Supporting Information

An Amphiphilic Molecular Basket with Conformation Sensitive to Both Solvent Changes and UV Irradiation

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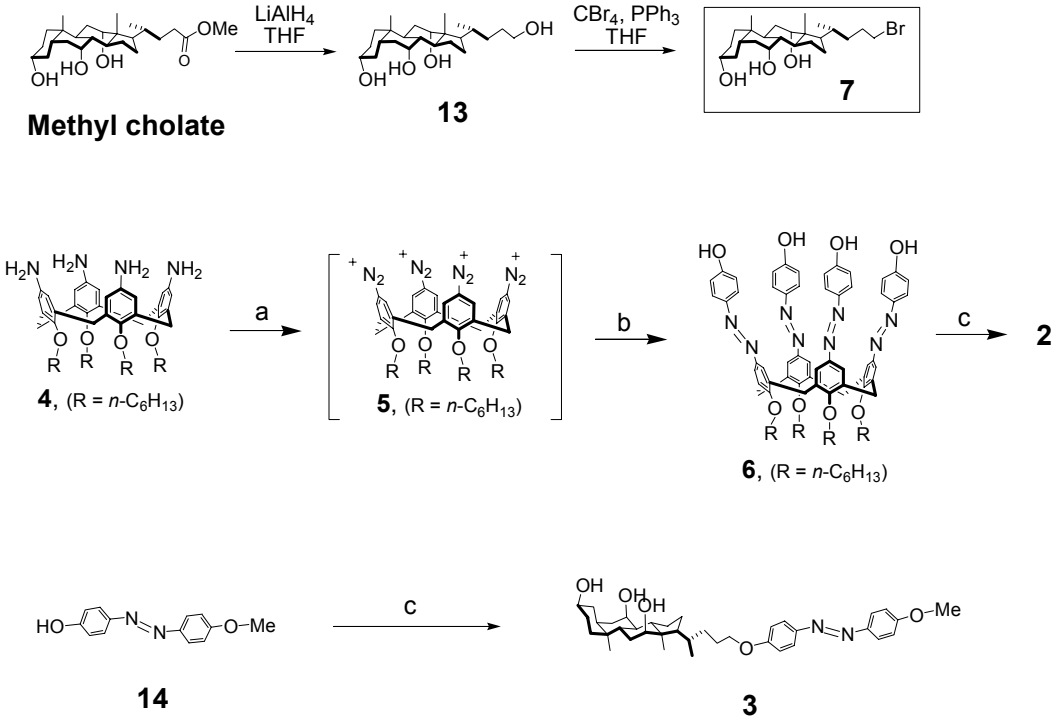
General Method

Anhydrous tetrahydrofuran (THF) and methylene chloride were dried by passage through a column of activated alumina under compressed nitrogen. Cholic acid was crystallized from 95% ethanol and dried at 90 °C under vacuum. All other reagents and solvents were of A.C.S. certified grade or higher, and were used as received from commercial suppliers. All glassware and syringes were dried in an oven at least overnight prior to use.

Synthesis



(a) $NaNO_2$, HCl, H_2O, THF; (b) phenol, pyridine, THF; (c) **7**, K_2CO_3, Bu_4NI, DMF

Compound 1. Synthesis of compound **1** was reported previously.[1]

Compound 13. Compound **13** was synthesized according to literature procedures.[2] mp 221-223 °C. ^{1}H NMR (300 MHz, CD_3OD, δ): 3.96 (s, 1H), 3.80 (m, 1H), 3.51 (t, 2H, J=6.3 Hz), 3.37 (m, 1H), 2.34-0.91 (m, 30H), 0.72 (s, 3H).

Compound 7. Compound **7** was synthesized according to modified literature procedures.[2] Compound **13** (1.10 g, 2.79 mmol) and Ph_3P (0.89 g, 3.38 mmol) were dissolved in anhydrous DMF (15 mL). CBr_4 (1.12 g, 3.38 mmol) was added slowly under N_2 flush. After 6 h at rt, the reaction mixture was poured into H_2O (100 mL). The precipitate formed was collected by suction filtration and washed with water (2 × 5 mL). The final product was purified by column chromatography over silica gel using CH_2Cl_2/acetone as the eluents to give a white powder (511 mg, 40% yield). mp 120-122 °C. ^{1}H NMR (300 MHz, CD_3OD, δ): 3.95 (s, 1H), 3.79 (m, 1H), 3.41 (m, 3H), 2.23-0.91 (m, 30H), 0.72 (s, 3H).

