Supplementary materials

A pH-activatable Copper-Axitinib coordinated multifunctional nanoparticles for synergistic chemo-chemodynamic therapy against aggressive cancers

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Experimental Section

Density Functional Theory (DFT) calculations

All DFT calculations for the estimation of Gibbs free energies were carried out with the Gaussian09 and GaussView5.0. Molecular geometries optimization and single point energy calculation were performed by using Becke's three-parameter hybrid functional and the LYP correlation functional (B3LYP) with D3 correction of Grimme et al, with the LanL2DZ basis set for Cu^{2+} and 6-31G* for other atoms. Frequency calculations were performed on the optimized geometries to verify that the geometries correspond to minima on the potential energy surface (PES). The solvation energies were estimated by single-point calculations using SCRF solvation model and the solvent was set to water or none for system in vacuum.

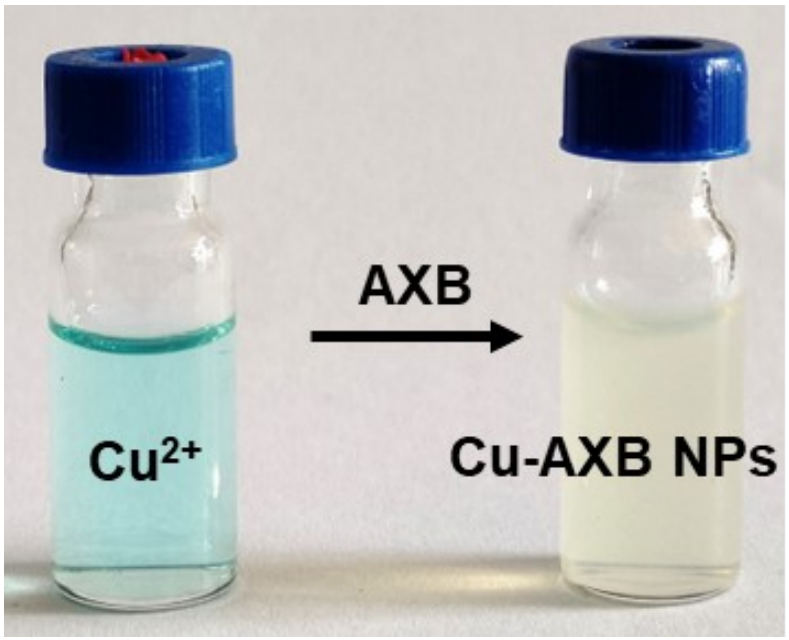

Fig.S1 Color changes before and after the formation of Cu-AXB NPs.

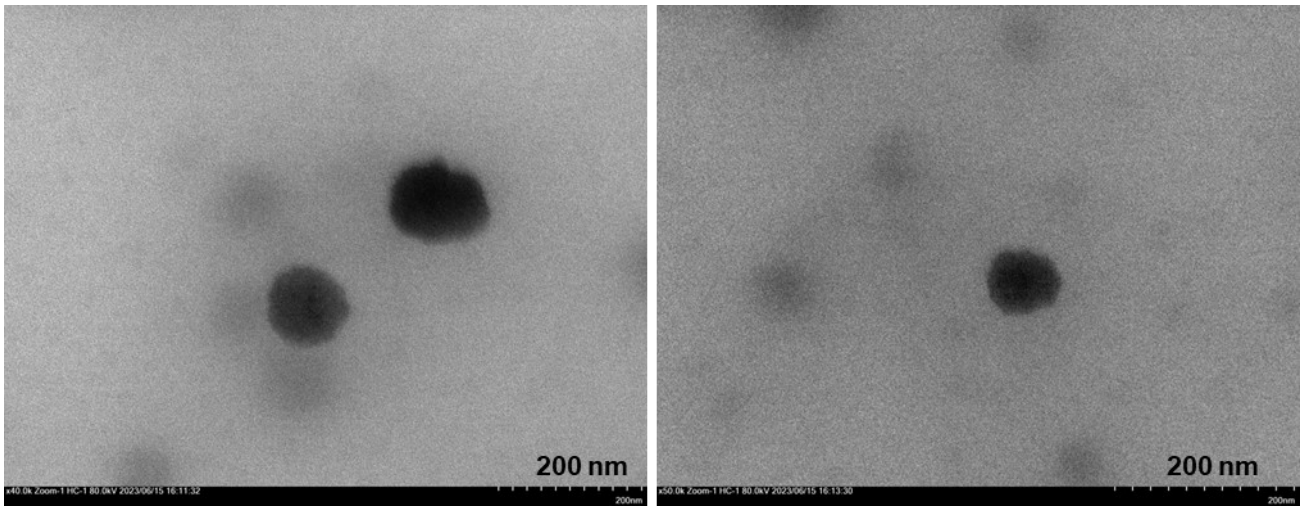

Fig.S2 TEM image of Cu-AXB NPs. scale bar=200 nm.

