Supporting Information

Phosphomolybdenum Blue Nano-photothermal Agent with Dual Peak Absorption and Biodegradable Properties Constructed Based on ssDNA in Near-Infrared Photothermal Therapy for Breast Cancer

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Table 1 Different experimental conditions for synthesizing PMB nanoparticles.

Group	Influencing factors	ssDNA (μM)	VC (%)	Time (h)	Temperature (°C)	HCl (mol/L)
a	Effect of ssDNA	**25**	10	6	95	1.2
b		**50**	10	6	95	1.2
c		**75**	10	6	95	1.2
d		**100**	10	6	95	1.2
e	Effect of VC	25	**5**	6	95	1.2
f		25	**10**	6	95	1.2
g		25	**15**	6	95	1.2
h		25	**20**	6	95	1.2
i	Effect of Time	25	10	**3**	95	1.2
j		25	10	**6**	95	1.2
k		25	10	**12**	95	1.2
l		25	10	**24**	95	1.2
m	Effect of Temperature	25	10	6	**25**	1.2
n		25	10	6	**37**	1.2
o		25	10	6	**60**	1.2
p		25	10	6	**95**	1.2
q	Effect of HCl	25	10	6	95	**0.6**
r		25	10	6	95	**1.2**
s		25	10	6	95	**1.8**
t		25	10	6	95	**2.4**