Compound 4. Compound **4** was synthesized according to literature procedures.[3] ^{1}H NMR (300 MHz, $CDCl_3$, δ): 6.07 (s, 8H), 4.29 (d, 4H, J = 13.2 Hz), 3.74 (t, 8H, J = 7.6 Hz), 2.90 (d, 4H, J = 13.2 Hz), 1.90-1.80 (m, 8H), 1.45-1.13 (m, 24H), 0.89 (t, 12H, J = 7.2 Hz).

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[1] Zhao, Y.; Ryu, E.-H. *J. Org. Chem.* **2005**, *70*, 7585–7591.

[2] Kihira, K.; Mikami, T.; Ikawa, S.; Okamoto, A.; Yoshii, M.; Miki, S.; Mosbach, E. H.; Hoshita, T. *Steroids* **1992**, *57*, 193–8.

[3] Jakobi, R. A.; Bohmer, V.; Grutter, C.; Kraft, D.; Vogt, W. *New J. Chem.* **1996**, *20*, 493-501.

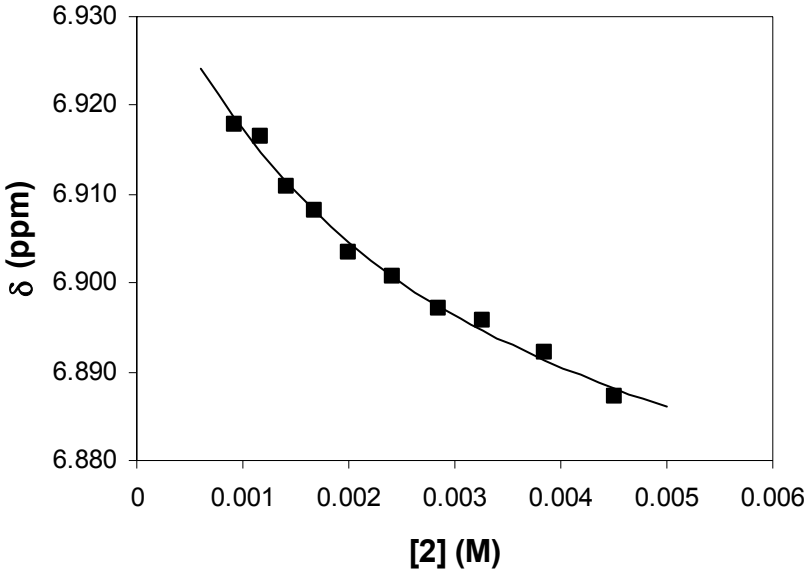

Figure 1S. Plot of the chemical shift of the *para* phenyl proton in **10** as a function of concentration of **2** in 95/5 of CCl_4/CD_3OD (vol/vol). Theoretical curve is nonlinear least-square fitting to a 1:1 binding isotherm.

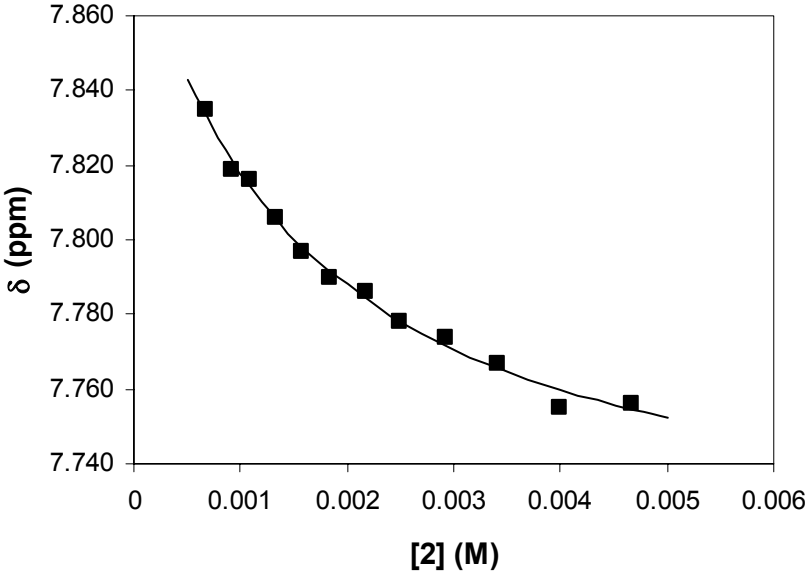

Figure 2S. Plot of the chemical shift of selected aromatic proton in **11** as a function of concentration of **2** in 95/5 of CCl_4/CD_3OD (vol/vol). Theoretical curve is nonlinear least-square fitting to a 1:1 binding isotherm.