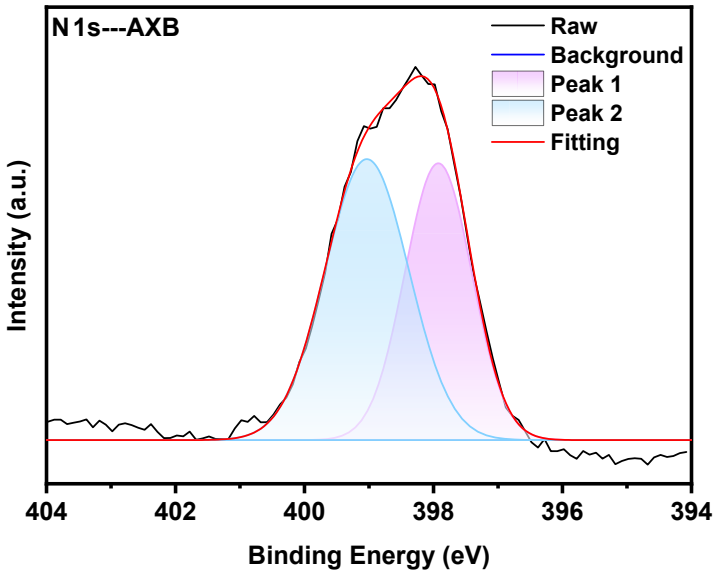

Fig.S3 High-resolution N 1s XPS spectra of AXB.

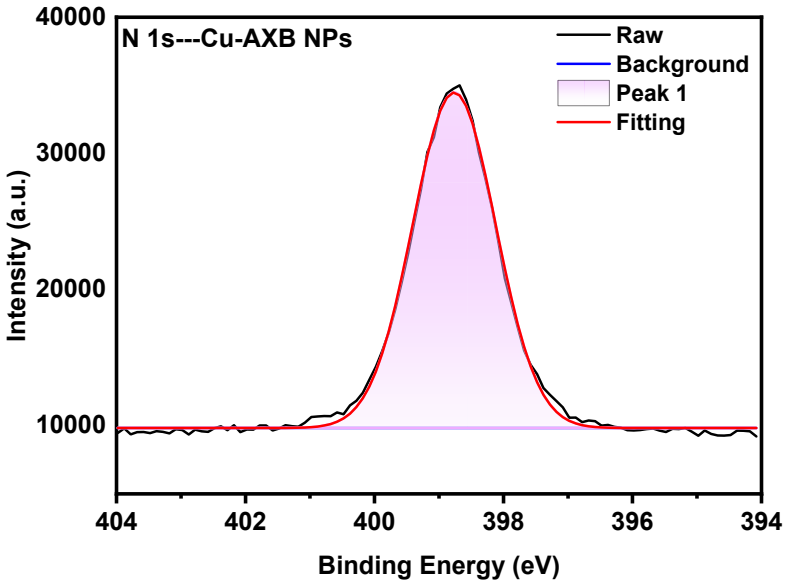

Fig.S4 High-resolution N 1s XPS spectra of Cu-AXB NPs.

