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Electronic supplementary information

A thermally stable pH-responsive "supramolecular buckle" based on the encapsulation of 4-(4-aminophenyl)-N-methylpyridinium by cucurbit[8]uril

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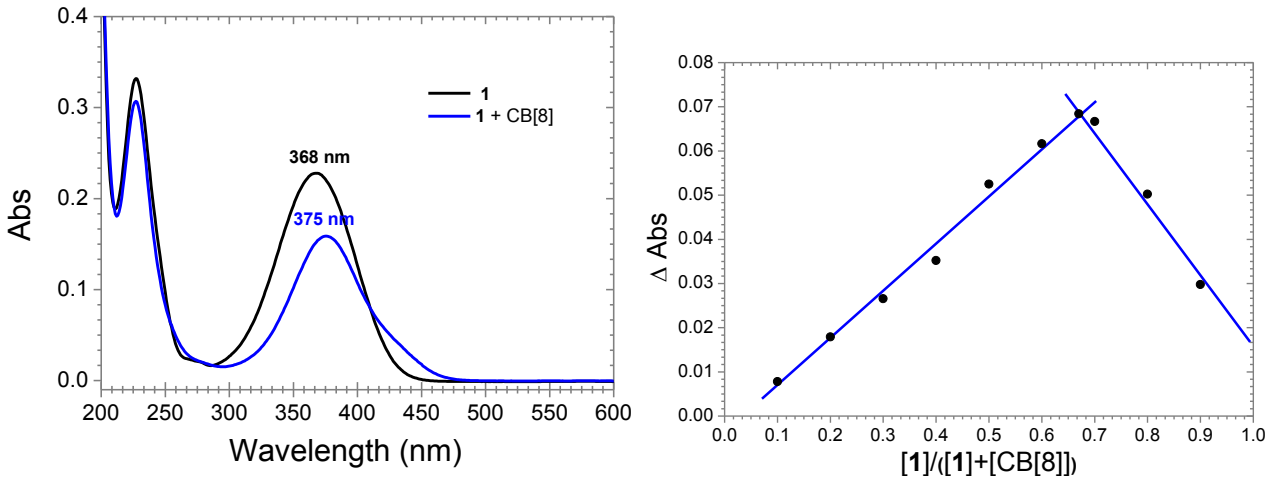

Figure S1. UV-vis spectra of **1** (13.3 μM) without and with CB[8] (6.7 μM) in water (pH = 7) at 25 °C (left), and Job's plot indicating a 1:2 stoichiometery for CB[8] and **1** (right). The total concentration used for generating the Job's plot was 20 μM.

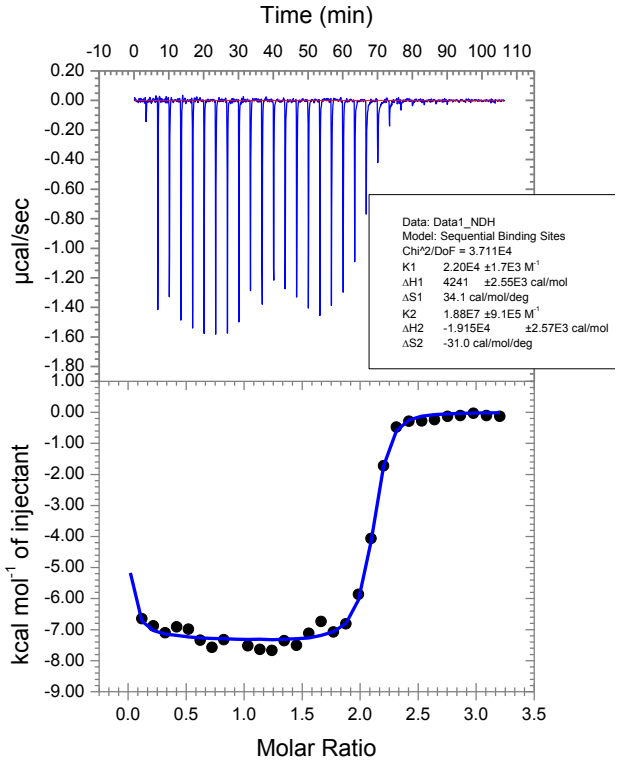

Figure S2. ITC data for the titration of CB[8] (0.1 mM) with **1** (2.0 mM) in a Tris-buffer solution (10 mM，pH 7.0) at 25 °C.

