Electronic Supplementary Information
for
Synthesis of (1-silyl)allylboronates by KO*t*Bu-catalyzed ring-opening *gem*-silylborylation of cyclopropenes

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I. General

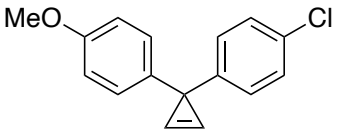
All reactions were carried out with standard Schlenk techniques under nitrogen unless otherwise noted. NMR spectra were recorded on JEOL JNM-ECS400, JEOL JNM-ECZL400S, or Agilent Unity-Inova500 spectrometer. High resolution mass spectra were recorded on JEOL JMS700 spectrometer. X-ray crystallographic analysis was performed by RIGAKU XTaLAB P200 with graphite-monochromated Mo-Kα (0.71075 Å) radiation. Preparative GPC was performed with JAI LaboACE LC-5060 equipped with JAIGEL-2HR columns using $CHCl_3$ as an eluent. Reversed-phase chromatography was performed with JAI LaboACE LC-5060 equipped with Mightysil RP-18GPII columns using MeCN as an eluent. Computations were performed using workstation at Research Center for Computational Science, National Institutes of Natural Sciences, Okazaki, Japan.

THF (Kanto Chemical; dehydrated), Et_2O (Wako Chemicals; dehydrated), CH_2Cl_2 (Kanto Chemical; dehydrated), toluene (Wako Chemicals), DMSO (Kanto Chemical; dehydrated), H_2O (Kishida Chemical), 4-bromoanisole (Wako Chemicals), 4-chloroacetophenone (TCI), $CHBr_3$ (Wako Chemicals), benzyltriethylammonium chloride (Wako Chemicals), (dimethylphenylsilyl)boronic acid pinacol ester (Wako Chemicals), 4-toluenesulfonic acid monohydrate (Wako Chemicals), TfOH (TCI), *n*BuLi (Kanto Chemical; 1.58 M solution in hexane), EtMgBr (Aldrich; 3.0 M solution in Et_2O), KO*t*Bu (TCI or Nacalai Tesque), NaO*t*Bu (TCI), LiO*t*Bu (Aldrich), Ti(O*i*Pr)$_4$ (Wako Chemicals), NaOH (Wako Chemicals), and $NaBO_3$•$4H_2O$ (Wako Chemicals) were used as received. **1a**,[1] **1b**,[1] **1d**,[2] **1e**,[1] **1i**,[3] **1j**,[3] **1k**,[3] **1l**,[4] **2b**,[5] **2c**,[5] and Cu(O*t*Bu)(IPr)[6] were synthesized following the literature procedures.

II. Synthesis of Substrates

Representative Procedures for Substrates:

3-(4-Chlorophenyl)-3-(4-methoxyphenyl)cyclopropene (1h)



*n*BuLi (7.80 mL, 12.5 mmol; 1.58 M solution in hexane) was added over 12 min to a solution of 4-bromoanisole (1.56 mL, 12.5 mmol) in THF (30 mL) at –78 °C, and the mixture was stirred for 30 min at –78 °C. 4-Chloroacetophenone (1.95 mL, 15.0 mmol) was then added to it, and the resulting mixture was stirred for 2 h at –78 °C and gradually warmed to room temperature over 1.5 h. The reaction was quenched with H_2O and this was extracted with CH_2Cl_2. The organic layer was washed with saturated NaClaq, dried over $MgSO_4$, filtered, and concentrated under vacuum. The residue was dissolved in toluene (30 mL) and 4-toluenesulfonic acid monohydrate (123 mg, 0.646 mmol) was added to it. The mixture was stirred for 2.5 h at 70 °C, and the reaction was quenched with H_2O and saturated NH_4Claq at room temperature. This was extracted with CH_2Cl_2, and the organic layer was washed with saturated NaClaq, dried over K_2CO_3, filtered and concentrated under vacuum. The residue was chromatographed on silica gel with hexane/CH_2Cl_2 = 1/1 to afford 1-(4-chlorophenyl)-1-(4-methoxyphenyl)ethylene as a white solid (2.62 g, 10.7 mmol; 86 % yield).

^{1}H NMR ($CDCl_3$): δ 7.33-7.26 (m, 4H), 7.24 (d, $^3J_{HH}$ = 8.7 Hz, 2H), 6.87 (d, $^3J_{HH}$ = 8.7 Hz, 2H), 5.40 (d, $^2J_{HH}$ = 0.9 Hz, 1H), 5.34 (d, $^2J_{HH}$ = 0.9 Hz, 1H), 3.83 (s, 3H).

A solution of NaOH (17.1 g, 428 mmol) in H_2O (17 mL) was added dropwise over 1 h to a solution of 1-(4-chlorophenyl)-1-(4-methoxyphenyl)ethylene (2.62 g, 10.7 mmol), benzyltriethylammonium chloride (424 mg, 1.86 mmol), and $CHBr_3$ (1.42 mL, 14.6 mmol) in CH_2Cl_2 (10 mL). The mixture was stirred for 21 h at 40 °C, and the reaction was quenched with H_2O and saturated NH_4Claq at room temperature. This was extracted with CH_2Cl_2, and the organic layer was washed with saturated NaClaq, dried over $MgSO_4$, passed through a pad of silica gel with EtOAc, and concentrated under vacuum. The residue was further passed through a pad of silica gel with CH_2Cl_2 and then with EtOAc to afford 1,1-dibromo-2-(4-chlorophenyl)-2-(4-methoxyphenyl)cyclopropane as a brown solid (4.10 g, 9.85 mmol; 92% yield).

^{1}H NMR ($CDCl_3$): δ 7.41 (d, $^3J_{HH}$ = 8.2 Hz, 2H), 7.38 (d, $^3J_{HH}$ = 9.2 Hz, 2H), 7.28 (d, $^3J_{HH}$ = 8.7 Hz, 2H), 6.84 (d, $^3J_{HH}$ = 8.7 Hz, 2H), 3.77 (s, 3H), 2.44 (d, $^2J_{HH}$ = 7.3 Hz, 1H), 2.40 (d, $^2J_{HH}$ = 7.8 Hz, 1H).

$Ti(O\textit{i}Pr)_4$ (146 μL, 0.493 mmol) was added to a solution of 1,1-dibromo-2-(4-chlorophenyl)-2-(4-methoxyphenyl)cyclopropane (4.10 g, 9.85 mmol) in THF (15 mL) and Et_2O (22 mL) at room temperature. EtMgBr (3.93 mL, 11.8 mmol; 3.0 M solution in Et_2O) was added dropwise to it over 2 h and the mixture was stirred for 2 h at room temperature. The reaction was slowly quenched with H_2O and 1 M HClaq at 0 °C. This was extracted with Et_2O, and the organic layer was washed with saturated

NaClaq, dried over $MgSO_4$, filtered, and concentrated under vacuum. The residue was chromatographed on silica gel with hexane/CH_2Cl_2 = 3/1 to afford 1-bromo-2-(4-chlorophenyl)-2-(4-methoxyphenyl)cyclopropane as a colorless oil (2.58 g, 7.63 mmol; 77 % yield, dr = 56/44).

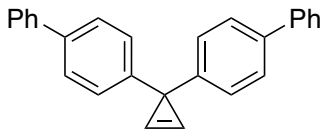
^{1}H NMR ($CDCl_3$): δ 7.35-7.29 (m, 2.24H), 7.28 (d, $^3J_{HH}$ = 8.7 Hz, 0.88H), 7.22 (d, $^3J_{HH}$ = 8.7 Hz, 0.88H), 7.17-7.10 (m, 2H), 6.89 (d, $^3J_{HH}$ = 8.7 Hz, 0.88H), 6.80 (d, $^3J_{HH}$ = 8.7 Hz, 1.12H), 3.81 (s, 1.32H), 3.76 (s, 1.68H), 3.67-3.58 (m, 1H), 1.88-1.70 (m, 2H).

KO*t*Bu (1.11 g, 9.92 mmol) was added portionwise to a solution of 1-bromo-2-(4-chlorophenyl)-2-(4-methoxyphenyl)cyclopropane (2.58 g, 7.63 mmol) in DMSO (18 mL) at room temperature. The mixture was stirred for 2 h at room temperature and the reaction was slowly quenched with H_2O at 15 °C. This was extracted with Et_2O/hexane, and the organic layer was washed with saturated NaClaq, dried over $MgSO_4$, filtered, and concentrated under vacuum. The residue was chromatographed on silica gel with hexane/CH_2Cl_2 = 2/1 to afford compound **1h** as a pale yellow solid (1.66 g, 6.47 mmol; 85% yield).

^{1}H NMR ($CDCl_3$): δ 7.47 (s, 2H), 7.23 (d, $^3J_{HH}$ = 8.2 Hz, 2H), 7.09 (d, $^3J_{HH}$ = 8.7 Hz, 2H), 7.07 (d, $^3J_{HH}$ = 8.7 Hz, 2H), 6.83 (d, $^3J_{HH}$ = 8.7 Hz, 2H), 3.80 (s, 3H). ^{13}C{^{1}H} NMR ($CDCl_3$): δ 158.0, 146.2, 138.7, 131.4, 129.5, 129.1, 128.2, 113.7, 113.6, 55.4, 30.9. HRMS (FAB) calcd for $C_{16}H_{13}ClO$ (M^+) 256.0649, found 256.0657.

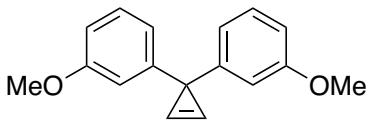
Analytical Data for Other substrate:

3,3-Di(4-phenylphenyl)cyclopropene (1c)



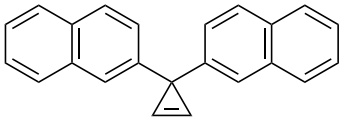
^{1}H NMR ($CDCl_3$): δ 7.63-7.57 (m, 4H), 7.56 (s, 2H), 7.54 (d, $^3J_{HH}$ = 8.2 Hz, 4H), 7.43 (t, $^3J_{HH}$ = 7.5 Hz, 4H), 7.36-7.30 (m, 2H), 7.30 (d, $^3J_{HH}$ = 8.7 Hz, 4H). ^{13}C{^{1}H} NMR ($CDCl_3$): δ 146.2, 141.1, 138.8, 128.8, 128.6, 127.2, 127.1, 127.0, 113.3, 31.5. HRMS (FAB) calcd for $C_{27}H_{20}$ (M^+) 344.1560, found 344.1562.

3,3-Di(3-methoxyphenyl)cyclopropene (1f)



^{1}H NMR ($CDCl_3$): δ 7.45 (s, 2H), 7.25-7.15 (m, 2H), 6.83-6.68 (m, 6H), 3.77 (s, 6H). ^{13}C{^{1}H} NMR ($CDCl_3$): δ 159.6, 148.8, 129.2, 120.7, 114.0, 113.0, 111.2, 55.2, 31.9. HRMS (FAB) calcd for $C_{17}H_{16}O_2$ (M^+) 252.1145, found 252.1144.

3,3-Di(2-naphthyl)cyclopropene (1g)

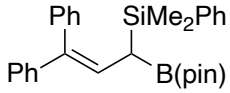


^{1}H NMR ($CDCl_3$): δ 7.87-7.81 (m, 2H), 7.79 (d, $^{3}J_{HH}$ = 8.7 Hz, 2H), 7.78-7.72 (m, 2H), 7.68 (s, 2H), 7.66 (s, 2H), 7.49-7.41 (m, 4H), 7.39 (dd, $^{3}J_{HH}$ = 8.7 Hz and $^{4}J_{HH}$ = 1.8 Hz, 2H). $^{13}C\{^{1}H\}$ NMR ($CDCl_3$): δ 144.7, 133.6, 132.1, 127.8, 127.7, 126.81, 126.79, 126.1, 125.5, 113.8, 32.4. HRMS (FAB) calcd for $C_{23}H_{16}$ (M^+) 292.1247, found 292.1247.

III. Catalytic Reactions and Derivatization

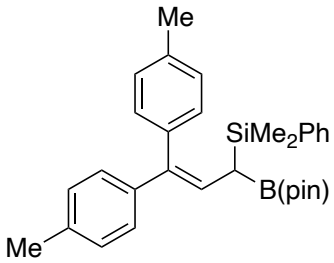
General Procedure for Table 2.

KO*t*Bu (3.4 mg, 30 μmol) was dissolved in THF (0.5 mL) at 40 °C. Silylboronate **2a** (98.1 μL, 0.360 mmol), cyclopropene **1** (0.300 mmol), and THF (1.0 mL) were added to it, and the resulting mixture was stirred for 20 h at 40 °C. This was passed through a pad of silica gel with EtOAc, and the solvent was removed under vacuum. The residue was chromatographed on silica gel and further purified by GPC with $CHCl_3$ to afford compound **3** (or **5**).



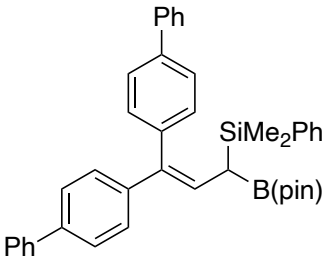
Compound 3aa. Hexane/EtOAc = 10/1 was used for silica gel chromatography. Pale yellow oil (92.3 mg, 0.216 mmol; 72% yield).

^{1}H NMR ($CDCl_3$): δ 7.46-7.40 (m, 2H), 7.35-7.07 (m, 11H), 6.93-6.87 (m, 2H), 6.22 (d, $^3J_{HH}$ = 12.4 Hz, 1H), 2.10 (d, $^3J_{HH}$ = 12.4 Hz, 1H), 1.20 (s, 6H), 1.17 (s, 6H), 0.34 (s, 3H), 0.32 (s, 3H). ^{13}C{^{1}H} NMR ($CDCl_3$): δ 143.7, 140.4, 138.5, 138.0, 134.1, 130.4, 129.1, 128.3, 128.0, 127.7, 127.2, 127.1, 126.5, 126.2, 83.1, 25.1, 24.9, 20.8, −2.5, −2.8. HRMS (FAB) calcd for $C_{29}H_{35}BO_2Si$ (M^+) 454.2494, found 454.2498.



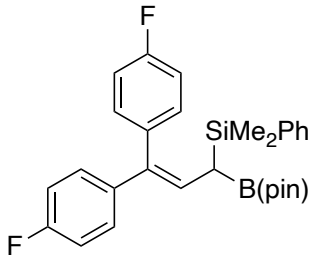
Compound 3ba. Hexane/EtOAc = 30/1 was used for silica gel chromatography. White solid (84.8 mg, 0.175 mmol; 58% yield).

^{1}H NMR ($CDCl_3$): δ 7.46-7.41 (m, 2H), 7.34-7.26 (m, 3H), 7.07 (d, $^3J_{HH}$ = 7.3 Hz, 2H), 7.00 (s, 4H), 6.80 (d, $^3J_{HH}$ = 7.8 Hz, 2H), 6.15 (d, $^3J_{HH}$ = 12.4 Hz, 1H), 2.35 (s, 3H), 2.29 (s, 3H), 2.08 (d, $^3J_{HH}$ = 12.8 Hz, 1H), 1.18 (s, 6H), 1.15 (s, 6H), 0.33 (s, 3H), 0.31 (s, 3H). ^{13}C{^{1}H} NMR ($CDCl_3$): δ 141.0, 138.3, 138.2, 137.6, 135.8, 135.7, 134.1, 130.2, 129.01, 128.98, 128.7, 127.6, 127.0, 126.0, 83.1, 25.0, 24.9, 21.4, 21.2, 20.5, −2.5, −2.7. HRMS (FAB) calcd for $C_{31}H_{39}BO_2Si$ (M^+) 482.2807, found 482.2819.



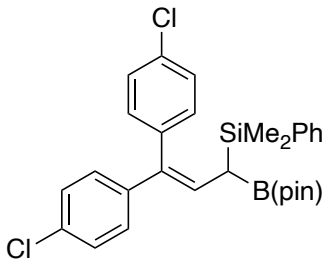
Compound 3ca. Hexane/CH_2Cl_2 = 3/1 was used for silica gel chromatography. Yellow oil (109 mg, 0.179 mmol; 60% yield).

^{1}H NMR ($CDCl_3$): δ 7.67-7.62 (m, 2H), 7.59-7.54 (m, 2H), 7.52 (d, $^3J_{HH}$ = 8.2 Hz, 2H), 7.49-7.38 (m, 8H), 7.38-7.26 (m, 5H), 7.21 (d, $^3J_{HH}$ = 8.2 Hz, 2H), 6.99 (d, $^3J_{HH}$ = 8.2 Hz, 2H), 6.33 (d, $^3J_{HH}$ = 12.8 Hz, 1H), 2.20 (d, $^3J_{HH}$ = 12.4 Hz, 1H), 1.22 (s, 6H), 1.19 (s, 6H), 0.39 (s, 3H), 0.35 (s, 3H). ^{13}C{^{1}H} NMR ($CDCl_3$): δ 142.6, 141.2, 141.1, 139.4, 139.2, 139.1, 138.0, 137.7, 134.1, 130.8, 129.1, 128.9, 128.8, 127.7, 127.5, 127.2, 127.1, 127.0, 126.8, 83.2, 25.1, 25.0, 21.1, −2.4, −2.8. HRMS (FAB) calcd for $C_{41}H_{43}BO_2Si$ (M^+) 606.3120, found 606.3130.



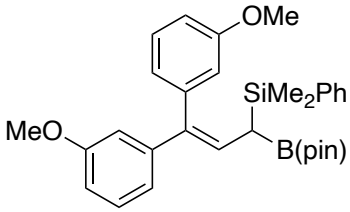
Compound 3da. Hexane/EtOAc = 30/1 was used for silica gel chromatography. White solid (104 mg, 0.213 mmol; 71% yield).

^{1}H NMR ($CDCl_3$): δ 7.44-7.37 (m, 2H), 7.36-7.26 (m, 3H), 7.00 (dd, $^3J_{HH}$ = 8.7 Hz and $^4J_{HF}$ = 5.5 Hz, 2H), 6.94 (t, ^3J = 8.7 Hz, 2H), 6.88 (t, ^3J = 8.7 Hz, 2H), 6.77 (dd, $^3J_{HH}$ = 8.7 Hz and $^4J_{HF}$ = 5.5 Hz, 2H), 6.13 (d, $^3J_{HH}$ = 12.4 Hz, 1H), 2.02 (d, $^3J_{HH}$ = 12.8 Hz, 1H), 1.21 (s, 6H), 1.19 (s, 6H), 0.36 (s, 3H), 0.32 (s, 3H). ^{13}C{^{1}H} NMR ($CDCl_3$): δ 161.8 (d, $^1J_{CF}$ = 245 Hz), 161.7 (d, $^1J_{CF}$ = 245 Hz), 139.7, 137.9, 136.5, 136.1, 134.1, 131.8 (d, $^3J_{CF}$ = 7.7 Hz), 129.2, 128.5 (d, $^3J_{CF}$ = 7.7 Hz), 127.7, 127.4, 115.3 (d, $^2J_{CF}$ = 21.1 Hz), 114.9 (d, $^2J_{CF}$ = 22.0 Hz), 83.3, 25.1, 25.0, 20.9, −2.4, −2.9. HRMS (FAB) calcd for $C_{29}H_{33}BF_2O_2Si$ (M^+) 490.2305, found 490.2322.



