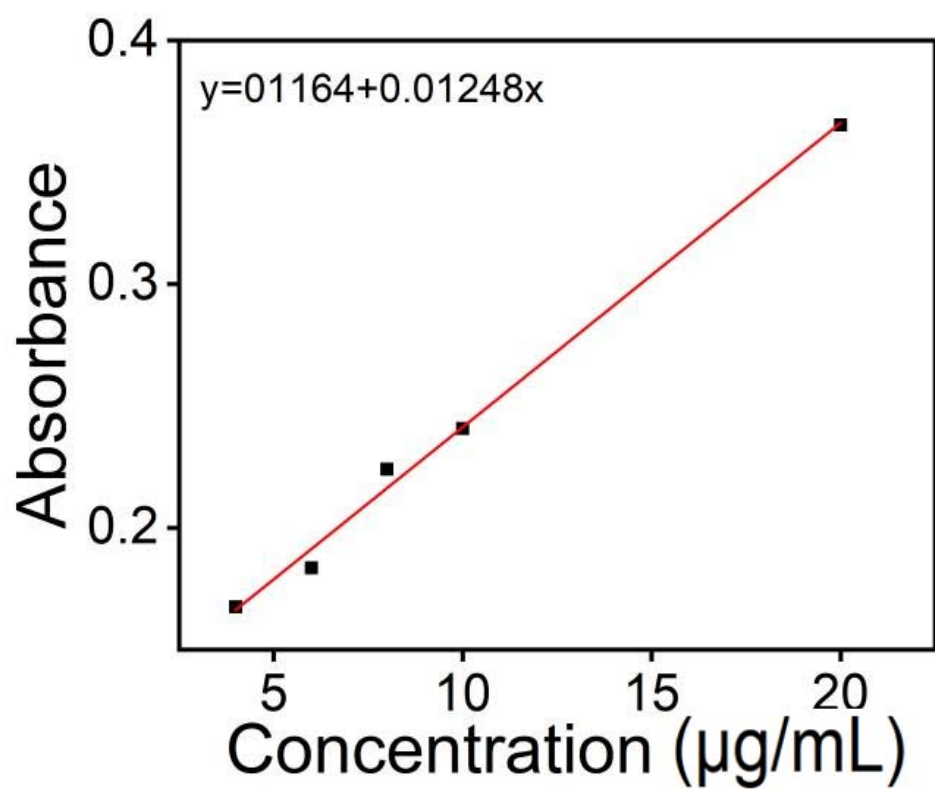


Figure S3. Standard curve of R837 in DMSO.

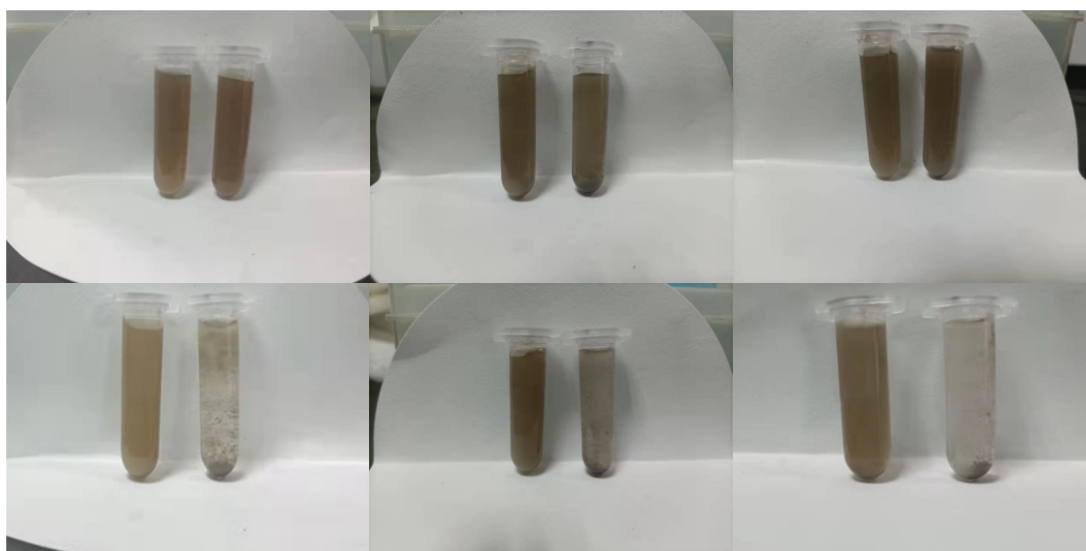


Figure S4. Nanoparticles aqueous solution changes during drug release in acidic conditions.



