Electronic Supporting Information

A selective and sensitive near-infrared fluorescent probe for *in vivo* real time tracking of exogenous and metabolized hydrazine, a genotoxic impurity

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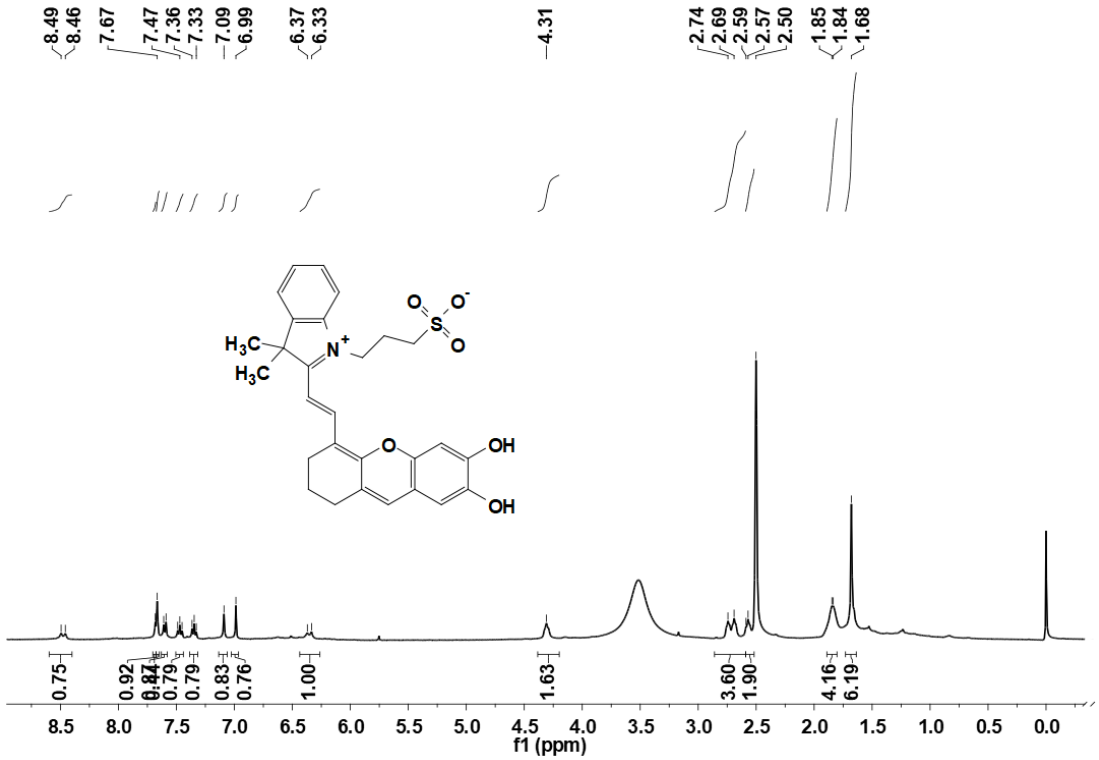

Fig. S1 ^{1}H NMR of **Hcy-DH** in DMSO-d_6.