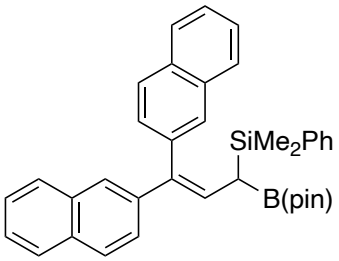
Compound 3ea. Hexane/EtOAc = 30/1 was used for silica gel chromatography. Yellow solid (70.5 mg, 0.135 mmol; 45% yield).

^{1}H NMR ($CDCl_3$): δ 7.43-7.36 (m, 2H), 7.36-7.26 (m, 3H), 7.22 (d, $^{3}J_{HH}$ = 8.7 Hz, 2H), 7.15 (d, $^{3}J_{HH}$ = 8.2 Hz, 2H), 6.96 (d, $^{3}J_{HH}$ = 8.7 Hz, 2H), 6.72 (d, $^{3}J_{HH}$ = 8.2 Hz, 2H), 6.20 (d, $^{3}J_{HH}$ = 12.8 Hz, 1H), 2.02 (d, $^{3}J_{HH}$ = 12.8 Hz, 1H), 1.21 (s, 6H), 1.19 (s, 6H), 0.37 (s, 3H), 0.32 (s, 3H). ^{13}C{^{1}H} NMR ($CDCl_3$): δ 141.6, 138.4, 137.7, 136.3, 134.0, 132.5, 132.2, 131.6, 129.2, 128.6, 128.5, 128.3, 128.2, 127.7, 83.3, 25.1, 25.0, 21.3, −2.4, −3.0. HRMS (FAB) calcd for $C_{29}H_{33}BCl_2O_2Si$ (M^+) 522.1714, found 522.1721.



Compound 3fa. Hexane/EtOAc = 10/1 was used for silica gel chromatography. Colorless oil (100 mg, 0.195 mmol; 65% yield).

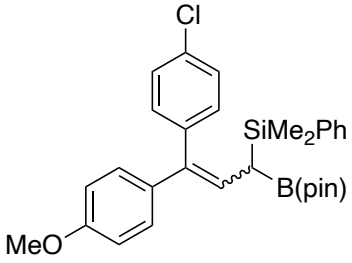
^{1}H NMR ($CDCl_3$): δ 7.49-7.42 (m, 2H), 7.36-7.26 (m, 3H), 7.19 (t, $^{3}J_{HH}$ = 7.8 Hz, 1H), 7.12 (t, $^{3}J_{HH}$ = 7.8 Hz, 1H), 6.78 (ddd, $^{3}J_{HH}$ = 8.2 Hz and $^{4}J_{HH}$ = 2.3 and 0.9 Hz, 1H), 6.75-6.68 (m, 2H), 6.66 (dd, $^{4}J_{HH}$ = 2.3 and 1.8 Hz, 1H), 6.52 (dd, $^{3}J_{HH}$ = 7.8 Hz and $^{4}J_{HH}$ = 1.4 Hz, 1H), 6.50 (dd, $^{4}J_{HH}$ = 2.8 and 1.4 Hz, 1H), 6.23 (d, $^{3}J_{HH}$ = 12.4 Hz, 1H), 3.74 (s, 3H), 3.73 (s, 3H), 2.11 (d, $^{3}J_{HH}$ = 12.4 Hz, 1H), 1.20 (s, 6H), 1.17 (s, 6H), 0.37 (s, 3H), 0.33 (s, 3H). ^{13}C{^{1}H} NMR ($CDCl_3$): δ 159.5, 159.4, 145.0, 141.7, 138.2, 138.1, 134.1, 129.3, 129.1, 128.9, 127.6, 122.9, 119.8, 115.5, 113.1, 112.6, 111.4, 83.1, 55.3, 55.2, 25.0, 20.9, −2.4, −2.7. HRMS (FAB) calcd for $C_{31}H_{39}BO_4Si$ (M^+) 514.2705, found 514.2711.



Compound 3ga. The reaction was conducted on a 2.00 mmol scale. Hexane/EtOAc = 30/1 was used

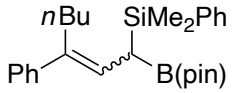
for silica gel chromatography. The solid thus obtained was washed with hexane and no GPC purification was performed. Pale yellow solid (758 mg, 1.37 mmol; 68% yield). The structure was confirmed by X-ray crystallographic analysis after recrystallization from CH_2Cl_2/MeOH.

^{1}H NMR ($CDCl_3$): δ 7.88-7.82 (m, 1H), 7.77 (d, $^3J_{HH}$ = 8.3 Hz, 1H), 7.77-7.69 (m, 2H), 7.68 (d, $^3J_{HH}$ = 8.3 Hz, 1H), 7.66-7.60 (m, 1H), 7.52-7.43 (m, 4H), 7.42-7.33 (m, 6H), 7.32-7.27 (m, 2H), 7.07 (dd, $^3J_{HH}$ = 8.3 Hz and $^4J_{HH}$ = 1.5 Hz, 1H), 6.45 (d, $^3J_{HH}$ = 12.2 Hz, 1H), 2.20 (d, $^3J_{HH}$ = 12.7 Hz, 1H), 1.24 (s, 6H), 1.21 (s, 6H), 0.41 (s, 3H), 0.34 (s, 3H). ^{13}C{^{1}H} NMR ($CDCl_3$): δ 141.0, 138.4, 138.1, 138.0, 134.2, 133.63, 133.56, 132.5, 132.4, 129.2, 129.0, 128.5, 128.2, 128.1, 127.9, 127.8, 127.7, 127.6, 127.5, 126.0, 125.9, 125.8, 125.7, 125.4, 83.2, 25.1, 25.0, 21.2, –2.4, –2.8. HRMS (FAB) calcd for $C_{37}H_{39}BO_2Si$ (M^+) 554.2807, found 554.2810.



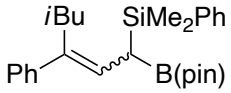
Compound 3ha. Hexane/EtOAc = 20/1 → 10/1 was used for silica gel chromatography. Yellow oil (86.5 mg, 0.167 mmol; 56% yield, dr = 52/48).

^{1}H NMR ($CDCl_3$): δ 7.47-7.38 (m, 2H), 7.36-7.26 (m, 3H), 7.21 (d, $^3J_{HH}$ = 8.7 Hz, 0.96H), 7.14 (d, $^3J_{HH}$ = 8.2 Hz, 1.04H), 7.03-6.94 (m, 2H), 6.85-6.71 (m, 4H), 6.14 (d, $^3J_{HH}$ = 12.4 Hz, 0.52H), 6.12 (d, $^3J_{HH}$ = 12.4 Hz, 0.48H), 3.82 (s, 1.56H), 3.77 (s, 1.44H), 2.11 (d, $^3J_{HH}$ = 12.4 Hz, 0.52H), 2.00 (d, $^3J_{HH}$ = 12.4 Hz, 0.48H), 1.20 (s, 6.24H), 1.18 (s, 5.76H), 0.36 (s, 1.44H), 0.35 (s, 1.56H), 0.32 (s, 1.44H), 0.31 (s, 1.56H). ^{13}C{^{1}H} NMR ($CDCl_3$): δ 158.4, 158.3, 142.4, 139.2, 138.0, 137.1, 136.8, 136.1, 134.1, 132.3, 132.2, 131.8, 131.7, 131.4, 129.1, 128.5, 128.4, 128.1, 128.0, 127.7, 127.6, 126.0, 113.8, 113.5, 83.2, 55.4, 55.3, 25.1, 25.0, 20.9, 20.6, −2.4, −2.5, −2.8, −3.0. HRMS (FAB) calcd for $C_{30}H_{36}BClO_3Si$ (M^+) 518.2210, found 518.2213.



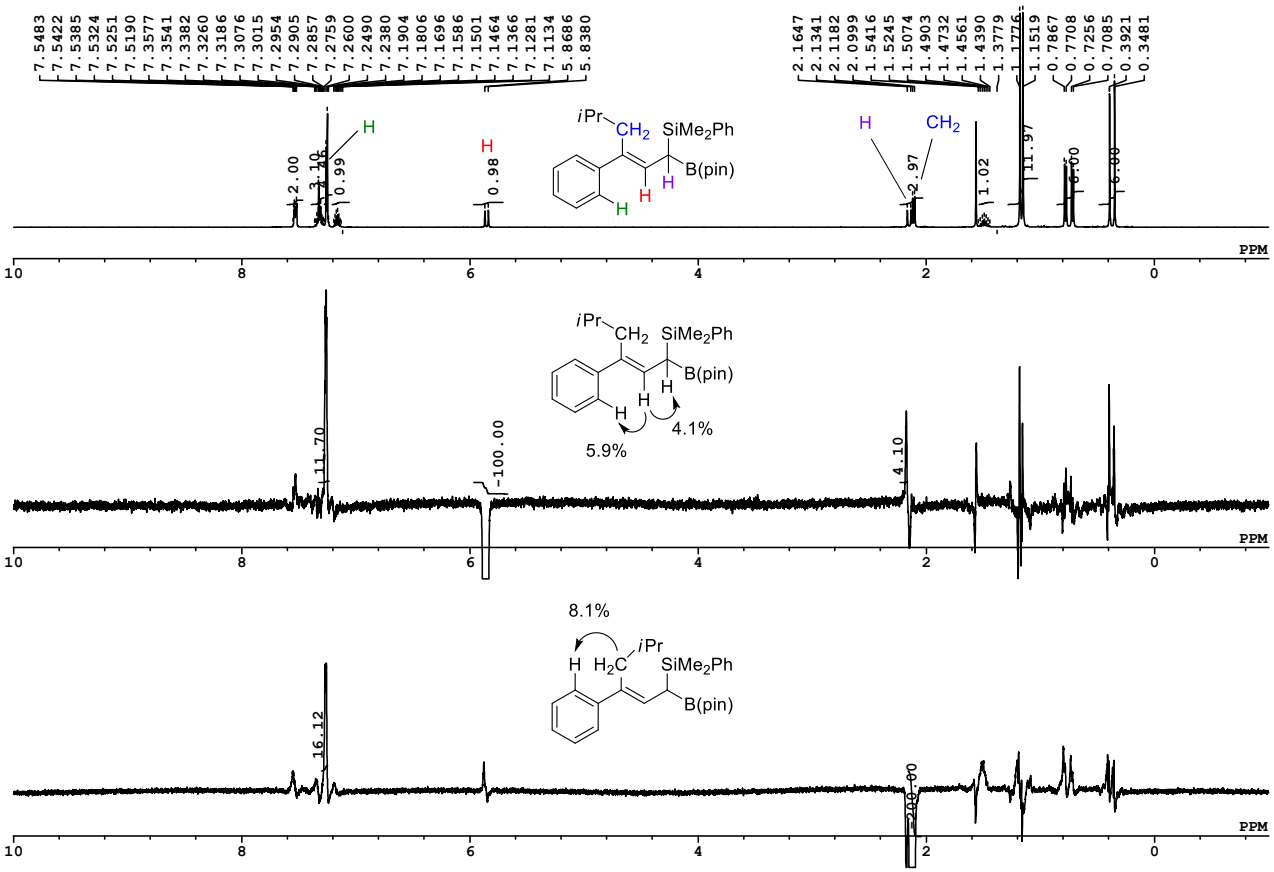
Compound 3ia. Hexane/EtOAc = 50/1 was used for silica gel chromatography. Reversed phase chromatography was performed with MeCN instead of GPC purification. Colorless oil (38.7 mg, 89.1 μmol; 30% yield, dr = 84/16). The stereochemistry was assigned by analogy with compound **3ja**.

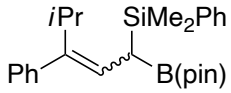
^{1}H NMR ($CDCl_3$): δ 7.58-7.50 (m, 1.68H), 7.44-7.38 (m, 0.32H), 7.37-7.11 (m, 7.68H), 6.88-6.83 (m, 0.32H), 5.82 (d, $^3J_{HH}$ = 11.9 Hz, 0.84H), 5.55 (d, $^3J_{HH}$ = 12.4 Hz, 0.16H), 2.36-2.06 (m, 2.84H), 1.86 (d, $^3J_{HH}$ = 11.9 Hz, 0.16H), 1.36-0.98 (m, 16H), 0.84 (t, $^3J_{HH}$ = 6.9 Hz, 0.48H), 0.80 (t, $^3J_{HH}$ = 7.1 Hz, 2.52H), 0.42 (s, 2.52H), 0.39 (s, 2.52H), 0.28 (s, 0.48H), 0.27 (s, 0.48H). ^{13}C{^{1}H} NMR ($CDCl_3$; *E*-isomer): δ 144.2, 138.4, 136.9, 134.1, 129.1, 128.1, 127.6, 126.4, 125.9, 125.5, 83.1, 30.7, 29.2, 25.0, 23.0, 19.9, 14.1, –2.7, –2.8. HRMS (FAB) calcd for $C_{27}H_{39}BO_2Si$ (M^+) 434.2807, found 434.2822.



Compound 3ja. The reaction was conducted on a 2.00 mmol scale. Hexane/EtOAc = 30/1 was used for silica gel chromatography. Reversed phase chromatography was performed with MeCN instead of GPC purification. Colorless oil (321 mg, 0.740 mmol; 37% yield, *E* pure (*E*/*Z* = 74/26 before purification)). The stereochemistry of the major isomer was determined by the NOE experiment.

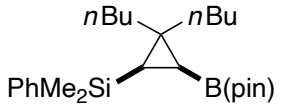
^{1}H NMR ($CDCl_3$; *E*-isomer): δ 7.56-7.50 (m, 2H), 7.37-7.28 (m, 3H), 7.28-7.22 (m, 4H), 7.20-7.12 (m, 1H), 5.85 (d, $^{3}J_{HH}$ = 12.2 Hz, 1H), 2.15 (d, $^{3}J_{HH}$ = 12.2 Hz, 1H), 2.11 (d, $^{3}J_{HH}$ = 7.3 Hz, 2H), 1.55-1.42 (m, 1H), 1.18 (s, 6H), 1.15 (s, 6H), 0.78 (d, $^{3}J_{HH}$ = 6.4 Hz, 3H), 0.72 (d, $^{3}J_{HH}$ = 6.8 Hz, 3H), 0.39 (s, 3H), 0.35 (s, 3H). ^{13}C{^{1}H} NMR ($CDCl_3$; *E*-isomer): δ 144.6, 138.5, 136.3, 134.1, 129.1, 128.1, 127.6, 126.71, 126.67, 125.9, 83.1, 38.1, 27.1, 25.0, 24.9, 23.2, 21.6, 20.1, –2.7, –2.8. HRMS (FAB) calcd for $C_{27}H_{39}BO_2Si$ (M^+) 434.2807, found 434.2798.





Compound 3ka. Hexane/EtOAc = 50/1 → 30/1 was used for silica gel chromatography. Reversed phase chromatography was performed with MeCN instead of GPC purification. Colorless oil (60.5 mg, 0.144 mmol; 48% yield, dr = 53/47). The stereochemistry was assigned by analogy with compound **3ja**.

^{1}H NMR ($CDCl_3$): δ 7.62-7.55 (m, 1.06H), 7.47-7.40 (m, 0.94H), 7.40-7.28 (m, 3H), 7.26-7.13 (m, 3H), 7.13-7.06 (m, 1.06H), 6.74 (d, $^3J_{HH}$ = 6.8 Hz, 0.94H), 5.54 (d, $^3J_{HH}$ = 11.9 Hz, 0.47H), 5.44 (d, $^3J_{HH}$ = 12.4 Hz, 0.53H), 2.79 (sept, $^3J_{HH}$ = 7.0 Hz, 0.53H), 2.52 (sept, $^3J_{HH}$ = 6.8 Hz, 0.47H), 2.17 (d, $^3J_{HH}$ = 11.9 Hz, 0.53H), 1.66 (d, $^3J_{HH}$ = 12.4 Hz, 0.47H), 1.25-1.12 (m, 12H), 1.03 (d, $^3J_{HH}$ = 6.9 Hz, 1.59H), 0.97 (d, $^3J_{HH}$ = 6.8 Hz, 1.41H), 0.94 (d, $^3J_{HH}$ = 6.9 Hz, 1.41H), 0.67 (d, $^3J_{HH}$ = 6.9 Hz, 1.59H), 0.44 (s, 1.59H), 0.42 (s, 1.59H), 0.31 (s, 1.41H), 0.29 (s, 1.41H). ^{13}C{^{1}H} NMR ($CDCl_3$): δ 144.5, 144.1, 143.4, 141.2, 138.6, 138.5, 134.2, 134.1, 129.5, 129.1, 129.0, 128.9, 127.8, 127.6, 127.5, 127.4, 125.9, 125.8, 125.1, 120.9, 83.1, 82.9, 36.5, 28.8, 25.0, 24.94, 24.92, 24.89, 22.7, 22.5, 22.1, 20.9, 18.41, 18.37, –2.6, –2.97, –2.99. HRMS (FAB) calcd for $C_{26}H_{37}BO_2Si$ (M^+) 420.2650, found 420.2656.

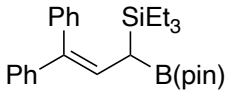


Compound 5la. Silica gel chromatography was not performed. Colorless oil (65.9 mg, 0.159 mmol; 53% yield). The stereochemistry was assigned based on the H–H coupling constant on the cyclopropane ring.

^{1}H NMR (acetone-d_6): δ 7.64-7.58 (m, 2H), 7.37-7.30 (m, 3H), 1.73 (ddd, $^2J_{HH}$ = 13.7 Hz and $^3J_{HH}$ = 10.3 and 4.9 Hz, 1H), 1.67-1.58 (m, 1H), 1.50 (td, J_{HH} = 12.4 Hz and $^3J_{HH}$ = 3.4 Hz, 1H), 1.45-1.19 (m, 8H), 1.17 (s, 6H), 1.14 (s, 6H), 1.04-0.95 (m, 1H), 0.90 (t, $^3J_{HH}$ = 7.3 Hz, 3H), 0.86 (t, $^3J_{HH}$ = 7.3 Hz, 3H), 0.40 (s, 3H), 0.36 (s, 3H), 0.07 (d, $^3J_{HH}$ = 11.2 Hz, 1H), 0.03 (d, $^3J_{HH}$ = 11.2 Hz, 1H). ^{13}C{^{1}H} NMR ($CDCl_3$): δ 141.9, 133.8, 128.4, 127.6, 82.9, 41.1, 33.6, 30.9, 30.1, 29.3, 25.3, 24.7, 23.5, 23.1, 20.0, 14.4, 14.3, 0.4, −0.6. Anal. Calcd for $C_{25}H_{43}BO_2Si$: C, 72.44; H, 10.46. Found: C, 72.67; H, 10.57.

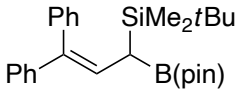
General Procedure for Equation 1.

KO*t*Bu (3.4 mg, 30 μmol) was dissolved in THF (0.5 mL) at 60 °C. Silylboronate **2** (0.360 mmol), cyclopropene **1a** (57.7 mg, 0.300 mmol), and THF (1.0 mL) were added to it, and the resulting mixture was stirred for 20 h at 60 °C. This was passed through a pad of silica gel with EtOAc, and the solvent was removed under vacuum. The residue was chromatographed on silica gel and further purified by GPC with $CHCl_3$ to afford compound **3**.



