Electronic Supplementary Material (ESI) for Nanoscale.

Supporting Information

Translocation, Biotransformation-Related Degradation, and Toxicity Assessment of Polyvinylpyrrolidone Modified 2H Nano-MoS_2

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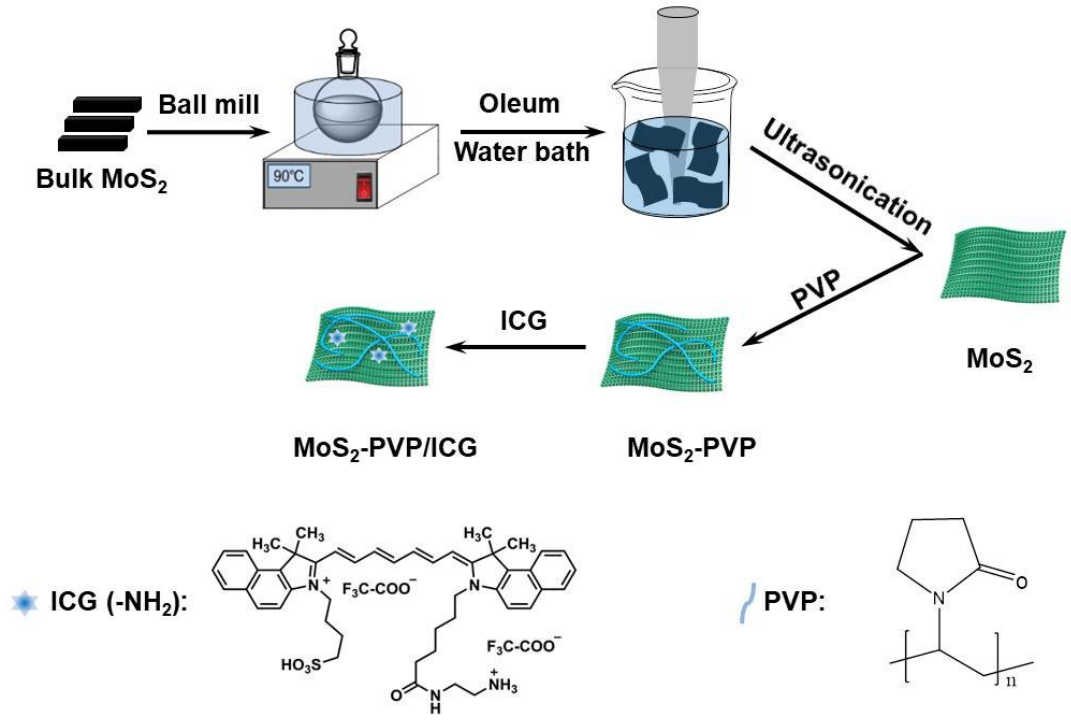
SUPPORTING FIGURES



Scheme S1. (A) Schematic illustration of synthesis of MoS_2-PVP/ICG NSs.

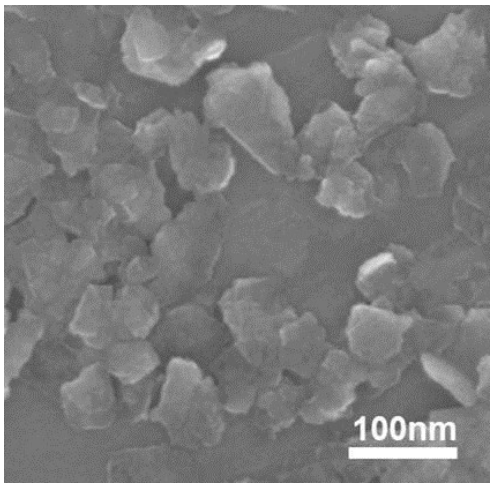


Figure S1. FE-SEM image of MoS_2-PVP NSs.

Figure S2. Stability tests of MoS_2-PVP NSs in water, DMEM, FBS, RPMI, and PBS solutions for 48 h (concentration: 80 μg mL^{-1}).

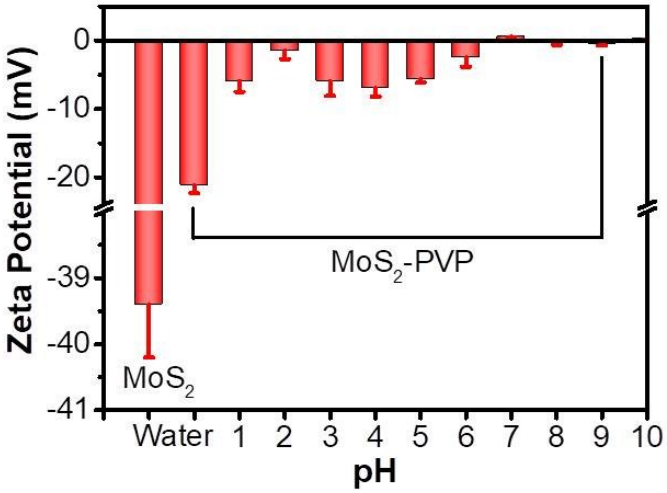


Figure S3. Zeta potential of nube MoS_2 NSs in water and MoS_2-PVP NSs in water and in PBS buffer with different pH values.

