

## Article

# Mitochondria-Targeted Fluorescent Nanoparticles with Large Stokes Shift for Long-Term BioImaging

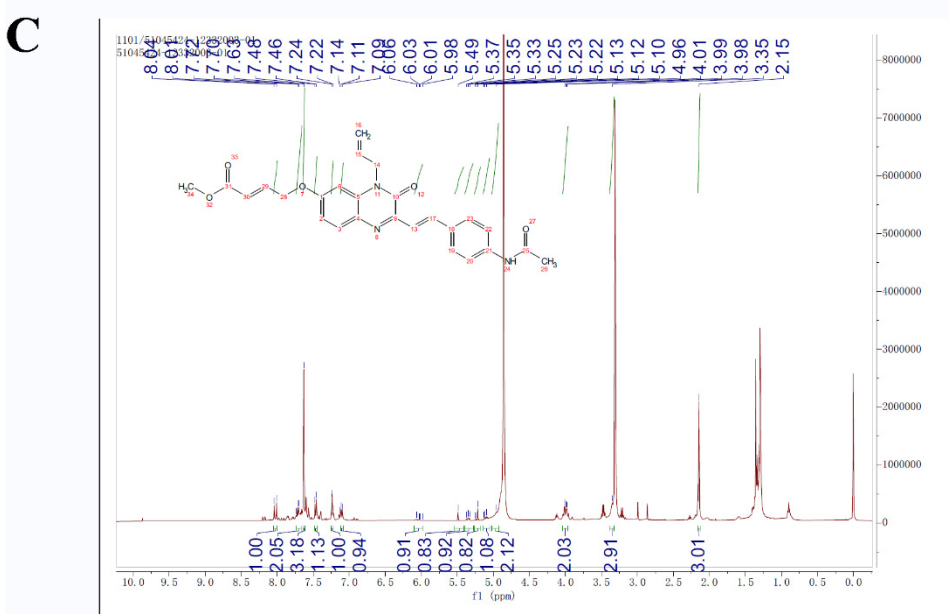