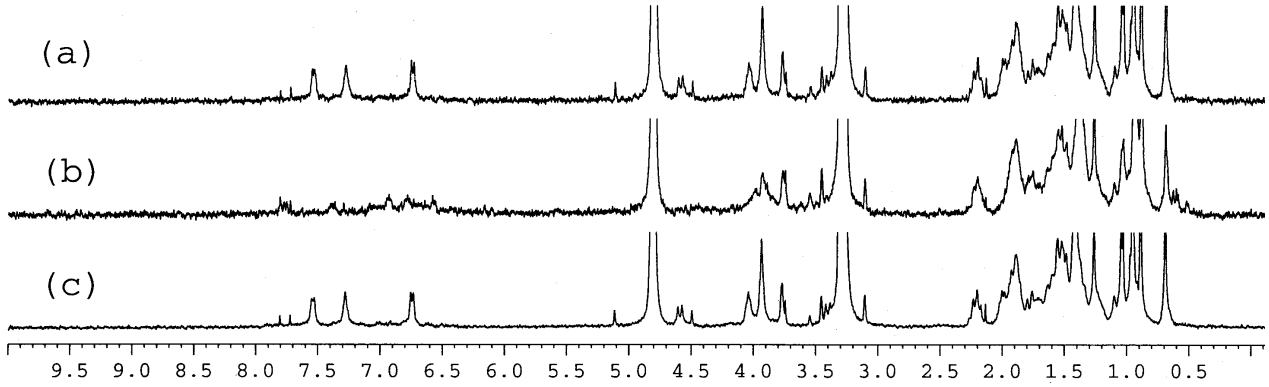

Figure 3S. ^{1}H NMR spectra of compound **2** a) before, b) immediately after, and c) 24 h in dark after irradiation. The peaks at between 3.3–4.1 ppm are from protons adjacent to OH and O in **2**. The large peaks at 3.3 and 4.8 ppm come from undeuterated solvents. Solvent = 5% CD_3CD/CCl_4.