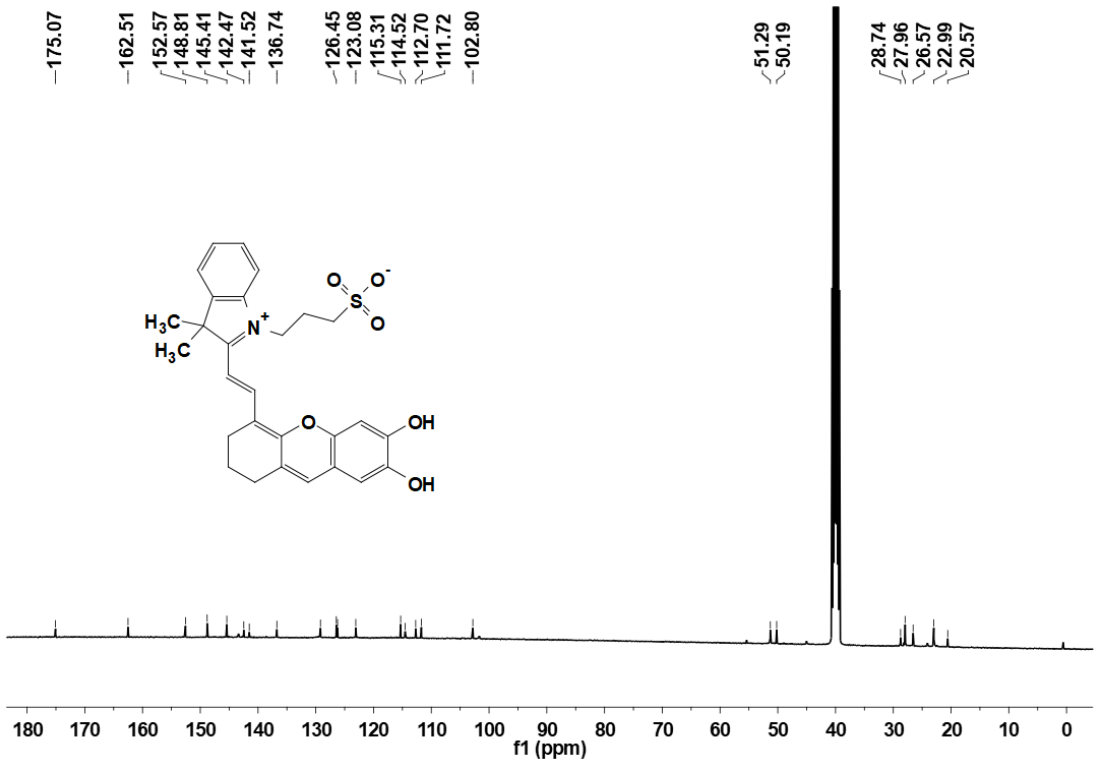

Fig. S2 ^{13}C NMR of **Hcy-DH** in DMSO-d_6.

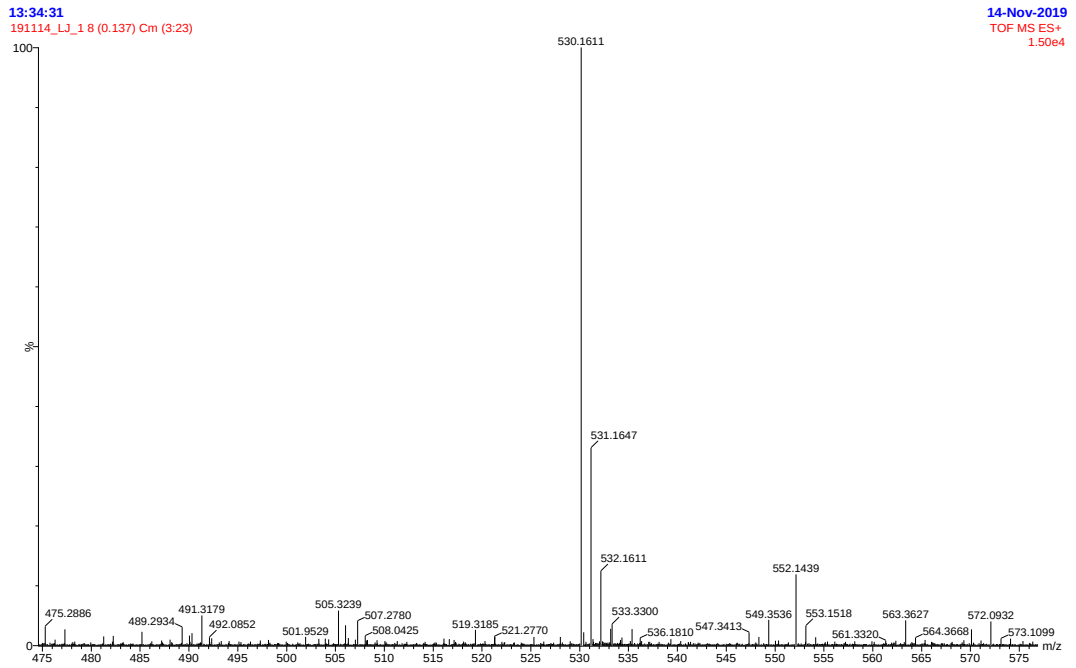

Fig. S3 HRMS of **Hcy-DH**.