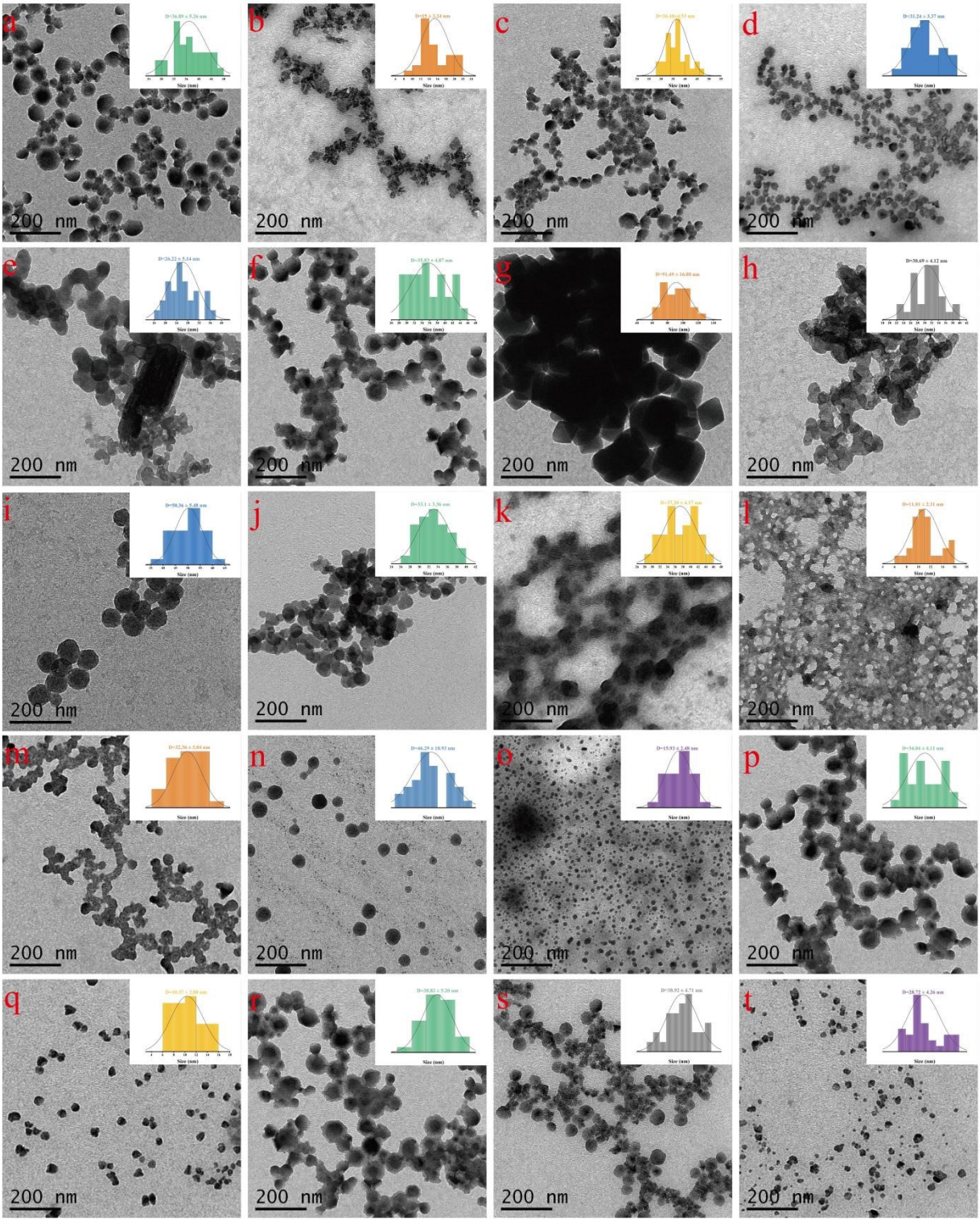

Figure S1 TEM images of as-prepared PMB with different experimental conditions. (a: 25 μM ssDNA; b: 50 μM ssDNA; c: 75 μM ssDNA; d: 100 μM ssDNA; e: 5 % VC; f: 10 % VC; g: 15 % VC; h: 20 % VC; i: 3 h; j: 6 h; k: 12 h; l: 24 h; m: 25℃; n:37℃; o: 60℃; p: 95℃; q: 0.6 mol/L HCl; r: 1.2 mol/L HCl; s: 1.8 mol/L HCl; t: 2.4 mol/L HCl).