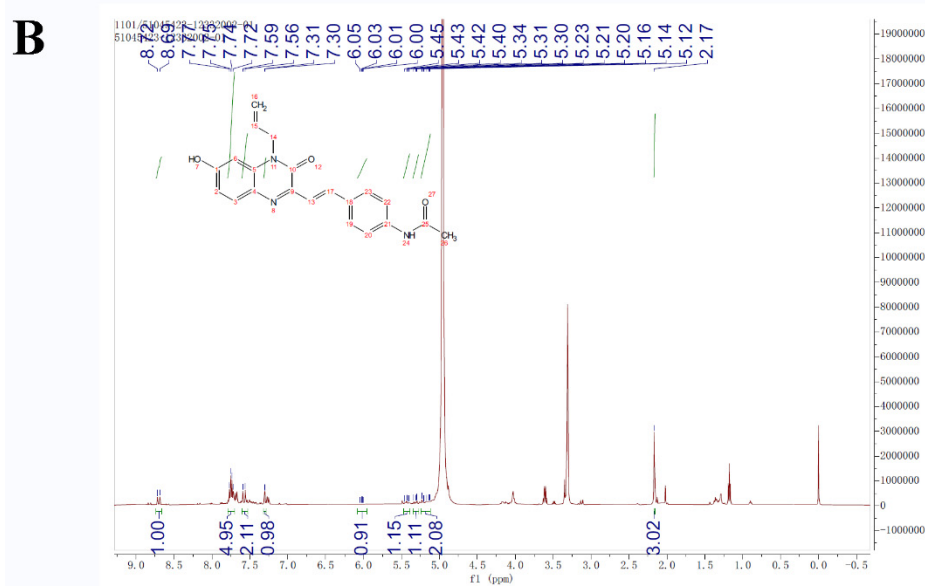
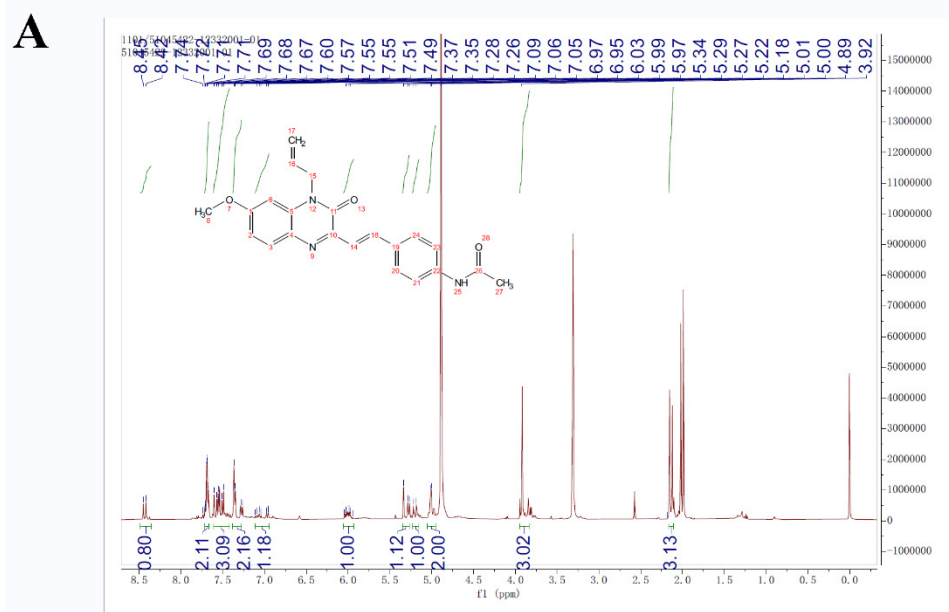
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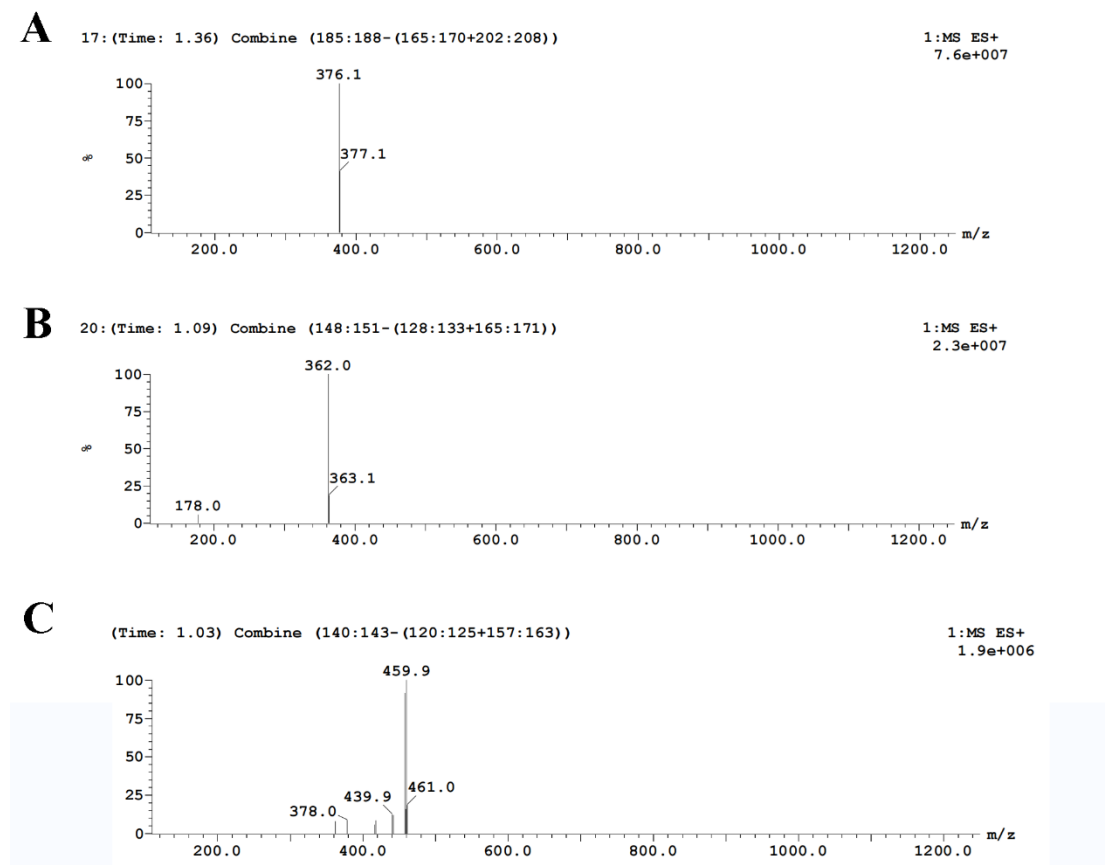
## Apparatus