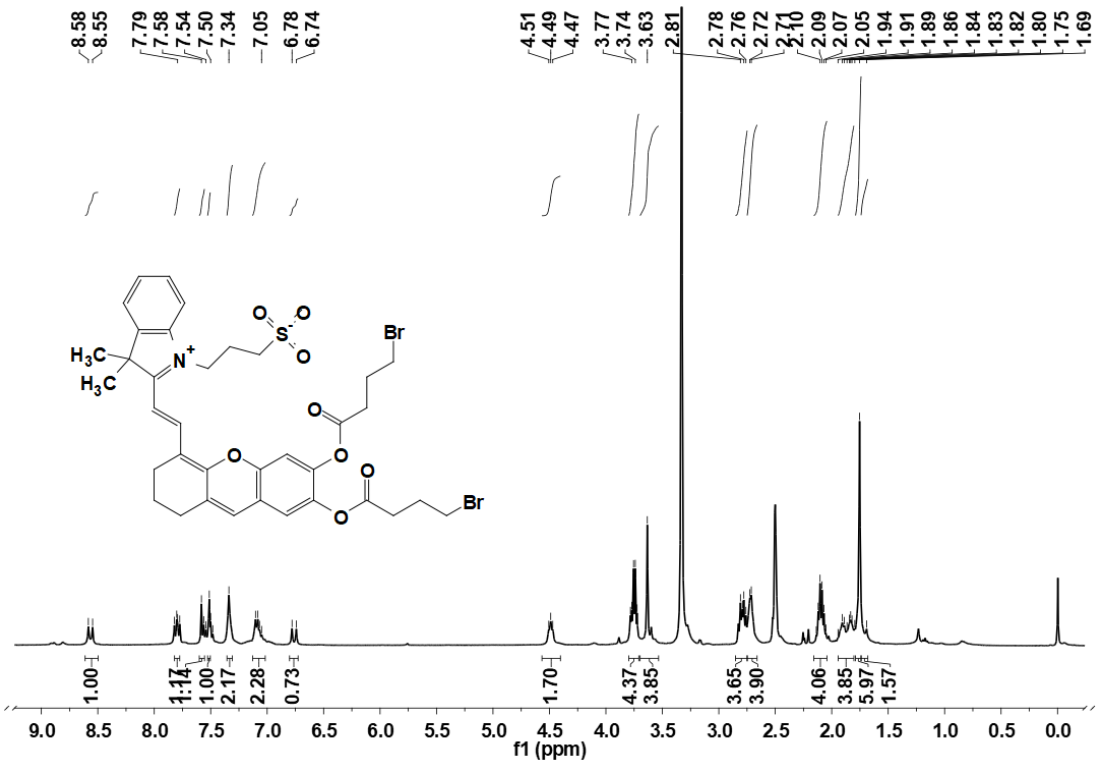

Fig. S4 ^{1}H NMR of **Hcy-DB** in DMSO-d_6.

