

Electronic Supplementary Material (ESI)

**Photo-induced synthesis of molybdenum oxide quantum dots for
surface-enhanced Raman scattering and photothermal therapy**

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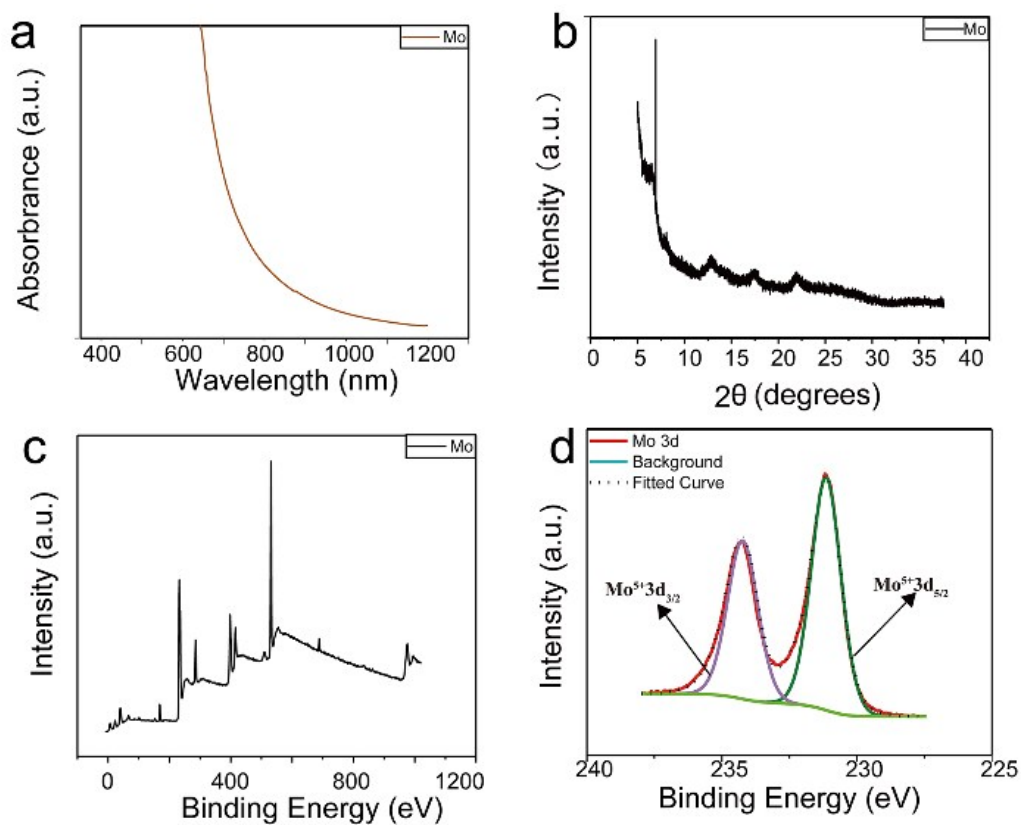


Fig. S1. The characterization of Y. a) UV-Vis-NIR, b) XRD, c) XPS and d) the high resolution XPS spectra of Y.

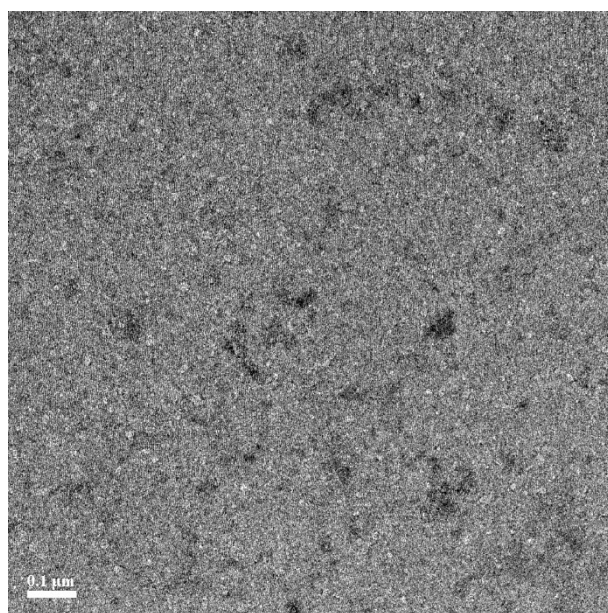


Fig. S2. TEM image of Y.

