Supplementary Information for

8-TQEN (*N,N,N',N'*-tetrakis(8-quinolylmethyl)ethylenediamine) Analogs as Fluorescent Cadmium Sensors: Strategies to Enhance Cd^{2+}-Induced Fluorescence and Cd^{2+}/Zn^{2+} Selectivity

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Experimental

6-Methoxy-8-methylquinoline. To the refluxing mixture of 4-methoxy-2-methylaniline (2.00 g, 14.6 mmol), glycerol (13.4 g, 146 mmol) and dry nitrobenzene (3.0 mL, 29.2 mmol) was added sulfuric acid (3.0 mL, 56.3 mmol) and further refluxed for 5 h. The resultant solution was cooled to r.t., added 30 mL of water and treated with activated carbon. The filtrate was washed with ether and resultant aqueous layer was made to alkaline (pH > 12) and extracted with dichloromethane. The organic layer was dried and evaporated to give 6-methoxy-8-methylquinoline (941 mg, 5.43 mmol, 37%).

^{1}H NMR ($CDCl_3$): δ (ppm) 8.79 (dd, *J* = 1.8, 4.3 Hz, 1H), 8.03 (dd, *J* = 1.8, 8.2 Hz, 1H), 7.35 (dd, *J* = 4.3, 8.2 Hz, 1H), 7.23 (dd, *J* = 1.1, 2.7 Hz, 1H), 6.92 (d, *J* = 2.7 Hz, 1H), 3.92 (s, 3H), 2.78 (s, 3H).

^{13}C NMR ($CDCl_3$): δ (ppm) 156.9, 146.5, 143.4, 138.5, 134.8, 129.2, 122.0, 121.0, 102.9, 55.4, 18.3.

6-Methoxyquinoline-8-carboaldehyde. The mixture of 6-methoxy-8-methylquinoline (975 mg, 5.60 mmol) and SeO_2 (1.25 g, 11.2 mmol) in diglyme (30 mL) was refluxed for 42 h. The resultant solution was cooled to r.t., filtered with celite and evaporated to give 6-methoxyquinoline-8-carboaldehyde (844 mg, 4.51 mmol, 80%).

^{1}H NMR ($CDCl_3$): δ (ppm) 11.40 (s, 1H), 8.90 (dd, *J* = 1.7, 4.3 Hz, 1H), 8.14 (dd, *J* = 1.7, 8.2 Hz, 1H), 7.98 (d, *J* = 3.1 Hz, 1H), 7.46 (dd, *J* = 4.3, 8.2 Hz, 1H), 7.38 (d, *J* = 3.1 Hz, 1H).

^{13}C NMR ($CDCl_3$): δ (ppm) 191.8, 156.8, 148.5, 143.2, 134.7, 132.4, 129.6, 121.8, 120.3, 112.3, 55.9.

Anal. Calcd for $C_{11}H_9NO_2$: C, 70.58; H, 4.85; N, 7.48. Found: C, 70.66; H, 4.82; N, 7.47.

8-Hydroxymethyl-6-methylquinoline. To the solution of 6-methoxyquinoline-8-carboaldehyde (844 mg, 4.51 mmol) in ethanol (70 mL) was added $NaBH_4$ (204 mg, 5.41 mmol) and stirred for 5 h at room temperature. Water was added and the solution was

extracted with dichloromethane, dried and evaporated to give 8-hydroxymethyl-6-mthoxyquinoline as white solid (725 mg, 3.83 mmol, 85%).

^{1}H NMR ($CDCl_3$) : δ (ppm) 8.70 (dd, *J* = 1.8, 4.3 Hz, 1H), 8.07 (dd, *J* = 1.8, 8.2 Hz, 1H), 7.39 (dd, *J* = 4.3, 8.5 Hz, 1H), 7.24 (d, *J* = 2.7 Hz, 1H), 6.99 (d, *J* = 2.7 Hz, 1H), 5.15 (s, 3H), 3.92 (s, 3H).

^{13}C NMR ($CDCl_3$): δ (ppm) 157.0, 146.1, 143.0, 139.4, 135.2, 129.5, 121.3, 120.2, 104.1, 64.5, 55.5.

Anal. Calcd for $C_{11}H_{11}NO_2$: C, 69.83; H, 5.86; N,7.40. Found: C,69.73; H, 5.83; N, 7.35.

8-Chloromethyl-6-methoxyquinoline. The solution of 8-hydroxymethyl-6-mthoxyquinoline (1.20 g, 6.34 mmol) and thionyl chloride (0.45 mL, 6.39 mmol) in dichloromethane (70 mL) was stirred for overnight at room temperature. The resultant solution was washed with saturated sodium carbonate. The organic layer was dried, evaporated and purified by column chromatography (Silica gel; eluent: ethyl acetate/hexane = 1/2) to give 8-chloromethyl-6-methoxyquinoline as white solid (747 mg, 3.60 mmol, 57%).

^{1}H NMR ($CDCl_3$): δ (ppm) 8.82 (dd, *J* = 1.5, 4.3 Hz, 1H), 8.05 (dd, *J* = 1.5, 8.2 Hz, 1H), 7.54 (d, *J* = 2.4 Hz, 1H), 7.39 (dd, *J* = 4.3, 8.2 Hz, 1H), 7.05 (d, *J* = 2.6 Hz, 1H), 5.28 (s, 2H), 3.94 (s, 3H).

^{13}C NMR ($CDCl_3$) : δ (ppm) 156.8, 147.2, 141.7, 136.8, 134.7, 129.3, 124.4, 121.5, 105.5, 55.6, 42.3.

HRMS (ESI-MS) *m/z*: $[M + Na]^+$ Calcd for $C_{11}H_{10}ClNONa$ 230.0349; Found 230.0312.

Anal. Calcd for $C_{11}H_{10.2}ClNO_{1.1}$ (with $0.1H_2O$): C, 63.08; H, 4.91; N, 6.69. Found: C, 62.89; H, 4.80; N, 6.53.

***N,N,N',N'*-Tetrakis(8-quinolylmethyl)ethylenediamine (8-TQEN, 1a).** To a dry CH_3CN solution (30 mL) of 8-bromomethylquinoline (1.72 g, 7.75 mmol) and ethylenediamine (0.13 mL, 1.94 mmol) was added potassium carbonate (1.74 g, 12.6 mmol) and potassium iodide

(573 mg, 3.45 mmol). The resulting reaction mixture was refluxed for 2 days under N_2. The resultant solution was cooled to room temperature and the solvent was evaporated. The residue was washed with $CHCl_3$ and water to give compound **1a** as a white solid (450 mg, 0.72 mmol, 37%). This material is insoluble to water, ethanol, chloroform, DMF, DMSO and other common organic solvents.

Anal. Calcd for $C_{42}H_{36}N_6$ (**1a**·0.2H_2O): C, 80.29; H, 5.84; N, 13.37. Found: C, 80.07; H, 5.78; N, 13.28.

***N,N,N',N'*-Tetrakis(6-methoxy-8-quinolylmethyl)ethylenediamine (6-MeO-8-TQEN, 1b).** To a dry CH_3CN solution (30 mL) of 6-methoxy-8-bromomethylquinoline (118 mg, 0.56 mmol) and ethylenediamine (9.5 μL, 0.14 mmol) was added potassium carbonate (196 mg, 1.40 mmol) and potassium iodide (236 mg, 1.40 mmol). The resulting reaction mixture was refluxed for 2 days under N_2, cooled to room temperature and the solvent was evaporated. The residue was extracted with $CHCl_3$/water and the organic layer was dried and evaporated to give compound **1b** as a white solid (109 mg, 0.14 mmol, quant.).

^{1}H NMR (DMSO-d_6): δ (ppm) 8.60 (dd, 4 H, J = 1.7, 4.1 Hz), 8.17 (dd, 4 H, J = 1.7, 8.1 Hz), 7.61 (d, 4 H, J = 2.4 Hz), 7.40 (dd, 4 H, J = 4.1, 8.1 Hz), 7.12 (d, 4 H, J = 2.4 Hz), 4.32 (s, 8 H), 3.74 (s, 12 H), 2.93 (s, 4 H).

^{13}C NMR (DMSO-d_6): δ (ppm) 156.7, 146.4, 142.0, 139.1, 134.8, 129.0, 121.3, 119.9, 103.8, 87.7, 55.2, 54.1.

HRMS (ESI-MS) *m/z*: $[M + Na]^+$ Calcd for $C_{46}H_{44}N_6O_4Na$ 745.3502; Found 745.3567.

Anal. Calcd for $C_{46}H_{45}N_6O_{4.5}$ (**1b**·0.5H_2O): C, 73.28; H, 6.01; N, 11.14. Found: C, 73.23; H, 6.04; N, 11.17.

***N,N,N',N'*-Tetrakis(3-hydroxypropyl)propanediamine hydrobromide (3d·2HBr).** The agitated mixture of 1,3-diaminopropane (2.08 mL, 25.0 mmol), 3-bromo-1-propanol (9.0 mL, 0.10 mol) and powdered sodium carbonate (9.24 g, 0.11 mol) in dry ethanol (50 mL) was

refluxed for three days under N_2. The resultant solution was cooled to r.t. and the solvent was evaporated. The residue was extracted with $CHCl_3$, dried and evaporated to give compound **3d**·2HBr as orange oil (9.58 g, 20.5 mmol, 82%).

^{1}H NMR (D_2O): δ (ppm) 3.48 (t, *J* = 6.3 Hz, 8H), 2.38-2.51 (m, 12H), 1.54-1.62 (m, 10H).

^{13}C NMR (D_2O): δ (ppm) 60.3, 51.5, 51.0, 27.9.

HRMS (ESI-MS) *m/z*: $[M + Na]^+$ Calcd for $C_{15}H_{34}N_2O_4Na$ 329.2416; Found 329.2416.

***N,N,N',N'*-Tetrakis(3-chloropropyl)ethylenediamine (4b).** The solution of *N,N,N',N'*-tetrakis(3-hydroxypropyl)ethylenediamine hydrobromide (**3b**·2HBr) (691 mg, 1.52 mmol) and thionyl chloride (2.0 mL, 28 mmol) in dichloromethane (30 mL) was refluxed for overnight under N_2. The resultant solution was cooled to r.t. and washed with 6*N* $NaOH_{aq}$. The organic layer was dried and evaporated to give compound **4b** as colorless oil (397 mg, 1.08 mmol, 71%).

^{1}H NMR ($CDCl_3$): δ (ppm) 3.61 (t, *J* = 6.3 Hz, 8H), 2.56 (t, *J* = 6.6 Hz, 8H), 2.49 (s, 4H), 1.88 (quint, *J* = 6.4 Hz, 8H).

^{13}C NMR ($CDCl_3$): δ (ppm) 52.7, 51.2, 43.2, 30.4.

Anal. Calcd for $C_{14}H_{28}Cl_4N_2$ (**4b**): C, 45.92; H, 7.71; N, 7.65. Found: C, 46.52; H, 7.73; N, 7.86.

***N,N,N',N'*-Tetrakis(3-chloropropyl)propanediamine (4d).** The solution of *N,N,N',N'*-tetrakis(3-hydroxypropyl)propanediamine hydrobromide (**3d**·2HBr) (943 mg, 2.01 mmol) and thionyl chloride (1.15 mL, 16 mmol) in dichloromethane (30 mL) was refluxed for overnight under N_2. The resultant solution was cooled to r.t. and washed with 6*N* $NaOH_{aq}$. The organic layer was dried and evaporated to give compound **4d** as orange oil (751 mg, 1.97 mmol, 98%).

^{1}H NMR ($CDCl_3$): δ (ppm) 3.60 (t, *J* = 6.3 Hz, 8H), 2.54 (t, *J* = 6.6 Hz, 8H), 2.39 (t, *J* = 7.2 Hz, 4H), 1.88 (quint, *J* = 6.4 Hz, 8H), 1.60 (m, 2H).

^{13}C NMR ($CDCl_3$):□δ (ppm) 48.5, 46.9, 43.2, 32.9, 30.3.

Anal. Calcd for $C_{15}H_{30.5}Cl_4N_2O_{0.25}$ (**4d**·0.25H_2O): C, 46.83; H, 7.99; N, 7.28. Found: C, 46.96; H, 7.94; N, 7.11.

***N,N,N',N'*-Tetrakis(2-(8-quinolyloxy)ethyl)ethylenediamine (8-TQOEEN, 2a).** To an agitated mixture of 8-quinolinol (2.18 g, 14.8 mmol) and powdered potassium hydroxide (830 mg, 14.8 mmol) in dry ethanol (30 mL) was added *N,N,N',N'*-tetrakis(2-chloroethyl)ethylenediamine (**4a**) (460 mg, 1.48 mmol) in 3 mL of ethanol. The resulting reaction mixture was refluxed overnight under N_2, cooled to room temperature and the solvent was evaporated. The residue was extracted with $CHCl_3$/water and the organic layer was washed with 3N NaOH, dried and evaporated. The residue was purified by column chromatography (alumina, $CHCl_3$/CH_3OH 99.5/0.5, R_f = 0.35) to give compound **2a** as a yellow oil (226 mg, 0.30 mmol, 20%).

^{1}H NMR ($CDCl_3$): δ (ppm) 8.91 (dd, *J* = 4.3, 1.8 Hz, 4 H), 8.14 (dd, *J* = 8.2, 1.5 Hz, 4 H), 7.40-7.45 (m, 12 H), 7.06 (dd, *J* = 7.3, 1.5 Hz, 4 H), 4.34 (t, *J* = 5.8 Hz, 8 H), 3.05 (t, *J* = 6.0 Hz, 8 H), 2.76 (s, 4 H).

^{13}C NMR ($CDCl_3$): δ (ppm) 154.0, 148.6, 139.5, 136.0, 129.3, 126.5, 121.6, 119.5, 64.2, 56.8, 52.5.

HRMS (ESI-MS) *m/z*: $[M + Na]^+$ Calcd for $C_{46}H_{44}N_6O_4Na$ 767.3322; Found 767.3434.

***N,N,N',N'*-Tetrakis(3-(8-quinolyloxy)propyl)ethylenediamine (8-TQOPEN, 2b).** To an agitated mixture of 8-quinolinol (1.88 g, 13.0 mmol) and powdered potassium hydroxide (788 mg, 14.0 mmol) in dry ethanol (30 mL) was added *N,N,N',N'*-tetrakis(3-chloropropyl)ethylenediamine (**4b**) (397 mg, 1.08 mmol) in 3 mL of ethanol. The resulting reaction mixture was refluxed overnight under N_2, cooled to room temperature and the solvent was evaporated. The residue was extracted with $CHCl_3$/water and the organic layer was washed with 3N NaOH, dried and evaporated. The residue was purified by column

chromatography (alumina, $CHCl_3/CH_3OH$ 99.5/0.5, R_f = 0.28) to give a yellow oil. This material was dissolved in small portions of acetonitrile and conc. hydrochloric acid was added to induce precipitation. After filtration, the obtained hydrochloride salt was dissolved in water and 6N NaOH was added to adjust the pH >12. The product was extracted into chloroform, dried and evaporated to give compound **2b** as a yellow oil (130 mg, 0.162 mmol, 15%).

^{1}H NMR ($CDCl_3$): δ (ppm) 8.89 (dd, *J* = 4.3, 1.5 Hz, 4 H), 8.05 (dd, *J* = 8.5, 1.5 Hz, 4 H), 7.27-7.38 (m, 12 H), 6.87 (dd, *J* = 7.3, 1.5 Hz, 4 H), 4.06 (t, *J* = 6.6 Hz, 8 H), 2.55 (t, *J* = 6.6 Hz, 8 H), 2.43 (s, 4 H), 1.88 (quint, *J* = 6.5 Hz, 8 H).

^{13}C NMR ($CDCl_3$): δ (ppm) 154.5, 148.9, 140.1, 135.5, 129.2, 126.5, 121.3, 119.1, 108.5, 66.7, 52.6, 50.7, 26.9.

