Supporting Information

Binding Uric Acid: A Pure Chemical Solution for the Treatment of Hyperuricemia

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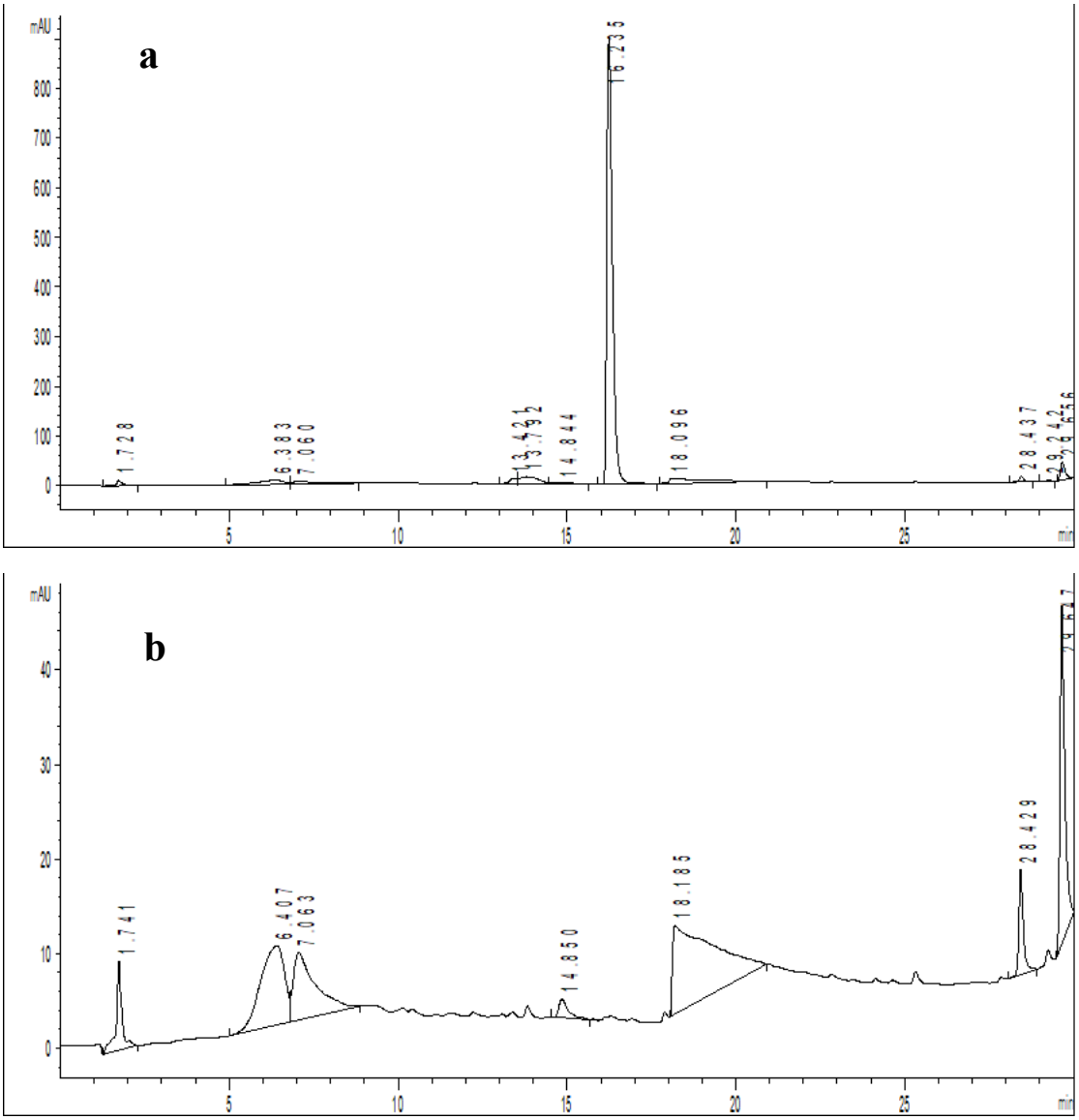

Figure S1. HPLC analysis for compound **1b** (purity ≥ 95.1%). **a**) HPLC chromatography of compound **1b**. **b**) HPLC chromatography of blank solvent. HPLC conditions: ZORBAX SB-C18, 5 μm (4.6 × 250 mm), 5%–95% methanol (added with 1‰ acetic acid), 30 min, flow rate 1 mL/min; UV detection 254 nm; injection volume, 20 μL; retention time, 16.24 min.

