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Electronic Supplementary Information

A novel theranostic agent based on porous bismuth nanosphere for CT imaging guided combined chemo-photothermal therapy and radiotherapy

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1. Supplementary Figures

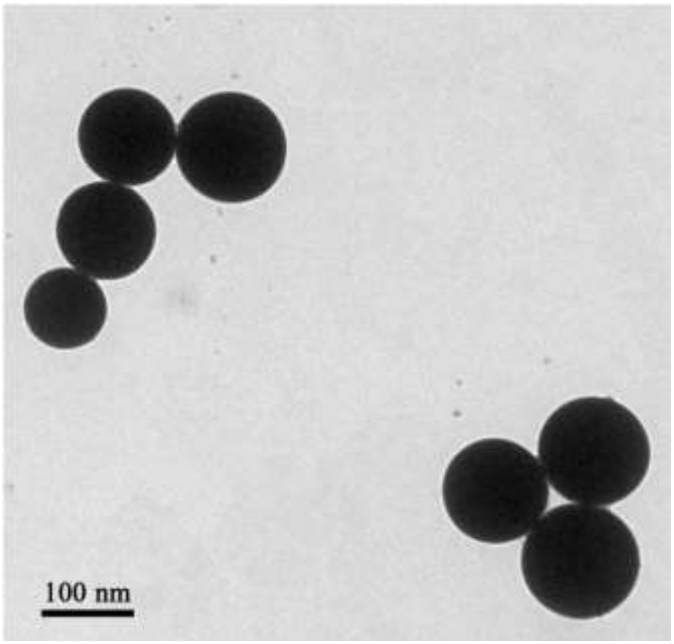

Fig. S1 TEM images of as-prepared Bi nanospheres.

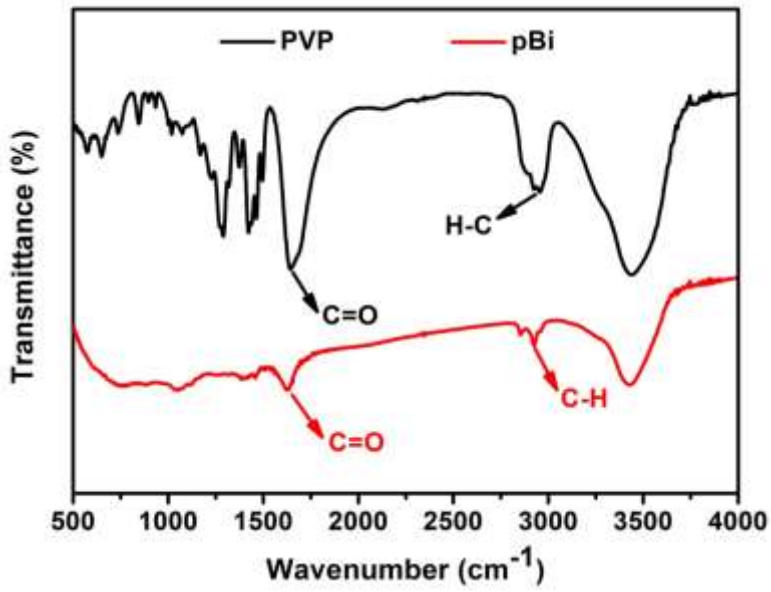

Fig. S2 Fourier transform infrared spectroscopy (FTIR) analysis of PVP and pBi nanospheres.

