Supplementary Information for

Photochemical Intramolecular Cyclization of *o*-Alkynylaryl Isocyanides with Organic Dichalcogenides Leading to 2,4-Bischalcogenated Quinoline Derivatives

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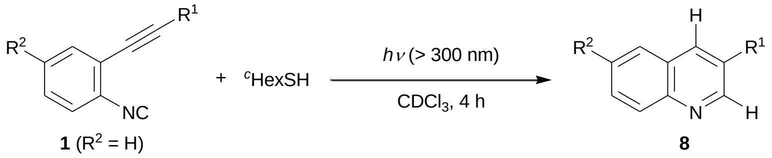
Contents

General Remarks.

^{1}H NMR spectra were recorded on a spectrometer (300 MHz or 400 MHz) using $CDCl_3$ as the solvent with tetramethylsilane (TMS) as the internal standard. ^{13}C NMR spectra were obtained on a spectrometer (75 MHz or 100 MHz) using $CDCl_3$ as the solvent. Chemical shifts in ^{13}C NMR were measured relative to $CDCl_3$ by using δ 77.0 ppm. Infrared spectra were determined on a FT-IR spectrometer. Melting points were determined on a micro melting point apparatus. Conventional mass spectra were recorded with a gas chromatograph mass spectrometer. High resolution mass spectra were obtained on a mass spectrometer. Terminal acetylenes (4-methylphenylacetylene,[S1] 4-methoxyphenylacetylene,[S1] 4-chlorophenylacetylene,[S1] 4-nitrophenylacetylene,[S2] and 4-cyanophenylacetylene[S2]), organic dichalcogenides (diphenyl diselenide (**4a**),[S3] bis(4-methylphenyl) diselenide (**4b**),[S3] bis(4-methoxyphenyl) diselenide (**4c**),[S3] bis(4-fluorophenyl) diselenide (**4e**),[S3] diphenyl ditelluride (**6a**),[S4] bis(4-methoxyphenyl) ditelluride (**6b**),[S5] bis(4-fluorophenyl) ditelluride (**6c**),[S6] and dibutyl ditelluride (**6d**)[S7]), and *o*-alkynylaryl isocyanides[S8] were prepared according to the literature. The formation of *o*-alkynylaryl isocyanides was determined by ^{1}H NMR with 1,3,5-trioxane as the internal standard because of their instability. Other reagents could be purchased commercially and used without further purification.

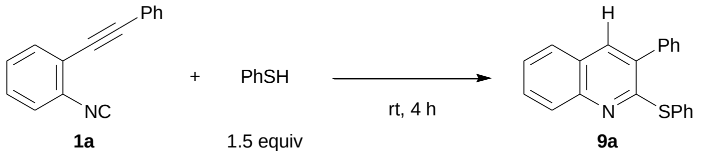
Table S1. Photochemical Reaction of Several Isocyanides **1** with Cyclohexanethiol[a]



entry	**1**	R^1	**8**	yield (%)[b]
1	**1a**	C_6H_5–	**8a**	82
2	**1b**	4-Me-C_6H_4–	**8b**	66
3	**1d**	4-Cl-C_6H_4–	**8d**	67
4	**1e**	4-F-C_6H_4–	**8e**	75
5	**1f**	*n*-Bu–	**8f**	72
6	**1g**	1-cyclohexenyl–	**8g**	64

[a] Reaction conditions: isocyanide (**1**, 0.10 mmol), thiol (0.20 mmol), $CDCl_3$ (0.50 mL), room temperature, *hυ* (> 300 nm: irradiation with a high pressure Hg lamp through Pyrex). [b] Isolated yield.

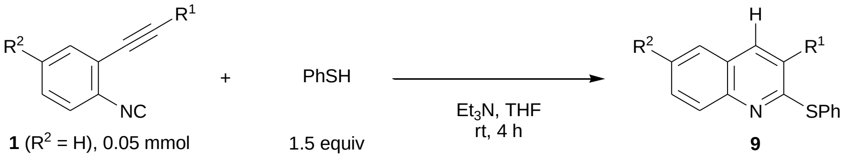
Table S2. Optimization of the Synthesis of 2-Sulfanylquinoline **9a**[a]

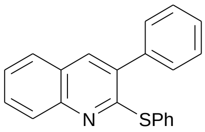
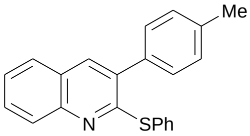
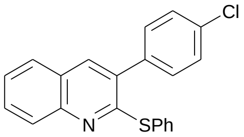
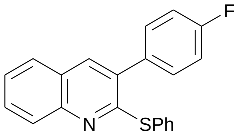
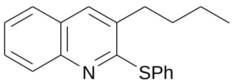


entry	solvent	additive	yield of **9a** (%)[b]
1	$CHCl_3$	—	29
2	$CHCl_3$	Et_3N	70
3	THF	Et_3N	85 (78)
4	$CHCl_3$	K_2CO_3	11

[a] Reaction conditions: isocyanide (**1a**, 0.05 mmol), benzenethiol, solvent (0.5 mL), room temperature, 4 h. [b] Determined by ^1H NMR. A value in parenthesis is isolated yield.

Table S3. Scope and Limitation of Several Isocyanides **1**[a]



entry	R^1	**1**	product	**9**	yield (%)[b]
1	C_6H_5-	**1a**		**9a**	78
2	4-Me-C_6H_4-	**1b**		**9b**	57
3	4-Cl-C_6H_4-	**1d**		**9d**	73
4	4-F-C_6H_4-	**1e**		**9e**	80
5	$CH_3(CH_2)_3$-	**1f**		**9f**	64

[a] Reaction conditions: isocyanide (**1**, 0.05 mmol), benzenethiol (0.075 mmol), THF (0.5 mL), Et_3N (0.5 mL), room temperature, 4 h. [b] Isolated yield.

UV-Vis Spectra of *o*-Alkynylaryl Isocyanides 1a and 1f

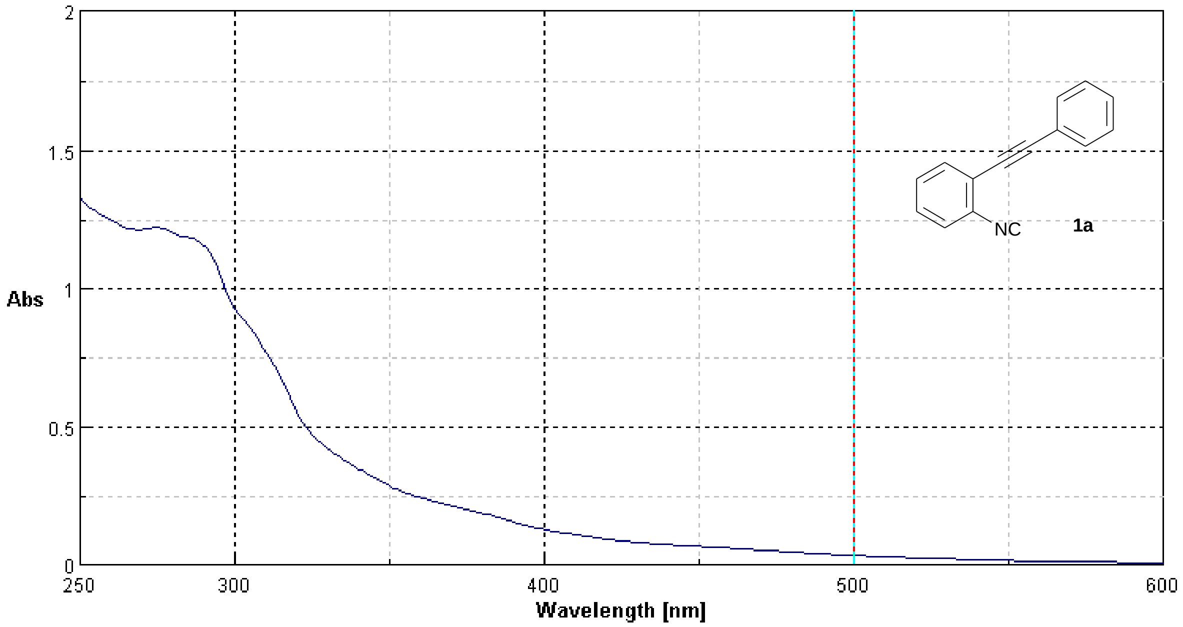


Figure S1. UV-Vis Spectrum of *o*-Alkynylaryl Isocyanide **1a** (1.2×10^{-5} M in $CHCl_3$).

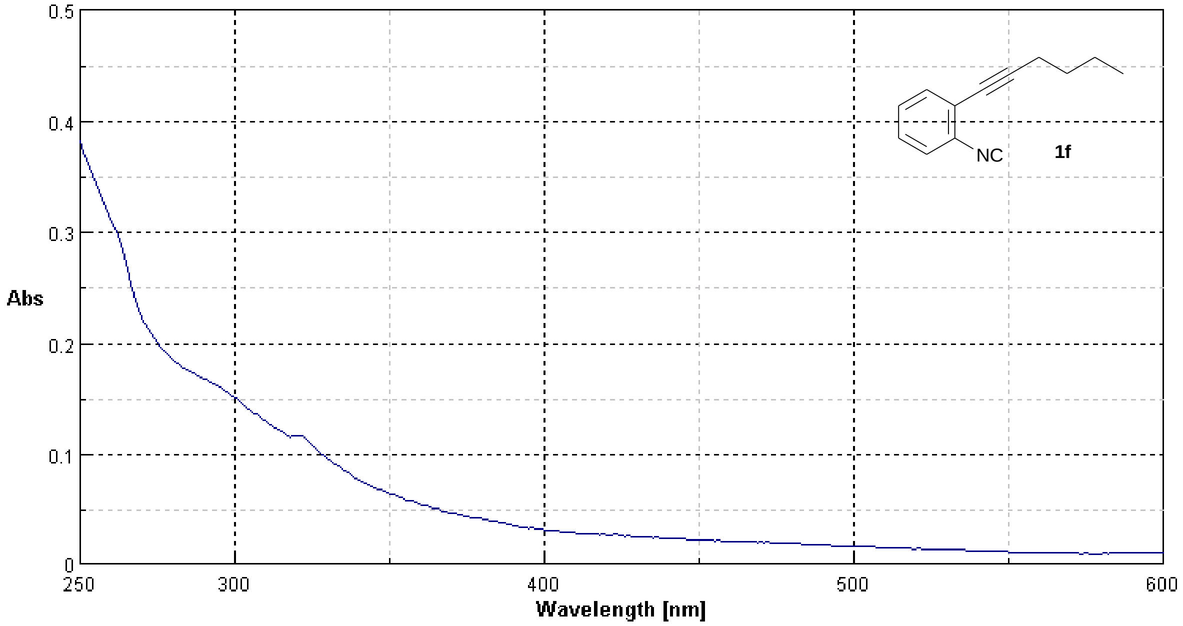


Figure S2. UV-Vis Spectrum of *o*-Alkynylaryl Isocyanide **1f** (4.7×10^{-6} M in $CHCl_3$).

Characterization Data.

3-(4-Methylphenyl)quinoline (8b):[S9] Quinoline **8b** (14.5 mg, 0.066 mmol, 66%) was obtained from **1b** (0.10 mmol) according to the general procedure. The crude mixture was purified by PTLC on silica gel (Hex:AcOEt = 9:1) and recycle GPC ($CHCl_3$). Slightly yellow oil; ^{1}H NMR (300 MHz, $CDCl_3$, ppm) δ 2.44 (s, 3H), 7.34 (d, *J* = 7.5 Hz, 2H), 7.57–7.64 (m, 3H), 7.71 (ddd, *J* = 1.5, 6.9, 8.4 Hz, 1H), 7.87 (d, *J* = 8.4 Hz, 1H), 8.13 (d, *J* = 8.4 Hz, 1H), 8.28 (d, *J* = 2.1 Hz, 1H), 9.18 (d, *J* = 2.1 Hz, 1H); ^{13}C NMR (75 MHz, $CDCl_3$, ppm) δ 21.2, 126.9, 127.2, 127.9, 128.1, 129.2, 129.7, 129.9, 132.8, 133.8, 135.0, 138.0, 147.2, 149.9; IR (NaCl, cm^{-1}) 3026, 2957, 2922, 2866, 1516, 1493, 1462, 1362, 1340, 1188, 1124, 1040, 1020, 953, 908, 816, 785, 750, 718; MS (FAB) *m/z* 220 ($[M+H]^+$, 100).

3-(4-Chlorophenyl)quinoline (8d):[S10] Quinoline **8d** (16.1 mg, 0.067 mmol, 67%) was obtained from **1d** (0.10 mmol) according to the general procedure. The crude mixture was purified by PTLC on silica gel (Hex:AcOEt = 9:1) and recycle GPC ($CHCl_3$). White solid; mp 130–132 °C (crystallized from acetone); ^{1}H NMR (400MHz, $CDCl_3$, ppm) δ 7.50 (d, *J* = 8.6 Hz, 2H), 7.60 (ddd, *J* = 1.4, 6.9, 7.8 Hz, 1H), 7.65 (d, *J* = 8.6 Hz, 2H), 7.75 (ddd, *J* = 1.4, 6.9, 8.2 Hz, 1H), 7.89 (d, *J* = 7.8 Hz, 1H), 8.16 (d, *J* = 8.2 Hz, 1H), 8.30 (d, *J* = 1.8 Hz, 1H), 9.14 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm) δ 127.2, 128.0, 128.6, 129.1, 129.4, 129.7, 132.6, 133.3, 134.4, 136.2, 139.9, 147.1, 149.2; MS (EI) *m/z* 239 (M^+, 100).

3-(4-Fluorophenyl)quinoline (8e):[S11] Quinoline **8e** (16.7 mg, 0.075 mmol, 75%) was obtained from **1e** (0.10 mmol) according to the general procedure. The crude mixture was purified by PTLC on silica gel (Hex:AcOEt = 9:1) and recycle GPC ($CHCl_3$). White solid; mp 100–102 ^{o}C (crystallized form acetone); ^{1}H NMR (300 MHz, $CDCl_3$, ppm) δ 7.22 (t, *J* = 8.6 Hz, 2H), 7.59 (dt, *J* = 1.0, 7.5 Hz, 1H), 7.65–7.78 (m, 3H), 7.88 (d, *J* = 7.9 Hz, 1H), 8.14 (d, *J* = 8.4 Hz, 1H), 8.27 (s, 1H), 9.14 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm) δ 116.2 (d, J_{CF} = 21.0 Hz), 127.2, 127.9, 127.9, 129.0, 129.0 (d, J_{CF} = 7.6 Hz), 129.6, 132.9, 133.3, 133.8 (d, J_{CF} = 3.8 Hz), 146.9, 149.3, 162.9 (d, J_{CF} = 245.8 Hz); IR (NaCl, cm^{-1}) 3076, 3052, 1508, 1497, 1231, 953, 905, 831, 785, 746; MS (EI) *m/z* 223 (M^+, 100).

3-*n*-Butylquinoline (8f):[S12] Quinoline **8f** (13.4 mg, 0.072 mmol, 72%) was obtained from **1f** (0.10 mmol) according to the general procedure. The crude mixture was purified by PTLC on silica gel (Hex:AcOEt = 9:1) and recycle GPC ($CHCl_3$). Colorless oil; ^{1}H NMR (300 MHz, $CDCl_3$, ppm) δ 0.96 (t, *J* = 7.1 Hz, 3H), 1.33–1.50 (m, 2H), 1.61–1.82 (m, 2H), 2.81 (hep, *J* = 7.8 Hz, 2H), 7.52 (t, *J* = 8.4 Hz, 1H), 7.65 (t, *J* = 8.4 Hz, 1H), 7.77 (d, *J* = 8.4 Hz, 1H), 7.91 (s, 1H), 8.07 (d, *J* = 8.4 Hz, 1H), 8.79 (s, 1H); ^{13}C NMR (75 MHz, $CDCl_3$, ppm) δ 13.9, 22.3, 32.9, 33.3, 126.5, 127.3, 128.2, 128.4, 129.1, 134.1, 135.3, 146.7, 152.1; HRMS (FAB) calcd for $C_{13}H_{16}N$ $[M+H]^+$ 186.1283, found 186.1279.

3-(1-Cyclohexenyl)quinoline (8g):[S13] Quinoline **8g** (13.3 mg, 0.064 mmol, 64%) was obtained from **1g** (0.10 mmol) according to the general procedure. The crude mixture was purified by PTLC on silica gel (Hex:AcOEt = 9:1) and recycle GPC ($CHCl_3$). Pale yellow oil; ^{1}H NMR

(300 MHz, $CDCl_3$, ppm) δ 1.63–1.78 (m, 2H), 1.80–1.93 (m, 2H), 2.24–2.35 (m, 2H), 2.46–2.58 (m, 2H), 6.32–6.42 (m, 1H), 7.51 (t, *J* = 8.4 Hz, 1H), 7.65 (t, *J* = 8.4 Hz, 1H), 7.79 (d, *J* = 8.4 Hz, 1H), 8.01 (s, 1H), 8.07 (d, *J* = 8.4 Hz, 1H), 9.04 (s, 1H); ^{13}C NMR (75 MHz, $CDCl_3$, ppm) δ 22.0, 22.9, 26.0, 27.1, 126.6, 127.2, 127.9, 128.7, 129.2, 129.9, 130.4, 133.6, 136.6, 146.5, 152.1; IR (NaCl, cm^{-1}) 3058, 2934, 2858, 1497, 1331, 1188, 1128, 957, 903, 787, 752; MS (EI) *m/z* 209 (M^+, 73).

General Procedures for the Synthesis of 2-Sulfanylquinolines.

To a solution of 2-(phenylethynyl)phenyl isocyanide (**1a**, 0.05 mmol), benzenethiol (0.075 mmol), and THF (0.5 mL) was added triethylamine (0.5 mL), and the mixture was stirred at room temperature for 4 h. After the reaction was complete, the resulting mixture was concentrated in vacuo, and purified by PTLC on silica gel (Hex; AcOEt = 9:1) and recycle GPC ($CHCl_3$) to give 3-phenyl-2-phenylsulfanylquinoline (**9a**, 12.2 mg, 0.039 mmol, 78%) as a colorless oil. Further purification was carried out by recycle GPC ($CHCl_3$) for all 2-sulfanylquinolines **9**.

3-Phenyl-2-phenylsulfanylquinoline (9a): Colorless oil; ^1H NMR (300 MHz, $CDCl_3$, ppm) δ 7.33–7.62 (m, 12H), 7.69–7.78 (m, 2H), 7.86 (s, 1H); ^{13}C NMR (75 MHz, $CDCl_3$, ppm) δ 125.8, 126.3, 127.4, 128.3, 128.4, 128.4, 128.7, 128.9, 129.4, 129.6, 130.2, 131.1, 134.9, 135.7, 138.0, 147.3, 158.3; IR (NaCl, cm^{-1}) 3057, 3030, 1614, 1592, 1516, 1475, 1439, 1385, 1362, 1337, 1132, 1084, 1024, 966, 910, 781, 748, 700, 689; HRMS (FAB) calcd for $C_{21}H_{16}NS$ $[M+H]^+$ 314.1003, found 314.0995.

3-(4-Methylphenyl)-2-phenylsulfanylquinoline (9b): Quinoline **9b** (9.3 mg, 0.029 mmol, 57%) was obtained from **1b** (0.10 mmol) according to the general procedure. The crude mixture was purified by PTLC on silica gel (Hex:AcOEt = 9:1) and recycle GPC ($CHCl_3$). Slightly yellow oil; ^1H NMR (300 MHz, $CDCl_3$, ppm) δ 2.45 (s, 3H), 7.31 (d, *J* = 7.7 Hz, 2H), 7.36–7.44 (m, 4H), 7.47 (d, *J* = 8.1 Hz, 2H), 7.52–7.60 (m, 3H), 7.70–7.76 (m, 2H), 7.84 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm) δ 21.4, 125.7, 126.3, 127.3, 128.3, 128.3, 128.7, 129.1, 129.2, 129.4, 131.1, 132.4, 134.6, 135.0, 135.6, 138.2, 147.2, 158.4; IR (NaCl, cm^{-1}) 3062, 3024, 2920, 2873, 1616, 1591, 1577, 1508, 1475, 1439, 1387, 1362, 1339, 1132, 1082, 1024, 968, 818, 748, 689; HRMS (FAB) calcd for $C_{22}H_{18}NS$ $[M+H]^+$ 328.1160, found 328.1168.

3-(4-Chlorophenyl)-2-phenylsulfanylquinoline (9d): Quinoline **9d** (12.7 mg, 0.037 mmol, 73%) was obtained from **1d** (0.10 mmol) according to the general procedure. The crude mixture was purified by PTLC on silica gel (Hex:AcOEt = 9:1) and recycle GPC ($CHCl_3$). Colorless oil; ^1H NMR (400 MHz, $CDCl_3$, ppm) δ 7.37–7.4 (m, 3H), 7.42–7.49 (m, 4H), 7.50–7.55 (m, 2H), 7.59 (ddd, *J* = 1.4, 6.8, 8.3 Hz, 1H), 7.71−7.78 (m, 2H), 7.84 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm) δ 126.0, 126.2, 127.4, 128.3, 128.4, 128.6, 128.8, 129.7, 130.8, 130.9, 133.5, 134.4, 134.8, 136.0, 136.3, 147.2, 158.0; IR (NaCl, cm^{-1}) 3057, 1616, 1583, 1558, 1491, 1475, 1387, 1360, 1339, 1134, 1096, 1082, 1016, 968, 829, 748, 689; HRMS (FAB) calcd for $C_{21}H_{14}ClNS$ $[M]^+$ 347.0535, found 347.0542.

3-(4-Fluorophenyl)-2-phenylsulfanylquinoline (9e): Quinoline **9e** (13.1 mg, 0.040 mmol, 80%) was obtained from **1e** (0.10 mmol) according to the general procedure. The crude mixture was purified by PTLC on silica gel (Hex:AcOEt = 9:1) and recycle GPC ($CHCl_3$). White solid; mp 103–104 °C (crystallized from acetone); ^{1}H NMR (400 MHz, $CDCl_3$, ppm) δ 7.17 (t, J = 8.7 Hz, 2H), 7.36–7.40 (m, 3H), 7.44 (ddd, J = 1.4, 6.9, 7.3 Hz, 1H), 7.49–7.55 (m, 4H), 7.58 (ddd, J = 1.4, 6.9, 7.3 Hz, 1H), 7.71–7.77 (m, 2H), 7.84 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm) δ 115.4 (d, J_{CF} = 21.0 Hz), 125.9, 126.2, 127.3, 128.3, 128.7, 129.5, 130.8, 131.3 (d, J_{CF} = 7.6 Hz), 131.9, 133.6, 133.8, 134.8, 135.8, 147.2, 158.1, 162.7 (d, J_{CF} = 247.7 Hz); IR (NaCl, cm^{-1}) 3057, 1593, 1558, 1508, 1475, 1387, 1362, 1339, 1223, 1159, 1134, 1082, 1067, 1016, 968, 835, 748, 689; HRMS (FAB) calcd for $C_{21}H_{15}FNS$ $[M+H]^+$ 332.0909, found 332.0905.

3-*n*-Butyl-2-phenylsulfanylquinoline (9f): Quinoline **9f** (9.3 mg, 0.032 mmol, 64%) was obtained from **1f** (0.10 mmol) according to the general procedure. The crude mixture was purified by PTLC on silica gel (Hex:AcOEt = 9:1) and recycle GPC ($CHCl_3$). Colorless oil; ^{1}H NMR (300 MHz, $CDCl_3$, ppm) δ 1.00 (t, J = 7.5 Hz, 3H), 1.48 (sex, J = 7.5 Hz, 2H), 1.77 (hep, J = 7.5 Hz, 2H), 2.86 (t, J = 7.5 Hz, 2H), 7.33–7.45 (m, 4H), 7.51 (ddd, J = 1.4, 6.8, 8.4 Hz, 1H), 7.57–7.63 (m, 2H), 7.64–7.74 (m, 2H), 7.78 (s, 1H); ^{13}C NMR (75 MHz, $CDCl_3$, ppm) δ 13.9, 22.6, 31.5, 32.1, 125.5, 126.8, 126.8, 128.2, 128.3, 128.5, 128.8, 131.1, 134.1, 134.2, 134.5, 146.7, 158.8; IR (NaCl, cm^{-1}) 3059, 2957, 2930, 2858, 1614, 1595, 1556, 1487, 1477, 1439, 1396, 1331, 1175, 1134, 1042, 1024, 953, 897, 858, 779, 748, 706, 687; HRMS (FAB) calcd for $C_{19}H_{19}NS$ $[M]^+$ 293.1238, found 293.1230.