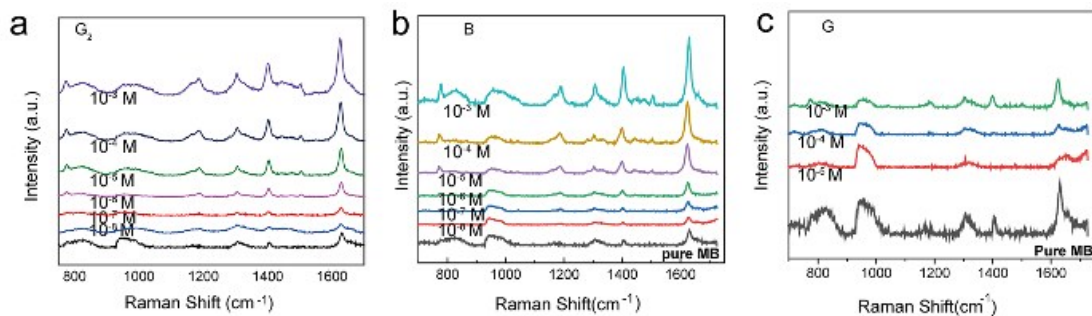


Fig. S3. SERS spectra of MB molecules at different concentrations deposited on a) G_2 , b) B, and c) G, respectively.

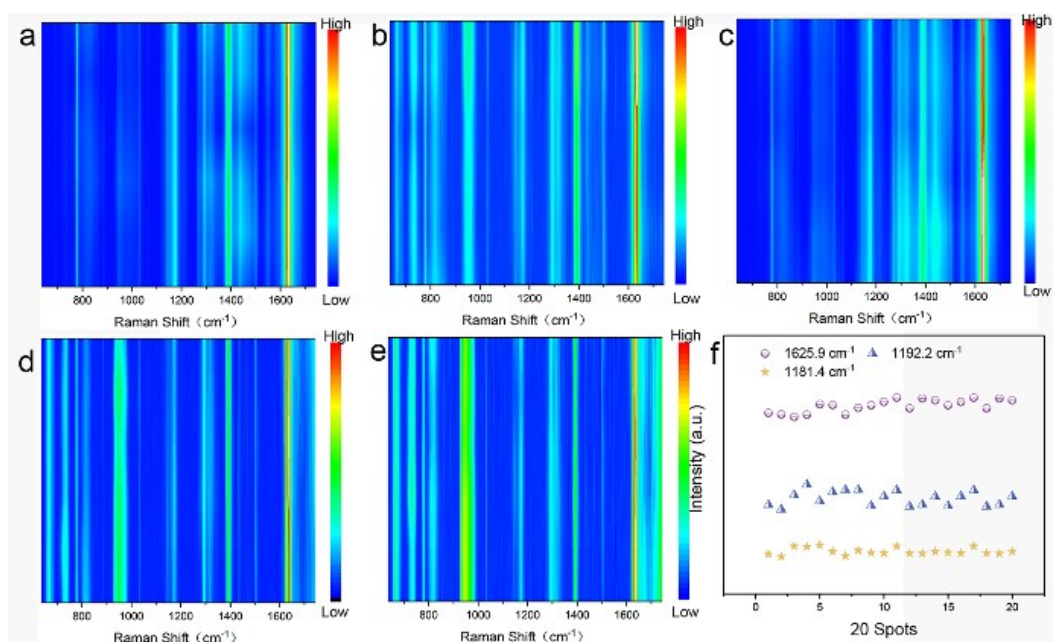


Fig. S4. Uniformity pseudo color maps about Raman spectra of MB molecules deposited on MoO_2 substrates. The MB concentration is a) 10^{-3} M, b) 10^{-4} M, c) 10^{-5} M, d) 10^{-6} M and e) 10^{-7} M. f) The SERS intensity distribution of three characteristic peaks of MB molecules (20 samples).