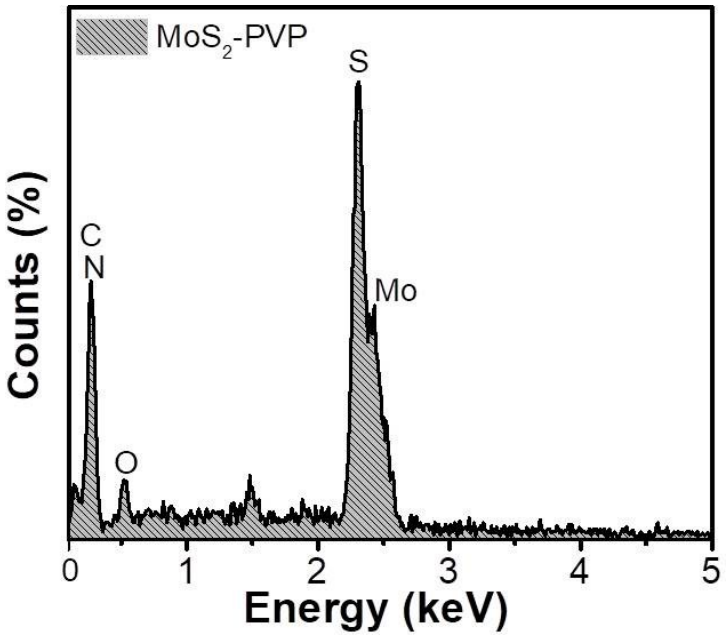


Figure S4. EDS spectrum of MoS_2-PVP NSs.

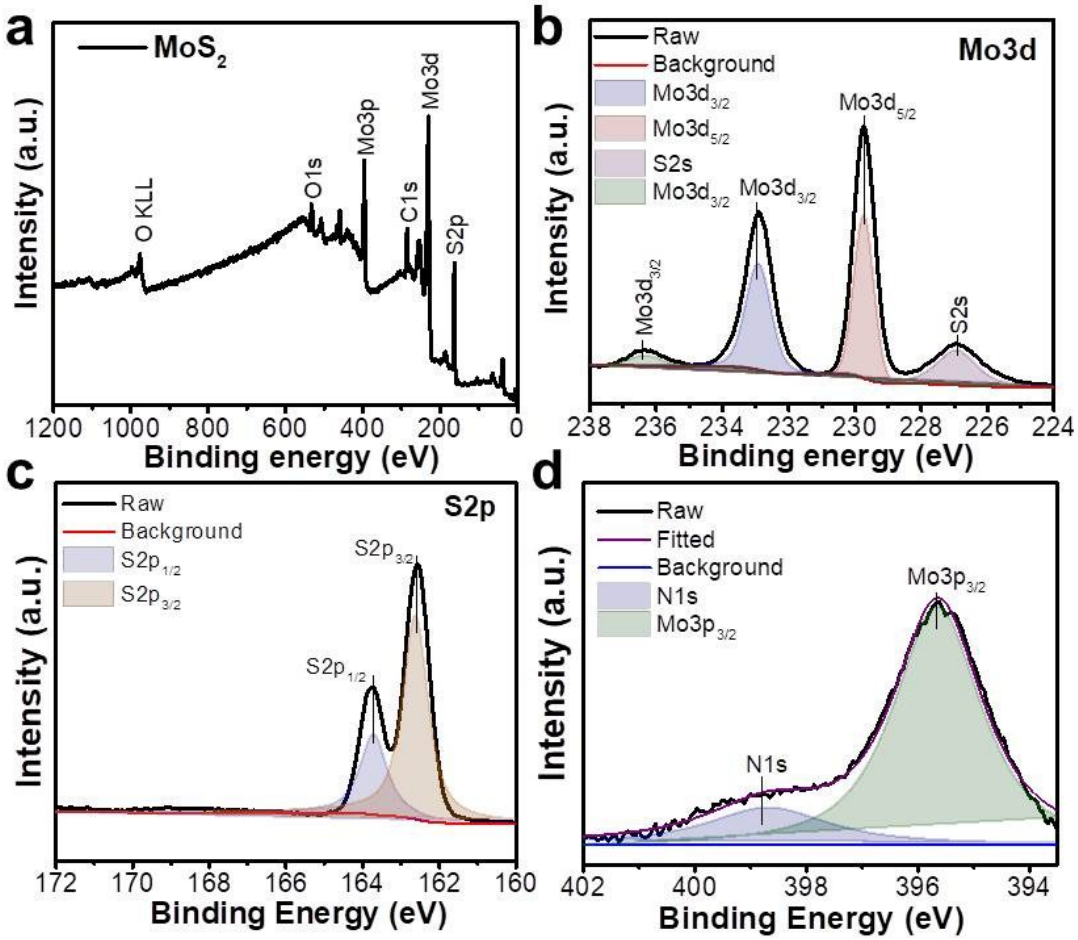


Figure S5. XPS survey spectrum (a) and high-resolution peak-fitting spectra of (b) Mo3d, (c) S2p and (d) Mo3p of nude MoS_2 NSs without any modification.