Nuclear magnetic resonance (NMR) spectra were recorded on Bruker AVANCE III 400 spectrometer with dimethyl sulfoxide-*d*<sub>6</sub> (DMSO-*d*<sub>6</sub>) as the solvents at 25°C. FTIR spectra were recorded on a Paragon 1000 instrument by the KBr sample holder method. DLS measurements were recorded on a Malvern Zetasizer Nano S device with a 4.0 mW laser operating at  $\lambda=633$  nm. All samples of 0.1 mg mL<sup>-1</sup> were tested with a scattering angle of 173° at 37°C. TEM studies were performed with a JEM-2010HT instrument operated at 200 kV to observe the shape and size of the micelles. Samples were prepared by directly dropping the solution onto carbon-coated copper grids and then air-drying at room temperature overnight before measurement. The UV-vis spectra were measured on a Perkin-Elmer Lambda 20/2.0 UV-vis spectrophotometer. At room temperature, the fluorescence spectra were recorded on a QM/TM/RM fluorescence spectrophotometer (Photon Technology International, Inc.). Molecular weight was determined through a MS system (Agilent).

## Materials

4-methoxy-o-Phenylenediamine (98%, Adamas), ethyl pyruvate (99%, Adamas),  $K_2CO_3$  (99.0%, Greagent), Acetone (99.5%, Adamas), 3-bromoprop-1-ene (95%, Matrix), ethyl acetate (99.8%, Adamas),  $MgSO_4$  (Fluka, 99.0%), N-(4-formylphenyl)acetamide (Aladdin, 99.0%), sulfuric acid (96%, Adamas), (E)-4-bromobut-2-enoic acid (Aladdin, 99.0%), N-hydroxysuccinimide (NHS, 99%, Adamas), 3-(4,5-dimethyl-thiazol-2-yl)-2,5-diphenyl tetrazolium bromide (MTT, Sigma), anhydrous ethanol and peptide (AC-Kr-(Cha)-r-(Cha)-r-(Cha)-r)(Remark:r is D-Arg),98%, GL Biochem) were used as received without purification. DMEM culture medium, and fetal bovine serum (FBS) were purchased from Gibco. L929 mouse fibroblast and IOSE-80 human ovarian epithelium cells were purchased from ATCC



**Figure S1.**  $^1\text{H}$  NMR spectra of Compound 7(A), Compound 8(B) and Compound 9(C) .**Figure S2.** MS spectra of Compound 7(A), Compound 8(B) and Compound 9(C) .

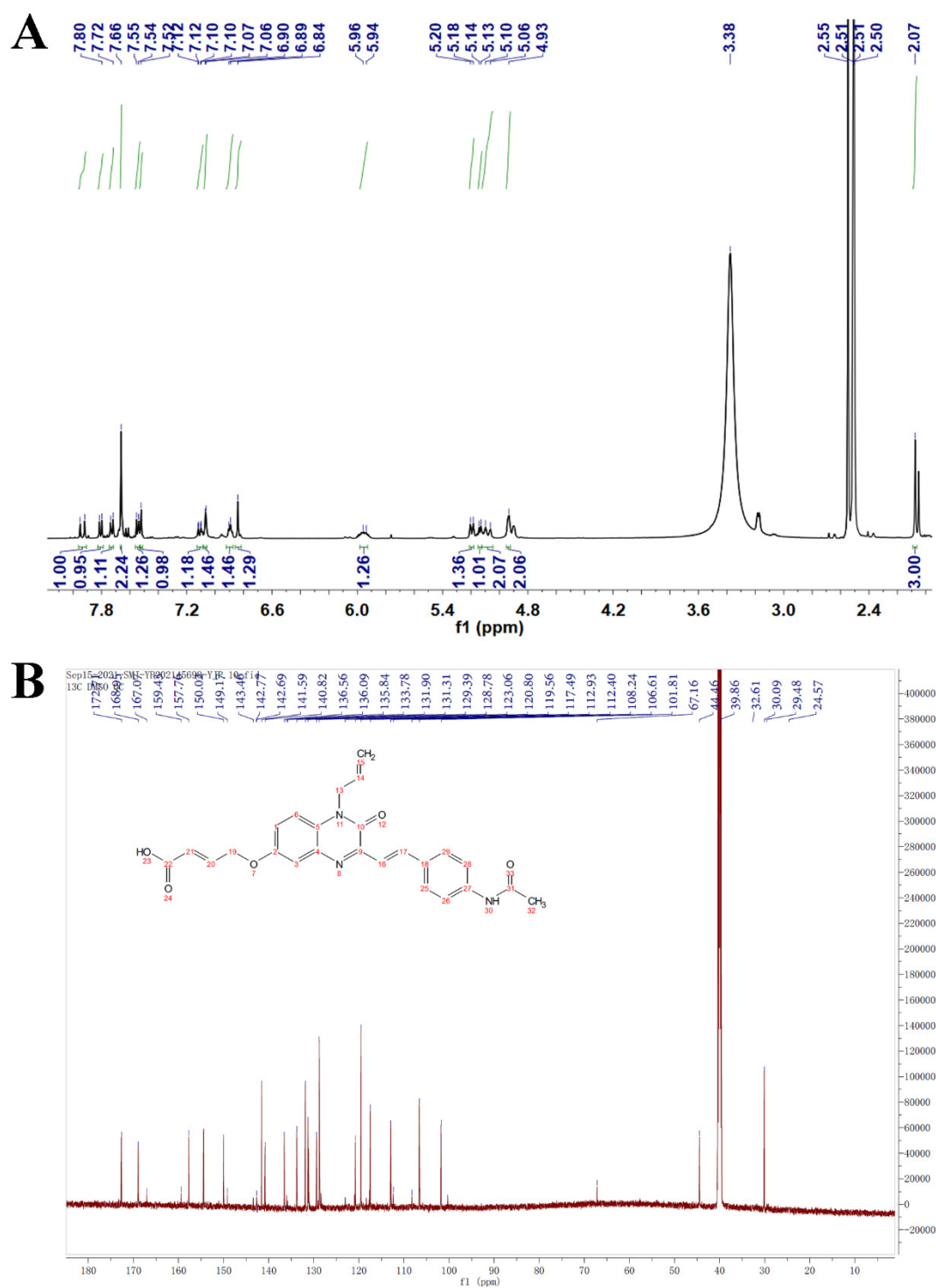


Figure S3.  $^1\text{H}$  NMR spectra of QC (A).  $^{13}\text{C}$  NMR spectra of QC (B).