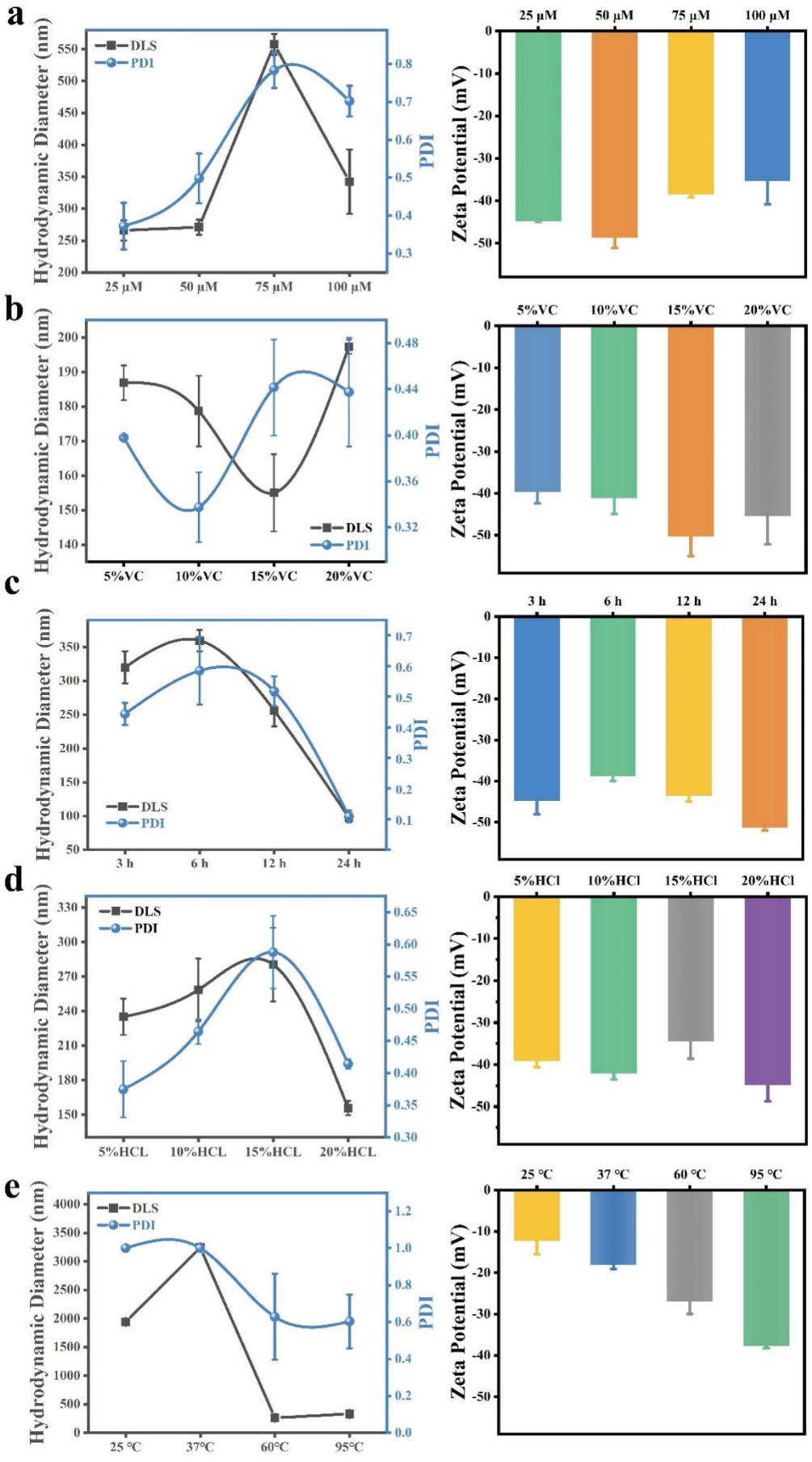

Figure S2 The DLS and Zeta potential of synthesized PMB under different conditions.

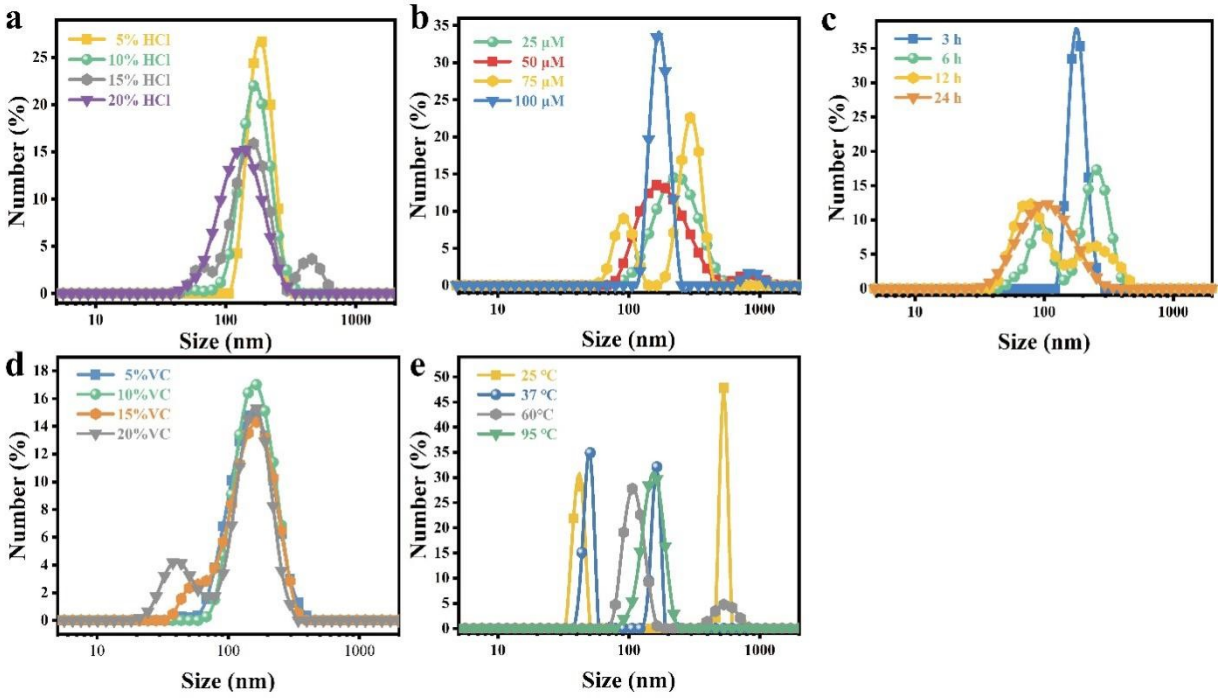

Figure S3 Particle size distribution of synthesized PMB under different conditions.

