Supporting Information

for

MoO_{3-x} Quantum Dot for Photoacoustic imaging Guided Photothermal/Photodynamic Cancer Treatment

Dandan Ding,[a, b#] Wei Guo[a, c#], Chongshen Guo,[a]*Jianzhe Sun,[a,b] Nannan Zheng,[a, c] Fei Wang,[a,c], Mei Yan,[a] Shaoqin Liu[a, c]*

[a] Key Lab of Microsystem and Microstructure (Ministry of Education), Harbin Institute of Technology, Harbin 150080, China.

[b] School of Chemistry and Chemical Engineering, Harbin Institute of Technology, Harbin 150080, China.

[c] School of Life and Technology, Harbin Institute of Technology, Harbin 150080, China.

[#] These two authors contributed equally to this work.

* **Corresponding authors**:

Dr. **Chongshen Guo**, Key Lab of Microsystem and Microstructure (Ministry of Education), Harbin Institute of Technology, Harbin 150080, China

E-mail: chongshenguo@hit.edu.cn; Fax: +86 451 86403493

Prof. **Shaoqin Liu**, Key Lab of Microsystem and Microstructure (Ministry of Education), Harbin Institute of Technology, Harbin 150080, China

E-mail: shaoqinliu@hit.edu.cn; Fax: +86 451 86403493