HRMS (ESI-MS) *m/z*: $[M + Na]^+$ Calcd for $C_{50}H_{52}N_6O_4Na$ 823.3948; Found 823.3985.

Anal. Calcd for $C_{50}H_{57}Cl_2N_6O_{5.5}$ (**2b**·2HCl·1.5H_2O): C, 66.66; H, 6.38; N, 9.33. Found: C, 66.77; H, 5.99; N, 9.23.

***N,N,N',N'*-Tetrakis(2-(8-quinolyloxy)ethyl)propanediamine (8-TQOEPN, 2c).** To an agitated mixture of 8-quinolinol (1.53 g, 10.6 mmol) and powdered potassium hydroxide (592 mg, 10.6 mmol) in dry ethanol (30 mL) was added *N,N,N',N'*-tetrakis(2-chloroethyl)propanediamine (**4c**) (285 mg, 1.06 mmol) in 3 mL of ethanol. The resulting reaction mixture was refluxed overnight under N_2, cooled to room temperature and the solvent was evaporated. The residue was extracted with $CHCl_3$/water and the organic layer was washed with 3N NaOH, dried and evaporated. The residue was purified by column chromatography (alumina, $CHCl_3/CH_3OH$ 99.5/0.5, R_f = 0.3) to give compound **2c** as a yellow oil (88 mg, 0.12 mmol, 9%).

^{1}H NMR ($CDCl_3$): δ (ppm) 8.88 (dd, *J* = 4.3, 1.8 Hz, 4 H), 8.06 (dd, *J* = 8.2, 1.5 Hz, 4 H), 7.29-7.40 (m, 12 H), 7.02 (dd, *J* = 6.4, 2.7 Hz, 4 H), 4.34 (t, *J* = 6.6 Hz, 8 H), 4.34 (t, *J* = 6.7 Hz, 8 H), 3.24 (t, *J* = 6.6 Hz, 8 H), 2.82 (t, *J* = 7.2 Hz, 8 H), 2.61 (s, 4 H), 1.85 (br., 2 H).

^{13}C NMR ($CDCl_3$): δ (ppm) 154.2, 148.9, 140.0, 135.5, 129.2, 126.5, 121.3, 119.3, 108.7, 77.2, 67.2, 53.6, 25.4.

HRMS (ESI-MS) *m/z*: $[M + Na]^+$ Calcd for $C_{47}H_{46}N_6O_4Na$ 781.3398; Found 781.3478.

Anal. Calcd for $C_{47}H_{50}N_6O_6$ (**2c**·$2H_2O$): C, 71.01; H, 6.34; N, 10.57. Found: C, 70.77; H, 6.35; N, 10.88.

***N,N,N',N'*-Tetrakis(3-(8-quinolyloxy)propyl)propanediamine (8-TQOPPN, 2d).** To an agitated mixture of 8-quinolinol (2.67 g, 18.4 mmol) and powdered potassium hydroxide (1.03 g, 18.4 mmol) in dry ethanol (30 mL) was added *N,N,N',N'*-tetrakis(3-chloropropyl)propanediamine (**4d**) (700 mg, 1.84 mmol) in 3 mL of ethanol. The resulting reaction mixture was refluxed overnight under N_2. The resultant solution was cooled to room temperature and the solvent was evaporated. The residue was extracted with $CHCl_3$/water and the organic layer was washed with 3N NaOH, dried and evaporated. The residue was purified by column chromatography (alumina, AcOEt/MeOH 98/2, R_f = 0.6) to give yellow oil. This material was dissolved in a small portion of ethanol and conc. hydrochloric acid was added to induce precipitation. After filtration, the hydrochloride salt was dissolved in water and 6N NaOH was added to adjust the pH >12. The product was extracted into chloroform, dried and evaporated to give compound **2d** as a yellow oil (195 mg, 0.239 mmol, 13%).

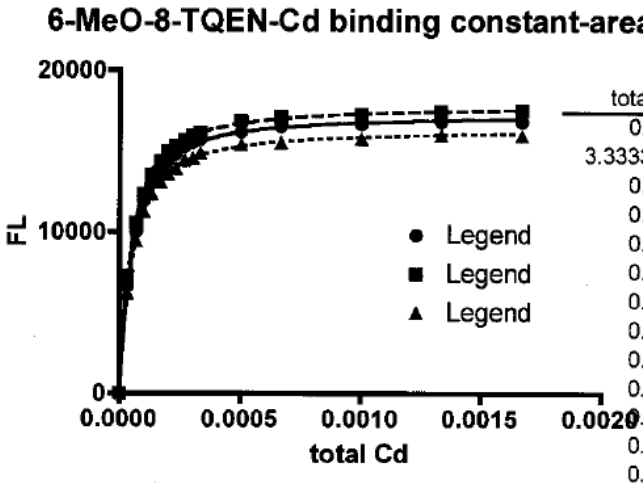
^{1}H NMR ($CDCl_3$): δ (ppm) 8.90 (dd, *J* = 4.3, 1.8 Hz, 4 H), 8.04 (dd, *J* = 8.2, 1.8 Hz, 4 H), 7.26-7.38 (m, 12 H), 6.89 (dd, *J* = 7.3, 1.5 Hz, 4 H), 4.10 (t, *J* = 6.7 Hz, 8 H), 2.57 (br., 8 H), 2.40 (br., 4 H), 2.06 (quint, *J* = 6.6 Hz, 8 H), 1.54 (br., 2 H).

^{13}C NMR ($CDCl_3$): δ (ppm) 154.5, 148.8, 140.0, 135.5, 129.1, 126.4, 121.2, 119.0, 108.4, 66.9, 52.3, 50.1, 26.8, 24.5.

HRMS (ESI-MS) *m/z*: $[M + H]^+$ Calcd for $C_{51}H_{55}N_6O_4$ 815.4286; Found 815.4285.

Anal. Calcd for $C_{51}H_{60}ClN_2O_{6.5}$ (**2d**·HCl·2.5H_2O): C, 68.32; H, 6.75; N, 9.37. Found: C, 68.51; H, 6.35; N, 9.26.

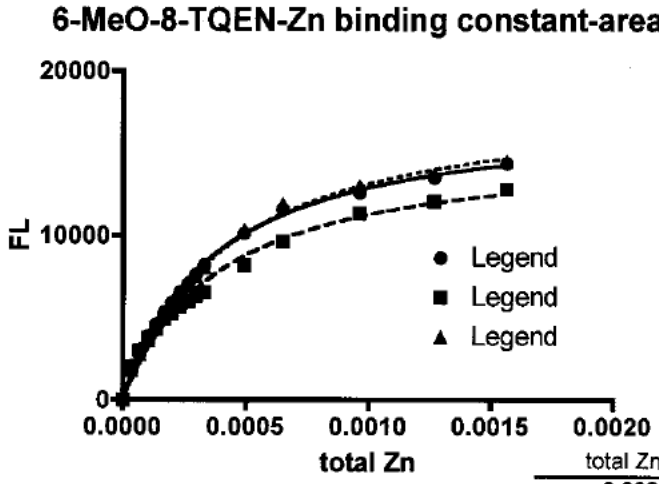
Measurements. Measurements for **1b** and **2c** were performed in DMF/HEPES buffer (1:1 (v/v), 50 mM HEPES, 100 mM KCl, pH = 8.0). Measurements for **2a**, **2b** and **2c** were performed in DMF/water (1:1). The reproducibility of all measurements has been confirmed. The values of the quantum yield are from single measurement. The K_d's are mean values of three independent measurements.



total Cd	Data Set-A	Data Set-B	Data Set-C
0.000000	0.0000	0.0000	0.0000
3.333300e-05	6642.7000	7249.9000	6194.1000
0.000067	10009.0000	10577.0000	9428.4000
0.000100	11927.0000	12324.0000	11249.0000
0.000133	13083.0000	13519.0000	12319.0000
0.000167	13838.0000	14364.0000	13100.0000
0.000200	14384.0000	14958.0000	13581.0000
0.000233	14846.0000	15329.0000	13940.0000
0.000267	15304.0000	15666.0000	14419.0000
0.000300	15531.0000	15995.0000	14575.0000
0.000333	15742.0000	16124.0000	14885.0000
0.000500	16209.0000	16891.0000	15403.0000
0.000667	16532.0000	17120.0000	15545.0000
0.001000	16683.0000	17254.0000	15771.0000
0.001333	16841.0000	17474.0000	15997.0000
0.001667	16819.0000	17530.0000	15977.0000

	Data Set-A	Data Set-B	Data Set-C
Best-fit values			
BMAX	17334	17881	16417
KD	3.4014e-005	3.2753e-005	3.4861e-005
L0	3.4000e-005	3.4000e-005	3.4000e-005
Std. Error			
BMAX	51.29	72.72	41.43
KD	6.7923e-007	9.1697e-007	5.8621e-007
95% Confidence Intervals			
BMAX	17224 to 17444	17725 to 18037	16328 to 16506
KD	3.2557e-005 to 3.5471e-005	3.0786e-005 to 3.4720e-005	3.3603e-005 to 3.6118e-005
Goodness of Fit			
Degrees of Freedom	14	14	14
R squared	0.9995	0.9990	0.9996
Absolute Sum of Squares	150547	308243	97076
Sy.x	103.7	148.4	83.27
Constraints			
L0	L0 = 3.4000e-005	L0 = 3.4000e-005	L0 = 3.4000e-005
Data			
Number of X values	16	16	16
Number of Y replicates	1	1	1
Total number of values	16	16	16
Number of missing values	0	0	0

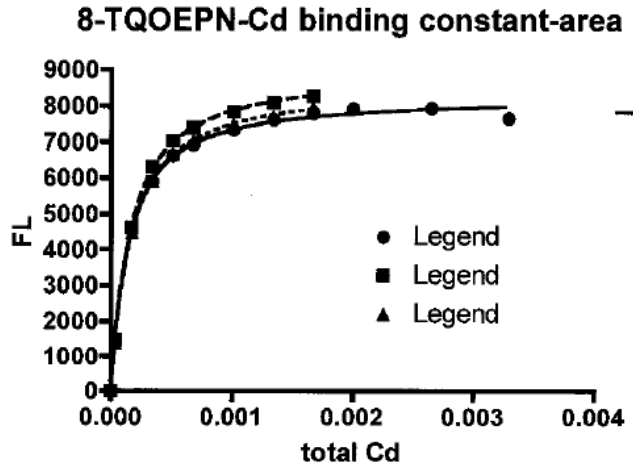
Figure S1. Estimation of dissociation constant of **1b** with Cd^{2+} ion.



total Zn	Data Set-A	Data Set-B	Data Set-C
0.000000	0.0000	0.0000	0.0000
3.328900e-05	2052.1000	1985.7000	1805.5000
0.000066	3071.7000	3003.7000	2765.1000
0.000100	3894.7000	3771.1000	3589.5000
0.000133	4615.1000	4360.8000	4340.9000
0.000166	5328.7000	4904.2000	5018.6000
0.000198	5939.3000	5268.7000	5694.0000
0.000231	6569.9000	5657.5000	6394.0000
0.000264	7062.8000	5955.8000	6972.8000
0.000296	7624.4000	6335.3000	7513.2000
0.000329	8194.3000	6558.0000	8067.8000
0.000490	10143.0000	8170.1000	10339.0000
0.000649	11616.0000	9620.8000	11916.0000
0.000962	12592.0000	11321.0000	13012.0000
0.001266	13508.0000	12061.0000	13686.0000
0.001563	14379.0000	12804.0000	14492.0000

	Data Set-A	Data Set-B	Data Set-C
Best-fit values			
BMAX	17450	15474	18373
KD	0.0003465	0.0003665	0.0003935
L0	3.4000e-005	3.4000e-005	3.4000e-005
Std. Error			
BMAX	339.0	600.4	377.1
KD	1.6786e-005	3.4830e-005	1.9338e-005
95% Confidence Intervals			
BMAX	16723 to 18177	14186 to 16762	17564 to 19182
KD	0.0003105 to 0.0003825	0.0002918 to 0.0004412	0.0003520 to 0.0004350
Goodness of Fit			
Degrees of Freedom	14	14	14
R squared	0.9962	0.9849	0.9963
Absolute Sum of Squares	1.0281e+006	2.9920e+006	1.0690e+006
Sy.x	271.0	462.3	276.3
Constraints			
L0	L0 = 3.4000e-005	L0 = 3.4000e-005	L0 = 3.4000e-005
Data			
Number of X values	16	16	16
Number of Y replicates	1	1	1
Total number of values	16	16	16
Number of missing values	0	0	0

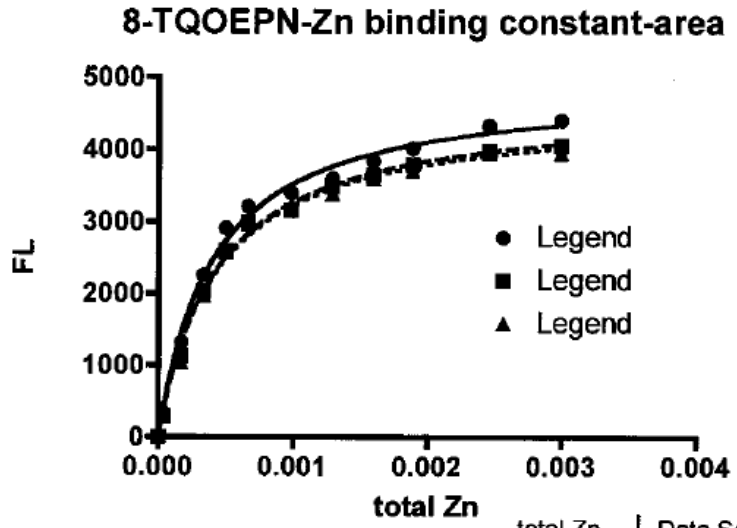
Figure S2. Estimation of dissociation constant of **1b** with Zn^{2+} ion.



total Cd	Data Set-A	Data Set-B	Data Set-C
0.000000	0.0000	0.0000	0.0000
0.000034	1431.9000	1467.4000	1363.0000
0.000170	4559.1000	4615.7000	4471.9000
0.000339	5916.3000	6311.3000	5907.5000
0.000507	6609.1000	7029.4000	6654.9000
0.000675	6911.0000	7396.9000	7039.0000
0.001010	7334.6000	7834.0000	7481.0000
0.001342	7620.7000	8091.0000	7691.7000
0.001672	7799.3000	8267.0000	7943.3000
0.001999	7922.0000		
0.002648	7936.4000		
0.003288	7648.6000		

	Data Set-A	Data Set-B	Data Set-C
Best-fit values			
BMAX	8269	8985	8584
KD	0.0001237	0.0001395	0.0001421
L0	3.4000e-005	3.4000e-005	3.4000e-005
Std. Error			
BMAX	69.43	47.46	35.71
KD	6.6485e-006	3.5958e-006	2.8592e-006
95% Confidence Intervals			
BMAX	8114 to 8424	8873 to 9097	8500 to 8669
KD	0.0001089 to 0.0001385	0.0001310 to 0.0001480	0.0001354 to 0.0001489
Goodness of Fit			
Degrees of Freedom	10	7	7
R squared	0.9981	0.9997	0.9998
Absolute Sum of Squares	148768	19930	11095
Sy.x	122.0	53.36	39.81
Constraints			
L0	L0 = 3.4000e-005	L0 = 3.4000e-005	L0 = 3.4000e-005
Data			
Number of X values	12	9	9
Number of Y replicates	1	1	1
Total number of values	12	9	9
Number of missing values	0	0	0

Figure S3. Estimation of dissociation constant of **2c** with Cd^{2+} ion.



total Zn	Data Set-A	Data Set-B	Data Set-C
0.000000	0.0000	0.0000	0.0000
0.000034	329.2800	293.8100	407.4800
0.000169	1317.0000	1128.7000	1037.5000
0.000335	2248.0000	2023.2000	1968.9000
0.000500	2912.0000	2594.7000	2567.7000
0.000662	3205.9000	2984.1000	2956.9000
0.000980	3388.4000	3152.4000	3234.8000
0.001290	3590.1000	3480.1000	3385.8000
0.001592	3829.8000	3629.4000	3592.7000
0.001886	4009.8000	3783.4000	3696.3000
0.002453	4326.3000	3970.5000	3946.0000
0.002993	4403.6000	4041.6000	3938.5000

	Data Set-A	Data Set-B	Data Set-C
Best-fit values			
BMAX	4877	4621	4549
KD	0.0003781	0.0004089	0.0004056
L0	3.4000e-005	3.4000e-005	3.4000e-005
Std. Error			
BMAX	109.9	84.29	106.8
KD	3.1995e-005	2.7046e-005	3.4659e-005
95% Confidence Intervals			
BMAX	4633 to 5122	4433 to 4808	4311 to 4787
KD	0.0003069 to 0.0004494	0.0003487 to 0.0004692	0.0003283 to 0.0004828
Goodness of Fit			
Degrees of Freedom	10	10	10
R squared	0.9945	0.9967	0.9944
Absolute Sum of Squares	137459	73971	119994
Sy.x	117.2	86.01	109.5
Constraints			
L0	L0 = 3.4000e-005	L0 = 3.4000e-005	L0 = 3.4000e-005
Data			
Number of X values	12	12	12
Number of Y replicates	1	1	1
Total number of values	12	12	12
Number of missing values	0	0	0

Figure S4. Estimation of dissociation constant of **2c** with Zn^{2+} ion.

