

Supplementary Information Available

Light-Up Bioprobe with Aggregation-Induced Emission Characteristics for Real-Time Apoptosis Imaging in Target Cancer Cells

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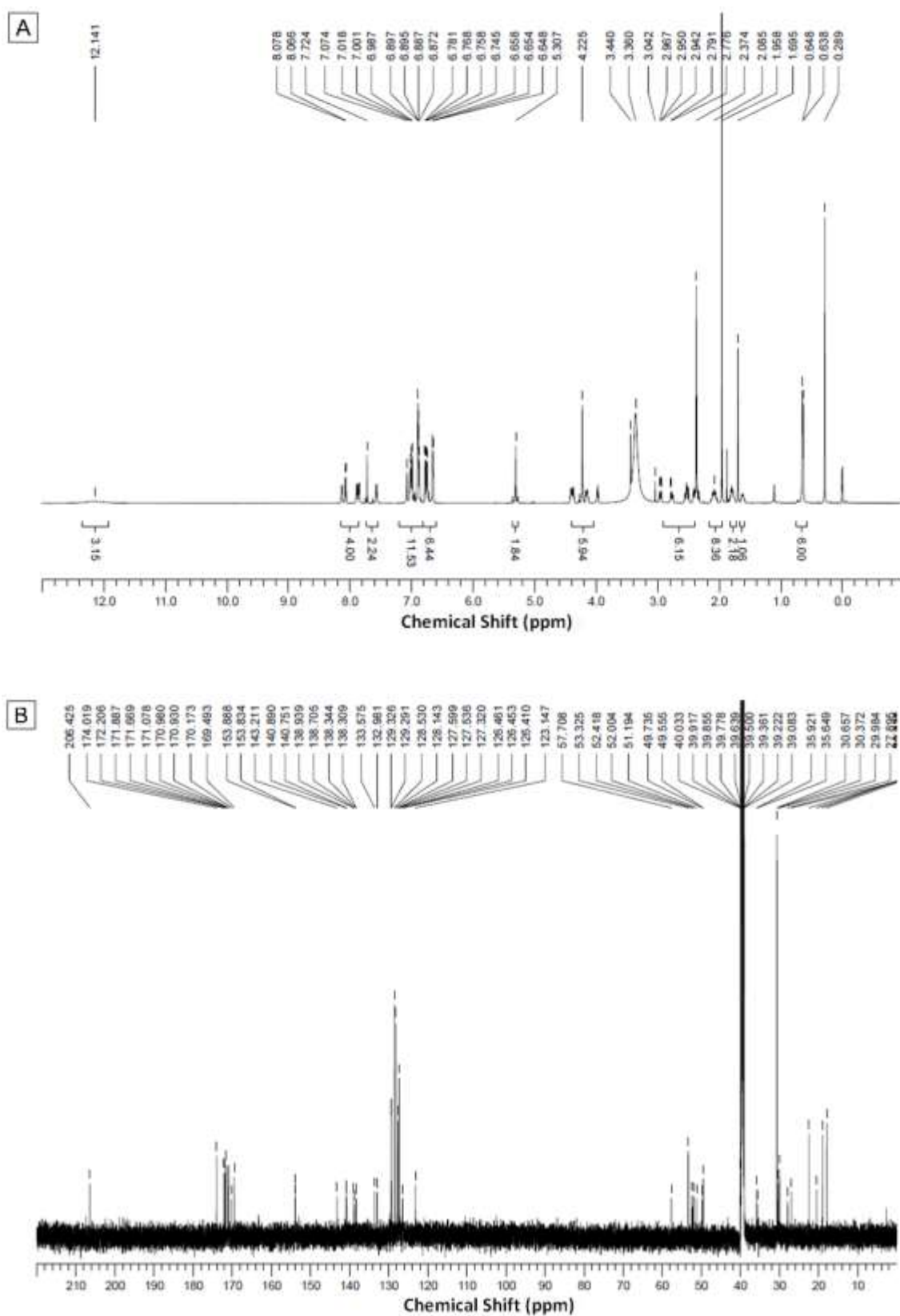


Fig. S1 (A) ^1H and (B) ^{13}C NMR spectra of Ac-DEVD-TPS- N_3 in $\text{DMSO-}d_6$.