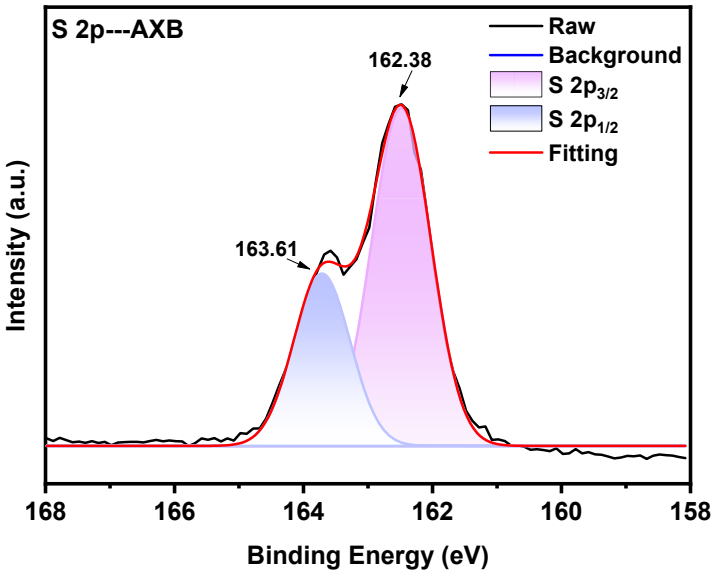

Fig.S5 High-resolution S 2p XPS spectra of AXB.

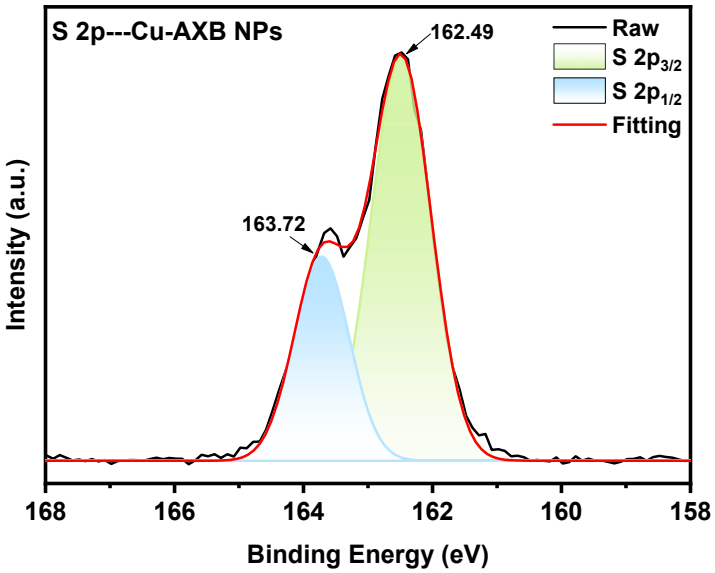

Fig.S6 High-resolution S 2p XPS spectra of Cu-AXB NPs.

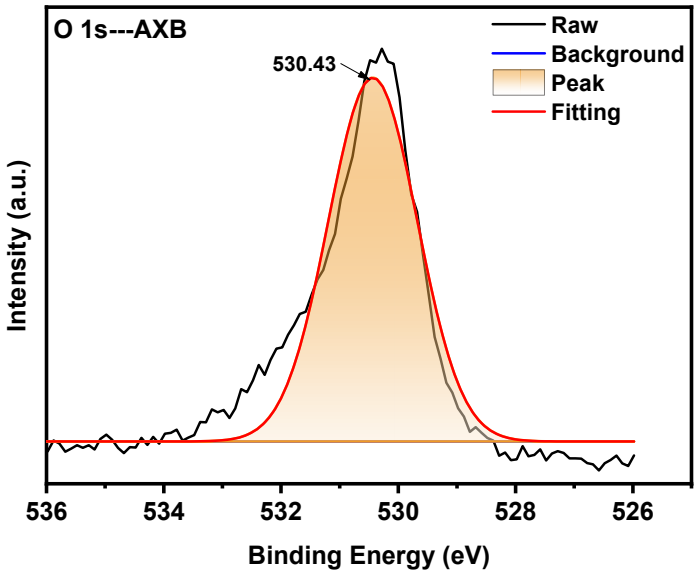

Fig.S7 High-resolution O 1s XPS spectra of AXB.