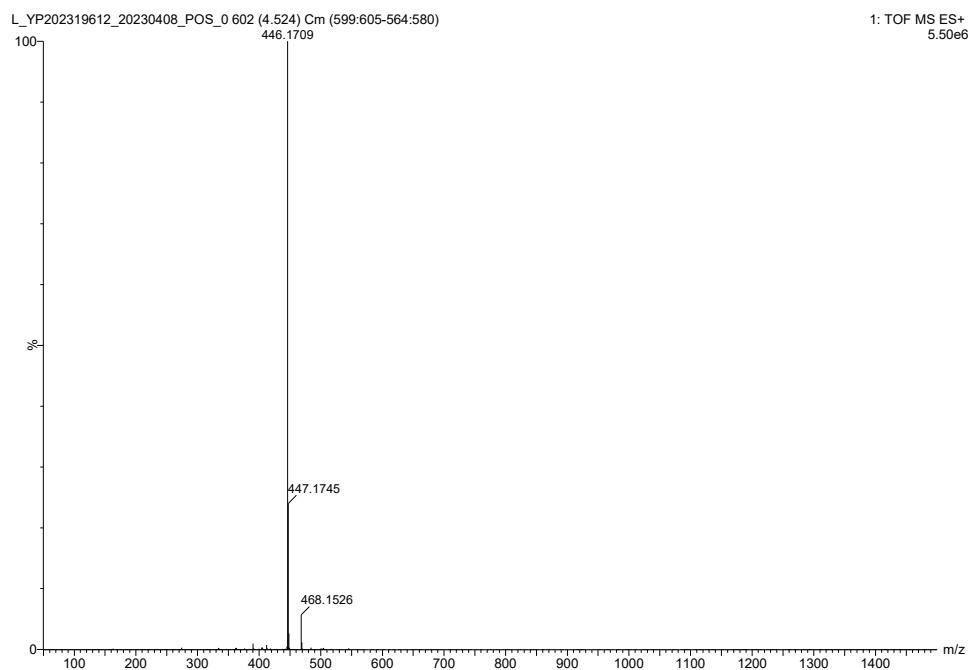


Figure S4. HRMS spectra of QC.

