Supporting Information

Boosting the Photothermal Performance of Vacancy $MoSe_{2-x}$ Nanoflowers for Photoacoustic Imaging Guided Tumor Chemo-photothermal Therapy

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S1. Photothermal conversion efficiencies

The photothermal conversion efficiencies were calculated as follows. The total energy balance was described as:

$$\sum_i m_i C_{p,\ i} \frac{dT}{dt} = Q_{in,\ np} + Q_{in,\ surr} - Q_{out} \quad 1$$

where m and C_p are the mass and heat capacity of the solvent (water), T is the temperature of the solution respectively. $Q_{in,\ np}$ is the photothermal energy inputted by the $MoSe_2$ nanoflowers (MNFs), which can be determined by:

$$Q_{in,\ np} = I\left(1 - 10^{\left(-A_\lambda\right)}\right)\eta \quad 2$$

Where I is the laser power used in the experiment, and the A_λ is the absorbance of the nanoparticles at the used wavelength (808 nm). The η is the photothermal conversion efficiency.

In addition, $Q_{in,\ surr}$ expressed the heat imput absorbed by the solvent and the container (cuvette), which is descirbed as follows:

$$Q_{in,\ surr} = Q_{Dis} = hS_{buff} \times \left(T_{max} - T_{surr}\right)_{buff} \quad 3$$

where h is heat transfer coefficient and S_{buff} is the surface area of the contained. T_{max} is the maximum steady temperature of the solvent, and T_{Surr} is the ambient surrounding temperature. The Q_{Dis} was measured independently to be 0.1452 mW.

Besides, Q_{out} is the heat loss to the surrounding:

$$Q_{out} = hS\left(T - T_{surr}\right) \quad 4$$

In the equation, hS can be calculated by determining the rate of temperature decrease when removing the laser. Without the light source, combining eq. (4) with eq. (1) can deduce:

$$\sum_i m_i C_{p,\ i} \frac{dT}{dt} = -Q_{out} = -hS(T - T_{surr}) \quad (5)$$

With carefully rearrangement and deducement, *t* is expressed as the following equation:

$$t = -\left(\frac{m_{buff} C_{p,buff}}{hS}\right) \ln\left(\frac{T - T_{surr}}{T_{max} - T_{surr}}\right) \quad (6)$$

Where two rate constants are defined as τ_s

$$\tau_S = \frac{m_{buff} C_{p,buff}}{hS} \quad (7) \quad \text{and} \quad \theta = \left(\frac{T - T_{surr}}{T_{max} - T_{surr}}\right) \quad (8)$$

Combining eq. (6), eq. (7) and eq. (8) yields:

$$t = -\tau_S \ln(\theta) \quad (9)$$

In order to get the *hS*, we measured the cooling curve and τ_s can be determined.

At the maximum steady temperature, eq. (10) is 0 and the following is obtained

$$Q_{in,\ np} + Q_{in,\ surr} = I\left(1 - 10^{(-A_\lambda)}\right)\eta + Q_{Dis} = hS(T_{max} - T_{surr}) \quad (10)$$

Therefore, the final photothermal coversion efficiency can be determined as

$$\eta = \frac{hS(T_{max} - T_{surr}) - Q_{Dis}}{I\left(1 - 10^{(-A_\lambda)}\right)\eta} \quad (11)$$

I is the laser power used during the experiment and A_{808} is the absorbance of the nanoparticles at the wavelength of 808 nm. The absorbance of MNFs at 808 nm is 1.215. In addition, the *m* is 0.5 g and the *C* is 4.2 J/g. The 808 nm laser photothermal conversion efficiency (η) of MNFs can be calculated to be 41.7 %.

