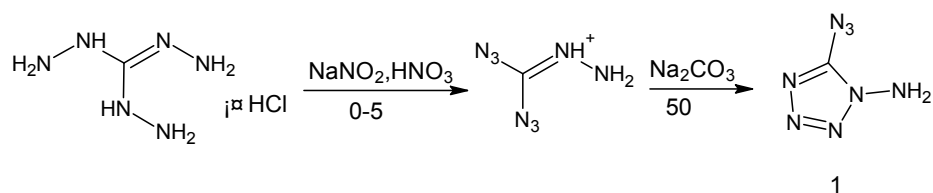


Supporting Information

Caution! 1-amino-5-azidotetrazole is extremely sensitive towards friction, impact, and electrostatic discharge. It should be synthesized only in 1~2 millimole amounts, and safety equipment such as thick gloves, leather coats, face shields, and ear plugs are recommended.

Synthesis of 1-amino-5-azidotetrazole (1)

Triaminoguanidinium chloride (0.282 g, 2 mmol) was dissolved in water (30 mL) and nitric acid (65%, 0.28 mL, 4mmol) was added. The reaction was cooled by ice-bath.. A solution of sodium nitrite (0.278 g, 4 mmol) in water (30 mL) was added dropwise at 0 °C over a period of 30 min. After complete addition, the reaction was stirred for an additional 30 min at 0 °C. Then the temperature was raised to 50°C and sodium carbonate (0.3g, 2.83mmol) was added fast in one portion. The mixture was stirred for an additional 1 hour at ambient temperature and extracted with ethyl acetate (50 mL×3). The combined organic extracts were allowed to evaporate until dryness. The residue was purified by a silica gel column (PE: EA=3:1, V/V, Rf=0.217) and 32 mg of 1-amino-5-azidotetrazole was obtained (11% yield).



Scheme 1 Synthesis route of 1-amino-5-azidotetrazole^[25]

Instrumentation and Measurement. ¹³C NMR and ¹⁵N NMR were recorded on a 400MHz (Varian mercury-plus 400) and 500MHz (Agilent DDR2) nuclear magnetic resonance spectrometers operating at 101 and 50.67 MHz, by using CD₃SOCD₃ as solvent. Chemical shifts in ¹³C NMR is relative to Me₄Si and ¹⁵N NMR to MeNO₂. The mass spectra was recorded with ESI ion source on a Agilent 500-MS mass spectrometer.

^{13}C NMR(DMSO- d_6 , 101MHz, ppm):150.6

^{15}N NMR(DMSO- d_6 , 50.67MHz, ppm):0.81, -8.38, -77.26, -141.91, -145.73, -155.13, -300.60, -309.93

MS(ESI $^+$): 127.08(M+H $^+$)

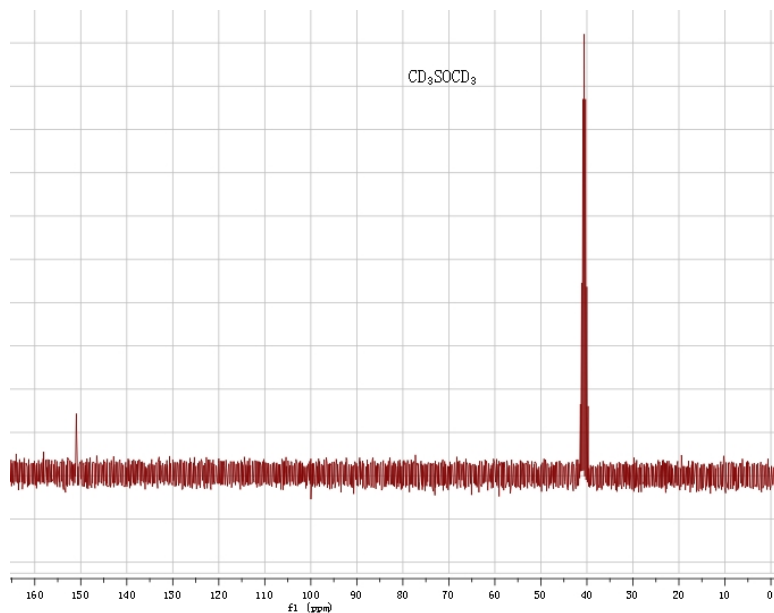


Fig. 1 The ^{13}C NMR spectroscopy of 1-amino-5-azidotetrazole

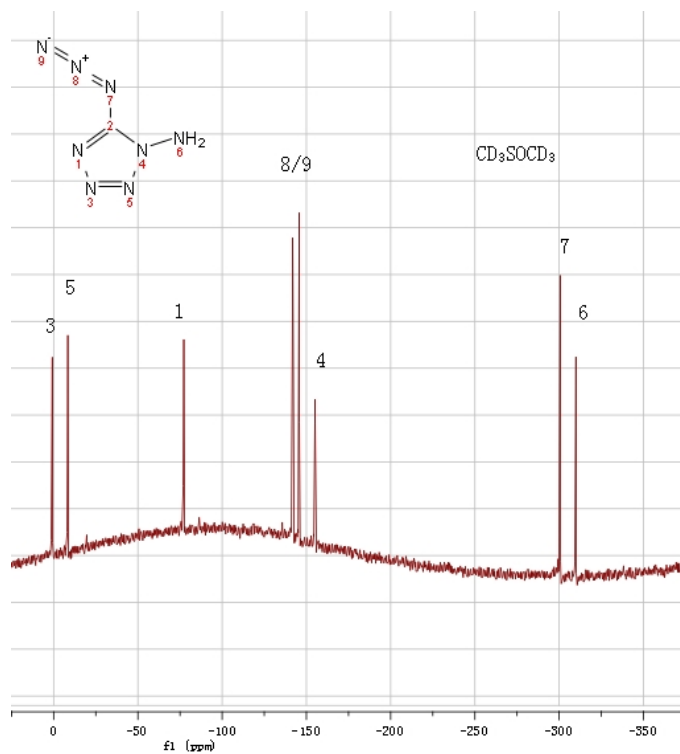


Fig. 2 The ^{15}N NMR spectroscopy of 1-amino-5-azidotetrazole