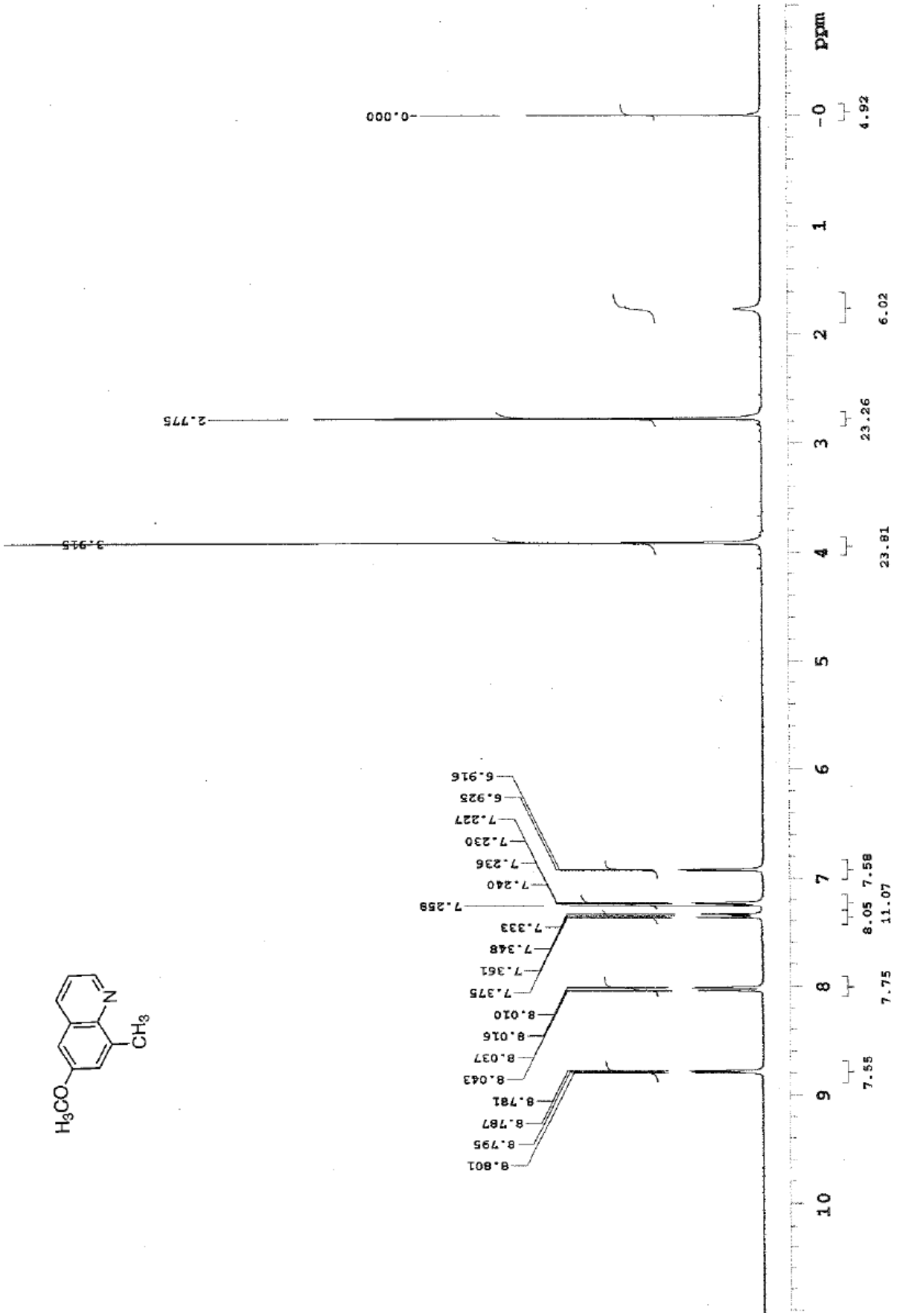


Figure S5. ^{1}H NMR spectrum of 6-methoxy-8-methylquinoline in $CDCl_3$.

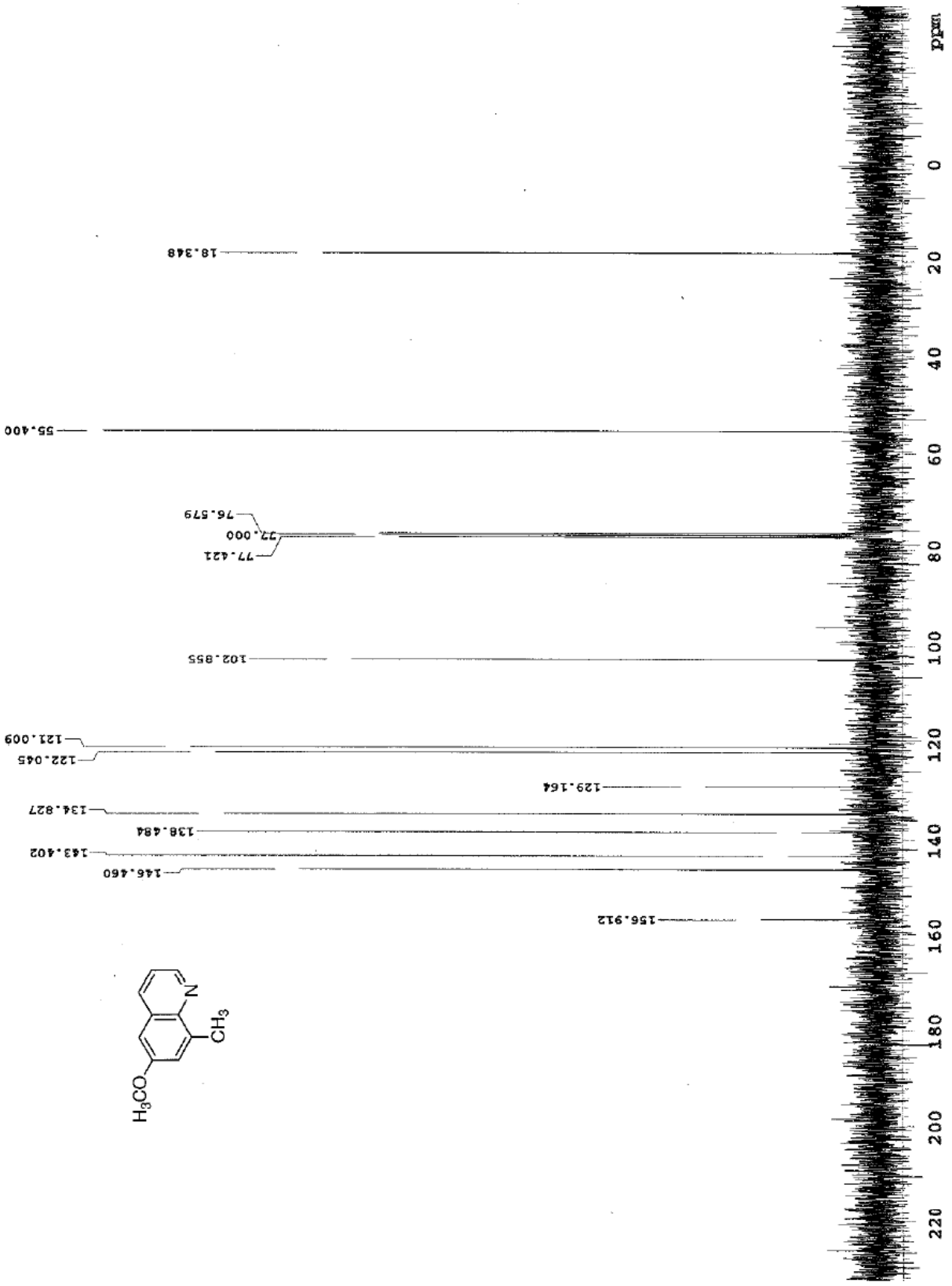


Figure S6. ^{13}C NMR spectrum of 6-methoxy-8-methylquinoline in $CDCl_3$.

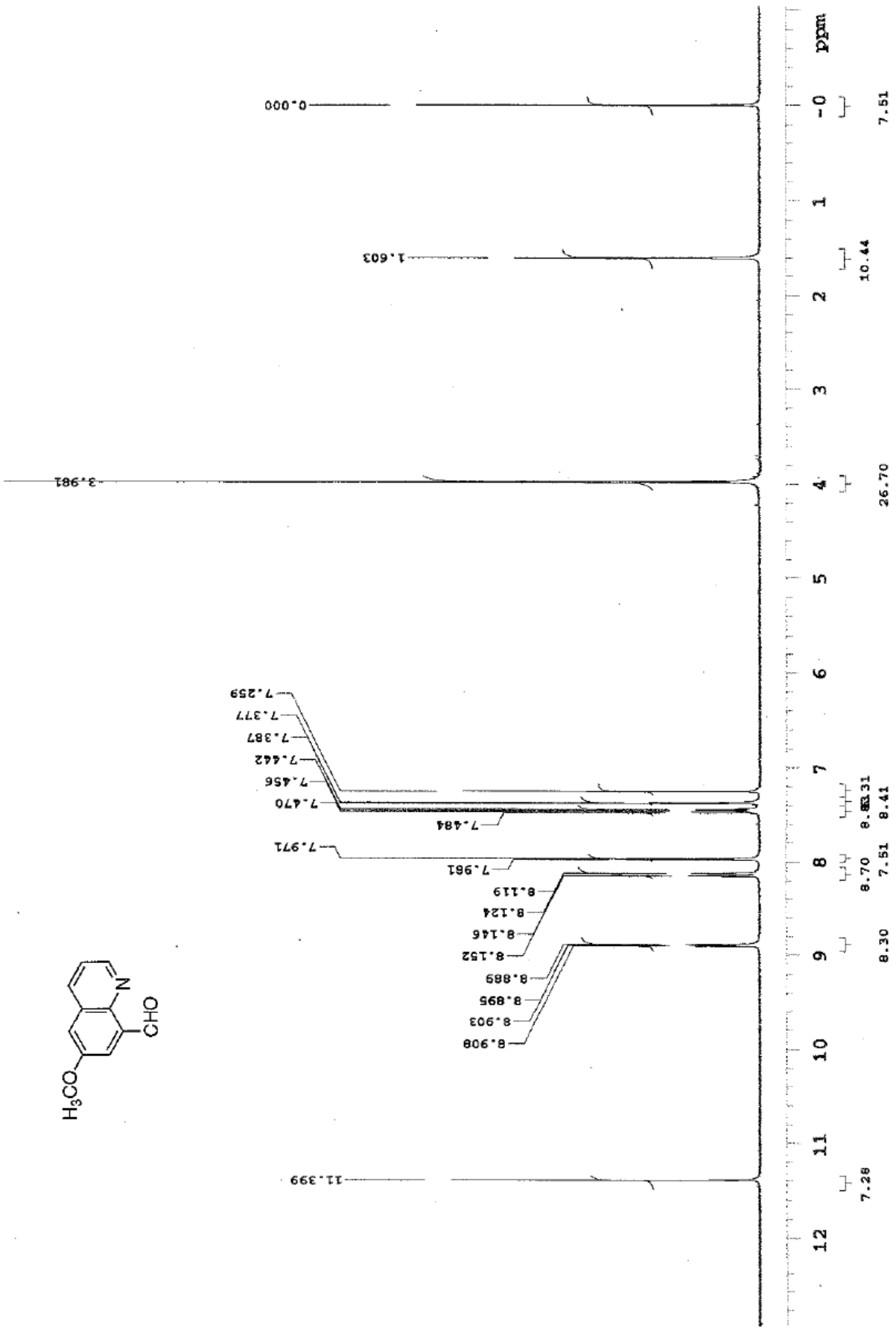


Figure S7. ^{1}H NMR spectrum of 6-methoxyquinoline-8-carboaldehyde in $CDCl_3$.

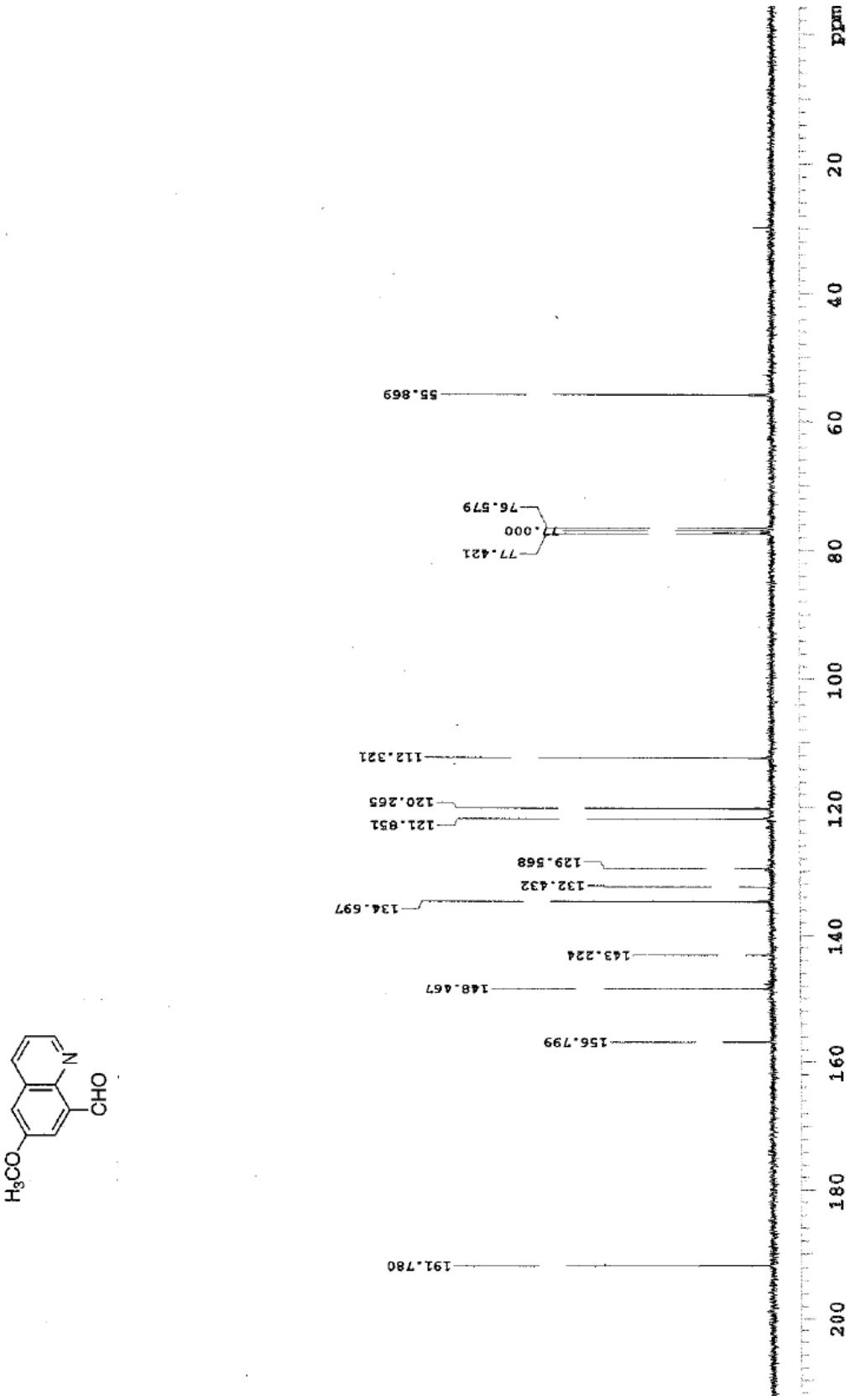


Figure S8. ^{13}C NMR spectrum of 6-methoxyquinoline-8-carboaldehyde in $CDCl_3$.