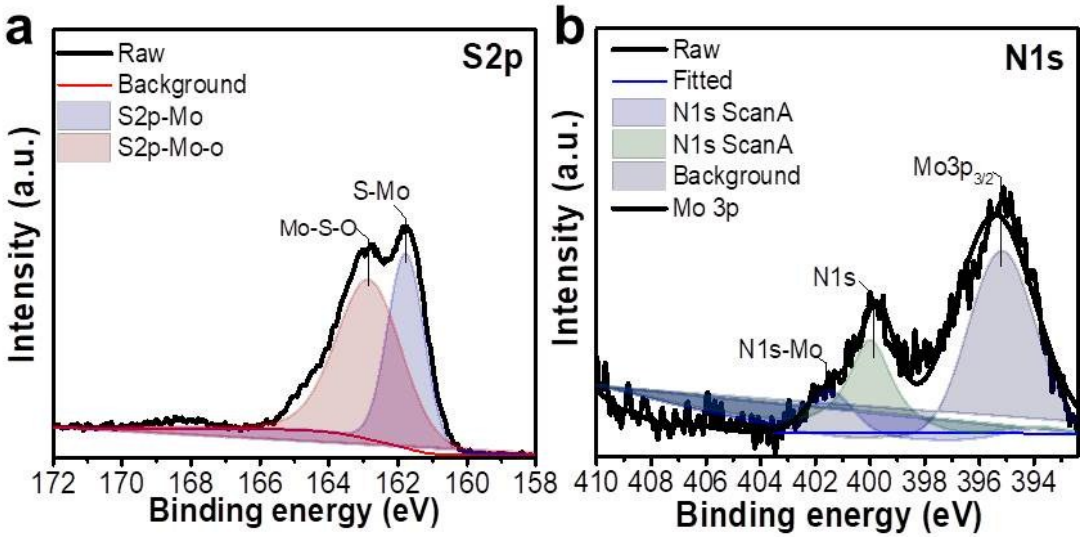


Figure S6. High-resolution XPS peak-fitting spectra of (a) S2p, and (b) N1s of MoS_2-PVP NSs.

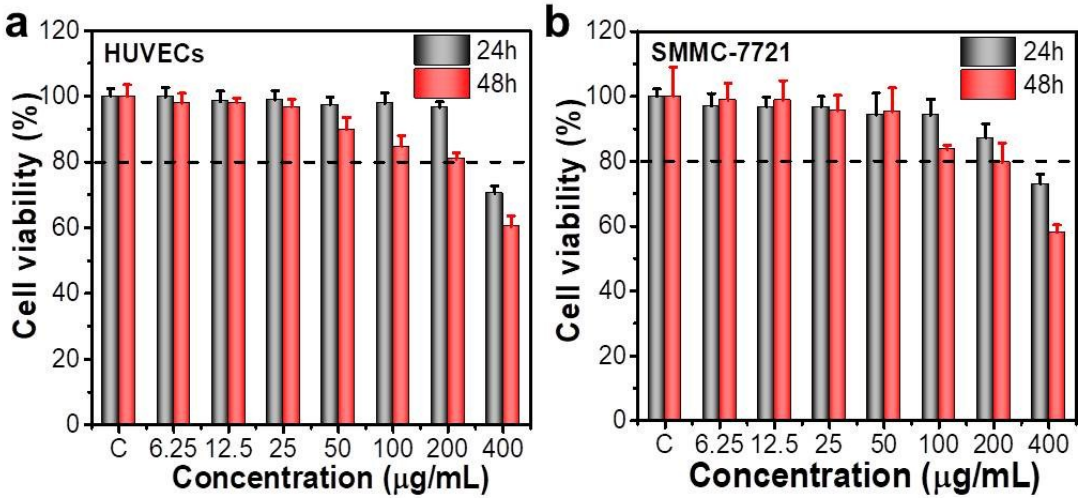


Figure S7. Cell viabilities of (a) HUVECs and (b) SMMC-7721 cells incubated with various concentrations of MoS_2-PVP NSs for 24 h and 48 h.

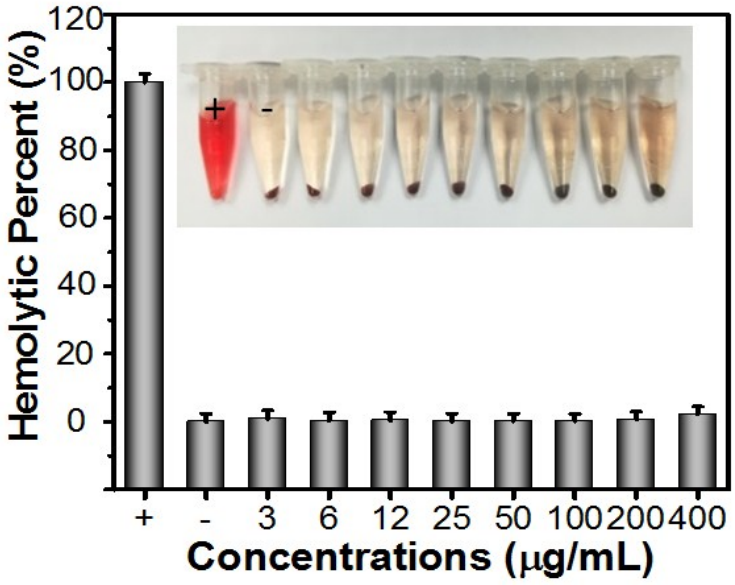


Figure S8. Hemolysis analysis of RBCs incubated with MoS_2-PVP NSs at different concentrations for 4 h using PBS and water as negative (−) and positive (+) controls, respectively. Inset: Corresponding photograph of hemolysis analysis.

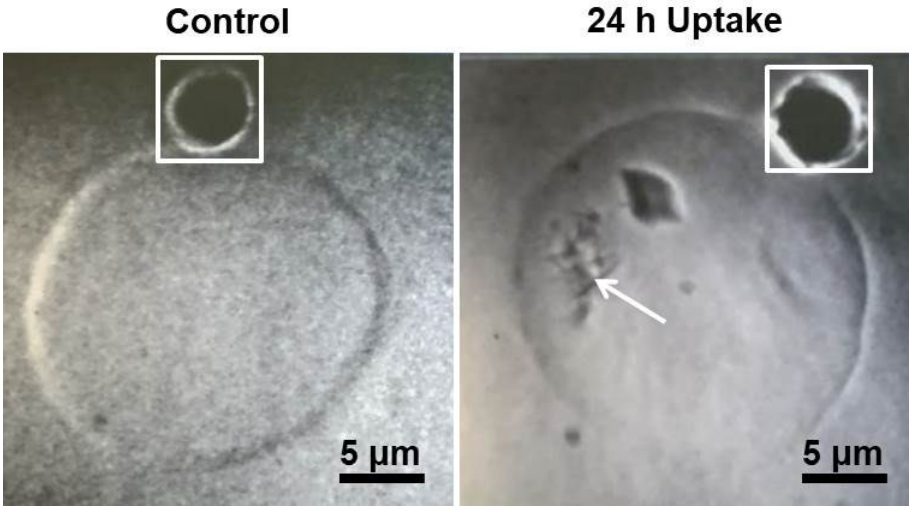


Figure S9. The raw data for phase contrast SR-TXM images. Raw SR-TXM phase contrast image showed MoS_2-PVP NSs in a single cell at 24 h uptake The bright edges indicate the cell membrane, the white arrowhead are MoS_2-PVP NSs and the larger black particles in the square white frames are gold particles. The image showed that most of MoS_2-PVP NSs remained inside of the cell.