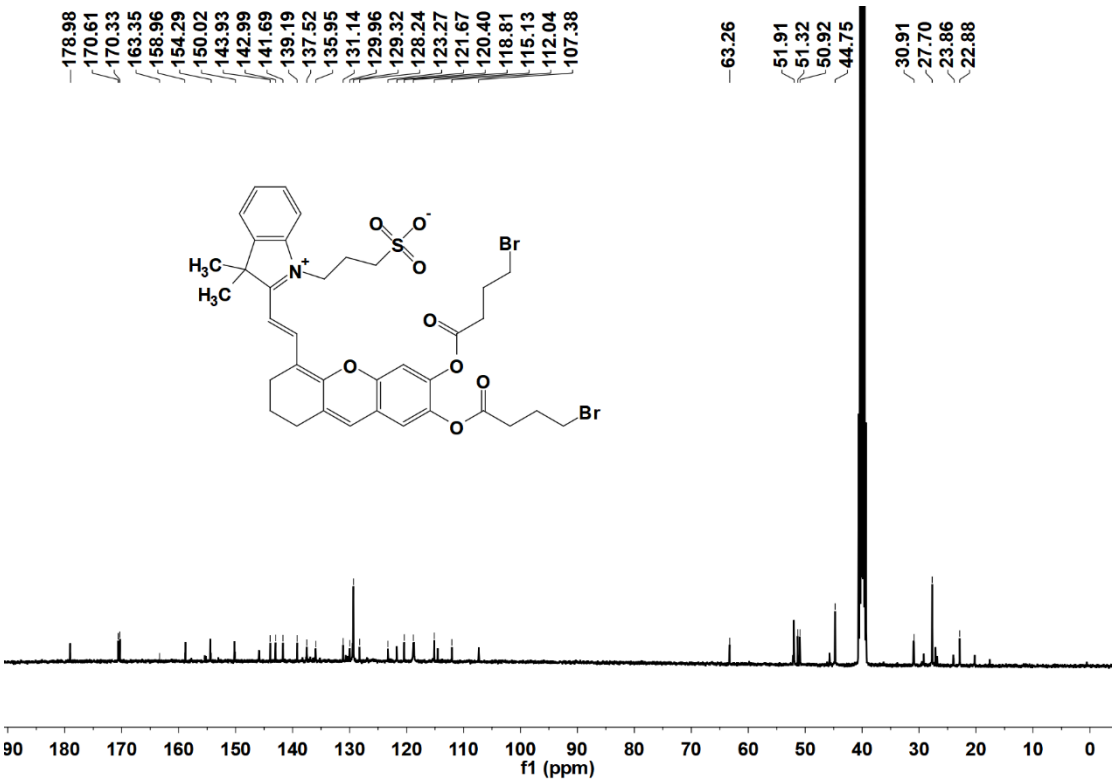

Fig. S5 ^{13}C NMR of **Hcy-DB** in DMSO-d_6.

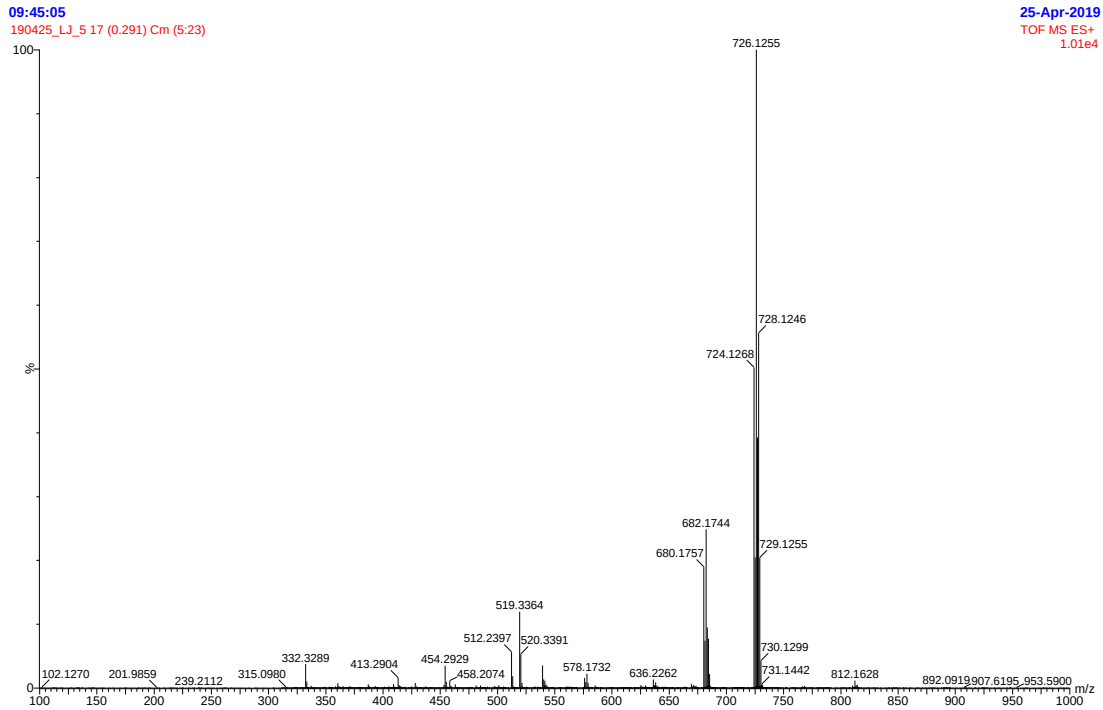

Fig. S6 HRMS of **Hcy-DB**.