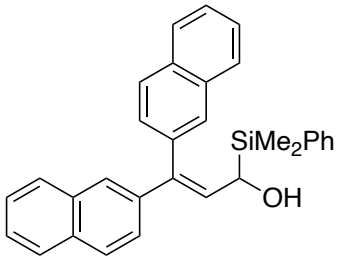
Compound 3ab. Hexane/EtOAc = 30/1 was used for silica gel chromatography. White solid (113 mg, 0.259 mmol; 86% yield).

^{1}H NMR ($CDCl_3$): δ 7.37-7.30 (m, 2H), 7.27-7.11 (m, 8H), 6.29 (d, $^3J_{HH}$ = 12.8 Hz, 1H), 1.98 (d, $^3J_{HH}$ = 12.8 Hz, 1H), 1.26 (s, 6H), 1.25 (s, 6H), 0.87 (t, $^3J_{HH}$ = 7.8 Hz, 9H), 0.64-0.52 (m, 6H). ^{13}C{^{1}H} NMR ($CDCl_3$): δ 143.9, 140.6, 137.7, 130.6, 128.4, 128.3, 128.1, 127.2, 126.6, 126.1, 83.0, 25.2, 25.0, 17.8, 7.6, 3.8. HRMS (FAB) calcd for $C_{27}H_{39}BO_2Si$ (M^+) 434.2807, found 434.2821.



Compound 3ac. Hexane/EtOAc = 20/1 was used for silica gel chromatography. Orange solid (90.1 mg, 0.207 mmol; 69% yield).

^{1}H NMR ($CDCl_3$): δ 7.38-7.31 (m, 2H), 7.29-7.10 (m, 8H), 6.29 (d, $^{3}J_{HH}$ = 12.4 Hz, 1H), 1.98 (d, $^{3}J_{HH}$ = 12.4 Hz, 1H), 1.26 (s, 6H), 1.25 (s, 6H), 0.78 (s, 9H), 0.12 (s, 3H), −0.00 (s, 3H). ^{13}C{^{1}H} NMR ($CDCl_3$): δ 143.7, 140.6, 137.2, 130.5, 128.6, 128.4, 128.1, 127.2, 126.7, 126.1, 83.1, 26.9, 25.3, 24.8, 18.5, 18.0, −4.9, −5.9. HRMS (FAB) calcd for $C_{27}H_{39}BO_2Si$ (M^+) 434.2807, found 434.2812.



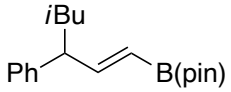
Procedure for Scheme 2a.

A mixture of compound **3ga** (55.5 mg, 0.100 mmol) and $NaBO_3$•$4H_2O$ (46.2 mg, 0.300 mmol) in THF (0.5 mL) and H_2O (0.5 mL) was stirred for 13 h at room temperature. The reaction was quenched with 5% $Na_2S_2O_3$aq and this was extracted with Et_2O. The solvent was removed under vacuum and the residue was purified by silica gel preparative TLC with hexane/EtOAc = 10/1. This was further purified by GPC with $CHCl_3$ to afford compound **6** as a white amorphous (30.3 mg, 68.1 μmol; 68% yield).

^{1}H NMR ($CDCl_3$): δ 7.90-7.83 (m, 1H), 7.82-7.77 (m, 2H), 7.77-7.69 (m, 2H), 7.69-7.63 (m, 1H), 7.58-7.53 (m, 2H), 7.53-7.47 (m, 3H), 7.47-7.40 (m, 5H), 7.40-7.33 (m, 2H), 7.15 (dd, $^{3}J_{HH}$ = 8.3 Hz and $^{4}J_{HH}$ = 1.5 Hz, 1H), 6.39 (d, $^{3}J_{HH}$ = 11.2 Hz, 1H), 4.41 (d, $^{3}J_{HH}$ = 11.2 Hz, 1H), 1.40 (bs, 1H), 0.412 (s, 3H), 0.408 (s, 3H). ^{13}C{^{1}H} NMR ($CDCl_3$): δ 141.9, 139.7, 137.1, 136.2, 134.5, 133.41, 133.39, 132.9, 132.7, 130.3, 129.7, 128.8, 128.33, 128.27, 128.10, 128.08, 127.9, 127.8, 127.6, 126.9, 126.3, 126.24, 126.16, 126.1, 125.4, 65.9, −5.2, −5.3. HRMS (FAB) calcd for $C_{31}H_{27}OSi$ ($M–H^–$) 443.1826, found 443.1829.

Procedure for Scheme 2b.

KO*t*Bu (3.4 mg, 30 μmol) was dissolved in THF (1.5 mL) at 40 °C. Silylboronate **2a** (98.1 μL, 0.360 mmol) and cyclopropene **1g** (87.4 mg, 0.299 mmol) were added to it, and the resulting mixture was stirred for 20 h at 40 °C. This was cooled to 0 °C, and 1 M NaOHaq (0.60 mL) and 30 wt% H_2O_2aq (0.60 mL) were added to it. The mixture was stirred for 3 h at 0 °C and the reaction was quenched with 5 wt% Na_2SO_3aq. This was extracted with EtOAc and the solvent was removed under vacuum. The residue was purified by preparative TLC with hexane/EtOAc = 15/1 → 10/1 and further purified by GPC with $CHCl_3$ to afford compound **6** as a colorless viscous oil (68.4 mg, 0.154 mmol; 51% yield).



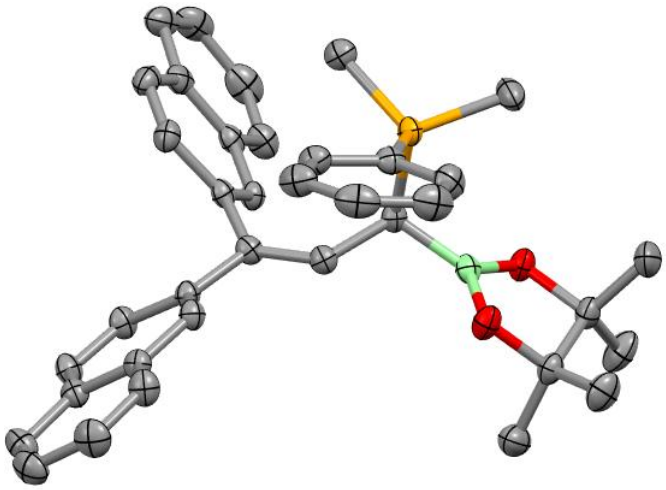
Procedure for Scheme 2c.

TfOH (9.70 μL, 0.111 mmol) was added to a solution of compound **3ja** (43.6 mg, 0.100 mmol) in CH_2Cl_2 (1.0 mL) at 0 °C, and the mixture was stirred for 1 h at 0 °C. The reaction was quenched with saturated $NaHCO_3$aq, and this was extracted with Et_2O. The organic layer was dried over $MgSO_4$, filtered, and concentrated under vacuum. The residue was purified by GPC with $CHCl_3$ and further chromatographed on silica gel with hexane/EtOAc = 20/1 to afford compound **7** as a colorless oil (20.2 mg, 67.3 μmol; 67% yield).

^{1}H NMR ($CDCl_3$): δ 7.31-7.25 (m, 2H), 7.22-7.15 (m, 3H), 6.69 (dd, $^3J_{HH}$ = 18.1 and 7.3 Hz, 1H), 5.40 (dd, $^3J_{HH}$ = 17.6 Hz and $^4J_{HH}$ = 1.4 Hz, 1H), 3.42 (q, $^3J_{HH}$ = 7.3 Hz, 1H), 1.66-1.57 (m, 2H), 1.54-1.41 (m, 1H), 0.88 (d, $^3J_{HH}$ = 6.8 Hz, 3H), 0.86 (d, $^3J_{HH}$ = 6.8 Hz, 3H). ^{13}C{^{1}H} NMR ($CDCl_3$): δ 157.4, 143.8, 128.6, 128.0, 126.3, 83.2, 49.7, 44.4, 25.4, 24.9, 22.8, 22.6. HRMS (FAB) calcd for $C_{19}H_{30}BO_2$ ($M+H^+$) 301.2333, found 301.2338.

IV. X-ray Crystal Structure

Compound 3ga



A colorless CH_2Cl_2 solution of compound **3ga** was prepared. Crystals suitable for X-ray analysis were obtained by layering MeOH and slow diffusion of the solvents at room temperature. The crystal structure has been deposited at the Cambridge Crystallographic Data Centre (deposition number: CCDC 2340586). The data can be obtained free of charge via the Internet at https://www.ccdc.cam.ac.uk/structures/.

Crystal Data and Structure Refinement.

Empirical Formula	$C_{37}H_{39}BO_2Si$	
Formula Weight	554.63	
Temperature	113 ± 2 K	
Wavelength	0.71075 Å	
Crystal System	Monoclinic	
Space Group	C2/c	
Unit Cell Dimensions	a = 16.206 (4) Å	α = 90°
	b = 14.988 (3) Å	β = 99.955 (6)°
	c = 26.246 (5) Å	γ = 90°

Volume	6279(2) $Å^3$
Z Value	8
Calculated Density	1.173 g/cm^3
Absorption coefficient	0.106 mm^{-1}
F(000)	2369.872
Crystal size	0.240 x 0.130 x 0.100 mm
Theta Range for Data Collection	3.14–27.50°
Index Ranges	$-20 \leq h \leq 19$, $0 \leq k \leq 19$, $0 \leq l \leq 34$
Reflections Collected	54311
Independent Reflections	7169 [R(int) = 0.0475]
Completeness to Theta = 25.2425°	99.74%
Absorption Correction	Semi-empirical from equivalents
Max. and Min. Transmission	1.000 and 0.857
Refinement Method	Full-matrix least-squares on F^2
Data / Restraints / Parameters	7169 / 67 / 417
Goodness-of-Fit on F^2	1.0505
Final R Indices [I>2sigma(I)]	R1 = 0.0427, wR2 = 0.1058
R Indices (All Data)	R1 = 0.0566, wR2 = 0.1112
Largest Diff. Peak and Hole	0.4525 and –0.2832 $e^-/Å^3$

V. Theoretical Calculations

All calculations were performed with the Gaussian 16 package.[7] Geometrical optimizations were conducted using the DFT-M06 functional.[8] The 6-31+G(d) basis set was used for all atoms. Frequency analyses were carried out to confirm that each structure is a local minimum (no imaginary frequency) or a transition state (only one imaginary frequency). The energies were evaluated by single-point calculations using the same level of theory as the geometry optimization, including solvation effect by SCRF-SMD model[9] using THF as solvent. Natural bond orbital (NBO) calculations were performed using NBO 3.1.[10] Energy diagrams were created with EveRplot.[11] The 3D optimized structures were displayed by the CYLview visualization program.[12] The output files were uploaded at https://doi.org/10.5281/zenodo.11212804.

We assessed the Gibbs energy changes at standard conditions (298.15 K and 1 atm), and the resulting Gibbs energy profiles are depicted in Figure S1.

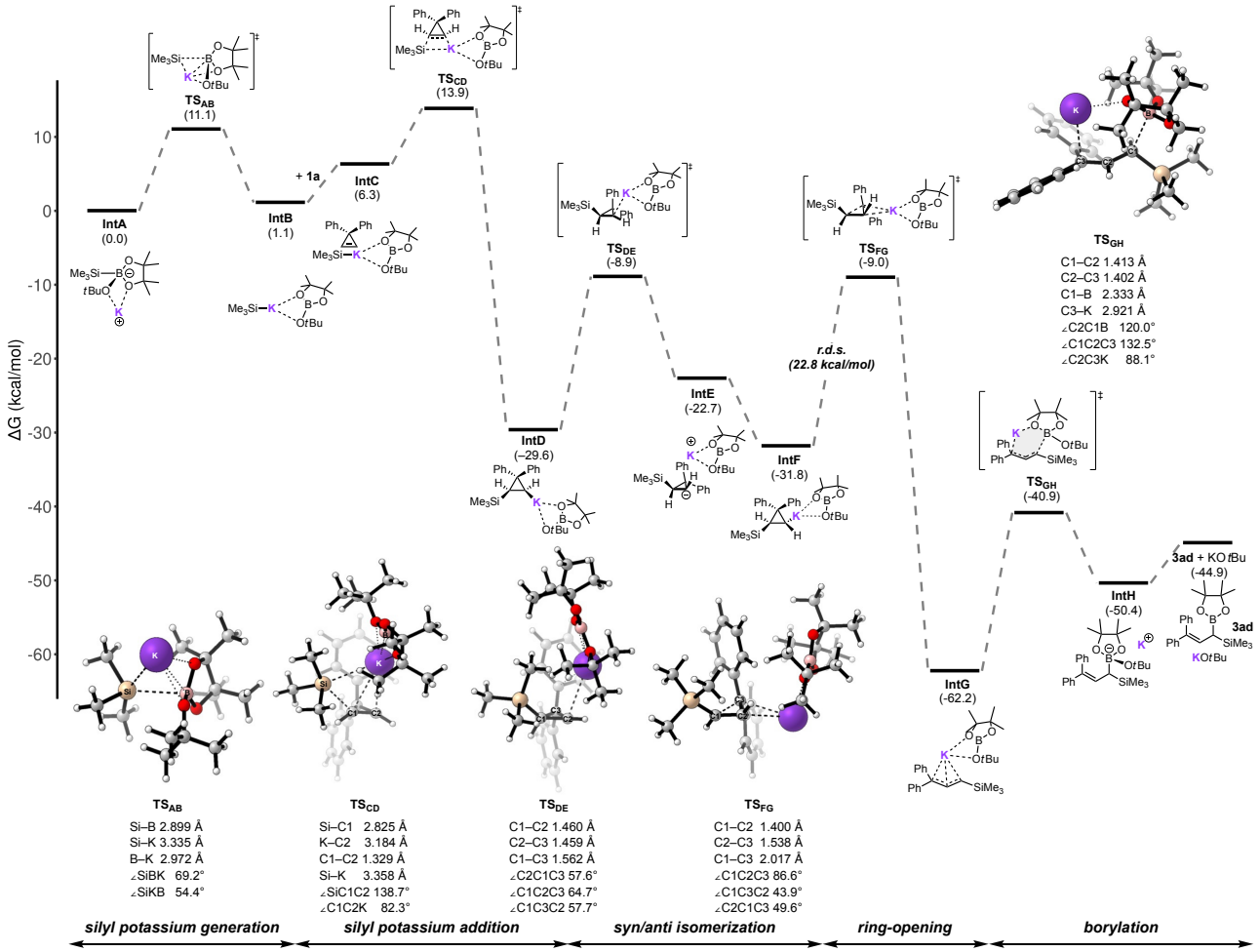


Figure S1. Calculated energy diagram for the KO*t*Bu-catalyzed *gem*-silylborylation of **1a** with trimethylsilylboronic acid pinacol ester.

We theoretically examined the ring-opening step of *syn*-isomer **IntD** and *anti*-isomer **IntF** to afford *π*-allylpotassium **IntG** (Figure S2). As a result, the *syn*-isomer **IntD** (0 kcal/mol) was found to be energetically unfavorable for direct ring-opening process through $\mathbf{TS_{syn\text{-}opening}}$ ($\Delta G^{\circ\ddagger}_{\text{syn-opening}}$ = 27.8 kcal/mol). Therefore, the *syn*/*anti*-isomerization of **IntD** could undergo through $\mathbf{TS_{DE}}$ to yield *anti*-isomer **IntF** ($\Delta G^{\circ\ddagger}_{DE}$ = 20.7 kcal/mol; ΔG°_{DF} = –2.2 kcal/mol). The ring-opening process $\mathbf{TS_{FG}}$ of *anti*-isomer **IntF** (–2.2 kcal/mol) exhibited a lower energy barrier ($\Delta G^{\circ\ddagger}_{FG}$ = 22.8 kcal/mol) than that of the *syn*-isomer. From the results of natural population analysis, the transition-state of the *anti*-isomer has more delocalized negative charge on the cyclopropane ring, leading to a lower activation energy barrier for $\mathbf{TS_{FG}}$. These results indicated that the ring-opening process proceeds via the *syn*-to-*anti* isomerization of **IntD**.

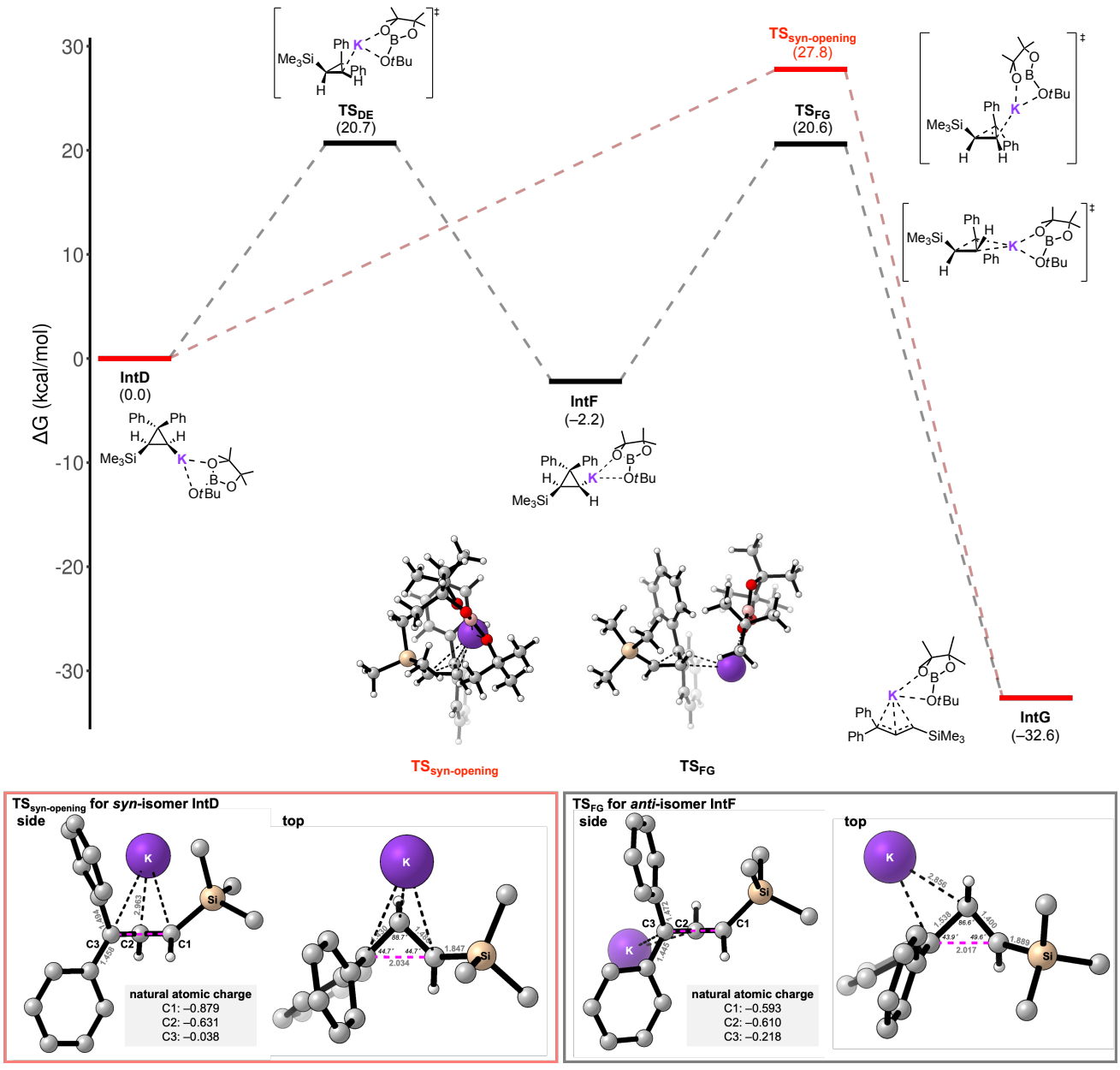


Figure S2. Calculated energy diagram for the ring-opening process of **IntD** and **IntF**.