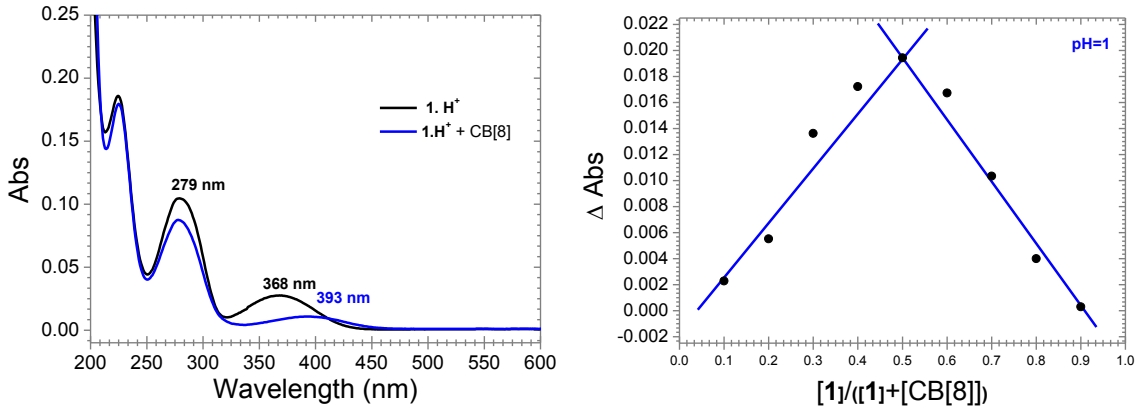

Figure S3. UV-vis spectra of **1** (13.3 μM) without and with CB[8] (6.7 μM) in an aqueous hydrochloric acid solution (pH = 1.0) at 25 °C (left), and Job's plot indicating a 1:1 stoichiometery for **1** H^+ and CB[8] (right). The total concentration used for generating the Job's plot was 20 μM.