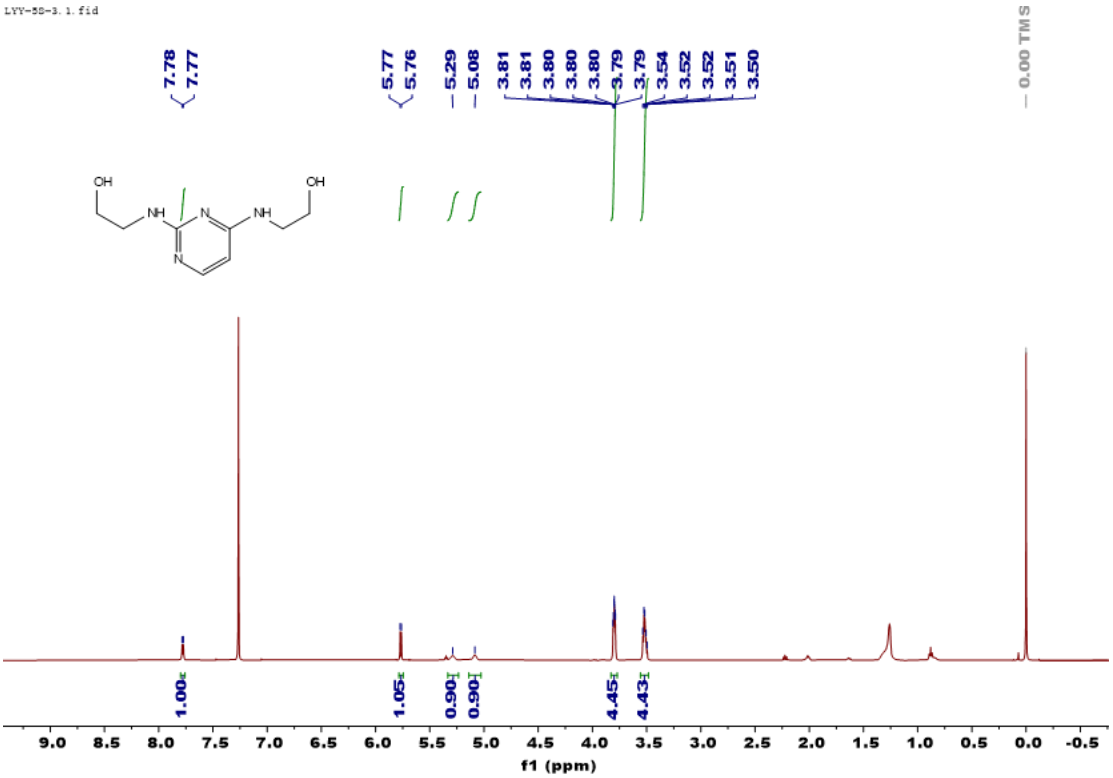

Figure S2. ^{1}H NMR spectrum of compound **1a** (500 MHz, chloroform-*d*).