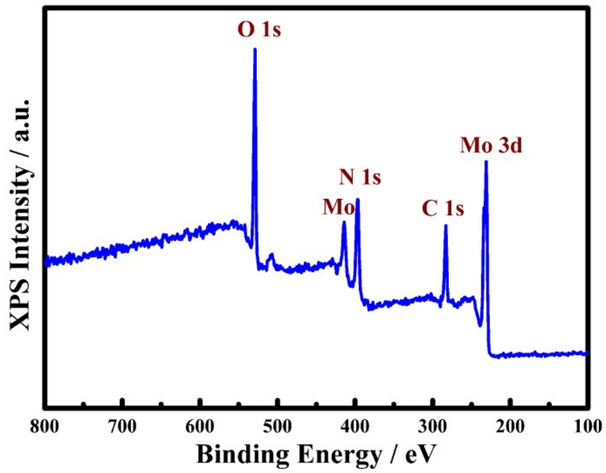

Figure S1 Full range XPS spectra of MoO_{3-x} quantum dot

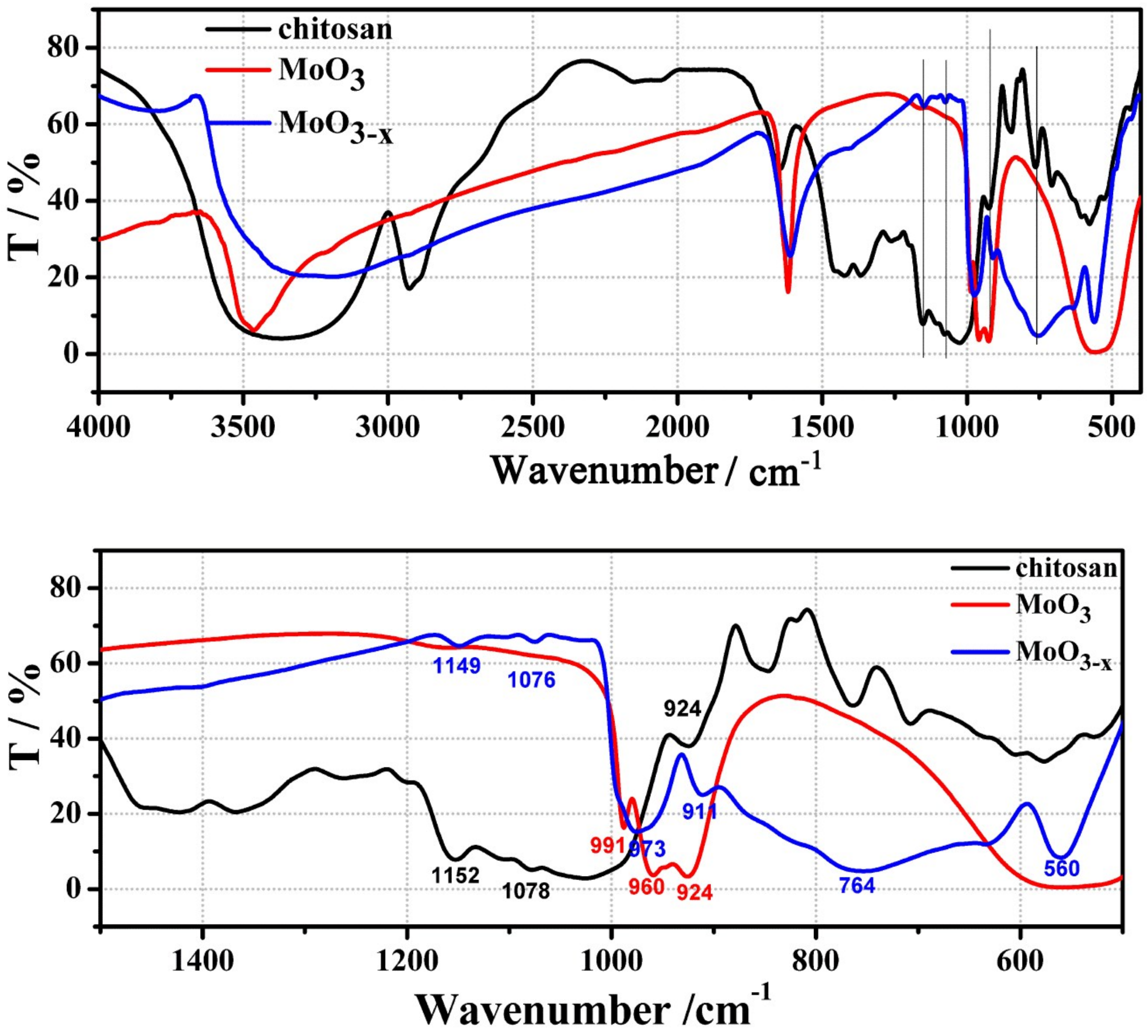

Figure S2 FT-IR spectra of MoO_{3-x} quantum dot. Chitosan and MoO_3 were used as control.

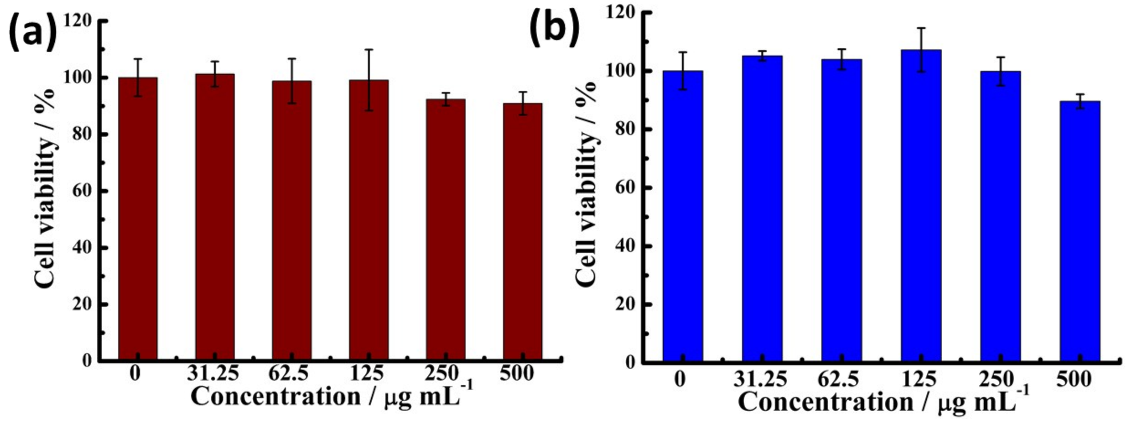

Figure S3 Cytotoxicity assay. The cells were coincubated with MoO_{3-x} nanocubes for 24 h, and then examined for cellular viability by MTT assay. (a) HeLa, (b) L02.

Calculation of the photothermal conversion efficiency

The photothermal conversion efficiency, η, can be determined by following eqution:

η**= [hS (T_{max}- T_{surr}) - Q_{dis}]/ I(1-$10^{-A_{880}}$)   Equ.S1**

where **h** is heat transfer coefficient;

S is the surface area of the container;

T_{max} is the equilibrium temperature;

T_{surr} is ambient temperature of the surroundings;

Q_{dis} is heat dissipated from light absorbed by the quartz sample cell itself (it was measured independently to be 11.34 mW using a quartz cell containing pure water)

I is incident laser power (2 W/cm^2)

A_{880} is the optical absorbance of nanocubes at 880 nm (0.47)

