

# Supplementary Materials

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

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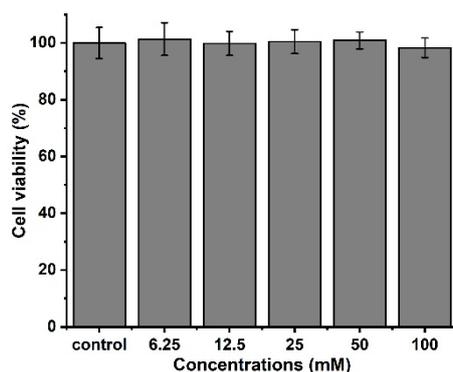
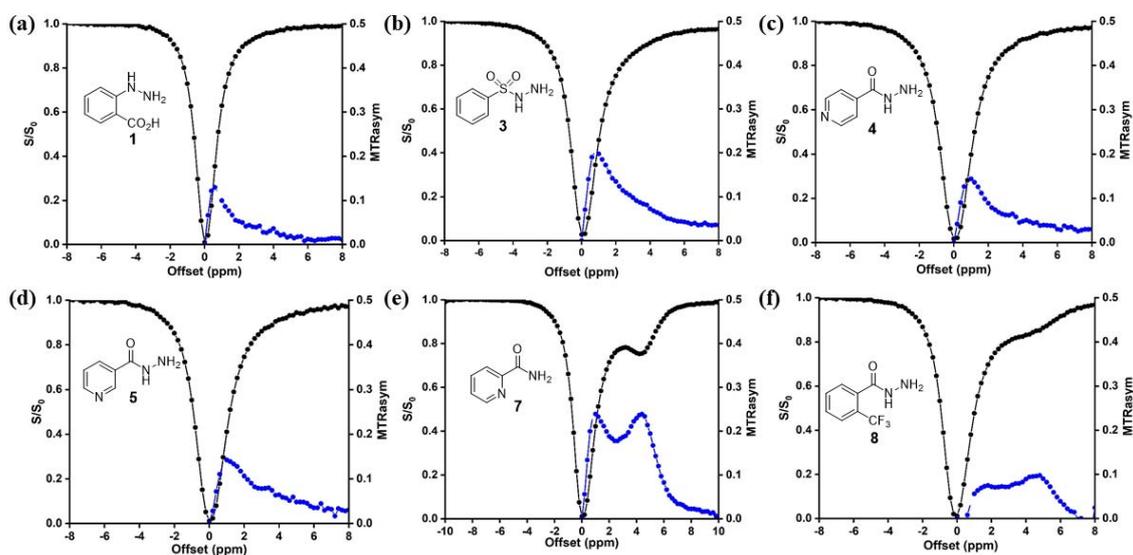
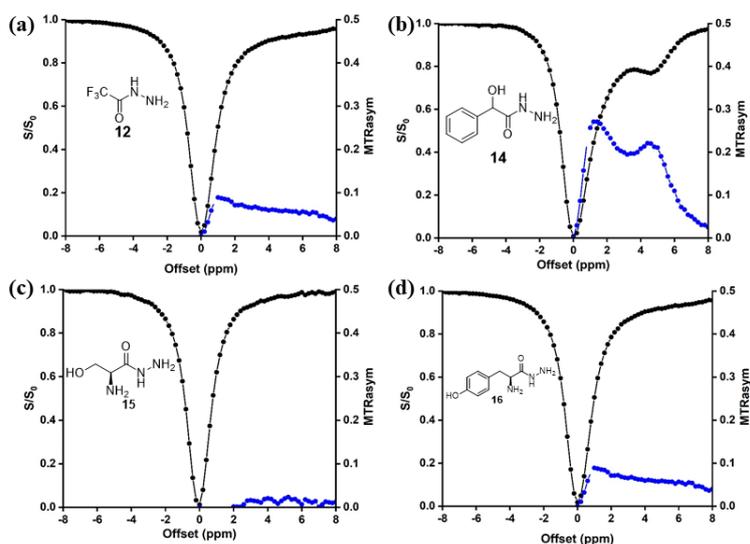