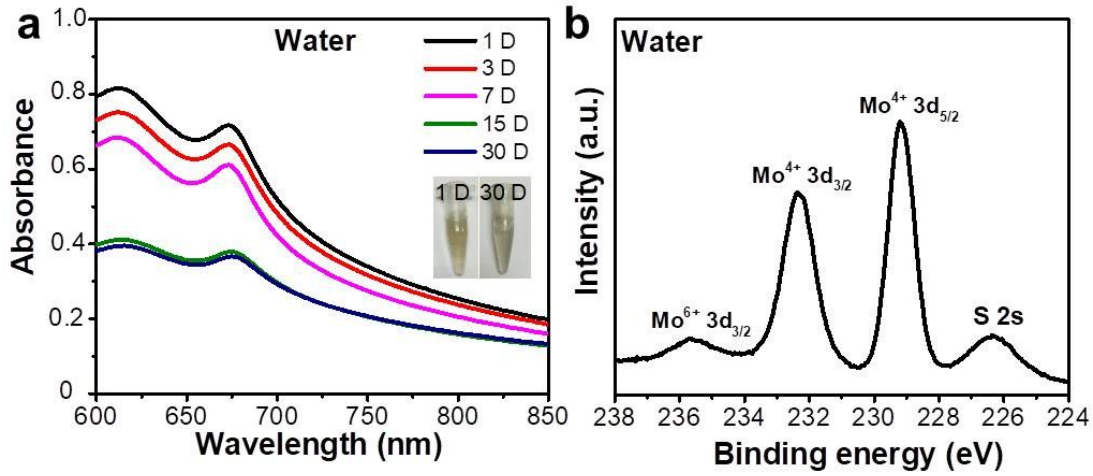


Figure S10. (a) UV–vis-NIR absorption spectra (Inset: color change in 1D and 30 D) and (b) high-resolution Mo3d XPS of MoS_2-PVP NSs treated in water for 30 days. (final concentration: 100 μg mL^{-1}).

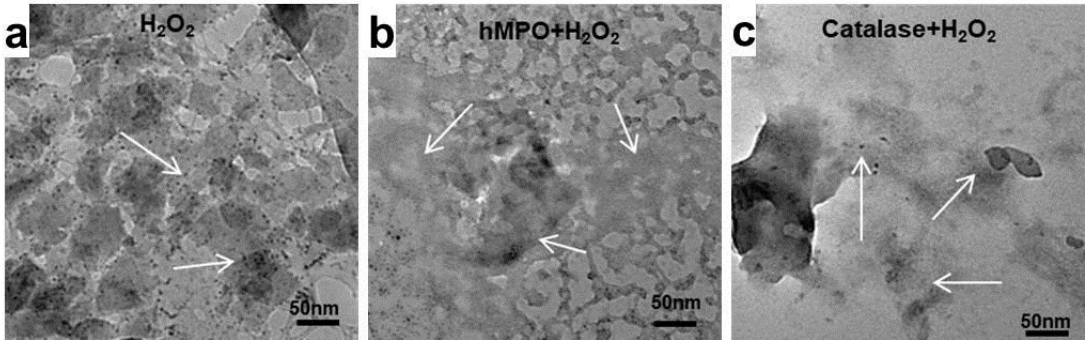


Figure S11. TEM images of MoS_2-PVP NSs after treated with (a) H_2O_2, (b) hMPO+H_2O_2, and (c) catalase+H_2O_2 for 30 days. The white arrows showing the biodegraded nanodots.

