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## SUPPLEMENTARY INFORMATION



Figure S1. Synthetic route of DEVD-Cy-OH



Figure S2. Mass spectrum of Cy-OH.



Figure S3. Mass spectrum of compound 2.



Figure S4. Mass spectrum of Compound 3.



Figure S5. Mass spectrum of Compound 4.



Figure S6. Mass spectrum of DEVD-Cy-OH.



Figure S7. <sup>1</sup>H-NMR (CD4O) of the Cy-OH.



Figure S8. <sup>1</sup>H-NMR (CD4O) of the DEVD-Cy-OH.



Figure S9. (a) Relative viability of HUCMSCs incubated with PAC-1 at various concentrations for 12 h (\*p < 0.05; n = 6 per group). (b) Relative viability of HUCMSCs incubated with the probe at various concentrations for 12 h. (c) Probe fluorescence in the absence or presence of apoptotic cell lysate at 37 °C.



Figure S10. (a) Confocal microscope images of bioorthogonally labeled HUCMSCs with Ac<sub>4</sub>ManNAz (+)/DBCO-Cy7(+) at different incubation times. (b) Fluorescence imaging of different numbers of cells. (c) Linear fit of cell number-fluorescence intensity.



Figure S11. (a) Bioluminescence intensity, (b) Cy7 fluorescence intensity, and (c) apoptosis probe fluorescence intensity of the healthy mice (control) and the CCl<sub>4</sub>-induced acute liver injury mice (model) within 7 days (168 h) after transplantation with labeled HUCMSCs. (d) Grey values of MRI images of the livers of the healthy mice (control) and the CCl<sub>4</sub>-induced acute liver injury mice (model) within 7 days (168 h) after transplantation with after transplantation with labeled HUCMSCs. Healthy mice (model) within 7 days (168 h) after transplantation with labeled HUCMSCs. Healthy mice without HUCMSCs transplatation were set as blank.



Figure S12. Cy7 fluorescence intensity of the lungs (a) and the livers (b), and apoptosis probe fluorescence intensity of the lungs (c) and the livers (d) of the healthy mice (control) and the CCl<sub>4</sub>-induced acute liver injury mice (model) within 7 days after transplantation with L-HUCMSCs.