Cartesian Coordinates of Optimized Species

IntA

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) x	y	z
1	14	0	0.979394	-1.84415	-0.5142
2	6	0	2.816099	-1.95598	0.037202
3	1	0	3.489081	-1.27056	-0.49754
4	1	0	2.945456	-1.75907	1.115364
5	1	0	3.186979	-2.97926	-0.13835
6	6	0	0.240827	-3.31934	0.457291
7	1	0	0.164426	-3.10967	1.536911
8	1	0	-0.76647	-3.59033	0.110401
9	1	0	0.881512	-4.20851	0.33831
10	6	0	-2.16403	0.718151	-0.76062
11	6	0	-2.29587	-0.14838	0.527642
12	5	0	-0.02182	-0.02528	-0.15401
13	8	0	-0.89413	0.334687	-1.27003
14	8	0	-0.95797	-0.21143	1.001727
15	8	0	0.911107	1.041804	0.315242
16	6	0	1.837115	1.783287	-0.46136
17	6	0	0.955549	-2.43016	-2.32616
18	1	0	-0.08263	-2.51487	-2.68374
19	1	0	1.474104	-1.73363	-3.00164
20	1	0	1.429039	-3.41926	-2.43494
21	6	0	-3.22028	0.439213	-1.8168
22	1	0	-4.23461	0.614449	-1.42742
23	1	0	-3.07086	1.110364	-2.67465
24	1	0	-3.16166	-0.59145	-2.18757
25	6	0	-2.16807	2.214223	-0.45181
26	1	0	-1.88636	2.763956	-1.36104
27	1	0	-3.16324	2.567364	-0.14306
28	1	0	-1.44285	2.464224	0.332646
29	6	0	-3.17734	0.45269	1.610211
30	1	0	-4.20313	0.613014	1.245899
31	1	0	-3.23478	-0.23394	2.467603
32	1	0	-2.78552	1.411844	1.970597
33	6	0	-2.79189	-1.56031	0.225512
34	1	0	-2.65386	-2.18616	1.118527
35	1	0	-3.86042	-1.57176	-0.03343
36	1	0	-2.23187	-2.0191	-0.59983
37	6	0	2.120623	1.17057	-1.8302
38	1	0	1.194213	1.053546	-2.40682
39	1	0	2.79912	1.827121	-2.39473
40	1	0	2.605544	0.189452	-1.74755
41	6	0	1.289491	3.194779	-0.6607
42	1	0	0.38299	3.174368	-1.2796
43	1	0	1.033418	3.64718	0.308748
44	1	0	2.03025	3.840233	-1.15647
45	6	0	3.130285	1.862045	0.346698
46	1	0	3.536834	0.85624	0.530835
47	1	0	3.900181	2.448337	-0.17598
48	1	0	2.945971	2.348752	1.318142
49	19	0	0.908924	0.124022	2.745381

TS_{AB}

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) x	y	z
1	14	0	1.555	-1.59755	-0.54601
2	6	0	3.487899	-1.32709	-0.49153
3	1	0	3.809305	-0.35704	-0.90421
4	1	0	3.873898	-1.3772	0.542652
5	1	0	4.015057	-2.11315	-1.06333
6	6	0	1.553334	-3.44123	0.089475
7	1	0	1.844872	-3.51399	1.151933
8	1	0	0.565636	-3.92068	-0.00391
9	1	0	2.270229	-4.05782	-0.48362
10	6	0	-2.46101	0.153341	-0.66555
11	6	0	-2.24565	-0.70101	0.623919
12	5	0	-0.34869	0.484588	0.122444
13	8	0	-1.11728	0.521709	-1.03766
14	8	0	-1.0668	-0.09967	1.189108
15	8	0	0.573088	1.440265	0.523506
16	6	0	1.166107	2.465527	-0.28847
17	6	0	1.29354	-1.91613	-2.43382
18	1	0	0.267546	-2.26255	-2.64149
19	1	0	1.449436	-1.00622	-3.03482
20	1	0	1.986801	-2.68882	-2.81225
21	6	0	-3.10922	-0.58991	-1.8148
22	1	0	-4.10469	-0.95869	-1.528
23	1	0	-3.23538	0.087781	-2.67004
24	1	0	-2.5037	-1.44128	-2.14658
25	6	0	-3.22263	1.444996	-0.39638
26	1	0	-3.17611	2.077895	-1.2928
27	1	0	-4.28138	1.255854	-0.17149
28	1	0	-2.78458	2.007985	0.439595
29	6	0	-3.36965	-0.60571	1.636373
30	1	0	-4.31806	-0.94838	1.198321
31	1	0	-3.14786	-1.25104	2.497738
32	1	0	-3.50523	0.417352	2.005966
33	6	0	-1.96056	-2.1661	0.326952
34	1	0	-1.59473	-2.65166	1.242984
35	1	0	-2.87055	-2.69056	0.003862
36	1	0	-1.18973	-2.28349	-0.44432
37	6	0	1.595346	1.942539	-1.65095
38	1	0	0.73647	1.594098	-2.23694
39	1	0	2.090764	2.748764	-2.21085
40	1	0	2.305224	1.111296	-1.54709
41	6	0	0.163662	3.599301	-0.44424
42	1	0	-0.7169	3.262734	-1.00767
43	1	0	-0.16838	3.958703	0.540159
44	1	0	0.615403	4.442986	-0.98553
45	6	0	2.38287	2.931126	0.495593
46	1	0	3.099176	2.103871	0.619825
47	1	0	2.898134	3.749052	-0.02623
48	1	0	2.087269	3.292484	1.491309
49	19	0	1.310483	-0.22536	2.483668

IntB

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) x	y	z
1	14	0	3.178466	-0.94672	-0.17665
2	6	0	4.291366	0.483157	-0.88981
3	1	0	3.704136	1.335846	-1.26934
4	1	0	4.974125	0.882322	-0.12172
5	1	0	4.915123	0.117582	-1.72699
6	6	0	4.565933	-2.29242	0.036281
7	1	0	5.269033	-2.03101	0.843748
8	1	0	4.145161	-3.28042	0.28402
9	1	0	5.1565	-2.40791	-0.89181
10	6	0	-2.9518	-0.58509	-0.67774
11	6	0	-2.18352	-1.47905	0.344431
12	5	0	-1.28932	0.601354	0.293335
13	8	0	-2.0509	0.546219	-0.84008
14	8	0	-1.46195	-0.48793	1.128575
15	8	0	-0.40229	1.553053	0.671003
16	6	0	0.068734	2.658182	-0.14927
17	6	0	2.41506	-1.60157	-1.84321
18	1	0	1.924794	-2.57932	-1.70254
19	1	0	1.659243	-0.91901	-2.26699
20	1	0	3.201218	-1.73673	-2.60968
21	6	0	-3.17787	-1.22503	-2.02884
22	1	0	-3.77098	-2.14416	-1.92339
23	1	0	-3.73593	-0.53626	-2.67657
24	1	0	-2.23477	-1.47308	-2.52882
25	6	0	-4.258	-0.03458	-0.13016
26	1	0	-4.63482	0.735438	-0.81564
27	1	0	-5.02132	-0.81948	-0.05005
28	1	0	-4.12782	0.425331	0.858757
29	6	0	-3.06556	-2.29101	1.264986
30	1	0	-3.69724	-2.9765	0.683046
31	1	0	-2.44418	-2.8979	1.93695
32	1	0	-3.71393	-1.65609	1.879369
33	6	0	-1.13687	-2.36756	-0.30809
34	1	0	-0.50588	-2.81587	0.47202
35	1	0	-1.60032	-3.18459	-0.87628
36	1	0	-0.4833	-1.80001	-0.98587
37	6	0	0.640764	2.108163	-1.44444
38	1	0	-0.13625	1.655841	-2.07413
39	1	0	1.117869	2.915921	-2.01639
40	1	0	1.404224	1.346048	-1.2255
41	6	0	-1.07556	3.624881	-0.39256
42	1	0	-1.88158	3.155782	-0.97057
43	1	0	-1.48848	3.983061	0.560677
44	1	0	-0.71506	4.495507	-0.9571
45	6	0	1.161876	3.313897	0.674748
46	1	0	1.998383	2.618215	0.840619
47	1	0	1.558607	4.193207	0.150566
48	1	0	0.772492	3.641528	1.648769
49	19	0	1.04699	-0.14519	2.322278

IntC

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) x	y	z
1	6	0	-6.684033	-1.85531	0.492757
2	6	0	-7.555395	-0.77231	0.590512
3	6	0	-7.136804	0.482717	0.152301
4	6	0	-5.859057	0.652815	-0.37465
5	6	0	-4.9761	-0.42861	-0.48355
6	6	0	-5.409904	-1.68296	-0.04154
7	6	0	-3.611135	-0.25991	-1.09601
8	6	0	-2.960697	1.08263	-0.8933
9	6	0	-2.510809	1.838741	-1.97934
10	6	0	-1.872423	3.06609	-1.78574
11	6	0	-1.671328	3.550636	-0.494
12	6	0	-2.114019	2.802063	0.5989
13	6	0	-2.753157	1.580843	0.400215
14	6	0	-3.27041	-1.0528	-2.32826
15	6	0	-2.716565	-1.46339	-1.23339
16	1	0	-6.99487	-2.84077	0.838369
17	1	0	-8.553053	-0.90464	1.007219
18	1	0	-7.808506	1.337908	0.222183
19	1	0	-5.545164	1.642706	-0.70844
20	1	0	-4.738845	-2.54048	-0.11361
21	1	0	-2.664124	1.462399	-2.99266
22	1	0	-1.538048	3.644678	-2.64634
23	1	0	-1.17393	4.507121	-0.33745
24	1	0	-1.955555	3.169135	1.612474
25	1	0	-3.092667	0.99917	1.258826
26	1	0	-3.473189	-1.15698	-3.38812
27	19	0	0.292352	0.684449	-0.82932
28	1	0	-2.095203	-2.15514	-0.67282
29	14	0	-0.090294	-1.67862	1.586489
30	6	0	1.231629	-1.91332	2.999119
31	1	0	1.212602	-1.07215	3.711857
32	1	0	1.038979	-2.83554	3.578935
33	1	0	2.262649	-1.97654	2.609527
34	6	0	-1.692562	-1.68559	2.69356
35	1	0	-2.61264	-1.77844	2.091065
36	1	0	-1.686321	-2.52873	3.409839
37	1	0	-1.787787	-0.75717	3.280778
38	6	0	-0.160626	-3.54045	0.995285
39	1	0	0.803838	-3.86963	0.573827
40	1	0	-0.387217	-4.20887	1.846842
41	1	0	-0.924835	-3.73427	0.223449
42	6	0	3.737402	-1.32761	-1.52628
43	6	0	4.988784	-1.04165	-0.63505
44	8	0	4.470103	-0.10407	0.347027
45	8	0	2.99073	-0.08433	-1.41573
46	6	0	2.845428	-2.42835	-0.97868
47	1	0	1.912881	-2.45701	-1.56003
48	1	0	3.323334	-3.41364	-1.06023
49	1	0	2.575743	-2.2527	0.072549
50	6	0	4.050502	-1.5861	-2.98333
51	1	0	4.697311	-2.46886	-3.08462
52	1	0	3.121626	-1.78688	-3.53352
53	1	0	4.549333	-0.73262	-3.45634
54	6	0	6.103666	-0.32166	-1.37626
55	1	0	6.853063	0.015739	-0.64838
56	1	0	6.602613	-0.9837	-2.09591
57	1	0	5.733572	0.561624	-1.91493
58	6	0	5.535246	-2.25091	0.089894
59	1	0	5.849615	-3.02128	-0.6281
60	1	0	6.41444	-1.9625	0.680947
61	1	0	4.796356	-2.68827	0.771363
62	8	0	2.687918	1.572183	0.215017
63	6	0	2.96598	2.341048	1.415836
64	6	0	1.840611	3.3567	1.485377
65	1	0	1.823433	3.981382	0.581331
66	1	0	0.869425	2.847812	1.584115
67	1	0	1.967085	4.012585	2.356723
68	6	0	2.928821	1.426336	2.626842
69	1	0	3.738185	0.686037	2.60316
70	1	0	3.033219	2.019922	3.545452
71	1	0	1.968659	0.891727	2.669353
72	6	0	4.309316	3.031818	1.262505
73	1	0	4.502985	3.673273	2.132975
74	1	0	5.128363	2.304514	1.189472
75	1	0	4.318843	3.663598	0.363398
76	5	0	3.391812	0.504448	-0.23221

TS_{CD}

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) x	y	z
1	6	0	-6.63694	-2.14793	-0.50193
2	6	0	-7.52995	-1.08315	-0.38464
3	6	0	-7.03273	0.217082	-0.35766
4	6	0	-5.66132	0.451168	-0.44244
5	6	0	-4.75026	-0.60834	-0.55757
6	6	0	-5.269	-1.91241	-0.59041
7	6	0	-3.26761	-0.38168	-0.65245
8	6	0	-2.81951	1.054604	-0.59665
9	6	0	-2.54775	1.749545	-1.77937
10	6	0	-2.062	3.058102	-1.74958
11	6	0	-1.84595	3.691146	-0.52473
12	6	0	-2.1365	3.017024	0.661328
13	6	0	-2.62428	1.710691	0.623308
14	6	0	-2.41985	-1.34581	-1.42945
15	6	0	-2.36936	-1.47095	-0.10772
16	1	0	-7.00838	-3.17223	-0.52663
17	1	0	-8.60164	-1.26635	-0.31771
18	1	0	-7.71585	1.061757	-0.27003
19	1	0	-5.29732	1.478375	-0.4198
20	1	0	-4.58941	-2.75884	-0.69101
21	1	0	-2.70391	1.245599	-2.73593
22	1	0	-1.85295	3.582658	-2.68168
23	1	0	-1.45617	4.708261	-0.4946
24	1	0	-1.97254	3.50621	1.621521
25	1	0	-2.85467	1.184514	1.549708
26	1	0	-2.45288	-1.91904	-2.35153
27	19	0	0.186008	0.415423	-0.93318
28	1	0	-2.49584	-2.22455	0.666304
29	14	0	-0.52598	-1.06712	1.994213
30	6	0	0.973877	-0.3629	3.008346
31	1	0	0.897861	0.732063	3.113885
32	1	0	1.011913	-0.79075	4.027593
33	1	0	1.941565	-0.57802	2.523643
34	6	0	-1.96116	-0.70434	3.237129
35	1	0	-2.95444	-0.99662	2.856796
36	1	0	-1.80158	-1.24769	4.185364
37	1	0	-2.00891	0.368499	3.485049
38	6	0	-0.28108	-2.96383	2.292409
39	1	0	0.665853	-3.32465	1.860288
40	1	0	-0.2516	-3.18393	3.374562
41	1	0	-1.08719	-3.57845	1.859875
42	6	0	3.530381	-1.92765	-1.03865
43	6	0	4.927286	-1.34389	-0.65932
44	8	0	4.573549	-0.15937	0.108156
45	8	0	2.716273	-0.72654	-1.12368
46	6	0	2.920665	-2.79488	0.049694
47	1	0	1.86869	-2.98995	-0.2014
48	1	0	3.435349	-3.76127	0.131181
49	1	0	2.949687	-2.3026	1.032101
50	6	0	3.485981	-2.64626	-2.36806
51	1	0	4.173914	-3.50314	-2.36346
52	1	0	2.473451	-3.03082	-2.54926
53	1	0	3.75563	-1.98737	-3.20127
54	6	0	5.723179	-0.86034	-1.86083
55	1	0	6.588677	-0.28599	-1.50524
56	1	0	6.095997	-1.70009	-2.46164
57	1	0	5.126418	-0.20591	-2.51146
58	6	0	5.775641	-2.25125	0.20202
59	1	0	5.974252	-3.19801	-0.31943
60	1	0	6.74123	-1.77126	0.40847
61	1	0	5.295201	-2.47495	1.161122
62	8	0	2.647811	1.352275	-0.04787
63	6	0	3.179207	2.549026	0.580056
64	6	0	1.986521	3.480914	0.688144
65	1	0	1.570133	3.695989	-0.30685
66	1	0	1.199779	3.028864	1.310838
67	1	0	2.280963	4.433246	1.148528
68	6	0	3.727389	2.219059	1.956602
69	1	0	4.588341	1.542016	1.898216
70	1	0	4.050795	3.142791	2.455605
71	1	0	2.953619	1.748097	2.578445
72	6	0	4.248772	3.135039	-0.32546
73	1	0	4.623502	4.078642	0.093786
74	1	0	5.101545	2.450315	-0.43162
75	1	0	3.839476	3.342999	-1.32384
76	5	0	3.329586	0.214087	-0.31856