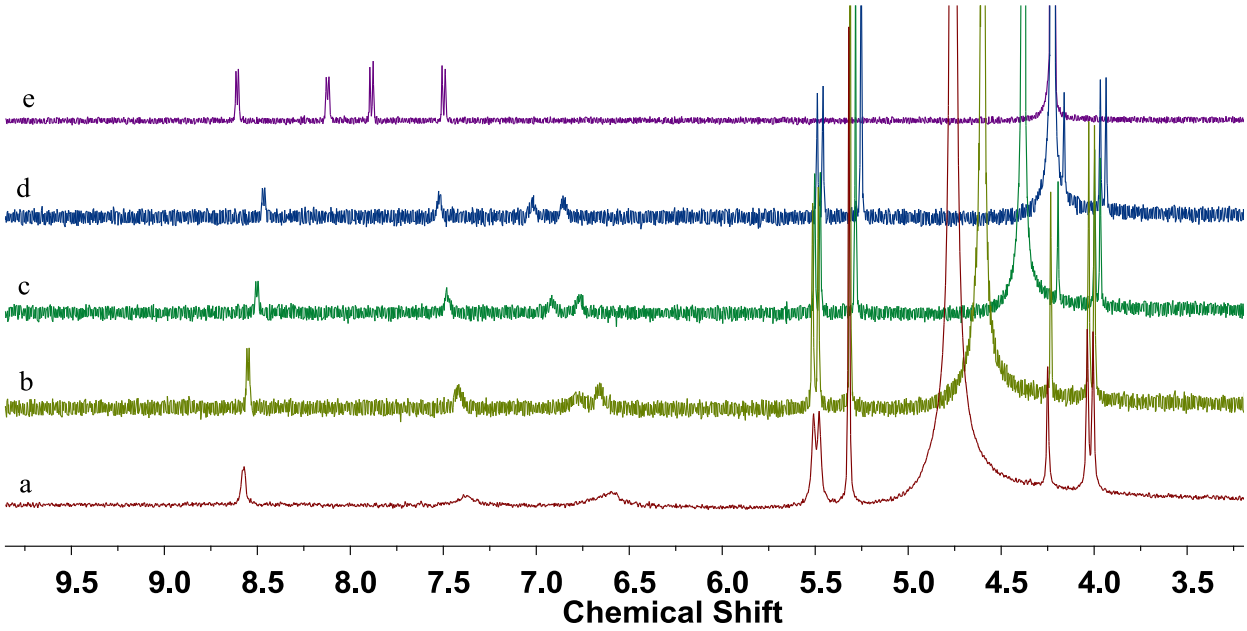

Figure S4. Partial ^{1}H NMR spectra (500 MHz) of CB[8]–**1** H^+ at (a) 25 °C, (b) 40 °C, (c) 60 °C and (d) 75 °C, and (e) **1** H^+ at 75 °C in D_2O. The spectra were calibrated by the temperature dependence of HDO chemical shifts reported by H. E. Gottlieb et al. *(J. Org. Chem.* **1997**, *61*, 7512-7515.).

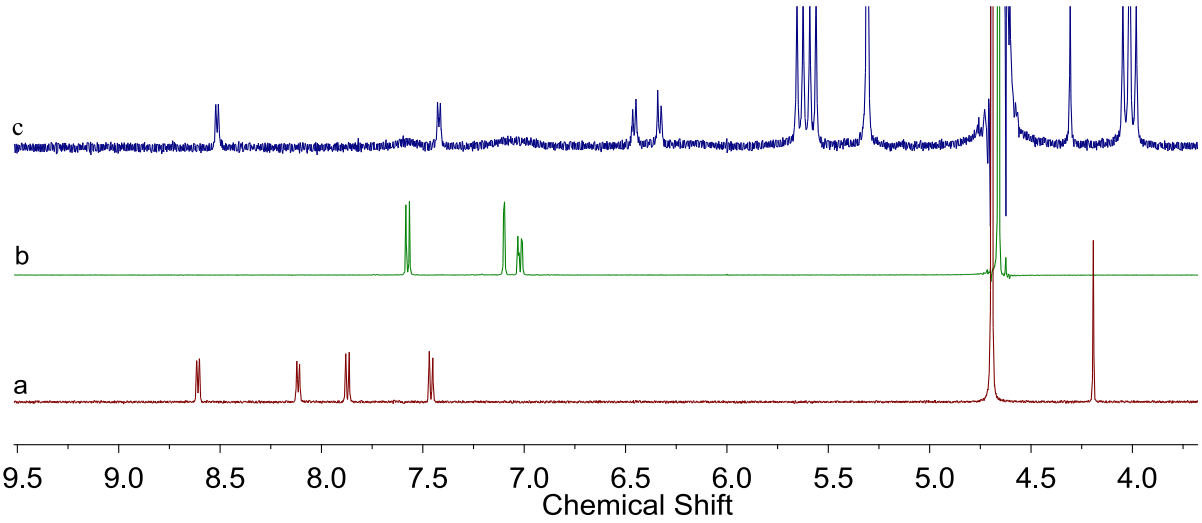

Figure S5. ^{1}H NMR spectra (500 MHz) of (a) **1** H^{+}, (b) 2,6-dihydroxynaphthalene, and (c) mixture of **1** H^{+}, 2,6-dihydroxynaphthalene and CB[8] (1:1:1) in D_2O at pD=1.