References and Notes for Supplementary Information

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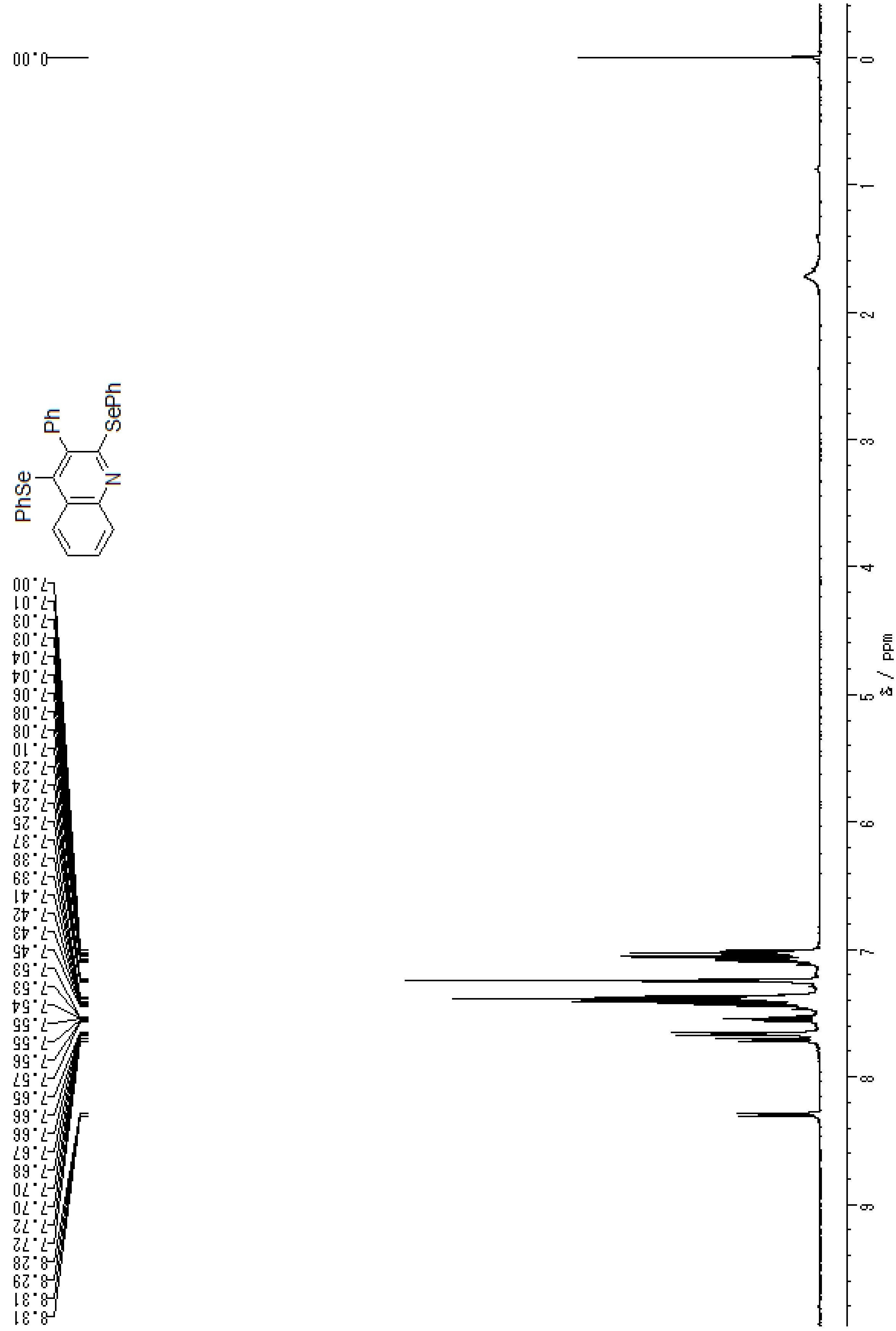
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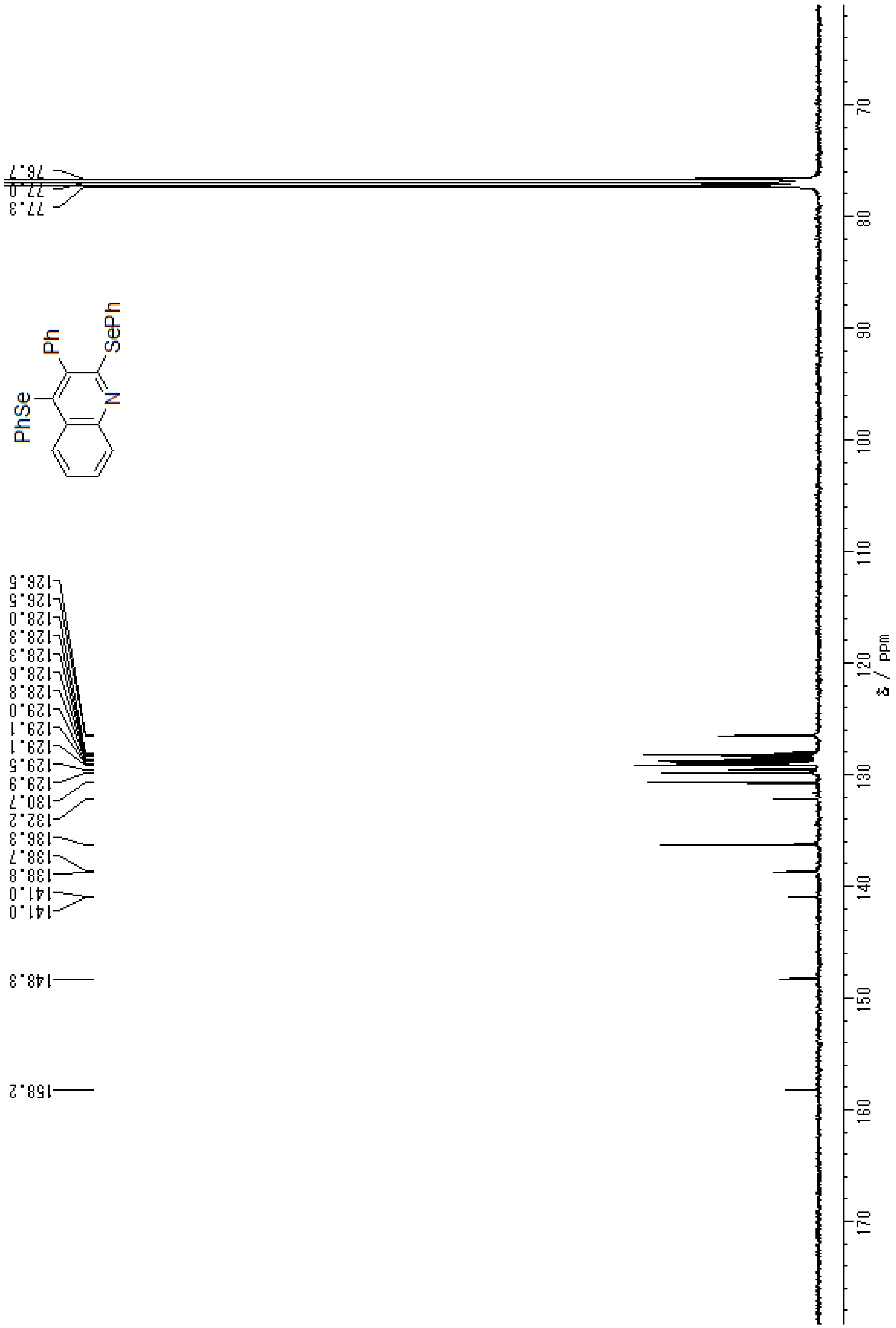
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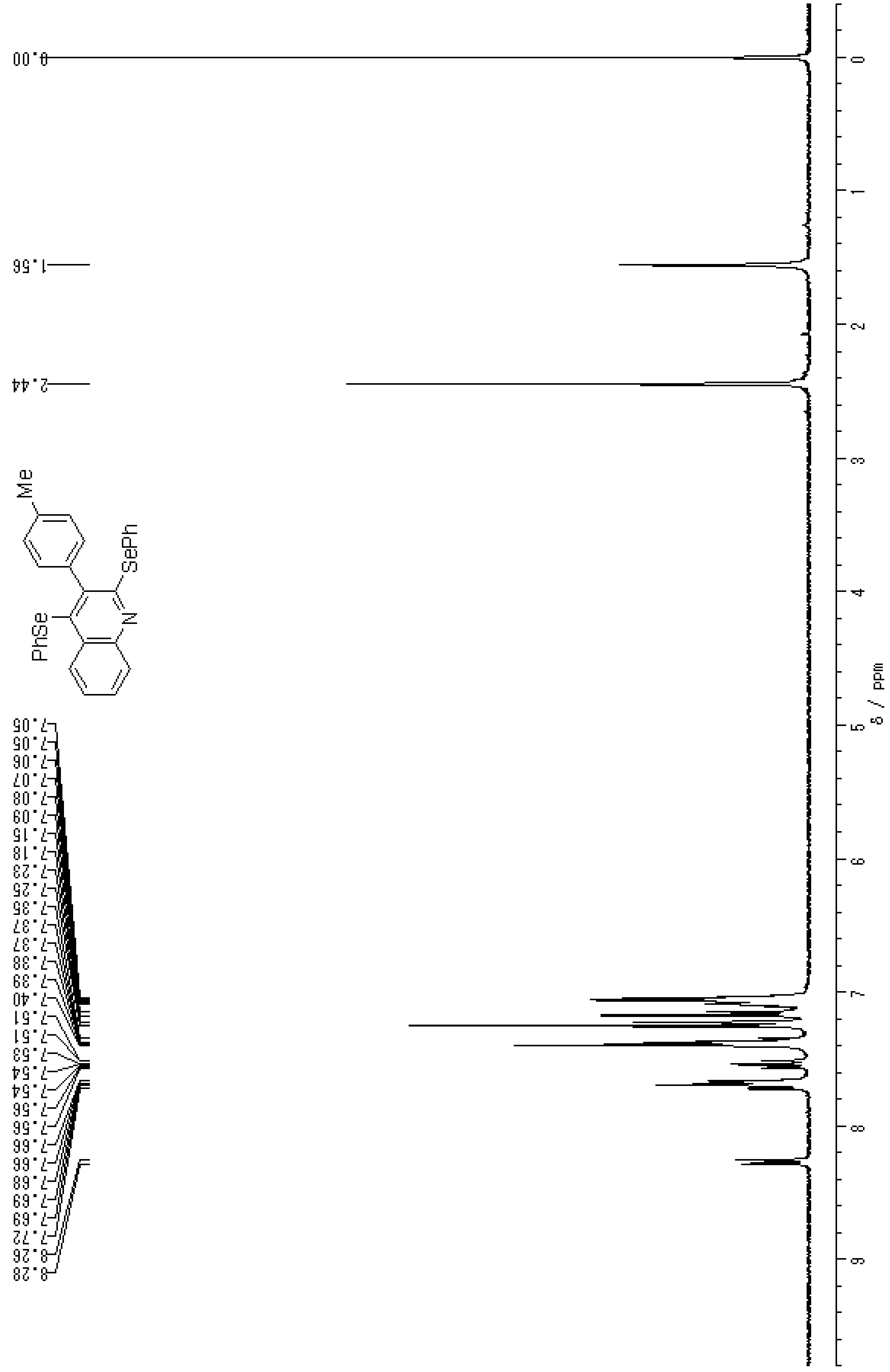
δ / ppm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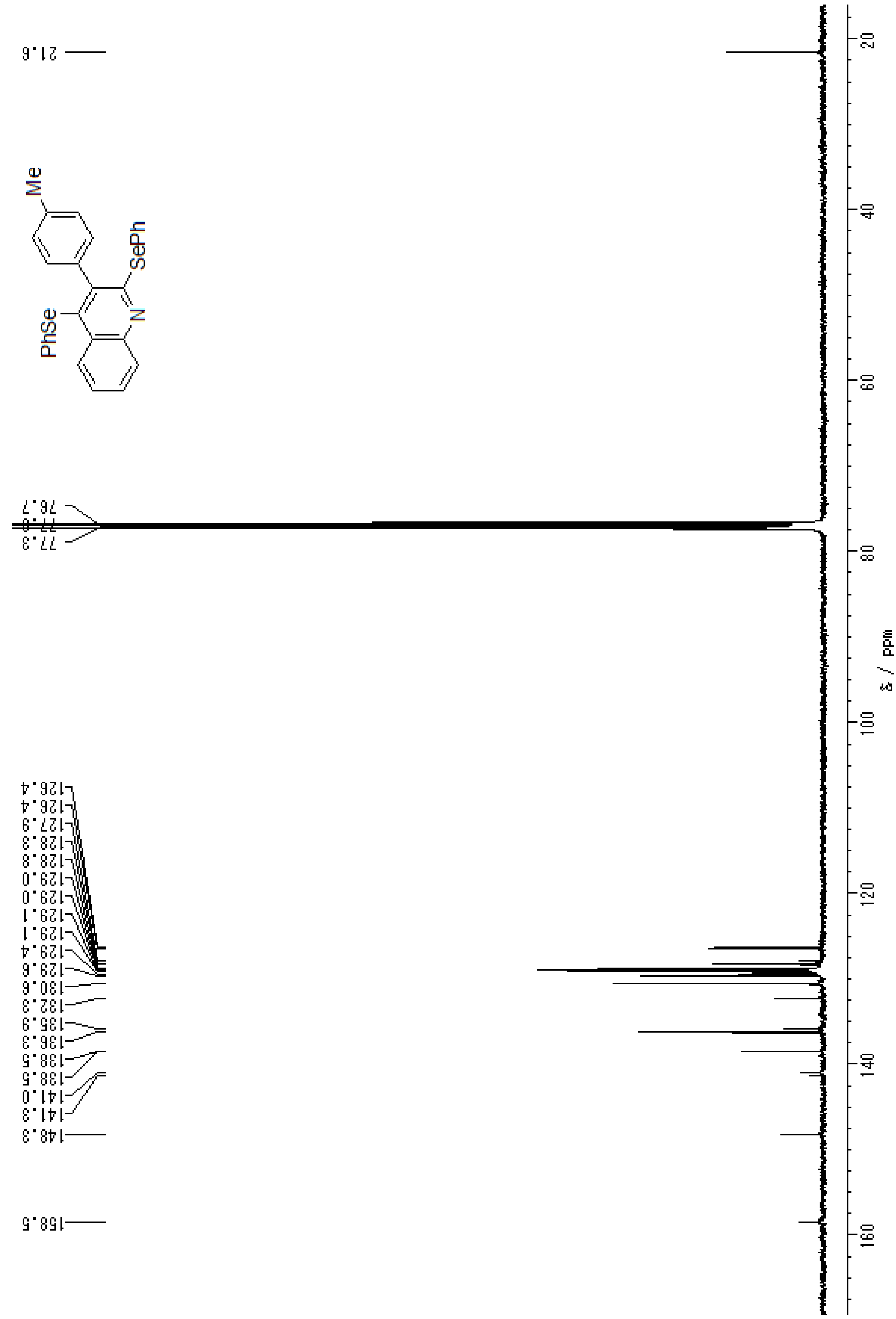
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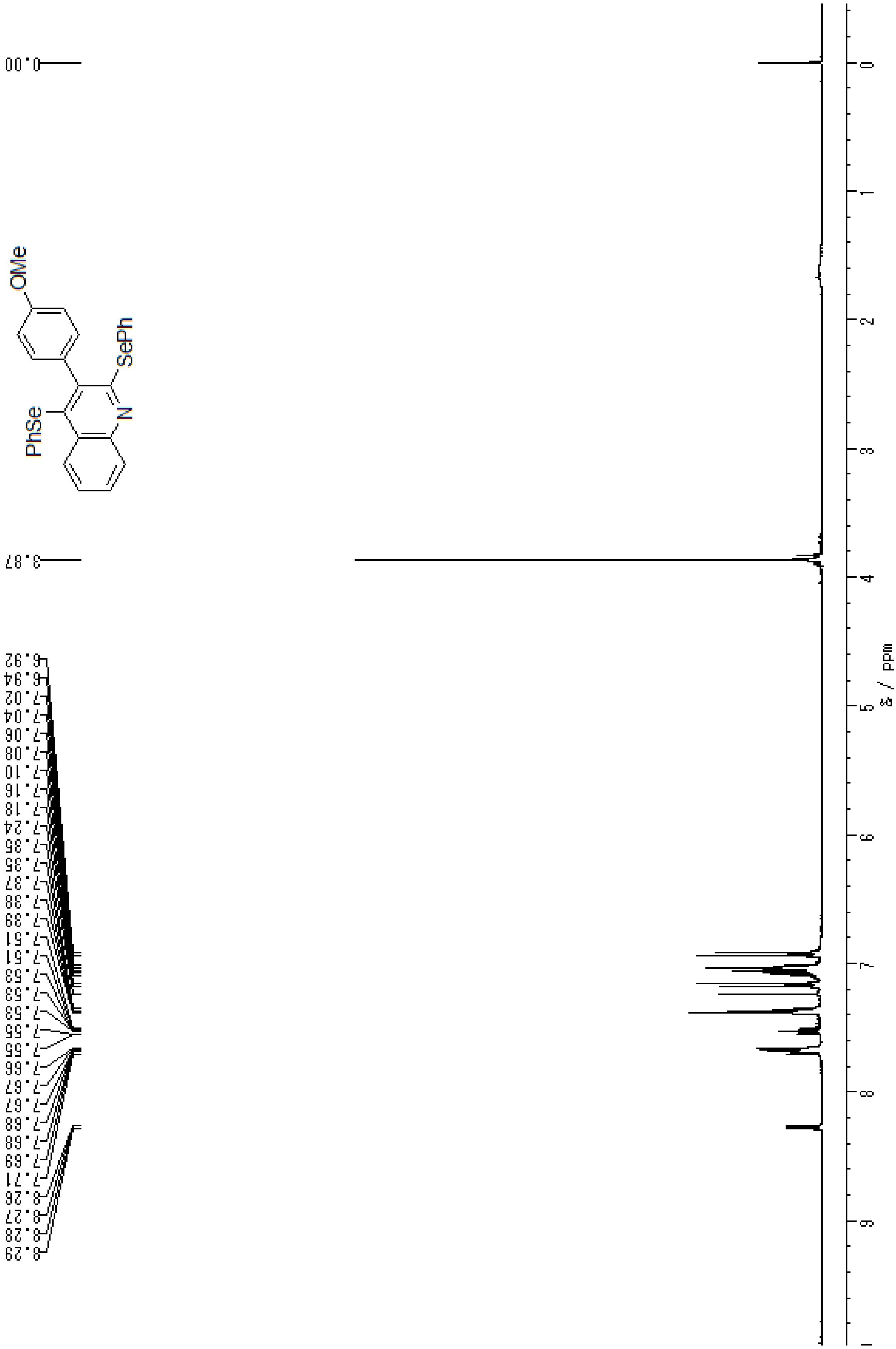
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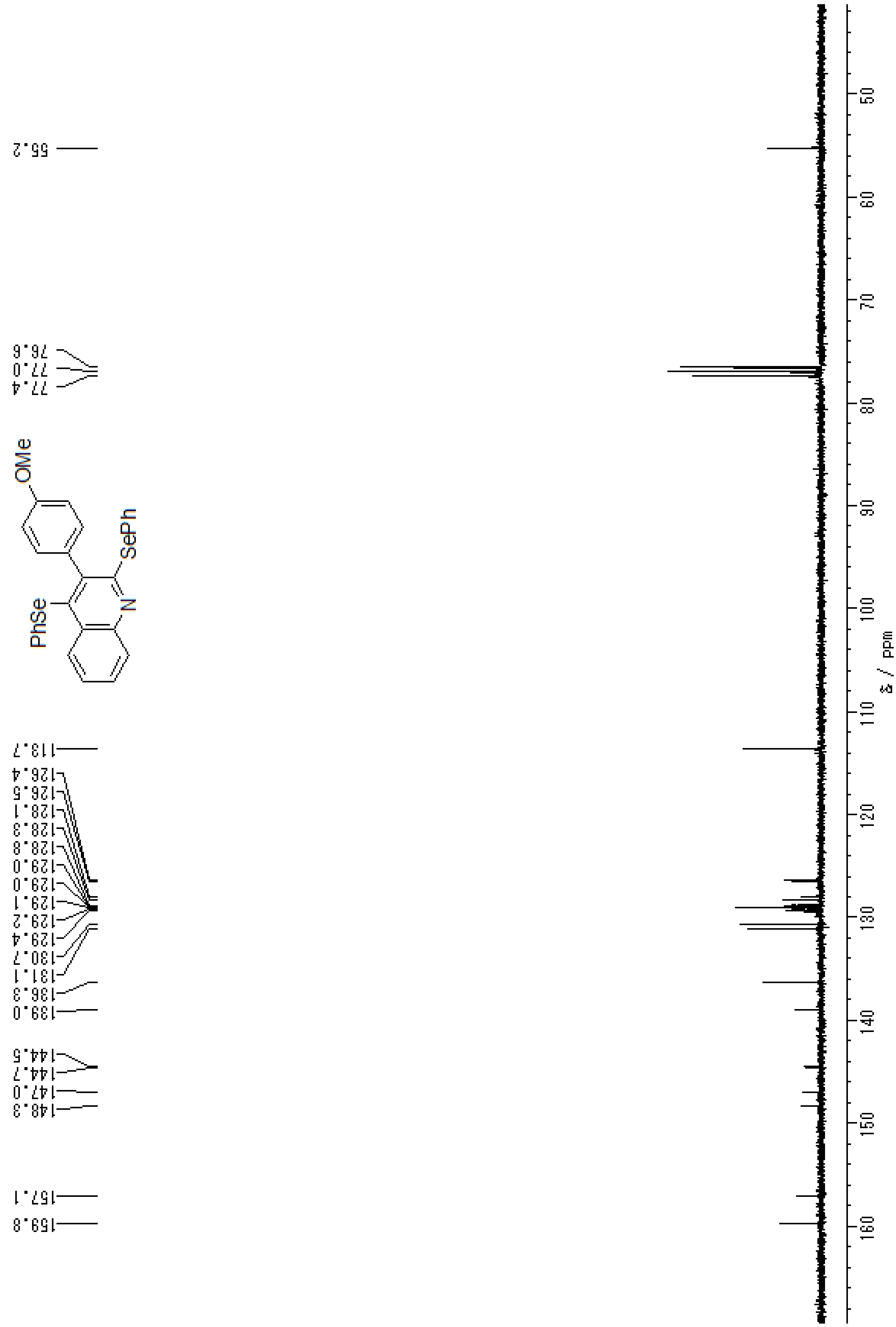
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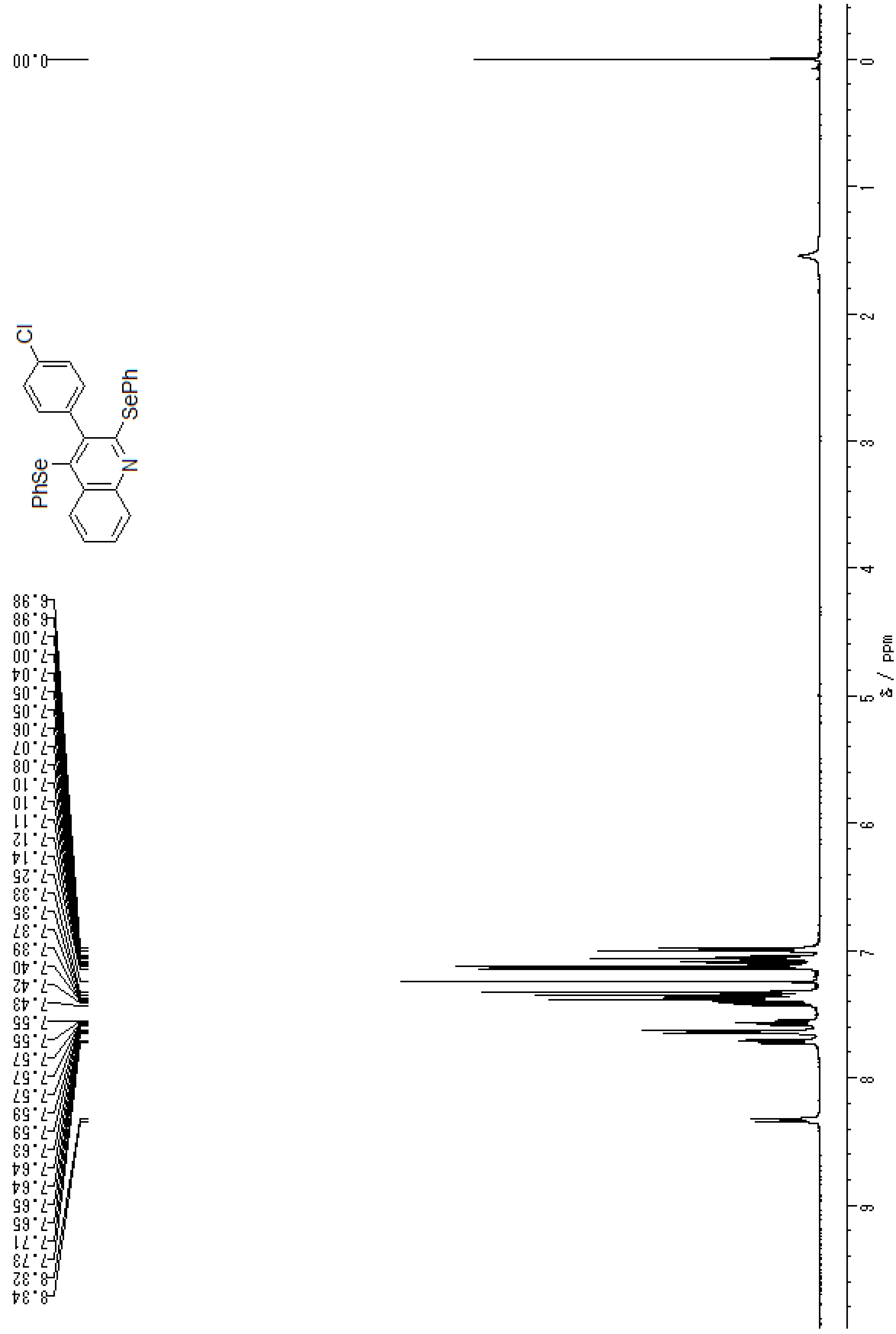
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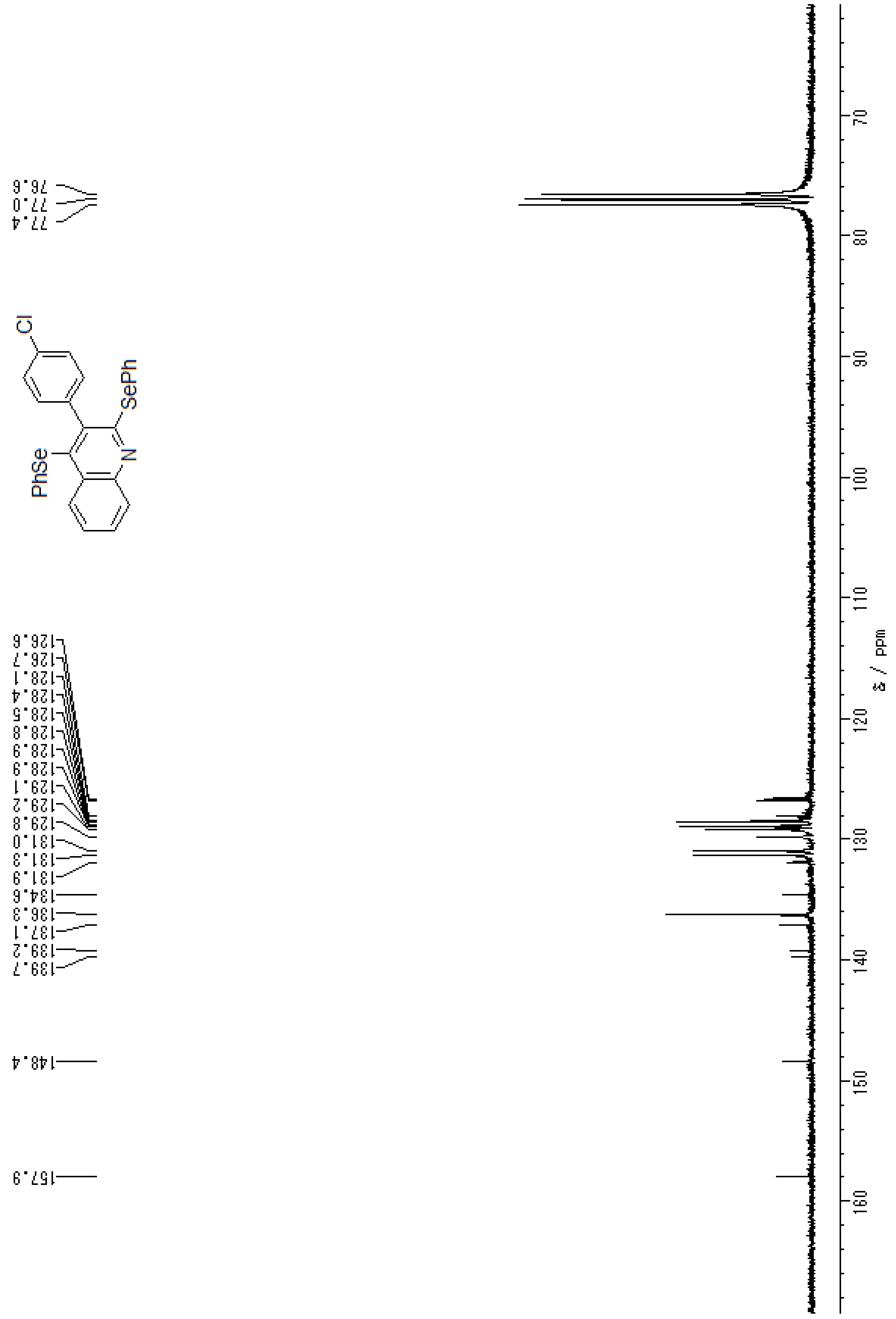
δ / ppm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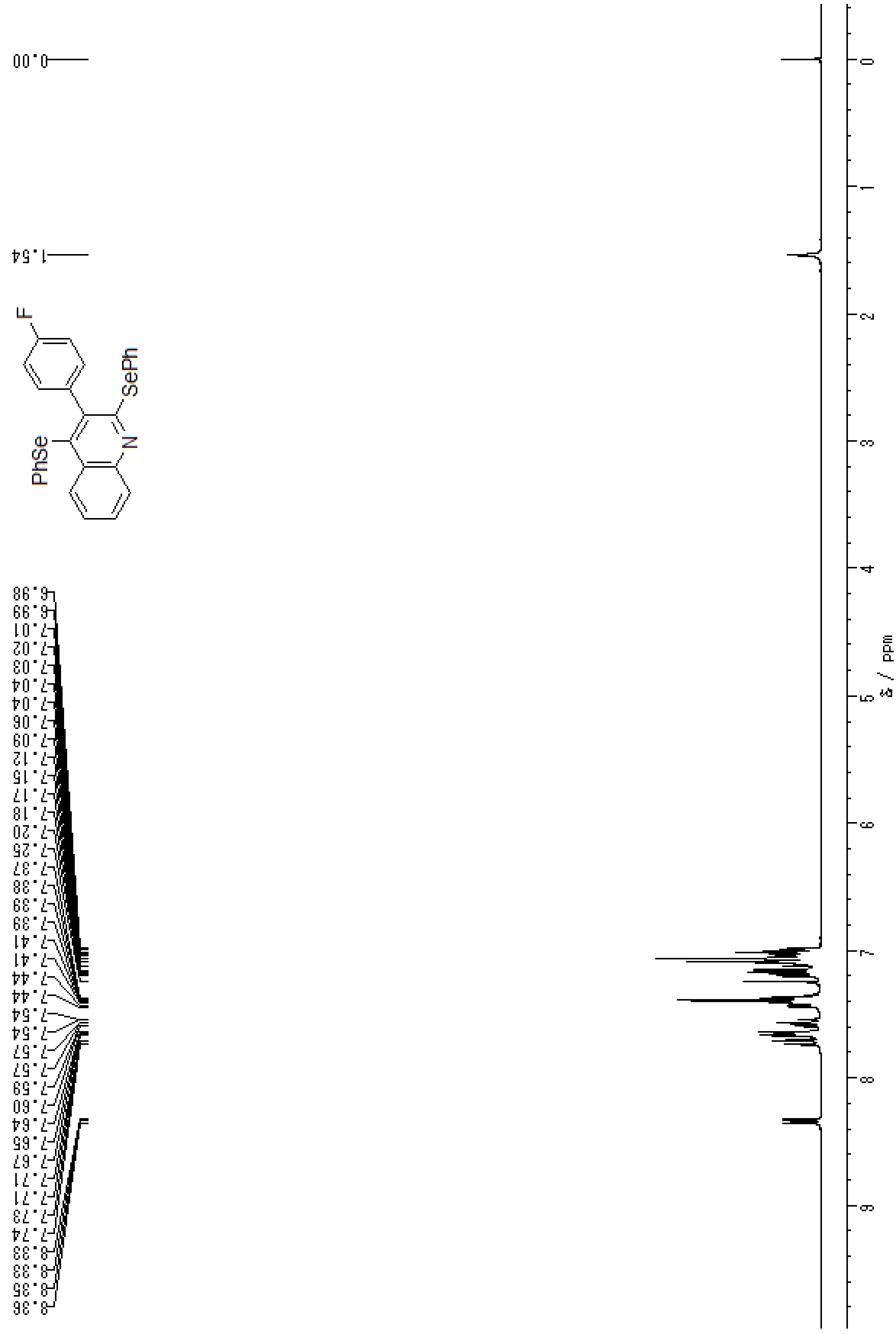
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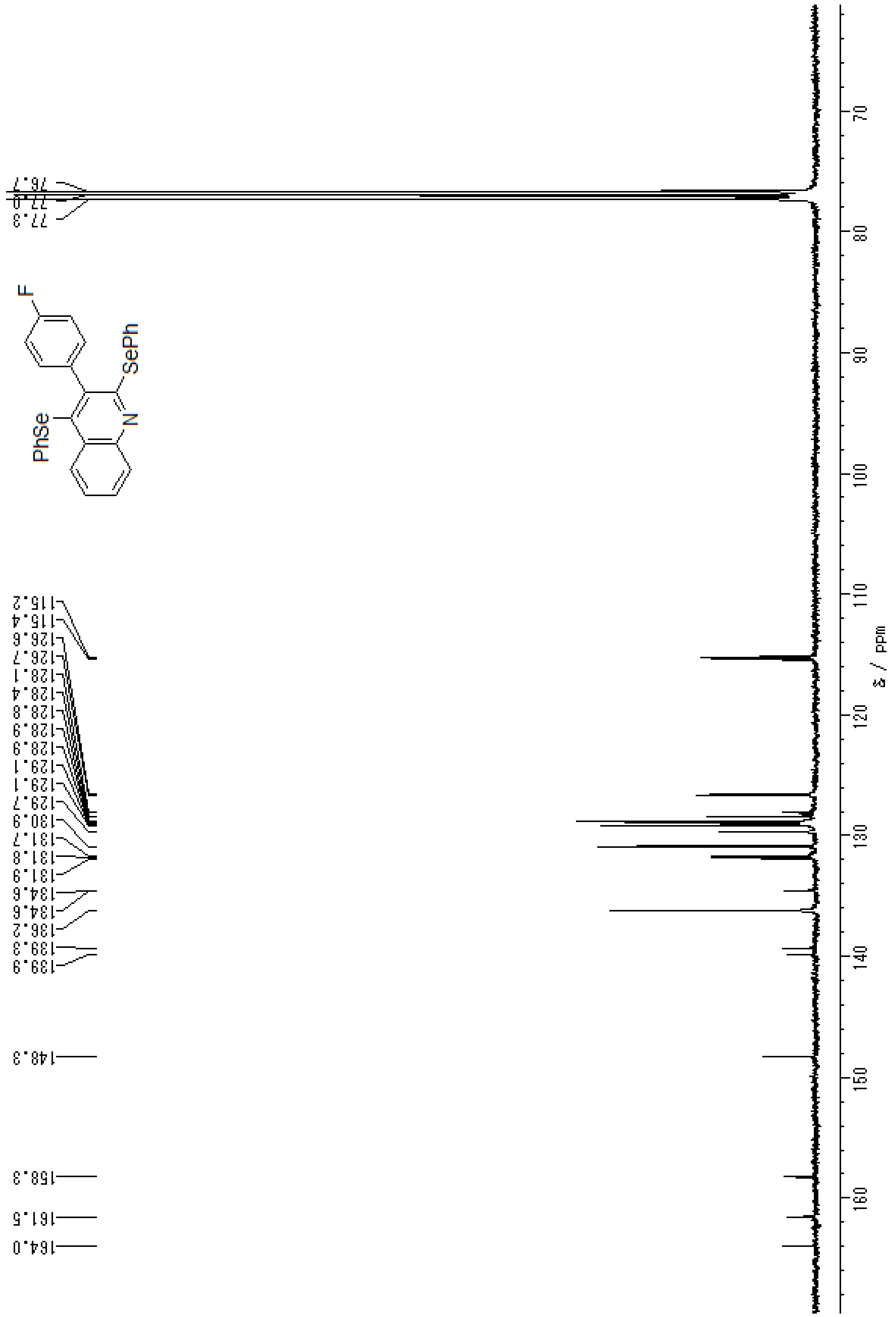
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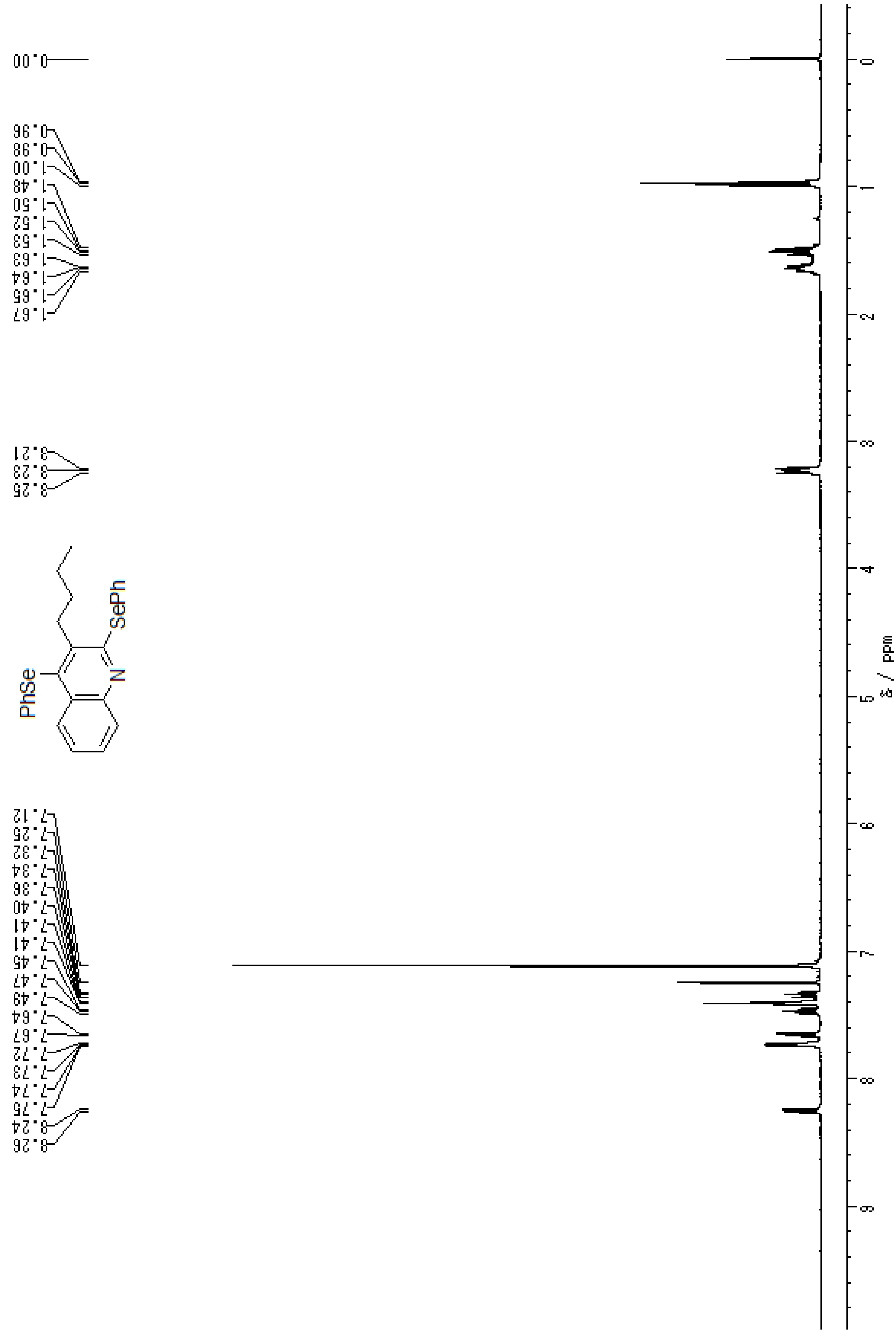
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7.45
7.47
7.49
7.64
7.67
7.72
7.73
7.74
7.75
8.24
8.26
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6
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δ / ppm