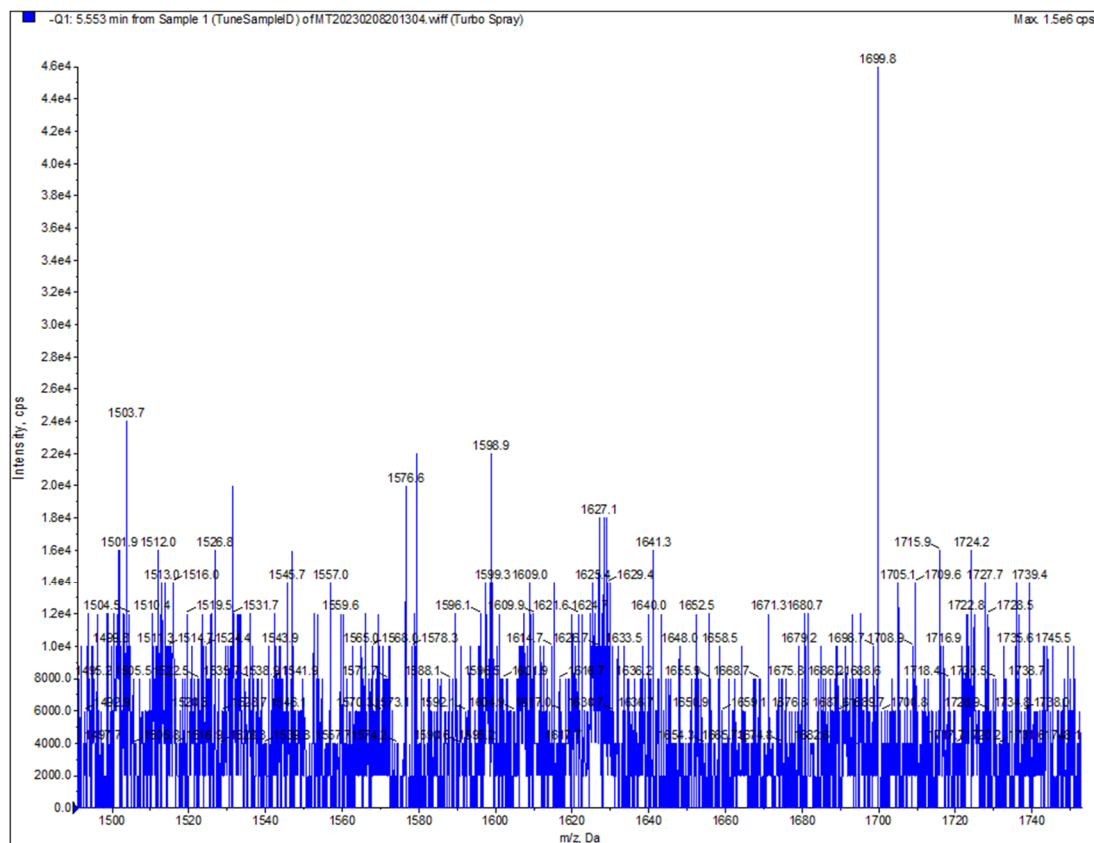
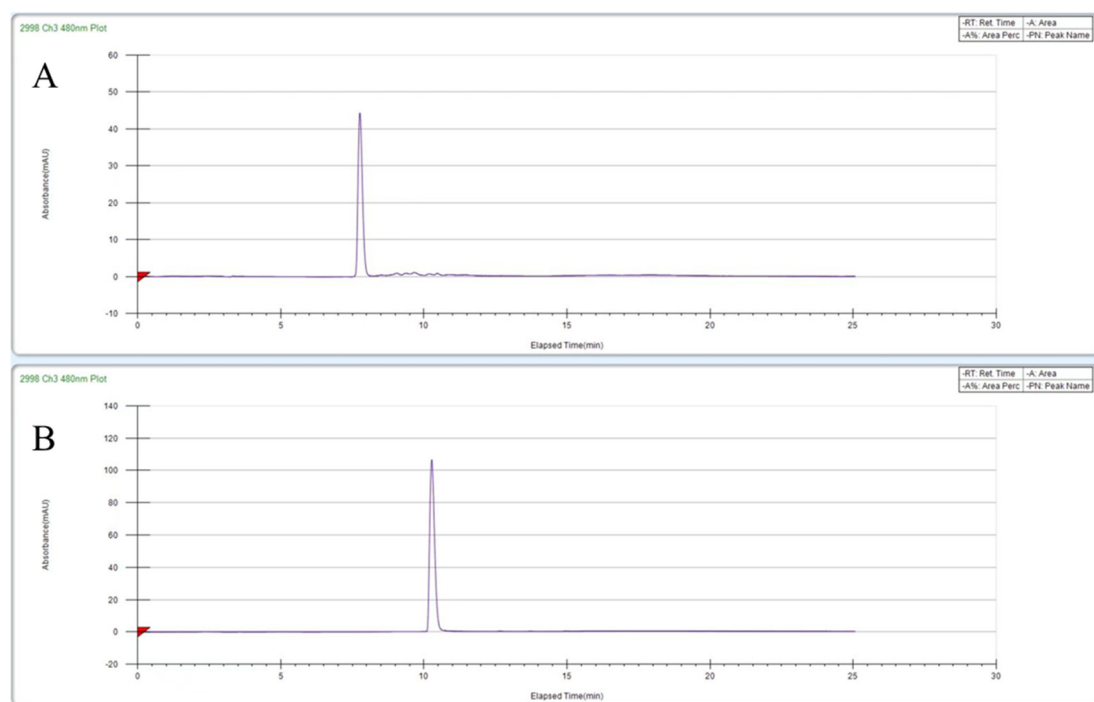


Figure S5. MS spectra of AC-QC nanoparticles.



**Figure S6.** HPLC spectra of AC peptide (A) and AC-QC (B).

## MS Analysis Report

Ion Source: ESI  
Desolvation(L/hr):800  
Cone(V): 30~50  
Capillary(KV):±(2500~3000)  
Desolvation Temp:450℃  
Run Time: 1min