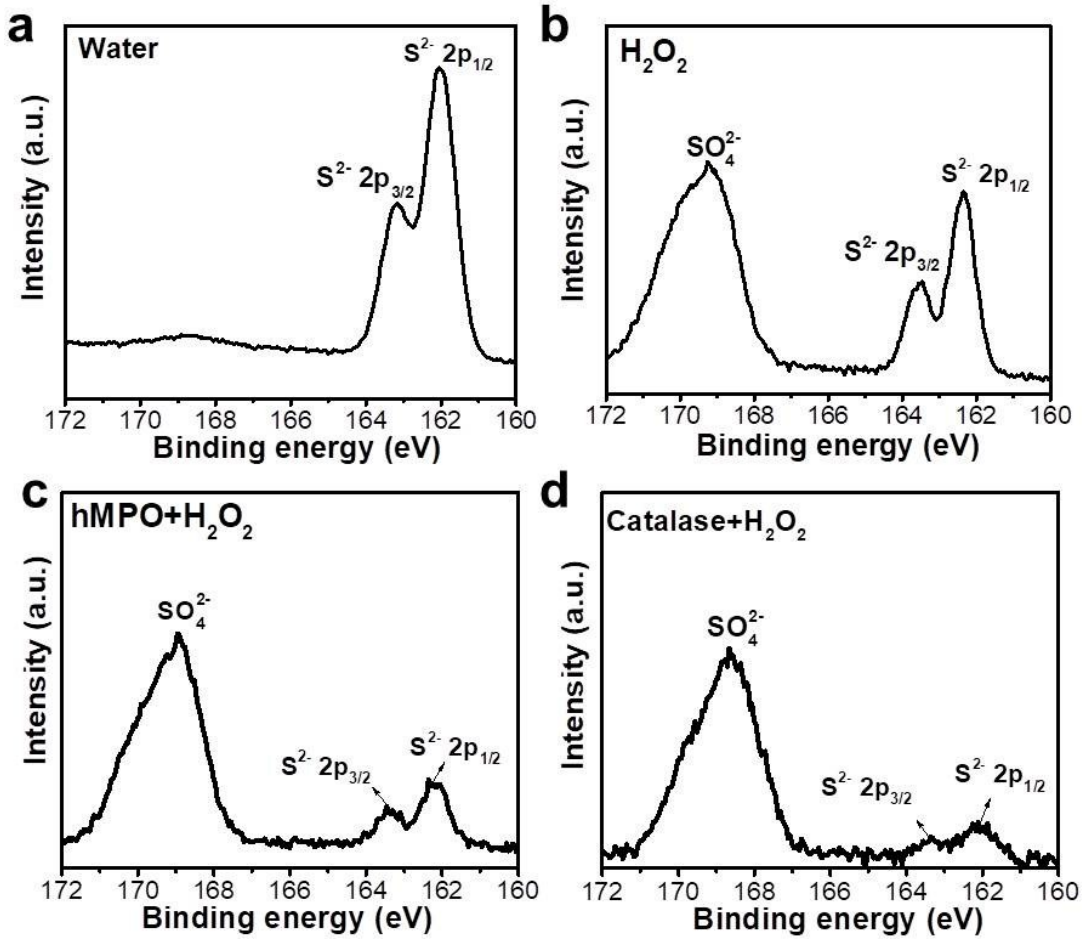


Figure S12. High-resolution XPS spectra analyses of S2p binding energy in MoS_2-PVP NSs treated with (a) water, (b) H_2O_2, (c) hMPO+H_2O_2, and (d) Catalase+H_2O_2 after 30 days.

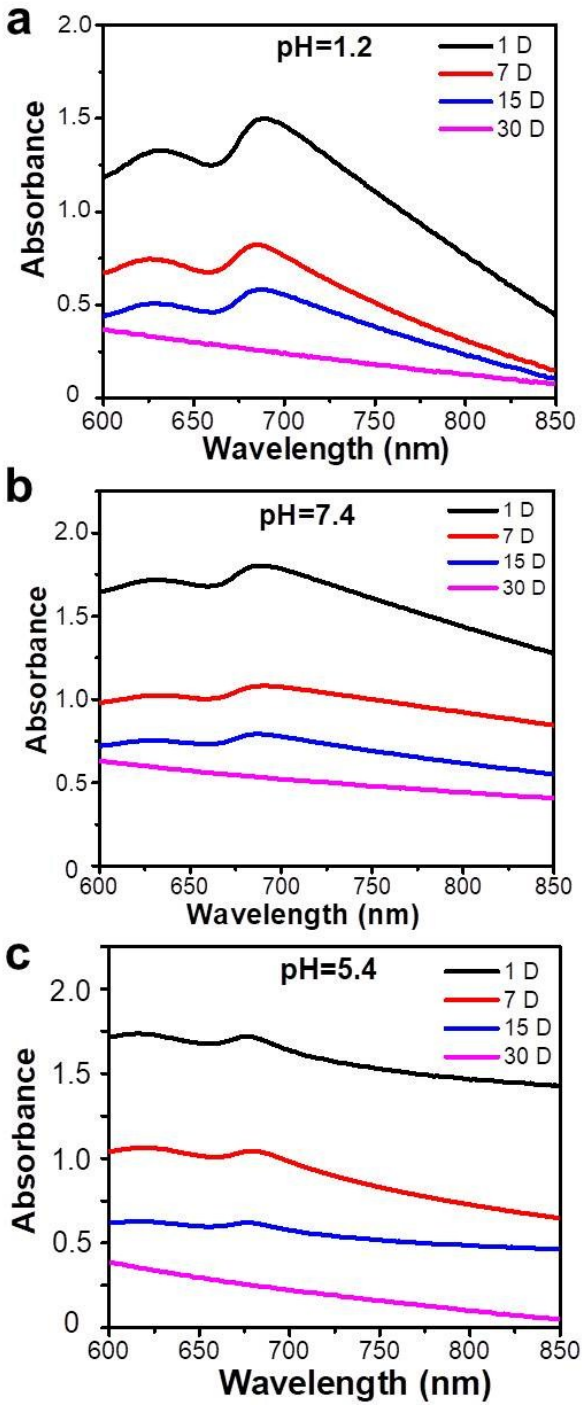


Figure S13. UV–vis-NIR spectra of MoS_2-PVP NSs treated with PBS in different pH values at (a) 1.2, (b) 7.4, and (c) 5.4 for 30 days.