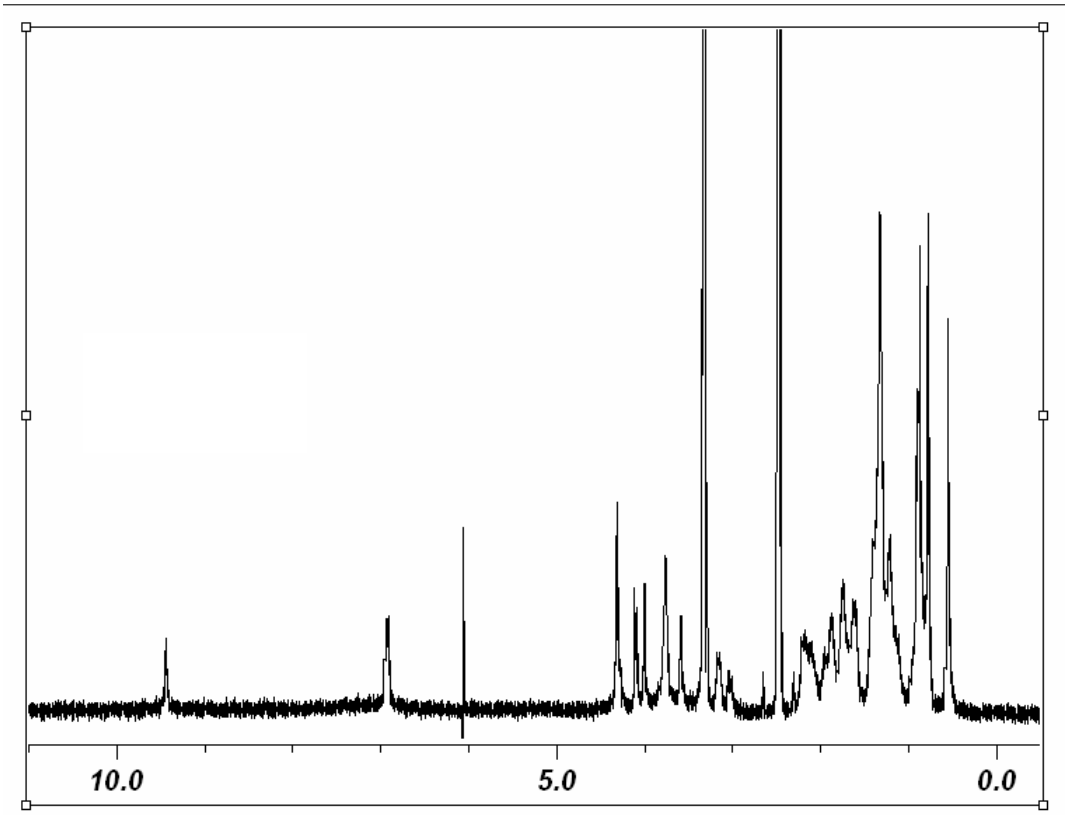

Figure 4S. ^{1}H NMR (400 MHz) spectra of compound **1** in DMSO-d_6.

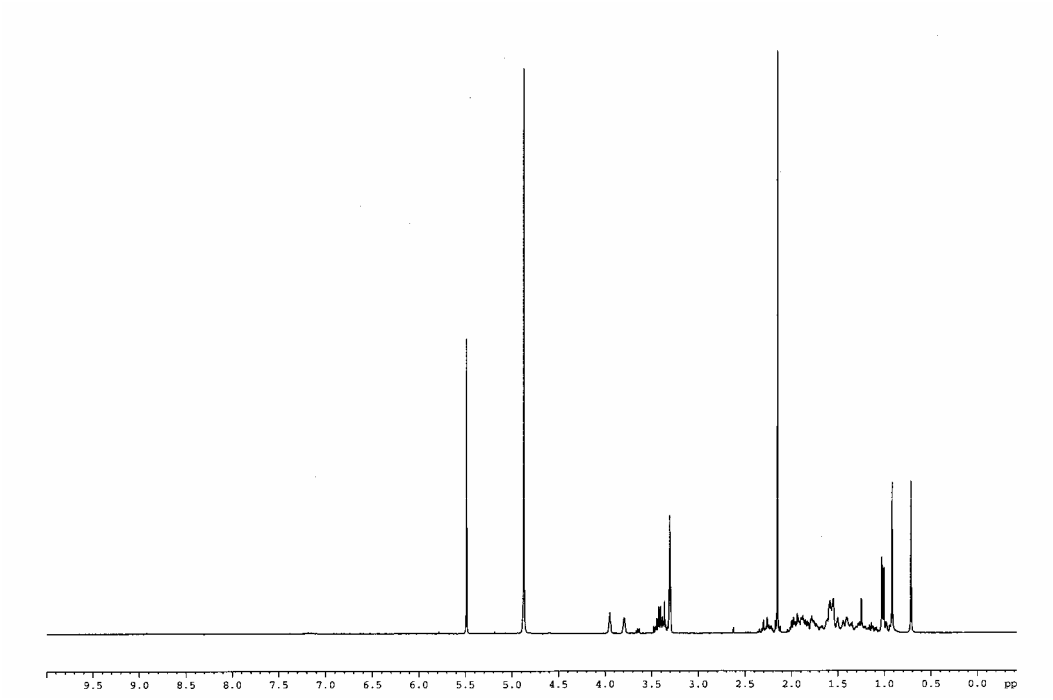

Figure 5S. ^{1}H NMR (400 MHz) spectra of compound **7** in CD_3OD.

