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(ESI)

## Synergistic TME-manipulation Effects of a Molybdenum-based

## **Polyoxometalate Enhanced the PTT Effects on Cancer Cells**

Gang Chen,<sup>ab</sup> Yu Wang,<sup>ab</sup> Xueping Kong,<sup>a</sup> Hongwei Li,<sup>ab</sup> Bao Li,<sup>a</sup> Xianghui Yu,<sup>c</sup> Lixin Wu,<sup>a</sup> and Yuqing Wu,<sup>\*ab</sup>

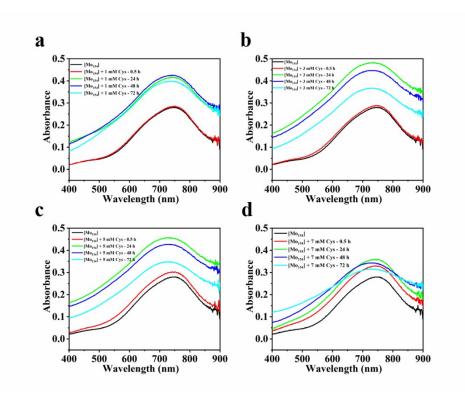
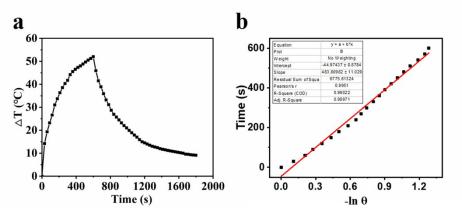
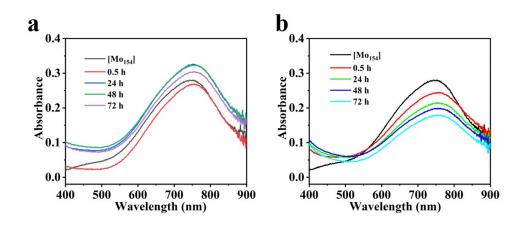


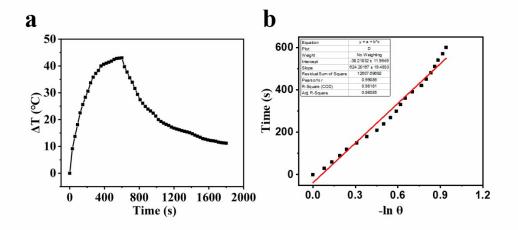
Fig. S1 Time-dependent UV-vis absorption spectra of  $[Mo_{154}]$  in the presence of different amounts of Cys between 1-7 mM.



**Fig. S2** (a) The temporal temperature variation of 5  $\mu$ M [Mo<sub>154</sub>] and 3 mM cysteine after 24 h incubated. The volume of solution is 1 mL. The solution is irradiated for 10 min using a laser of 808 nm (1.4 W/cm<sup>2</sup>), and then cooled to the room temperature at the ambient environment. (b) Time constant for heat transfer from the system is calculated to be  $\tau_s = 483.80982$  s by applying the linear time data from the cooling period *versus* negative natural logarithm of driving force temperature, which is obtained from Fig. S2a.



**Fig. S3** UV-vis absorption spectra of 5  $\mu$ M [Mo<sub>154</sub>] in the presence of 3 mM Cys after incubation for different times (at 4 °C), at (a) pH 5.0 and (b) 6.0, respectively.



**Fig. S4.** (a) The temporal temperature variation of 5  $\mu$ M [Mo<sub>154</sub>] and 3 mM Cys after 48 h incubation (pH 5.0). The volume of solution is 1 mL, being irradiated for 10 min (808 nm, 1.4 W/cm<sup>2</sup>); followed being cooled at ambient environment. (b) Time constant for heat transfer from the system is calculated to be  $\tau_s = 624.20212$  s by applying the linear time from the cooling period *versus* negative natural logarithm of driving force temperature, which is obtained from Fig. S4a.

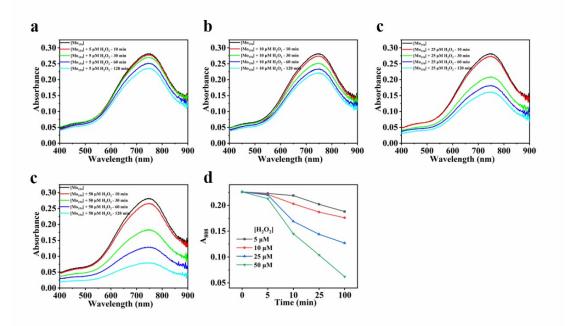


Fig. S5. UV-vis absorption spectra of 5  $\mu$ M [Mo<sub>154</sub>] in the presence of the different amounts of H<sub>2</sub>O<sub>2</sub>, being measured at 120 min after mixing.

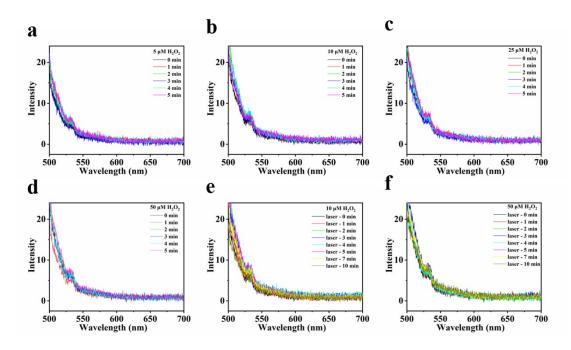


Fig. S6. The fluorescence spectra of 5  $\mu$ M [Mo<sub>154</sub>] in solution after treated with H<sub>2</sub>O<sub>2</sub> and DCFH-DA, respectively, which shows no fluorescence intensity at 525 nm for DCF, no matter it was irradiated by 808 nm or not.