

Supplementary Materials

Acyl hydrazides and acyl hydrazone as high performance chemical exchange saturation transfer MRI contrast agents

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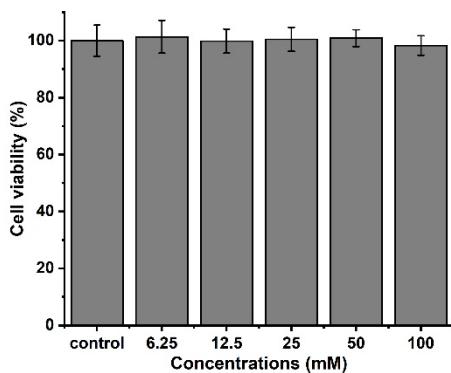


Figure S1. Cytotoxicity assay of ADH on 4T1 cells with different concentration range.

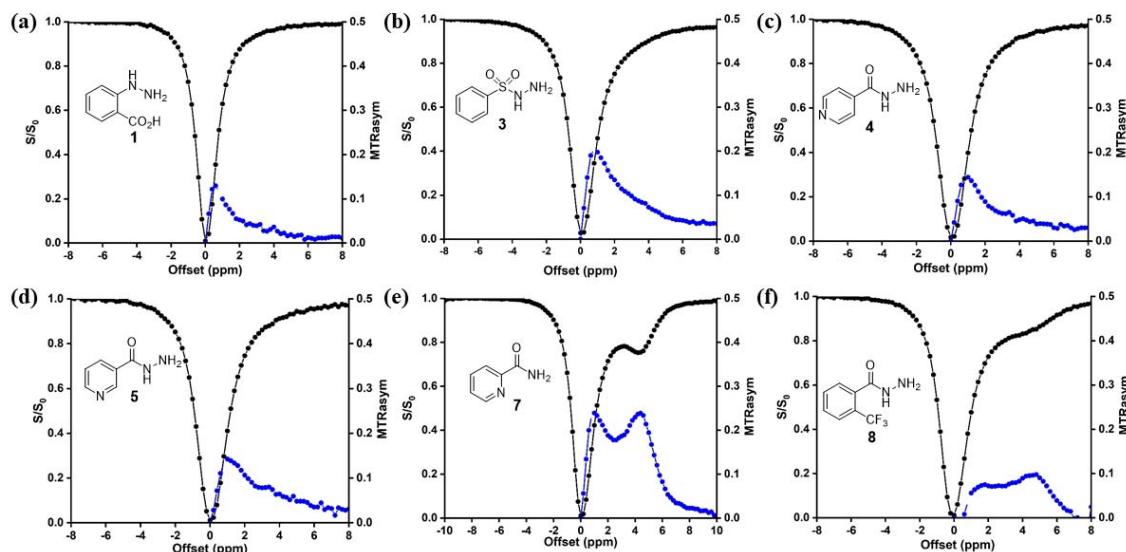


Figure S2. Z spectra and MTR_{asym} spectra of acyl hydrazide **1** (a), **3** (b), **4** (c), **5** (d), **7** (e) and **8** (f). Experimental conditions: CEST data were obtained at 40 mM concentration; pH 7.2, tsat = 3 s, B₁ = 3.6 μT, 37 °C.

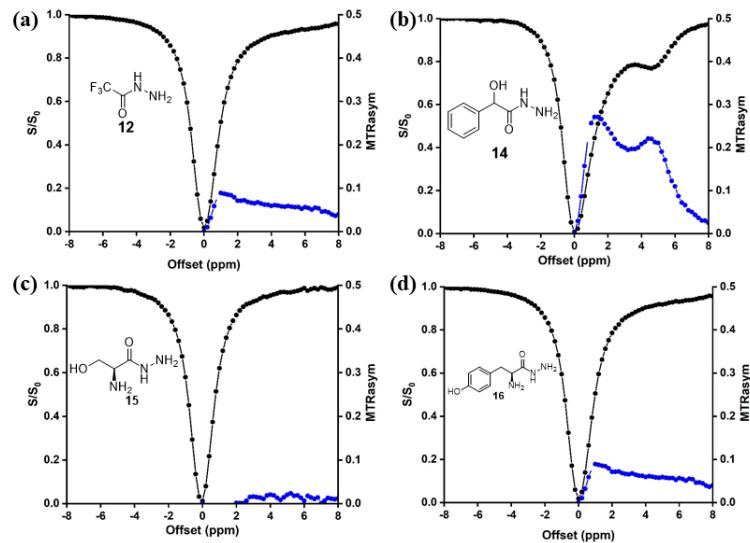


Figure S3. Z spectra and MTR_{asym} of acyl hydrazide **12** (a), **14** (b), **15** (c), and **16** (d). Experimental conditions: CEST data were obtained at 40 mM concentration; pH 7.2, tsat = 3 s, B₁ = 3.6 μT, 37 °C.

