Supplementary Data

Sn_xWO₃ as a Theranostic Platform for Realizing Multi-imaging-guided Photothermal/Photodynamic Combination Therapy

Yan Gao,^{a#} Fei Wang,^b Weicheng Huang,^c Chunyu Yang,^a Wei Guo,^b Chuanqi Song,^a Qun Zhang,^a Bin Yang,^c Yanling Xu,* ^a Chongshen Guo* ^{a,b}

^a School of Chemistry and Chemical Engineering, Harbin Institute of Technology, Harbin, 150001, China

^b Key Lab of Microsystem and Microstructure Manufacturing (Ministry of Education), Academy of Fundmental and Interdisciplinary Sciences, Harbin Institute of Technology, Harbin, 150080,

China

^c Condensed Matter Science and Technology Institute, Department of Physics, Harbin Institute of Technology, Harbin 150080, China.

^d Department of Chemistry, City University of Hong Kong, Hong Kong SAR, China

Corresponding author: xuyanling@hit.edu.cn (Y. L. Xu)

chongshenguo@hit.edu.cn (C. S. Guo)

Calculation of thermal conversion efficiency

The photothermal conversion efficiency (η) is calculated with following equation:

$$\eta = \frac{hA(T_{max} - T_{surr}) - Q_{dis}}{I(1 - 10^{-A_{1064}})}$$
Equation S1

h is heat transfer coefficient; A is the surface area of the container;

 T_{max} and T_{surr} are the equilibrium temperature and ambient temperature, respectively;

 \mathbf{Q}_{dis} is heat dissipated from light absorbed by the quartz cell.

I is incident laser power (2 W/cm²); A1064 is the optical absorbance of nanoparticles at 1064 nm (0.49).

hA is unknown and could be obtained by following equation.

$$hA = \frac{\sum mC}{\tau s}$$
 Equation S2

Where m, C, τ_s are the mass, heat capacity of water and time constant, respectively. For determining the τ_s , θ is introduced as in Equation 3.

$$\theta = \frac{T - T_{surr}}{T_{max} - T_{surr}}$$

At the cooling stage of the aqueous dispersion (see Figure 2d), the cooling time t and θ abide by the following Equation 4:

Equation S3

$$t = -\tau s \ln(\theta)$$
 Equation 4

Time constant for heat transfer from the system could be determined by plotting linear time from the cooling stage against negative natural logarithm of θ . (Figure. 2e) By this way, τ_s is determined as 224.8 s. (m=0.5 g, C 4.2 J g⁻¹ °C⁻¹, hA = 9.34 mW/ °C)

Thus, the photothermal conversion efficiency (η) is calculated to be 18.6%.

Calculation of synergy index

HepG2 cells seeded 96-well plates were incubated with 250 or 500 µg mL⁻¹ of Sn_xWO₃@BSA for 24 h, respectively. Then, 880 nm NIR irradiation (2.0 W cm⁻²) was applied for 10 min. For the PTT process, sodium azide (50 µL, 10×10^{-6} M) was introduced into each well before NIR irradiation. As to the PDT group, the phototherapy was carried out under ice bath, while kept other operations unchanged. MTT assay was performed for quantifying cell viabilities after above treatments. The data of *in vitro* PDT, PTT and synergetic PDT/PTT effect were inputted into the CompuSyn software and the synergy index was 0.243.

Table S1 The therapeutic efficiency of PDT, PTT and PDT/PTT with regard to the concentrationof $Sn_xWO_3@BSA$

Concentration	PDT (Inhibition rate)	PTT (Inhibition rate)	PTT/PDT (Inhibition rate)
250 mg/mL	0.121	0.388	0.46
500 mg/mL	0.171	0.45	0.52



Fig. S1. Zeta potential of Sn_xWO₃, Sn_xWO₃@PAH and Sn_xWO₃@PAH/BSA.



Fig. S2. Absorbance of DPBF solutions after different treatment.



Fig. S3. Detection of mitochondrial potential changes by JC-1 staining.



Fig. S4. Histology staining of major organs harvested from different groups of mice at 14th days.



Fig. S5. Haematological data were collected from the control nude mice or mice injected with $Sn_xWO_3@BSA$ (1 mg mL⁻¹) at 1, 3, 7 and 14 days after injection.