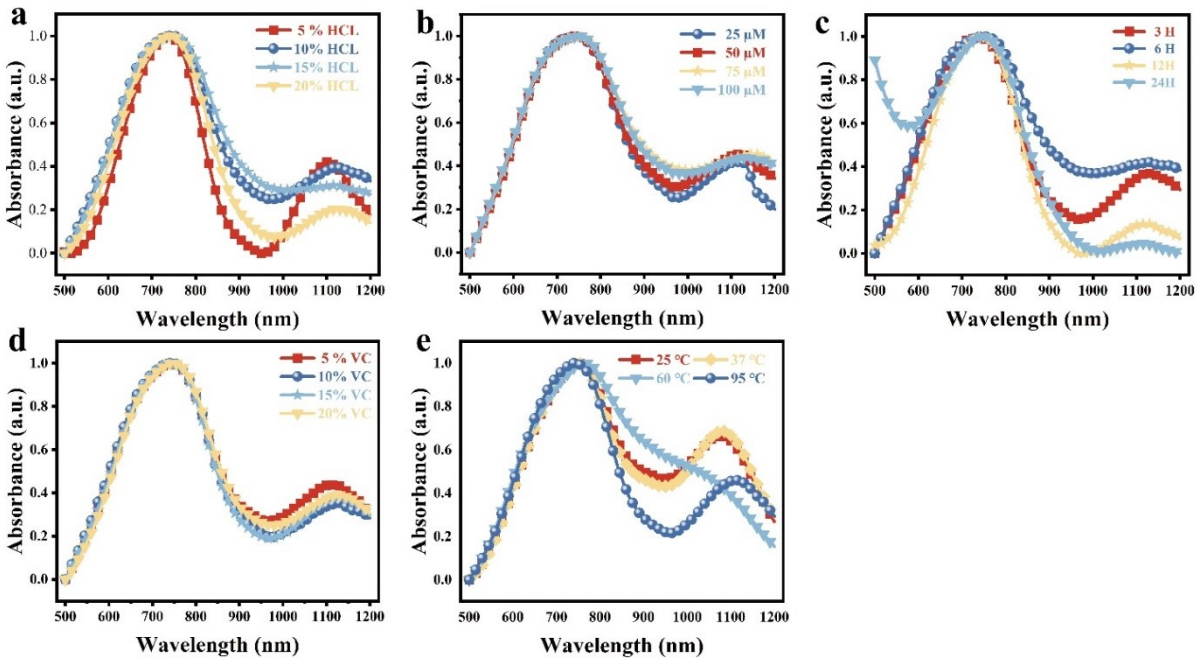

Figure S4 Visible - Near infrared absorption spectra of PMB nanoparticles synthesized under different experimental conditions.

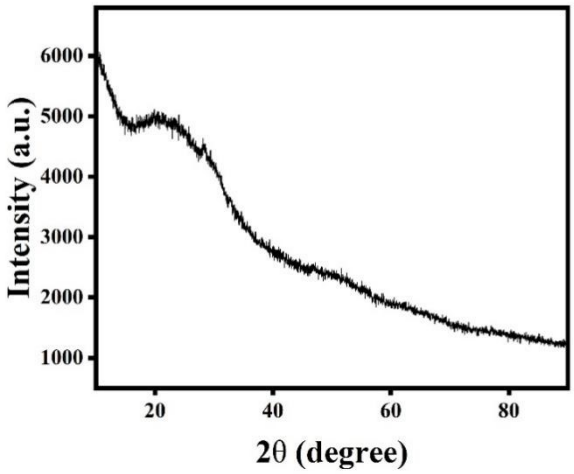

Figure S5 XRD pattern of PMB powder.