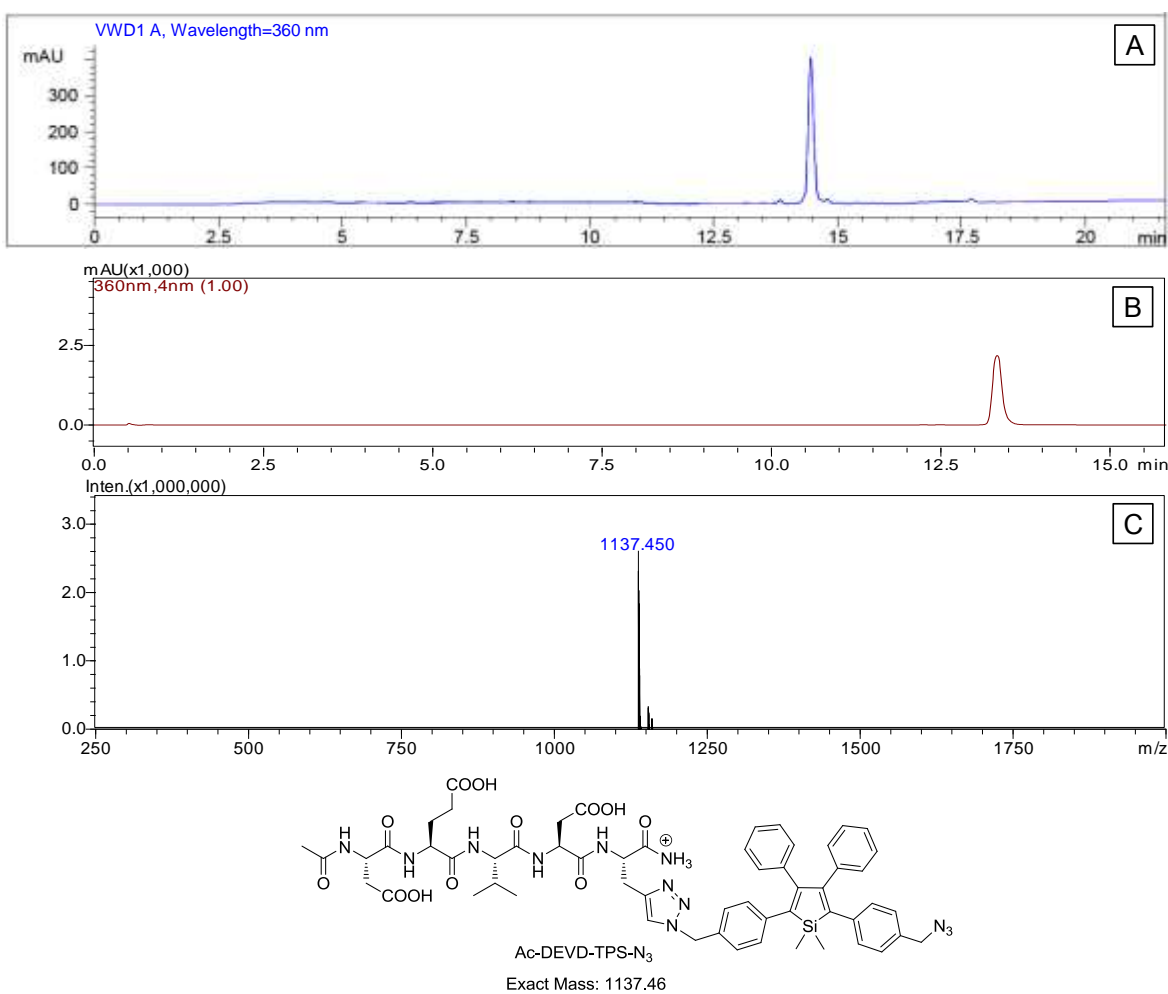


Fig. S2 (A) HPLC spectrum and (B and C) LC-MS spectra of Ac-DEVD-TPS-N₃. The difference in retention time for A and B is due to the different columns used for separation and analysis.