IntD

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) x	y	z
1	6	0	6.686325	1.208826	-1.0436
2	6	0	7.343877	-0.02092	-1.12813
3	6	0	6.611651	-1.18195	-0.90712
4	6	0	5.251012	-1.11778	-0.60281
5	6	0	4.569189	0.107683	-0.51154
6	6	0	5.330509	1.269021	-0.74889
7	6	0	3.098653	0.177729	-0.22625
8	6	0	2.468235	-1.15801	0.054078
9	6	0	1.900911	-1.9127	-0.97823
10	6	0	1.301705	-3.14657	-0.73096
11	6	0	1.267589	-3.65709	0.56754
12	6	0	1.866044	-2.93757	1.600896
13	6	0	2.467721	-1.70738	1.339089
14	6	0	2.238068	1.237099	-0.92119
15	6	0	2.61075	1.38281	0.556153
16	1	0	7.236835	2.134555	-1.21354
17	1	0	8.40657	-0.06785	-1.36336
18	1	0	7.09779	-2.15607	-0.96833
19	1	0	4.713321	-2.05007	-0.43088
20	1	0	4.850325	2.246911	-0.70423
21	1	0	1.962137	-1.52733	-1.99965
22	1	0	0.866041	-3.71552	-1.55304
23	1	0	0.787763	-4.61469	0.769003
24	1	0	1.865235	-3.33617	2.615695
25	1	0	2.950628	-1.15341	2.146486
26	1	0	2.905567	1.868553	-1.5347
27	1	0	3.435537	2.063983	0.832421
28	14	0	1.265529	1.510745	1.848058
29	6	0	-0.3314	0.55831	1.497988
30	1	0	-0.171078	-0.50081	1.242875
31	1	0	-0.948944	0.584801	2.410629
32	1	0	-0.933269	1.032479	0.708804
33	6	0	1.826171	1.039243	3.594134
34	1	0	2.870419	1.335171	3.774843
35	1	0	1.203261	1.551186	4.343806
36	1	0	1.74653	-0.04057	3.785637
37	6	0	0.812062	3.344165	1.905217
38	1	0	0.514603	3.712351	0.911559
39	1	0	-0.014626	3.539392	2.605131
40	1	0	1.672118	3.94749	2.233742
41	6	0	-3.536952	-2.02787	-0.40414
42	6	0	-4.495063	-1.29417	0.586435
43	8	0	-4.539356	0.05289	0.037851
44	8	0	-2.66287	-0.94943	-0.83538
45	6	0	-4.241132	-2.55074	-1.64474
46	1	0	-3.486841	-2.86733	-2.37689
47	1	0	-4.870502	-3.41927	-1.41106
48	1	0	-4.870233	-1.78248	-2.11405
49	6	0	-2.697289	-3.11848	0.22261
50	1	0	-3.341698	-3.89071	0.665785
51	1	0	-2.079313	-3.5998	-0.54712
52	1	0	-2.031287	-2.72988	1.002413
53	6	0	-3.925887	-1.16973	1.990408
54	1	0	-4.552952	-0.47776	2.567982
55	1	0	-3.917856	-2.13658	2.510233
56	1	0	-2.900737	-0.77237	1.981914
57	6	0	-5.899359	-1.85132	0.636596
58	1	0	-5.883225	-2.90145	0.959968
59	1	0	-6.497163	-1.28499	1.362699
60	1	0	-6.400801	-1.7934	-0.33604
61	8	0	-2.807207	1.375168	-1.08759
62	6	0	-3.276084	2.723253	-0.80753
63	6	0	-2.252536	3.626983	-1.46893
64	1	0	-1.250643	3.456778	-1.04687
65	1	0	-2.213088	3.443844	-2.55186
66	1	0	-2.510887	4.681926	-1.30869
67	6	0	-4.647903	2.913008	-1.42928
68	1	0	-5.396982	2.264782	-0.95707
69	1	0	-4.973245	3.954861	-1.3058
70	1	0	-4.618114	2.69051	-2.50482
71	6	0	-3.302493	2.95292	0.694464
72	1	0	-3.627808	3.980557	0.905894
73	1	0	-3.996874	2.266607	1.1971
74	1	0	-2.301319	2.820903	1.129046
75	5	0	-3.359016	0.225264	-0.63011
76	19	0	-0.337279	0.263289	-1.80161

TS_{DE}

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) x	y	z
1	6	0	6.78688	0.99306	-0.89901
2	6	0	7.44874	-0.15695	-0.46344
3	6	0	6.699933	-1.22457	0.024674
4	6	0	5.307409	-1.14258	0.077217
5	6	0	4.629592	-0.00051	-0.3671
6	6	0	5.398677	1.062163	-0.85525
7	6	0	3.115609	0.119281	-0.2963
8	6	0	2.411289	-1.20823	-0.2348
9	6	0	2.381856	-1.9954	-1.40357
10	6	0	1.639148	-3.16885	-1.47382
11	6	0	0.899056	-3.59972	-0.36621
12	6	0	0.960443	-2.86328	0.81538
13	6	0	1.72892	-1.69828	0.885429
14	6	0	2.40576	1.23497	-0.91222
15	6	0	2.597237	1.337765	0.53146
16	1	0	7.359627	1.839256	-1.28044
17	1	0	8.53596	-0.21863	-0.50645
18	1	0	7.199764	-2.13093	0.367892
19	1	0	4.741555	-1.9876	0.47312
20	1	0	4.864732	1.944319	-1.21906
21	1	0	2.938366	-1.65186	-2.2792
22	1	0	1.629013	-3.74973	-2.39632
23	1	0	0.305532	-4.51173	-0.41946
24	1	0	0.418978	-3.20368	1.699069
25	1	0	1.797662	-1.1614	1.831258
26	1	0	1.90142	1.602426	-1.7956
27	1	0	3.473251	1.943077	0.897984
28	14	0	1.295785	1.592913	1.868356
29	6	0	-0.432506	0.861371	1.619347
30	1	0	-0.478764	-0.23677	1.642065
31	1	0	-1.066235	1.228975	2.442734
32	1	0	-0.903769	1.223158	0.693054
33	6	0	1.910501	1.11993	3.591597
34	1	0	2.926582	1.511023	3.752258
35	1	0	1.263206	1.553625	4.369151
36	1	0	1.94636	0.033554	3.757821
37	6	0	1.033729	3.465129	1.876096
38	1	0	0.71415	3.821295	0.884462
39	1	0	0.268413	3.766406	2.607749
40	1	0	1.965167	3.994103	2.128458
41	6	0	-3.732543	-1.8785	0.198016
42	6	0	-4.737202	-0.83985	0.789698
43	8	0	-4.566282	0.301305	-0.09742
44	8	0	-2.700648	-1.01791	-0.35635
45	6	0	-4.305997	-2.68213	-0.95666
46	1	0	-3.492287	-3.23649	-1.44314
47	1	0	-5.049411	-3.41028	-0.60733
48	1	0	-4.778416	-2.03814	-1.71048
49	6	0	-3.107572	-2.80203	1.219675
50	1	0	-3.885714	-3.38176	1.735771
51	1	0	-2.438057	-3.51424	0.718882
52	1	0	-2.527002	-2.25445	1.971243
53	6	0	-4.35734	-0.3628	2.182201
54	1	0	-4.985787	0.497895	2.446373
55	1	0	-4.517684	-1.14526	2.935252
56	1	0	-3.306519	-0.0426	2.23213
57	6	0	-6.184309	-1.27482	0.758383
58	1	0	-6.320857	-2.19206	1.348025
59	1	0	-6.81689	-0.49357	1.199684
60	1	0	-6.535611	-1.46117	-0.26279
61	8	0	-2.571293	1.140601	-1.25338
62	6	0	-2.910768	2.546987	-1.40971
63	6	0	-1.703154	3.15611	-2.09763
64	1	0	-0.799624	3.03951	-1.48023
65	1	0	-1.527494	2.678328	-3.07204
66	1	0	-1.859091	4.229463	-2.26727
67	6	0	-4.14759	2.662818	-2.2818
68	1	0	-5.02522	2.218677	-1.7949
69	1	0	-4.367599	3.720373	-2.48087
70	1	0	-3.988109	2.16033	-3.24574
71	6	0	-3.125234	3.178136	-0.0438
72	1	0	-3.338231	4.249117	-0.16291
73	1	0	-3.971967	2.721235	0.485119
74	1	0	-2.226092	3.082034	0.581953
75	5	0	-3.295139	0.2069	-0.58946
76	19	0	-0.245589	-0.35782	-1.44089

IntE

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) x	y	z
1	6	0	6.833943	0.941592	-0.80977
2	6	0	7.460142	-0.2458	-0.42994
3	6	0	6.678357	-1.30611	0.023054
4	6	0	5.291662	-1.17931	0.093315
5	6	0	4.64637	0.004294	-0.29275
6	6	0	5.449296	1.061818	-0.74229
7	6	0	3.15543	0.165462	-0.16966
8	6	0	2.405077	-1.12536	-0.20051
9	6	0	2.415197	-1.87378	-1.39454
10	6	0	1.70119	-3.06285	-1.51402
11	6	0	0.943583	-3.53946	-0.43858
12	6	0	0.945126	-2.82663	0.759286
13	6	0	1.683606	-1.64689	0.878775
14	6	0	2.50168	1.380558	-0.84917
15	6	0	2.702968	1.344892	0.672229
16	1	0	7.430107	1.782133	-1.16643
17	1	0	8.544212	-0.3419	-0.48489
18	1	0	7.148427	-2.24168	0.327277
19	1	0	4.702808	-2.02174	0.459508
20	1	0	4.956725	1.983309	-1.05515
21	1	0	2.993366	-1.4981	-2.24161
22	1	0	1.729669	-3.6197	-2.45079
23	1	0	0.375804	-4.46476	-0.5301
24	1	0	0.382454	-3.19796	1.616347
25	1	0	1.708351	-1.12851	1.836931
26	1	0	1.433329	1.119317	-1.02322
27	1	0	3.568024	1.939308	1.017179
28	14	0	1.30818	1.671475	1.87045
29	6	0	-0.381309	0.952856	1.418155
30	1	0	-0.442174	-0.14266	1.484457
31	1	0	-1.122107	1.363783	2.123033
32	1	0	-0.702776	1.274681	0.415883
33	6	0	1.705074	1.185483	3.650471
34	1	0	2.674944	1.604298	3.956983
35	1	0	0.942061	1.579025	4.339436
36	1	0	1.756086	0.096956	3.797166
37	6	0	1.080523	3.543929	1.82106
38	1	0	0.847287	3.875873	0.797571
39	1	0	0.261836	3.870812	2.480071
40	1	0	1.994708	4.069159	2.1351
41	6	0	-3.784109	-1.83591	0.348159
42	6	0	-4.696123	-0.71361	0.939799
43	8	0	-4.524514	0.36906	-0.01872
44	8	0	-2.752992	-1.0642	-0.32693
45	6	0	-4.473971	-2.6755	-0.71315
46	1	0	-3.726042	-3.30557	-1.21264
47	1	0	-5.230409	-3.3366	-0.2709
48	1	0	-4.960594	-2.05308	-1.476
49	6	0	-3.127996	-2.72659	1.379471
50	1	0	-3.89019	-3.24538	1.977484
51	1	0	-2.518897	-3.49078	0.877598
52	1	0	-2.478628	-2.16144	2.05836
53	6	0	-4.208981	-0.18483	2.278877
54	1	0	-4.773192	0.723472	2.528072
55	1	0	-4.367351	-0.91526	3.082866
56	1	0	-3.141568	0.076878	2.252671
57	6	0	-6.162895	-1.0698	1.018779
58	1	0	-6.310297	-1.944	1.668095
59	1	0	-6.724243	-0.23125	1.451054
60	1	0	-6.586769	-1.29122	0.032879
61	8	0	-2.571311	1.028534	-1.35333
62	6	0	-2.853296	2.435493	-1.60363
63	6	0	-1.643366	2.934224	-2.37138
64	1	0	-0.724639	2.821167	-1.77563
65	1	0	-1.523283	2.380537	-3.31363
66	1	0	-1.755904	3.998688	-2.61496
67	6	0	-4.113409	2.538309	-2.44333
68	1	0	-4.991055	2.169613	-1.89658
69	1	0	-4.297961	3.586231	-2.71546
70	1	0	-4.00772	1.958598	-3.3706
71	6	0	-2.995019	3.177243	-0.28496
72	1	0	-3.187251	4.240497	-0.48234
73	1	0	-3.829131	2.787232	0.313043
74	1	0	-2.072627	3.108253	0.308733
75	5	0	-3.29828	0.17967	-0.58743
76	19	0	-0.424761	-0.66667	-1.63457

IntF

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) x	y	z
1	6	0	-2.403739	0.168459	0.51111
2	6	0	-1.265597	-0.66641	-0.01467
3	6	0	-2.192116	1.661803	0.549707
4	14	0	-1.369051	-2.20826	-1.05453
5	6	0	-1.580942	-0.63661	1.497469
6	1	0	-0.377563	-0.08537	-0.33277
7	6	0	-3.817735	-0.19078	0.140331
8	6	0	-1.537947	2.355682	-0.47395
9	6	0	-2.619617	2.391649	1.668376
10	6	0	-1.472224	-1.82771	-2.90488
11	6	0	0.243504	-3.13133	-0.71464
12	6	0	-2.786956	-3.37432	-0.6287
13	1	0	-2.135331	-1.55803	1.756318
14	6	0	-4.323263	0.104939	-1.13332
15	6	0	-4.677806	-0.79412	1.062699
16	6	0	-1.287306	3.726798	-0.37222
17	1	0	-1.209361	1.810042	-1.36177
18	6	0	-2.381987	3.75882	1.773185
19	1	0	-3.125783	1.859331	2.476747
20	1	0	-0.741251	-1.0615	-3.20572
21	1	0	-1.275671	-2.72794	-3.50739
22	1	0	-2.471506	-1.45896	-3.18048
23	1	0	1.123793	-2.51683	-0.96387
24	1	0	0.322542	-4.07303	-1.27839
25	1	0	0.302481	-3.37203	0.358817
26	1	0	-2.658565	-4.31206	-1.19165
27	1	0	-2.808553	-3.63173	0.440027
28	1	0	-3.768743	-2.95841	-0.89679
29	6	0	-5.628842	-0.22387	-1.48622
30	1	0	-3.671076	0.589835	-1.86329
31	6	0	-5.989853	-1.12102	0.718792
32	1	0	-4.306581	-1.02071	2.063324
33	6	0	-1.702853	4.432283	0.754146
34	1	0	-0.767775	4.243824	-1.17947
35	1	0	-2.719423	4.302755	2.655499
36	6	0	-6.468822	-0.84399	-0.5594
37	1	0	-5.993542	0.00116	-2.48865
38	1	0	-6.639444	-1.59651	1.453877
39	1	0	-1.50511	5.500398	0.838122
40	1	0	-7.49083	-1.10483	-0.83289
41	19	0	0.57084	1.162634	1.949063
42	8	0	2.643577	-0.62198	1.407097
43	8	0	2.296542	1.00655	-0.24132
44	6	0	3.38275	-1.62281	2.157881
45	5	0	2.985301	-0.10629	0.203824
46	6	0	2.693685	1.203905	-1.62512
47	6	0	2.535305	-1.87716	3.390282
48	6	0	3.528256	-2.89325	1.339738
49	6	0	4.734949	-1.04141	2.533837
50	8	0	3.953084	-0.53082	-0.66488
51	6	0	2.699303	2.684967	-1.92773
52	6	0	1.665308	0.49373	-2.48951
53	6	0	4.097304	0.523074	-1.65663
54	1	0	1.537282	-2.23851	3.103574
55	1	0	2.418117	-0.95713	3.981757
56	1	0	3.006789	-2.63364	4.031392
57	1	0	4.029913	-3.66248	1.942648
58	1	0	2.543469	-3.28085	1.045553
59	1	0	4.124233	-2.72619	0.434267
60	1	0	5.288585	-1.75002	3.1647
61	1	0	4.611755	-0.10666	3.098582
62	1	0	5.343979	-0.83506	1.642719
63	1	0	1.672459	3.073983	-1.89397
64	1	0	3.094709	2.868933	-2.93641
65	1	0	3.302556	3.250345	-1.2082
66	1	0	0.668433	0.896221	-2.26085
67	1	0	1.64677	-0.58838	-2.29733
68	1	0	1.859813	0.653219	-3.55829
69	6	0	4.467865	-0.0994	-2.98342
70	6	0	5.215699	1.429586	-1.16813
71	1	0	5.470501	-0.54195	-2.91826
72	1	0	4.487257	0.664099	-3.77351
73	1	0	3.766844	-0.88869	-3.27729
74	1	0	6.12352	0.828539	-1.02676
75	1	0	4.970107	1.902867	-0.20701
76	1	0	5.440917	2.219957	-1.89603

TS_{FG}

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) x	y	z
1	6	0	-0.136199	-1.2957	2.610707
2	6	0	-0.436	-0.5852	3.773308
3	6	0	-1.151804	0.610098	3.654808
4	6	0	-1.561005	1.077797	2.411308
5	6	0	-1.261603	0.384799	1.215808
6	6	0	-0.5247	-0.8116	1.365708
7	6	0	-1.669804	0.848498	-0.11989
8	6	0	-1.736807	2.251698	-0.45909
9	6	0	-1.10171	3.288599	0.281408
10	6	0	-1.091813	4.604498	-0.15469
11	6	0	-1.729114	4.979498	-1.34539
12	6	0	-2.369913	3.990696	-2.08719
13	6	0	-2.384109	2.663996	-1.65839
14	6	0	-2.017701	-0.1826	-1.20639
15	6	0	-3.261701	-0.30391	-0.57539
16	14	0	-4.036498	-1.82291	0.237908
17	6	0	-4.194599	-1.55141	2.094608
18	6	0	-5.763596	-2.05811	-0.47859
19	6	0	-2.981794	-3.34361	-0.09409
20	19	0	0.326495	1.056603	-2.26749
21	6	0	3.279193	1.17821	0.601808
22	6	0	4.087798	-0.11709	0.941008
23	8	0	3.2257	-1.17419	0.438608
24	8	0	2.523295	0.767908	-0.57259
25	6	0	2.271392	1.559707	1.670308
26	6	0	4.13029	2.374313	0.237507
27	6	0	5.395598	-0.23018	0.174008
28	6	0	4.321198	-0.34259	2.417708
29	8	0	1.6658	-1.23209	-1.45039
30	6	0	1.736603	-2.63999	-1.80939
31	6	0	0.779004	-2.7896	-2.97689
32	6	0	1.295005	-3.49789	-0.63669
33	6	0	3.157705	-2.96949	-2.23659
34	5	0	2.453599	-0.61069	-0.53679
35	1	0	0.428602	-2.2287	2.667208
36	1	0	-0.1237	-0.9533	4.750008
37	1	0	-1.419606	1.173399	4.549908
38	1	0	-2.167707	1.982896	2.365207
39	1	0	-0.244098	-1.3695	0.471707
40	1	0	-0.56931	3.0426	1.199208
41	1	0	-0.568316	5.354	0.440808
42	1	0	-1.727418	6.017197	-1.67659
43	1	0	-2.882014	4.251895	-3.01459
44	1	0	-2.901808	1.912295	-2.25299
45	1	0	-1.413599	-1.1014	-1.23559
46	1	0	-3.913203	0.586291	-0.59909
47	1	0	-4.705401	-0.60241	2.314808
48	1	0	-3.211799	-1.52371	2.586907
49	1	0	-4.779897	-2.36161	2.555008
50	1	0	-5.731697	-2.26221	-1.55809
51	1	0	-6.280794	-2.89831	0.008307
52	1	0	-6.376799	-1.15771	-0.32739
53	1	0	-2.773593	-3.47281	-1.16659
54	1	0	-3.495992	-4.25081	0.255807
55	1	0	-2.020294	-3.285	0.437407
56	1	0	1.632091	2.364706	1.282907
57	1	0	2.769291	1.928808	2.576608
58	1	0	1.624695	0.714406	1.941308
59	1	0	4.78169	2.650014	1.078608
60	1	0	3.484589	3.235211	0.018107
61	1	0	4.757592	2.185214	-0.64109
62	1	0	5.8084	-1.23678	0.322408
63	1	0	6.136896	0.497218	0.529408
64	1	0	5.251396	-0.08028	-0.90549
65	1	0	4.897796	0.488415	2.847608
66	1	0	4.897701	-1.26519	2.565107
67	1	0	3.378998	-0.43699	2.971008
68	1	0	1.100803	-2.1724	-3.82799
69	1	0	-0.237896	-2.4863	-2.68829
70	1	0	0.741607	-3.8353	-3.30959
71	1	0	1.934205	-3.33709	0.240807
72	1	0	1.355508	-4.55949	-0.91319
73	1	0	0.252806	-3.2831	-0.36089
74	1	0	3.204506	-3.99769	-2.61989
75	1	0	3.862105	-2.88889	-1.39799
76	1	0	3.486003	-2.29259	-3.03809

