## **Supporting Information**

# Multifunctional theranostic graphene oxide nanoflakes as MR imaging agents with enhanced photothermal and radiosensitizing properties

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## Calculation of photothermal conversion efficiency

The photothermal conversion efficiency  $(\eta)$  of NFs was calculated according to the following formulas (1, 2):

$$\eta = \frac{hS (T_{max} - T_{sur}) - Q_{dis}}{I(1 - 10^{-A_{808}})}$$
(1)

where *h* is the heat transfer coefficient, *S* is the surface area of the container,  $T_{max}$  and  $T_{sur}$  are the maximum equilibrium temperature and the ambient temperature, I is the laser power,  $A_{808}$  is the absorbance of NFs at 808 nm, and  $Q_{dis}$  is heat dissipation due to light absorbance of the solvent. *hS* can be calculated according to the following equation:

$$hS = \frac{m_s C_s}{\tau}$$
(2)

where  $\tau$  is the sample system time constant, and  $m_s$  and  $C_s$  are the mass and the heat capacity of the solvent (water), respectively.

	$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	1 0.5 0.2 0.1 0.05 0 TE= 36 ms	1 0.5 0.2 0.1 0.05 0 TE= 48 ms	$ \begin{array}{cccccccccccccccccccccccccccccccccccc$
IE= 12 ms	TE- 24 IIIs	TE- 38 IIIs	1E- 48 IIIS	IE- 80 IIIs
	1 0.5 0.2	1 0.5 0.2	1 0.5 0.2	1 0.5 0.2
0.1 0.05 0	0.1 0.05 0	0.1 0.05 0	0.1 0.05 0	0.1 0.05 0
TE= 72 ms	TE= 84 ms	TE= 96 ms	TE= 108 ms	TE= 120 ms
1 0.5 0.2 0.1 0.05 0	1 0.5 0.2 0 0 0 0.1 0.05 0	1 0.5 0.2 0.1 0.05 0	1 0.5 0.2 0.1 0.05 0	
TE= 132 ms	TE= 144 ms	TE= 156 ms	TE= 168 ms	

[Fe] concentration/ mM

**Figure S1.** T2-weighted MR images of NF solutions containing 0-1.0 mM Fe. Images were obtained for various TE values, with the TR value fixed at 2,000 ms.



**Figure S2.** Temperature changes of the NF solution (50  $\mu$ g/mL) during NIR heating (laser on, 1.8 W/cm<sup>2</sup>) and cooling (laser off) cycles.



**Figure S3.** Temperature increase of CT26 cells incubated with various concentrations of NFs for 4 h. Temperatures were recorded after 808 nm laser irradiation for 1 or 2 min at  $1.5 \text{ W/cm}^2$ .



**Figure S4.** Representative H&E images from the combined NF + PTT/RT group at day 2 post-treatment, showing marked vascular hemorrhaging (R: red blood cells; N: necrotic zone).

### References

S1. Bhana S, Lin G, Wang L, Starring H, Mishra SR, Liu G, et al. Near-infrared-absorbing gold nanopopcorns with iron oxide cluster core for magnetically amplified photothermal and photodynamic cancer therapy. ACS applied materials & interfaces. 2015;7(21):11637-47.

S2. Hu Y, Wang R, Wang S, Ding L, Li J, Luo Y, et al. Multifunctional Fe<sub>3</sub>O<sub>4</sub>@ Au core/shell nanostars: a unique platform for multimode imaging and photothermal therapy of tumors. Scientific Reports. 2016;6.