Supplementary Material (ESI) for Organic & Biomolecular Chemistry
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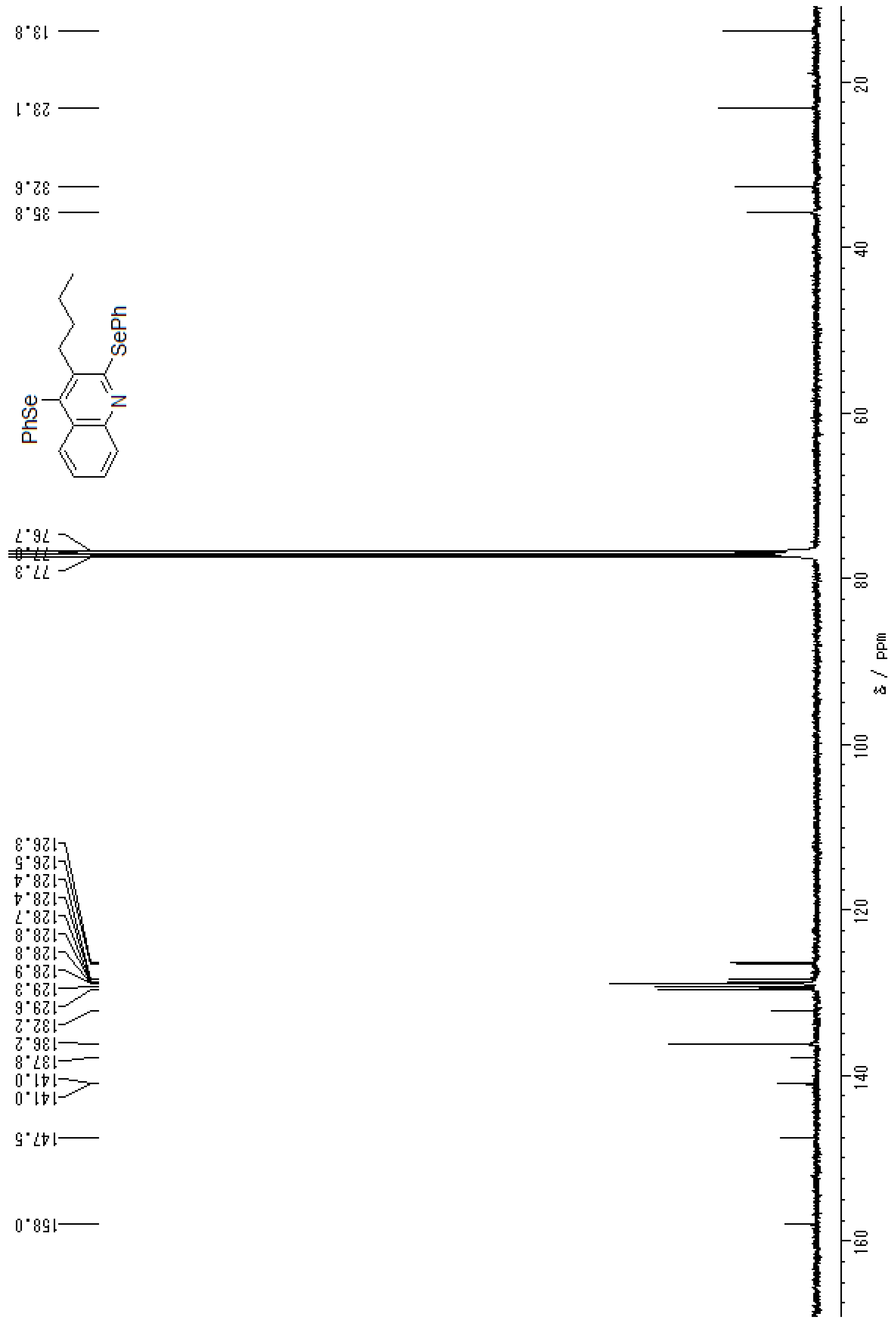