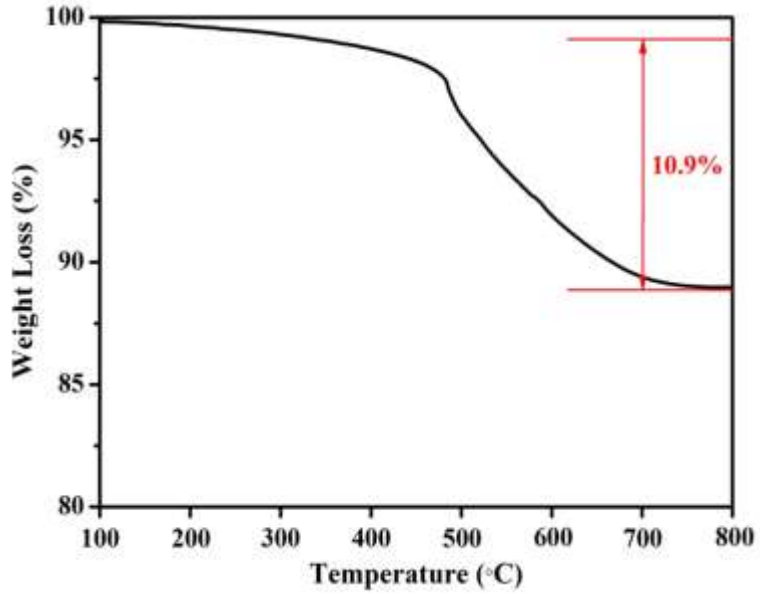

Fig. S3 Thermo-gravimetric (TG) analysis of PVP content in Bi nanospheres.

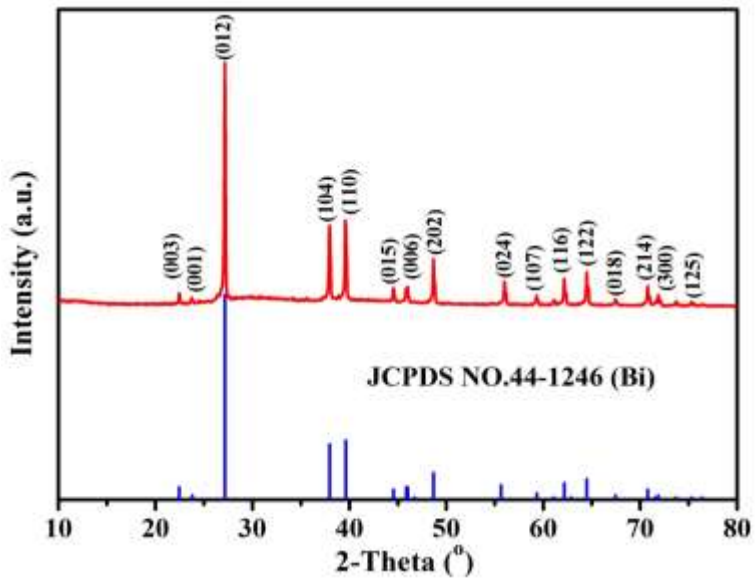

Fig. S4 Powder XRD patterns of pBi nanospheres.

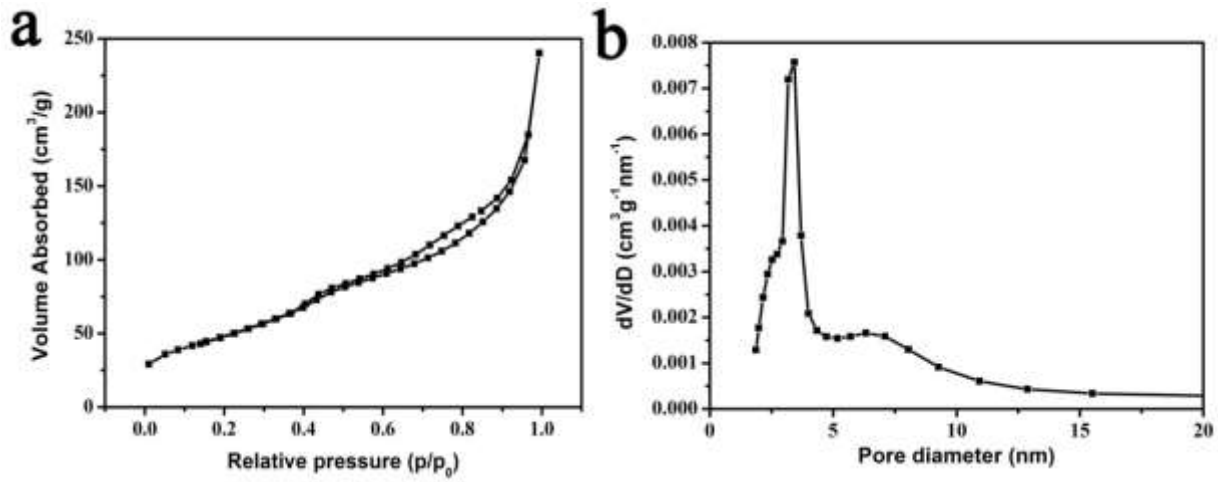

Fig. S5 (a) N_2 adsorption-desorption isotherms. (b) The pore diameter distribution of pBi nanospheres.