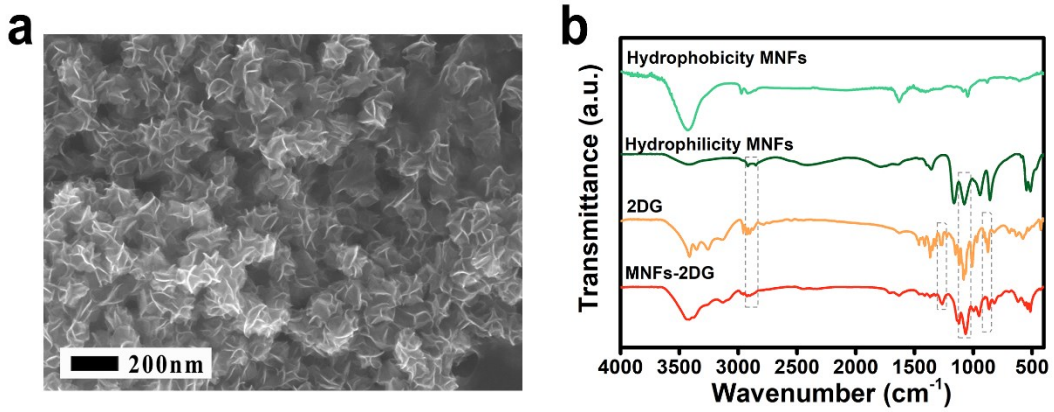

Figure S1. (a) SEM images of hydrophilic MNFs and (b) FT-IR spectra of hydrophobicity MNFs, hydrophilicity MNFs, 2DG and MNFs-2DG.

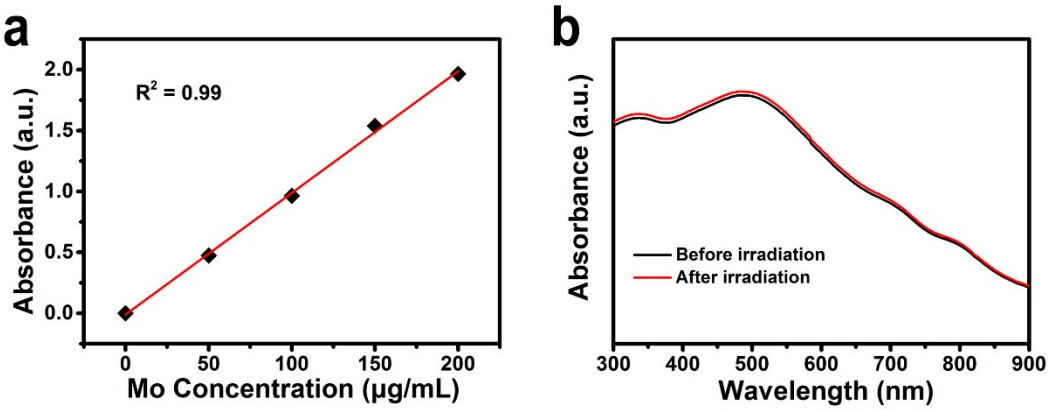

Figure S2. (a) The concentration-dependent absorbance of MNFs at 808 nm. (b) The UV-vis-NIR absorption spectra of MNFs before and after NIR irradiation five laser on/off cycles.

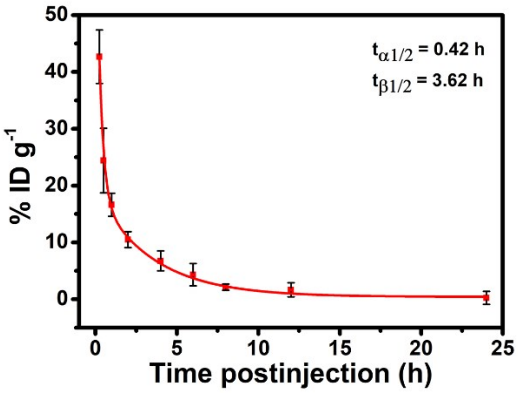

Figure S3. (a) Blood circulation curve of MNFs in mice by measuring the Mo concentration in the blood at different time points after intravenous injection.