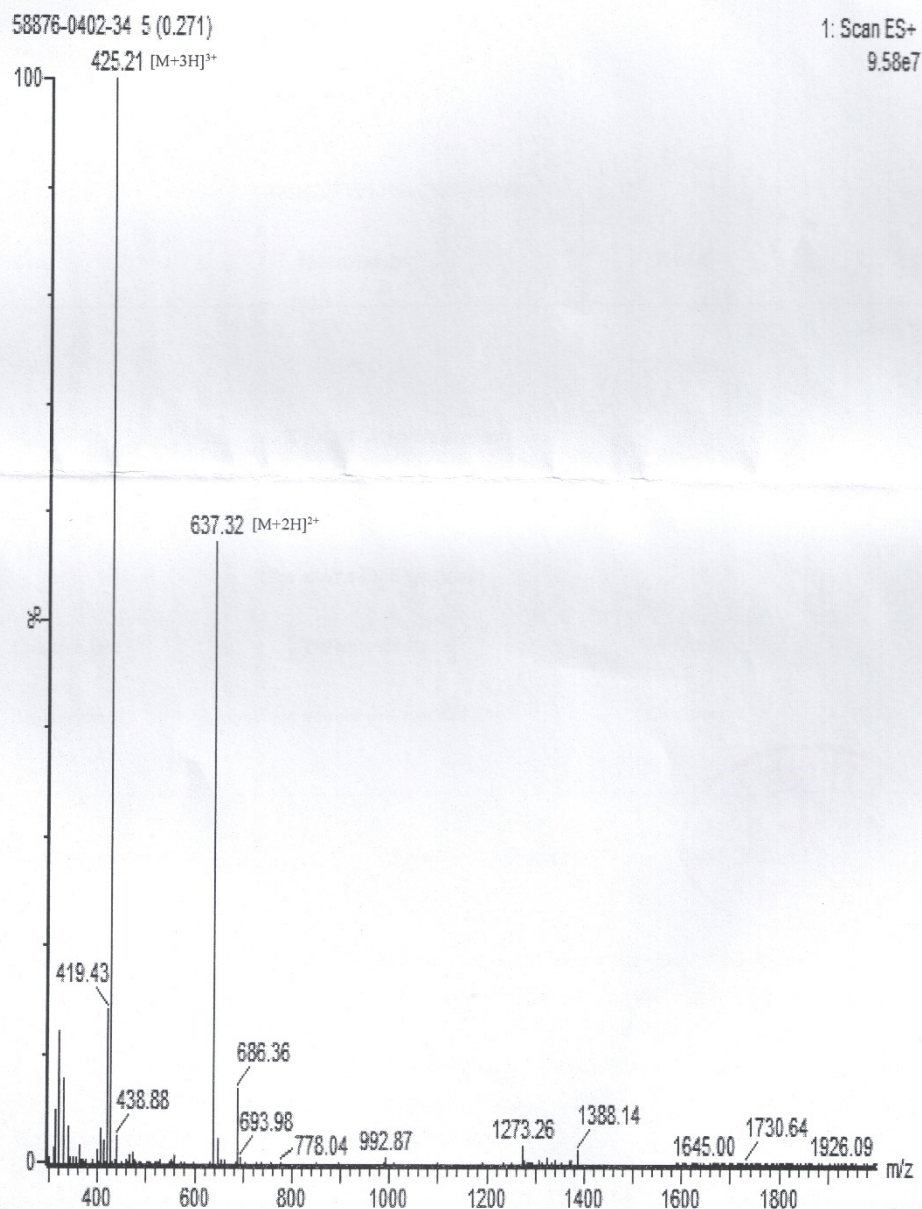
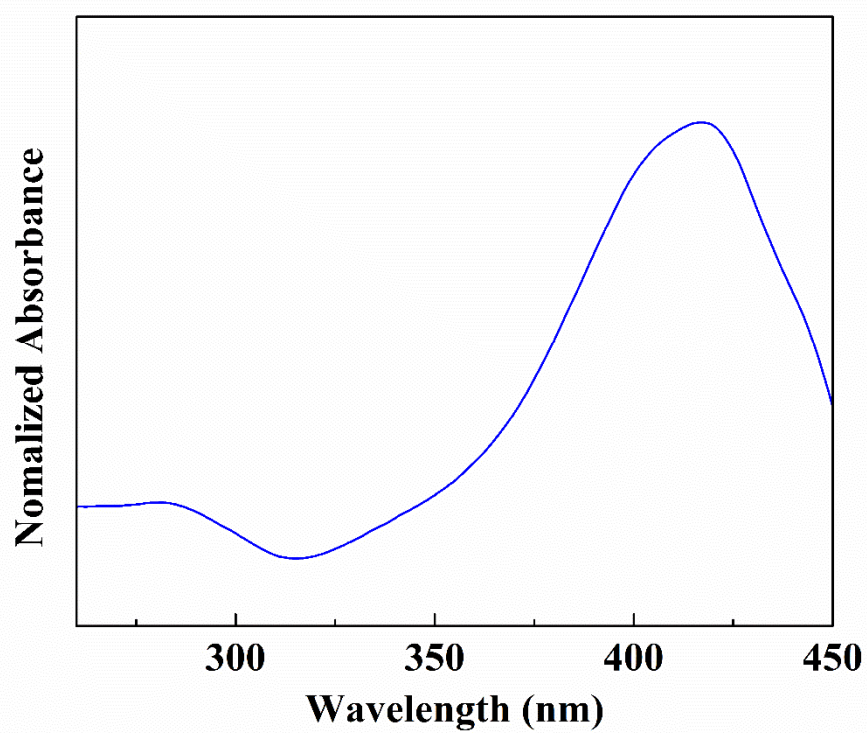


Figure S7. MS spectra of AC peptide.