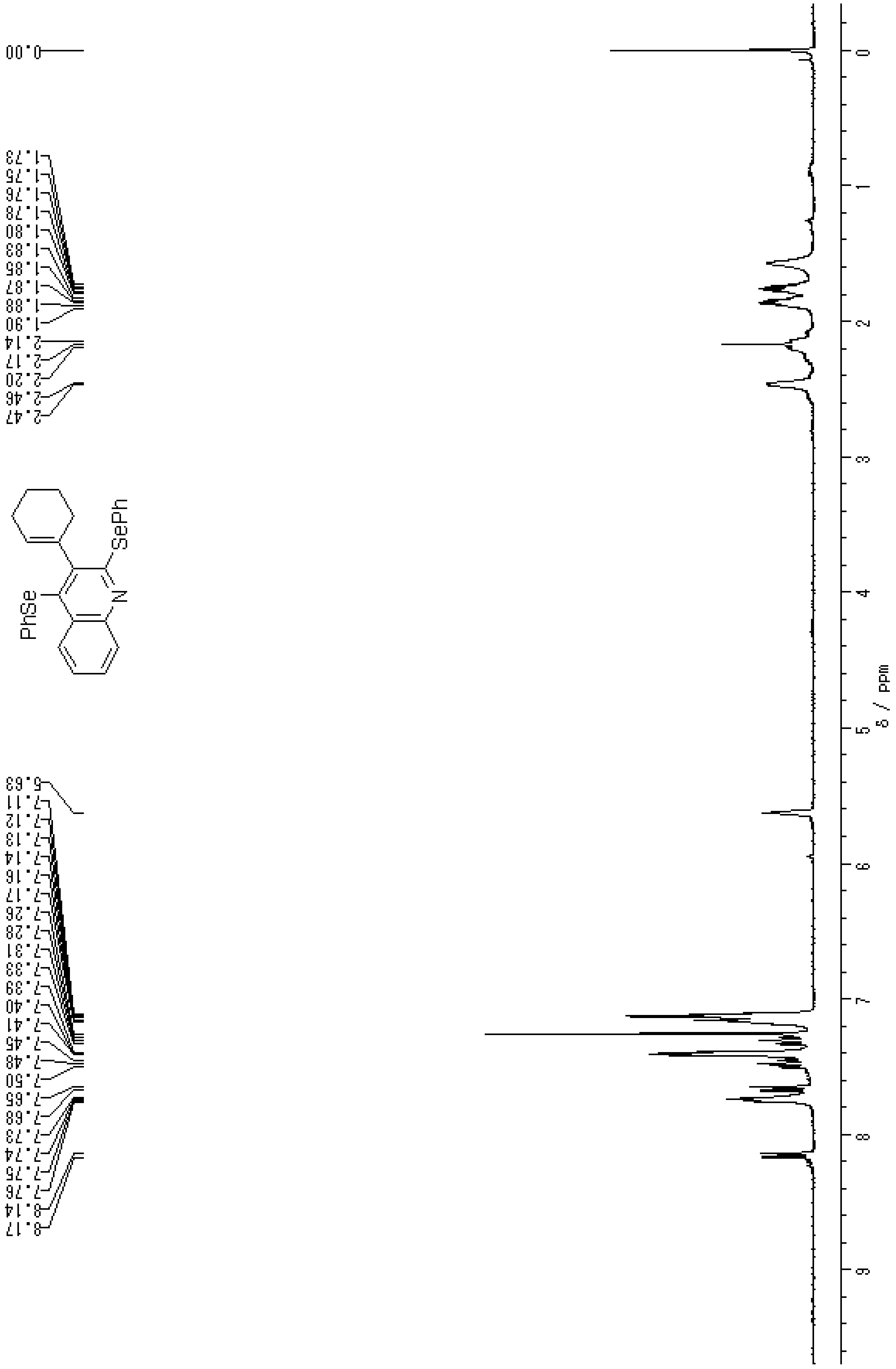
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SePh
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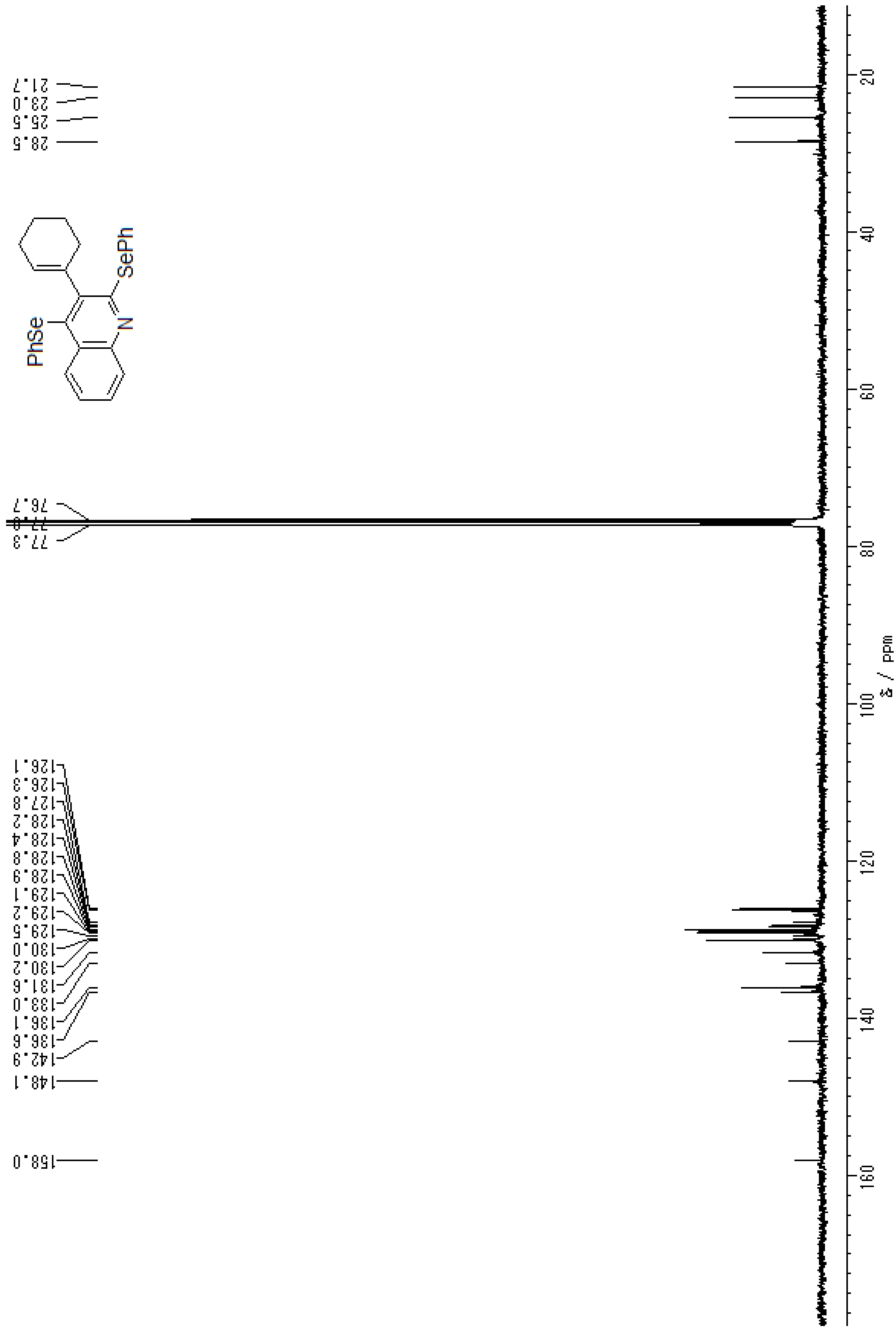
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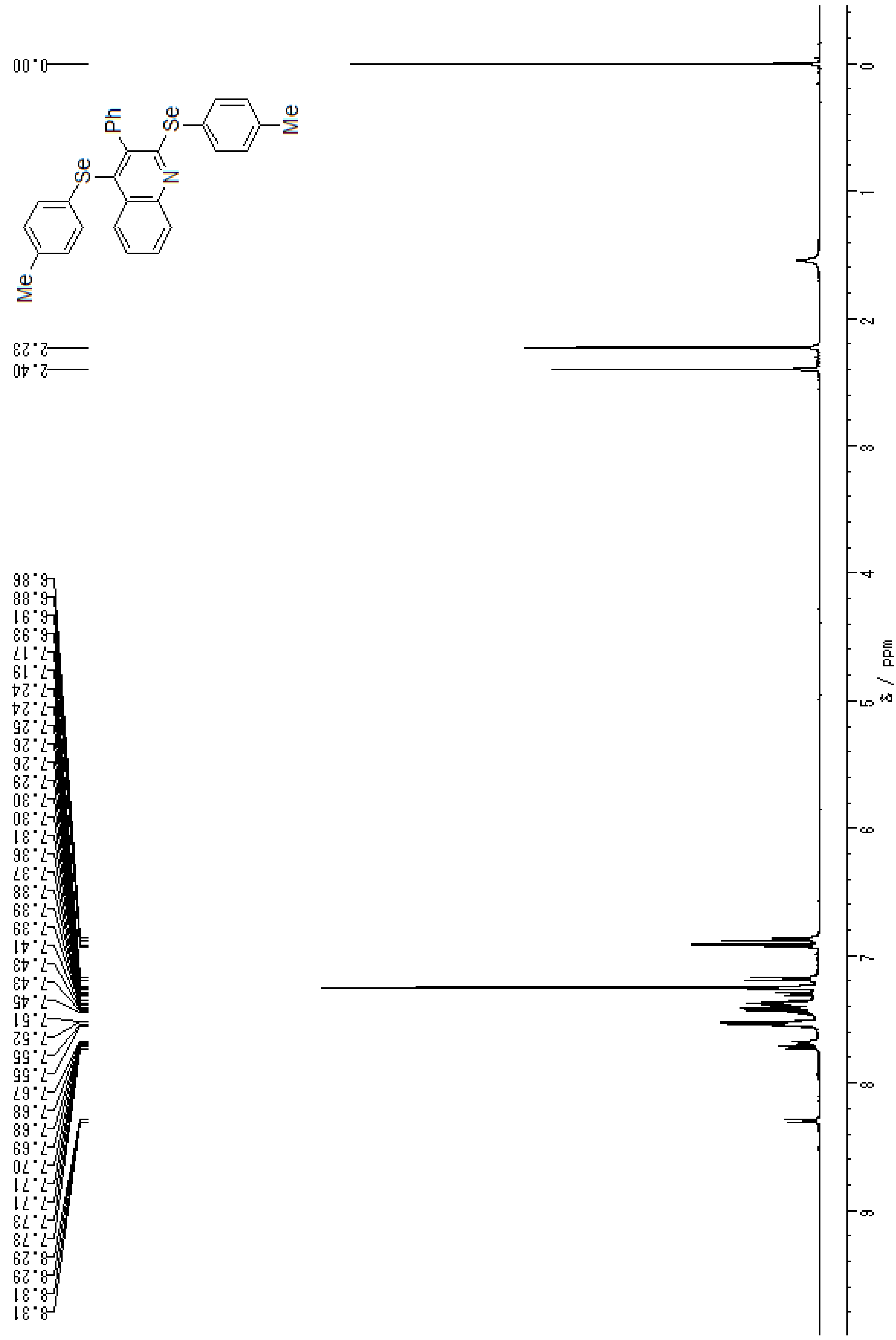
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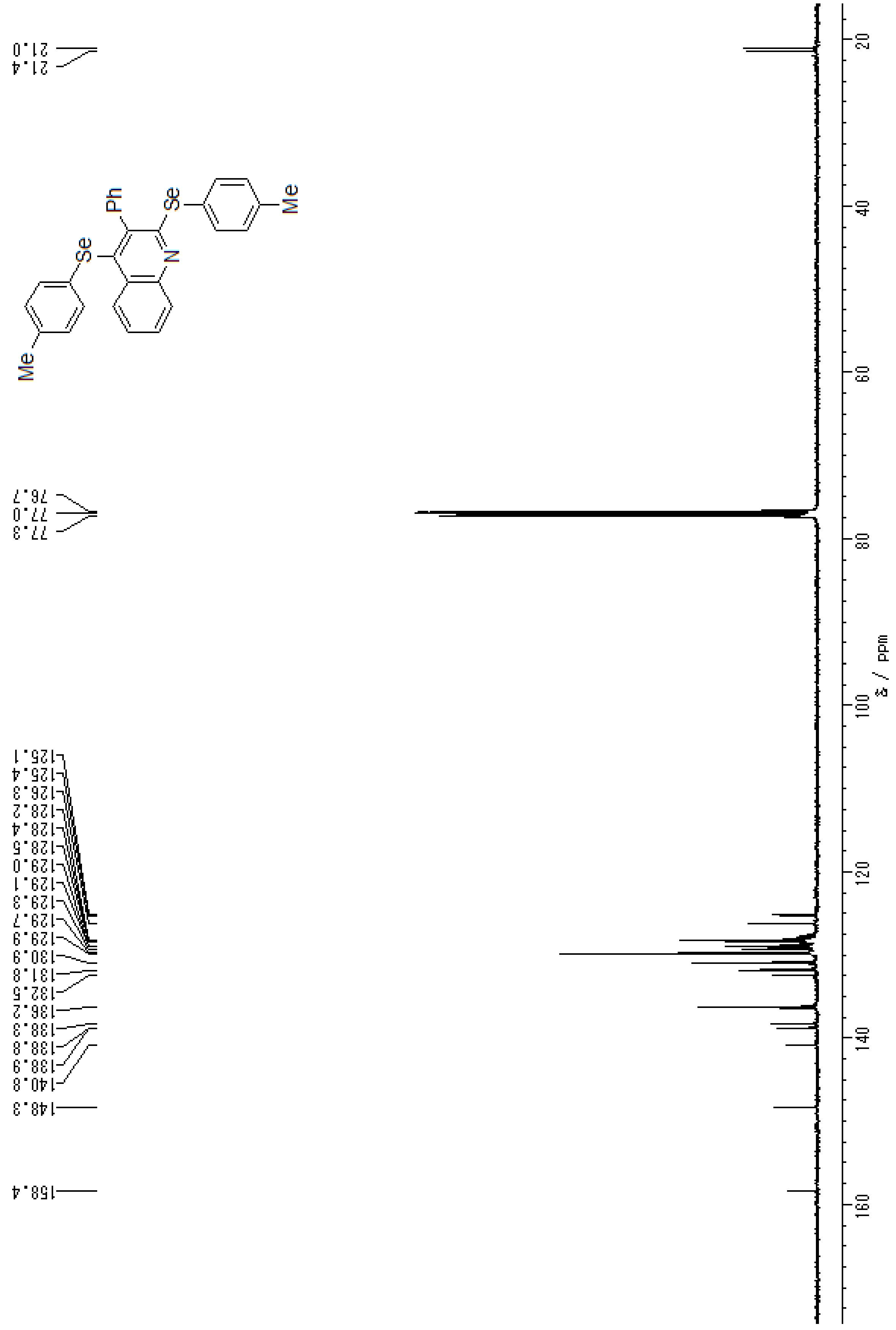
δ / ppm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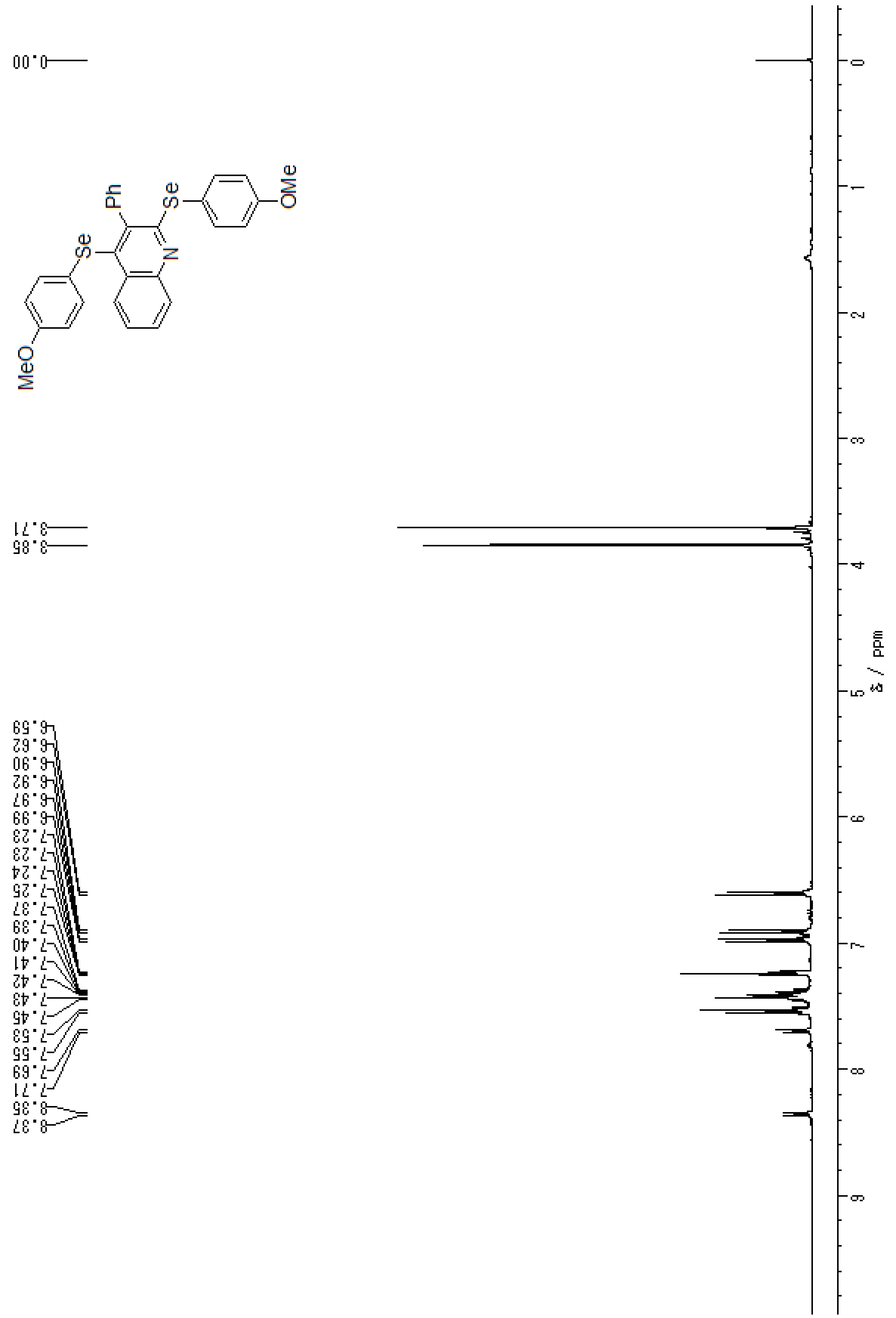
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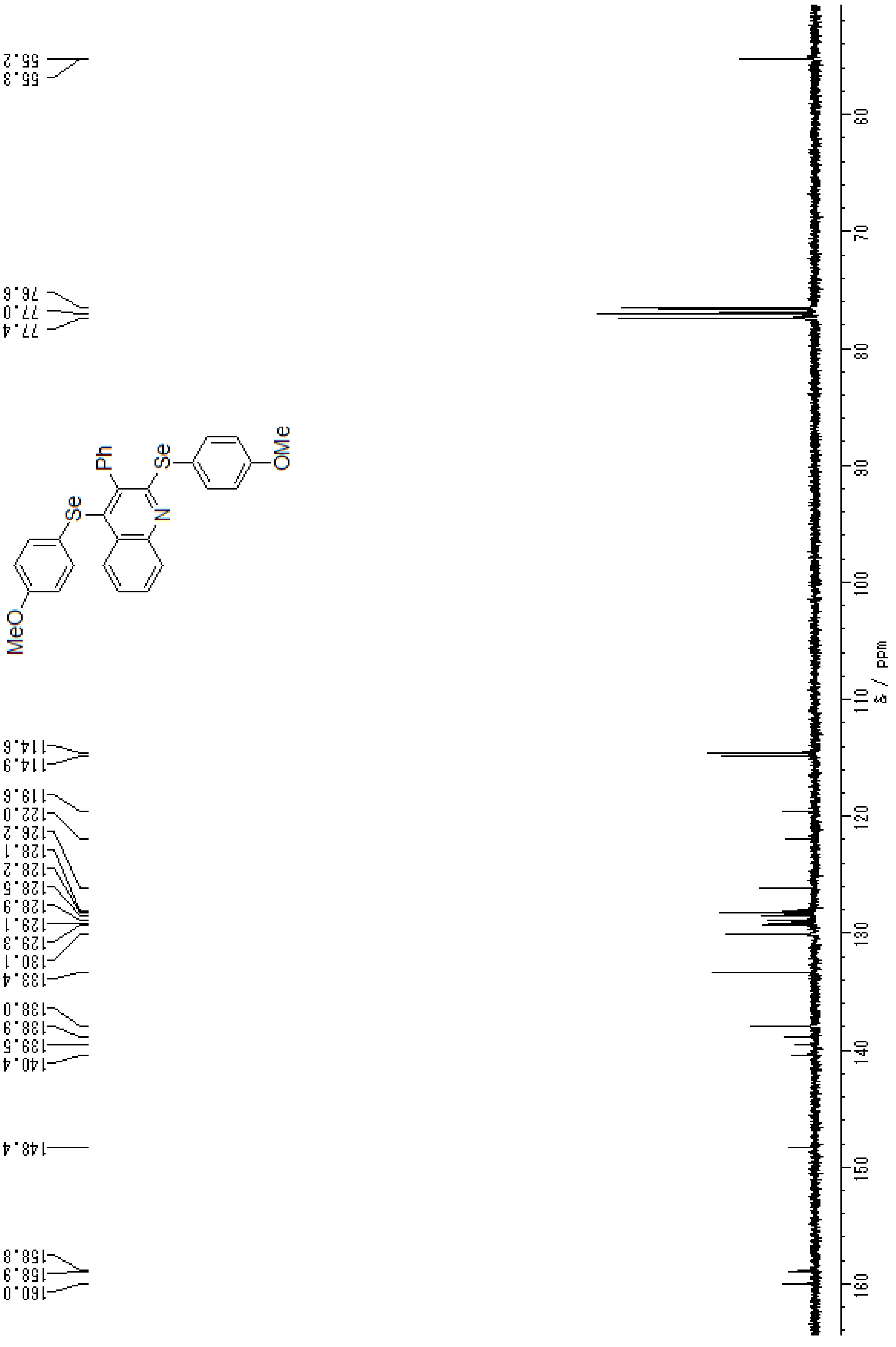
δ / ppm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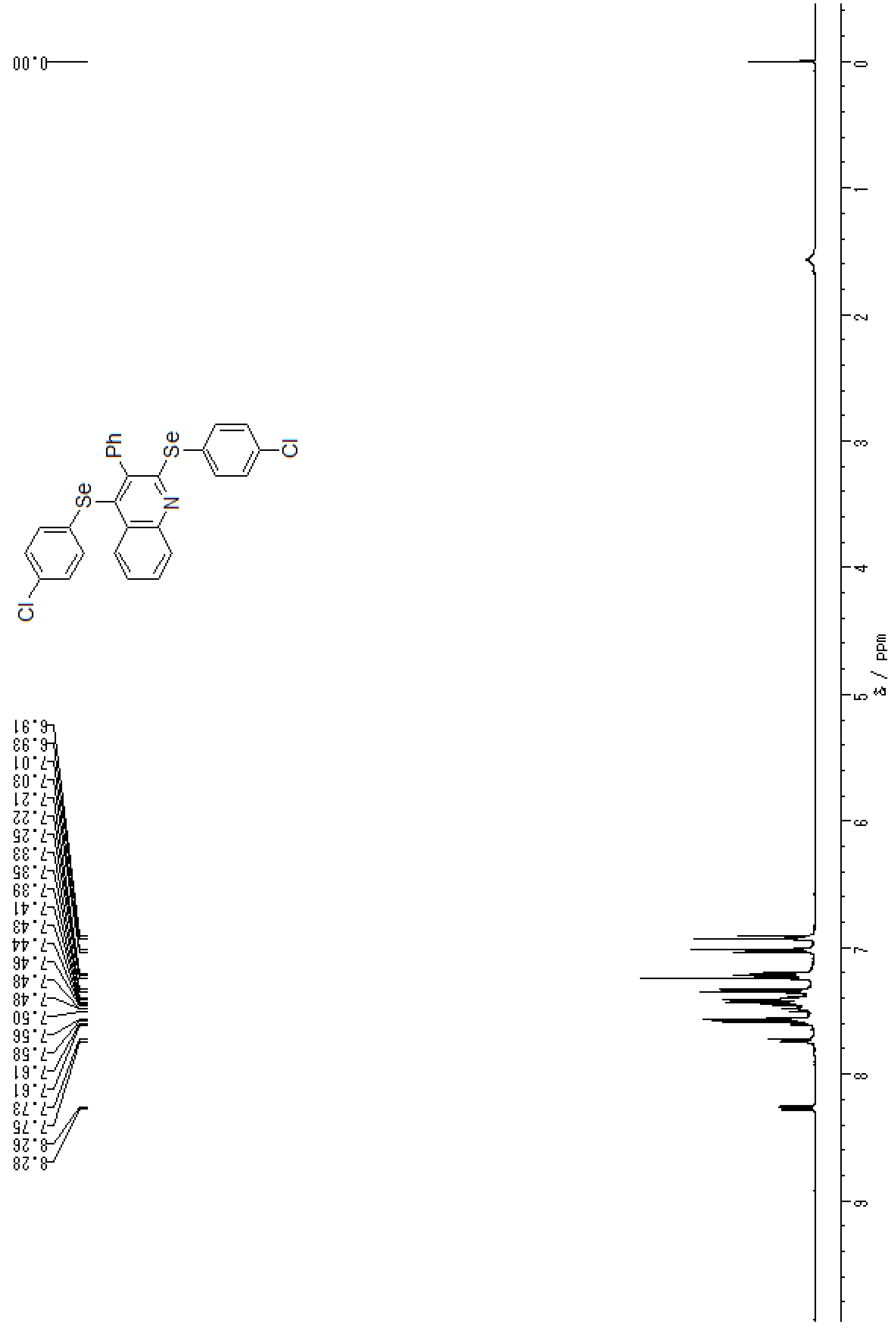
δ / ppm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Ph
Se
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Cl
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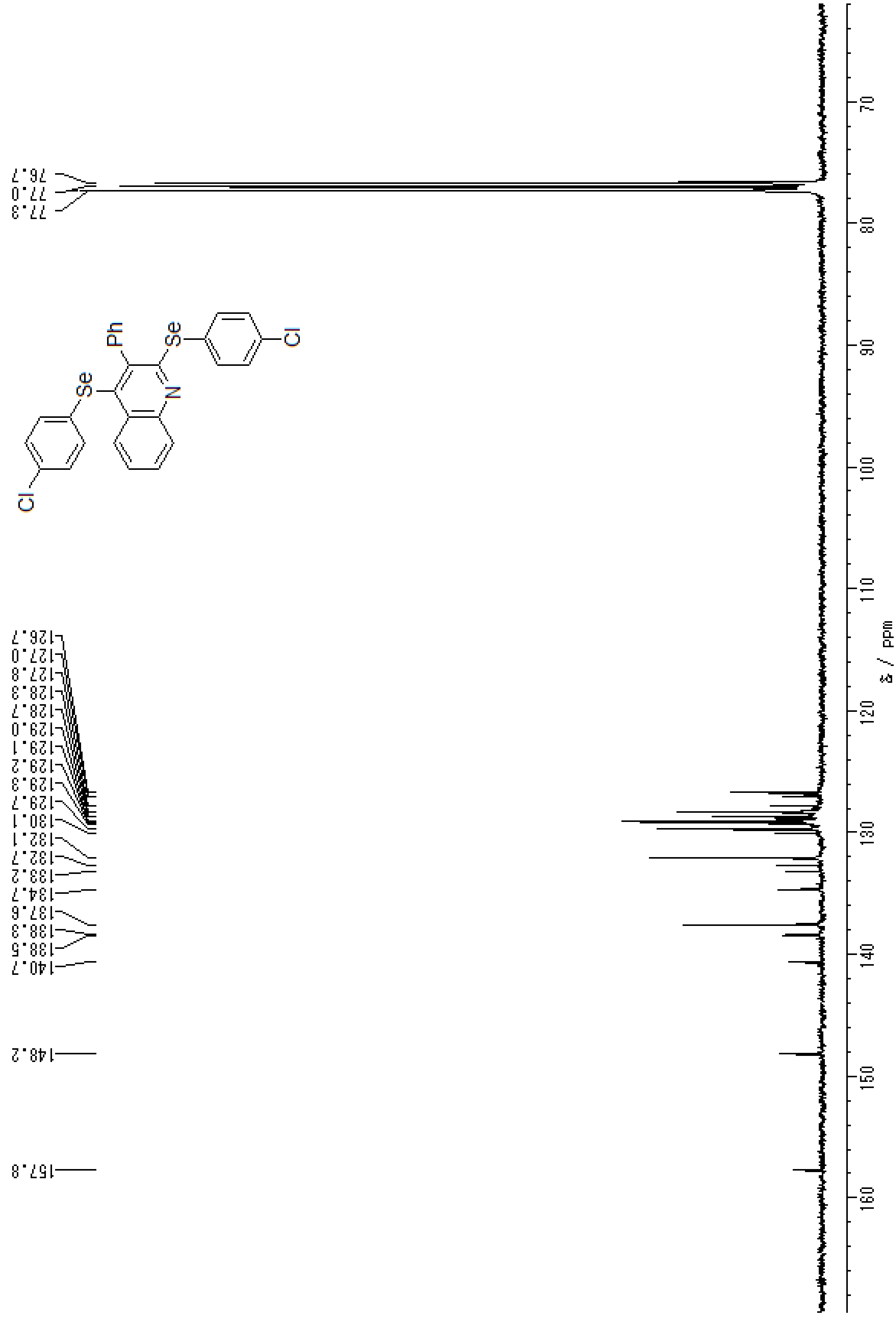
δ / ppm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N
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Cl
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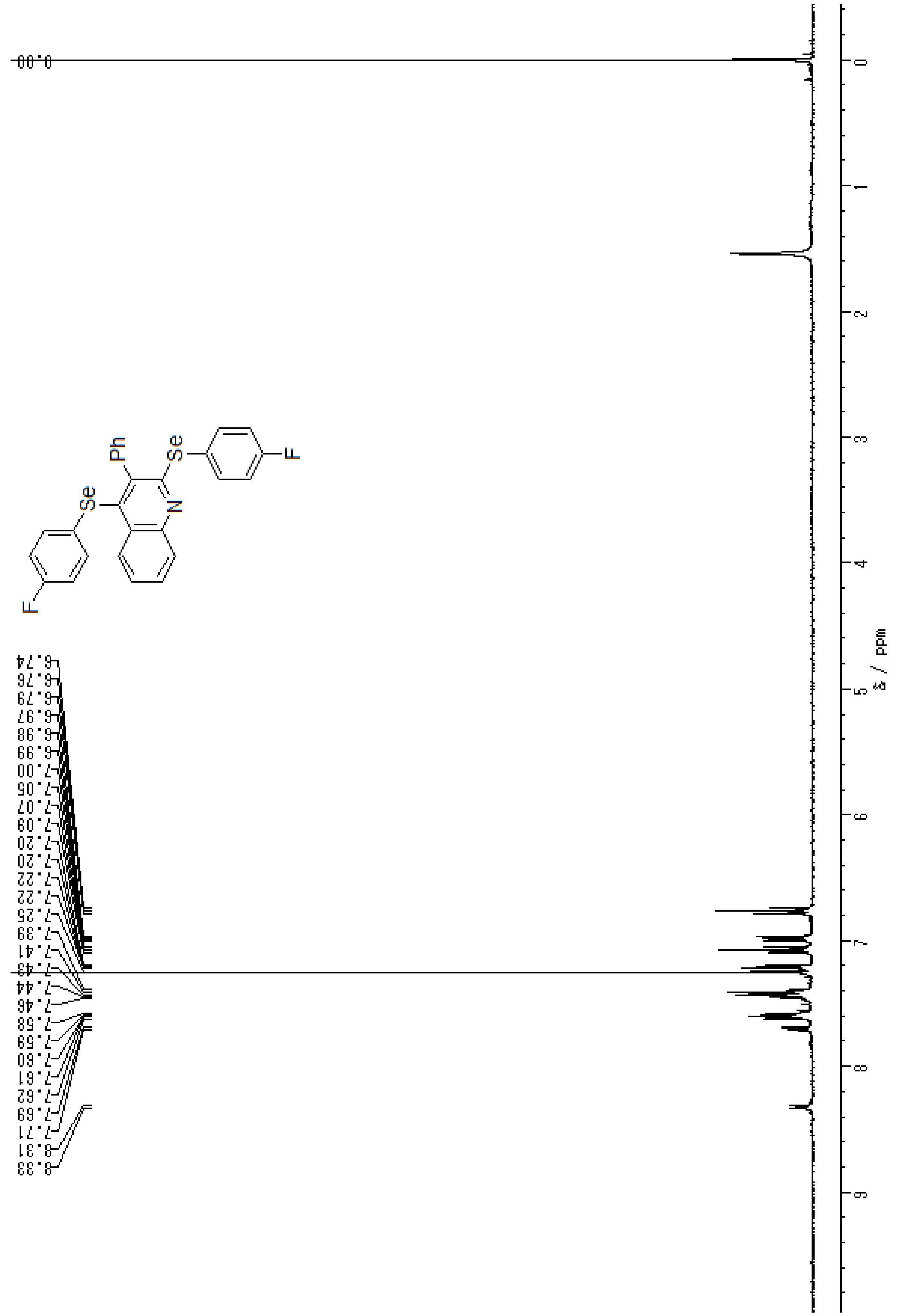
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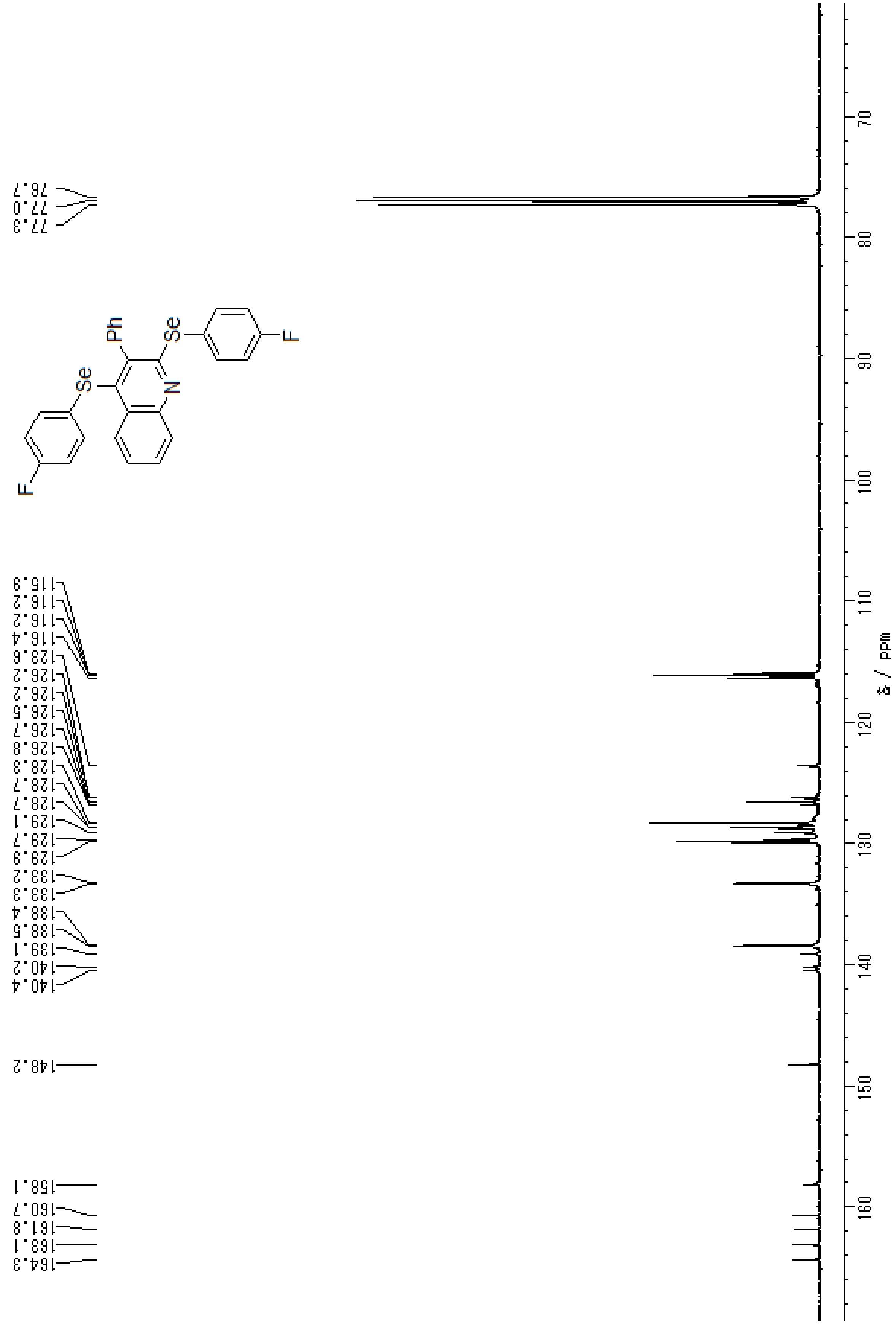
δ / ppm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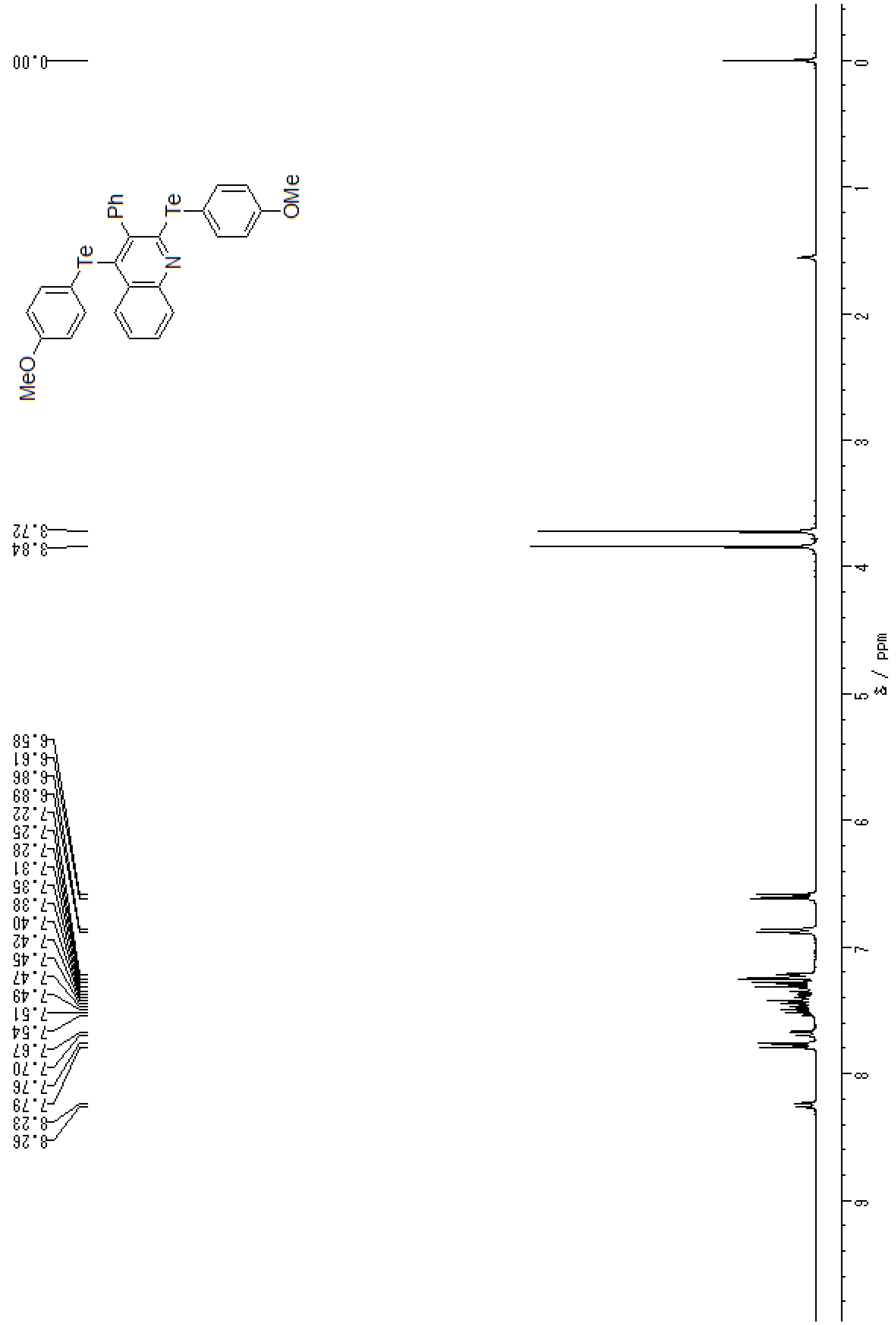
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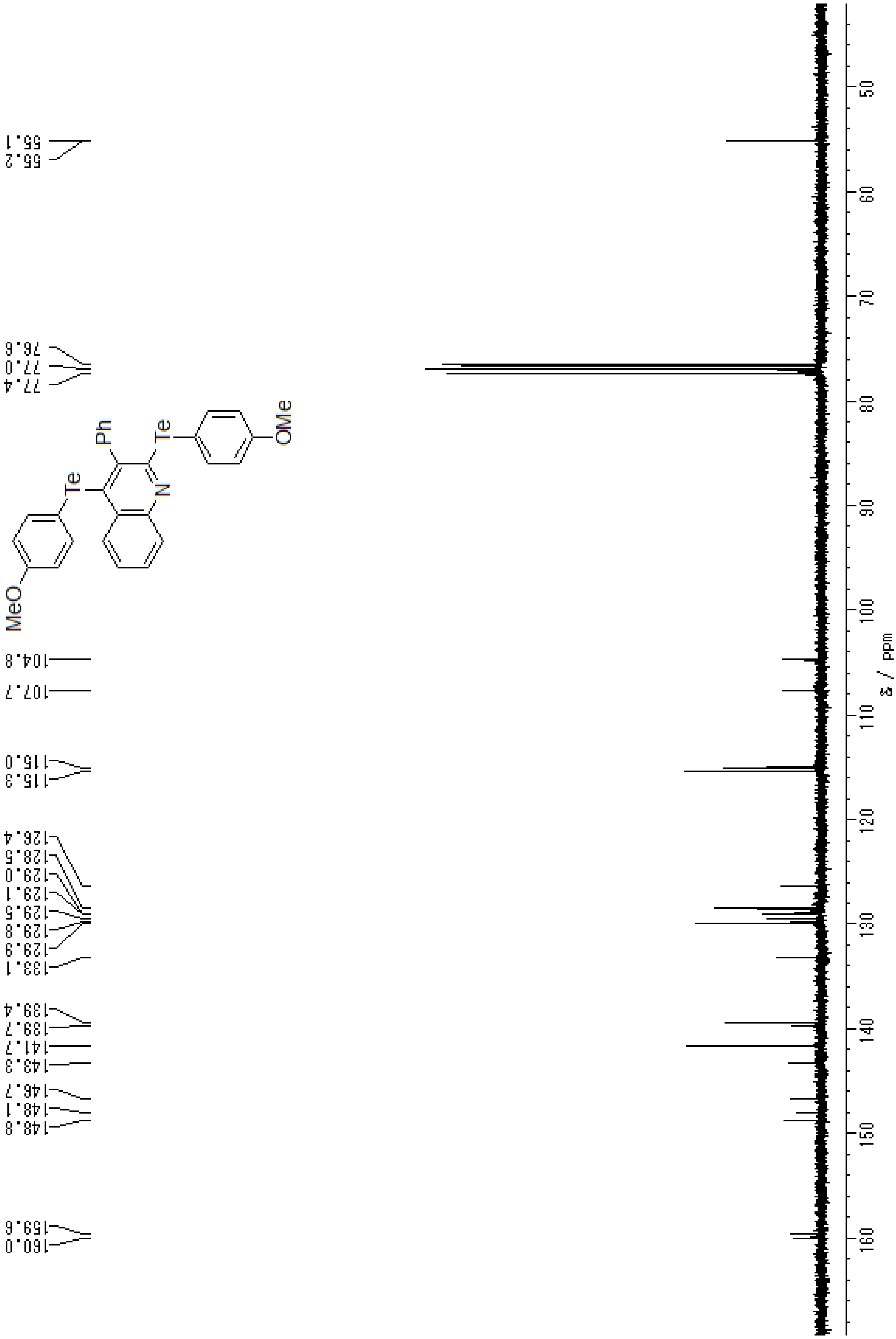
δ / ppm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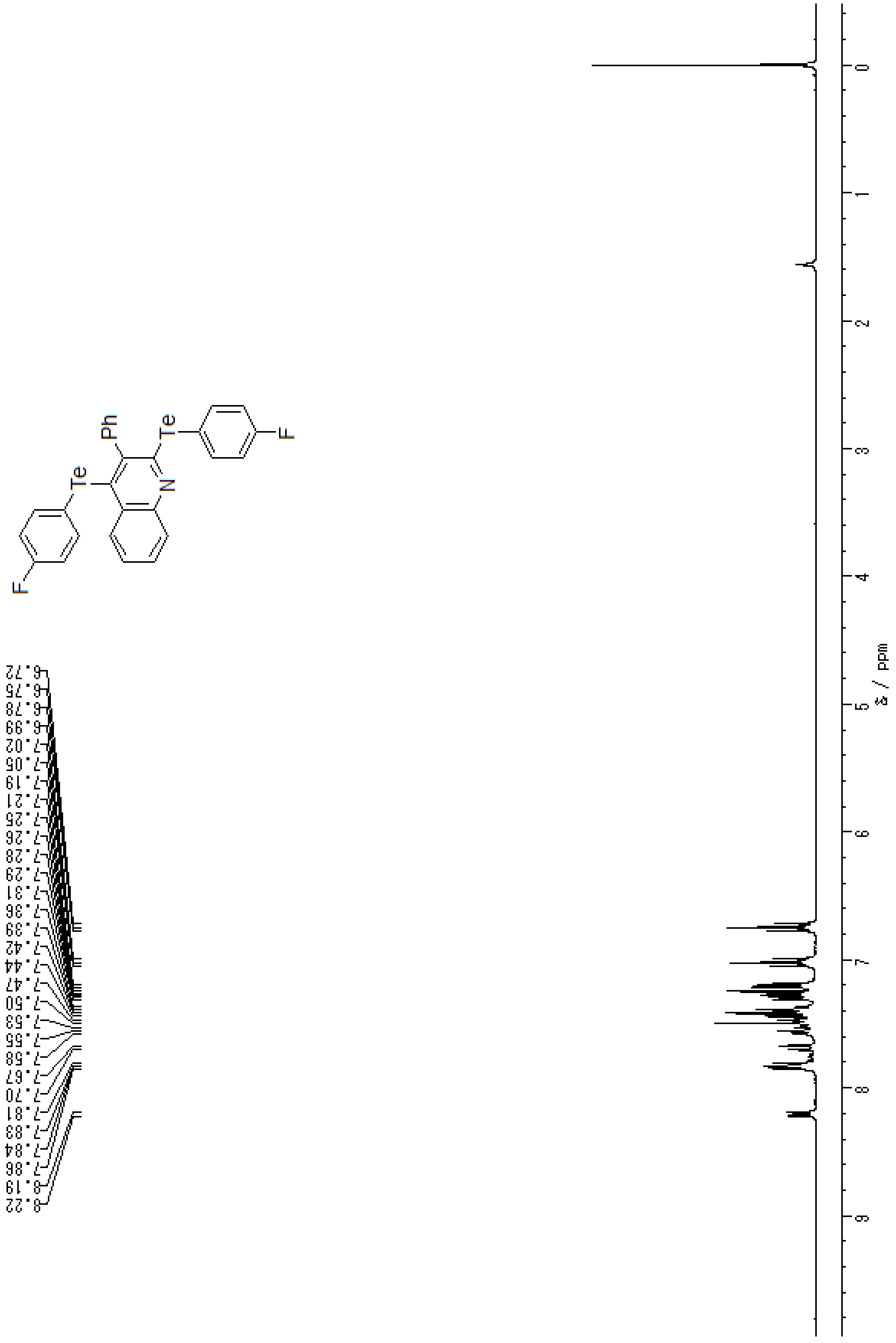
δ / ppm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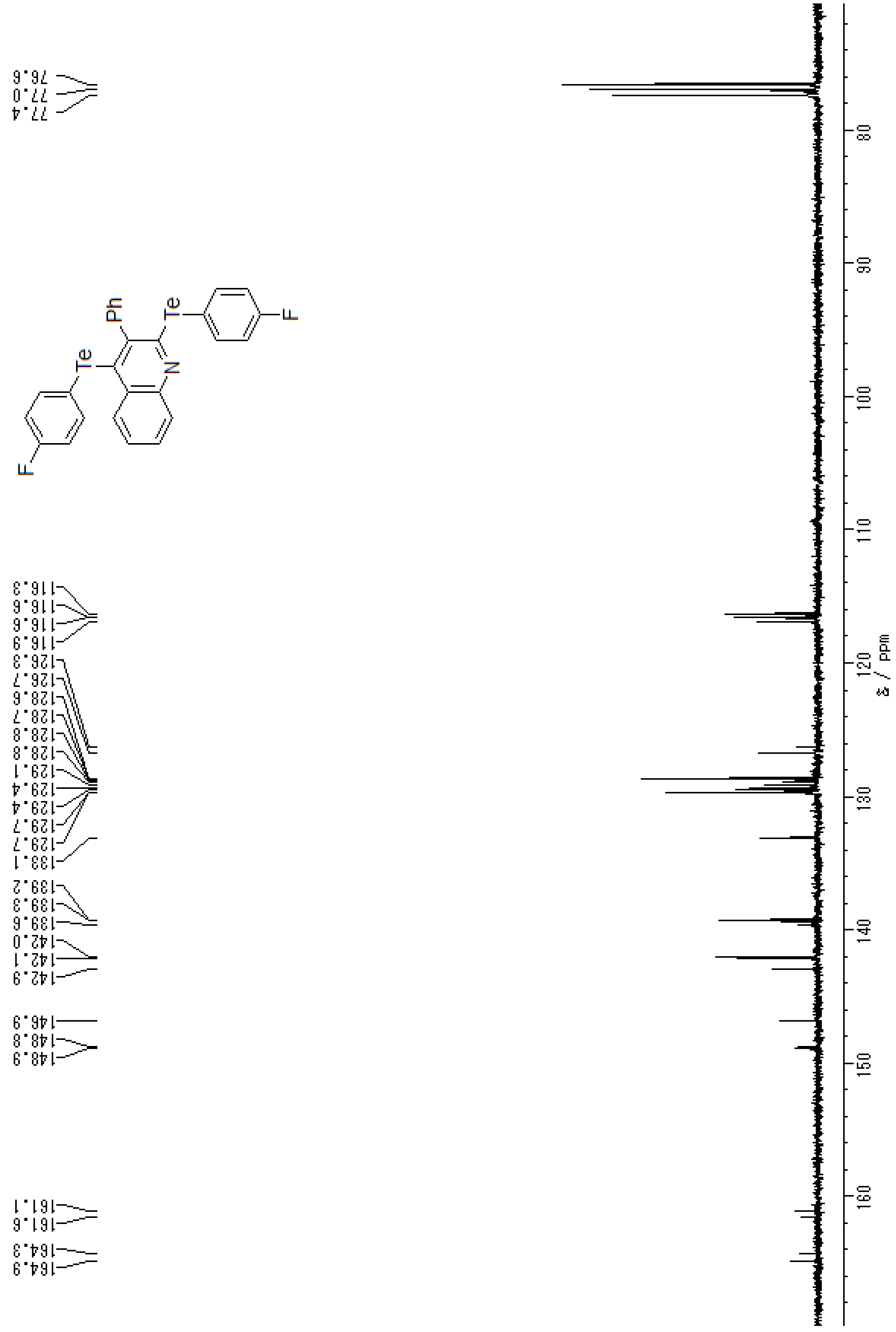
δ / ppm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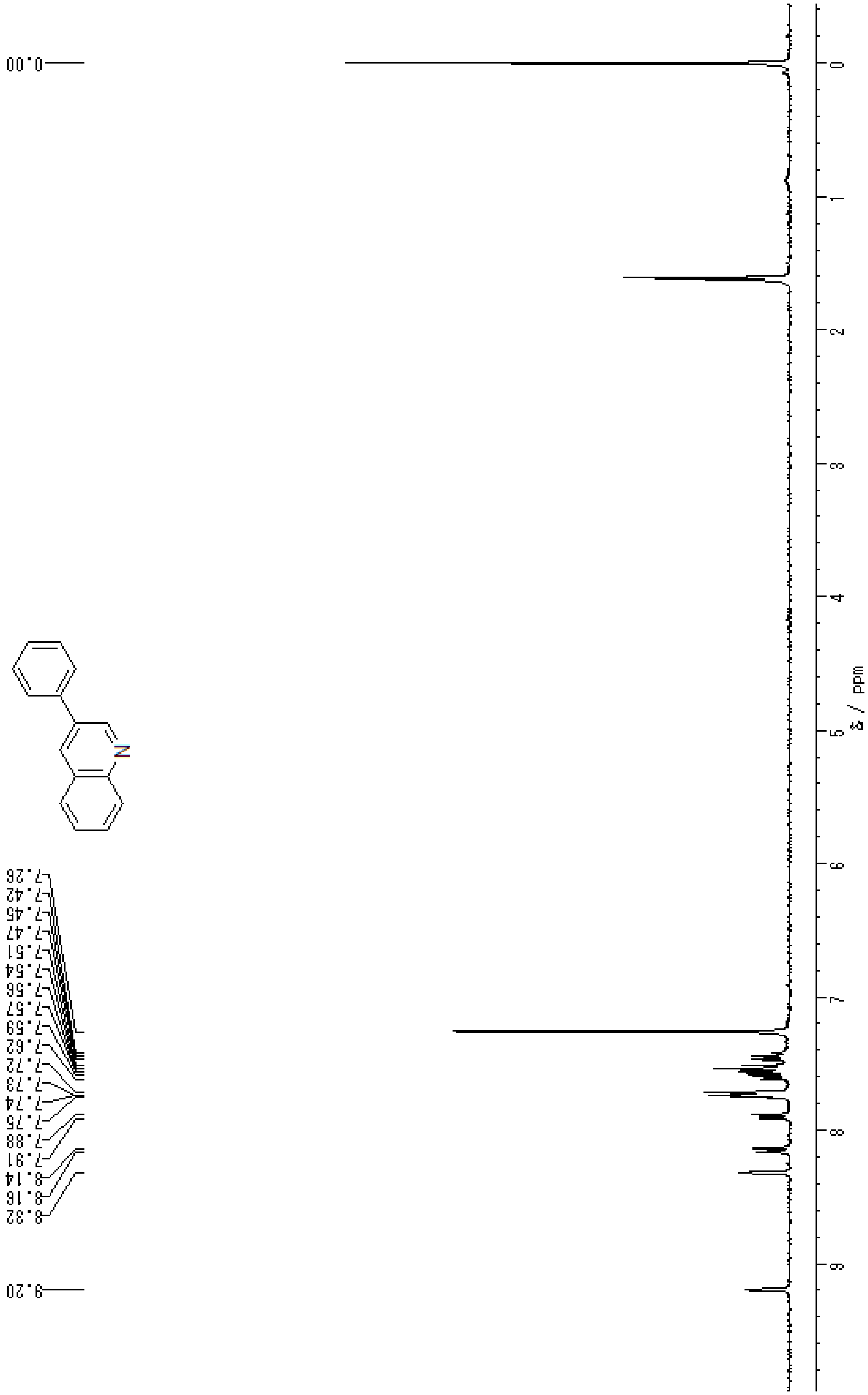
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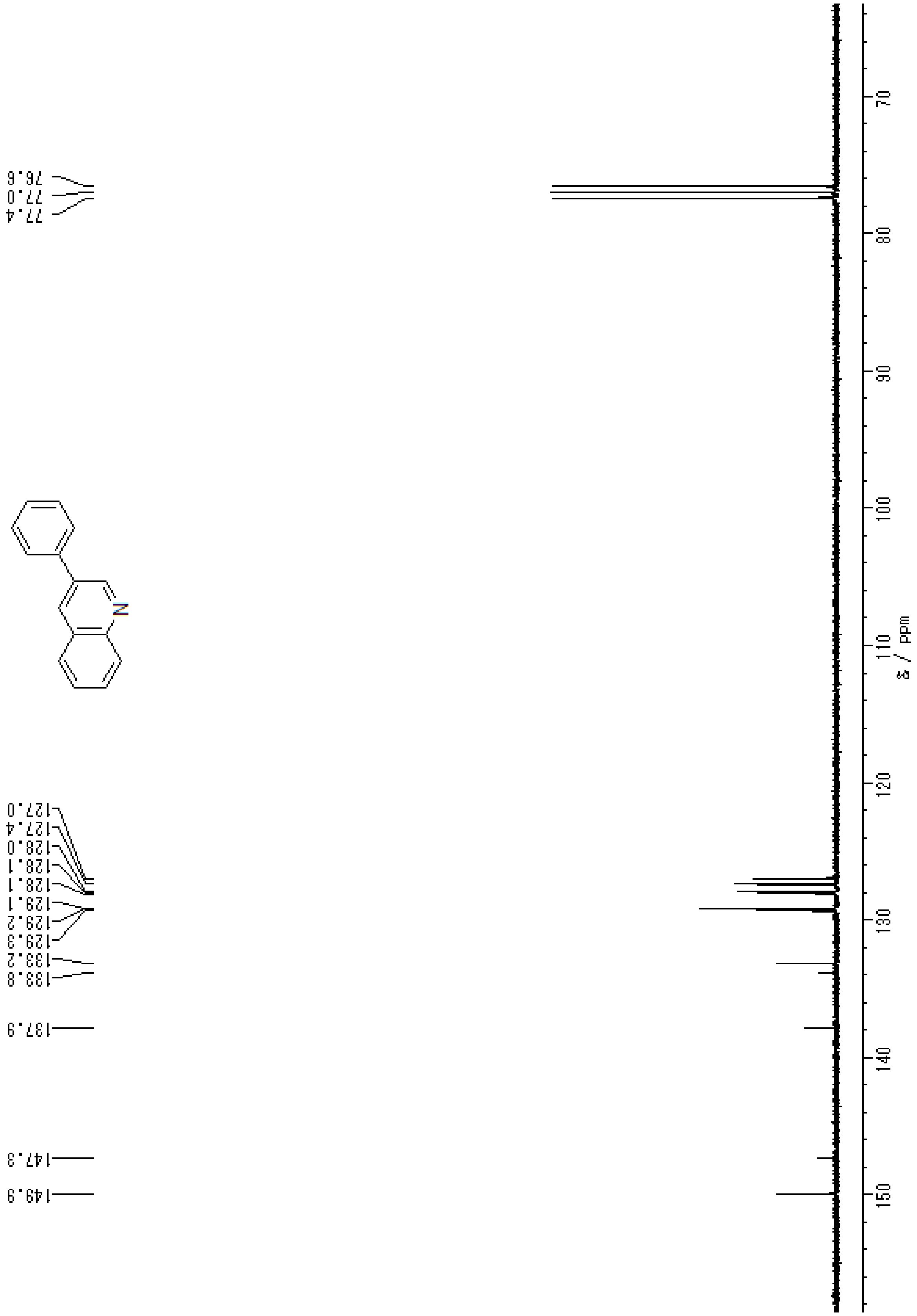