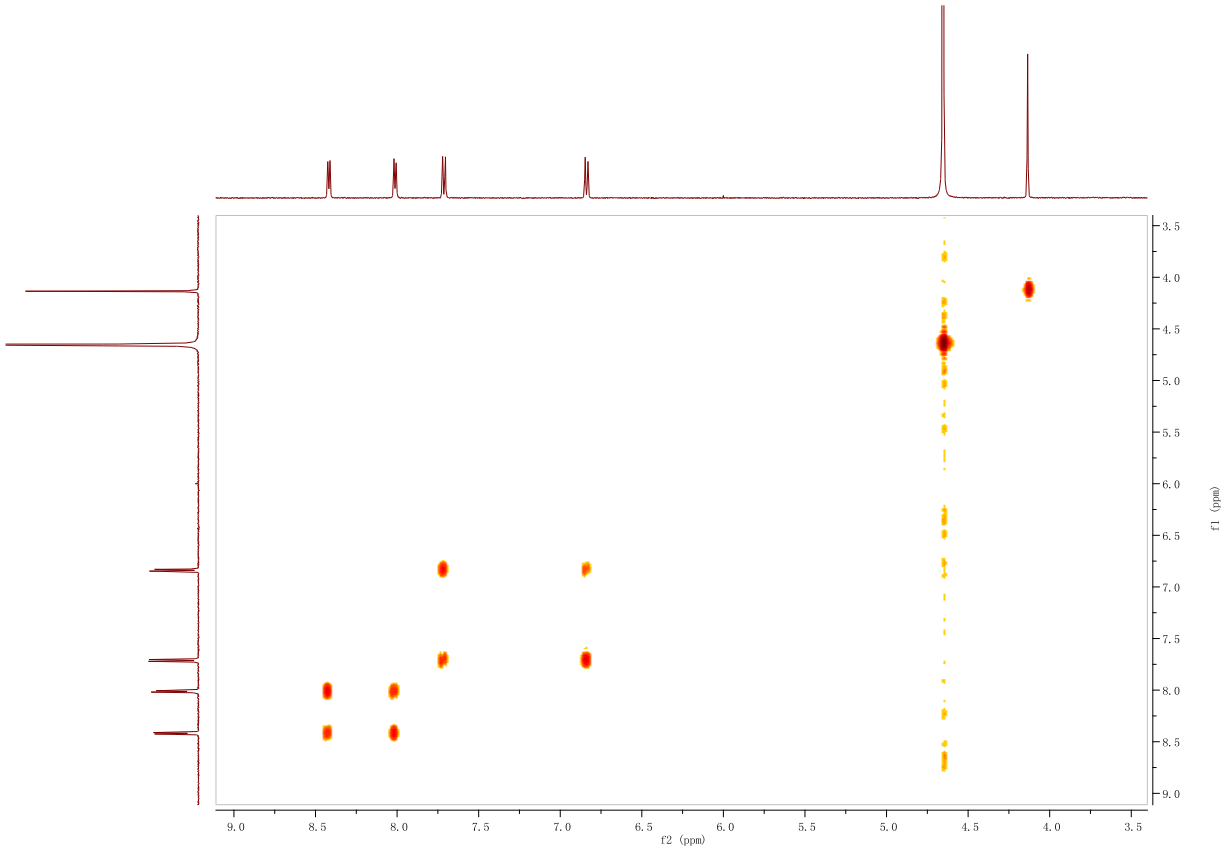

Figure S6. 2D ^{1}H NMR COSY spectrum (400 MHz, 293 K) of **1** in D_2O.