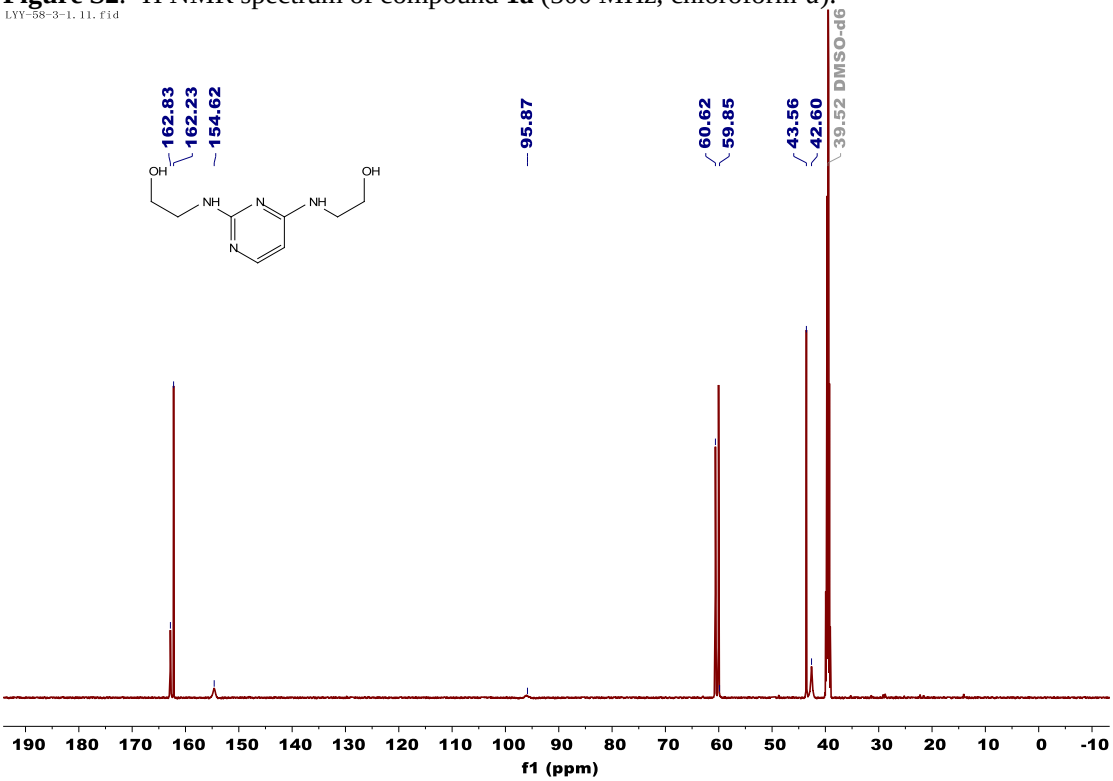

Figure S3. ^{13}C NMR spectrum of compound **1a** (150 MHz, DMSO-d_6).

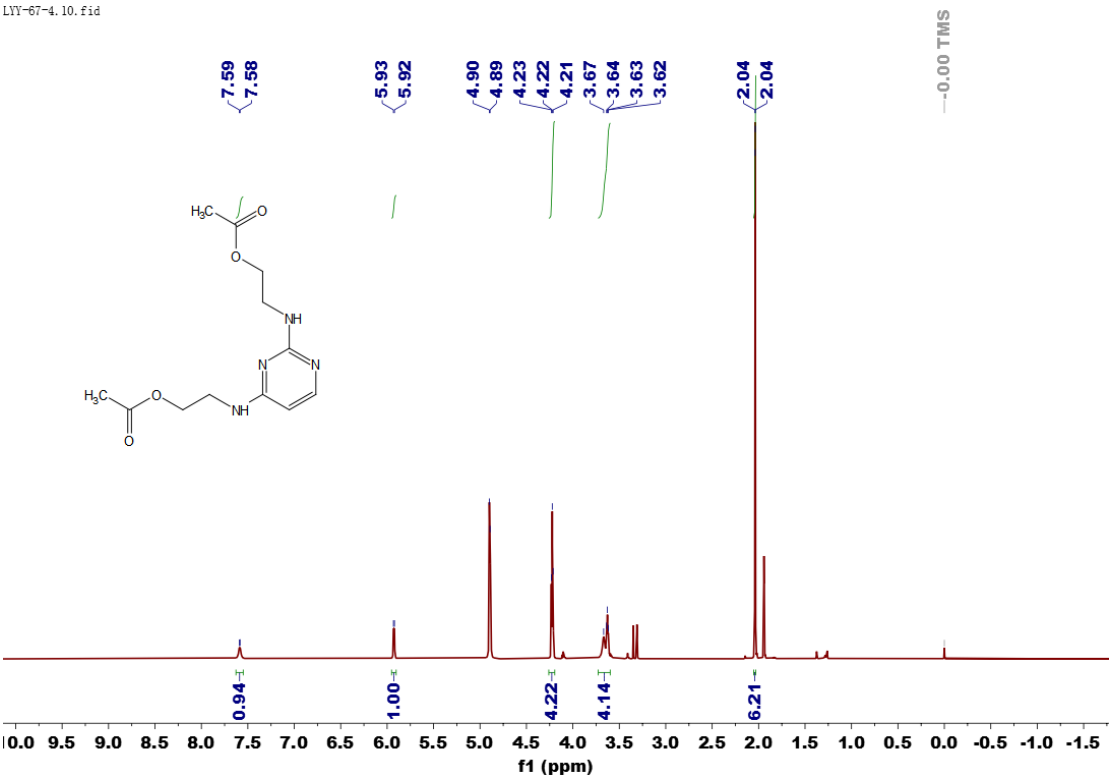

Figure S4. ^{1}H NMR spectrum of compound **1b** (600 MHz, methanol-d_4).