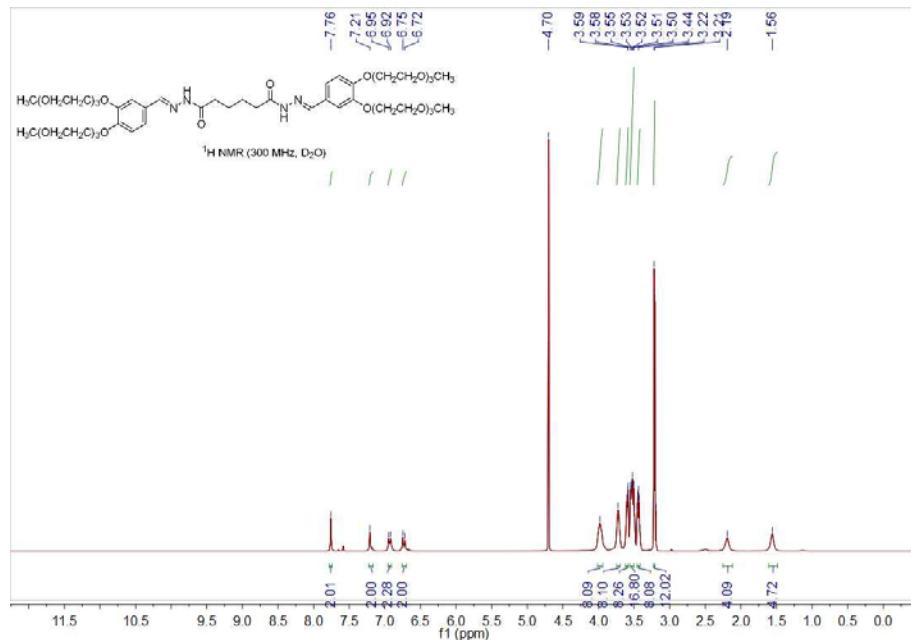


Figure S4. ¹H NMR of acyl hydrazone **17**

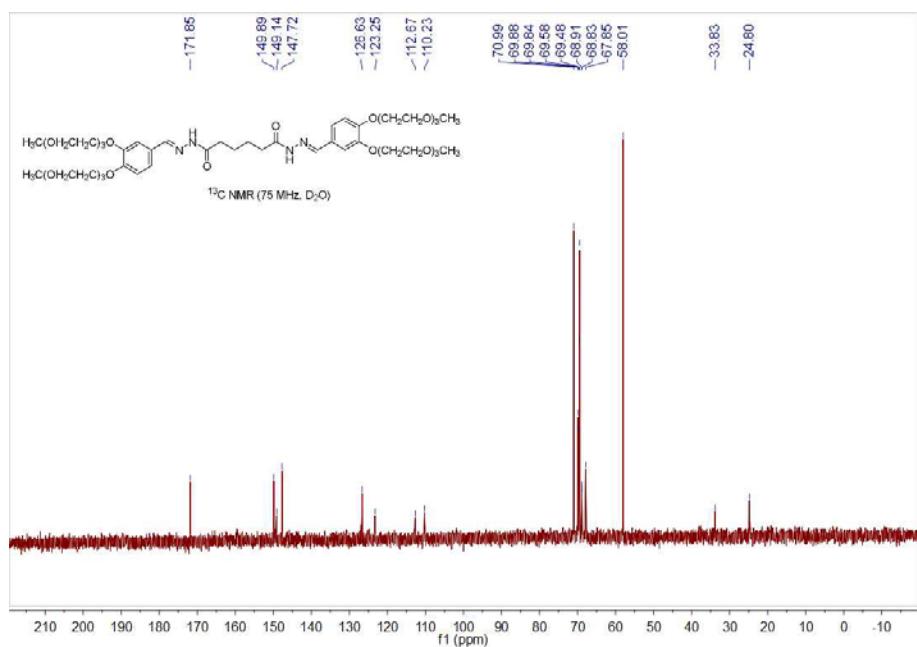


Figure S5. ^{13}C NMR of acyl hydrazone **17**

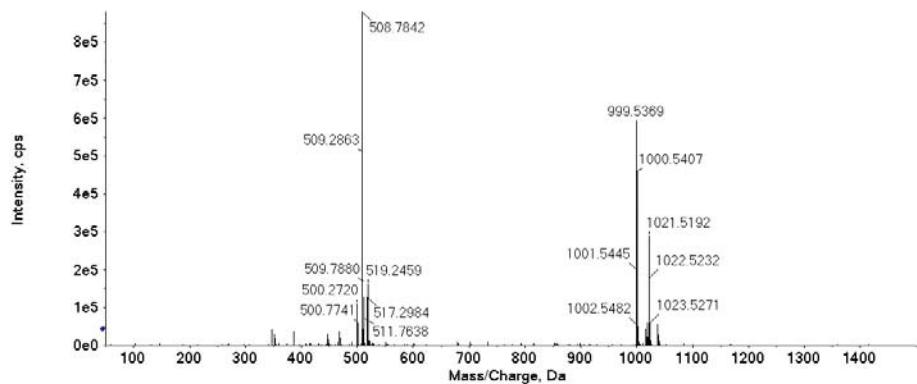


Figure S6. HRMS of acyl hydrazone **17**, calcd for $\text{C}_{48}\text{H}_{79}\text{N}_4\text{O}_{18}^+$ ($[\text{M}+\text{H}]^+$) 999.5384, found 999.5369.