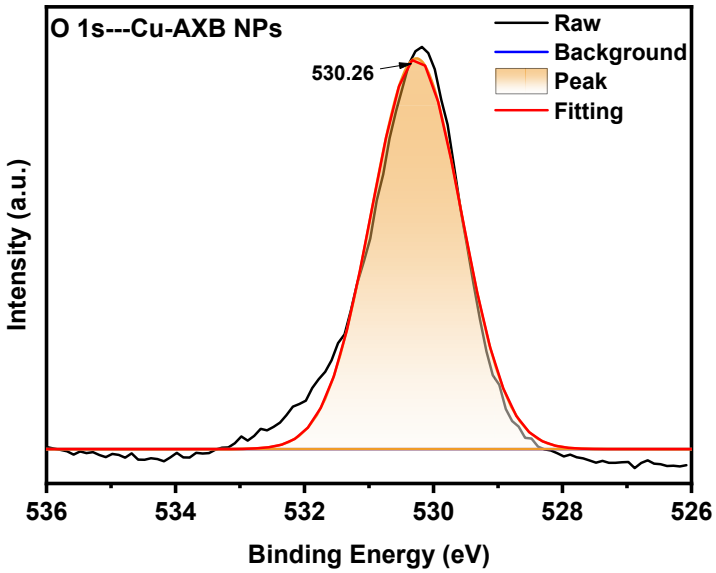

Fig.S8 High-resolution O 1s XPS spectra of Cu-AXB NPs.

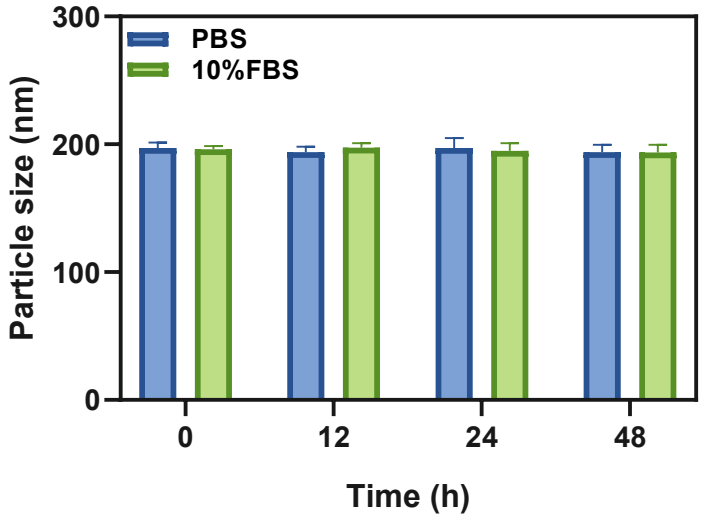

Fig.S9 The particle size of Cu-AXB NPs in the PBS and 10%FBS.

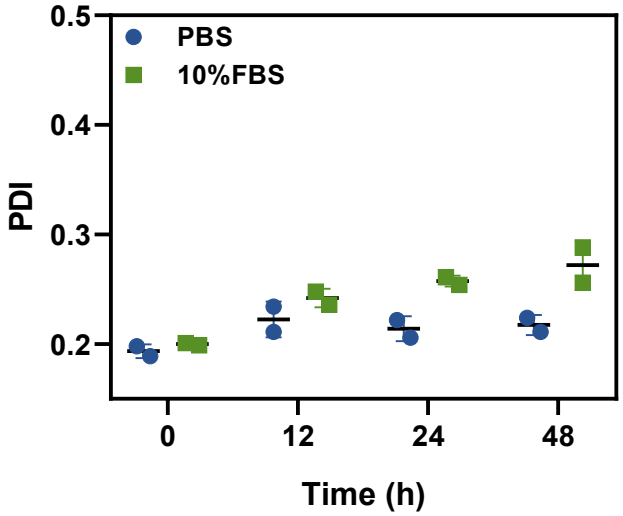

Fig.S10 The PDI of Cu-AXB NPs in the PBS and 10%FBS.