δ / ppm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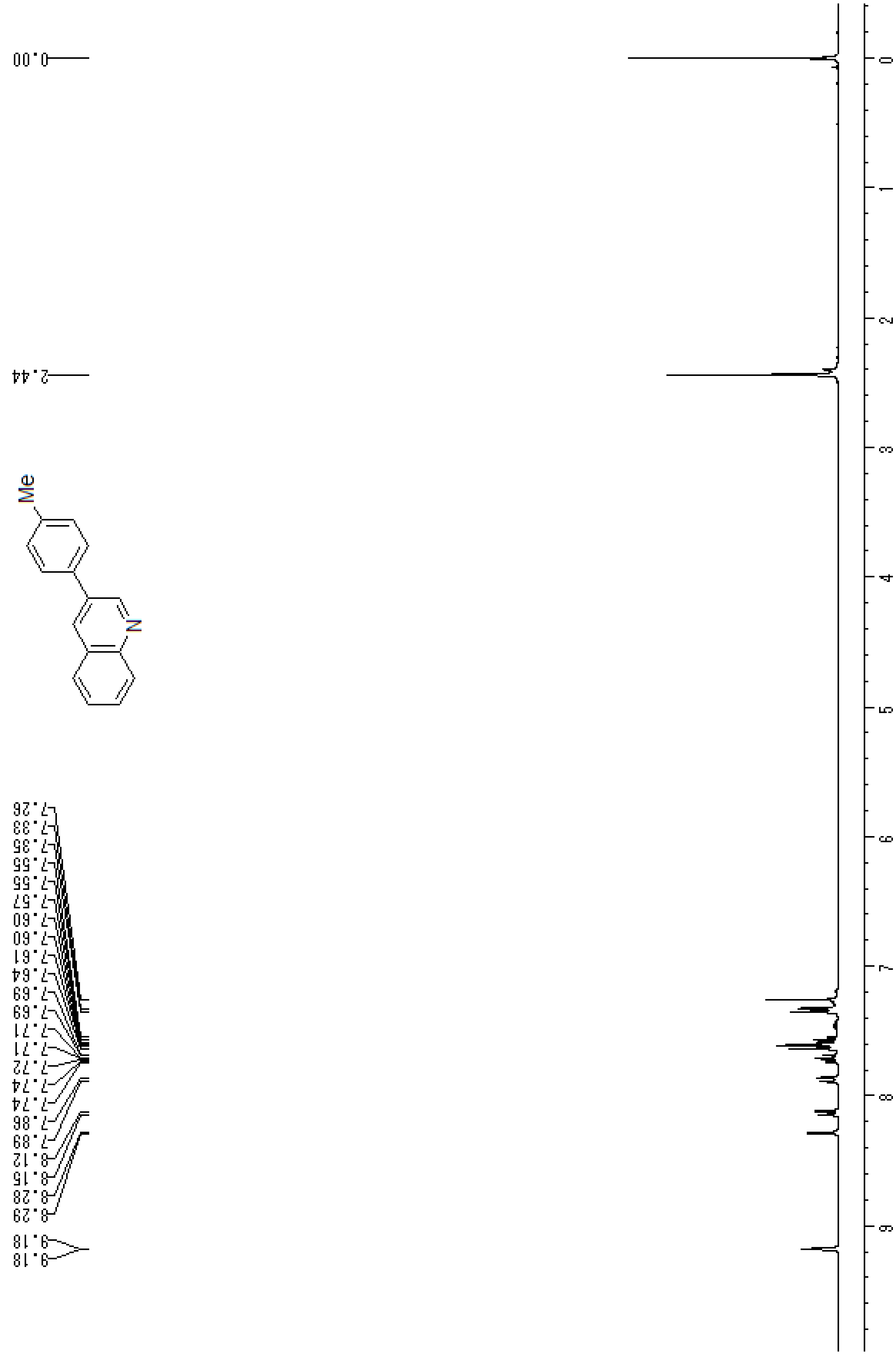
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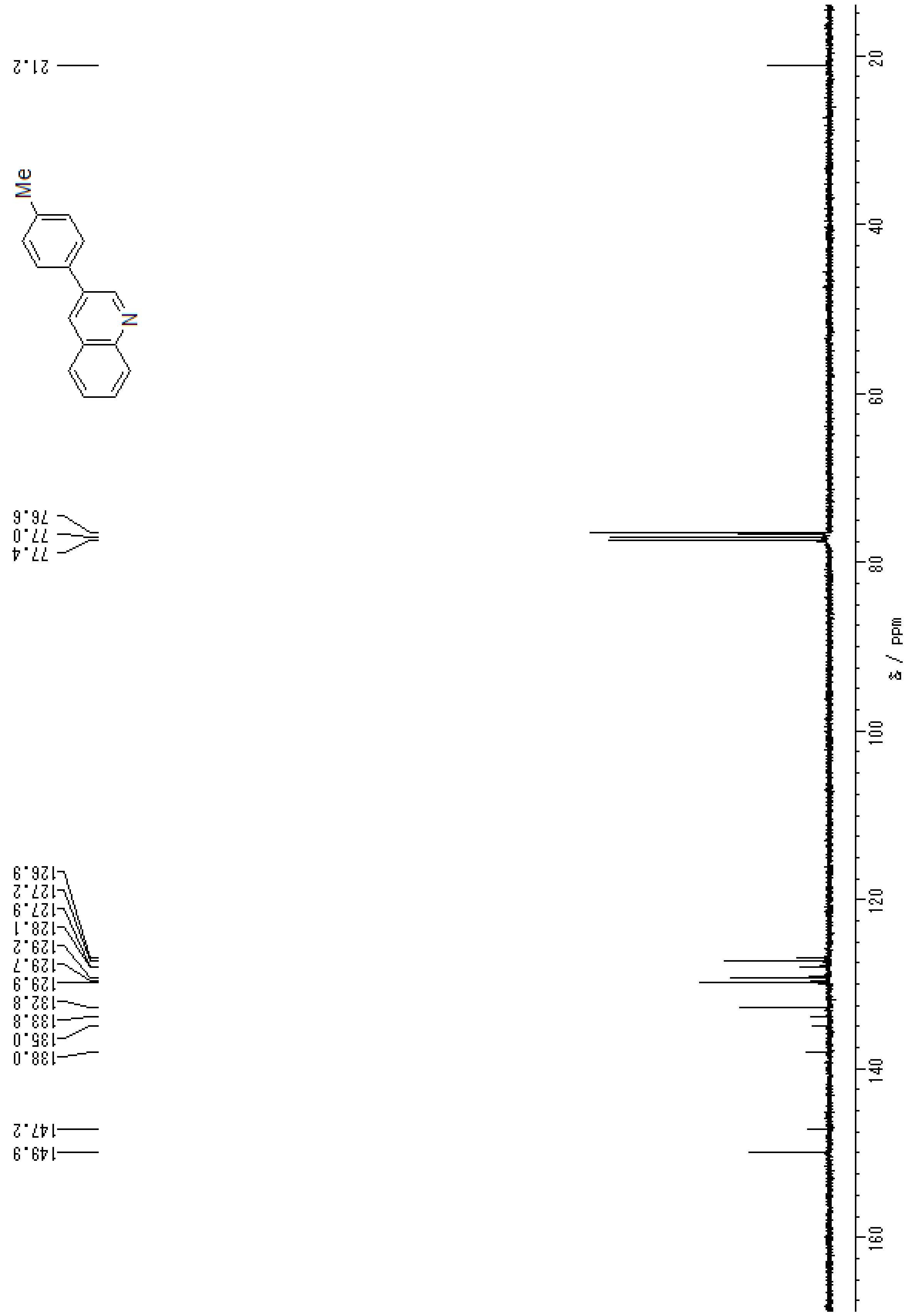
δ / ppm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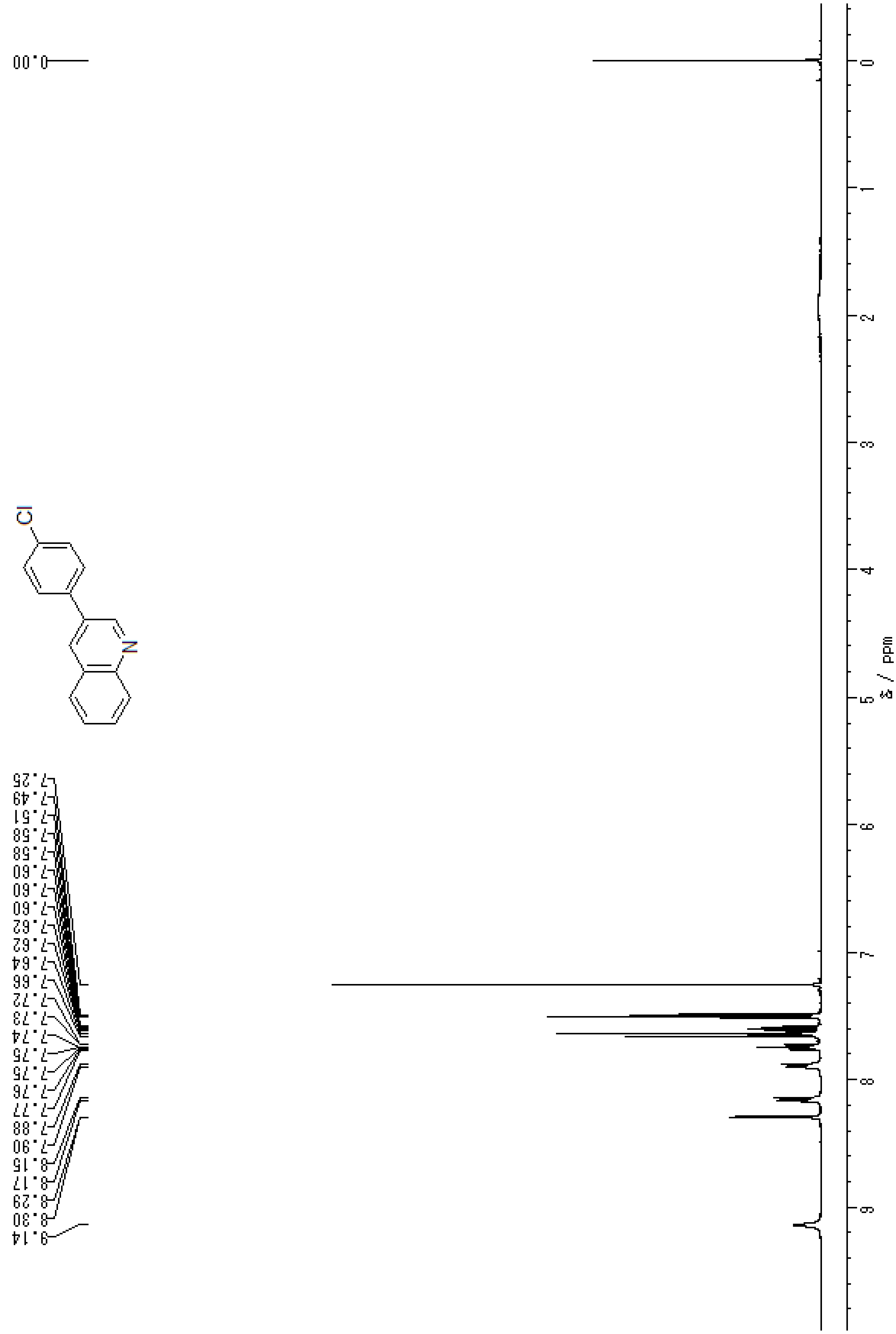
δ / ppm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7.66
7.72
7.73
7.74
7.75
7.75
7.76
7.77
7.88
7.90
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8.17
8.29
8.30
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4
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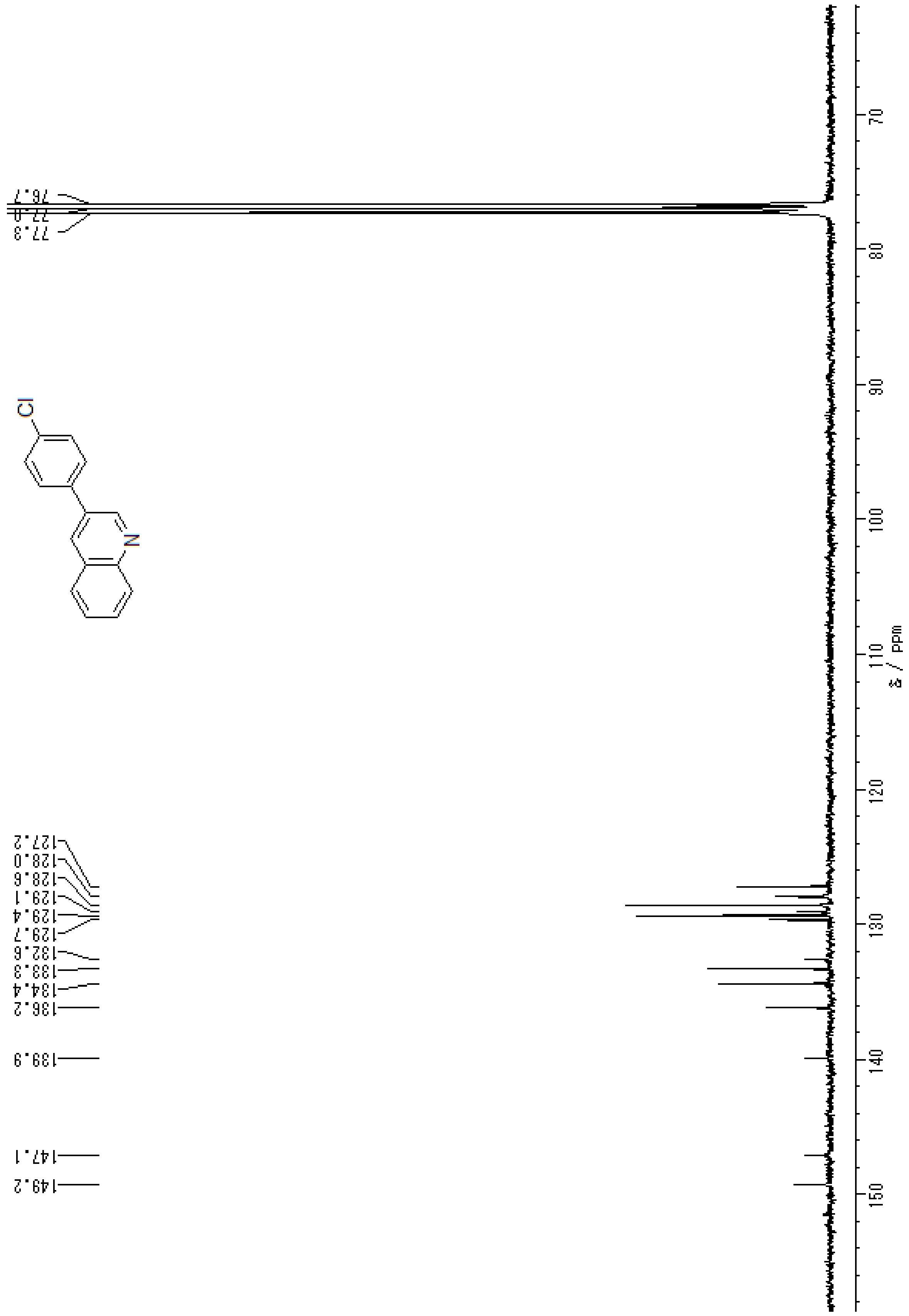
δ / ppm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132.6
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139.9
147.1
149.2
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90
100
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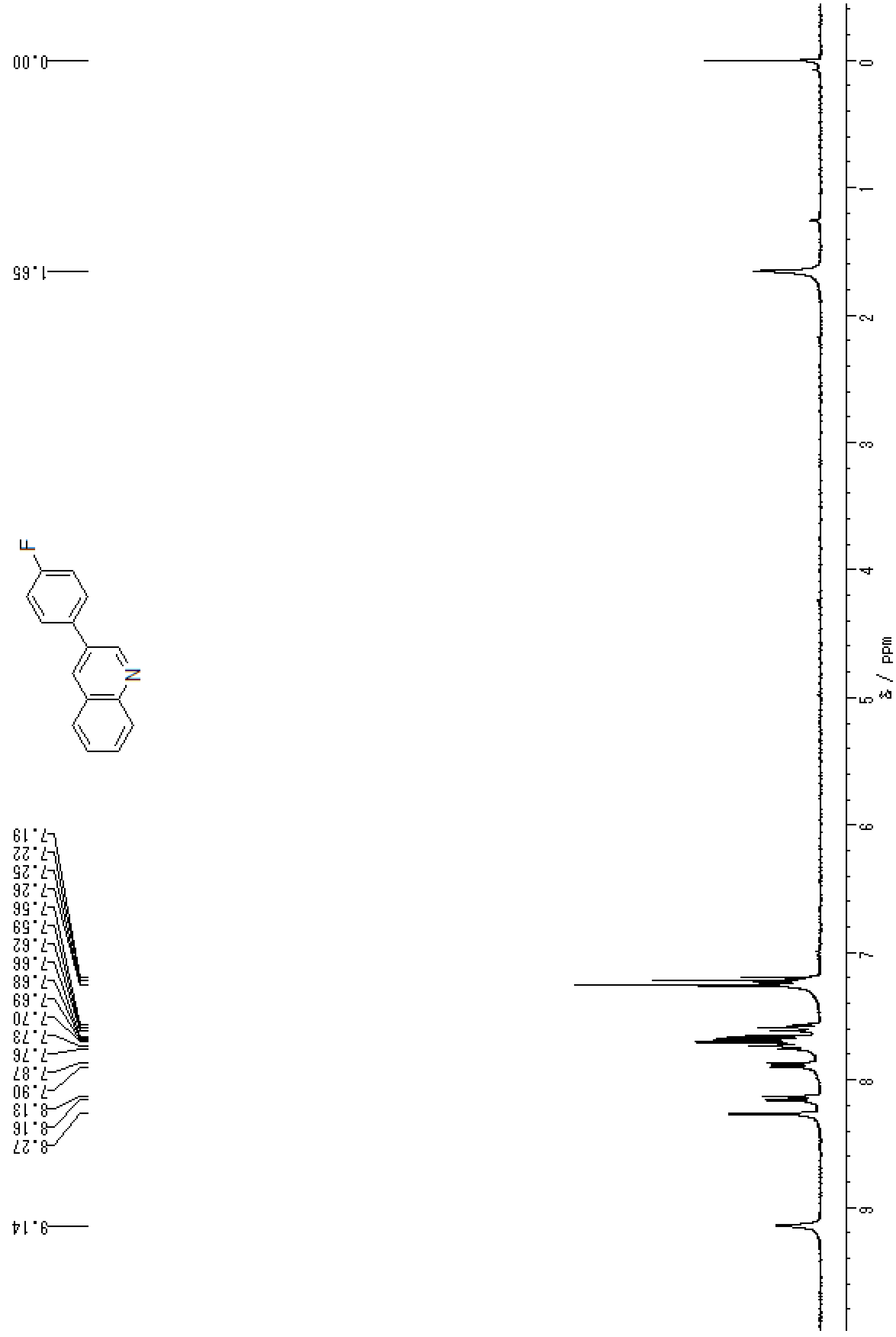
130
140
150
δ / ppm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7.59
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7.66
7.68
7.69
7.70
7.73
7.76
7.87
7.90
8.13
8.16
8.27
9.14
F
N
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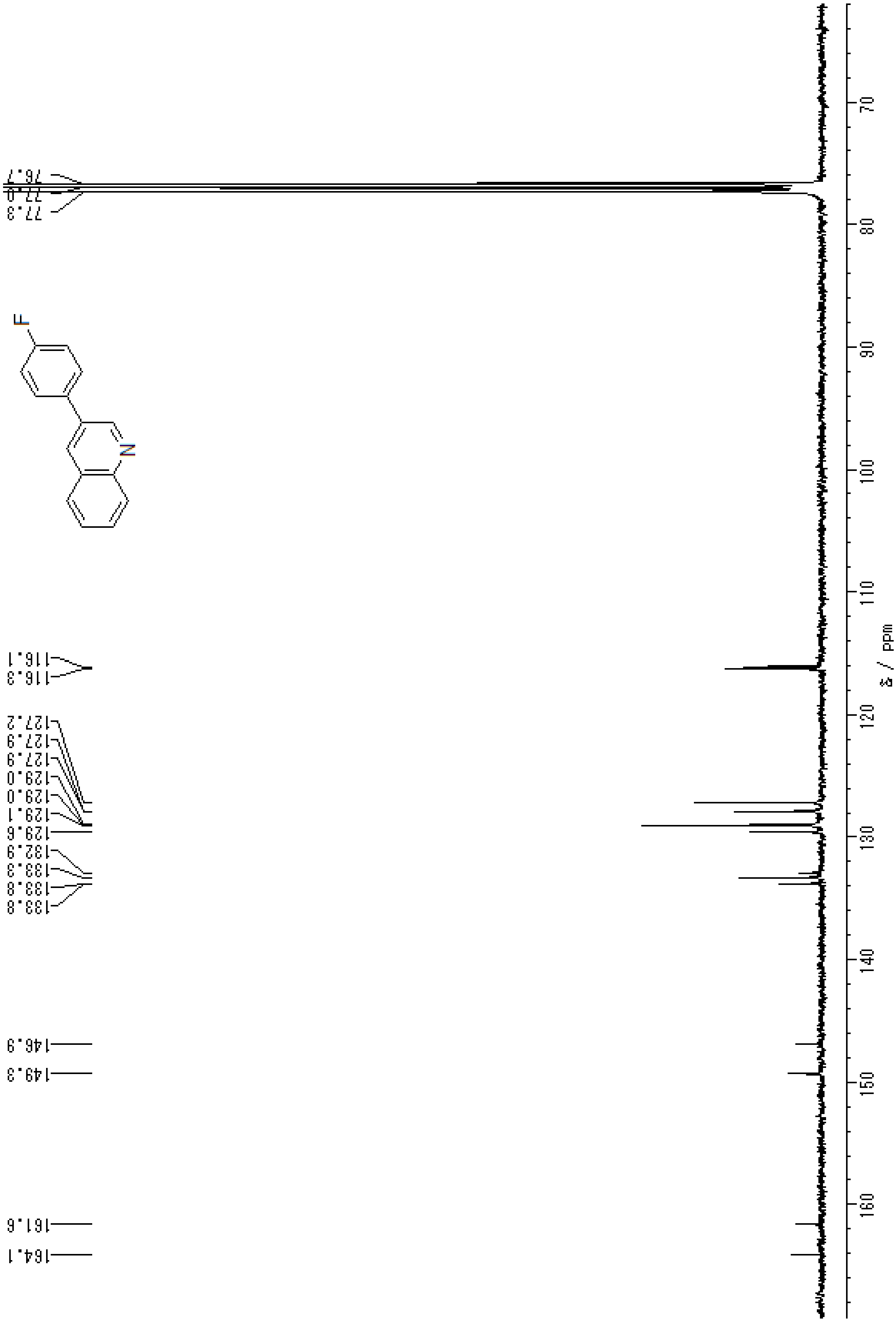
3
4
5
6
7
8
9
δ / ppm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129.0
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129.6
132.9
133.3
133.8
133.8
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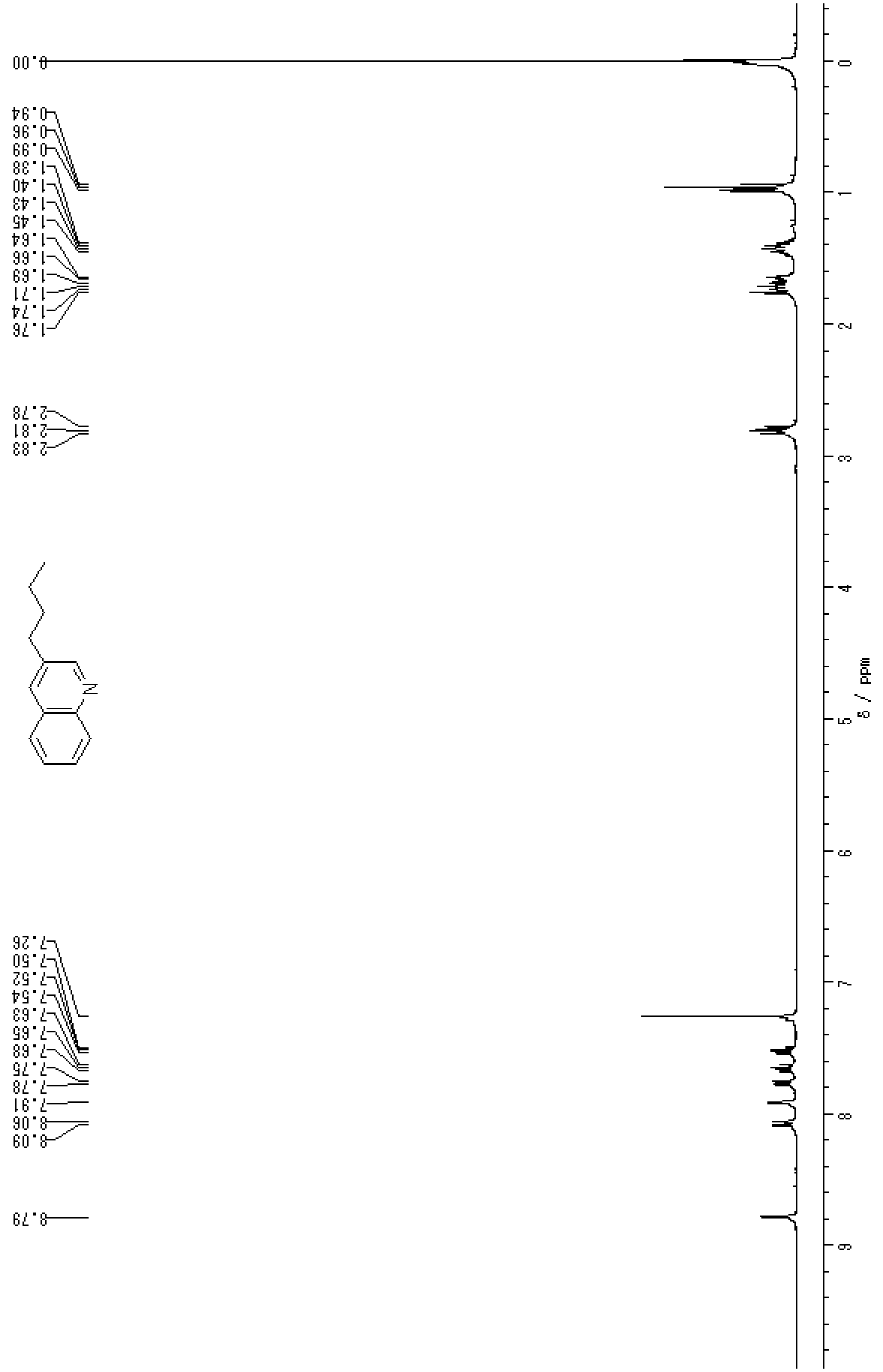
149.3
161.6
164.1
70
80
90
100
110
120
130
140
150
160
δ / ppm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1.66
1.69
1.71
1.74
1.76
2.78
2.81
2.83
7.26
7.50
7.52
7.54
7.63
7.65
7.68
7.75
7.78
7.91
8.06
8.09
8.79
N
0
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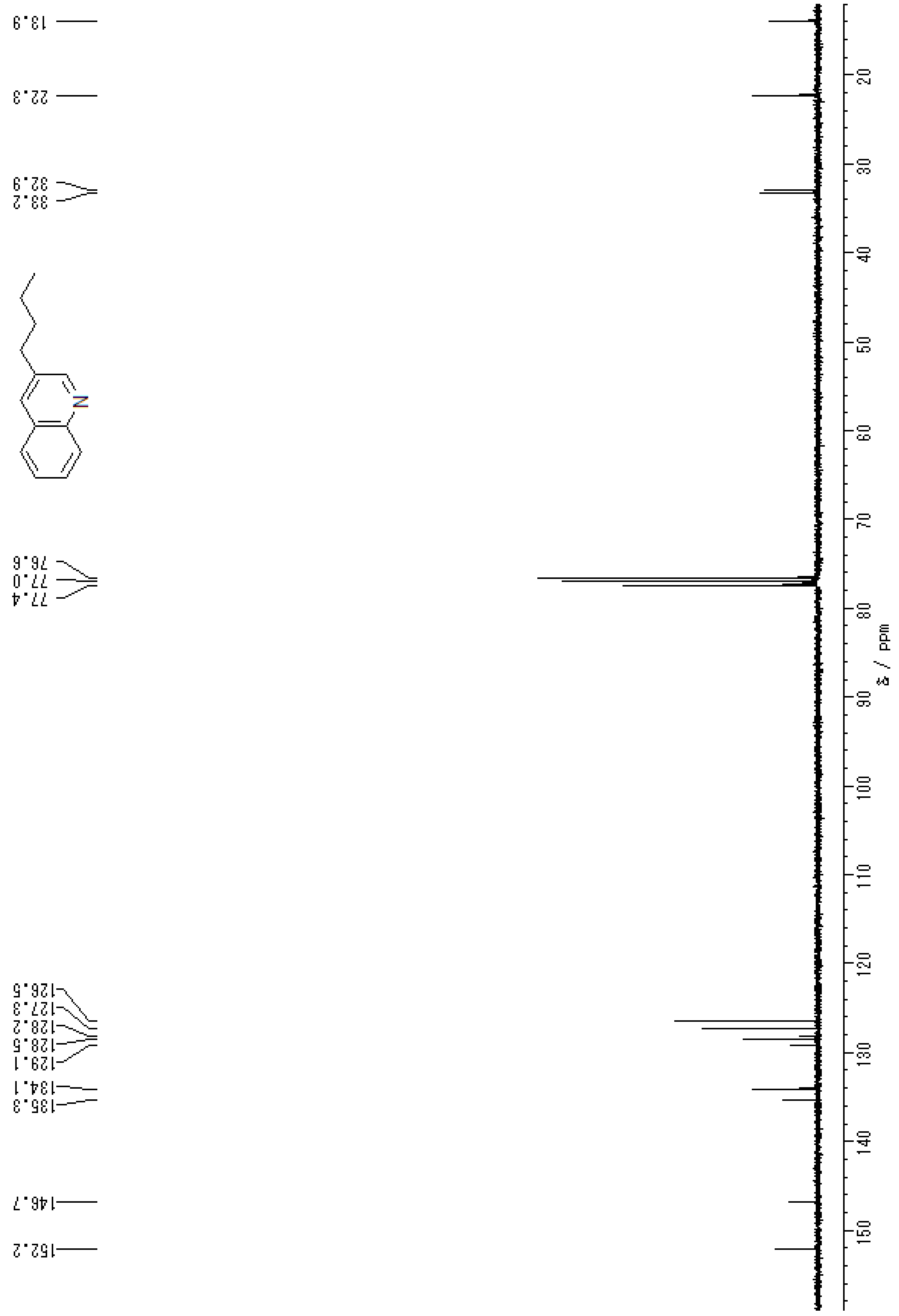