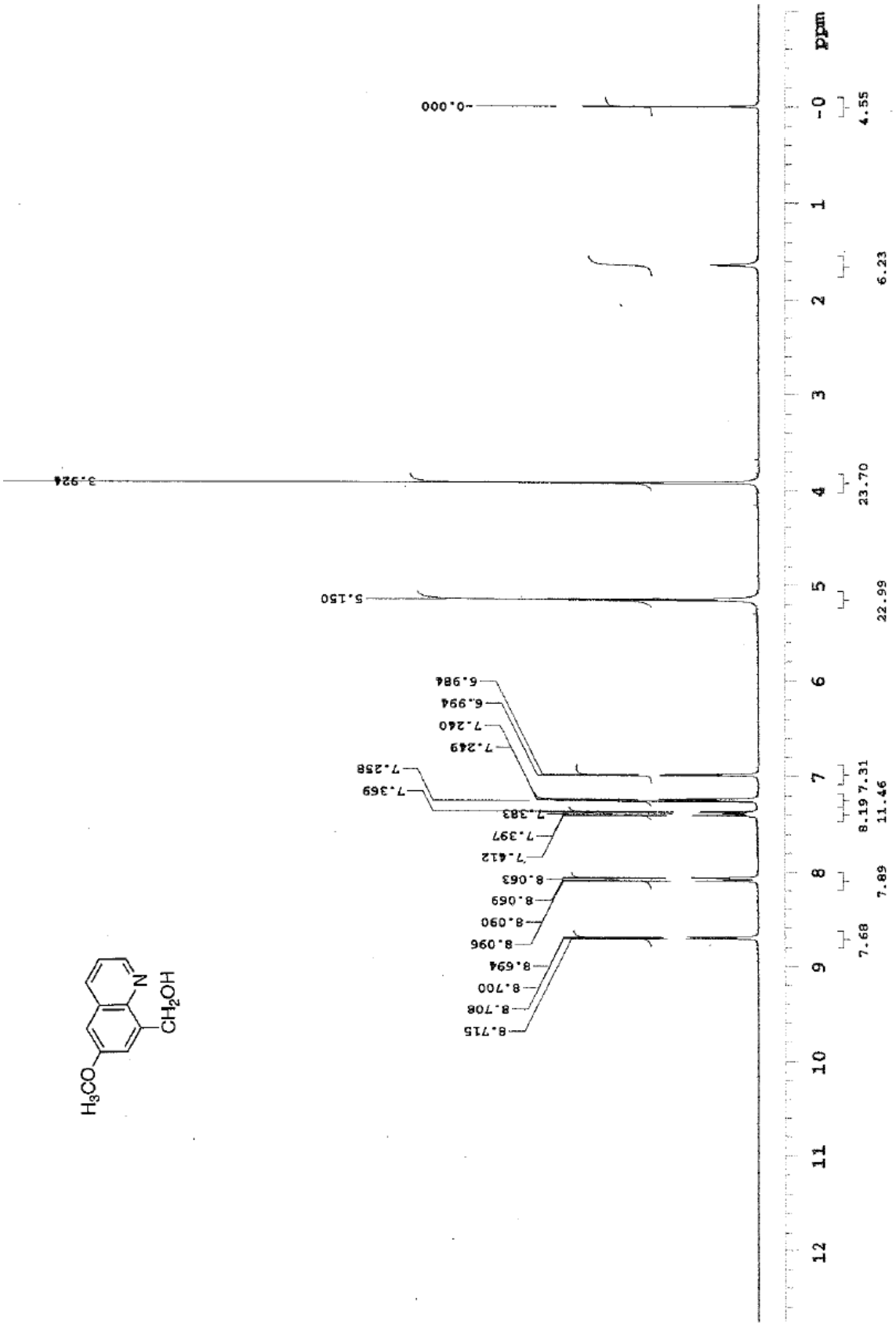


Figure S9. ^{1}H NMR spectrum of 8-hydroxymethyl-6-methoxyquinoline in $CDCl_3$.

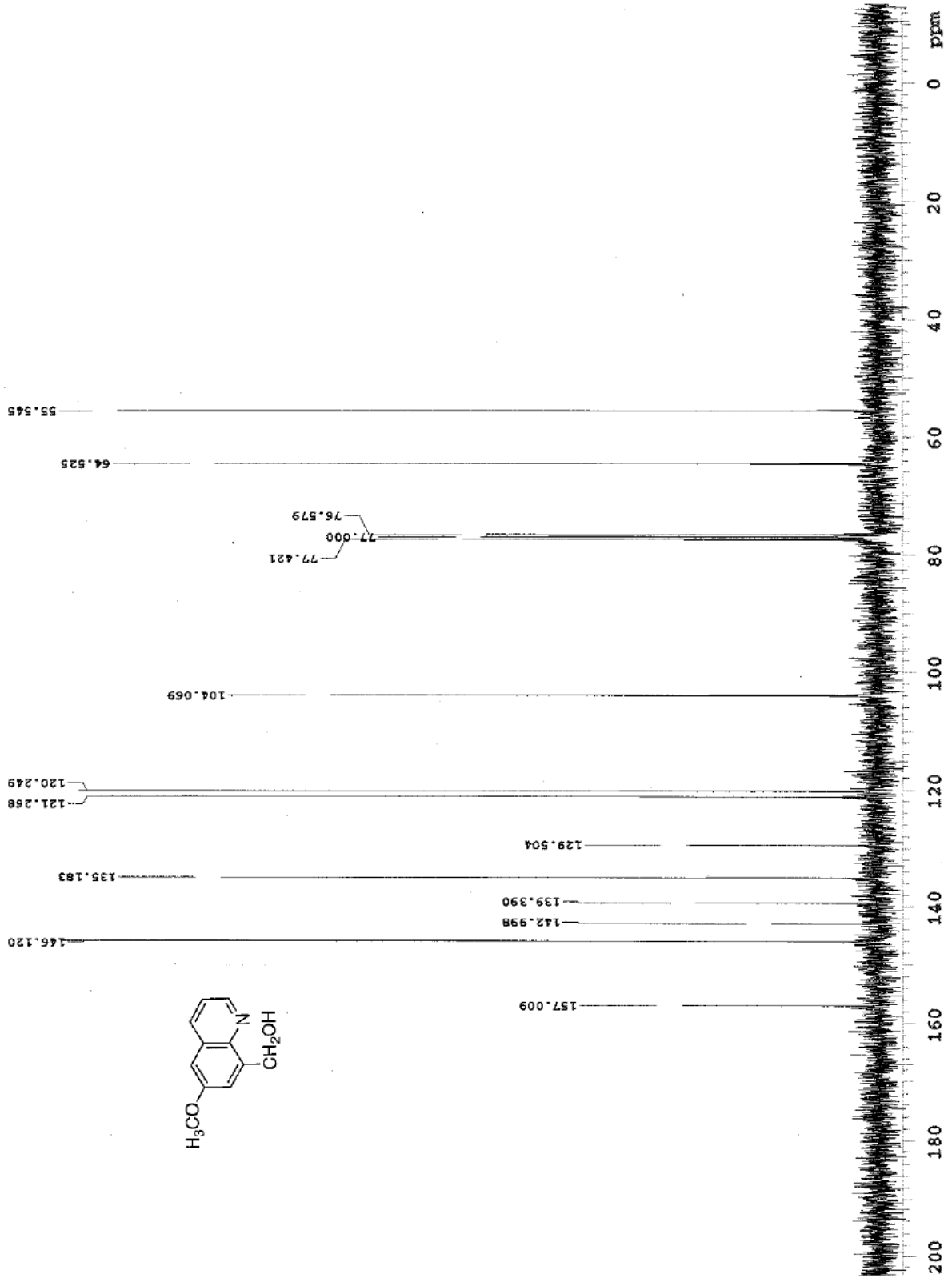


Figure S10. ^{13}C NMR spectrum of 8-hydroxymethyl-6-methoxyquinoline in $CDCl_3$.

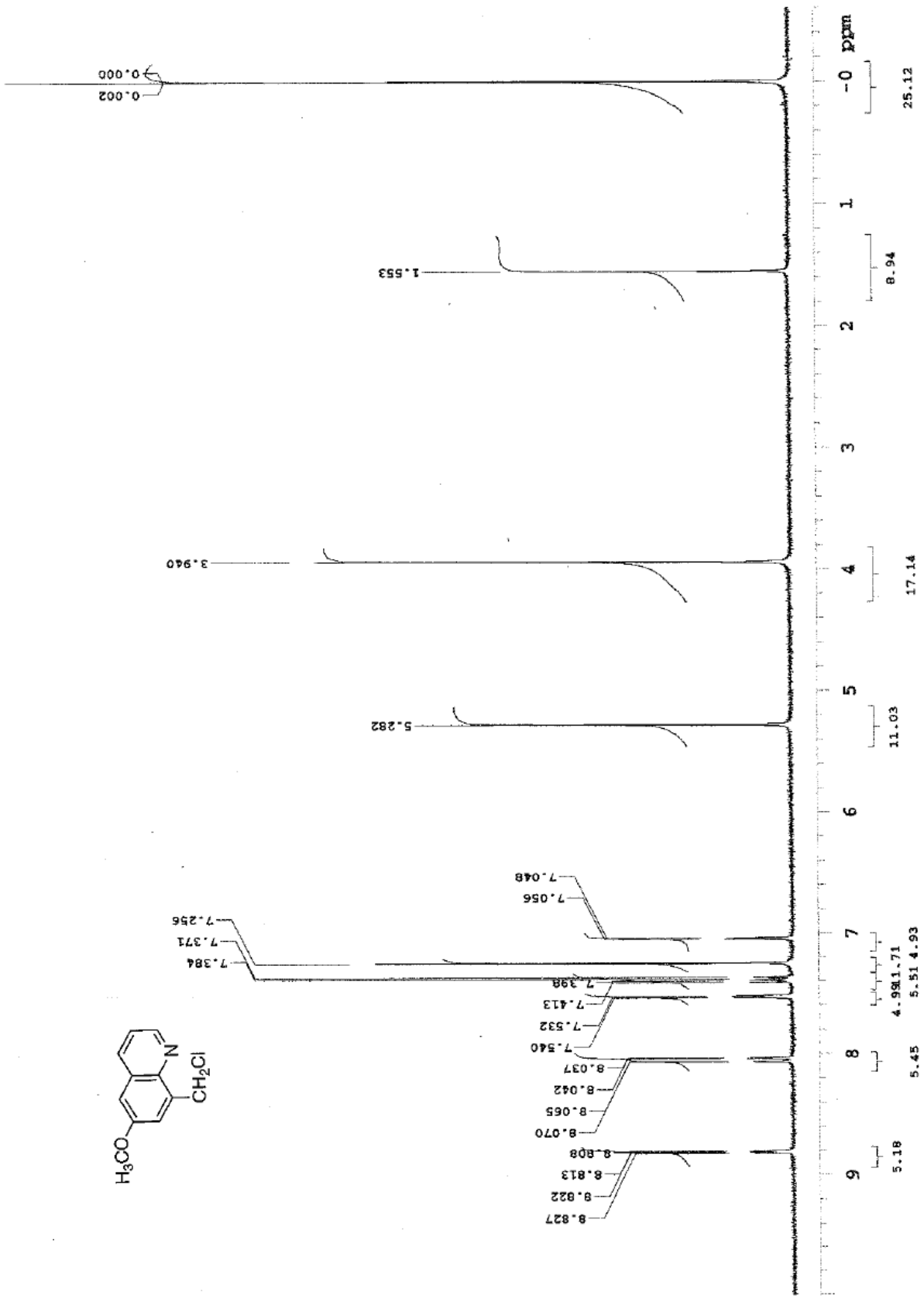


Figure S11. ^{1}H NMR spectrum of 8-chloromethyl-6-methoxyquinoline in $CDCl_3$.

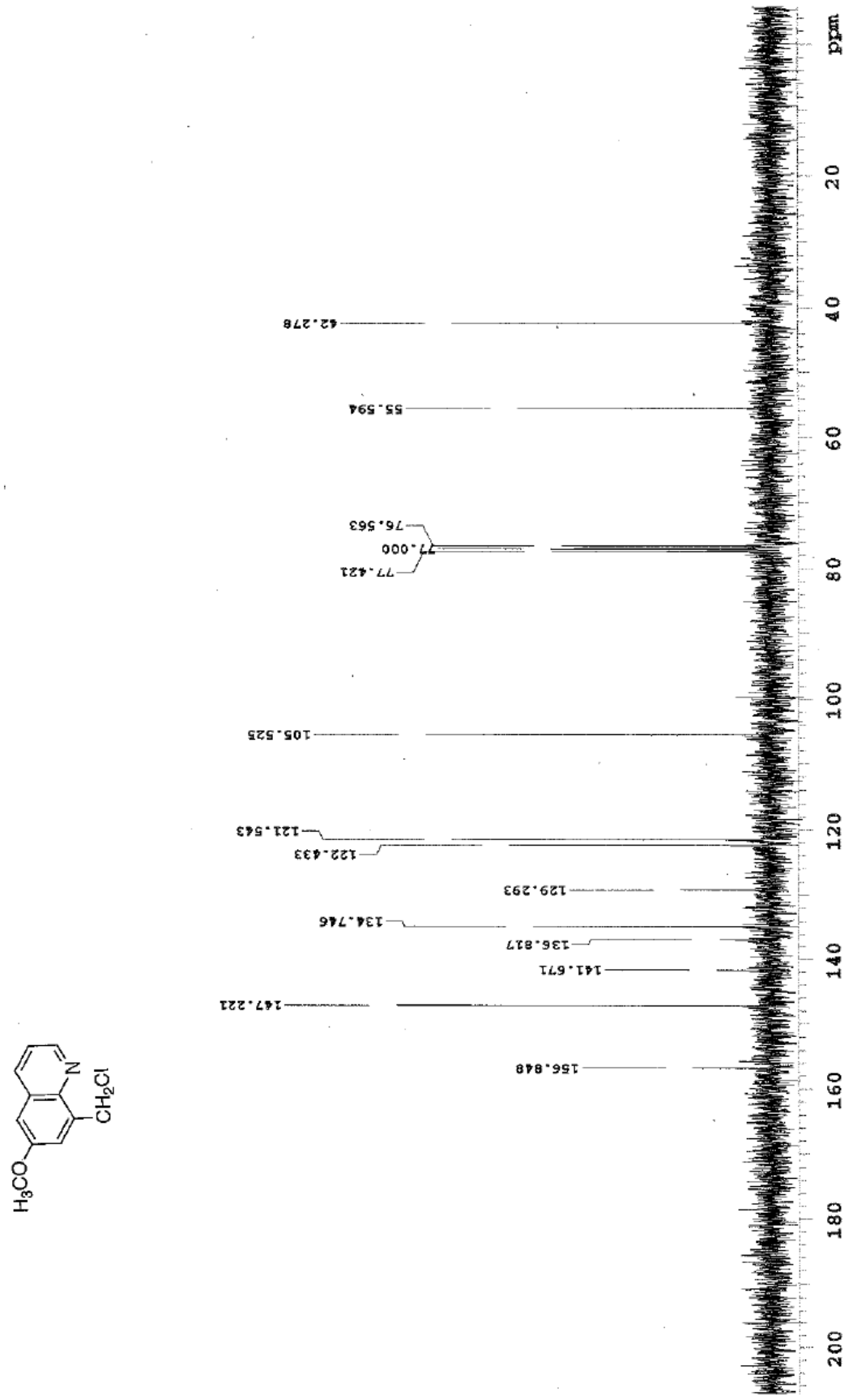


Figure S12. ^{13}C NMR spectrum of 8-chloromethyl-6-methoxyquinoline in $CDCl_3$.