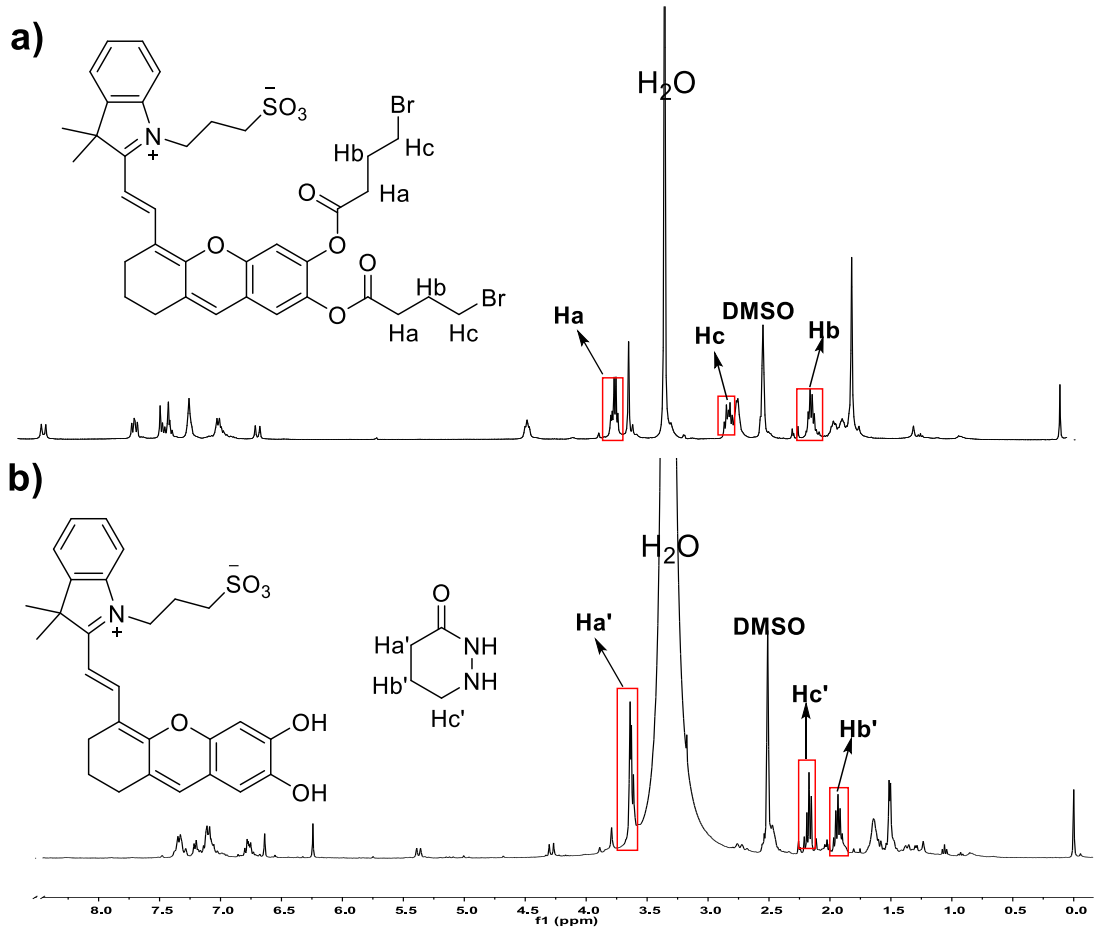

Fig. S7 ^{1}H NMR spectra of **Hcy-DB** in the absence (a) and presence (b) of N_2H_4 (20 equiv) in DMSO-d_6.