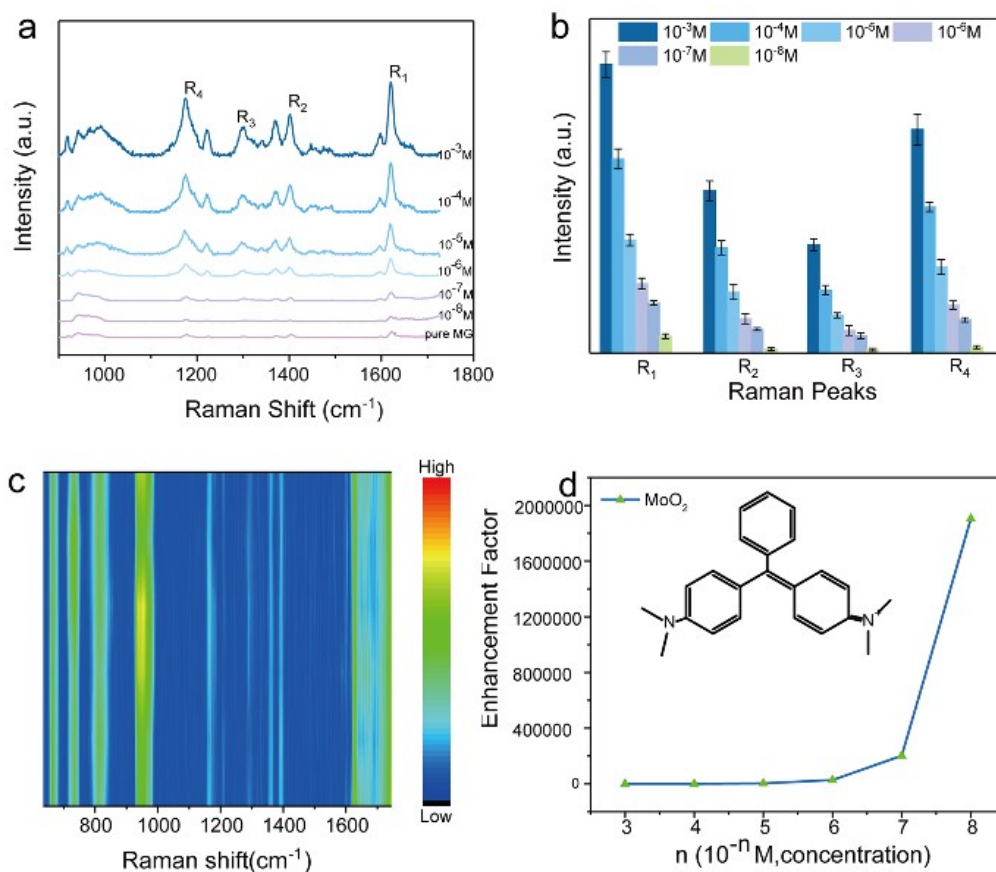


Fig. S5. SERS measurement of MG (Malachite Green) molecules deposited on MoO_2 substrates. a) Raman spectrums of MG molecules with different concentrations deposited on MoO_2 substrates. b) The intensity of four typical Raman peaks extract from panel. c) Uniformity pseudo color map about Raman spectrums of MG molecules deposited on MoO_2 substrates with 10^{-8}M concentrations. d) Broken line diagram of Raman enhancement factor of MB molecules deposited on three molybdenum oxide substrates with the change of concentration.