IntG

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			x	y	z
1	6	0	-3.439146	3.46052	0.384828
2	6	0	-4.690932	3.636774	-0.20048
3	6	0	-5.402992	2.500828	-0.59892
4	6	0	-4.880431	1.228676	-0.41263
5	6	0	-3.613149	1.015165	0.182063
6	6	0	-2.9103	2.184459	0.561865
7	6	0	-3.061626	-0.32536	0.385366
8	6	0	-3.340228	-1.38524	-0.59065
9	6	0	-3.485236	-1.11556	-1.97221
10	6	0	-3.699935	-2.12728	-2.90373
11	6	0	-3.774122	-3.46024	-2.49987
12	6	0	-3.632622	-3.75513	-1.14279
13	6	0	-3.418343	-2.74399	-0.21305
14	6	0	-2.12619	-0.51942	1.435136
15	6	0	-1.196001	-1.51341	1.698691
16	14	0	0.083261	-1.31441	3.013539
17	6	0	1.095511	0.254705	2.682604
18	6	0	1.252936	-2.79257	2.999625
19	6	0	-0.638169	-1.11995	4.748027
20	6	0	3.368859	-1.34883	-1.40443
21	6	0	4.488508	-0.62992	-0.59188
22	8	0	4.05381	0.76021	-0.63067
23	8	0	2.206633	-0.52759	-1.09822
24	6	0	3.577952	-1.27753	-2.90797
25	6	0	3.091057	-2.77247	-0.9818
26	6	0	4.522274	-1.03804	0.872811
27	6	0	5.86995	-0.72876	-1.19674
28	8	0	1.797581	1.729118	-0.63344
29	6	0	2.080558	3.104441	-0.25136
30	6	0	0.713875	3.737338	-0.0672
31	6	0	2.843063	3.771324	-1.38172
32	6	0	2.863092	3.139231	1.050109
33	5	0	2.695984	0.725531	-0.77377
34	19	0	-0.436075	0.078147	-0.90909
35	1	0	-2.852683	4.326879	0.695298
36	1	0	-5.103991	4.633927	-0.34689
37	1	0	-6.390005	2.609506	-1.05003
38	1	0	-5.4738	0.364242	-0.7129
39	1	0	-1.917331	2.096836	1.009054
40	1	0	-3.441436	-0.08163	-2.32249
41	1	0	-3.806498	-1.86905	-3.95796
42	1	0	-3.942257	-4.25344	-3.22726
43	1	0	-3.700974	-4.78836	-0.80064
44	1	0	-3.336939	-3.00094	0.842825
45	1	0	-2.089113	0.331142	2.13239
46	1	0	-1.163397	-2.40255	1.055597
47	1	0	1.537249	0.228574	1.673461
48	1	0	1.917908	0.392737	3.402606
49	1	0	0.453725	1.149132	2.738729
50	1	0	0.740249	-3.71242	3.317311
51	1	0	2.105457	-2.63457	3.676978
52	1	0	1.655865	-2.97461	1.99177
53	1	0	-1.336723	-0.27073	4.79154
54	1	0	0.151848	-0.93841	5.492818
55	1	0	-1.192819	-2.01863	5.054483
56	1	0	2.664772	-1.61926	-3.41248
57	1	0	4.402616	-1.92784	-3.22685
58	1	0	3.792462	-0.25494	-3.24636
59	1	0	3.989483	-3.39176	-1.1115
60	1	0	2.2954	-3.19963	-1.60638
61	1	0	2.774369	-2.83638	0.065195
62	1	0	5.17666	-0.34648	1.419733
63	1	0	4.919691	-2.0541	0.996681
64	1	0	3.526037	-0.99855	1.336923
65	1	0	6.179467	-1.78043	-1.27311
66	1	0	6.594307	-0.21049	-0.5549
67	1	0	5.915515	-0.27816	-2.19456
68	1	0	0.16577	3.241852	0.748157
69	1	0	0.118976	3.662899	-0.98917
70	1	0	0.813769	4.800175	0.189488
71	1	0	3.820982	3.296898	-1.53732
72	1	0	3.014467	4.830386	-1.1463
73	1	0	2.272689	3.717653	-2.31919
74	1	0	2.997071	4.182178	1.367926
75	1	0	3.856155	2.686468	0.940209
76	1	0	2.321386	2.608603	1.845477

TS_{GH}

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) x	y	z
1	6	0	3.500616	2.835191	-1.51028
2	6	0	3.133081	3.914966	-0.71037
3	6	0	2.503902	3.663701	0.509816
4	6	0	2.220642	2.361582	0.90628
5	6	0	2.543404	1.252591	0.100416
6	6	0	3.215393	1.532453	-1.10798
7	6	0	2.169763	-0.12776	0.485072
8	6	0	3.134761	-1.21292	0.249257
9	6	0	0.922031	-0.42009	1.054207
10	6	0	4.529298	-0.98384	0.269336
11	6	0	5.445332	-2.00884	0.072709
12	6	0	5.016168	-3.31845	-0.15604
13	6	0	3.647362	-3.57357	-0.18543
14	6	0	2.727969	-2.54364	-0.0002
15	6	0	-0.242372	0.355503	1.251843
16	5	0	-2.054312	0.129651	-0.20007
17	14	0	-1.064243	0.142733	2.910188
18	8	0	-2.934548	-0.72039	0.500632
19	6	0	-3.400187	-1.69527	-0.43428
20	6	0	-2.168386	-1.87099	-1.37023
21	8	0	-1.584841	-0.5484	-1.36381
22	6	0	-3.818912	-2.94916	0.307343
23	6	0	-4.612258	-1.11404	-1.15664
24	6	0	-2.508471	-2.23934	-2.80101
25	6	0	-1.159318	-2.86432	-0.81045
26	6	0	-1.456124	-1.65955	3.310044
27	6	0	0.114712	0.733319	4.27882
28	6	0	-2.61453	1.19543	3.104453
29	6	0	-2.001117	2.541888	-1.07182
30	1	0	4.017715	3.003921	-2.45499
31	1	0	3.350844	4.935559	-1.02221
32	1	0	2.237787	4.492415	1.166364
33	1	0	1.747799	2.18939	1.872646
34	1	0	3.560107	0.710141	-1.74119
35	1	0	0.839	-1.4636	1.393604
36	1	0	4.898119	0.022436	0.469575
37	1	0	6.51167	-1.78444	0.110635
38	1	0	5.735938	-4.12129	-0.30943
39	1	0	3.283794	-4.58538	-0.36719
40	1	0	1.66411	-2.78644	-0.03845
41	1	0	-0.127266	1.416798	0.997457
42	1	0	-4.67961	-2.72227	0.951214
43	1	0	-4.124079	-3.73684	-0.39676
44	1	0	-3.018871	-3.34417	0.943629
45	1	0	-4.35624	-0.20641	-1.71966
46	1	0	-5.36603	-0.83851	-0.40735
47	1	0	-5.066975	-1.83725	-1.84768
48	1	0	-1.591312	-2.37901	-3.39316
49	1	0	-3.109864	-1.46363	-3.28945
50	1	0	-3.06444	-3.18716	-2.83666
51	1	0	-0.859657	-2.60529	0.21352
52	1	0	-0.258915	-2.89898	-1.44344
53	1	0	-1.563797	-3.88498	-0.80997
54	1	0	-2.235473	-2.04603	2.63976
55	1	0	-1.823458	-1.74214	4.344674
56	1	0	-0.571654	-2.30913	3.22804
57	1	0	1.079791	0.204689	4.231164
58	1	0	0.323417	1.810858	4.190214
59	1	0	-0.312418	0.56273	5.280056
60	1	0	-2.994111	1.119963	4.135541
61	1	0	-3.407685	0.886771	2.412299
62	1	0	-2.391789	2.255899	2.911236
63	19	0	0.944794	-0.47604	-2.14379
64	8	0	-2.343723	1.476261	-0.19194
65	6	0	-0.672948	2.343792	-1.79394
66	1	0	0.138145	2.131778	-1.08152
67	1	0	-0.761472	1.542373	-2.54002
68	1	0	-0.404358	3.263126	-2.3327
69	6	0	-1.922889	3.787875	-0.20099
70	1	0	-2.863125	3.923315	0.35102
71	1	0	-1.106237	3.698425	0.530155
72	1	0	-1.743552	4.684506	-0.81058
73	6	0	-3.120804	2.678853	-2.09551
74	1	0	-4.085708	2.82411	-1.59034
75	1	0	-2.943652	3.536899	-2.7602
76	1	0	-3.188434	1.773085	-2.71593

IntH

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) x	y	z
1	6	0	3.499609	2.728315	-1.84732
2	6	0	3.116867	3.874925	-1.15285
3	6	0	2.447404	3.741295	0.061277
4	6	0	2.137269	2.48005	0.56377
5	6	0	2.48262	1.312452	-0.13298
6	6	0	3.195578	1.468825	-1.33731
7	6	0	2.10029	-0.05031	0.328708
8	6	0	3.149016	-1.10029	0.231797
9	6	0	0.850438	-0.37138	0.777467
10	6	0	4.480792	-0.81005	0.572217
11	6	0	5.470919	-1.78487	0.512444
12	6	0	5.160403	-3.08113	0.101324
13	6	0	3.847335	-3.38572	-0.24892
14	6	0	2.857655	-2.40686	-0.189
15	6	0	-0.360317	0.445161	0.947089
16	5	0	-1.734847	-0.08502	0.129269
17	14	0	-0.77446	0.509505	2.804234
18	8	0	-2.37537	-1.17098	0.876109
19	6	0	-2.979609	-2.06216	-0.03464
20	6	0	-1.99108	-2.03639	-1.24841
21	8	0	-1.423964	-0.73202	-1.19168
22	6	0	-3.114791	-3.42363	0.631143
23	6	0	-4.383311	-1.57125	-0.39598
24	6	0	-2.648389	-2.2414	-2.60506
25	6	0	-0.865386	-3.0568	-1.09849
26	6	0	-0.68643	-1.19589	3.603558
27	6	0	0.497514	1.568363	3.728138
28	6	0	-2.440861	1.311237	3.147414
29	6	0	-2.724649	2.100008	-0.91911
30	1	0	4.04639	2.81207	-2.78609
31	1	0	3.354408	4.862249	-1.54624
32	1	0	2.1652	4.627413	0.62922
33	1	0	1.631695	2.399131	1.523723
34	1	0	3.541985	0.58279	-1.87702
35	1	0	0.723398	-1.42588	1.05344
36	1	0	4.739649	0.19667	0.90261
37	1	0	6.492666	-1.53138	0.793995
38	1	0	5.935845	-3.84439	0.051264
39	1	0	3.588823	-4.39101	-0.58087
40	1	0	1.837532	-2.66485	-0.47667
41	1	0	-0.164513	1.487569	0.662551
42	1	0	-3.829033	-3.35173	1.46386
43	1	0	-3.494467	-4.18155	-0.0707
44	1	0	-2.160581	-3.77564	1.042589
45	1	0	-4.356567	-0.59809	-0.89871
46	1	0	-4.954617	-1.44376	0.534688
47	1	0	-4.922092	-2.29157	-1.0295
48	1	0	-1.886852	-2.20508	-3.4011
49	1	0	-3.395167	-1.46809	-2.8204
50	1	0	-3.139086	-3.22434	-2.66813
51	1	0	-0.372275	-2.96769	-0.12169
52	1	0	-0.109059	-2.88634	-1.88245
53	1	0	-1.219443	-4.09082	-1.21615
54	1	0	0.344664	-1.58011	3.623822
55	1	0	-1.316997	-1.91704	3.066205
56	1	0	-1.034144	-1.13945	4.646708
57	1	0	1.528521	1.208657	3.589854
58	1	0	0.459484	2.626047	3.42503
59	1	0	0.282499	1.534658	4.808117
60	1	0	-2.45462	2.351864	2.790532
61	1	0	-2.629778	1.326985	4.232506
62	1	0	-3.257962	0.77771	2.64723
63	19	0	0.638848	0.032125	-2.47908
64	8	0	-2.675641	1.036399	-0.00491
65	6	0	-1.444077	2.939309	-0.95372
66	1	0	-1.183607	3.30624	0.050431
67	1	0	-0.57738	2.375919	-1.33391
68	1	0	-1.575677	3.81178	-1.61045
69	6	0	-3.863818	2.99759	-0.43852
70	1	0	-4.799663	2.421873	-0.39586
71	1	0	-3.652856	3.37313	0.573162
72	1	0	-4.014545	3.858818	-1.10608
73	6	0	-3.05148	1.631194	-2.34084
74	1	0	-4.003527	1.080942	-2.35424
75	1	0	-3.147416	2.491081	-3.0209
76	1	0	-2.279525	0.955965	-2.73285

3ad

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) x	y	z
1	6	0	-3.175861	-1.86374	-2.86734
2	6	0	-3.183101	-3.15949	-2.35123
3	6	0	-2.768039	-3.37783	-1.03973
4	6	0	-2.342194	-2.30937	-0.25247
5	6	0	-2.3209	-1.00548	-0.76002
6	6	0	-2.755445	-0.79861	-2.07659
7	6	0	-1.869298	0.149673	0.061723
8	6	0	-2.838108	1.258535	0.250806
9	6	0	-4.210412	0.993356	0.377826
10	6	0	-5.125808	2.020989	0.585145
11	6	0	-4.692775	3.343714	0.660167
12	6	0	-3.33499	3.62575	0.519037
13	6	0	-2.421052	2.597151	0.31052
14	6	0	-0.630166	0.226153	0.59529
15	6	0	0.509484	-0.71941	0.452736
16	14	0	1.057447	-1.37636	2.169833
17	5	0	1.758315	-0.03363	-0.19162
18	6	0	1.390532	0.078169	3.312312
19	6	0	-0.294944	-2.44328	2.918311
20	6	0	2.612131	-2.412	1.966335
21	8	0	2.689376	-0.71447	-0.93494
22	6	0	3.583901	0.273197	-1.50742
23	6	0	3.419413	1.477195	-0.53016
24	8	0	2.064419	1.297571	-0.04349
25	6	0	3.536049	2.840084	-1.17692
26	6	0	4.33549	1.399947	0.681556
27	6	0	4.98038	-0.30623	-1.57146
28	6	0	3.075914	0.564277	-2.91095
29	1	0	-3.50053	-1.68153	-3.89139
30	1	0	-3.515785	-3.99368	-2.96777
31	1	0	-2.780247	-4.38448	-0.62276
32	1	0	-2.03406	-2.48436	0.778512
33	1	0	-2.757248	0.213865	-2.48355
34	1	0	-4.563325	-0.03738	0.325658
35	1	0	-6.184582	1.78558	0.69001
36	1	0	-5.409002	4.149371	0.816619
37	1	0	-2.98448	4.656887	0.555741
38	1	0	-1.366866	2.837626	0.169322
39	1	0	-0.407806	1.119597	1.187548
40	1	0	0.245353	-1.60801	-0.14276
41	1	0	0.459142	0.586568	3.60018
42	1	0	2.050245	0.825741	2.848369
43	1	0	1.875372	-0.26905	4.236634
44	1	0	-1.24292	-1.8948	3.017033
45	1	0	-0.47918	-3.34873	2.32256
46	1	0	0.004992	-2.76729	3.926259
47	1	0	2.856814	-2.91795	2.912032
48	1	0	3.4823	-1.80612	1.675639
49	1	0	2.477889	-3.18612	1.196997
50	1	0	3.414543	3.62316	-0.41668
51	1	0	4.527633	2.966028	-1.6343
52	1	0	2.773962	2.996399	-1.94871
53	1	0	5.382074	1.587832	0.407706
54	1	0	4.032132	2.166527	1.406753
55	1	0	4.278707	0.421399	1.178832
56	1	0	5.002352	-1.14111	-2.28447
57	1	0	5.697792	0.451201	-1.91782
58	1	0	5.31488	-0.68441	-0.59828
59	1	0	3.739276	1.257842	-3.4445
60	1	0	3.039592	-0.37516	-3.47774
61	1	0	2.06359	0.990338	-2.89869

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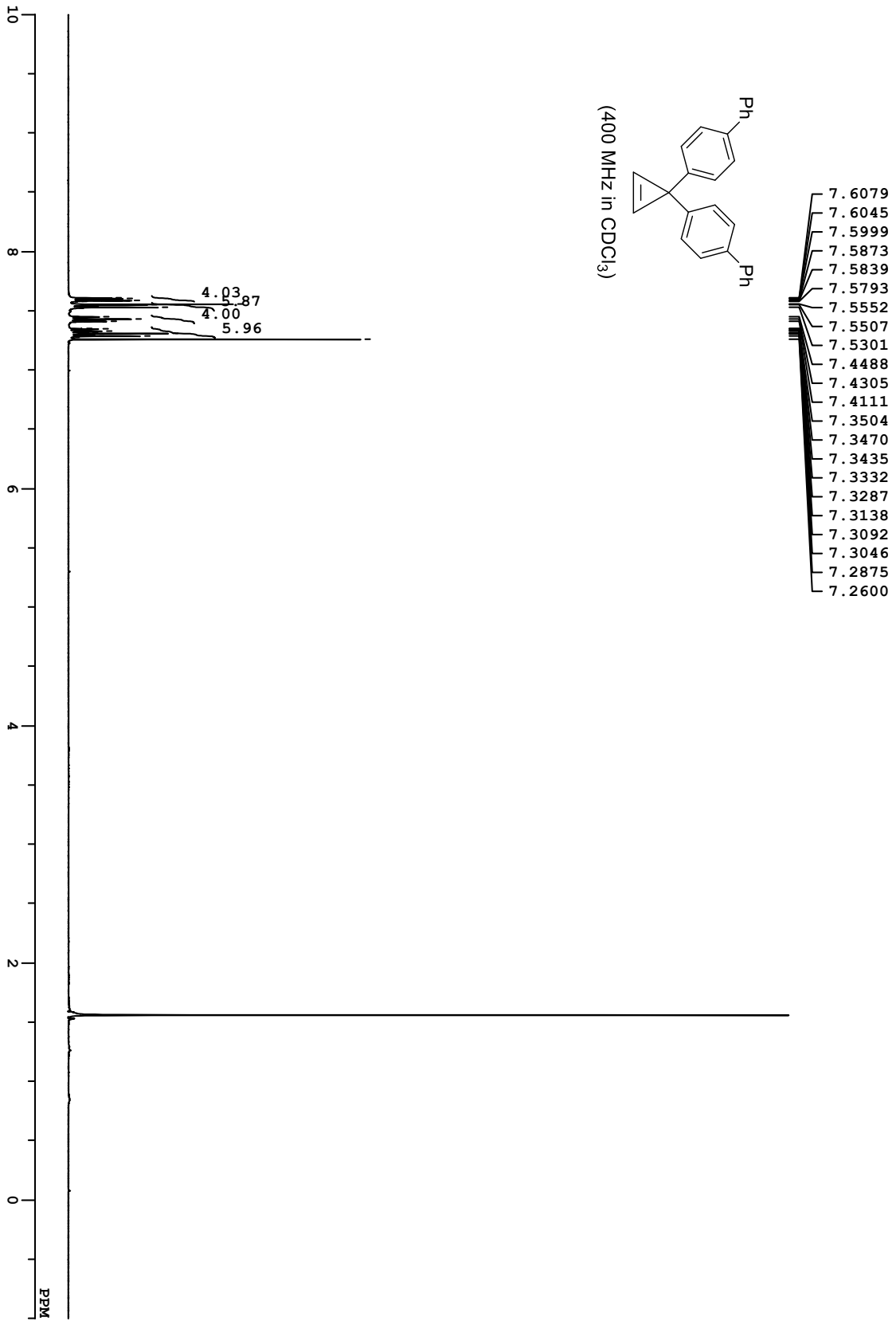
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			x	y	z
1	6	0	1.097377	-0.00015	0.000005
2	6	0	1.645195	0.739739	-1.23331
3	1	0	1.279948	0.253566	-2.1516
4	1	0	1.279978	1.778834	-1.23647
5	1	0	2.747462	0.763314	-1.2725
6	6	0	1.644821	-1.43833	-0.02387
7	1	0	2.747068	-1.48446	-0.02371
8	1	0	1.278544	-1.99031	0.856047
9	1	0	1.280053	-1.96047	-0.9224
10	6	0	1.645435	0.69841	1.257076
11	1	0	1.279914	1.736697	1.294836
12	1	0	1.280823	0.182118	2.158979
13	1	0	2.747699	0.721126	1.296587
14	8	0	-0.269719	-7.4E-05	0.000016
15	19	0	-2.629511	0.000113	0.000038