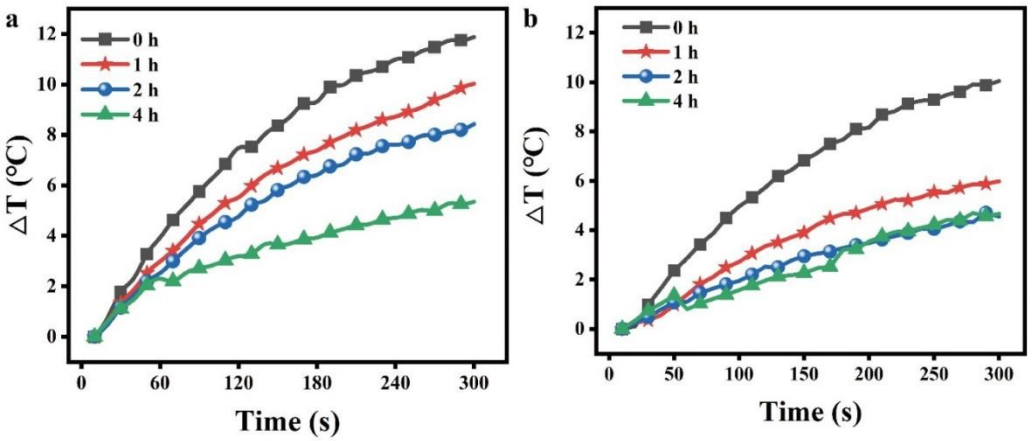

Figure S6 Photothermal temperature rise curves of PMB (140.6 μg/mL, 1.5 W, 808 nm laser) after degradation in (a) pH 6.0 and (b) pH 7.4 Saline irradiation with 808 nm laser for 5 min.

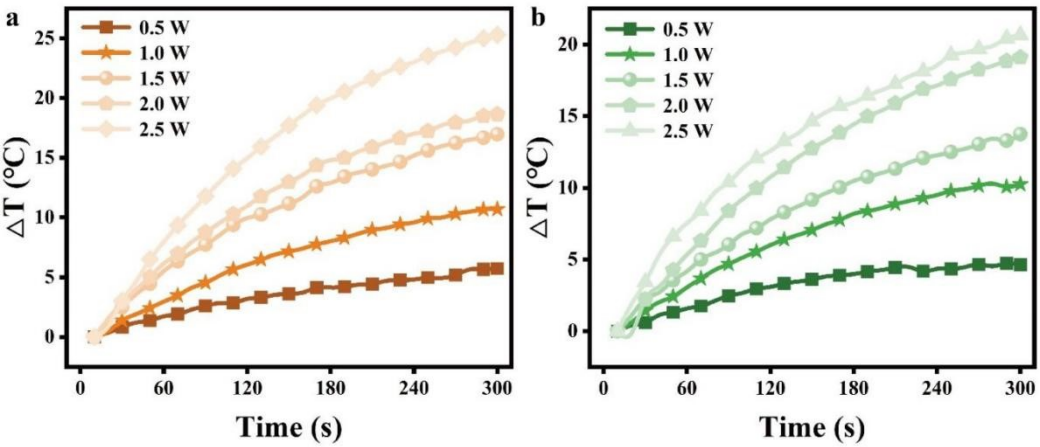

Figure S7 Photothermal temperature rise curves of PMB aqueous suspensions (140.6 μg/mL, 1 mL) under different irradiation power of (a) 808 nm and (b)1064 nm lasers.

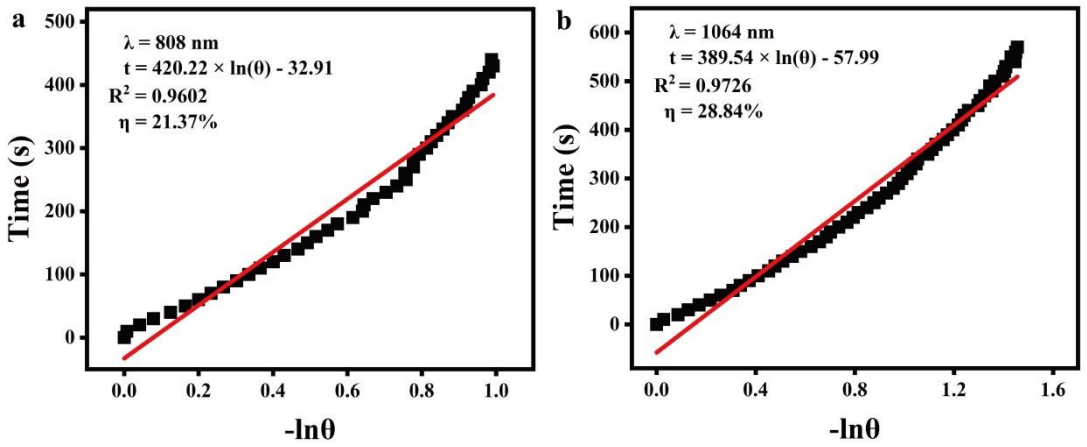

Figure S8 Line time data versus - lnθ from the cooling of PMB to obtain the *τ* and calculated the photothermal conversion efficiency under 808 nm (a) and 1064 nm (b) laser irradiation.