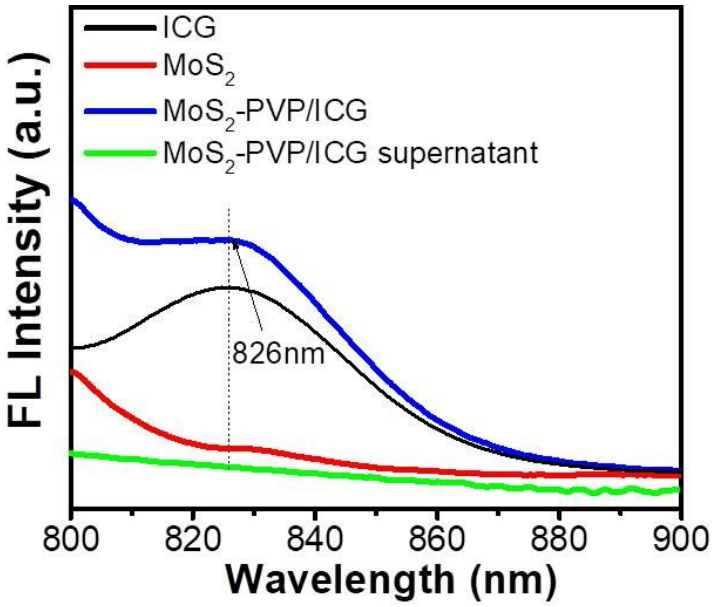


Figure S14. Fluorescence spectra of free ICG, MoS_2, MoS_2-PVP/ICG, and MoS_2-PVP/ICG supernatant after kept 7 days in dark.

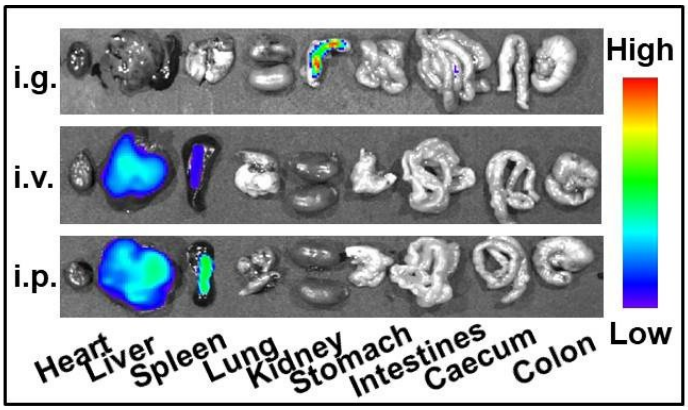


Figure S15. The Fluorescence images of major organs and gastrointestinal tract after injection of MoS_2-PVP/ICG NSs at 48 h (*i.g.*) and 7 days (*i.v.*, *i.p.*).

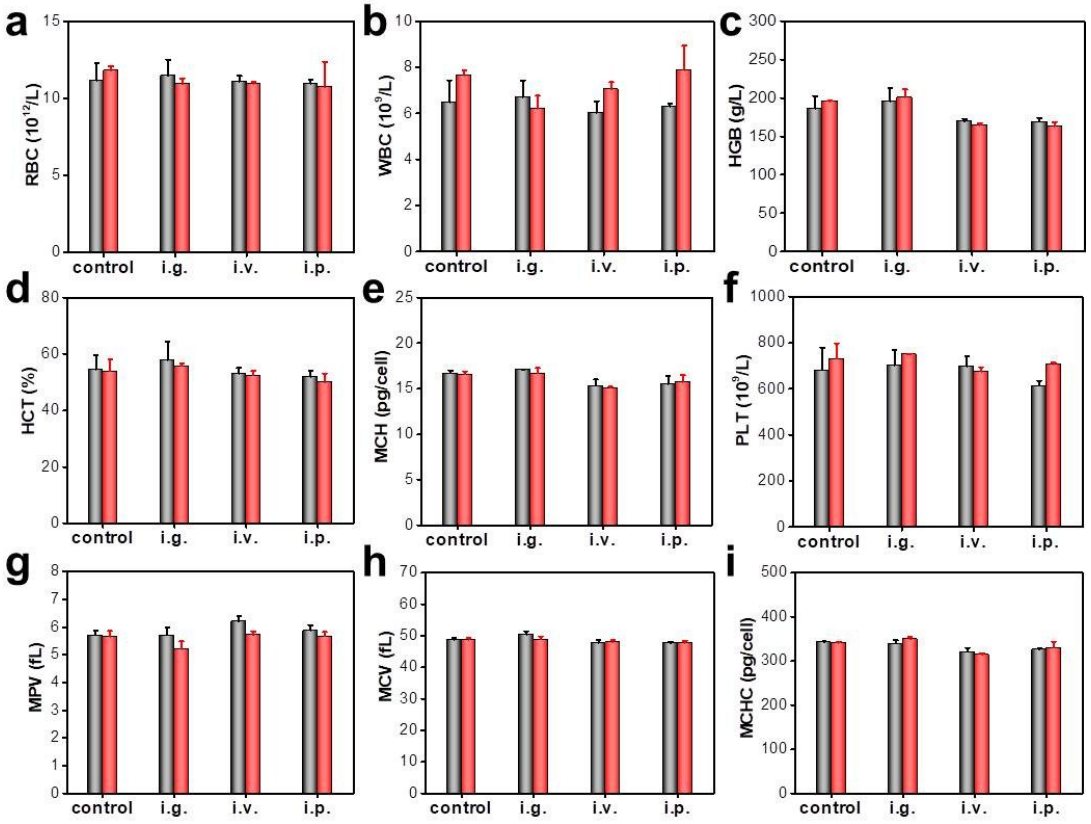


Figure S16. Haematological assay (a–i) of mice treated with MoS_2-PVP NSs after *i.p.* and *i.v.* injection for 15days (black) and 30 days (red), and *i.g.* administration for 24 h (black) and 48 h (red). Error bars represent standard deviation calculated from three mice. Untreated mice were used as control. (a) red blood cells (RBCs), (b) white blood cells (WBC), (c) hemoglobin (HGB), (d) hematocrit (HCT), (e) mean corpuscular hemoglobin (MCH), (f) platelets (PLT), (g) mean platelet volume (MPV), (h) mean corpuscular volume (MCV), and (i) mean corpuscular hemoglobin concentration (MCHC).