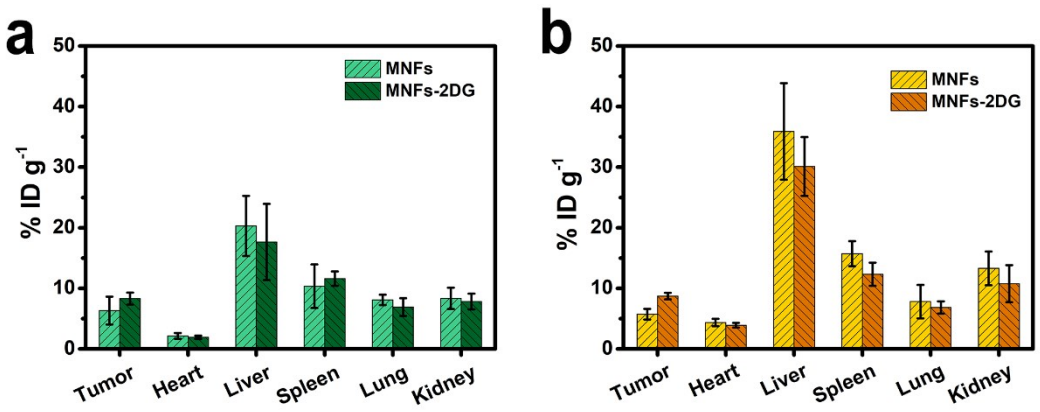

Figure S4. (a) Biodistribution in mice of MNFs and MNFs-2DG at 1 h and (b) at 24 h after intravenous injection.

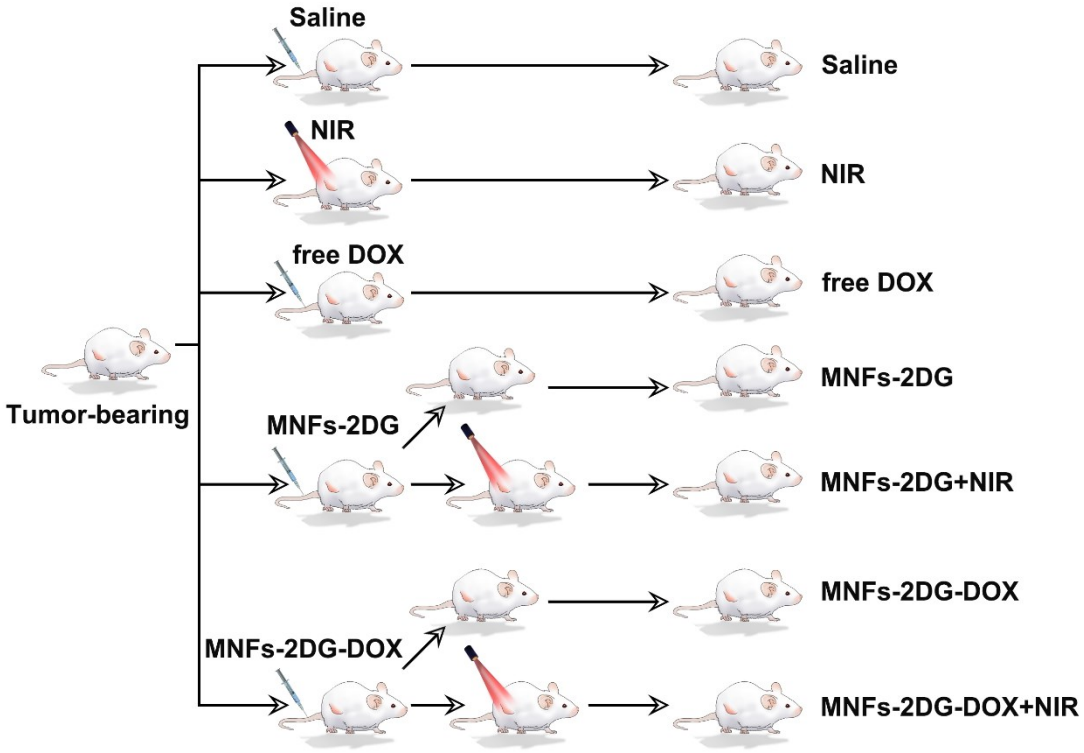

Figure S5. Experimental design of the antitumor study in mice bearing subcutaneous 4T1 tumors (n = 5).