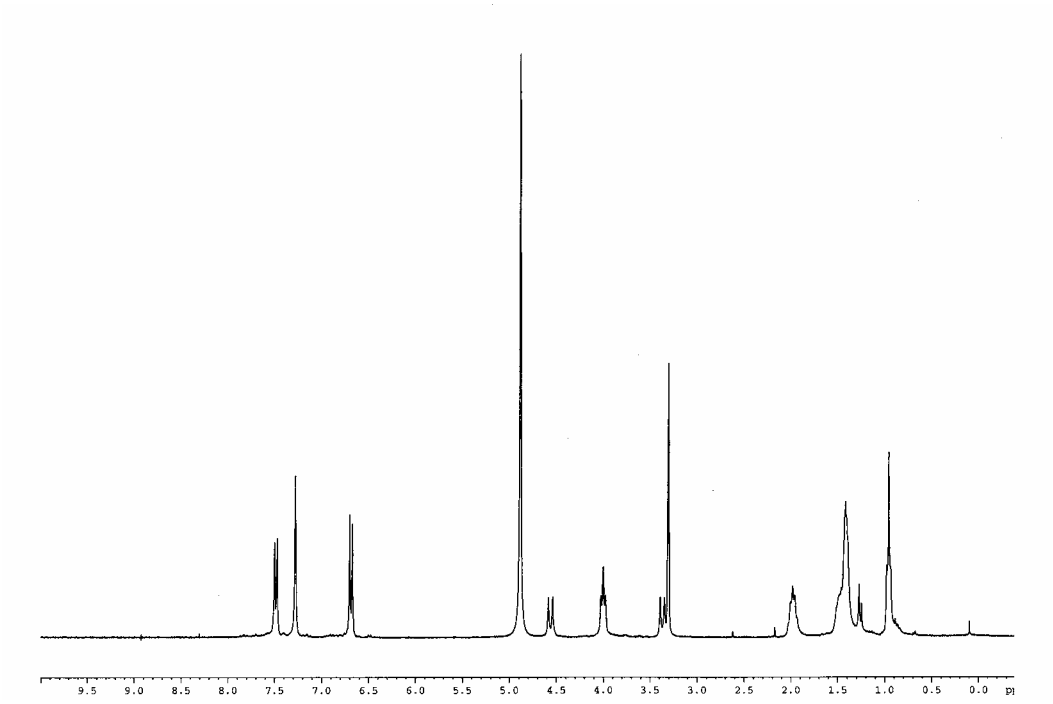

Figure 6S. ^{1}H NMR (400 MHz) spectra of compound **6** in CD_3OD.

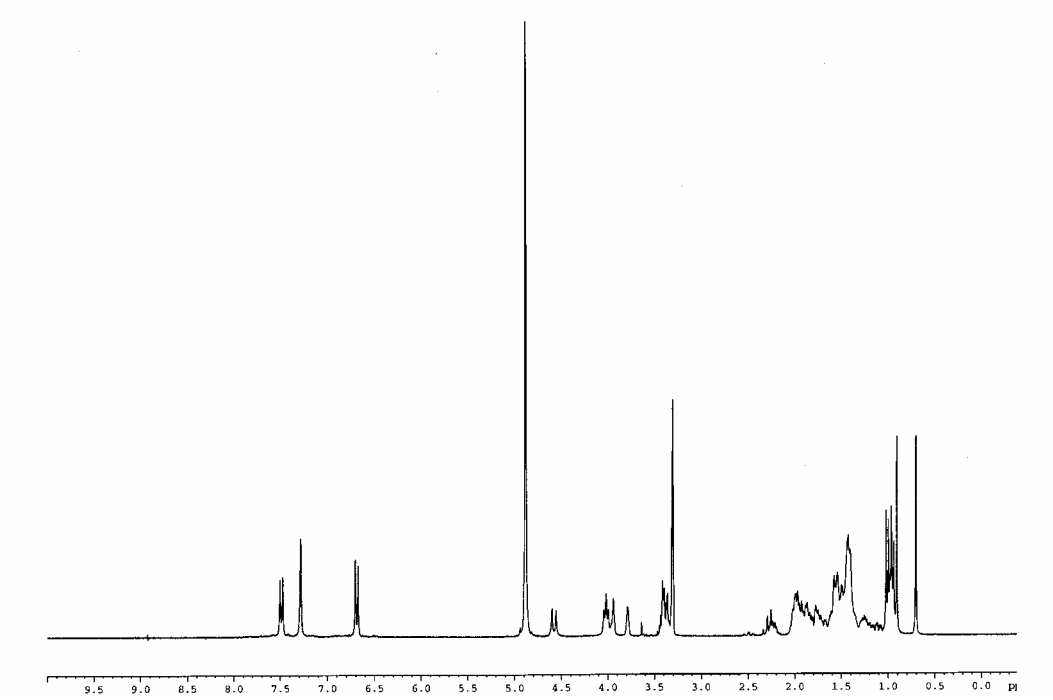

Figure 7S. ^{1}H NMR (400 MHz) spectra of compound **2** in CD_3OD.