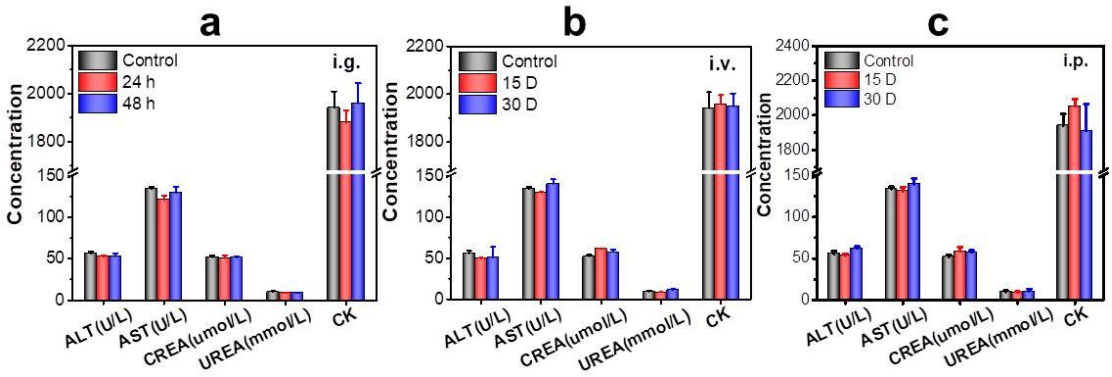


Figure S17. Blood biochemical analysis of mice after *i.g.* (a) administration with MoS_2-PVP NSs for 24 h and 48 h, and *i.v.* (b), *i.p.* (c) injected with MoS_2-PVP NSs for 15 days and 30 days.

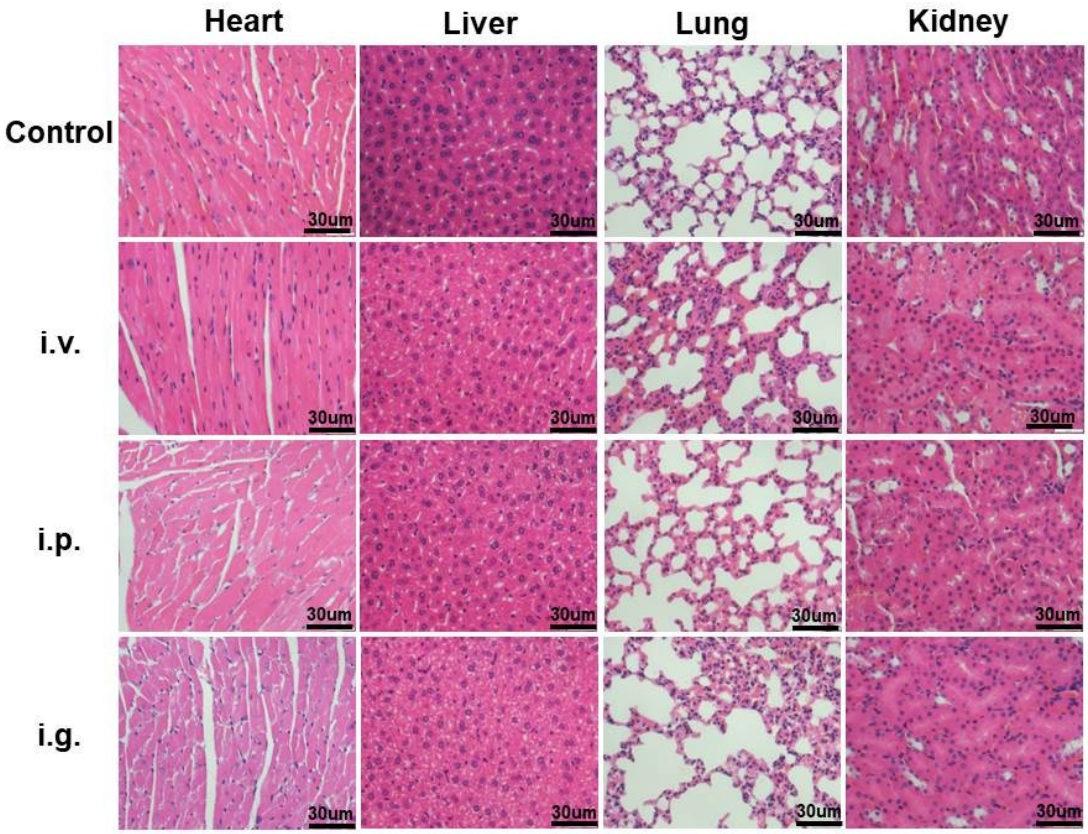


Figure S18. The H&E stained images of major organs slices of after *i.v.*, *i.p.*, and *i.g.* injected with MoS_2-PVP NSs at the dose of 10 mg kg^{-1}. The mice were sacrificed at 30 days after *i.v.* and *i.p.* injection, and 48 h after *i.g.* administration. No appreciable abnormality was observed in these major organs.