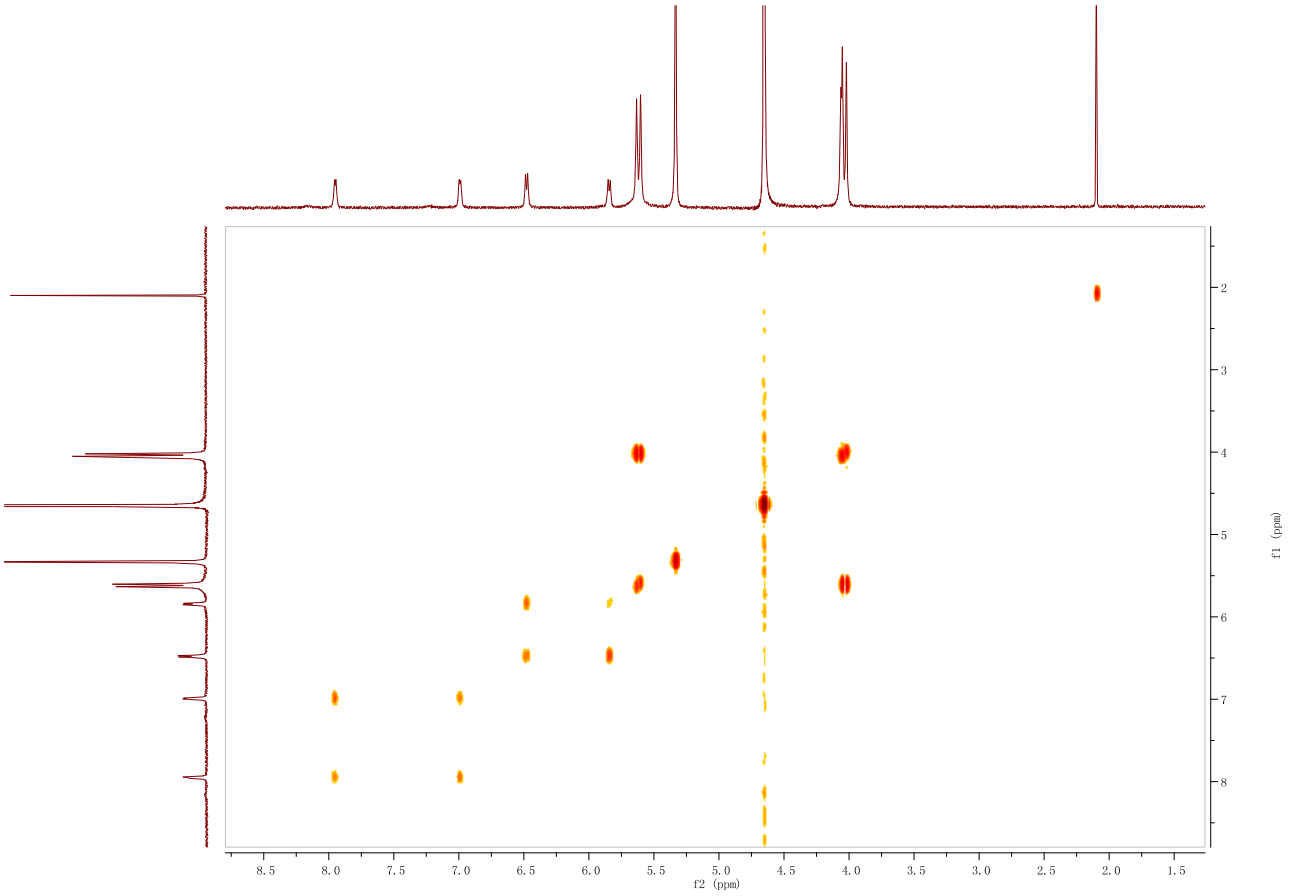

Figure S7. 2D ^{1}H NMR COSY spectrum (400 MHz, 293 K) of the solution of **1** and CB[8] (2:1) in D_2O.