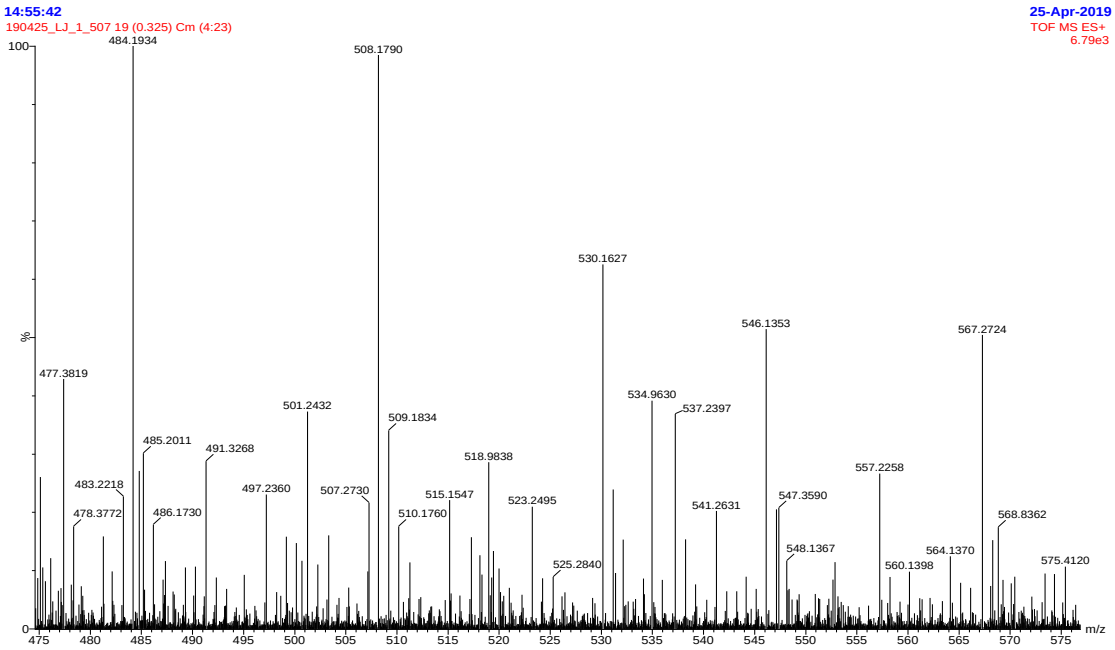

Fig. S8 HRMS of **Hcy-DB** upon the addition of hydrazine.

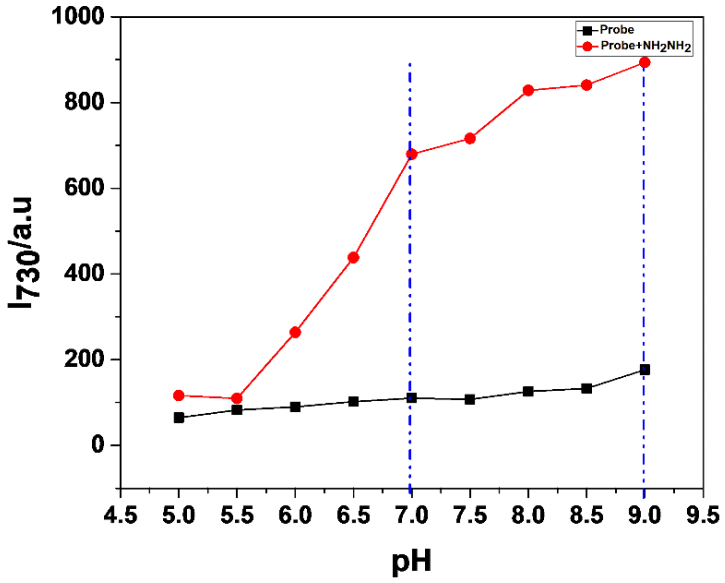

Fig. S9 The effect of pH on the response of **Hcy-DB** (10 μM) to hydrazine (200 μM).