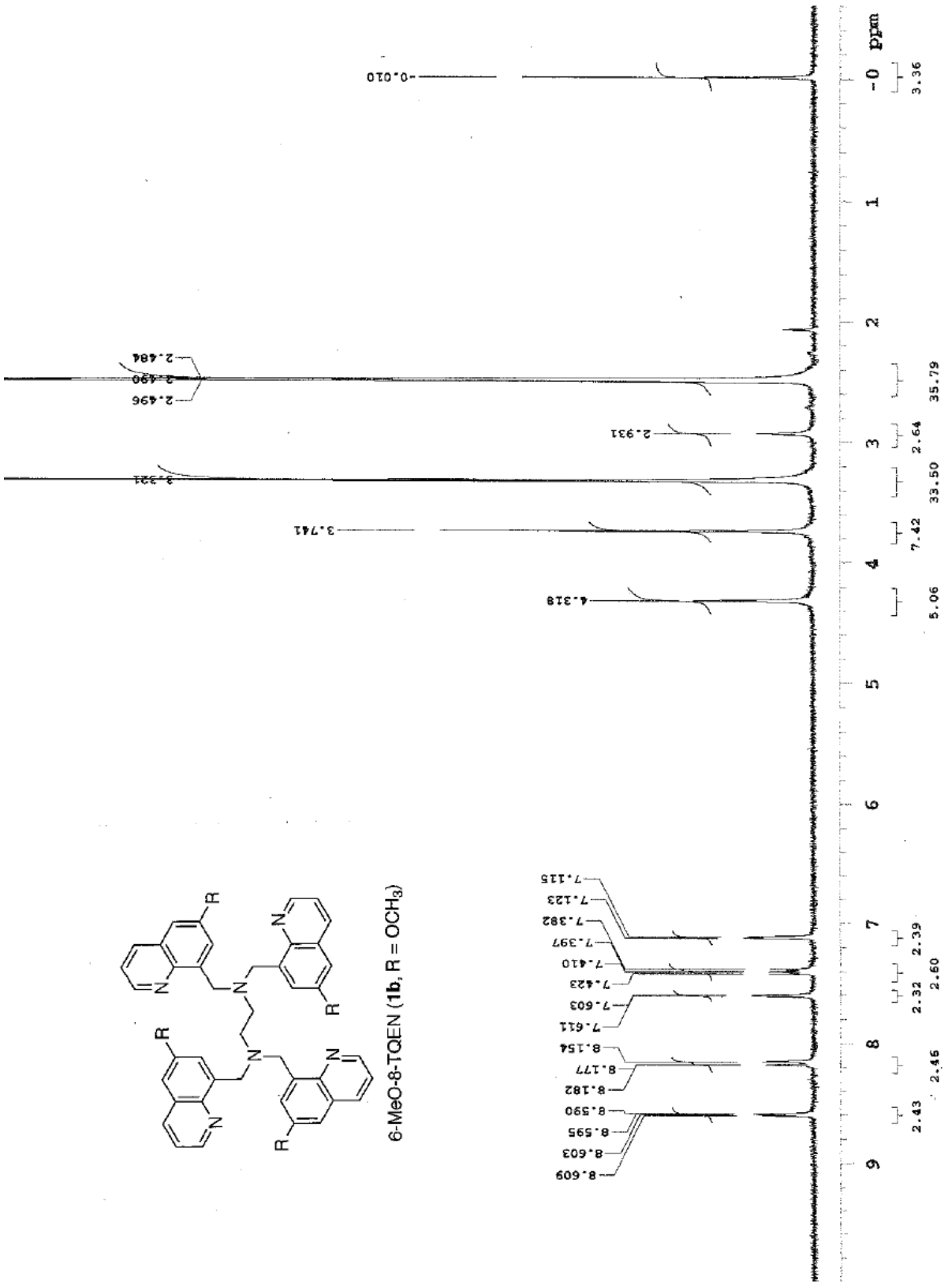


Figure S13. ^{1}H NMR spectrum of **1b** in DMSO-d_6.

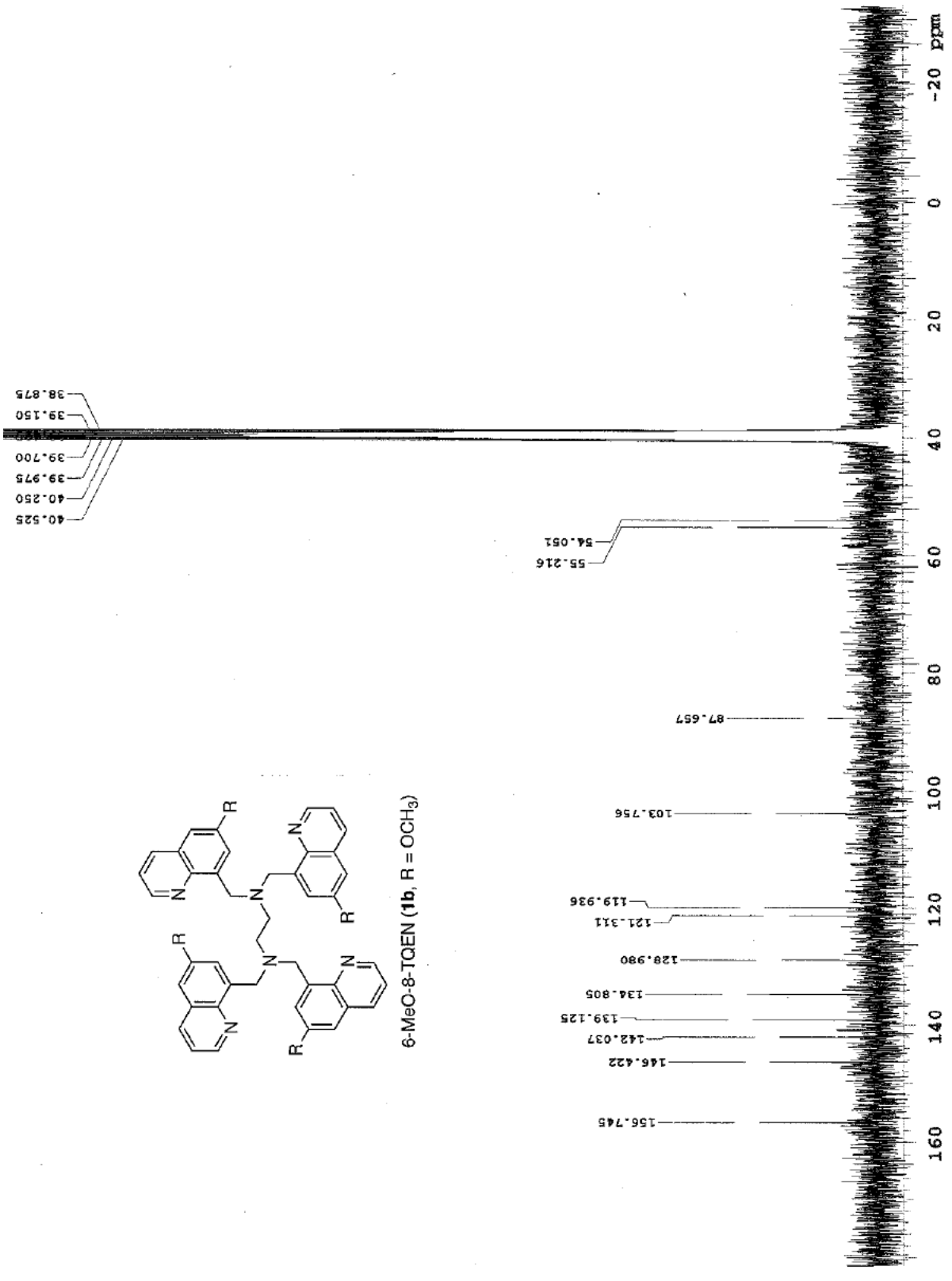


Figure S14. ^{13}C NMR spectrum of **1b** in DMSO-d_6.

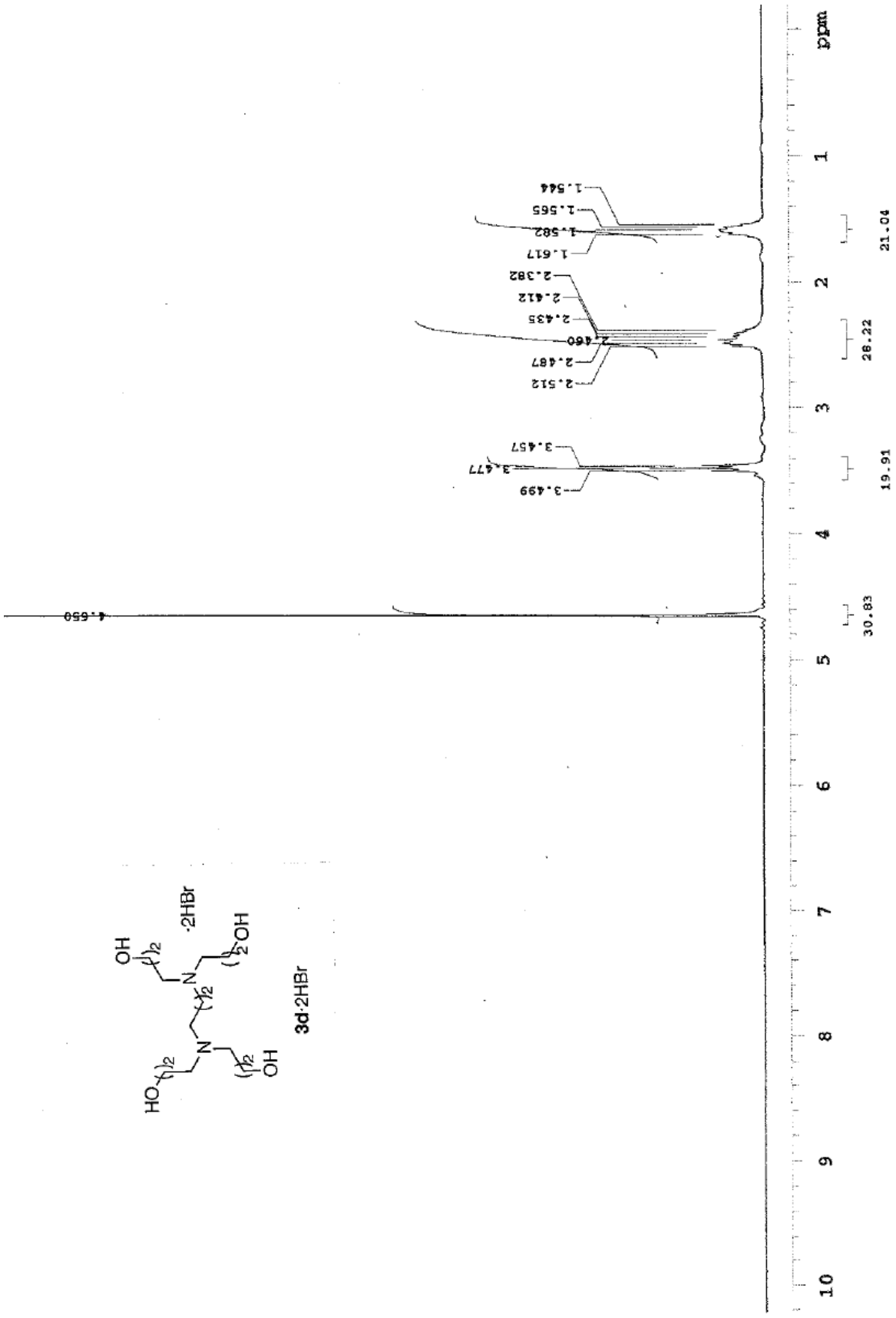


Figure S15. ^{1}H NMR spectrum of **3d**·2HBr in D_2O.

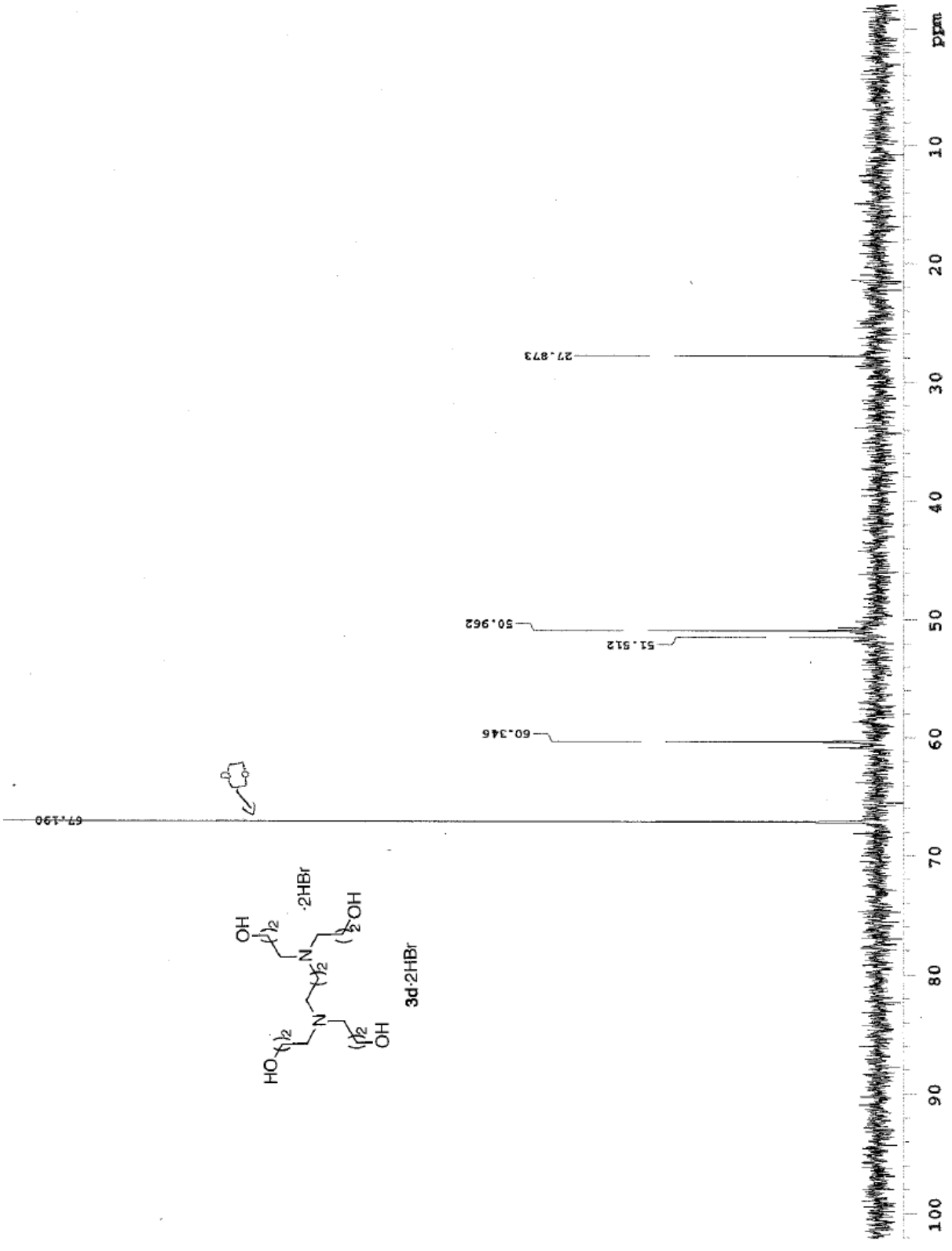


Figure S16. ^{13}C NMR spectrum of **3d**·2HBr in D_2O.