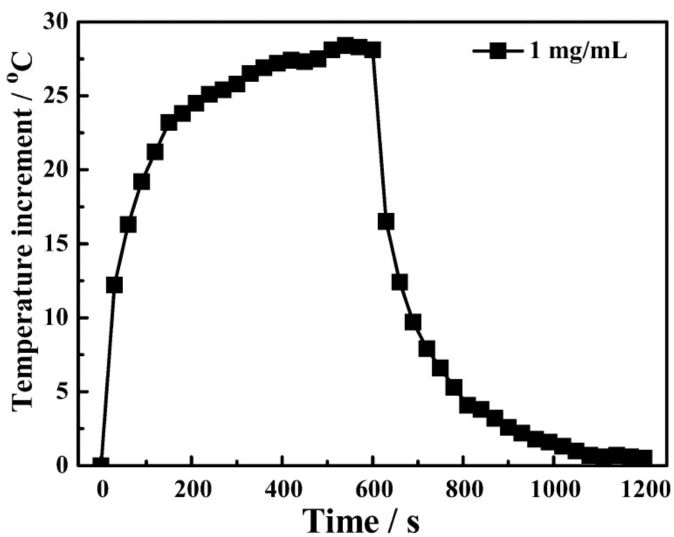

Figure S4. Temperature variations of solution containing 1 mg/ml nanocube. The NIR laser irradiation lasted 10 min and then was turned off.

It easily found that only the hS remains unknown for calculating η. To obtain the value of hS, a dimensionless driving force temperature, θ is introduced using the maximum system temperature.

$\Theta = (T-T_{surr})/(T_{max}-T_{surr})$ **Equ.S2**

At the cooling stage of the aqueous dispersion, the cooling time t and θ abide by the following equationS3;

$t=\tau_s \ln(\Theta)$ **Equ.S3**

Therefore, time constant for heat transfer from the system could be determined by plotting linear time data from the cooling period against negative natural logarithm of driving force temperature.

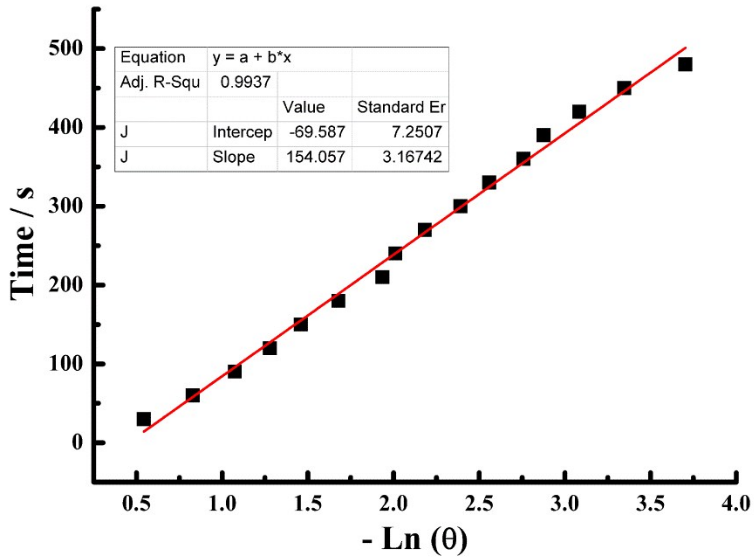

Figure S5. Linear relation between the t and lnθ.

The $\boldsymbol{\tau_s}$ is calculated to be 154 s.

$hS = \Sigma m_i C_{p,\,1} / \boldsymbol{\tau}_s$ **Equ.S4**

Where m, Cp, τ_s are the mass, heat capacity of water and time constant, respectively.

The m is 0.45 g and C is 4.2 J/g. The hS is determined to 12.27 mW/ ^{o}C according to Equ.S4. Substituting hS =12.27 mW/ ^{o}C into Equ.S1 produces η=25.5%.