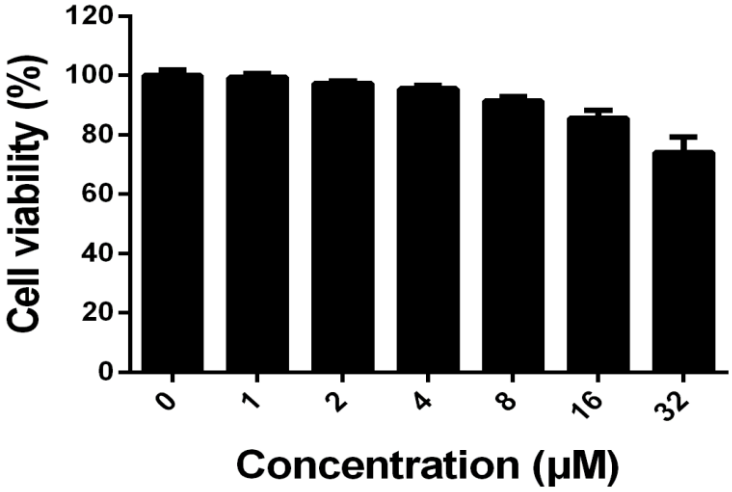

Fig. S10 Cell viability of H1975 cells after incubation with different concentrations of **Hcy-DB** (0-32 μM) for 24 h.

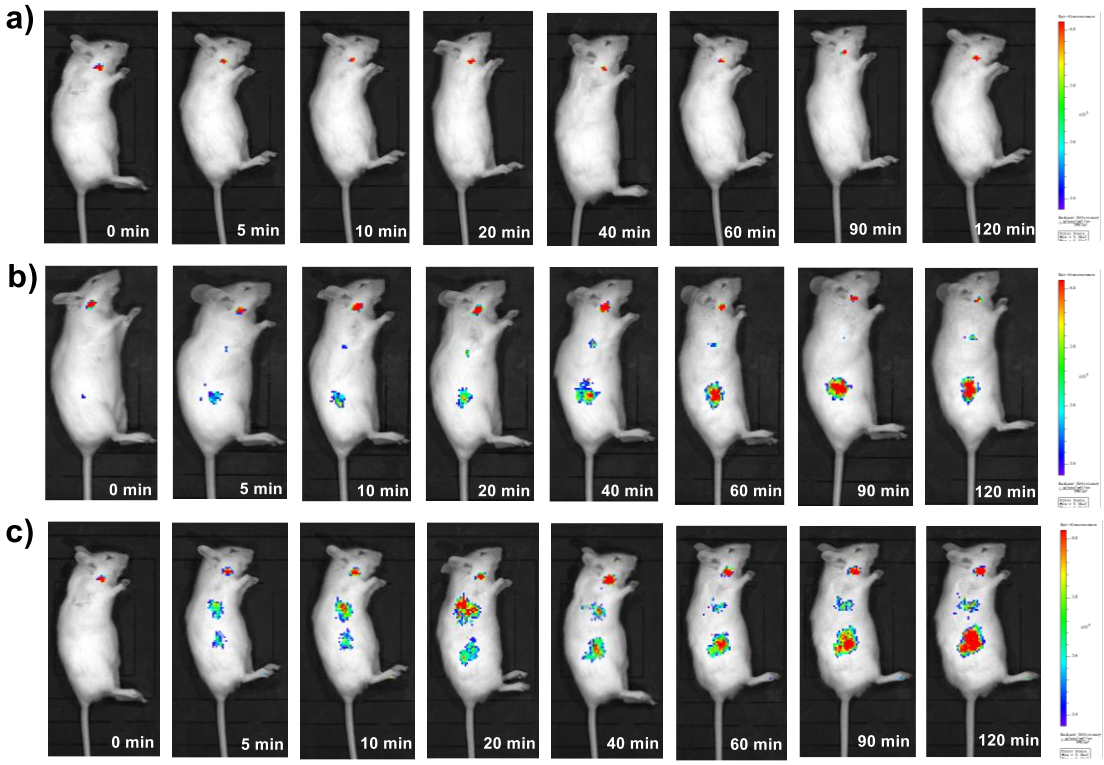

Fig. S11 Fluorescence images (pseudocolor) of Kunming mice. (a) the mouse was given a tail-vein injection of **Hcy-DB** (50 μL, 50 μM); (b) the mouse was given a tail-vein injection of **Hcy-DB** (50 μL, 50 μM) followed by hydrazine (50 μL, 500 μM); (c) the mouse was given a tail-vein injection of **Hcy-DB** (50 μL, 50 μM) followed by an intragastric administration of isoniazid (5.4 mg) in 0.6 mL 20% DMSO-PBS buffer (pH = 7.4, 10 mM, v/v). The mice were imaged with an excitation filter of 600 nm and an emission filter of 730 nm. Images were taken at 0, 5, 10, 20, 40, 60, 90 and 120 min.