1a

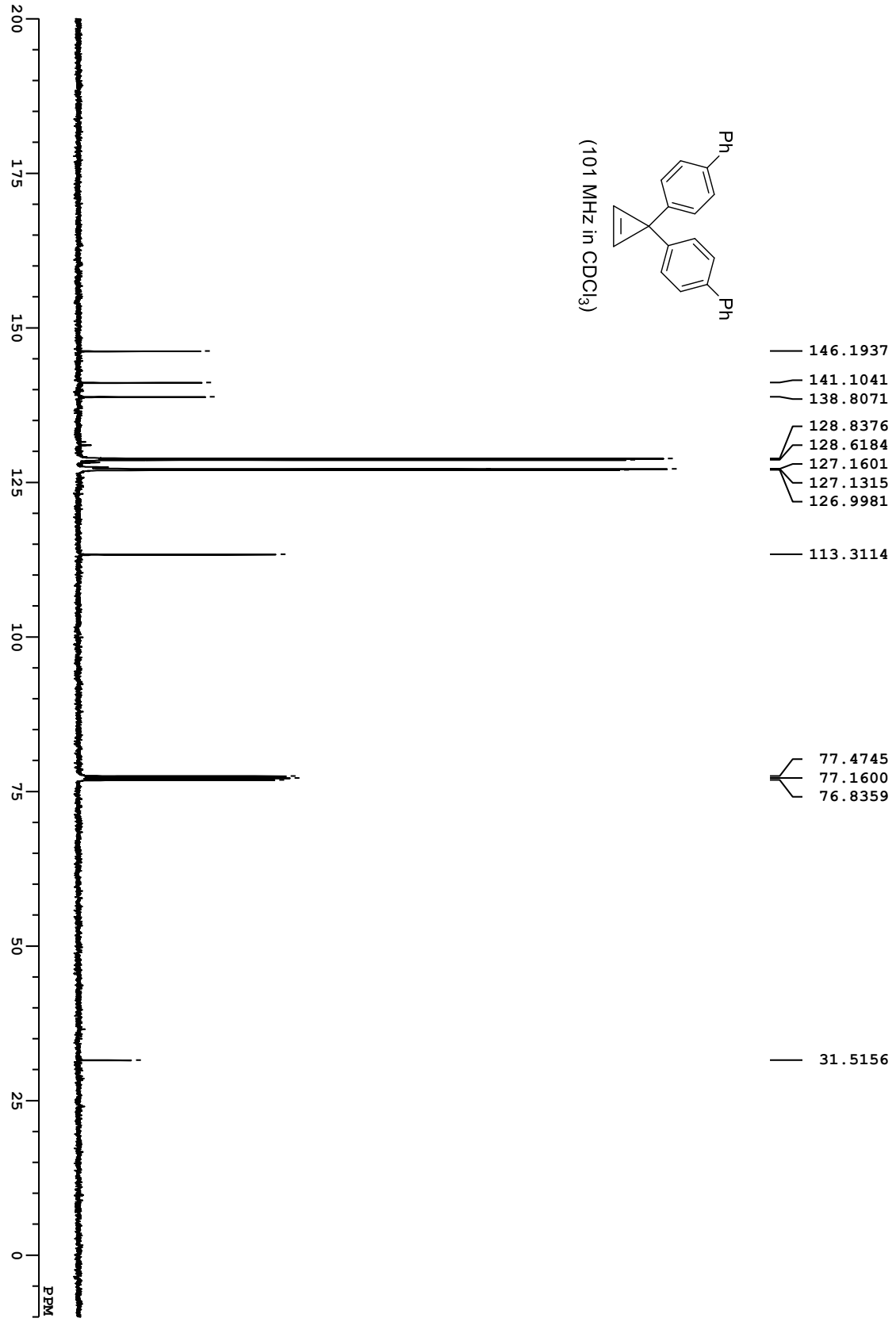
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			x	y	z
1	6	0	-0.002322	2.405483	0.645903
2	6	0	0.00222	2.405343	-0.64608
3	6	0	0.00002	1.04574	0.000056
4	6	0	1.278676	0.250763	0.039782
5	6	0	-1.278664	0.250774	-0.03961
6	6	0	-1.392817	-0.88356	-0.85311
7	6	0	-2.588824	-1.59148	-0.92952
8	6	0	-3.696008	-1.18299	-0.18643
9	6	0	-3.594877	-0.05754	0.627975
10	6	0	-2.397435	0.65205	0.695418
11	6	0	2.397505	0.652241	-0.69509
12	6	0	3.59493	-0.05735	-0.62779
13	6	0	3.696001	-1.18304	0.186336
14	6	0	2.588809	-1.59172	0.929281
15	6	0	1.392778	-0.88375	0.852958
16	1	0	-0.532625	-1.21605	-1.43589
17	1	0	-2.656532	-2.46782	-1.57365
18	1	0	-4.631059	-1.73897	-0.24272
19	1	0	-4.451368	0.270757	1.216262
20	1	0	-2.331872	1.536499	1.331588
21	1	0	2.33197	1.536905	-1.33097
22	1	0	4.4515	0.270985	-1.21593
23	1	0	4.631065	-1.73902	0.242487
24	1	0	2.656429	-2.46822	1.573191
25	1	0	0.53265	-1.21654	1.435678
26	1	0	-0.000075	2.922397	-1.5986
27	1	0	-0.000031	2.923225	1.598047

VI. ^{1}H and ^{13}C NMR Spectra

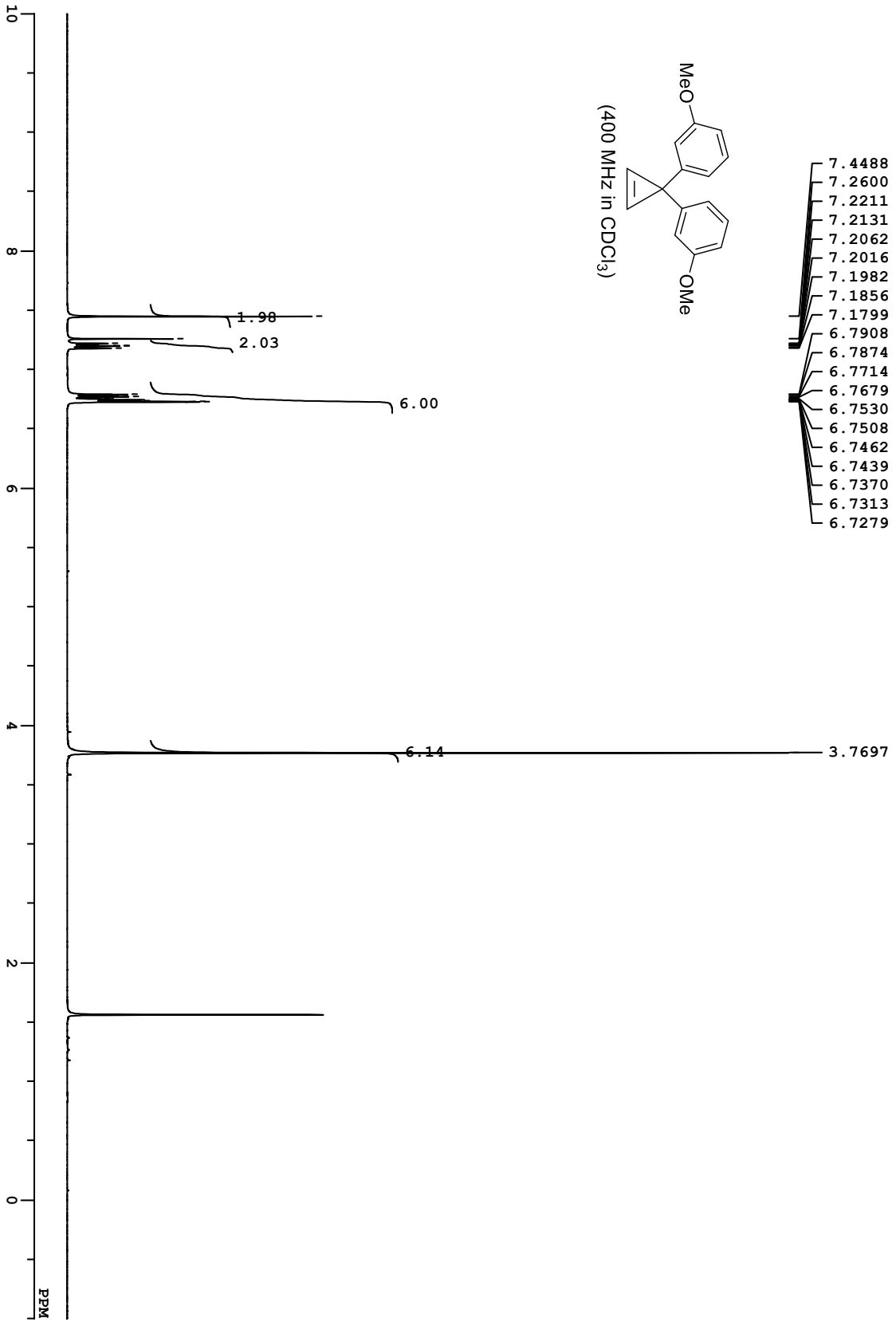
compound **1c**



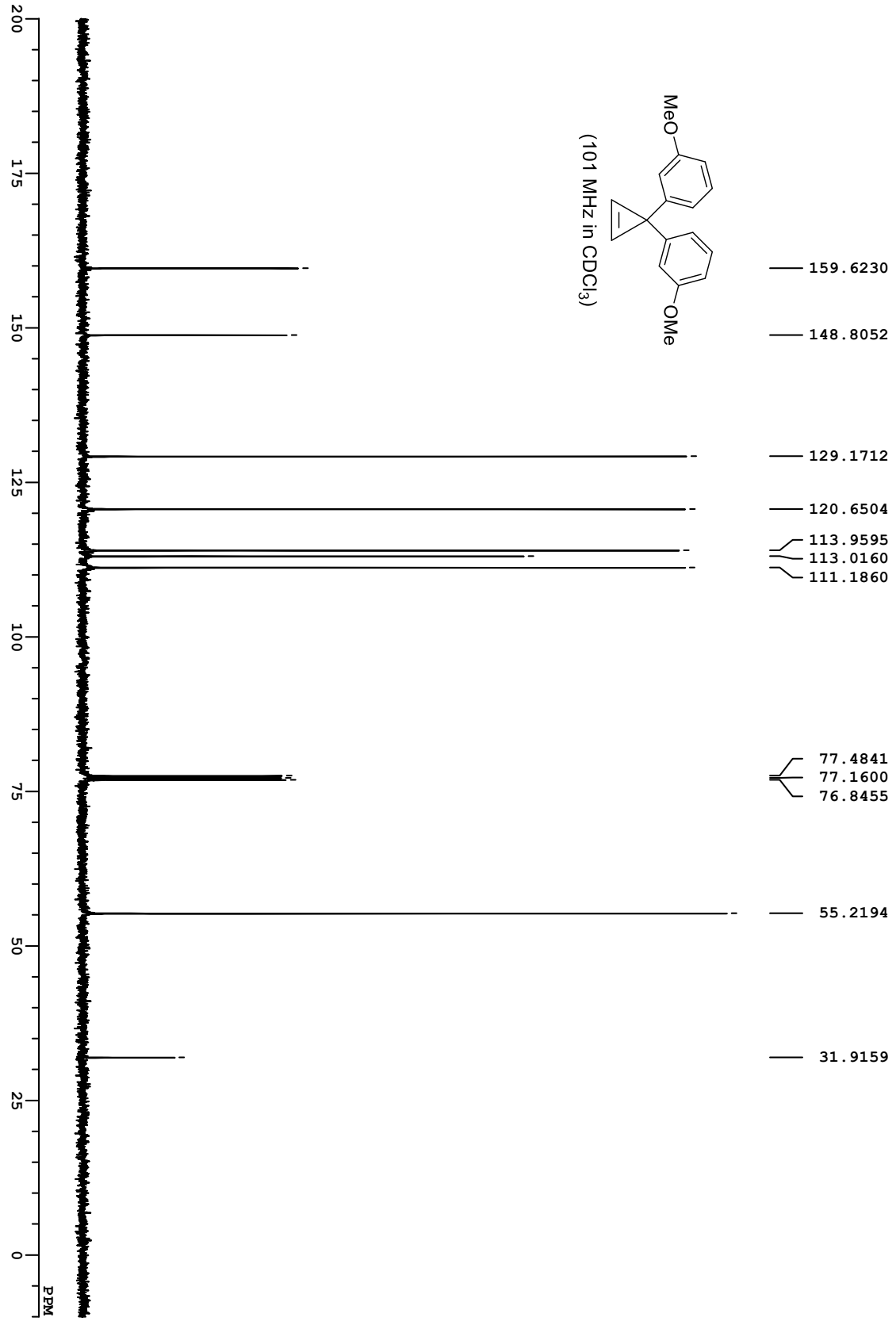
compound **1c**


(101 MHz in CDCl3)
Ph
Ph
146.1937
141.1041
138.8071
128.8376
128.6184
127.1601
127.1315
126.9981
113.3114
77.4745
77.1600
76.8359
31.5156
200
175
150
125
100
75
50
25
0
PPM

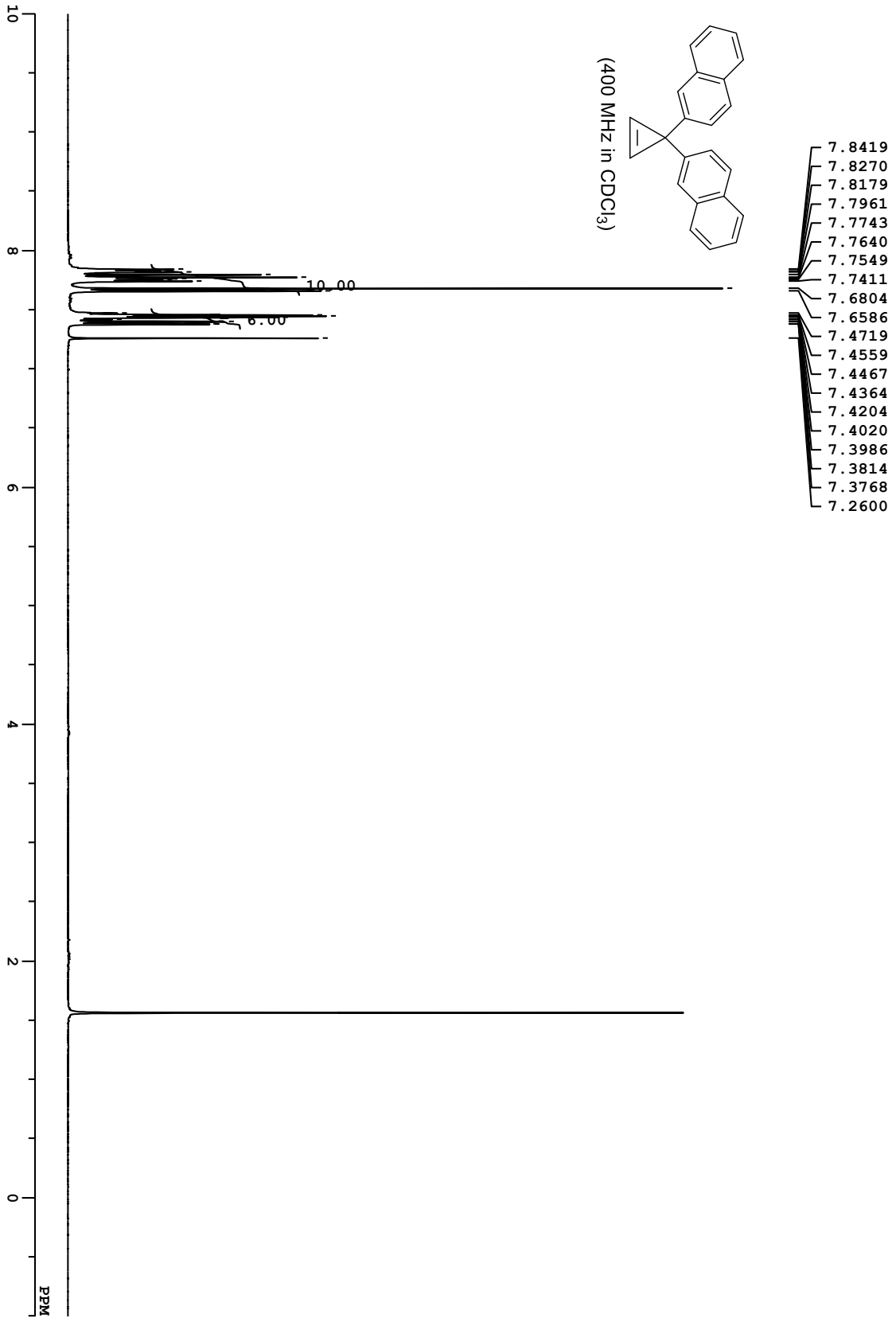
compound **1f**


(400 MHz in CDCl3)
MeO
OMe
7.4488
7.2600
7.2211
7.2131
7.2062
7.2016
7.1982
7.1856
7.1799
6.7908
6.7874
6.7714
6.7679
6.7530
6.7508
6.7462
6.7439
6.7370
6.7313
6.7279
1.98
2.03
6.00
6.14
3.7697
PPM