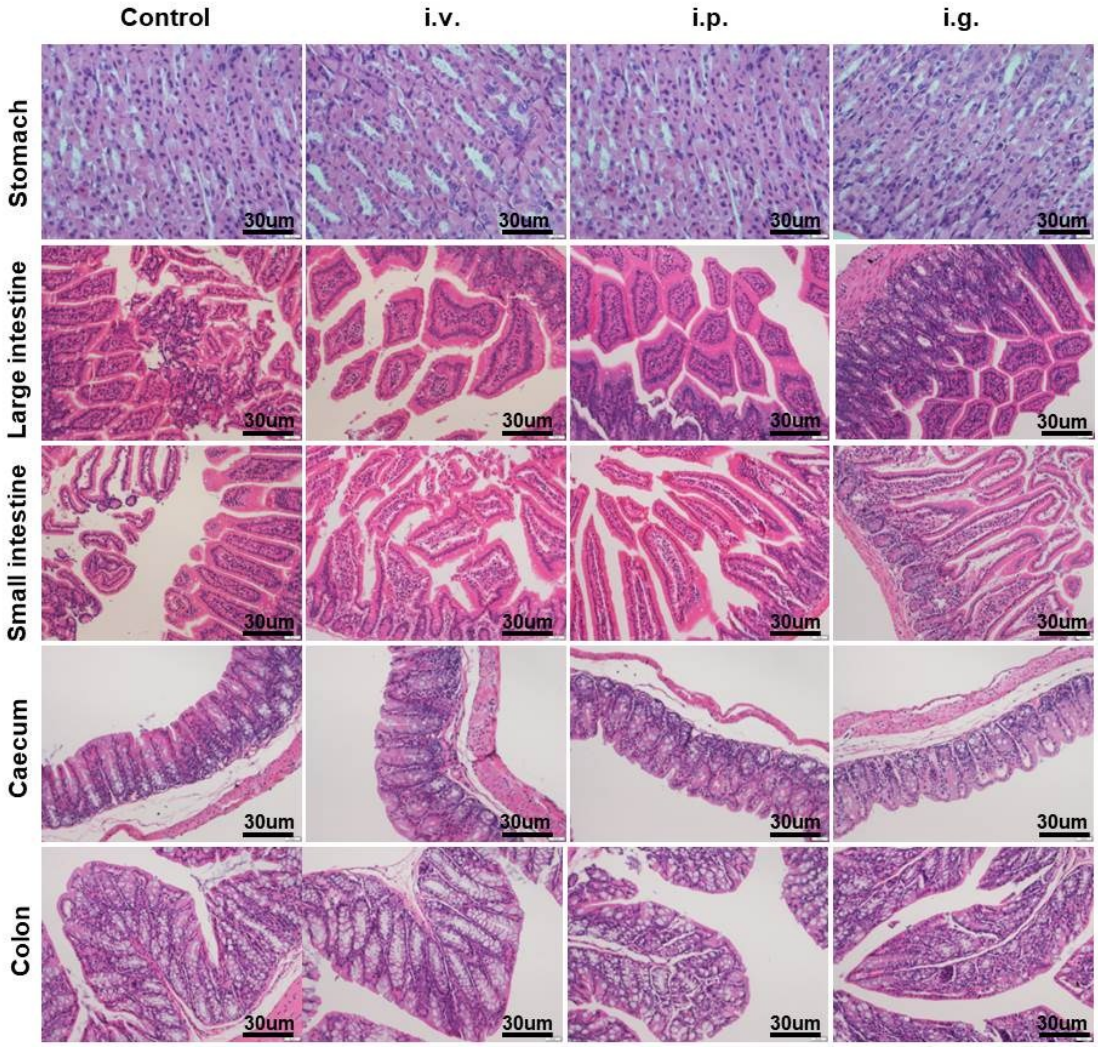


Figure S19. The photographs of H&E stained of gastrointestinal organs after *i.v.*, *i.p.*, and *i.g.* injected with MoS_2-PVP NSs. The mice were sacrificed at 30 days after *i.v.* and *i.p.* injection, and 48 h after *i.g.* administration. The gastrointestinal organs did not show significant changes.

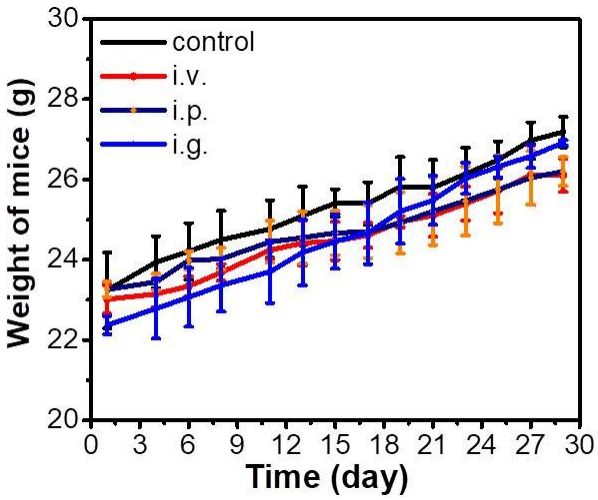


Figure S20. The body weight of mice after different administration and control groups in 30 days. No spontaneous animal death or body weight loss was observed within 30 days.

Table S1. Comparisons of relative peak areas in the XPS spectra of different Mo valence states of MoS_2-PVP NSs treated with pure water, H_2O_2, hMPO+H_2O_2, and Catalase+H_2O_2 after 30 days.

	Water	H_2O_2	hMPO + H_2O_2	Catalase + H_2O_2
Mo^{6+}	16.8%	40.9%	92.6%	94.9%
Mo^{4+}	93.2%	59.1%	7.4%	5.1%

Supporting Information Videos

Video S1

SR-TXM 3D imaging for a single SMMC-7721 cell without any treated as control group. The cell reveals a light blue color and the larger particles outside the cell are gold particles used as a reference for reconstruction.

Videos S2, S3

SR-TXM 3D imaging for a single SMMC-7721 cell after exposed to 24 h MoS_2-PVP NSs for 24 h and exocytosis for 12 h, respectively. Red, yellow, and green colors indicate MoS_2-PVP NSs-contained lysosome with increasing gradients of X-ray absorption intensity. The larger particles outside the cell are gold particles used as a reference for reconstruction.

Videos S4, S5

X-ray 3D CT imaging of BALB/c mice after *i.g.* and *i.v.* injected with MoS_2-PVP NSs for 48 h, respectively. The skeleton of mice reveals a white color. Blue, yellow, and red colors indicate MoS_2-PVP NSs located in different organs with increasing of X-ray intensity.