2
3
4
5
6
7
8
9
δ / ppm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126.5
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128.5
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134.1
135.8
146.7
152.2
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20
30
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50
60
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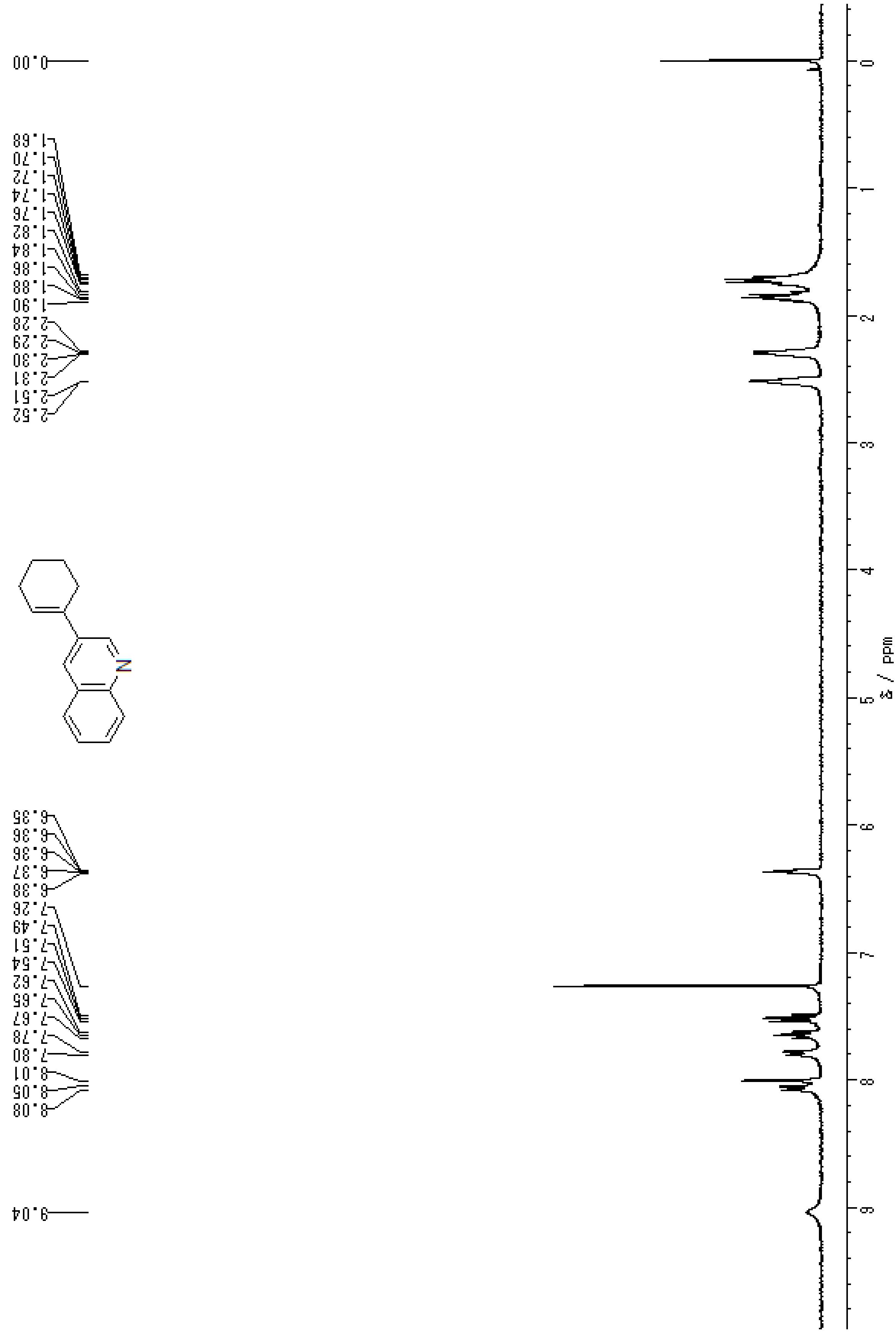
80
90
100
110
120
130
140
150
δ / ppm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1.84
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1.88
1.90
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2.29
2.30
2.31
2.51
2.52
6.35
6.36
6.36
6.37
6.38
7.26
7.49
7.51
7.54
7.62
7.65
7.67
7.78
7.80
8.01
8.05
8.08
9.04
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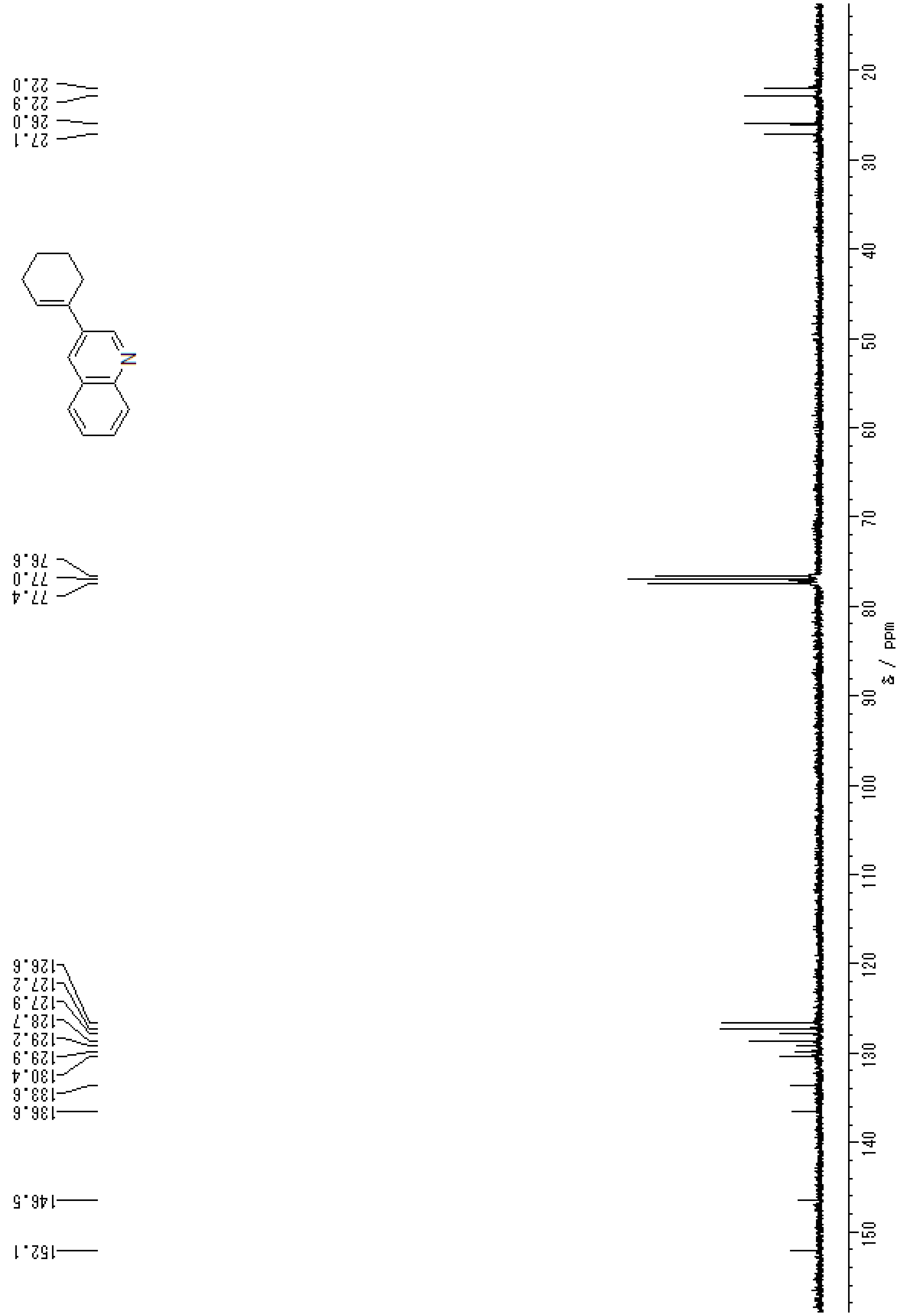
3
4
5
6
7
8
9
δ / ppm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77.0
77.4
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127.9
128.7
129.2
129.9
130.4
133.6
136.6
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152.1
N
20
30
40
50
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70
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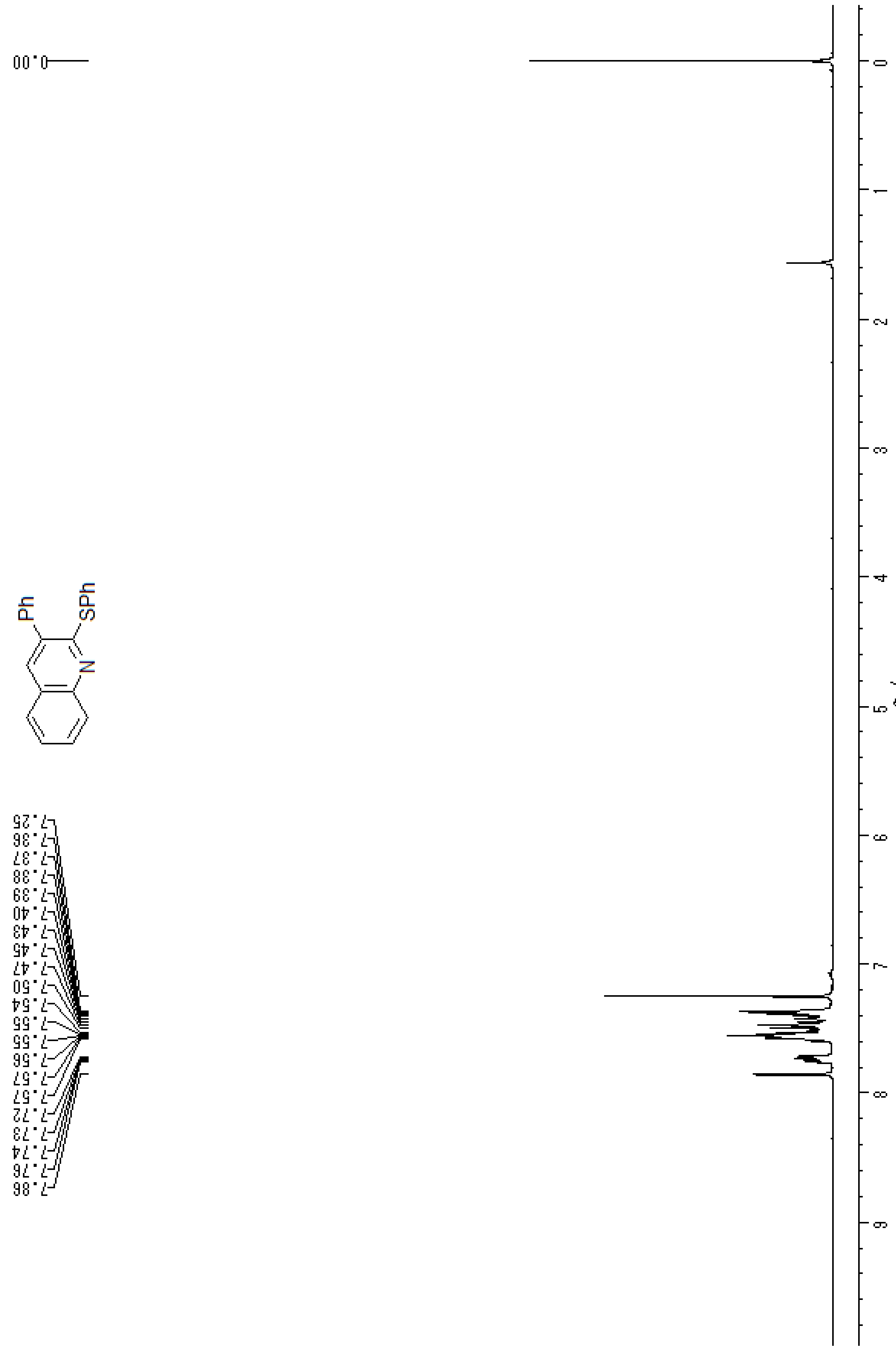
90
100
110
120
130
140
150
δ / ppm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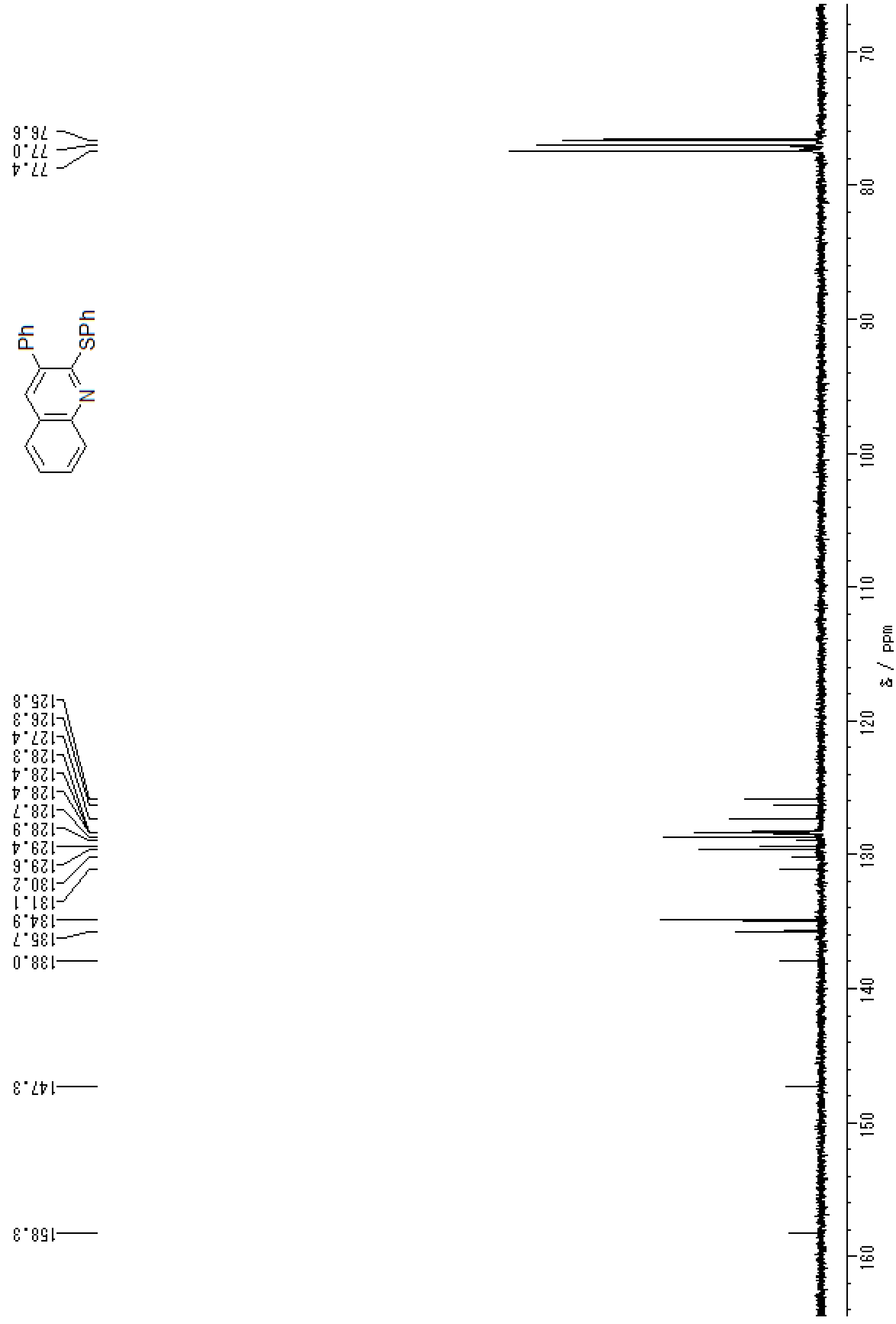
7.54
7.55
7.55
7.56
7.57
7.57
7.72
7.73
7.74
7.76
7.86
Ph
SPh
N
0
1
2
3
4
5
6
7
8
9
δ / ppm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77.4
Ph
SPh
N
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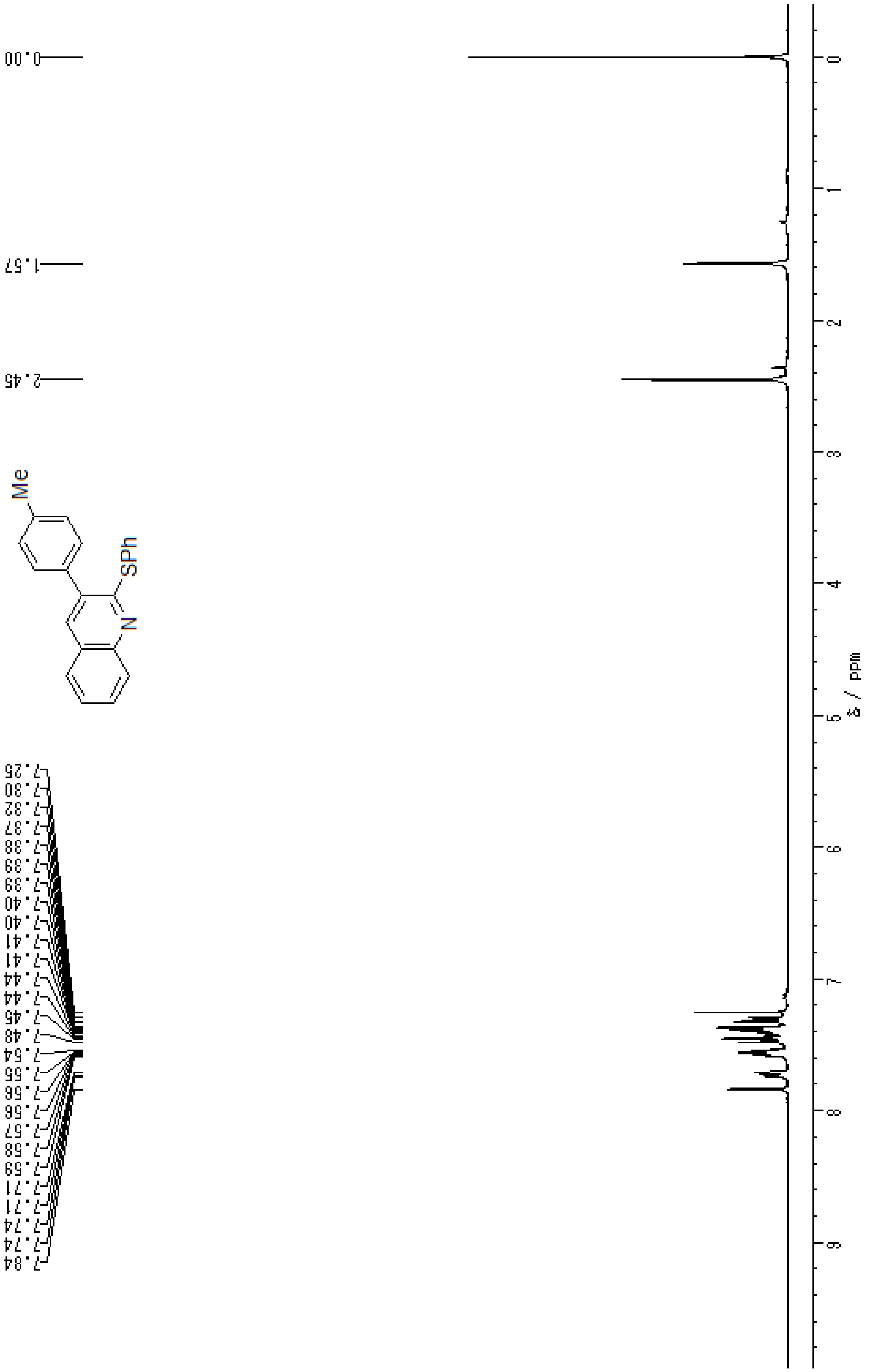
126.3
127.4
128.3
128.4
128.4
128.7
128.9
129.4
129.6
130.2
131.1
134.9
135.7
138.0
147.3