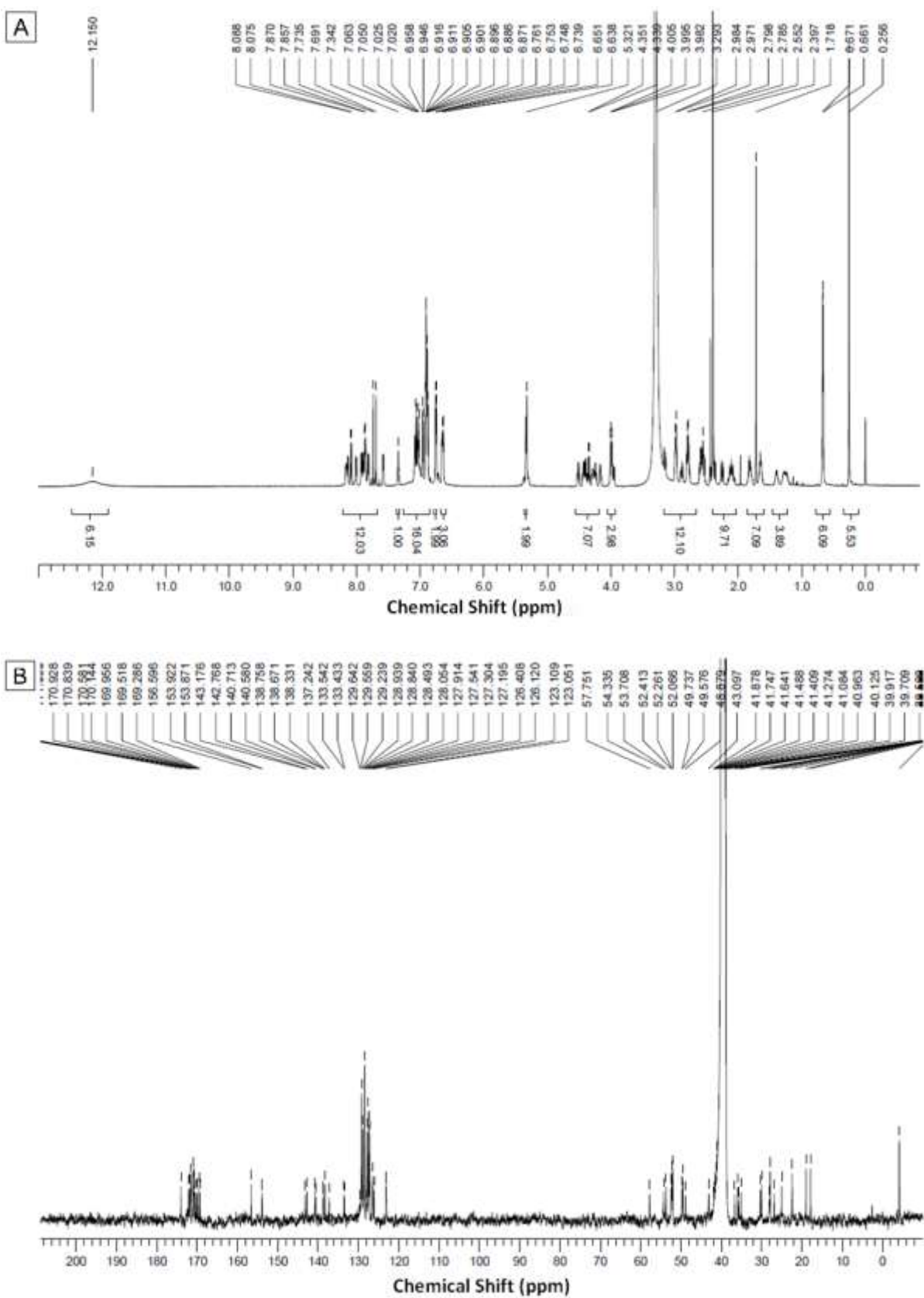


Fig. S3 (A) ^1H and (B) ^{13}C NMR spectra of Ac-DEVD-TPS-cRGD in $\text{DMSO-}d_6$.