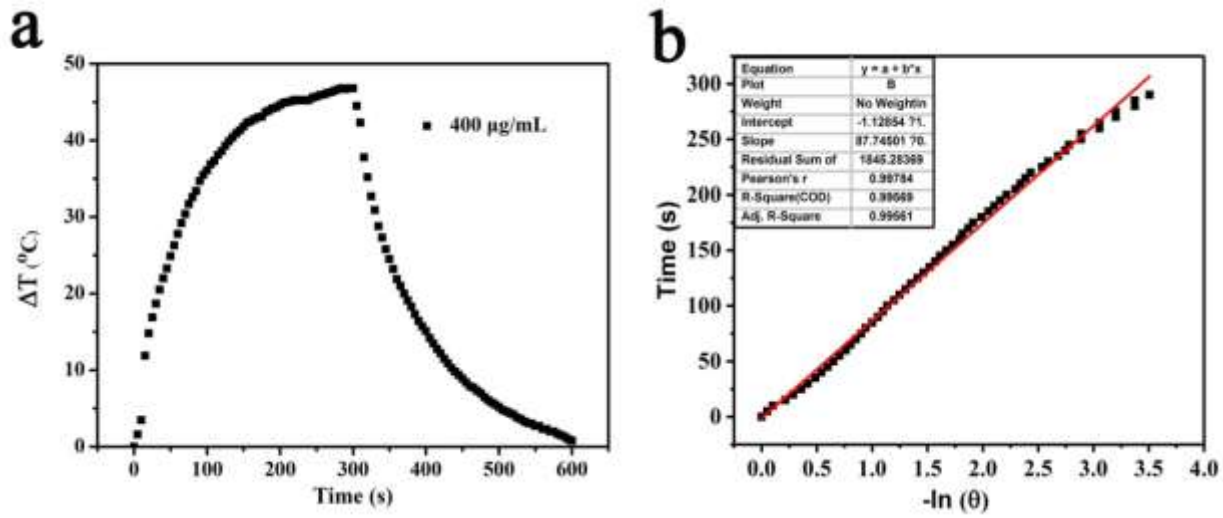

Fig. S6 (a) Photothermal effect of the irradiation of the pBi nanospheres aqueous solution for 300 s with the NIR laser (808 nm, 1.0 W/cm^2), and then the laser was shut off. (b) Linear time data versus –ln(θ) obtained from the cooling period of Fig. S5a.

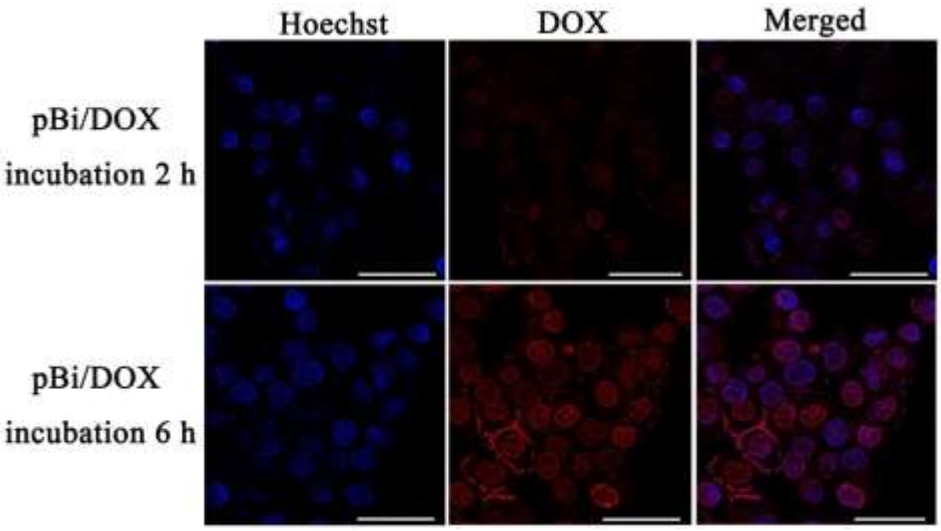

Fig. S7 CLSM images of HeLa cells incubated with pBi/DOX nanospheres for 2 h and 6 h, respectively (Scale bar = 50 μm).