Figure S5. The gel phenomenon of nanoparticles in calcium ion environment. A) GdOF @ PDA-HA-R837 HG was mixed with Ca^{2+} solution. B) The mixed solution of A) was tilted and shown a gel formation rather than a liquid. C) GdOF @ PDA-HA-R837 HG was added to Ca^{2+} solution, and gel formation appeared immediately.

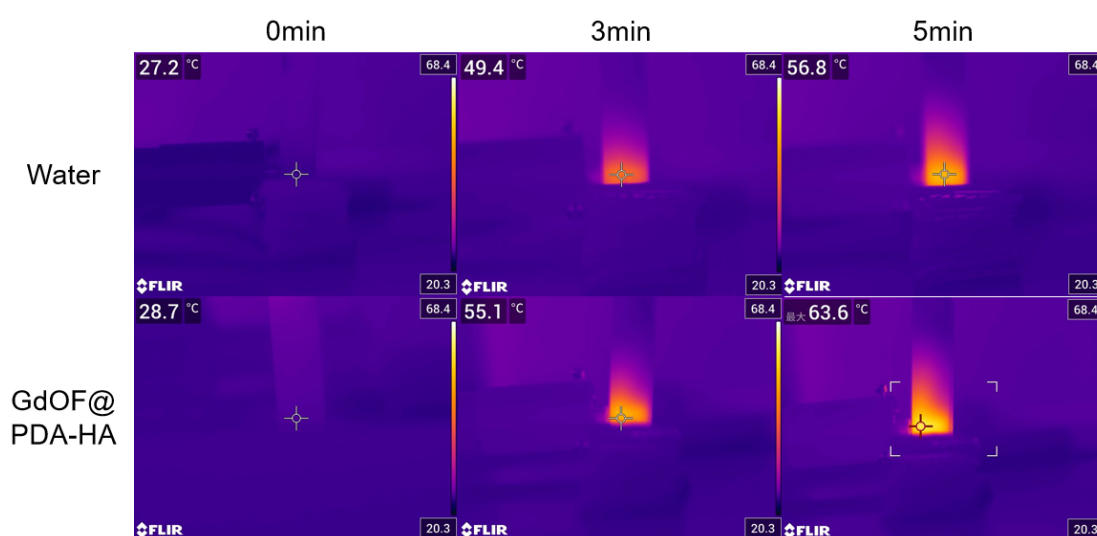


Figure S6. Temperature changes in water and GdOF@PDA-HA under laser irradiation (980 nm, $1.5\text{W}/\text{cm}^2$).