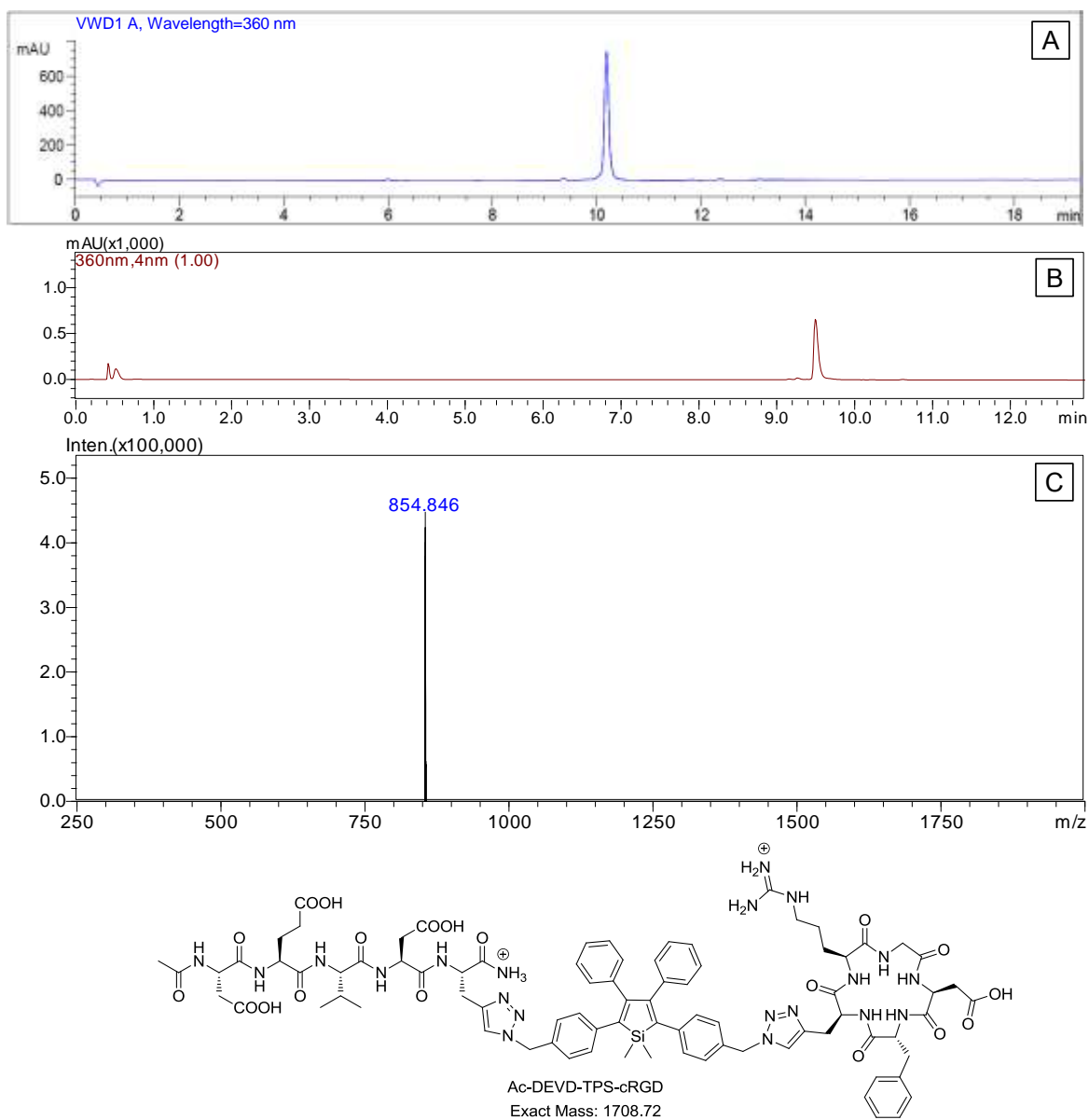


Fig. S4 (A) HPLC spectrum and (B and C) LC-MS spectra of Ac-DEVD-TPS-cRGD. The difference in retention time for A and B is due to the different columns used for separation and analysis.

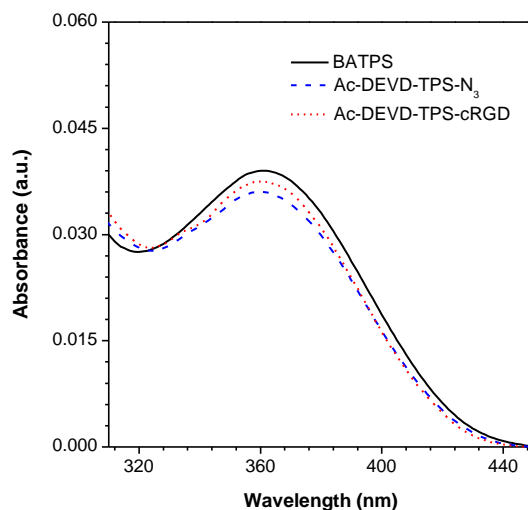


Fig. S5 UV-vis absorption spectra of BATPS, Ac-DEVD-TPS-N₃ and Ac-DEVD-TPS-cRGD in DMSO/water (v/v = 1: 199), [BATPS] = [Ac-DEVD-TPS-N₃] = [Ac-DEVD-TPS-cRGD] = 3.3 μM.