Table 2 The relevant experimental data and calculation results used to calculate the photothermal conversion efficiency under 808 nm and 1064 nm laser irradiation.

	τ	*h*S	$T_{max} - T_{sur}$	Q_{dis}	$-A_{808\,/\,1064\,nm}$	$10^{-A_{808\,/\,1064\,nm}}$	η
H_2O	1043.76	0.0040	0.81	0.0023			
PMB Under 808 nm laser	420.22	0.0099	24.89		-0.636	0.2312	21.38
PMB Under 1064 nm laser	389.55	0.0107	26.96		-0.477	0.3334	28.84

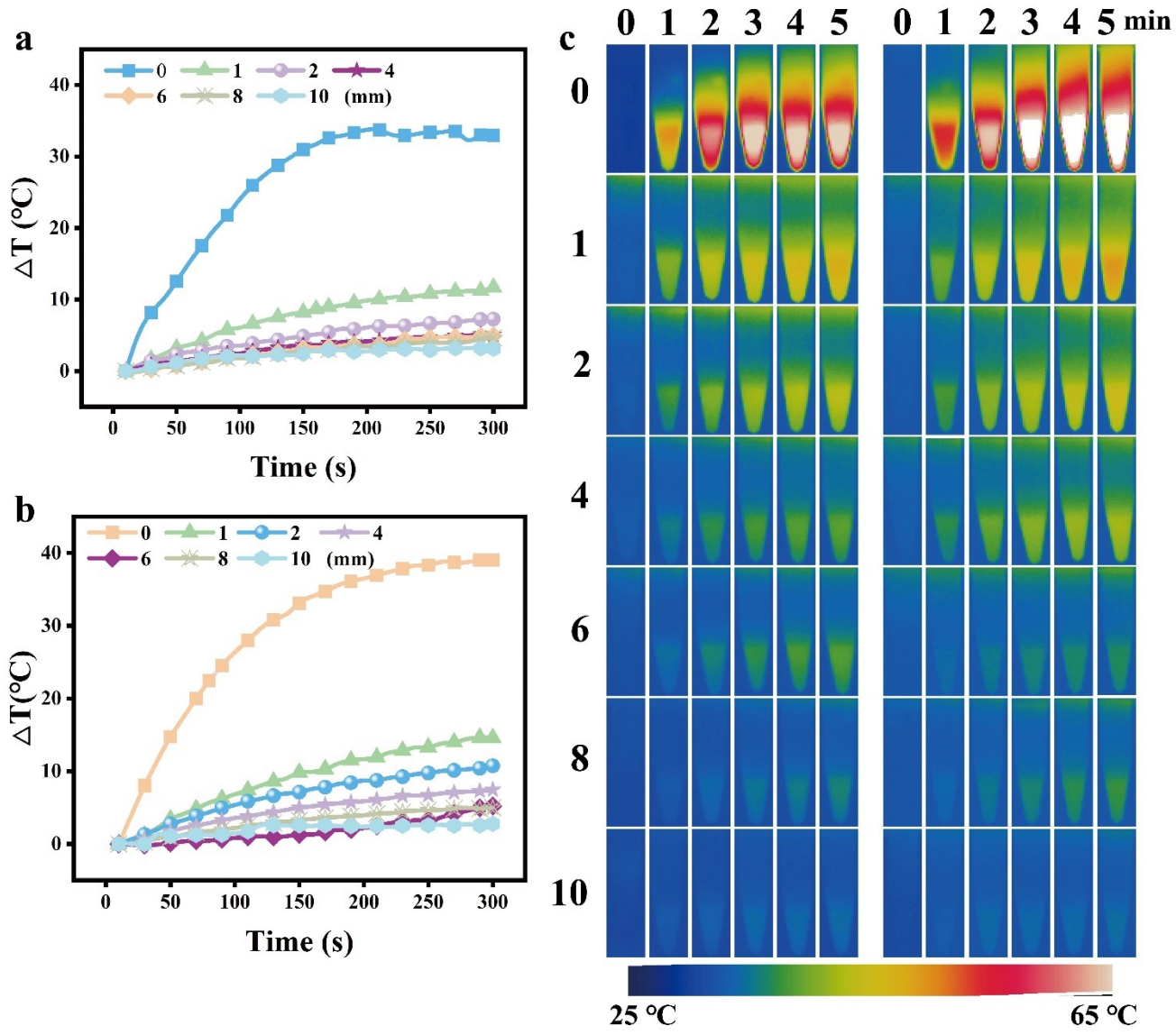

Figure S9 (a) 808 nm and (b) 1064 nm (*P* = 3 W) laser irradiation covering the temperature rise of PMB (140.6 μg/mL) in tumor tissue homogenates of different thickness within 5 min, and (c) corresponding thermograms (left 808 nm laser irradiation, right 1064 nm laser irradiation).