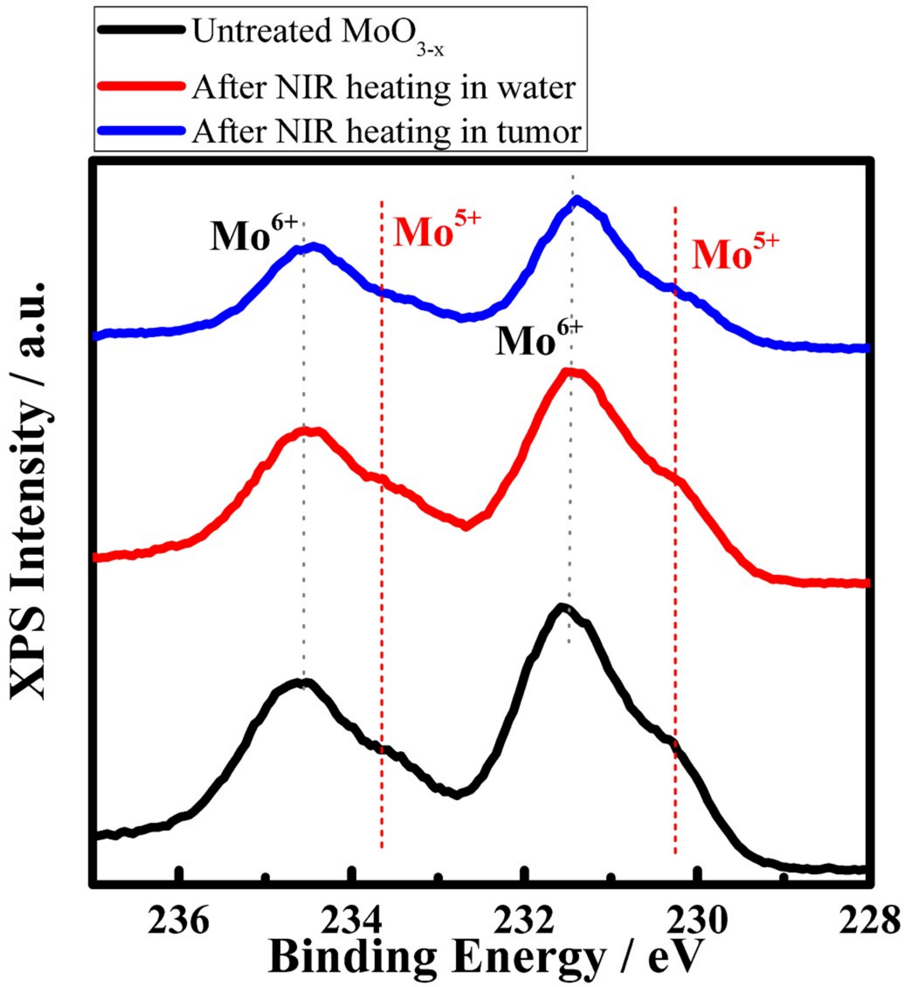

Figure S6 The XPS spectra of MoO_{3-x} QDs before and after heating treatment.

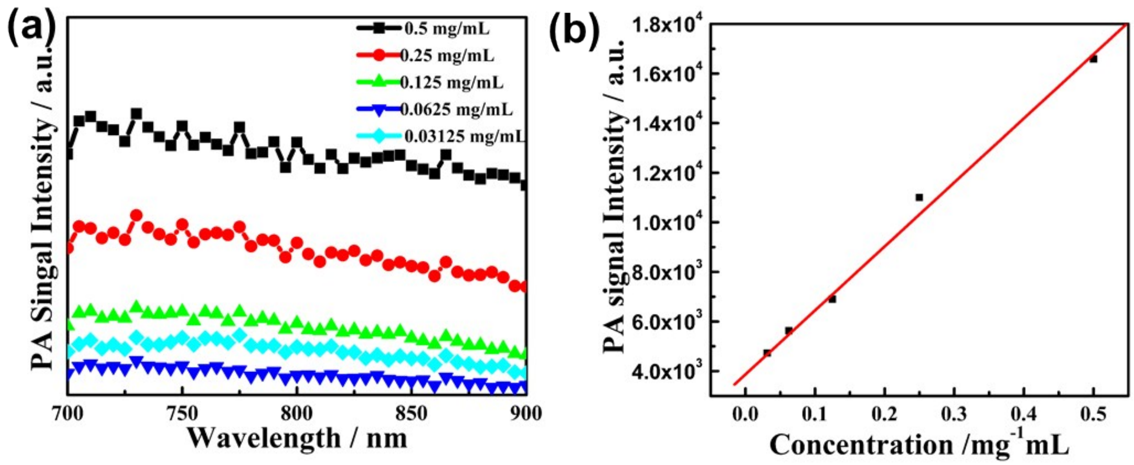

Figure S7 (a) Photoacoustic signal of MoO_{3-x} solutions with different concentrations. (b) Plot of photoacoustic signal at 880 nm versus MoO_{3-x} concentrations.