158.3
70
80
90
100
110
120
130
140
150
160
δ / ppm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7.32
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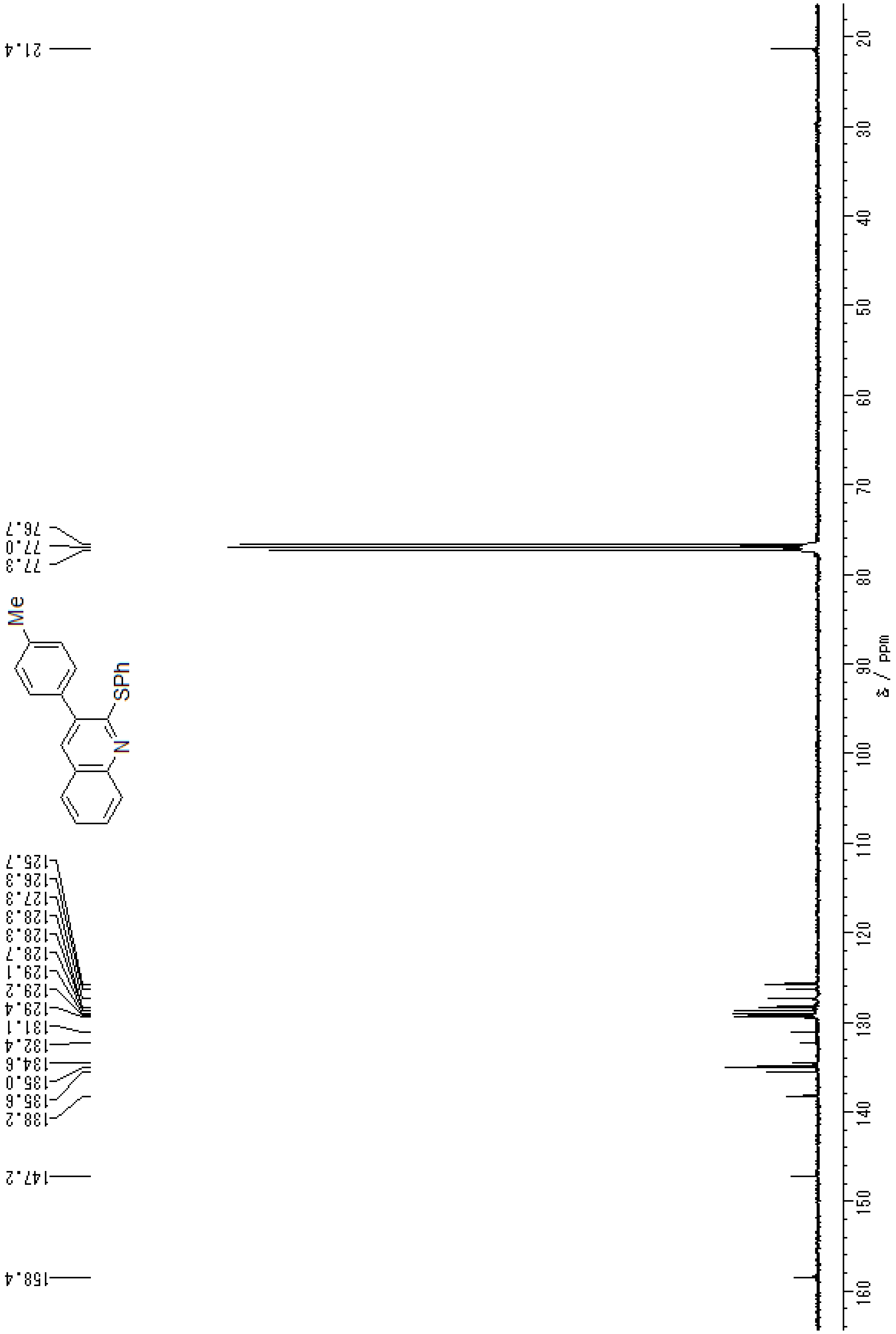
7.38
7.39
7.39
7.40
7.40
7.41
7.41
7.44
7.44
7.45
7.48
7.54
7.55
7.56
7.56
7.57
7.58
7.59
7.71
7.71
7.74
7.74
7.84
Me
SPh
N
0
1
2
3
4
5
6
7
8
9
δ / ppm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77.3
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SPh
N
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128.3
128.3
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129.1
129.2
129.4
131.1
132.4
134.6
135.0
135.6
138.2
147.2
158.4
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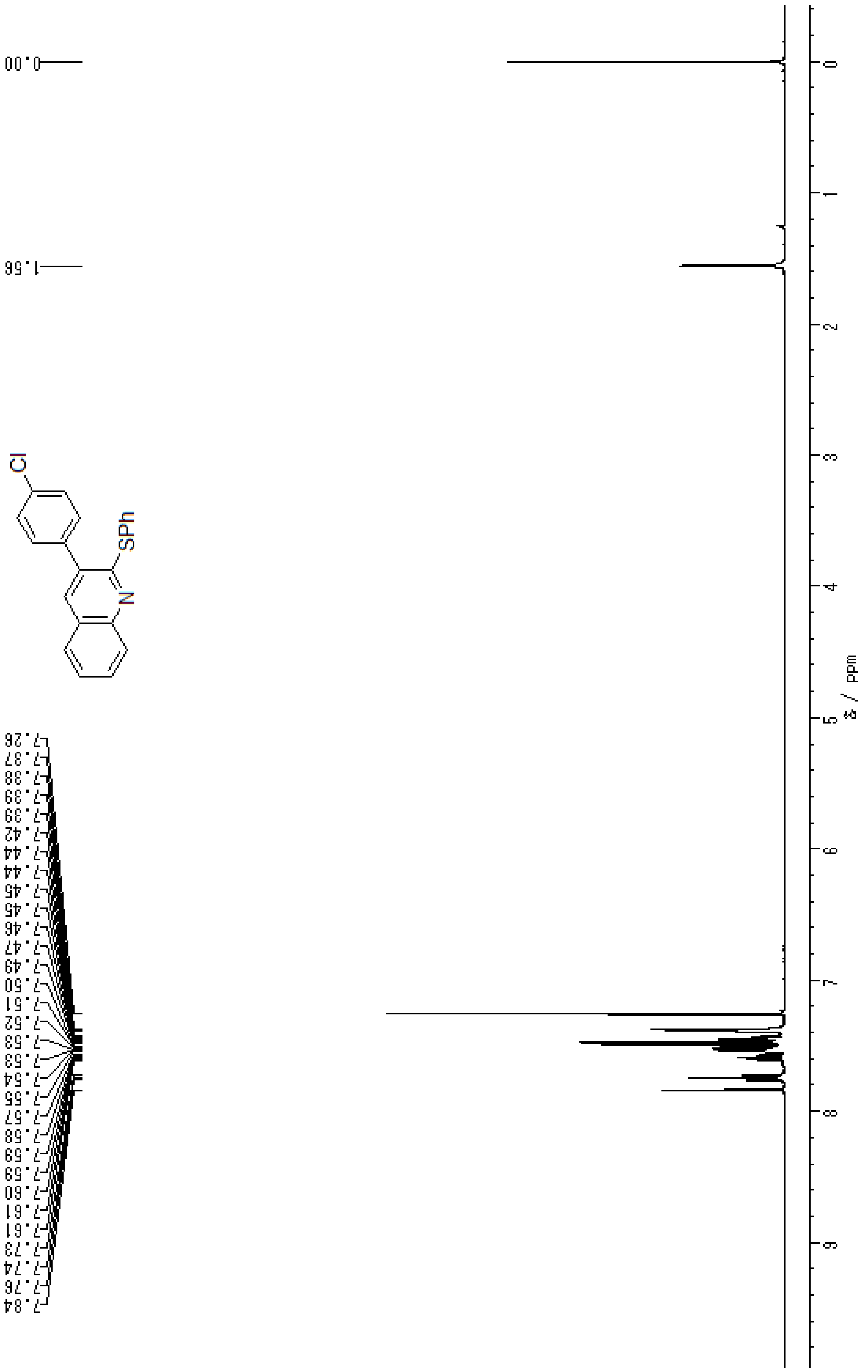
30
40
50
60
70
80
90
100
110
120
130
140
150
160
δ / ppm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1.56
Cl
SPh
N
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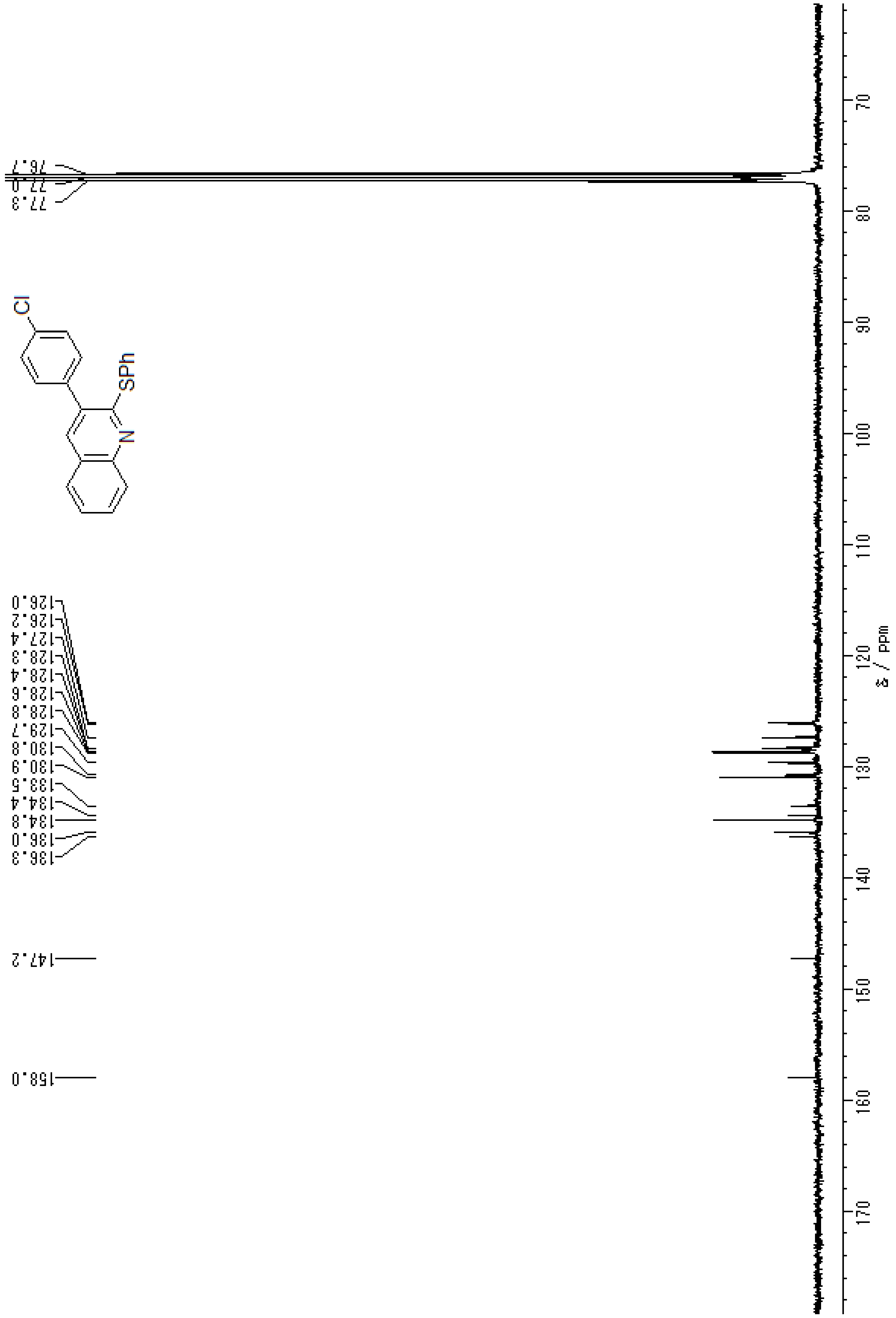
7.37
7.38
7.39
7.39
7.42
7.44
7.44
7.45
7.45
7.46
7.47
7.49
7.50
7.51
7.52
7.53
7.53
7.54
7.55
7.57
7.58
7.59
7.59
7.60
7.61
7.61
7.73
7.74
7.76
7.84
0
1
2
3
4
5
6
7
8
9
δ / ppm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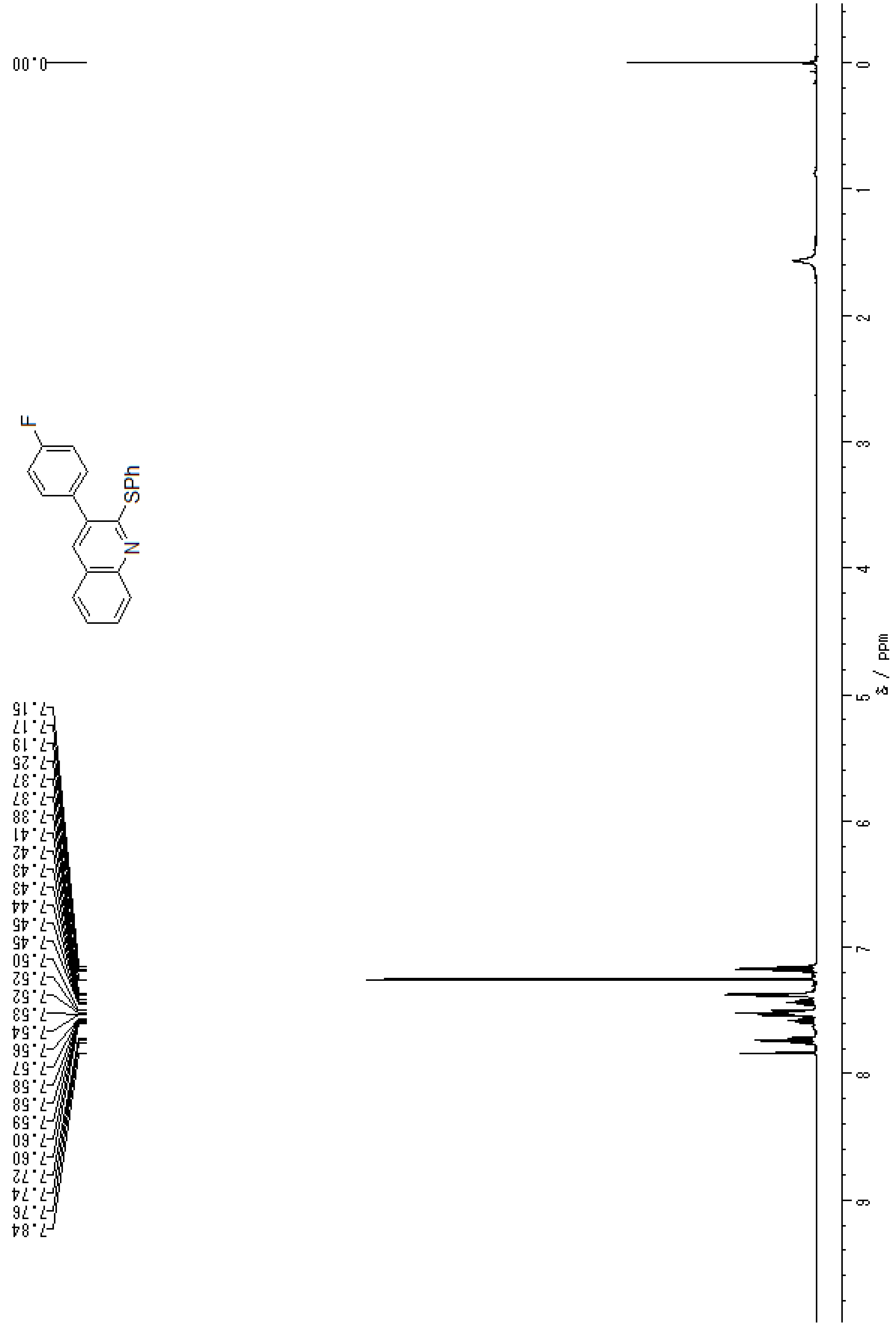
77.3
Cl
SPh
N
126.0
126.2
127.4
128.3
128.4
128.6
128.8
129.7
130.8
130.9
133.5
134.4
134.8
136.0
136.8
147.2
158.0
70
80
90
100
110
120
130
140
150
160
170
δ / ppm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F
SPh
N
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7.17
7.19
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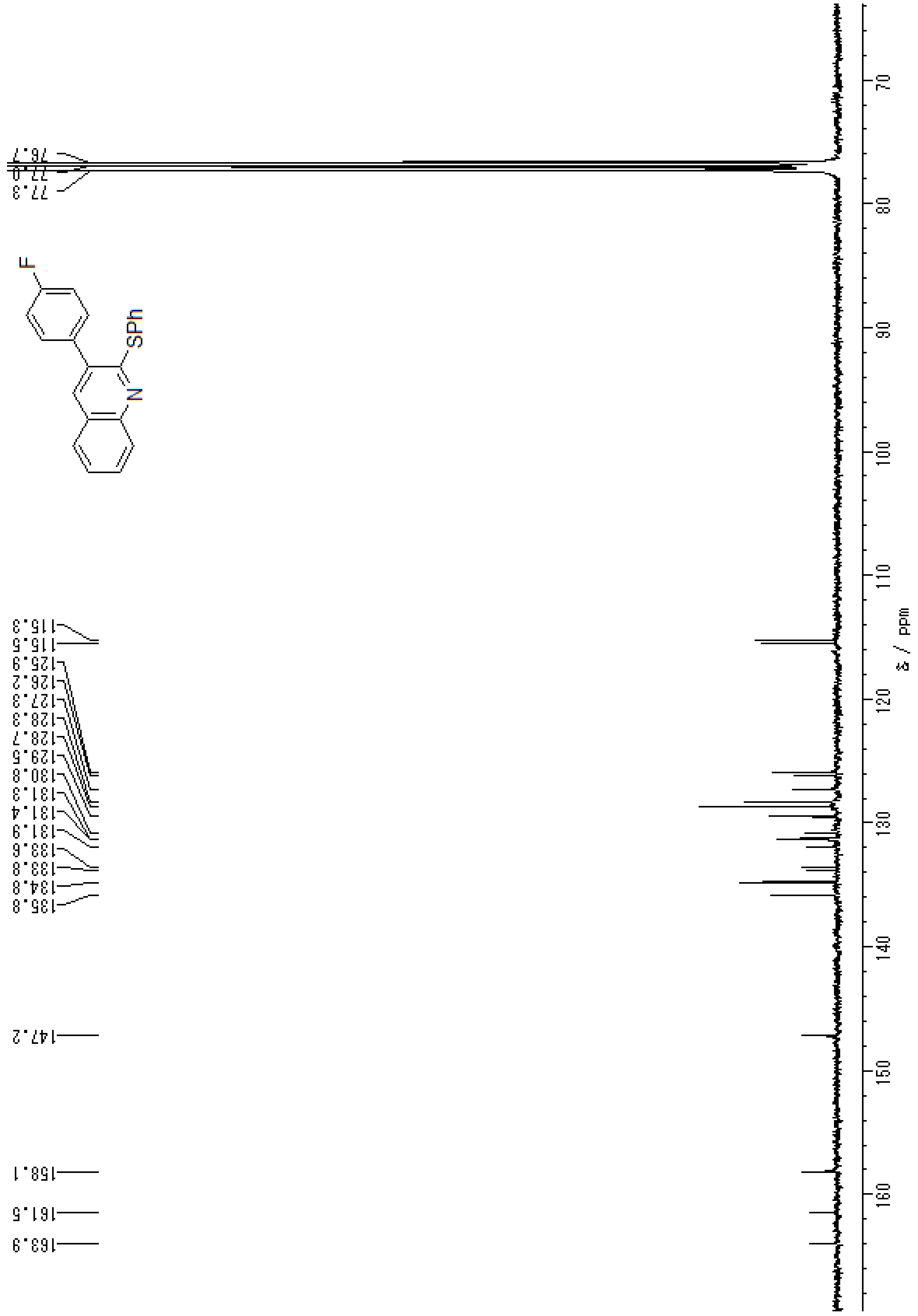
7.41
7.42
7.43
7.43
7.44
7.45
7.45
7.50
7.52
7.52
7.53
7.54
7.56
7.57
7.58
7.58
7.59
7.60
7.60
7.72
7.74
7.76
7.84
0
1
2
3
4
5
6
7
8
9
δ / ppm