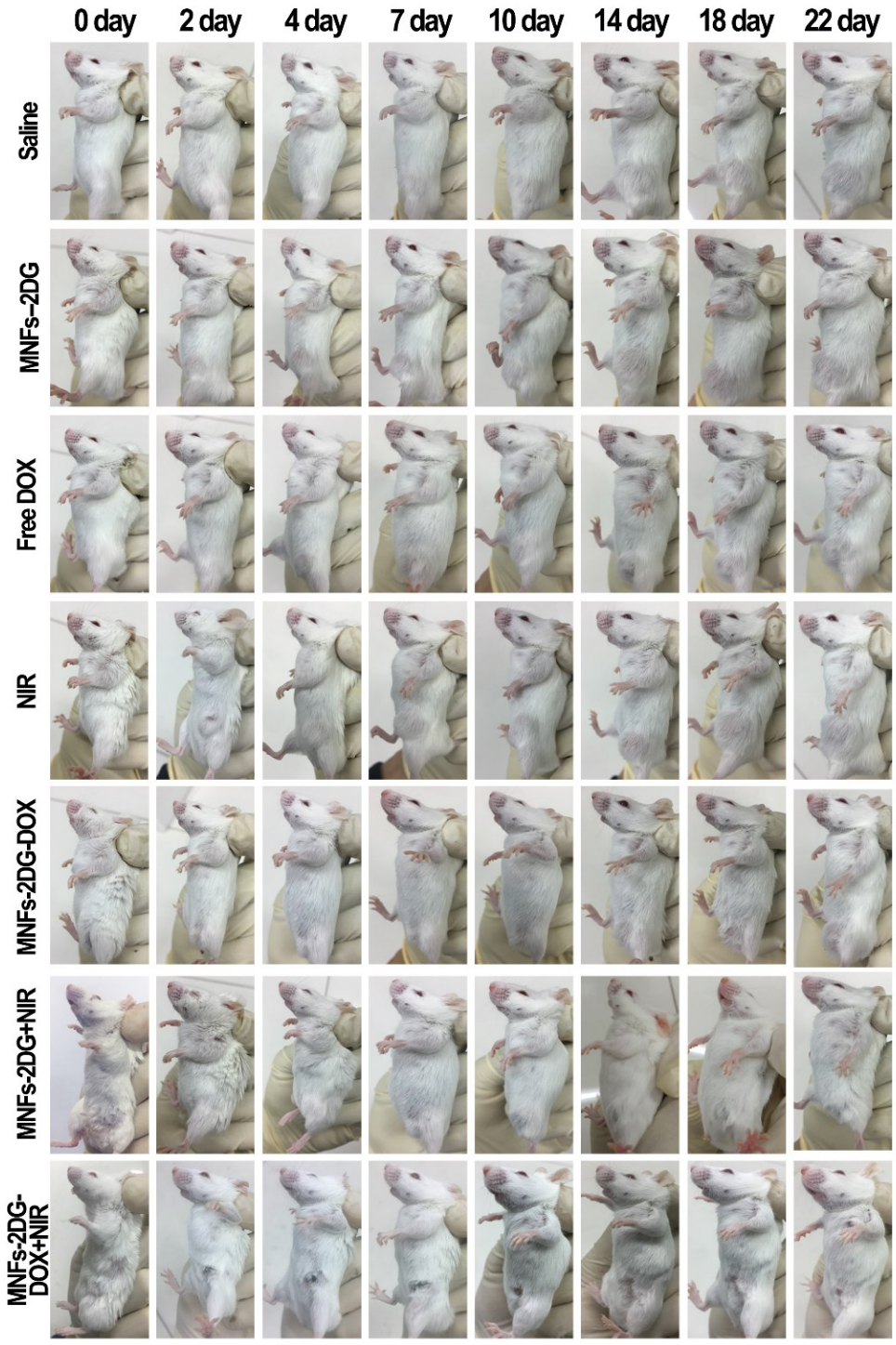

Figure S6. The photographs of representative mice for each group acquired at 0, 2, 4, 7, 10, 14, 18, and 22 days.