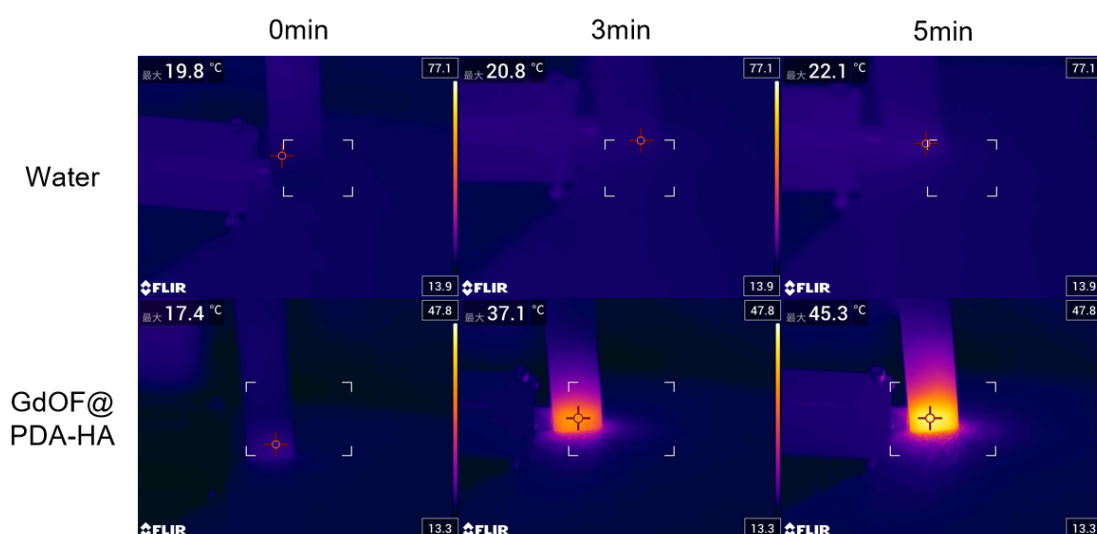


Figure S7. Temperature changes in water and GdOF@PDA-HA under laser irradiation (808 nm, $1.5\text{W}/\text{cm}^2$).

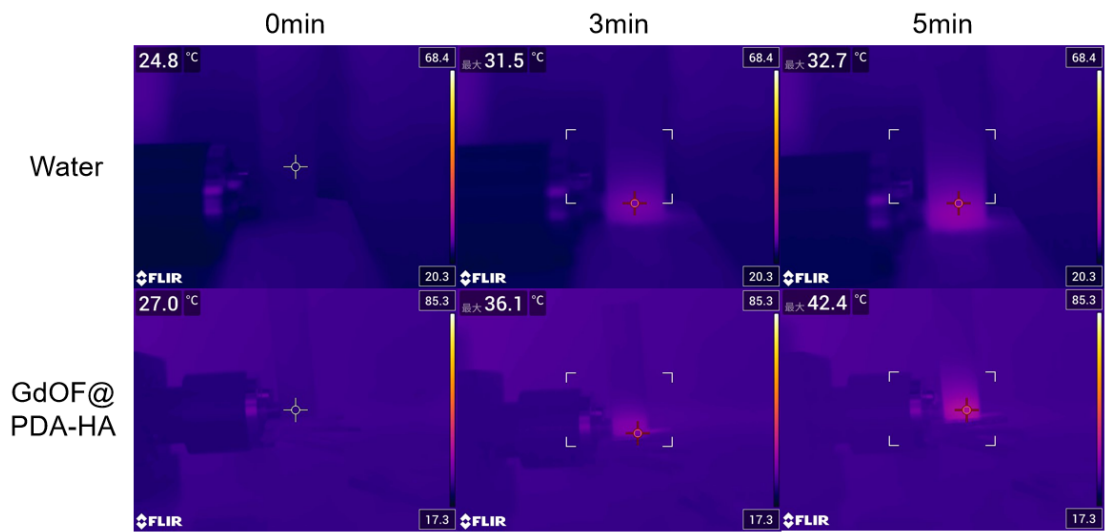


Figure S8. Temperature changes in water and GdOF@PDA-HA under laser irradiation (1064 nm, 1.5W/cm²).