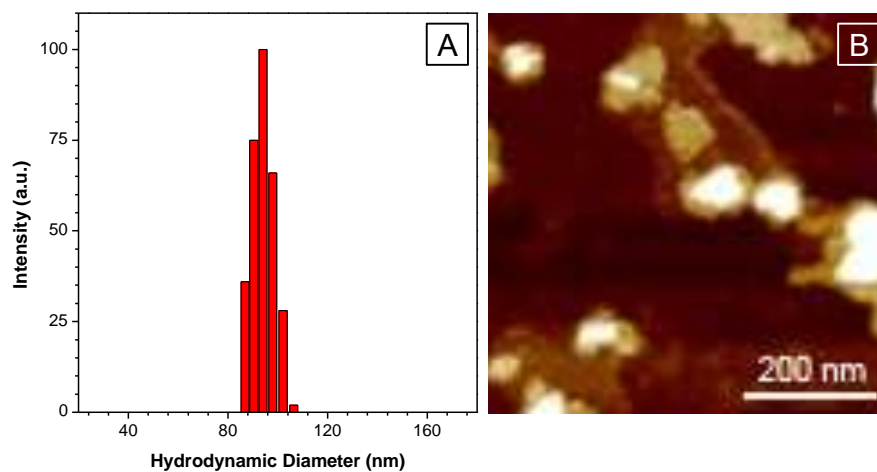


Fig. S6 (A) Hydrodynamic diameter and (B) atomic force microscopy (AFM) image of BATPS in DMSO/water (v/v = 1:199).