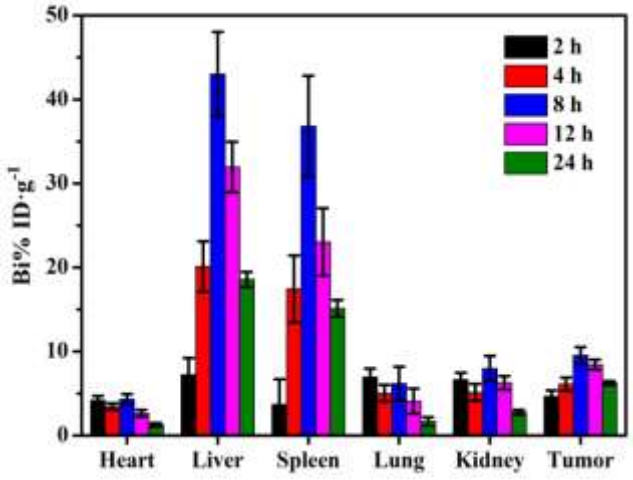

Fig. S8 Time-dependent biodistribution of Bi in mice after intravenous injection of pBi nanospheres.

2. Calculation of the photothermal conversion efficiency(η)

The photothermal conversion efficiency of the porous Bi nanospheres was calculated using the reported method.[1-3] The aqueous solution of the porous Bi nanospheres (400 μg/mL) was exposed to 808 nm laser (1.0 W/cm^2) until temperature tends to stabilize, and the laser was shut off. Then the temperature of the aqueous solution was gradually cooled to room temperature. The temperature change was recorded by the Fotric225 camera. (Fig. S5a). The η value was calculated as follows:

$$\eta = \frac{hs\,(T_{Max}-T_{Surr})-Q_{Dis}}{I\,(1-10^{-A_{808}})} \quad \text{Eq. 1}$$

Where **h** is the heat transfer coefficient, **s** is the surface area of the container, and the value of **hs** is obtained from the Eq.4 and Fig. S3b. The maximum steady temperature (T_{max}) and environmental temperature (T_{Surr}) was 69.8 °C and 23.1 °C, respectively. **I** stands for laser power was 396 mW. A_{808} stands for the absorbance of the porous Bi nanospheres at 808 nm was 2.66. Q_{Dis} is the heat associated with the light absorbance of the solvent and container. A dimensionless parameter θ is calculated as followed:

$$\theta = \frac{T-T_{Surr}}{T_{Max}-T_{Surr}} \quad \text{Eq. 2}$$

τ_s ,which a sample system time constant, can be calculated as Eq.3

$$t = -\tau_s \ln(\theta) \quad \text{Eq. 3}$$

As shown in Fig. 5b, τ_s was determined and calculated to be 87.745 s.

$$hs = \frac{m_D C_D}{\tau_s} \quad \text{Eq. 4}$$

In addition, m_D is 0.2 g and C_D is 4.2 J/g·°C. Thus, according to Eq. 4, **hs** is calculated to be 9.57 mW/°C.

Q_{Dis} is heat dissipated from the light absorbed by the container itself, and it was determined independently using a container containing pure water. Thus, substituting according values of each parameters to Eq. 1, the 808 nm laser photothermal conversion efficiency (η) of the porous Bi nanospheres can be calculated to be 48.5%.

References

1. X. Liu, Q. Ren, F. Fu, R. Zou, Q. Wang, G. Xin, Z. Xiao, X. Huang, Q. Liu and J. Hu, *Dalton Trans.*, 2015, **44**, 10343-10351.
2. C. M. Hessel, V. P. Pattani, M. Rasch, M. G. Panthani, B. Koo, J. W. Tunnell and B. A. Korgel, *Nano Lett.*, 2011, **11**, 2560-2566.
3. X. Liu, B. Li, F. Fu, K. Xu, R. Zou, Q. Wang, B. Zhang, Z. Chen and J. Hu, *Dalton Trans.*, 2014, **43**, 11709-11715.