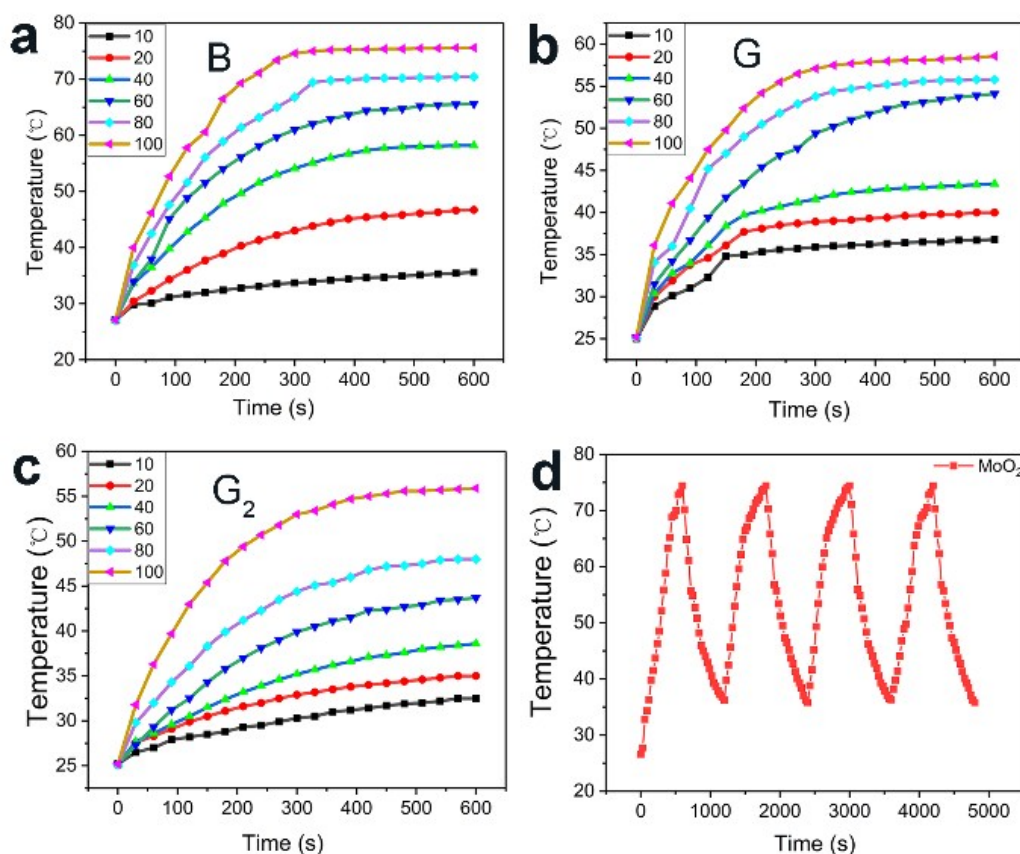


Fig. S6. Temperature changes with gradient concentrations (10-100 µg/mL) of the a) B, b) G, and c) G₂ aqueous solutions under irradiation at a wavelength of 808 nm laser with a power density of 2 W/cm² for 600 s. d) Temperature variation of MoO₂ QDs solution (1 mg/mL) with four cycles under NIR irradiation and natural cooling (the time interval between each cycle is about 20 min).

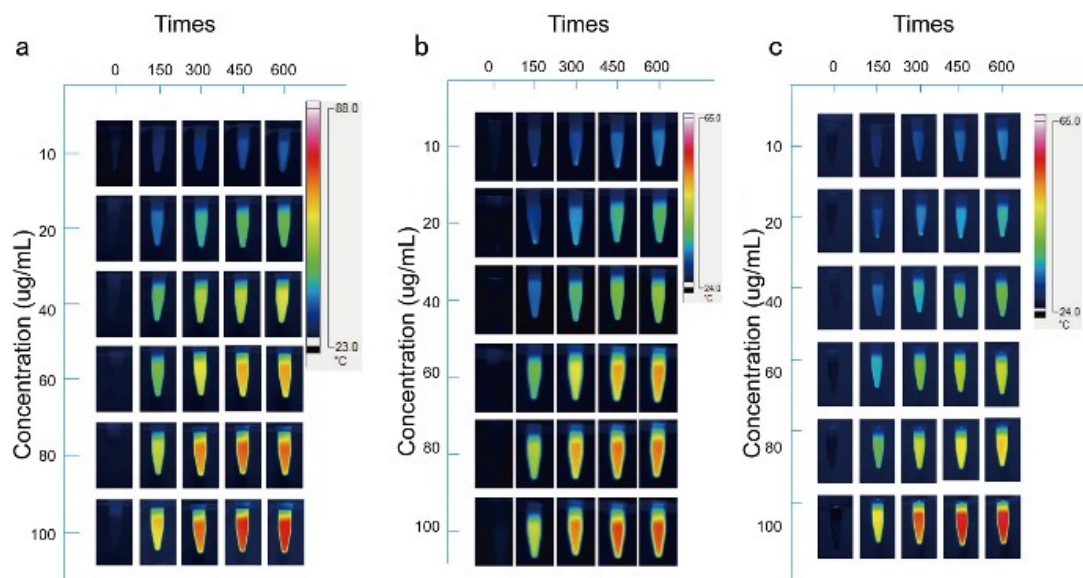


Fig. S7. Infrared thermal images a) B, b) G, and c) G_2 with different concentrations under NIR irradiation.

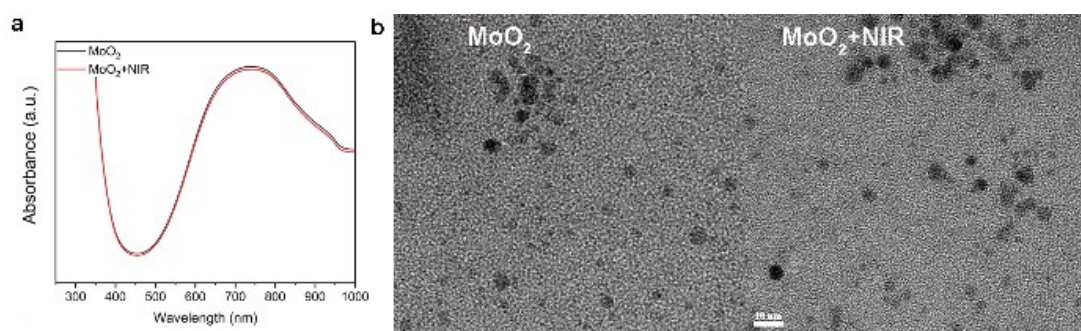


Fig. S8. a) UV-Vis-NIR absorption spectra and b) TEM images of MoO_2 QDs before and after NIR irradiation.