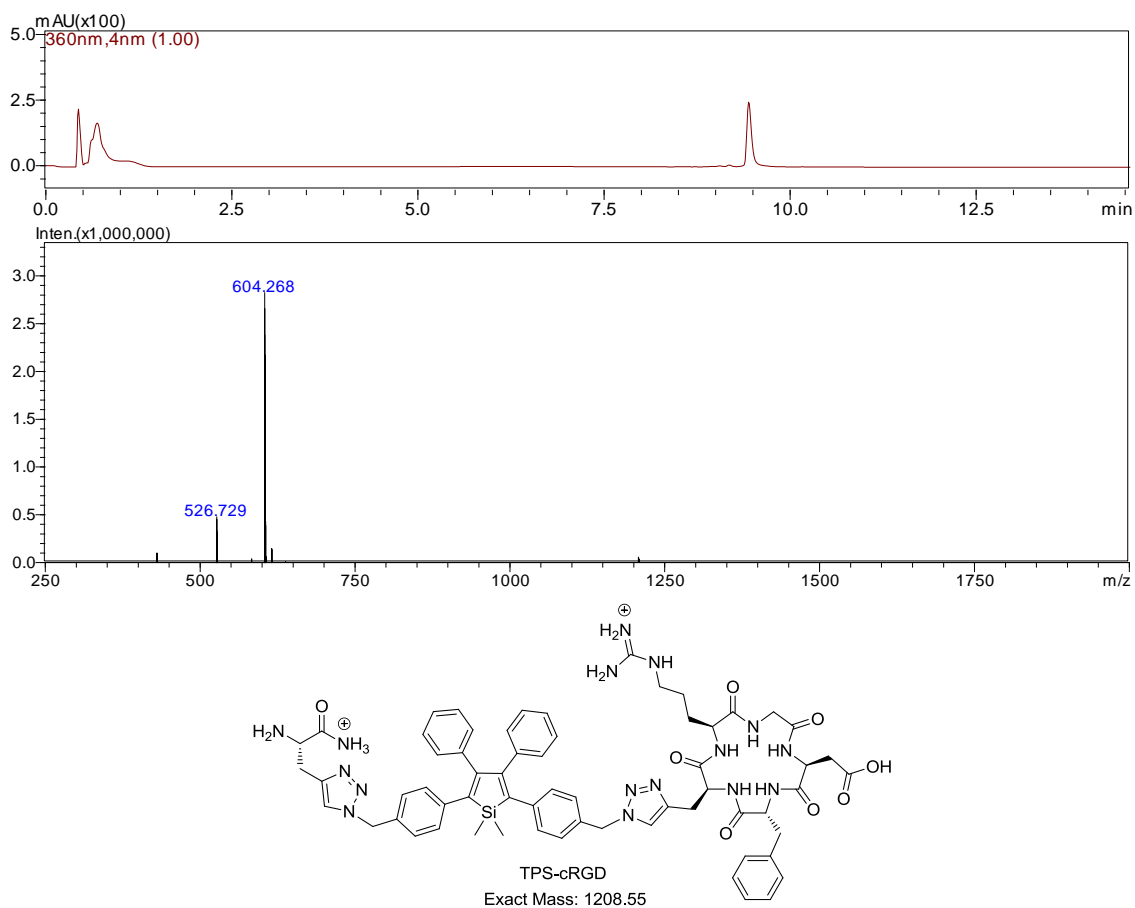


Fig. S7 The caspase-catalyzed hydrolysis of Ac-DEVD-TPS-cRGD ($t = 1$ h) to yield the residue of TPS-cRGD monitored by LC-MS, $[\text{Ac-DEVD-TPS-cRGD}] = 3.3 \mu\text{M}$, $[\text{Caspase-3}] = 80 \text{ ng mL}^{-1}$.

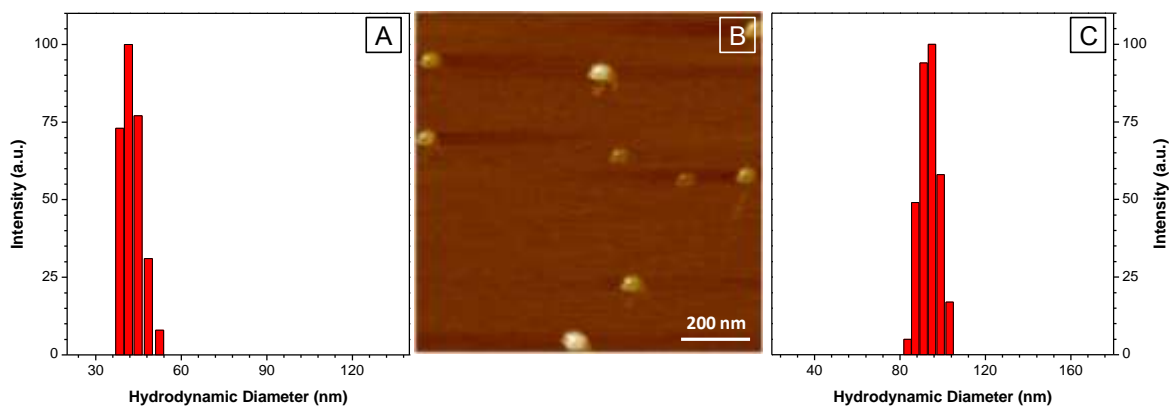


Fig. S8 (A) Hydrodynamic diameter and (B) AFM image of the residues of Ac-DEVD-TPS-cRGD after caspase-3 cleavage. (C) Hydrodynamic diameter of the residues of Ac-DEVD-TPS-N₃ after caspase-3 cleavage.