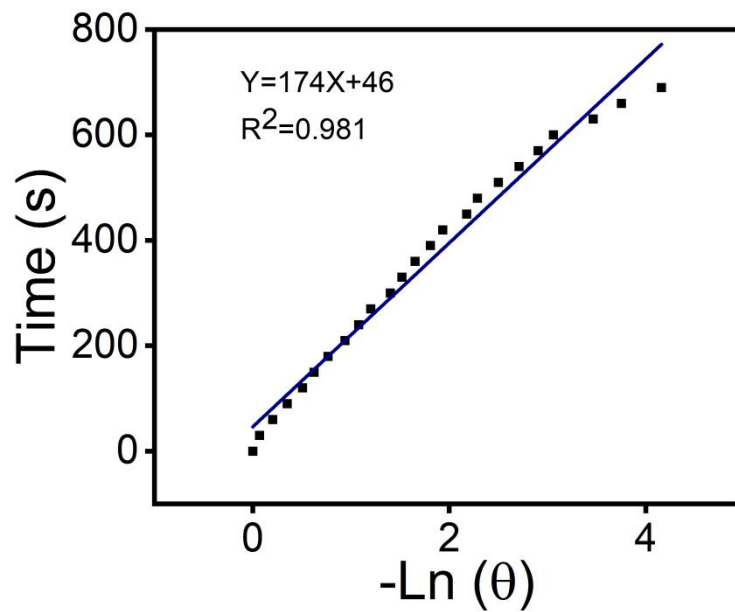


Figure S9. Linear time data versus $-\ln\theta$ obtained from the cooling stage.

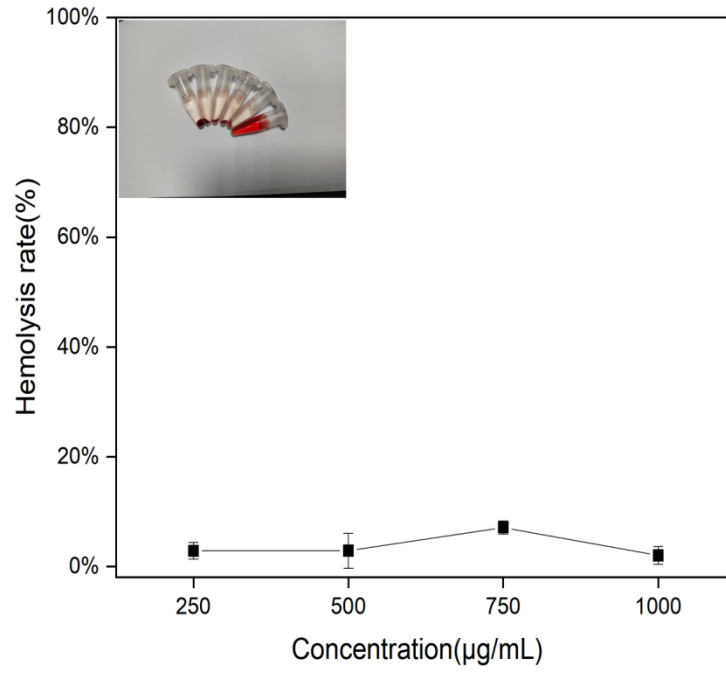


Figure S10. The result of the hemolysis experiment. From left to right in the insert figure are PBS, 250 µg/mL, 500 µg/mL, 750 µg/mL, 1000 µg/mL, and ultrapure water.

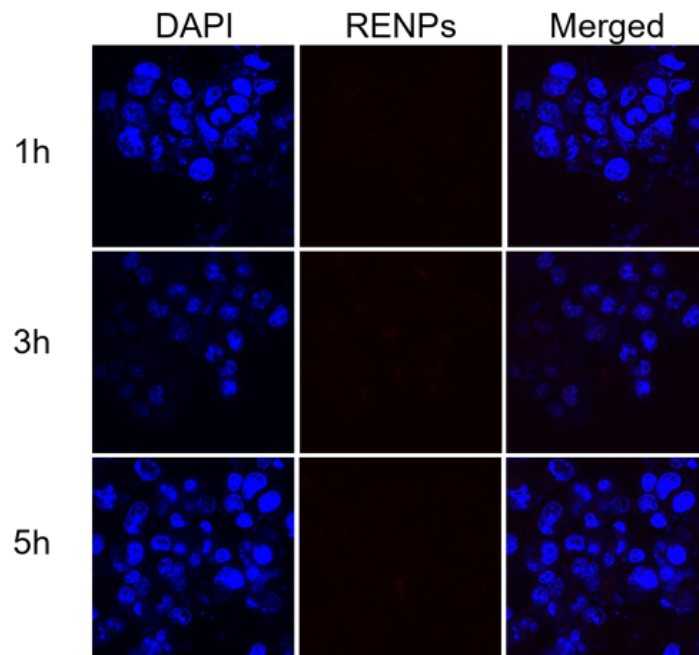


Figure S11. Cell uptake of GdOF@PDA.