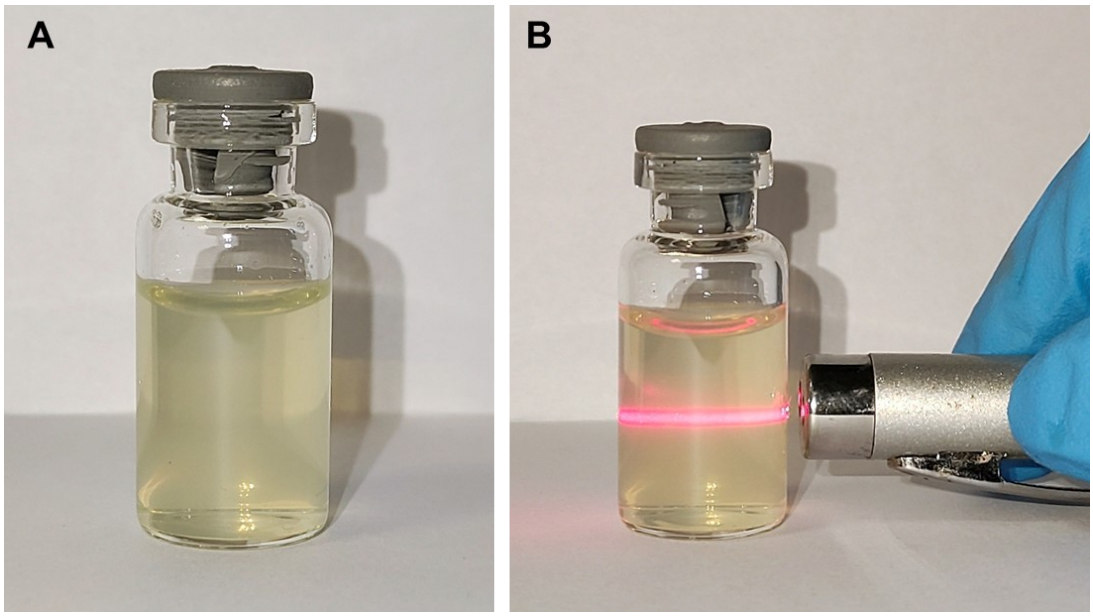

Fig.S11 (A)The appearance image of Cu-AXB NPs stored in 4° refrigerator for one month. (B) The Tyndall phenomenon of nanoparticles was apparent after storage for one month.

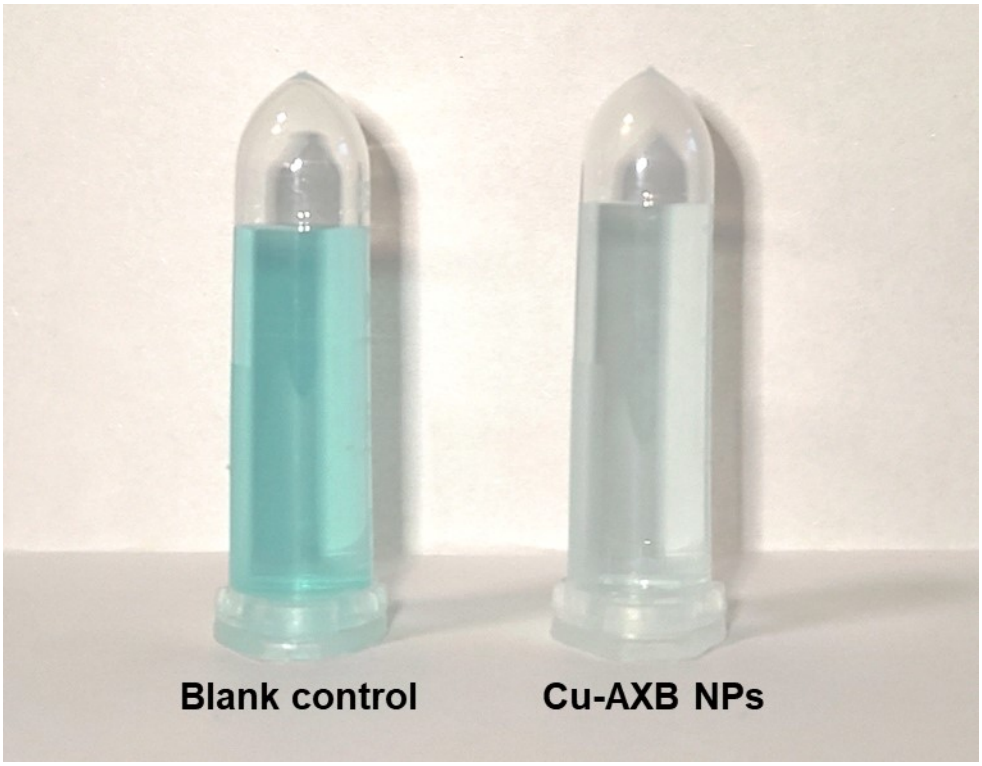

Fig.S12 The images of MB solutions color under different treatment.