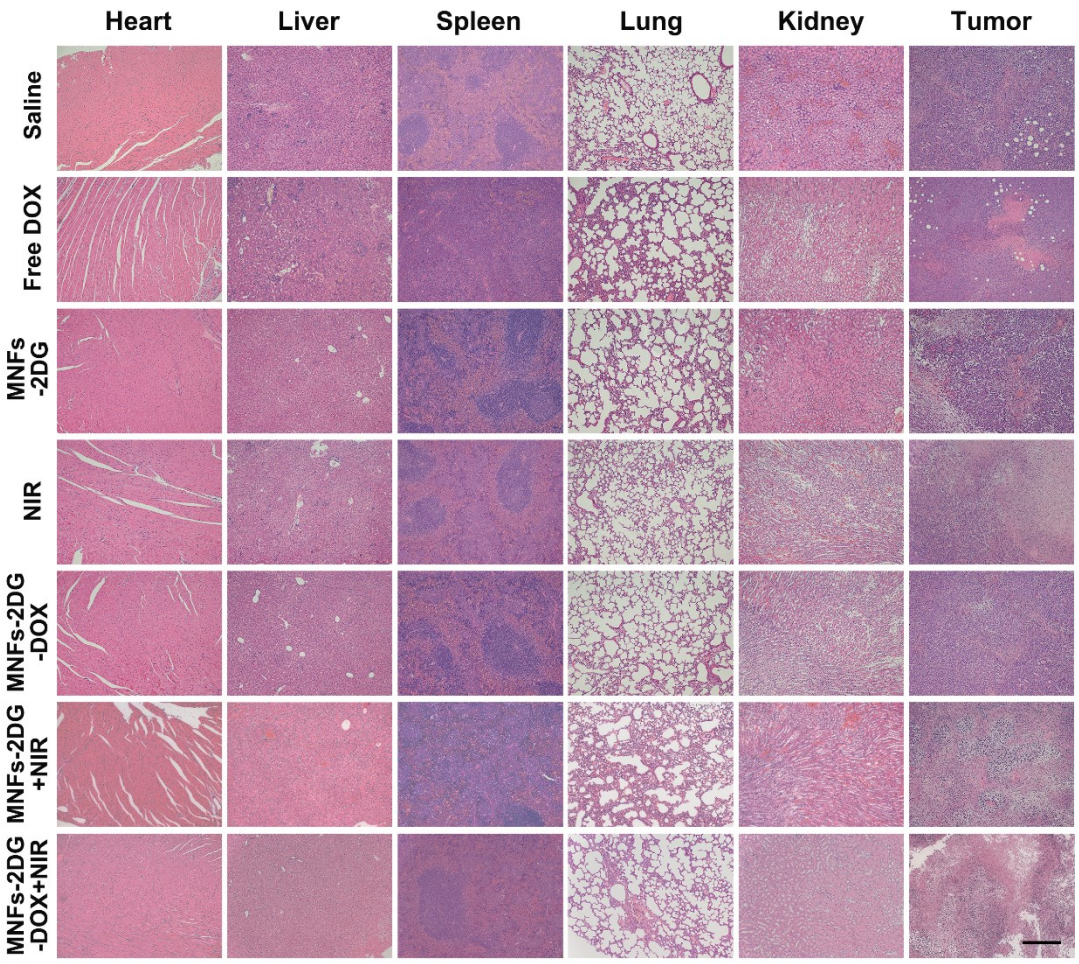

Figure S7. The H&E staining of tumor, heart, liver, spleen, lung, and kidney of mice from the different groups. Scale bar = 200 μm.