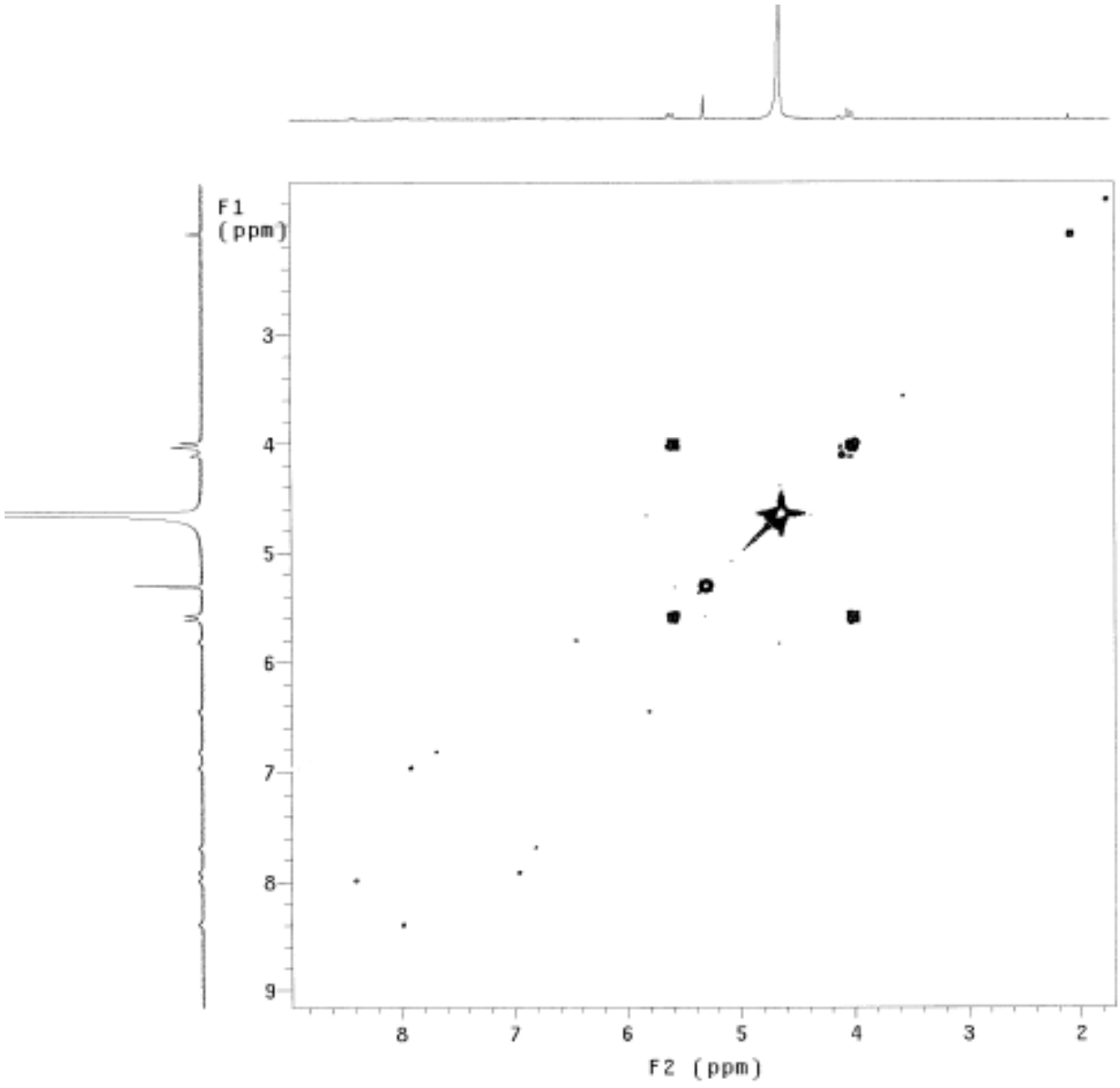

Figure S8. 2D ^{1}H NMR COSY spectrum (400 MHz, 293 K) of the solution of **1** and CB[8] (1:0.3) in D_2O.