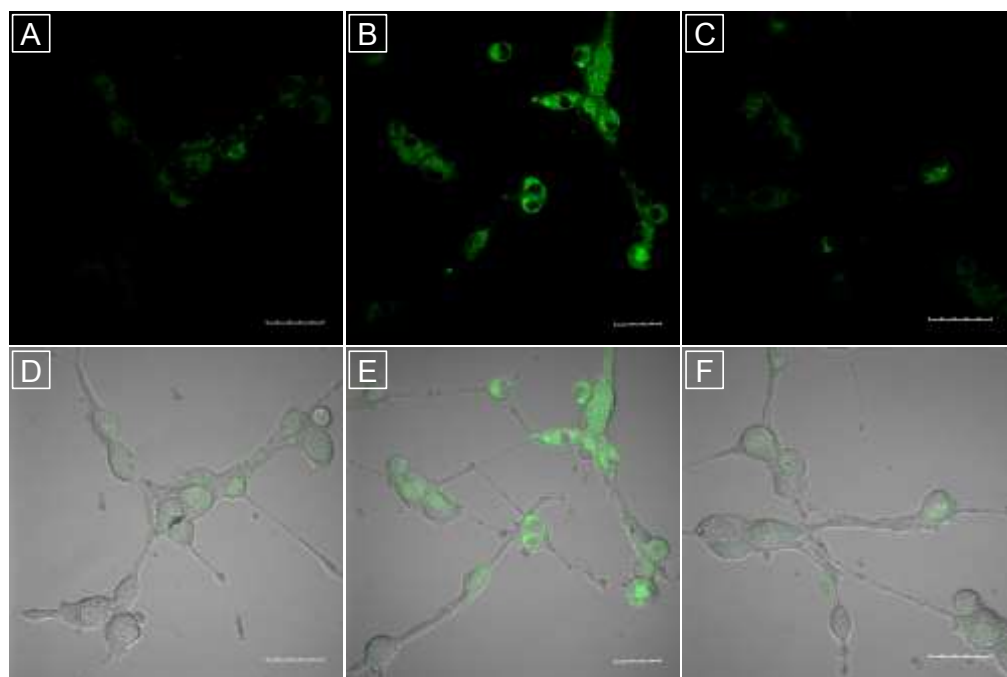


Fig. S9 CLSM images of (A) healthy and (B) apoptotic U87MG cells treated with Ac-DEVD-TPS-N₃. (C) CLSM image of STS-induced U87MG cells pretreated with caspase inhibitor before Ac-DEVD-TPS-N₃ staining. (D-F) are the corresponding fluorescence/transmission overlay images of (A-C). [Ac-DEVD-TPS-N₃] = 5 μ M, [STS] = 1 μ M, [Inhibitor] = 10 μ M. Scale bar: 30 μ m for all the images.

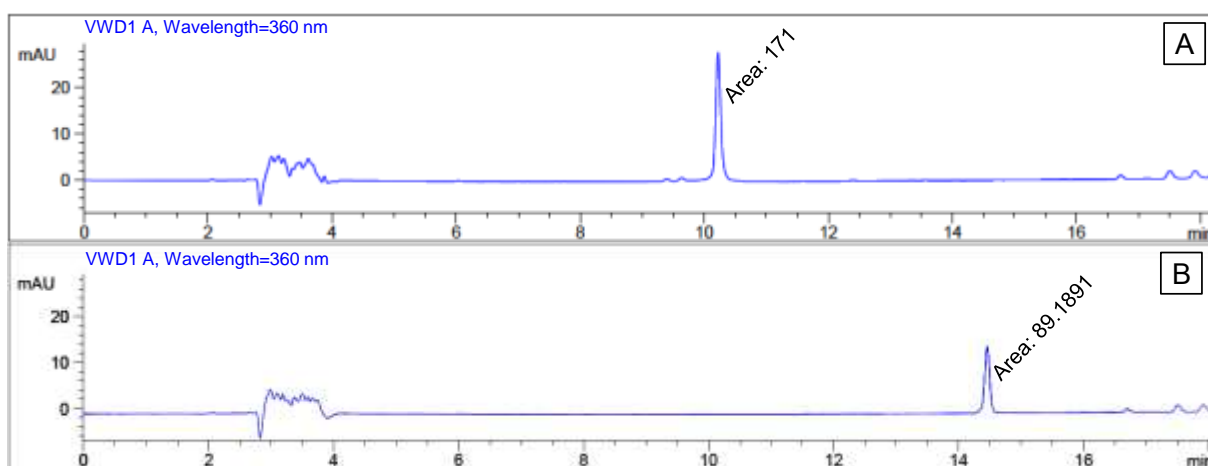


Fig. S10 HPLC spectra of (A) Ac-DEVD-TPS-cRGD and (B) Ac-DEVD-TPS-N₃ in U87MG cell lysates. The cells were incubated with both probes at 37 °C for 2 h, respectively.

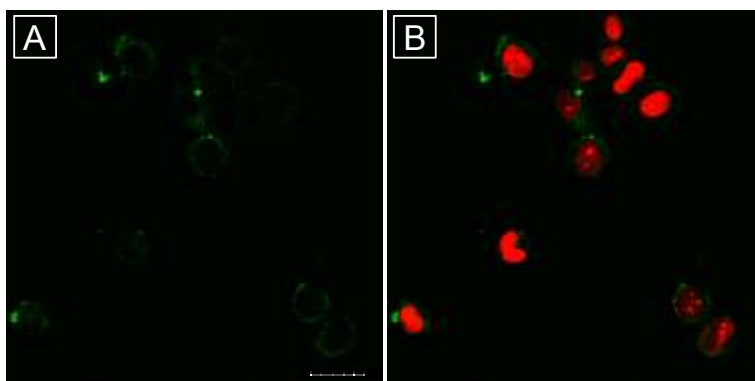


Fig. S11 (A, B) CLSM images of apoptotic 293T normal cells treated with Ac-DEVD-TPS-cRGD. The cellular nuclei were stained by propidium iodide (red). Scale bar: 30 μm for both images.