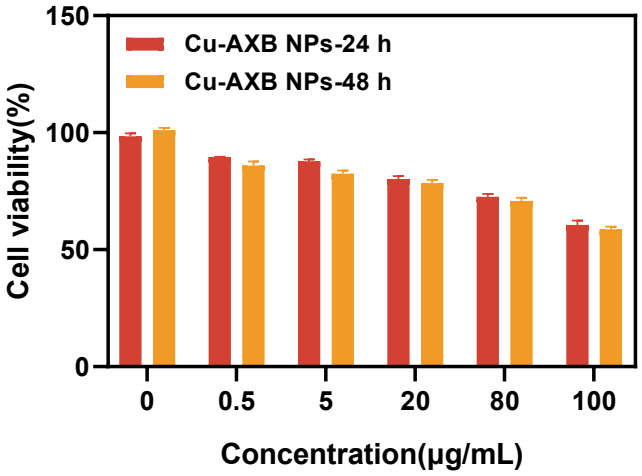

Fig.S13 Cell viability of 3T3-L1 cells after incubation with Cu-AXB NPs for 24 h and 48 h.

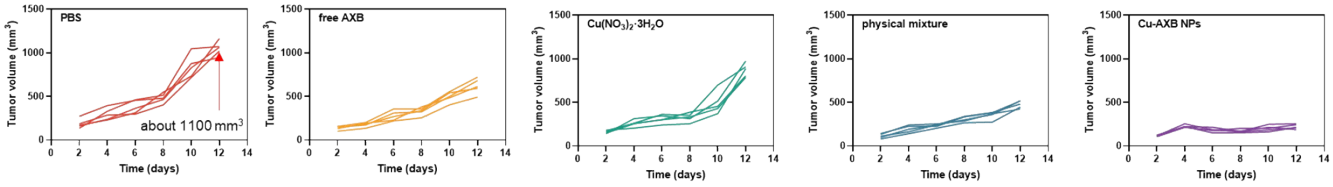

Fig.S14 Individual tumor growth curves of each 4T1 tumor-bearing mouse after different treatments.

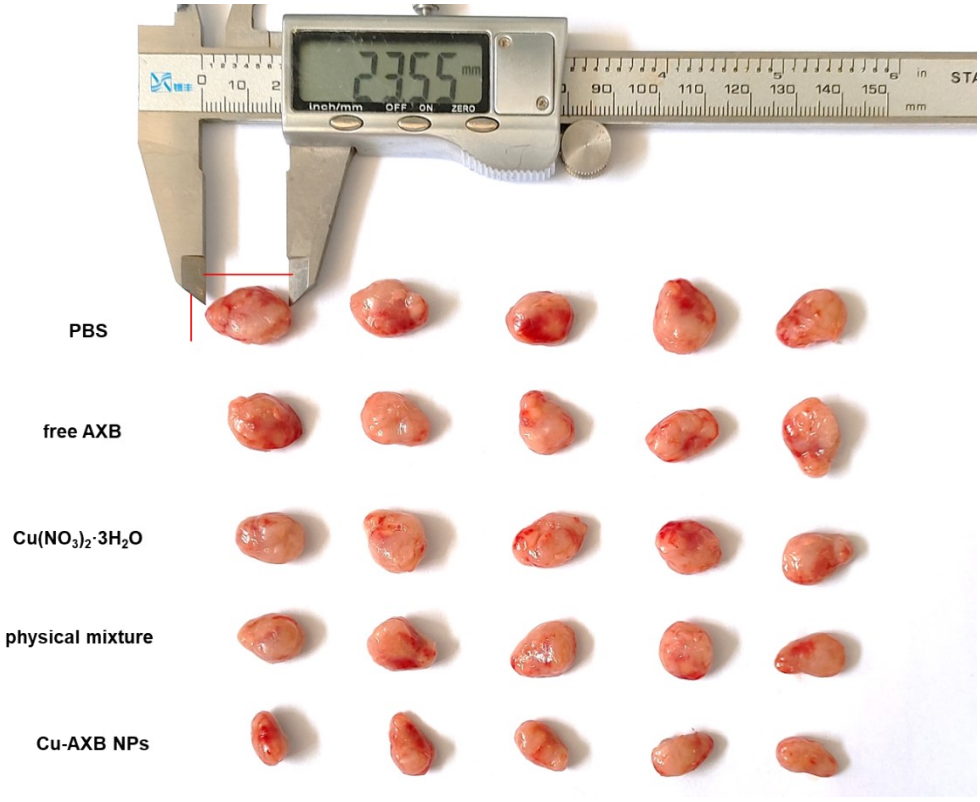

Fig.S15 The enlarged optical image of the tumors.