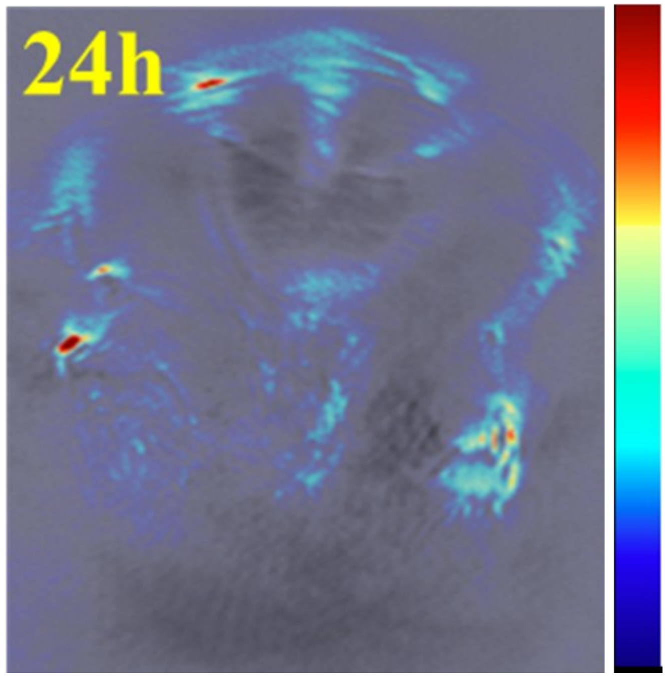

Figure S8 In vivo PA image via tail intravenous injection after 24h.

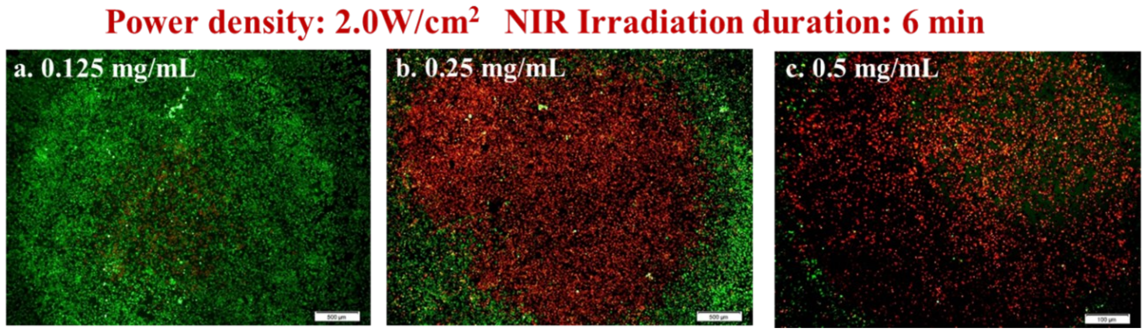

Figure S9 Fluorescence images and dead circle area of HeLa cells received different concentration of MoO_{3-x}.

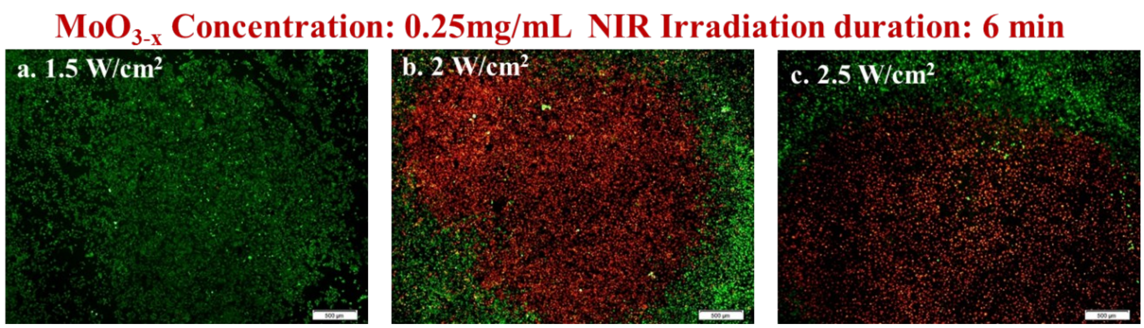

Figure S10 Fluorescence images and dead circle area of HeLa cells under different power density of NIR laser.