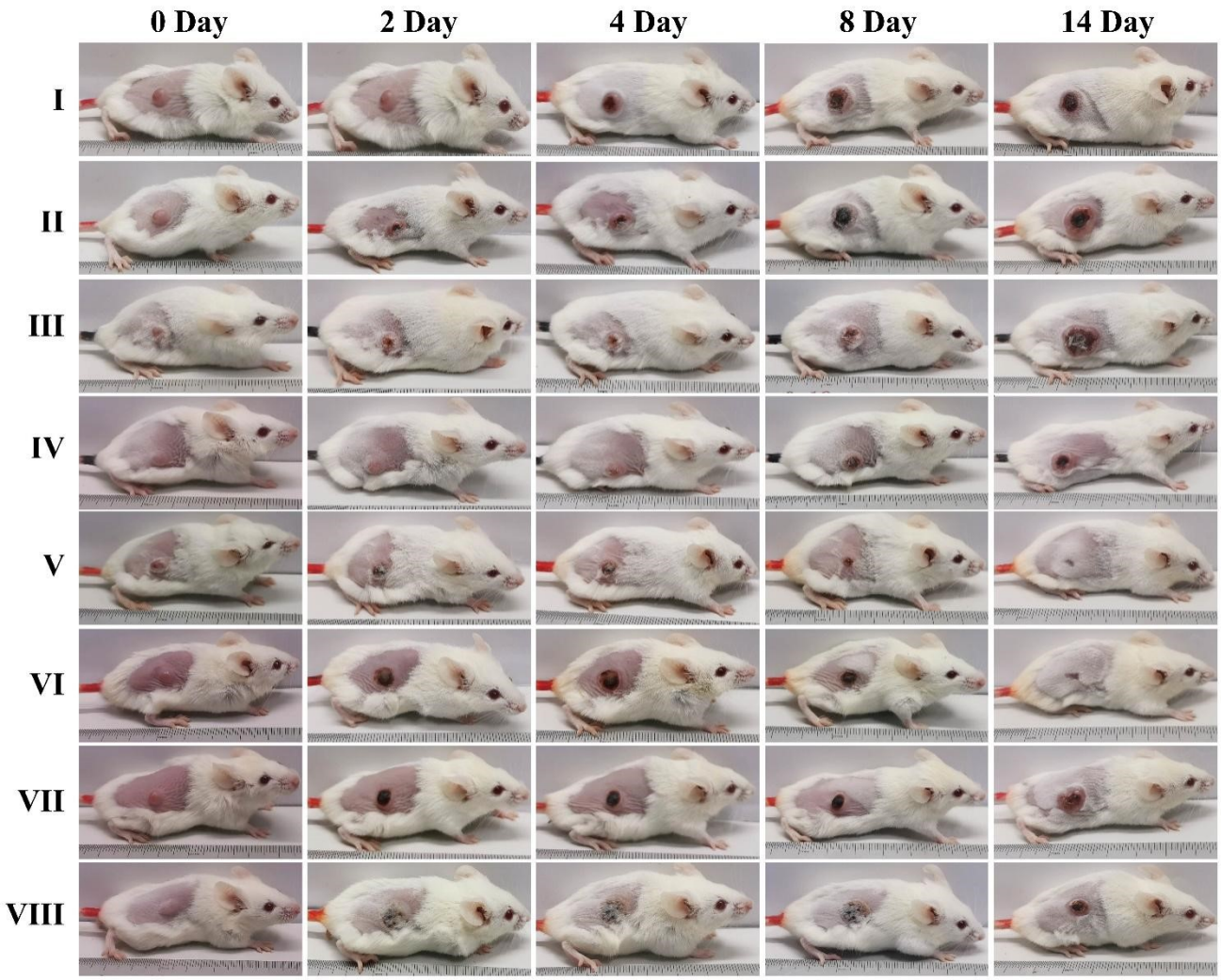

Figure S10 4T1 cells tumor-bearing mice images on the 0, 2, 4, 8, and 14 days after different treatments. (I: Saline; II: Saline + 808 nm; III: Saline + 1064 nm; IV: PMB; V: PMB + 808 nm; VI: PMB + 1064 nm; VII: PMB + 808 nm + cover; VIII: PMB + 1064 nm + cover).

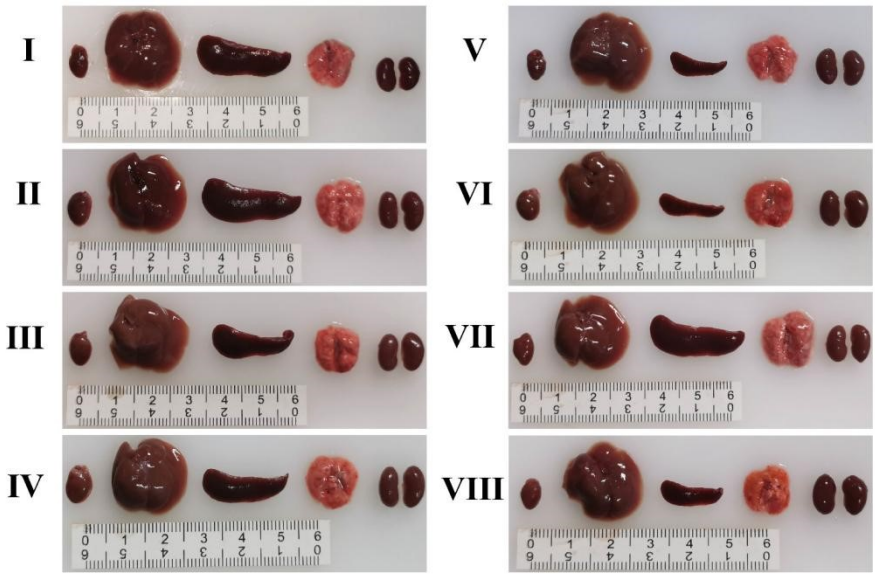

Figure S11 Major organ photographs (heart, liver, spleen, lungs, and kidneys) of tumor-bearing Balb/C mice dissected from different groups after 