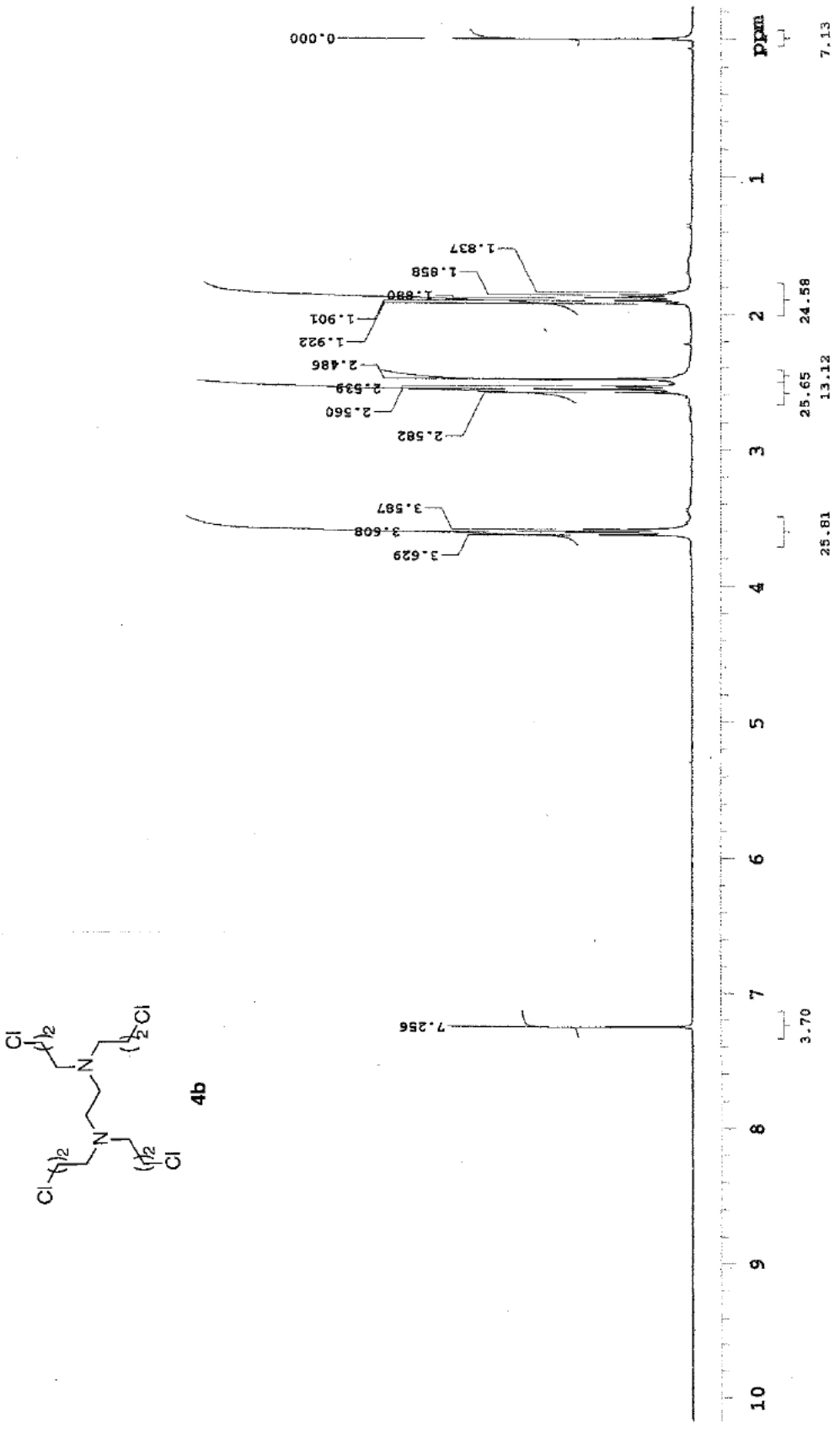


Figure S17. ^{1}H NMR spectrum of **4b** in $CDCl_3$.

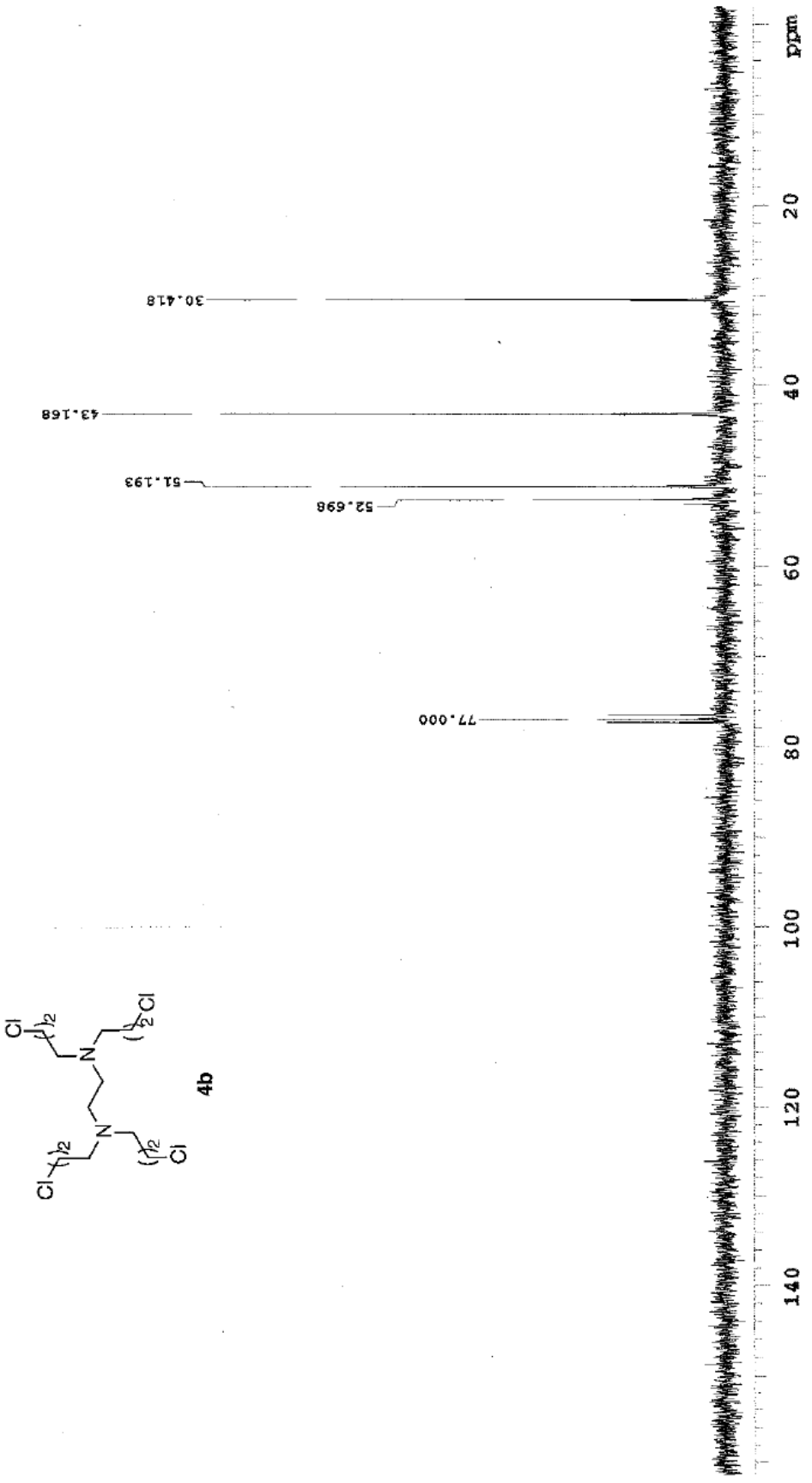


Figure S18. ^{13}C NMR spectrum of **4b** in $CDCl_3$.

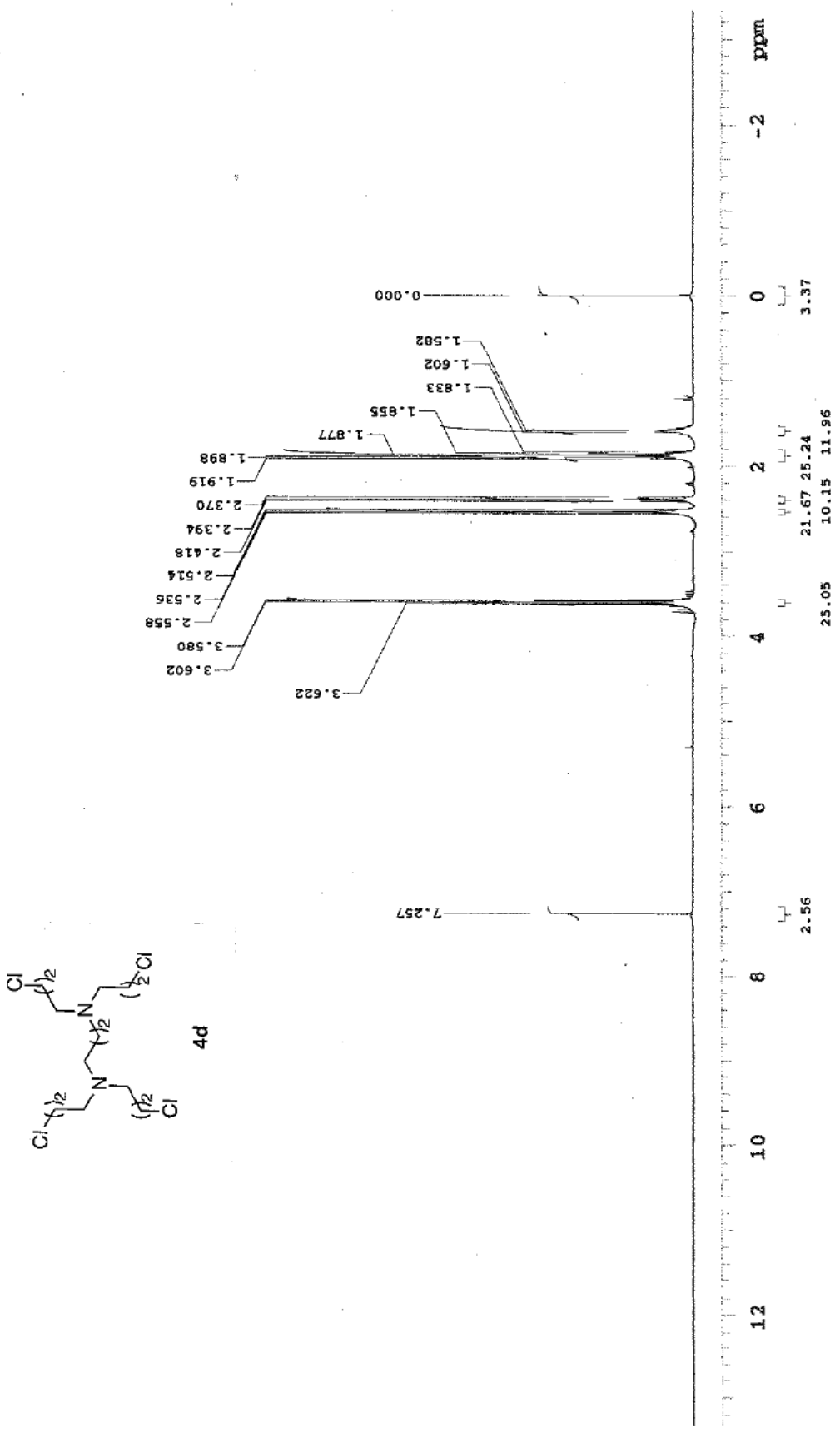


Figure S19. ^{1}H NMR spectrum of **4d** in $CDCl_3$.

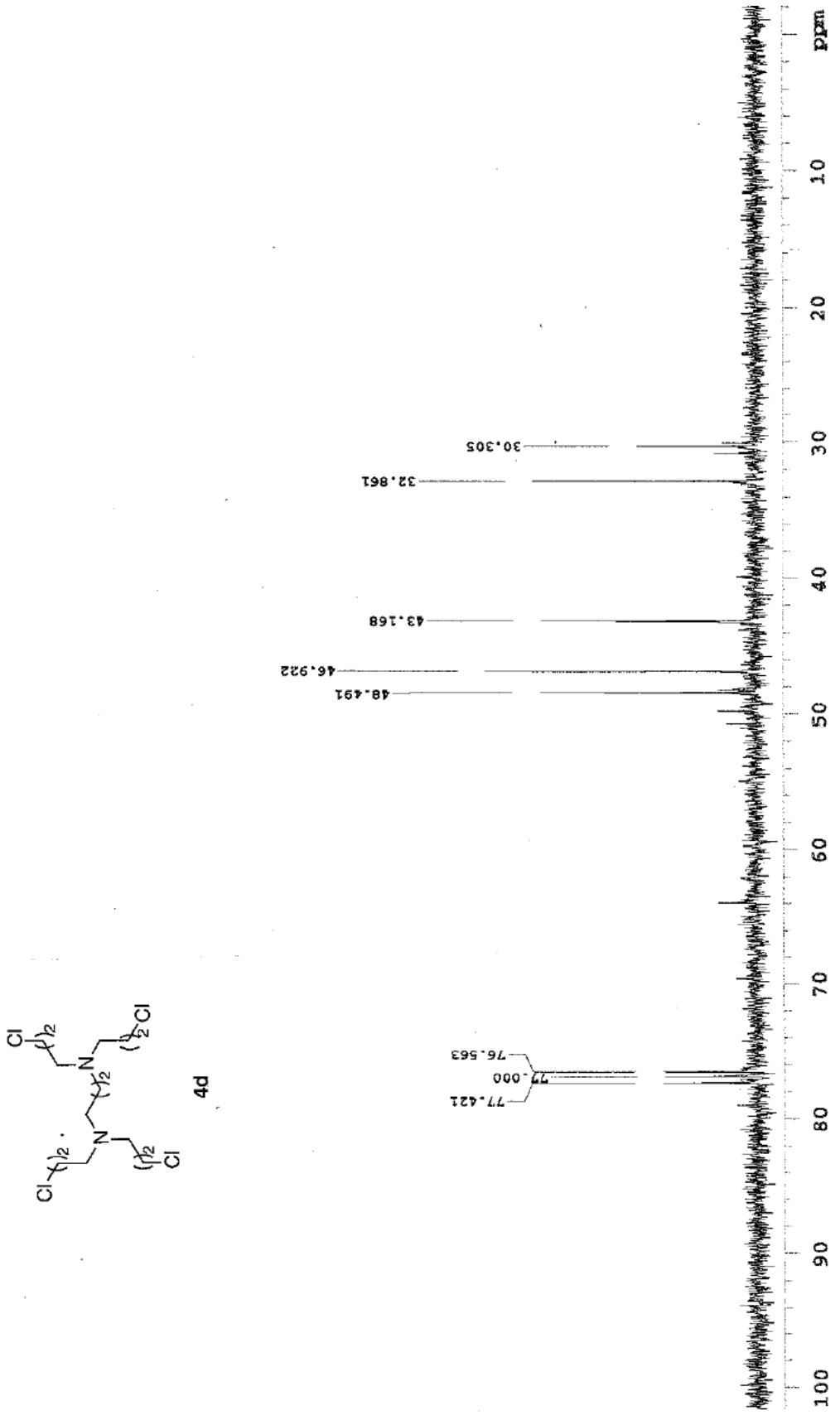


Figure S20. ^{13}C NMR spectrum of **4d** in $CDCl_3$.