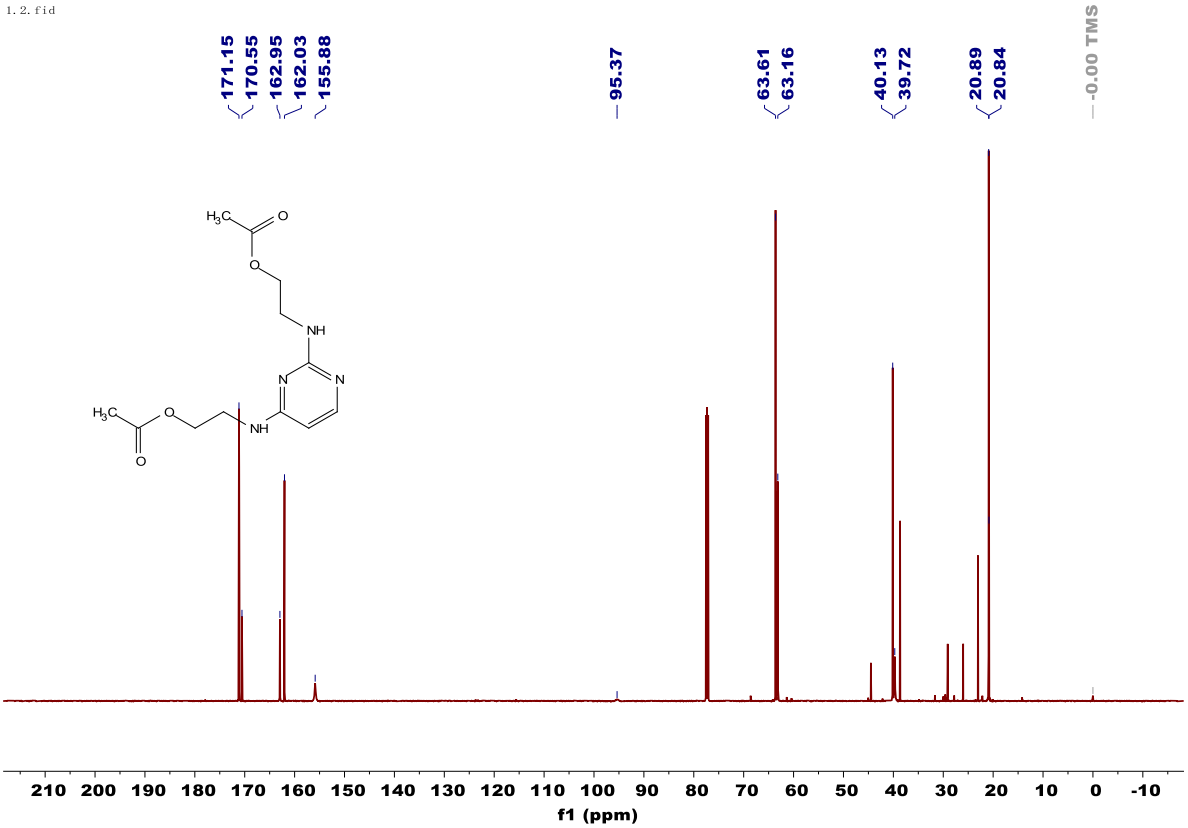

Figure S5. ^{13}C NMR spectrum of compound **1b** (150 MHz, chloroform-*d*).