76.7
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77.3
F
SPh
N
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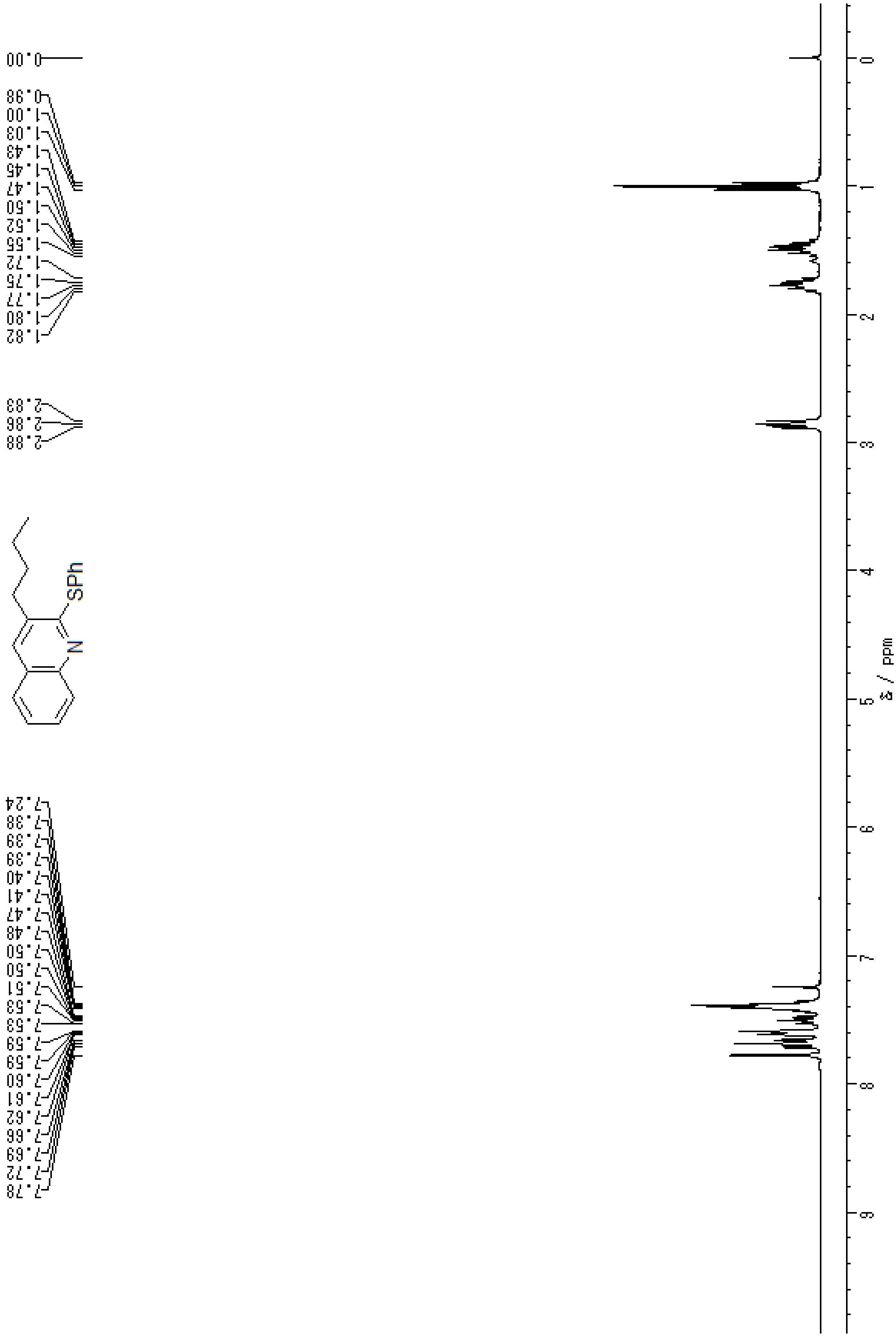
115.5
125.9
126.2
127.3
128.3
128.7
129.5
130.8
131.3
131.4
131.9
133.6
133.8
134.8
135.8
147.2
158.1
161.5
163.9
70
80
90
100
110
120
130
140
150
160
δ / ppm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1.03
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1.45
1.47
1.50
1.52
1.55
1.72
1.75
1.77
1.80
1.82
2.83
2.86
2.88
N
SPh
7.24
7.38
7.39
7.39
7.40
7.41
7.47
7.48
7.50
7.50
7.51
7.53
7.53
7.59
7.59
7.60
7.61
7.62
7.66
7.69
7.72
7.78
0
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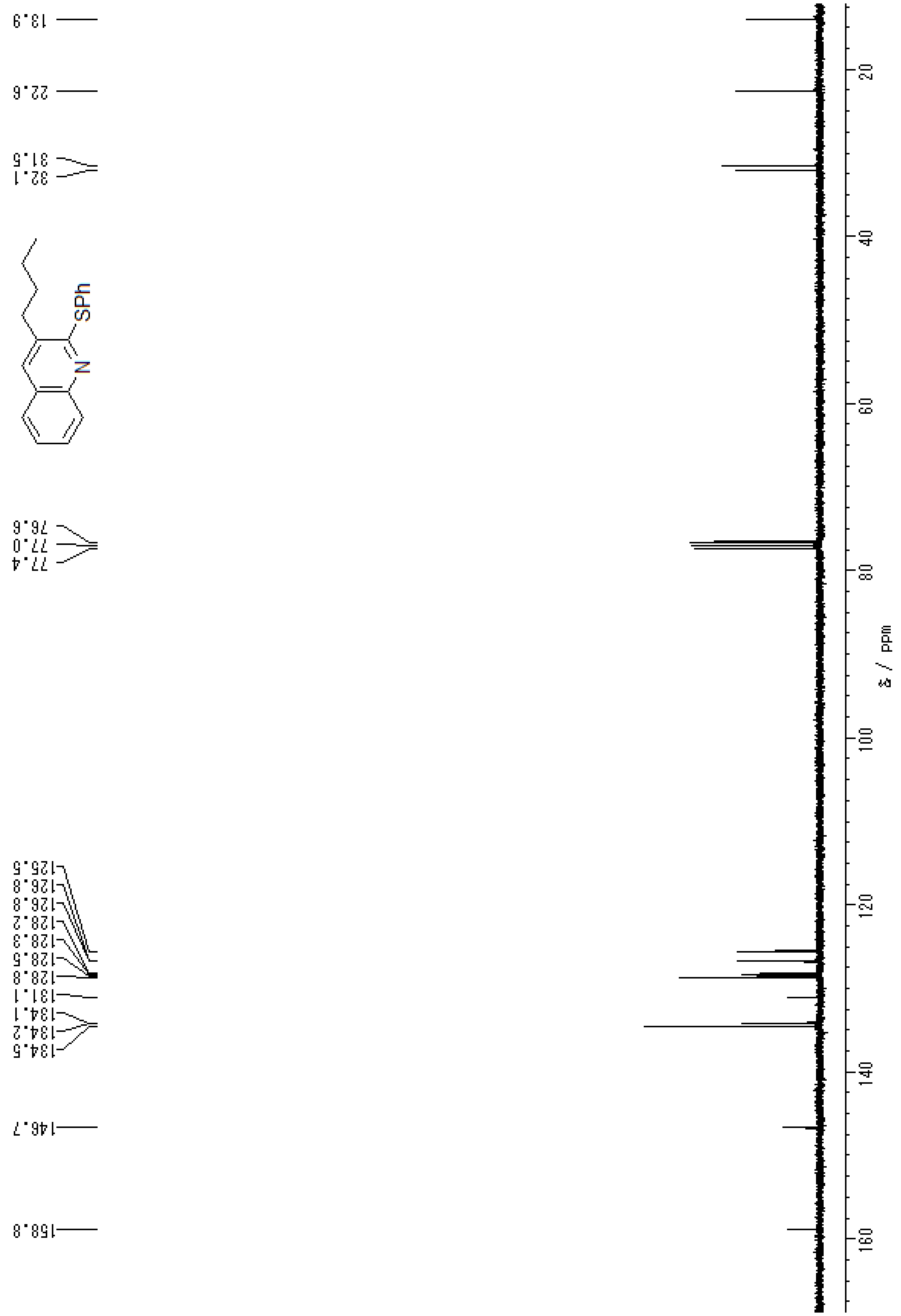
2
3
4
5
6
7
8
9
δ / ppm


13.9
22.6
31.5
32.1
N
SPh
76.6
77.0
77.4
125.5
126.8
126.8
128.2
128.3
128.5
128.8
131.1
134.1
134.2
134.5
146.7
158.8
20
40
60
80
100
120
140
160
δ / ppm