Figure S8. QC fluorescence spectra in PBS solvents.

Figure S9. AC-QC fluorescence spectra in various solvents.





**Figure S8** AC-QC conjugate of UV-vis absorption spectra in DMSO.

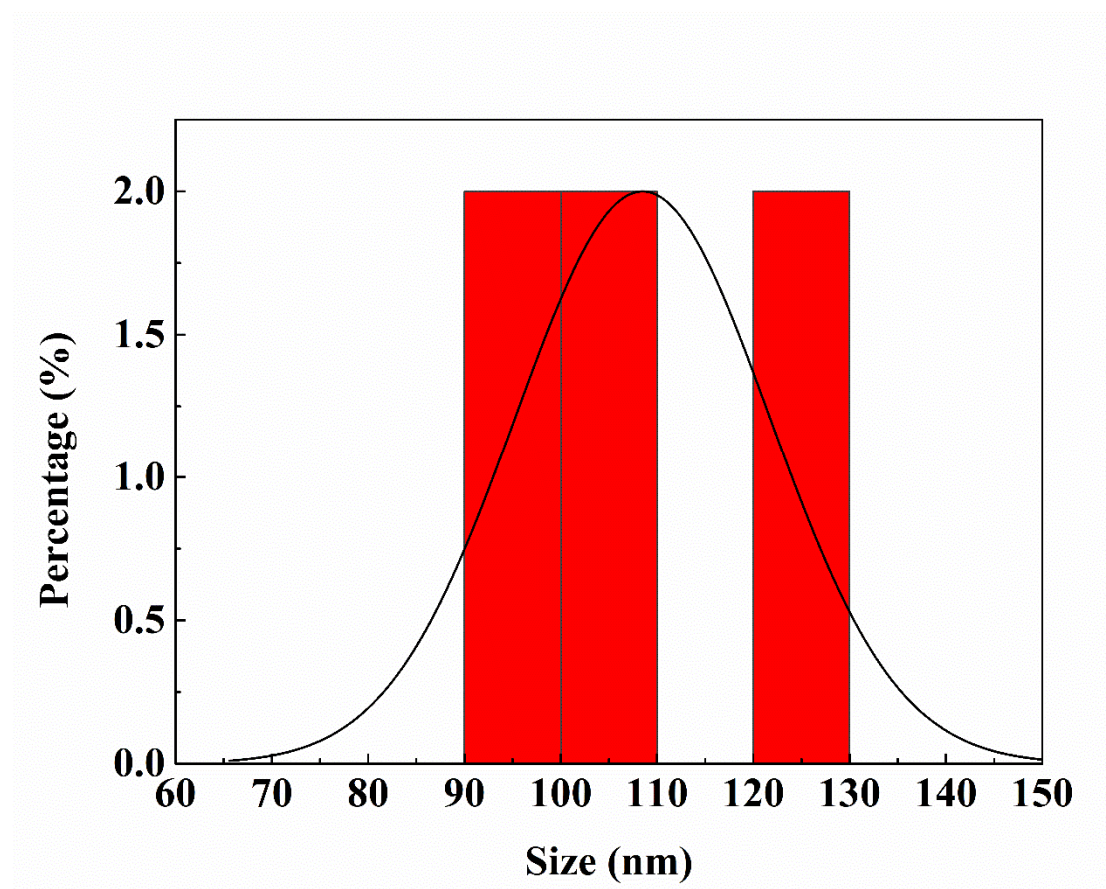


Figure S9. The size distribution of TEM.