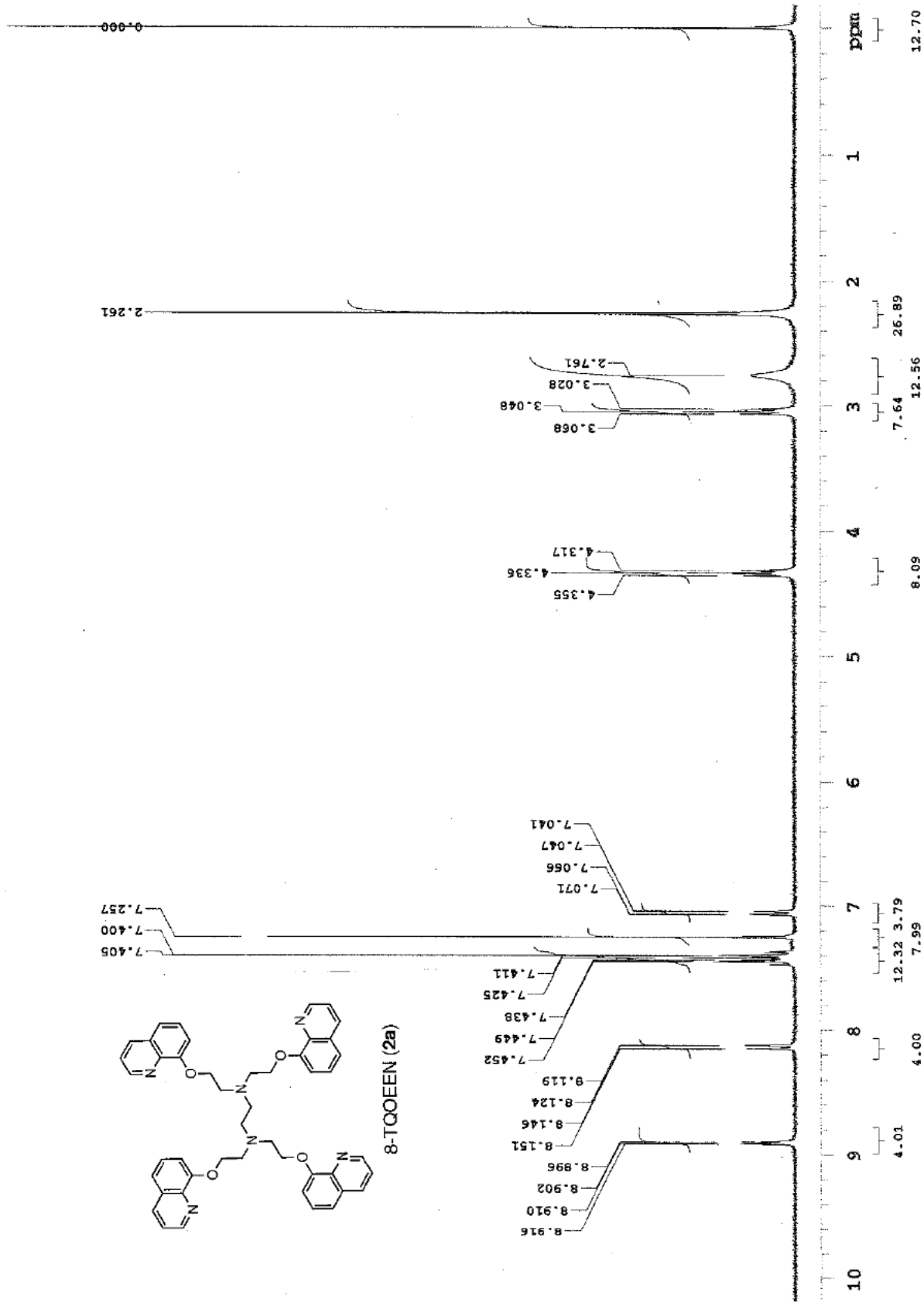


Figure S21. ^{1}H NMR spectrum of 8-TQOEEN (**2a**) in $CDCl_3$.

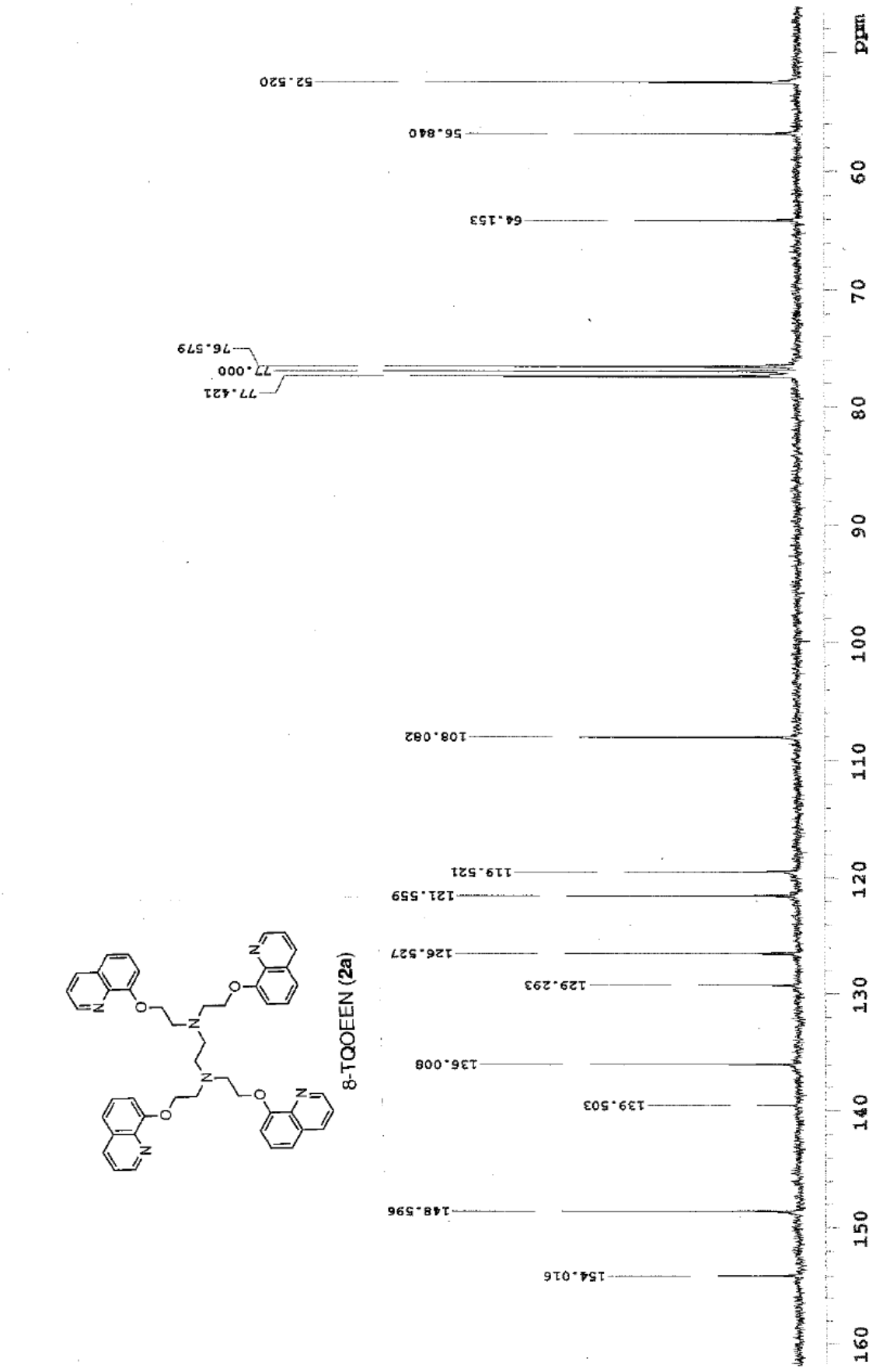


Figure S22. ^{13}C NMR spectrum of 8-TQOEEN (**2a**) in $CDCl_3$.

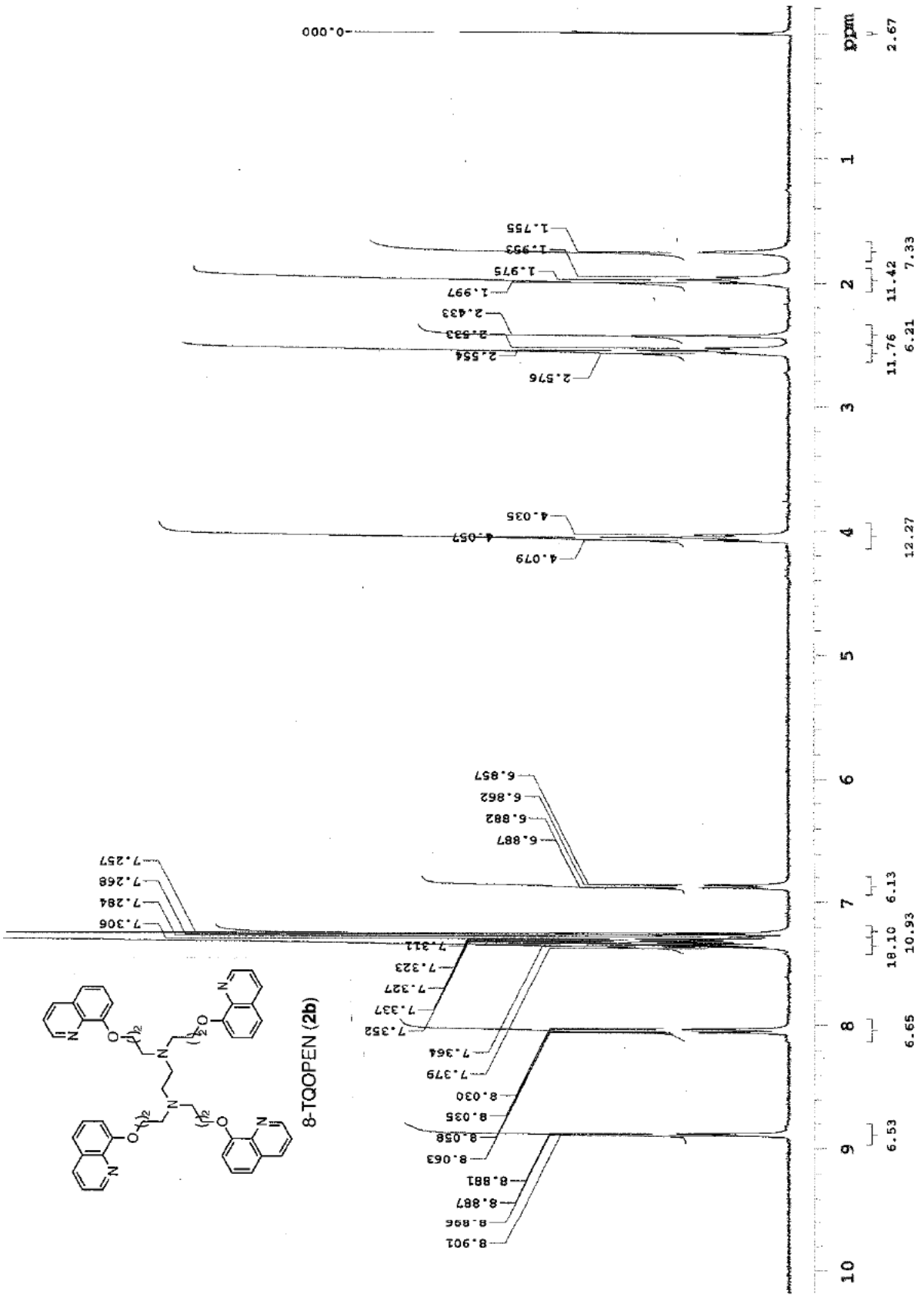


Figure S23. ^{1}H NMR spectrum of 8-TQOPEN (**2b**) in $CDCl_3$.

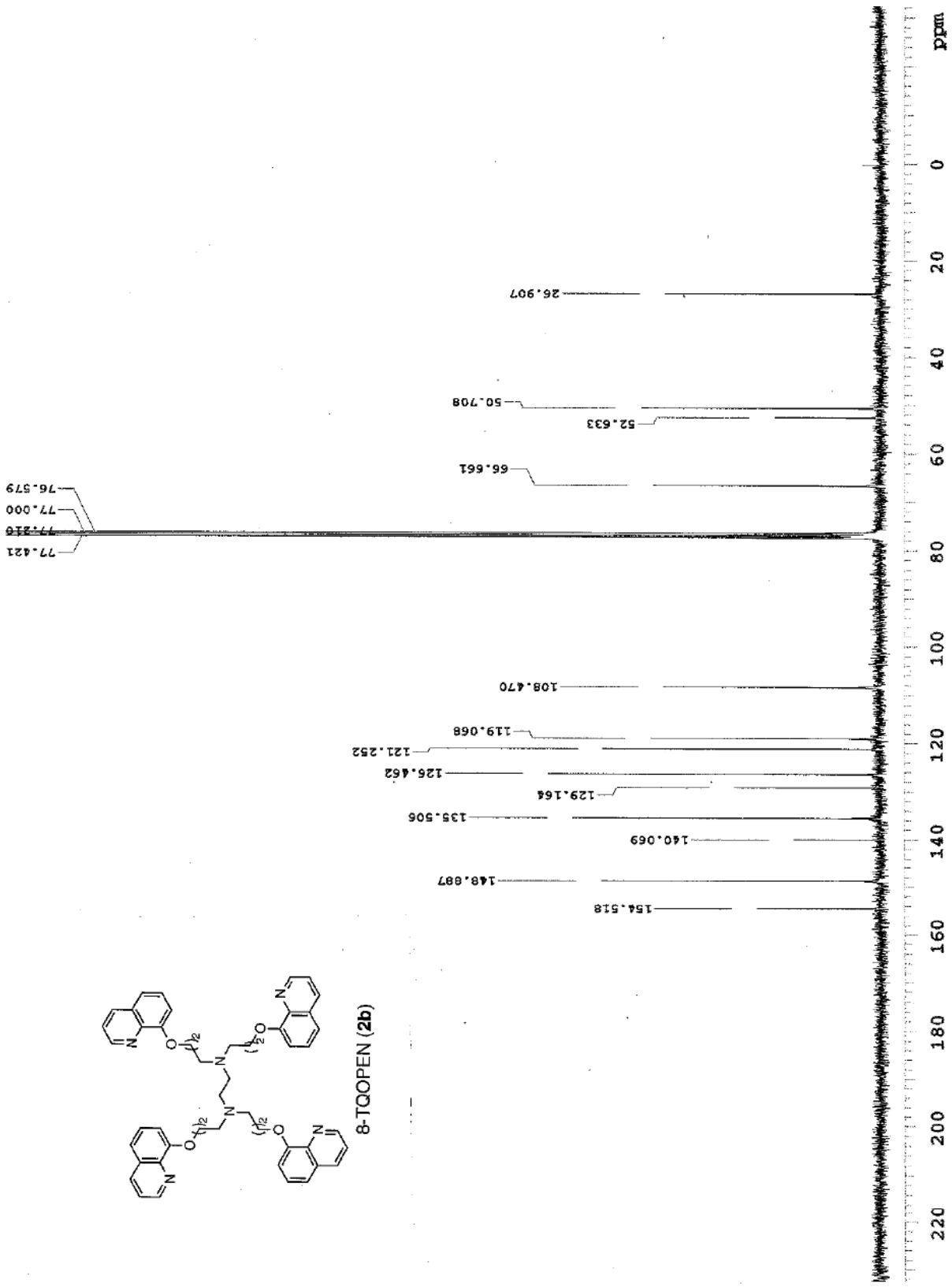


Figure S24. ^{13}C NMR spectrum of 8-TQOPEN (**2b**) in $CDCl_3$.