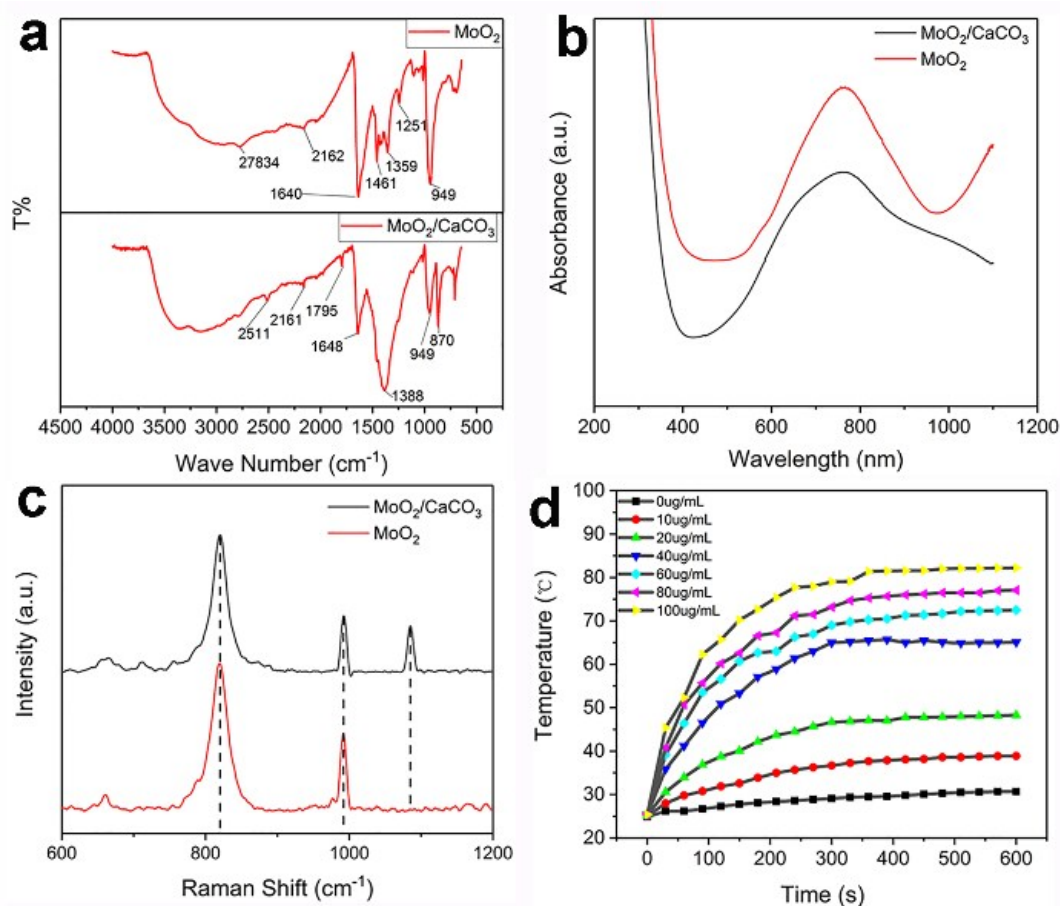


Fig. S9. a) FT-IR spectra and b) UV-Vis-NIR absorption spectra of MoO₂ and MoO₂ wrapped in CaCO₃. c) Raman analysis of MoO₂ and MoO₂ wrapped in CaCO₃. d) Temperature changes with gradient concentrations (10-100 µg/mL) of the MoO₂ QDs wrapped in CaCO₃ aqueous solutions under irradiation at a wavelength of 808 nm laser with a power density of 2 W/cm² for 600 s.