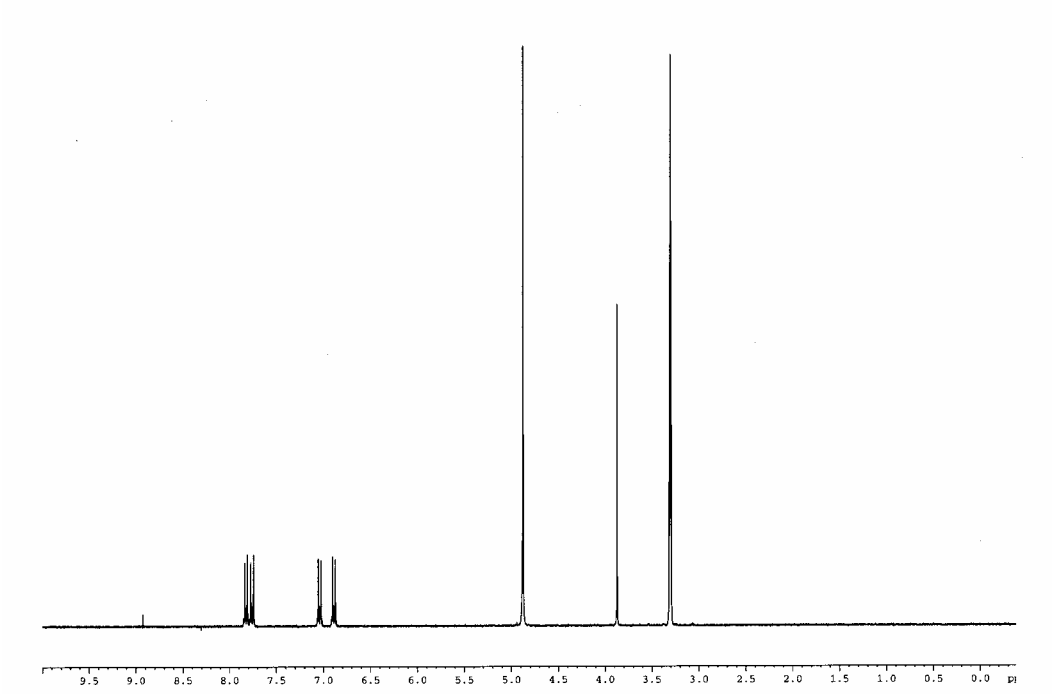

Figure 8S. ^{1}H NMR (400 MHz) spectra of compound **14** in CD_3OD.

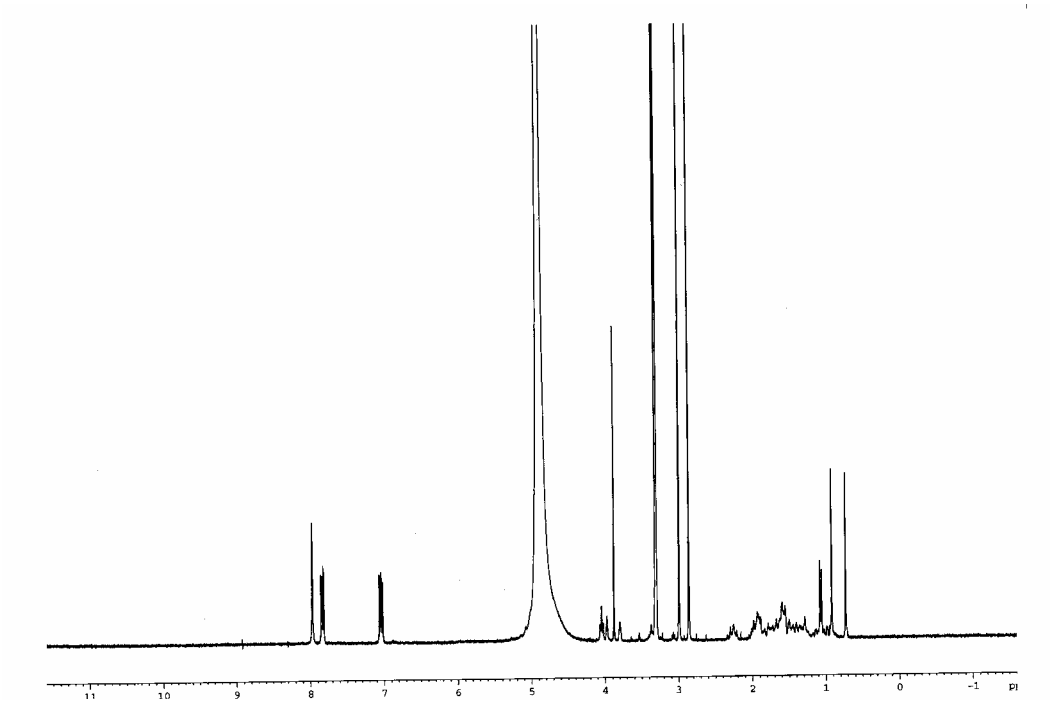

Figure 9S. ^{1}H NMR (400 MHz) spectra of compound **3** in CD_3OD.