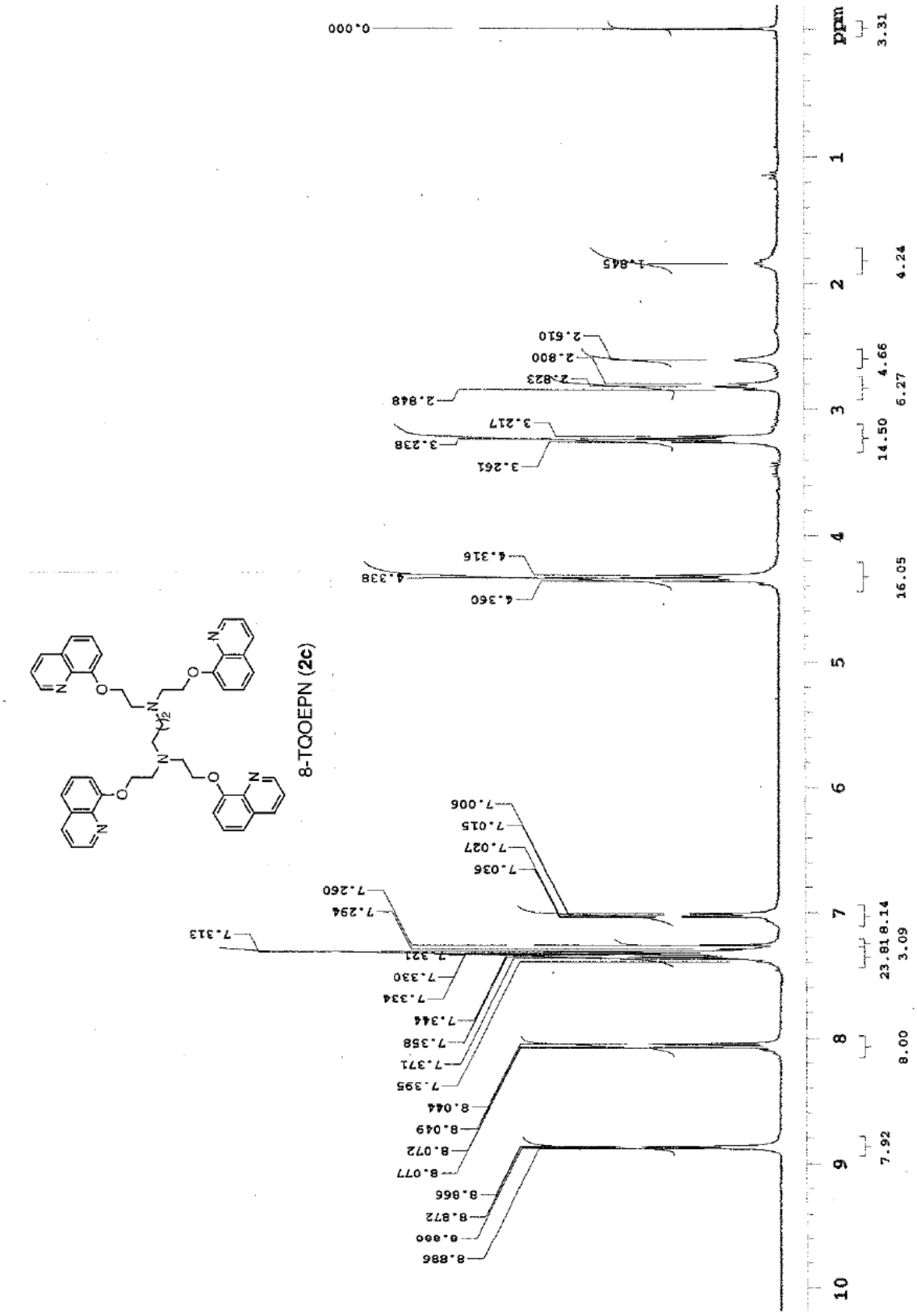


Figure S25. ^{1}H NMR spectrum of 8-TQOEPN (**2c**) in $CDCl_3$.

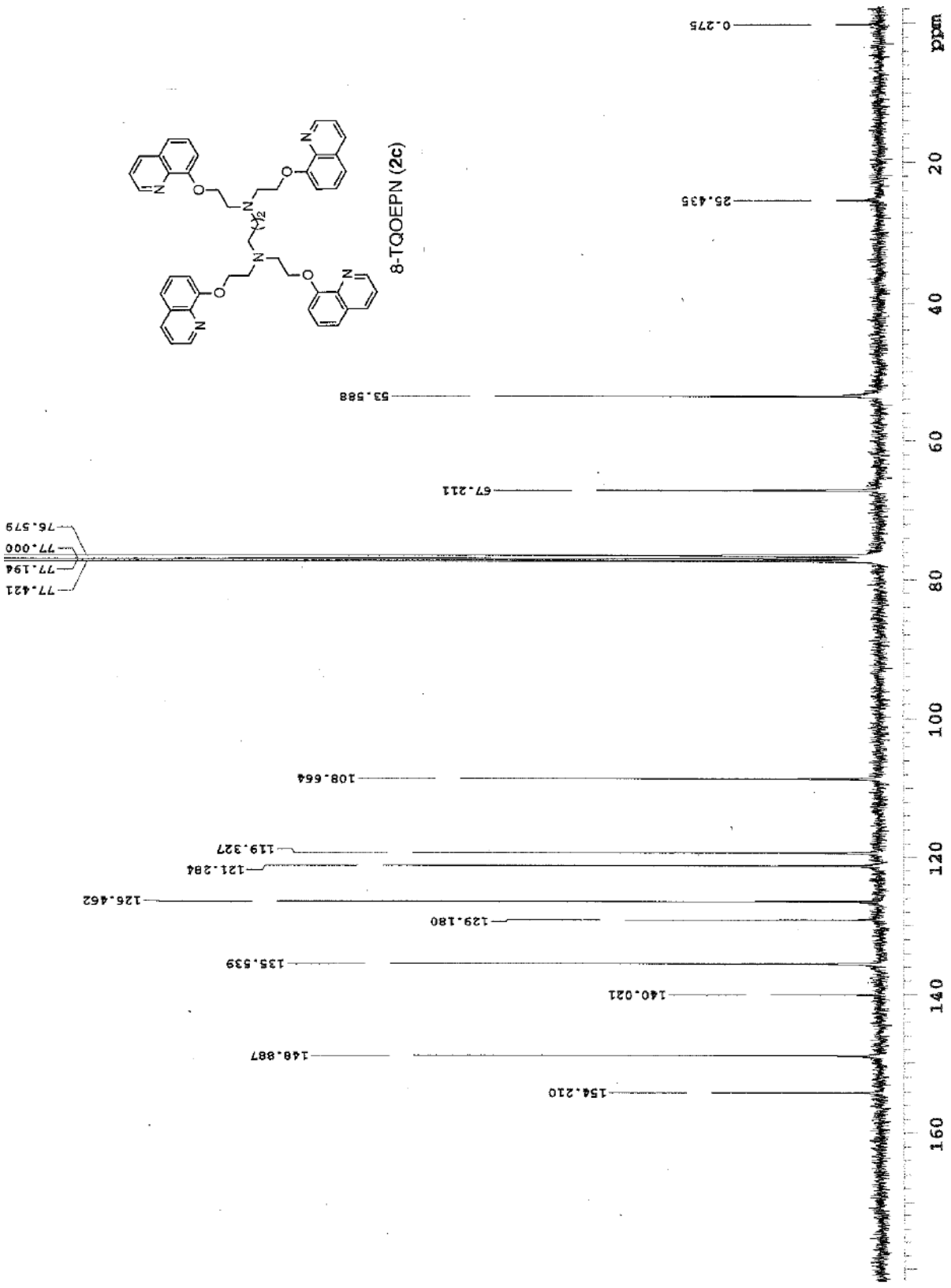


Figure S26. ^{13}C NMR spectrum of 8-TQOEPN (**2c**) in $CDCl_3$.

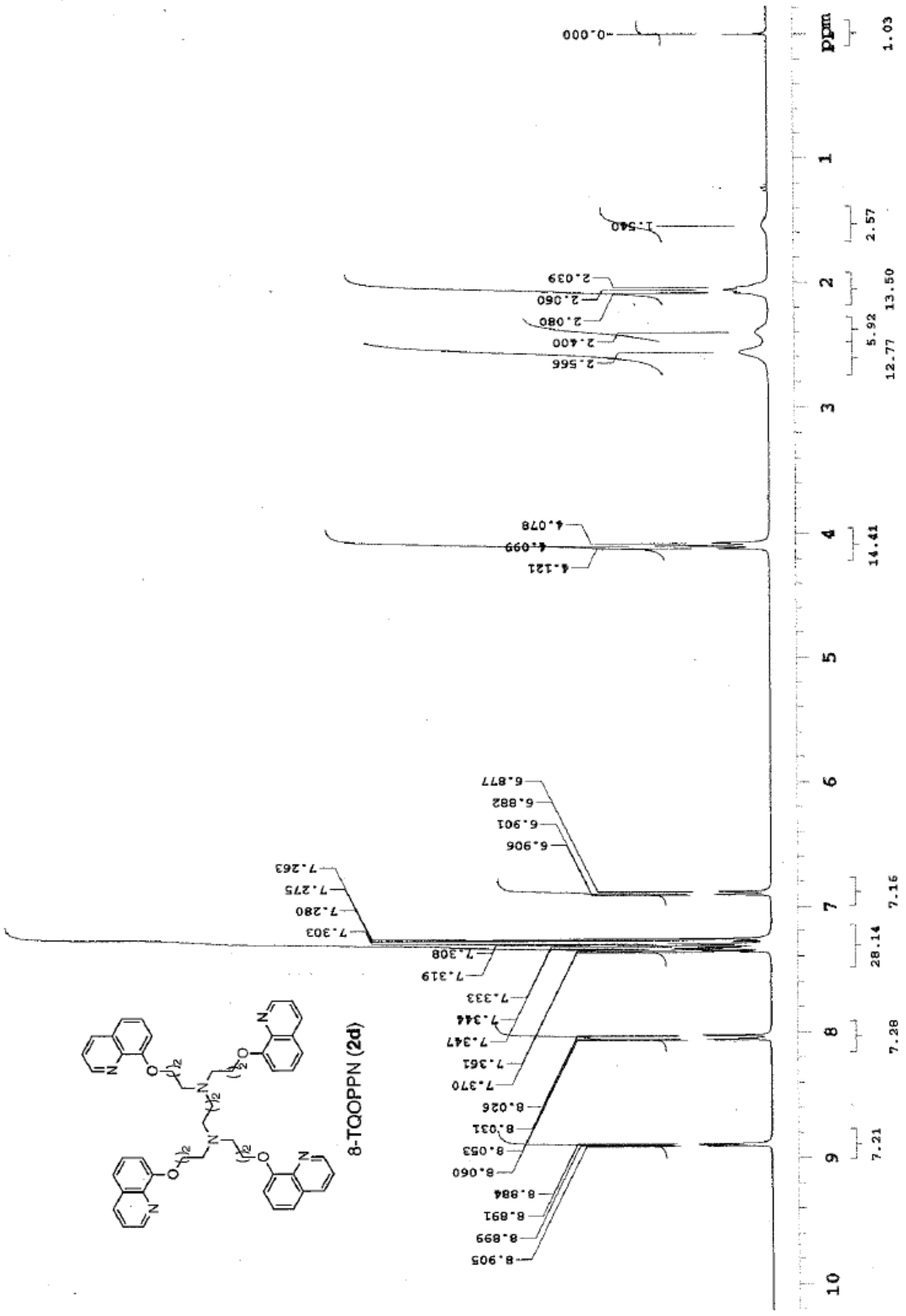


Figure S27. ^{1}H NMR spectrum of 8-TQOPPN (**2d**) in $CDCl_3$.

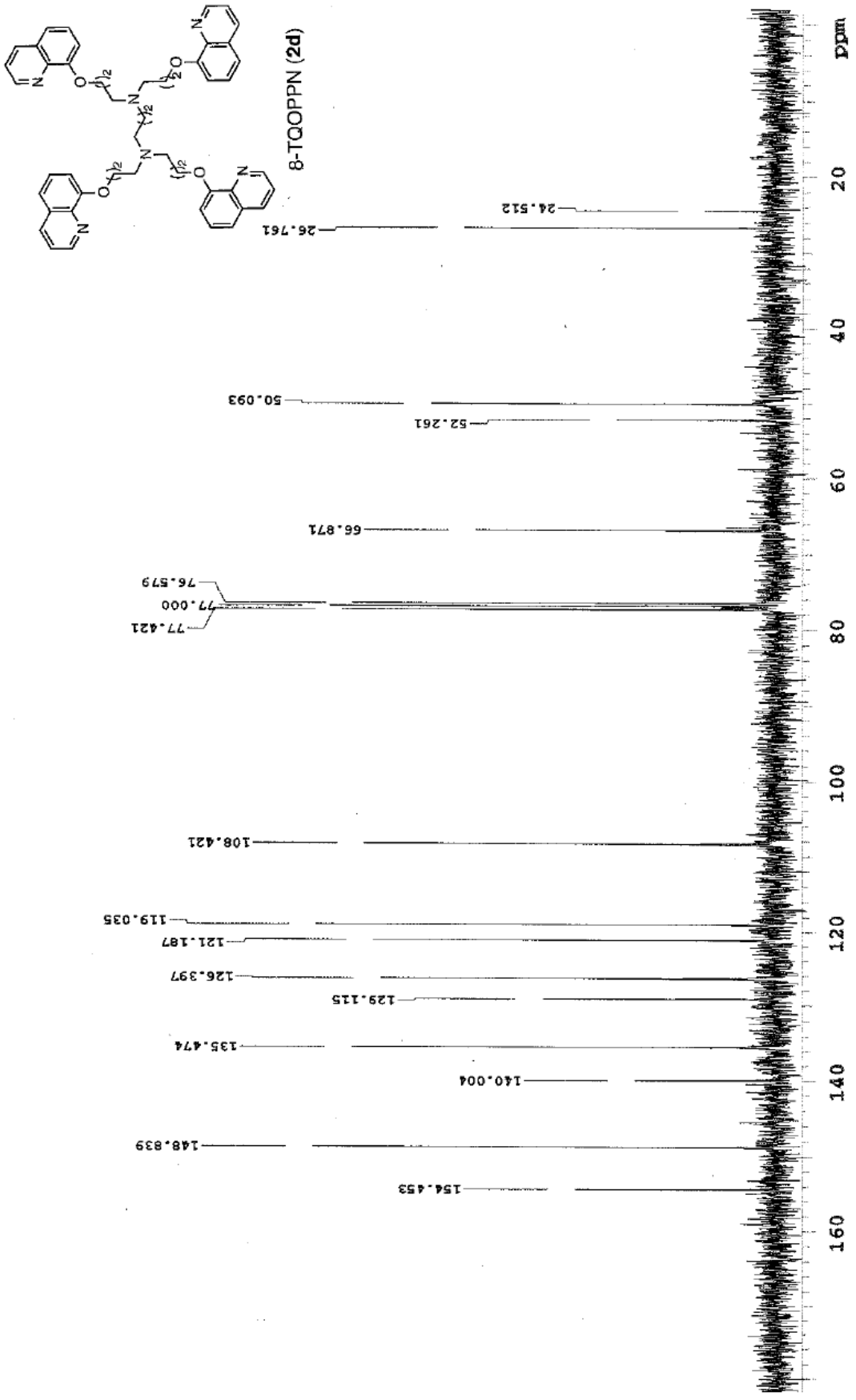


Figure S28. ^{13}C NMR spectrum of 8-TQOPPN (**2d**) in $CDCl_3$.