The Fig. S9a displays the FT-IR spectrum of MoO₂/CaCO₃, where the characteristic peak of calcium carbonate at 1388 cm⁻¹ (asymmetric C-O stretching mode) can be observed. The UV-Vis-NIR absorption spectrum of MoO₂/CaCO₃ shows a similar spectral pattern of that of MoO₂ (Fig. S9b). The Raman feature of MoO₂/CaCO₃ was also recorded (Fig. S9c), which illustrated the fingerprint signals of both MoO₂ (993 and 820 cm⁻¹) and CaCO₃ (1086 cm⁻¹, symmetric C-O stretching mode), indicating the successful coating of MoO₂ by calcium carbonate. Fig. S9d shows the photothermal heating curves of MoO₂/CaCO₃ at different concentrations, where the maximal temperature of MoO₂/CaCO₃ solution under NIR laser irradiation can reach 81 °C which is almost the same as that induced by MoO₂.

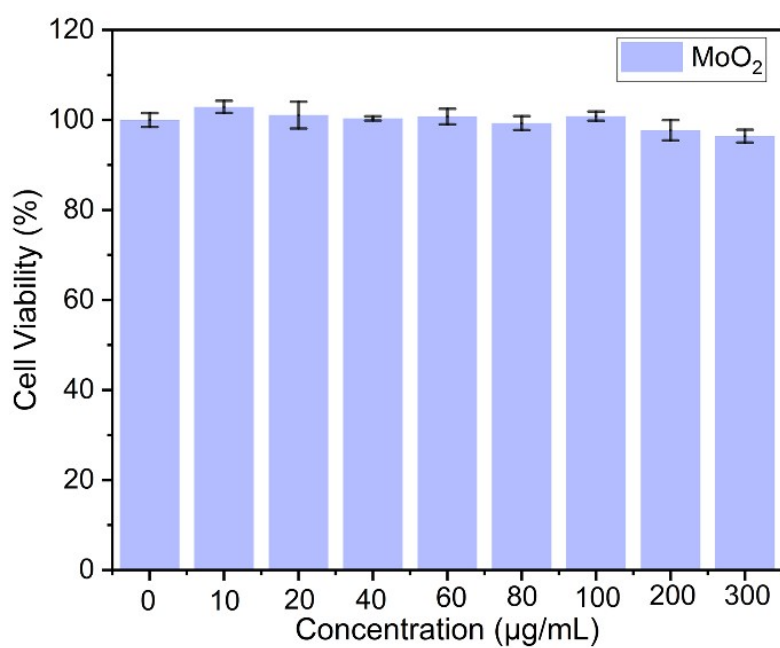


Fig. S10. MTT assay of the cell viabilities of normal hepatocytes, LO2 cells, treated with different concentrations of MoO₂ QDs

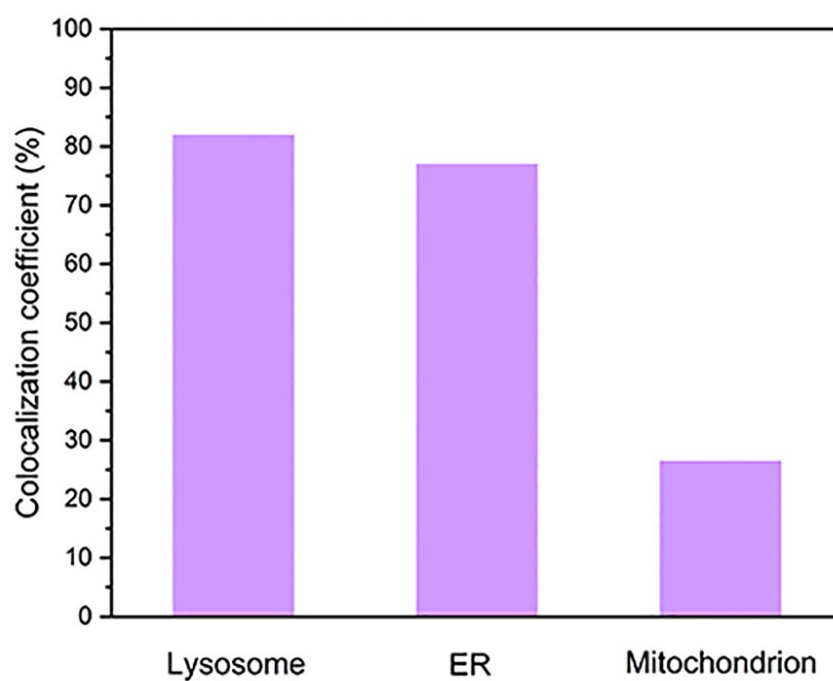


Fig. S11. The co-localization coefficients for MoO₂ QDs and different organelles.