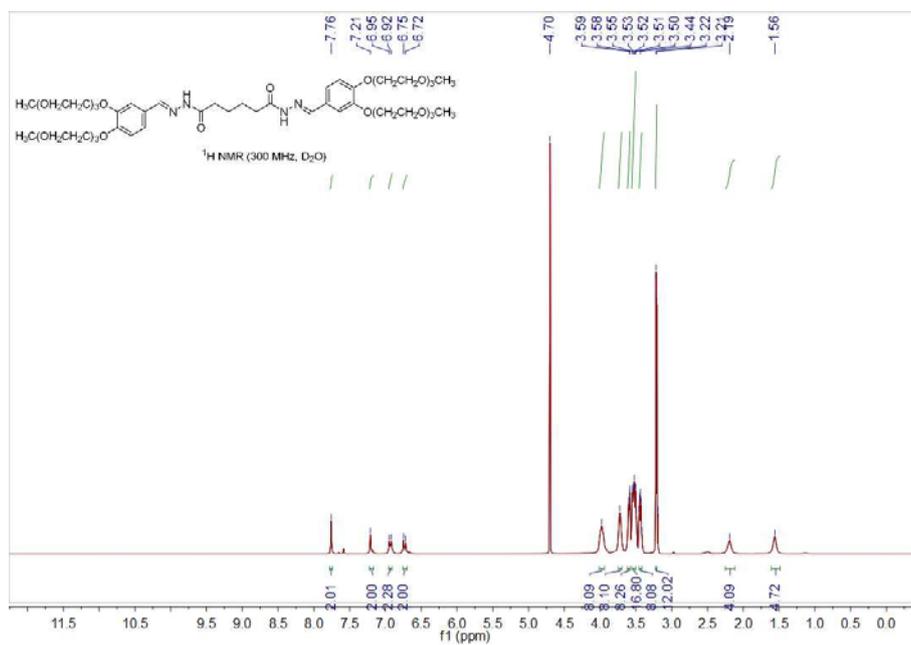
Figure S1. Cytotoxicity assay of ADH on 4T1 cells with different concentration range.



**Figure S2.** Z spectra and MTR<sub>asym</sub> 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, B<sub>1</sub> = 3.6 μT, 37 °C.



**Figure S3.** Z spectra and MTR<sub>asym</sub> 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, B<sub>1</sub> = 3.6 μT, 37 °C.



**Figure S4.** <sup>1</sup>H NMR of acyl hydrazide **17**

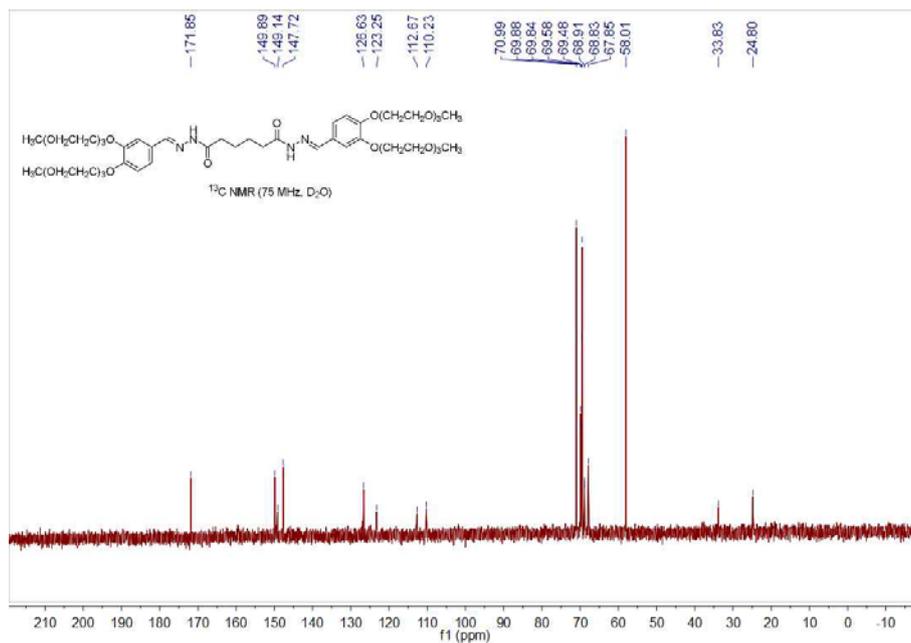


Figure S5. <sup>13</sup>C NMR of acyl hydrazone 17

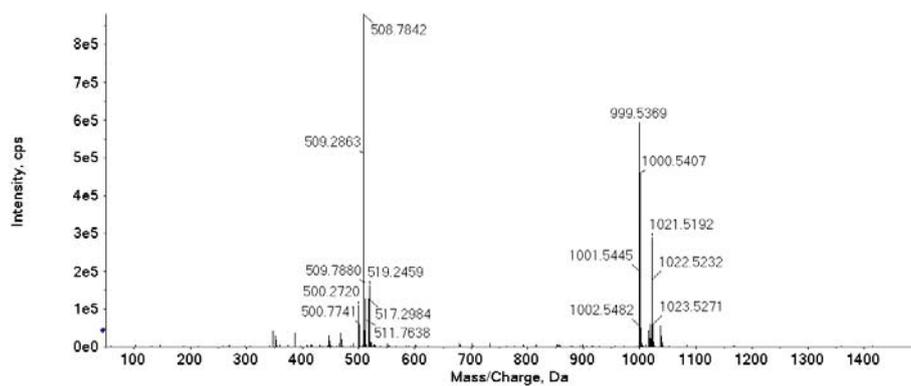


Figure S6. HRMS of acyl hydrazone 17, calcd for C<sub>48</sub>H<sub>79</sub>N<sub>4</sub>O<sub>18</sub><sup>+</sup> ([M+H]<sup>+</sup>) 999.5384, found 999.5369.