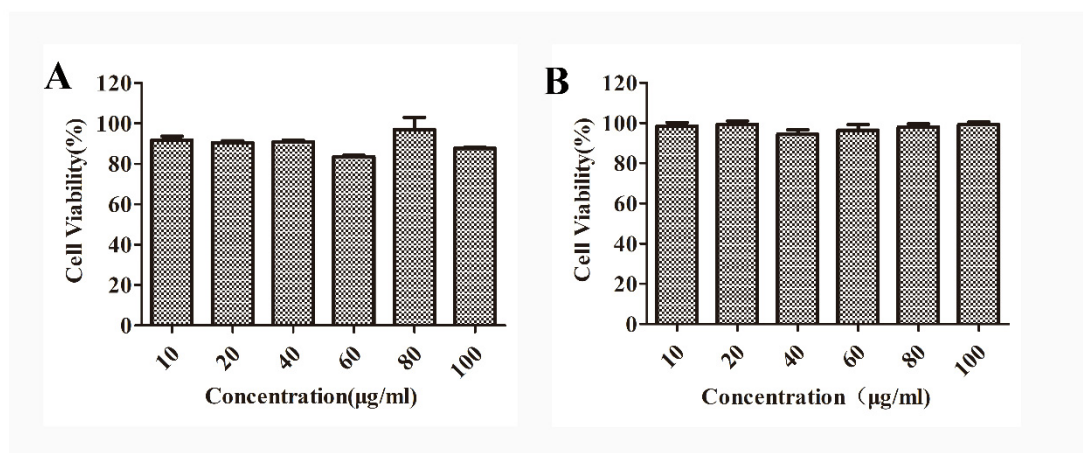
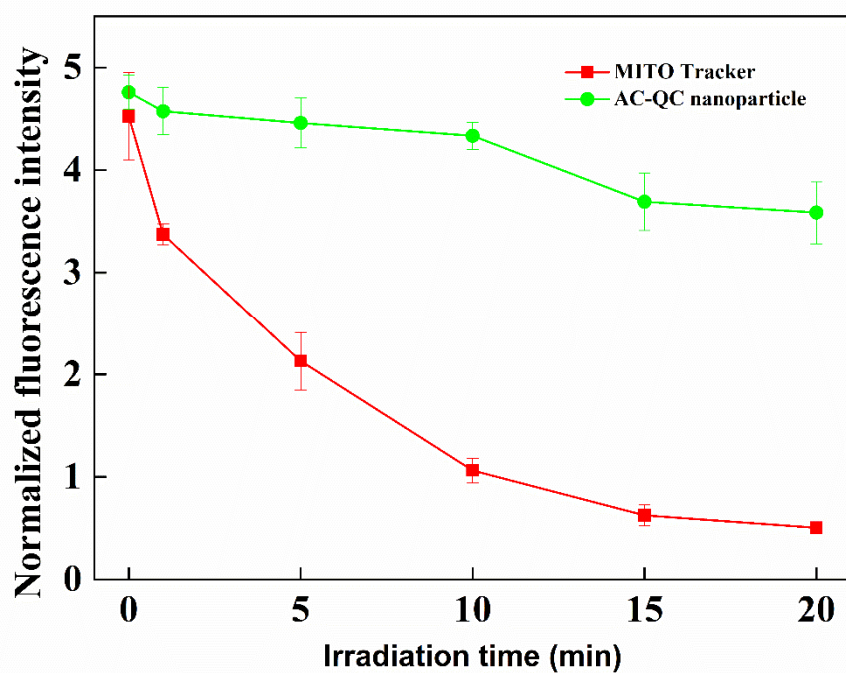
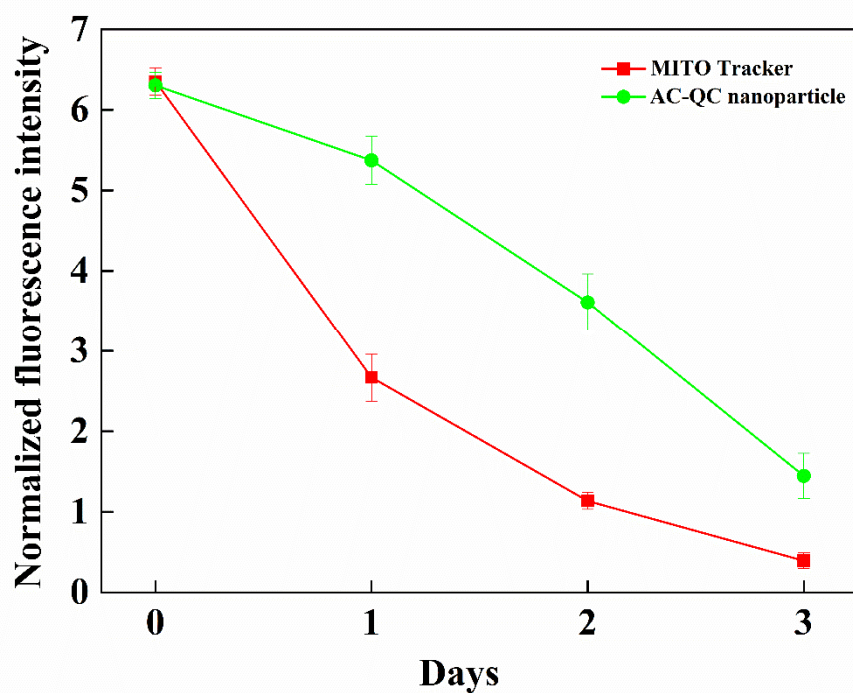


Figure S10. Relative cell viability of IOSE-80 cells (A) and L929 cells (B) against nanoparticle solution after cultured for 72 h with different nanoparticle concentrations.



**Figure S11.** Time-dependent peak fluorescence intensity of MITO Tracker and AC-QC nanoparticle after 20 min irradiation. Data represent mean values  $\pm$  standard deviation,  $n = 3$ , the statistical significance level is  $***p < 0.001$ . All experiments were carried out three times independently.



**Figure S12.** Long-term peak fluorescence intensity of MITO Tracker and AC-QC nanoparticle at 37 °C for 4 h and subculture for various time intervals from day 0 to day 3. Data represent mean values  $\pm$  standard deviation,  $n = 3$ , the statistical significance level is  $***p < 0.001$ . The experiment was carried out three times independently.