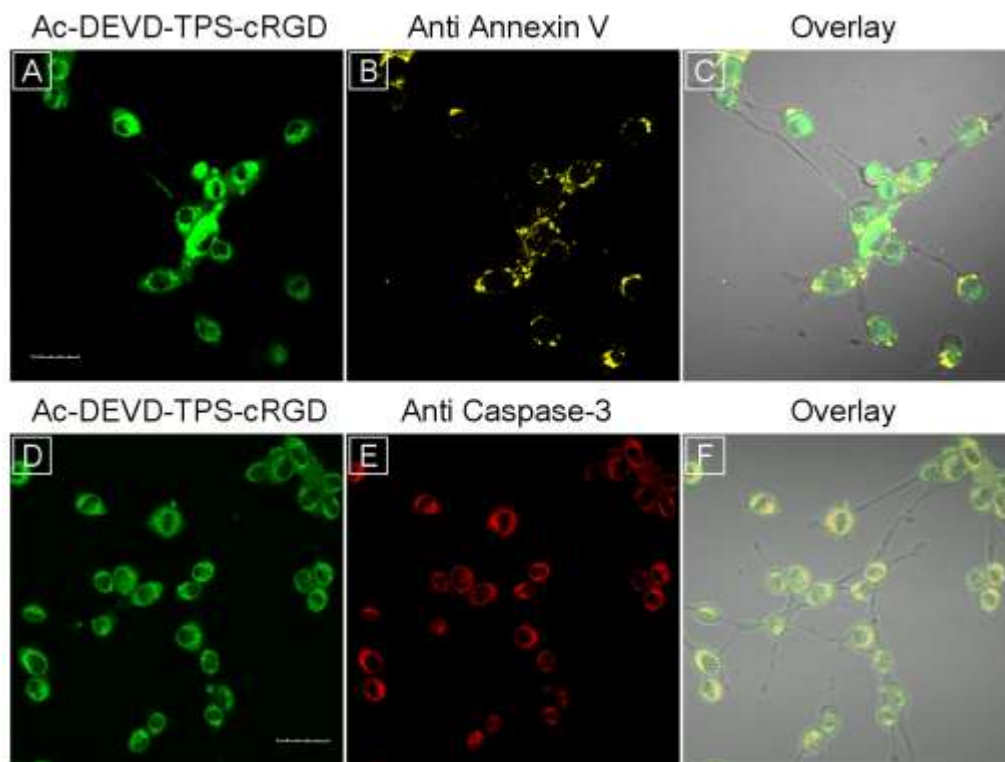


Fig. S12 CLSM images of apoptotic U87MG cells upon treatment with (A) Ac-DEVD-TPS-cRGD (green) and (B) Annexin V-Alexa Fluor 488 (yellow). (C) The overlay image of (A) and (B). CLSM images of apoptotic U87MG cells upon treatment with (D) Ac-DEVD-TPS-cRGD (green) and (E) anti-caspase-3 primary antibody followed by Texas Red-labeled secondary antibody (red). (F) The overlay image of (D) and (E). [Ac-DEVD-TPS-cRGD] = 5 μM. Scale bar: 30 μm for all the images.

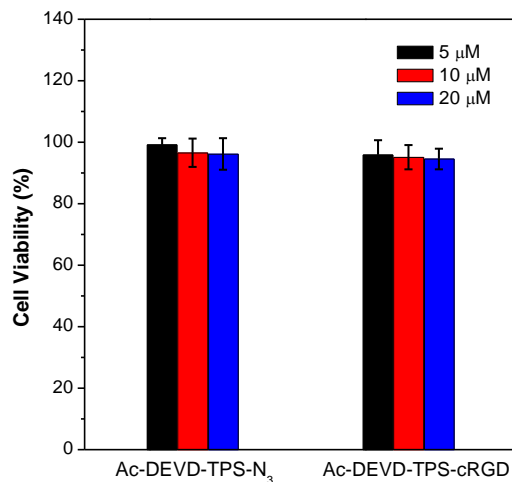


Fig. S13 Metabolic viability of U87MG cancer cells after incubation with Ac-DEVD-TPS-N₃ and Ac-DEVD-TPS-cRGD at different concentrations for 48 h, respectively. U87MG cells upon incubation with DMEM media only is used as the control.