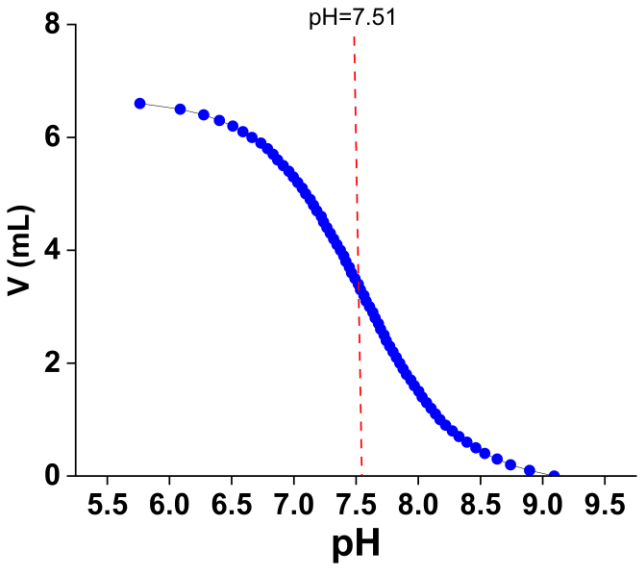

Figure S6. pH-V titration curve of compound **1a**

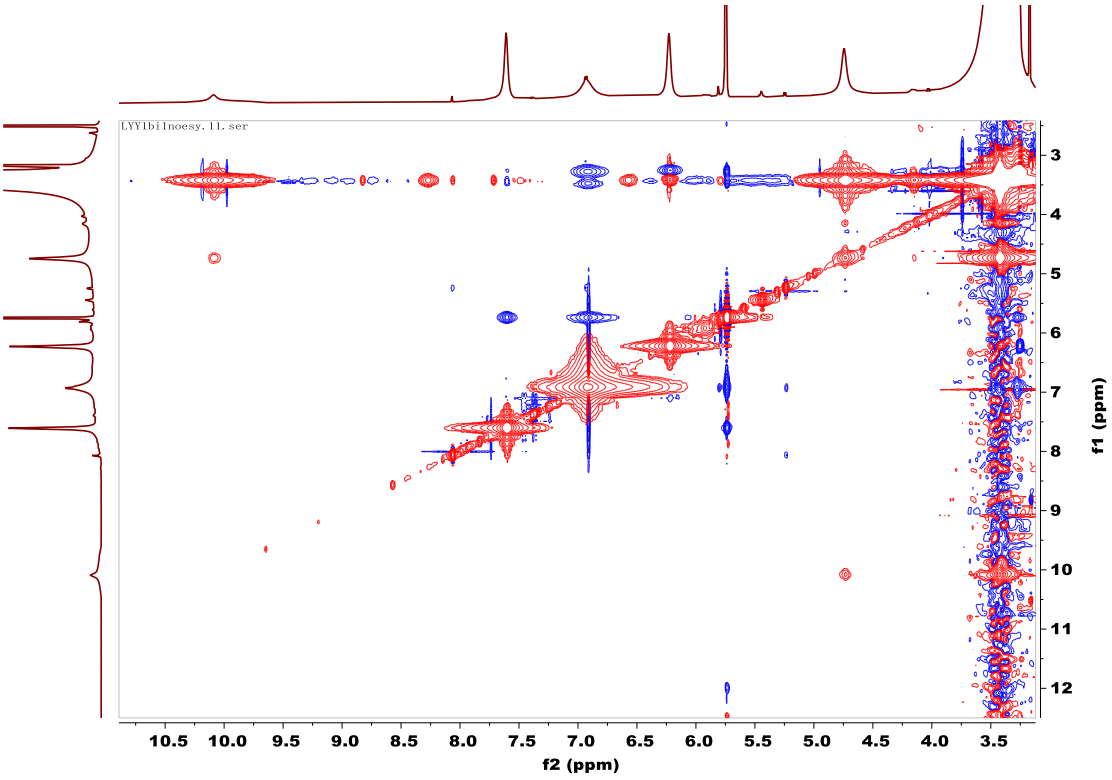

Figure 7S. NOESY of a 1:1 mixture of compound **1a** and uric acid (600 MHz, DMSO-d_6).

Table 1S. The amount, the percentage of the total administered dose, or concentration of compounds **1a**/**1b** in feces, urine and plasma 10.5 hours after the oral administration of compound **1b** (approximately 500 mg/kg, 80 mg per mouse).

	1a	**1b**
In urine (mg) / percentage (%)	23.7±3.5 / 42.3%	n. d. / n. d.
In feces (mg) / percentage (%)	1.4±0.7 / 2.5%	n. d. / n. d.
In plasma (mg/mL)	n. d.	n. d.

n. d. not detected.

In this experiment, 4 male Kunming mice aged 8 weeks (40±0.5 g) were used. After one week of environmental adaptation, the mice were intubated with compound **1b** (80 mg, dissolved in 0.3 mL 0.9% saline containing 0.5% CMC-Na). The mice were then placed in metabolic cages, respectively, to collect urine and feces over a period of 10.5 hours. Then, blood sample was collected from the orbital sinus of each mouse and stored in tubes with 1 mg/mL EDTA, and centrifugated at 3000 rpm for 10 minutes at 4 °C to yield the plasma. All collected urine and feces (ground in a mortar) were separately placed into 25 mL volumetric flasks, and diluted or extracted by 25 mL methanol. After 24 h, the supernatant in each flask was then centrifuged (10 min, 3000 rpm), diluted 50 times, and analyzed using HPLC (column: Supersil ODS2, 3 μm, 2.1 mm × 150 mm; 0~25 min, 5% to 100% acetonitrile in water, 254 nm, 0.2 mL/min). 100 μL plasma sample of each mouse was added with 900 μL methanol. After 24 h, they were centrifuged and analyzed with method mentioned above. The concentration of compound **1a**/**1b** in samples was calculated based on their peak area and the standard curve obtained by standard samples.