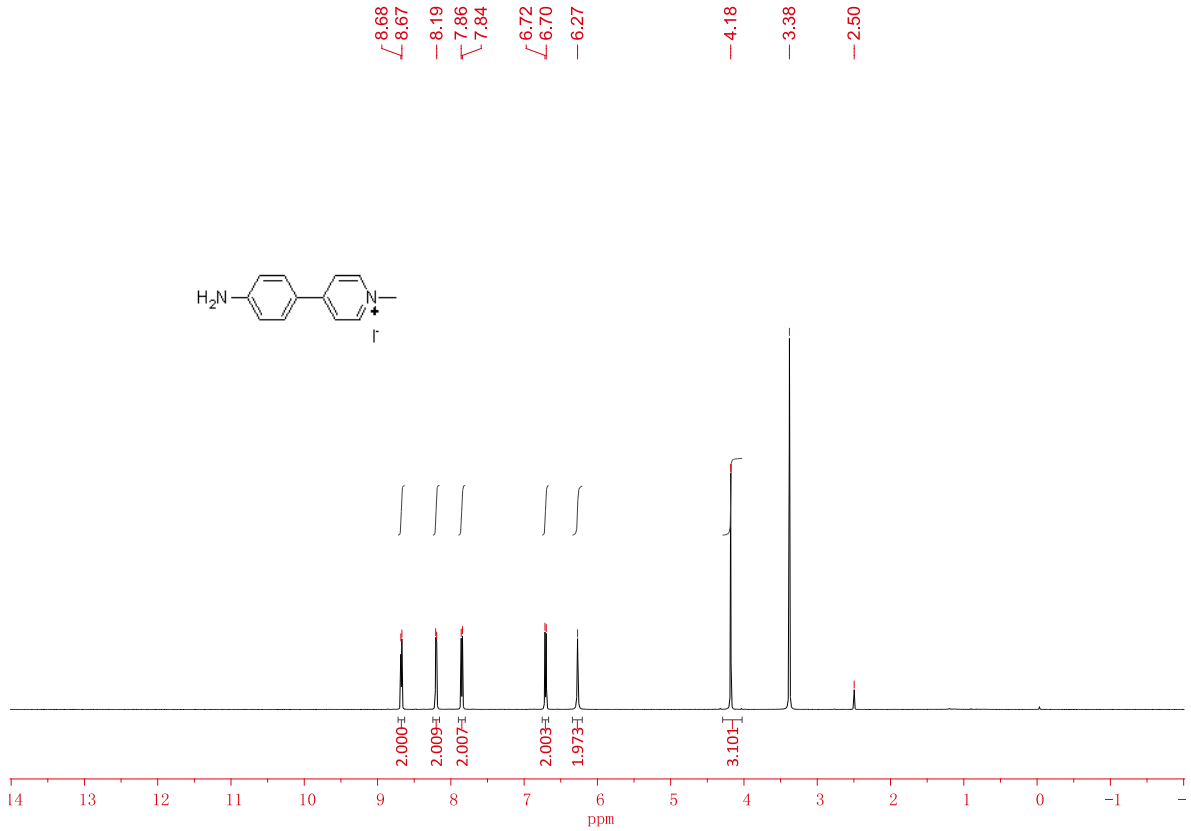

Figure S9. ^{1}H NMR spectrum (500 MHz, DMSO-d_6) of compound **1**.

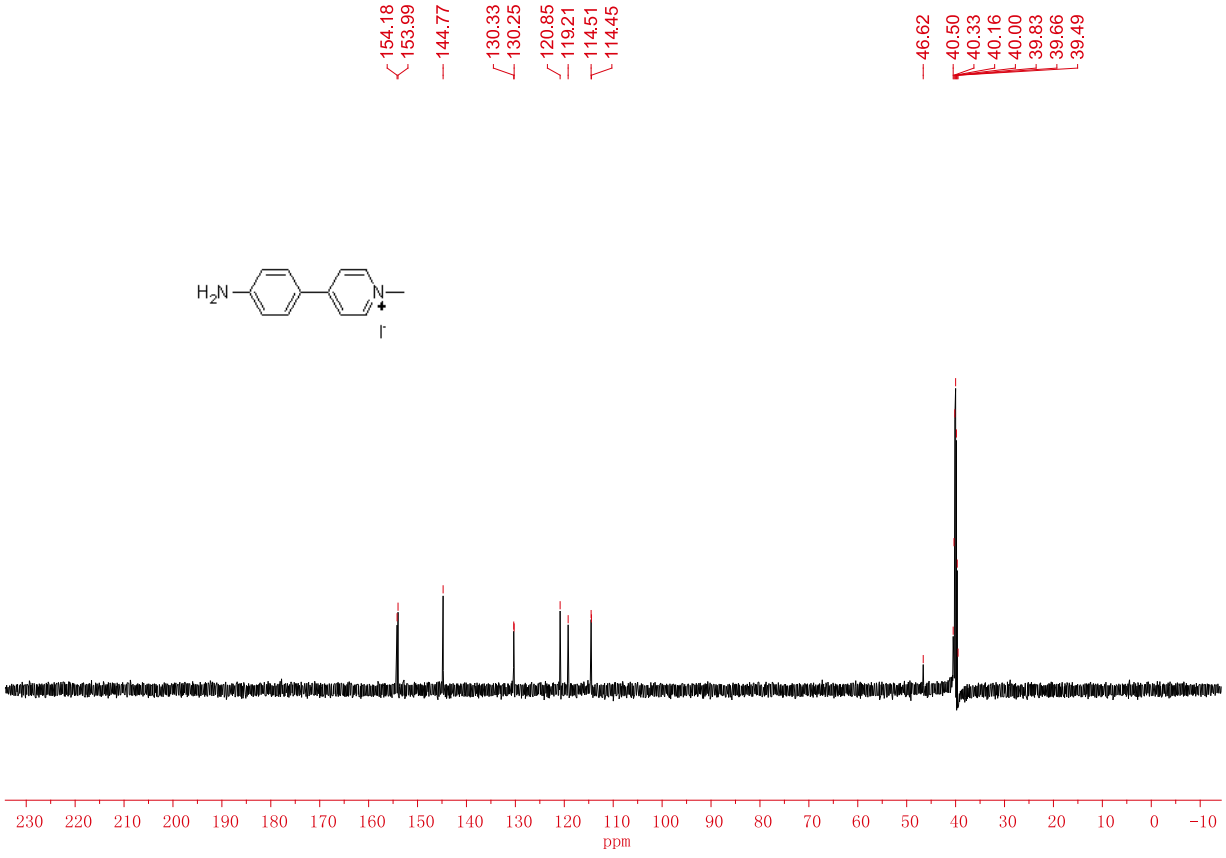

Figure S10. ^{13}C NMR spectrum (125 MHz, DMSO-d_6) of compound **1**.