14 days of different treatments. (I: Saline; II: Saline + 808 nm; III: Saline + 1064 nm; IV: PMB; V: PMB + 808 nm; VI: PMB + 1064 nm; VII: PMB + 808 nm + cover; VIII: PMB + 1064 nm + cover).

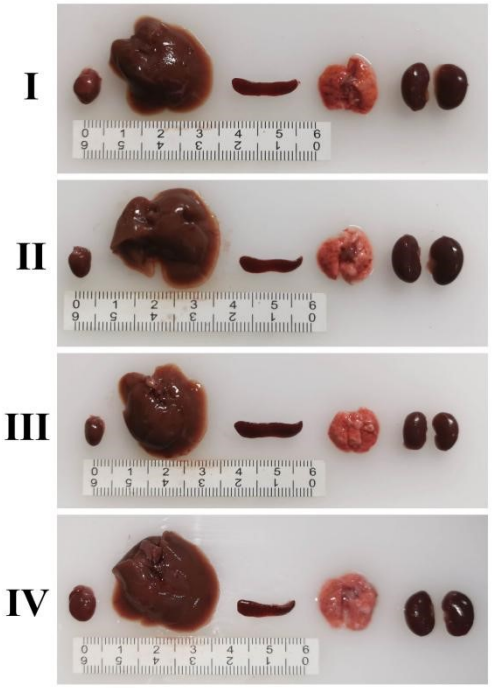

Figure S12 Major organs photographs (heart, liver, spleen, lung, and kidney) of healthy ICR mice after different concentrations of PMB were injected through the tail vein for acute toxicity assay (I: Saline; II: 10 mg/kg PMB; III: 25 mg/kg PMB; IV: 50 mg/kg PMB).