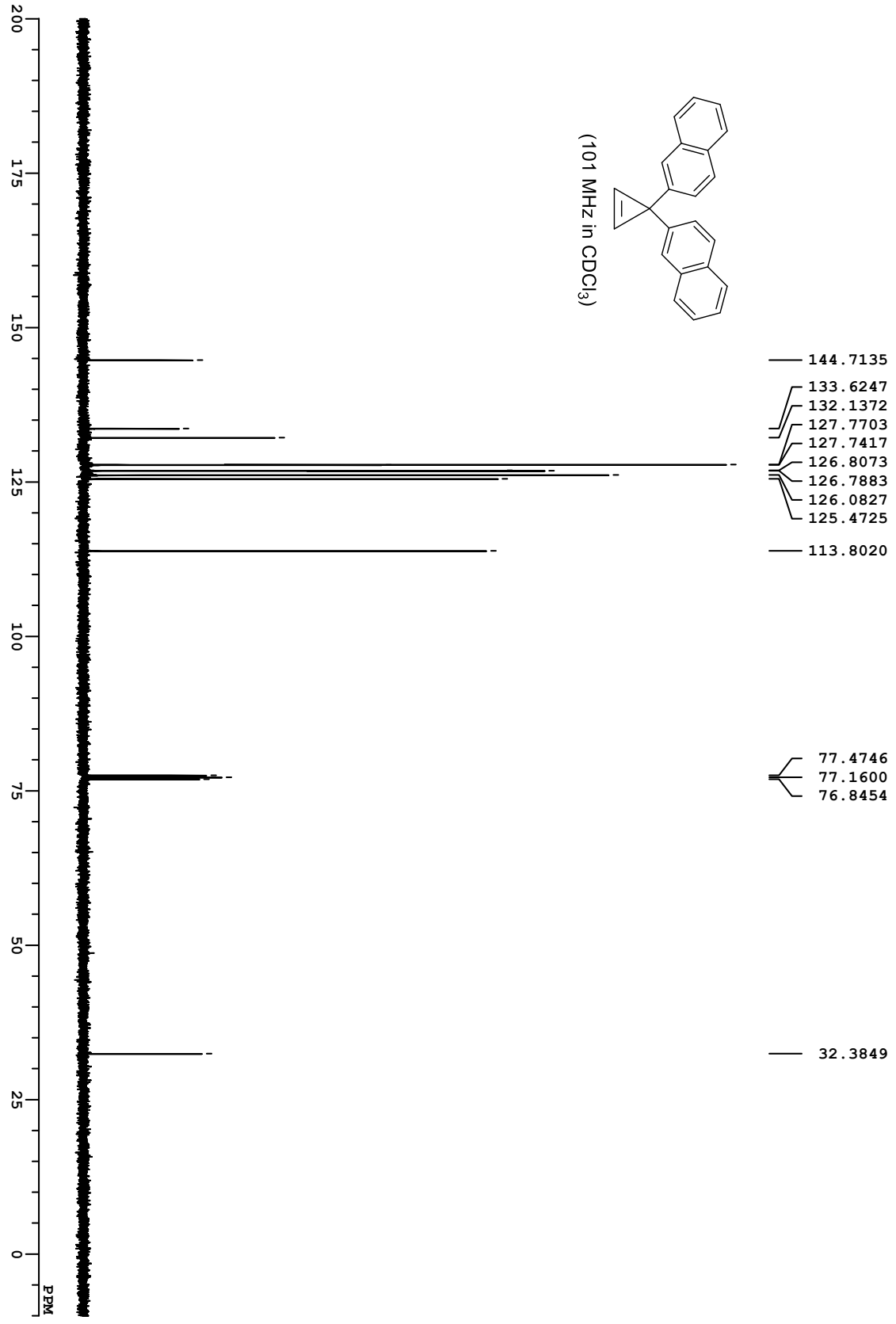
compound **1f**


(101 MHz in CDCl3)
MeO
OMe
159.6230
148.8052
129.1712
120.6504
113.9595
113.0160
111.1860
77.4841
77.1600
76.8455
55.2194
31.9159
200
175
150
125
100
75
50
25
0
PPM

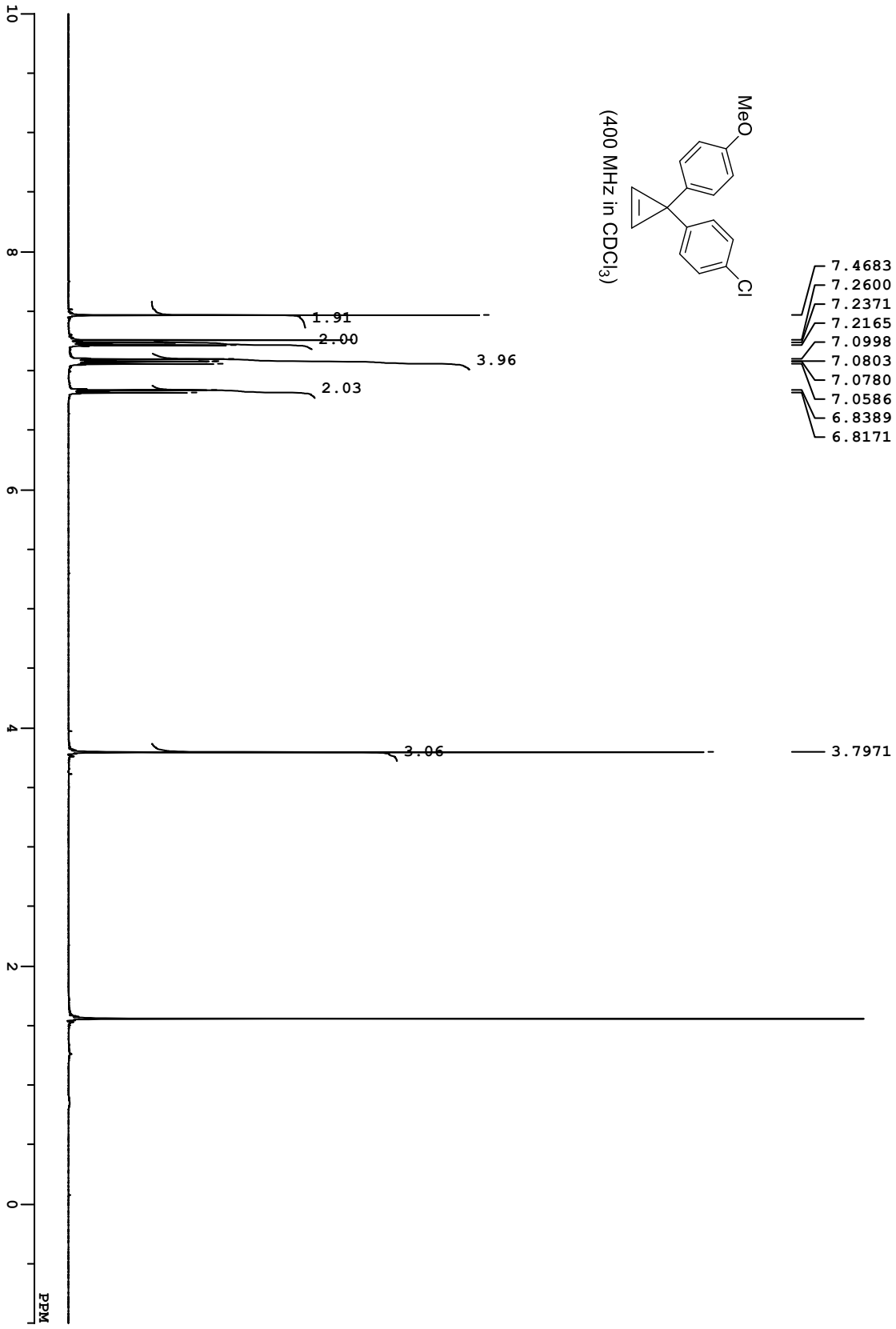
compound **1g**


(400 MHz in CDCl3)
7.8419
7.8270
7.8179
7.7961
7.7743
7.7640
7.7549
7.7411
7.6804
7.6586
7.4719
7.4559
7.4467
7.4364
7.4204
7.4020
7.3986
7.3814
7.3768
7.2600
10.00
6.00
PPM

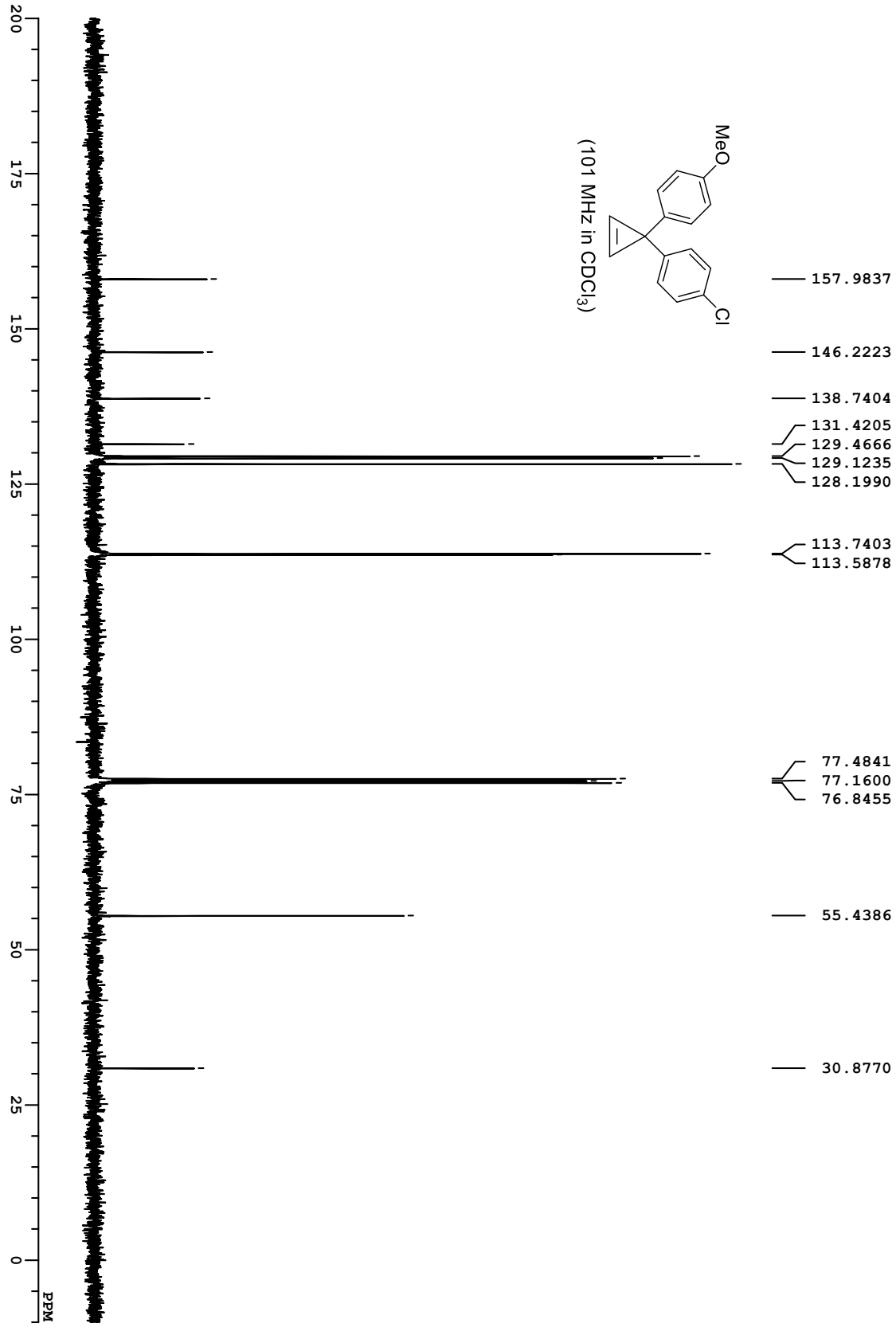
compound **1g**


(101 MHz in CDCl3)
144.7135
133.6247
132.1372
127.7703
127.7417
126.8073
126.7883
126.0827
125.4725
113.8020
77.4746
77.1600
76.8454
32.3849
200
175
150
125
100
75
50
25
0
PPM

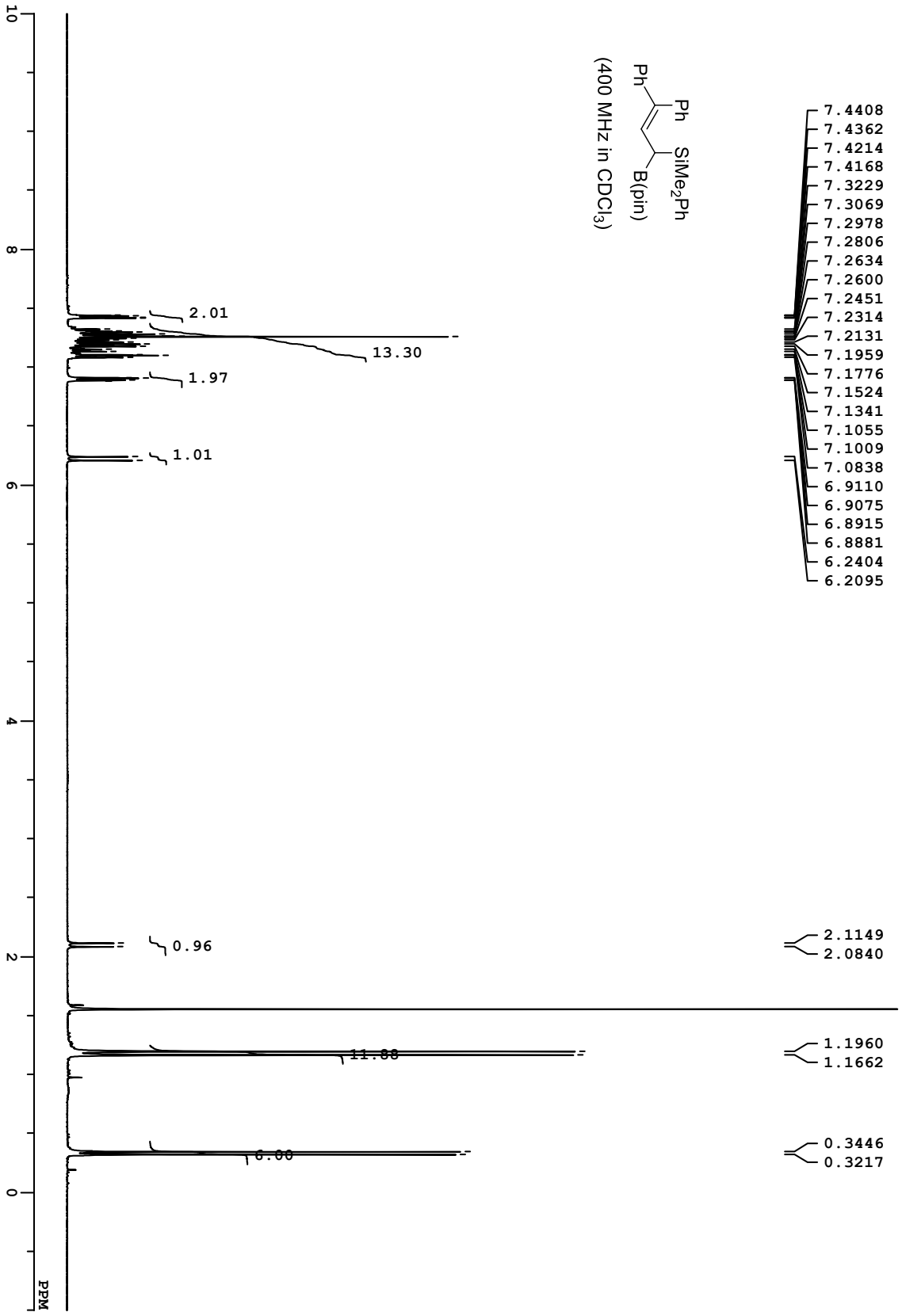
compound **1h**


(400 MHz in CDCl3)
MeO
Cl
7.4683
7.2600
7.2371
7.2165
7.0998
7.0803
7.0780
7.0586
6.8389
6.8171
3.7971
1.91
2.00
3.96
2.03
3.06
PPM

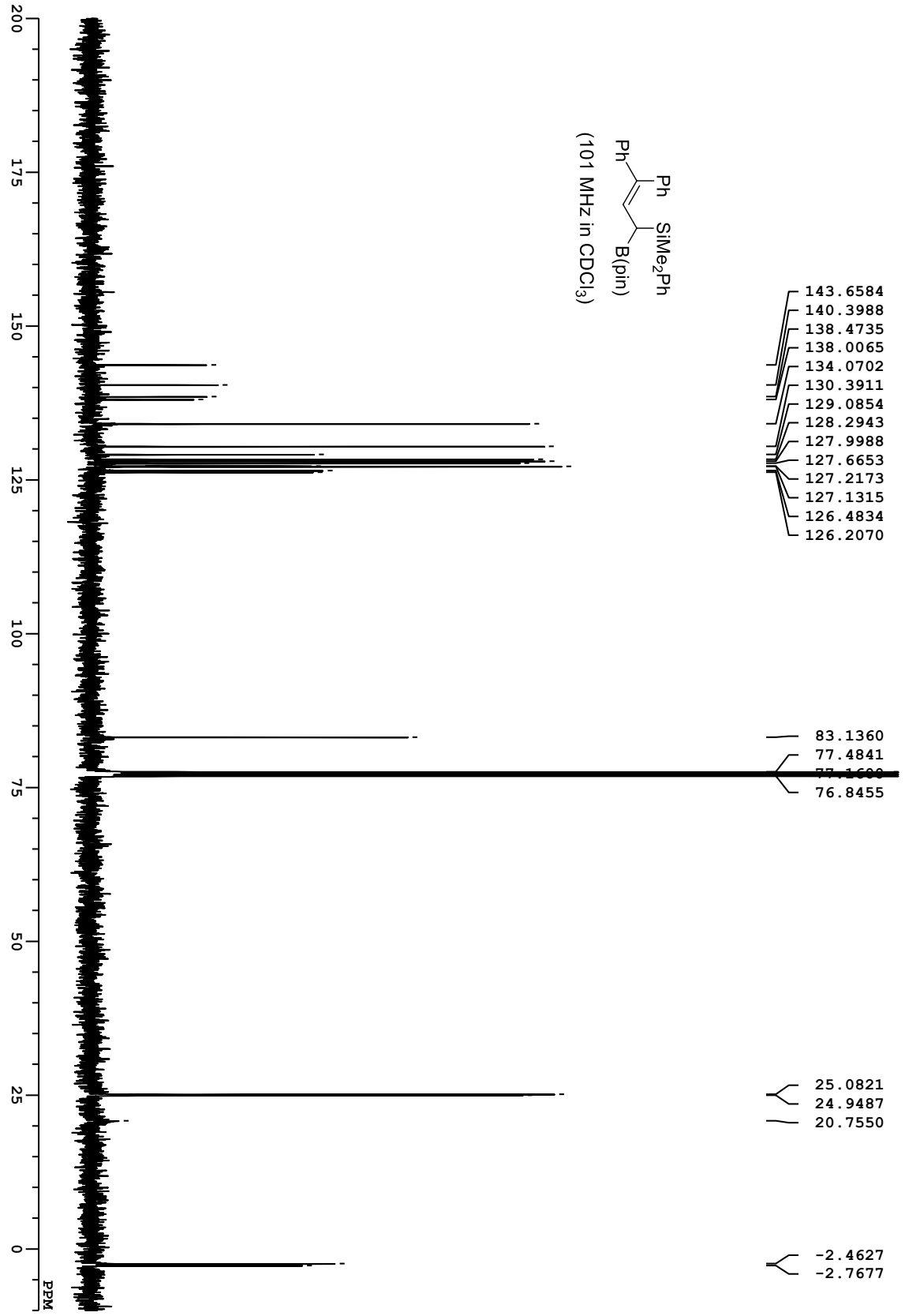
compound **1h**


(101 MHz in CDCl3)
MeO
Cl
157.9837
146.2223
138.7404
131.4205
129.4666
129.1235
128.1990
113.7403
113.5878
77.4841
77.1600
76.8455
55.4386
30.8770
PPM

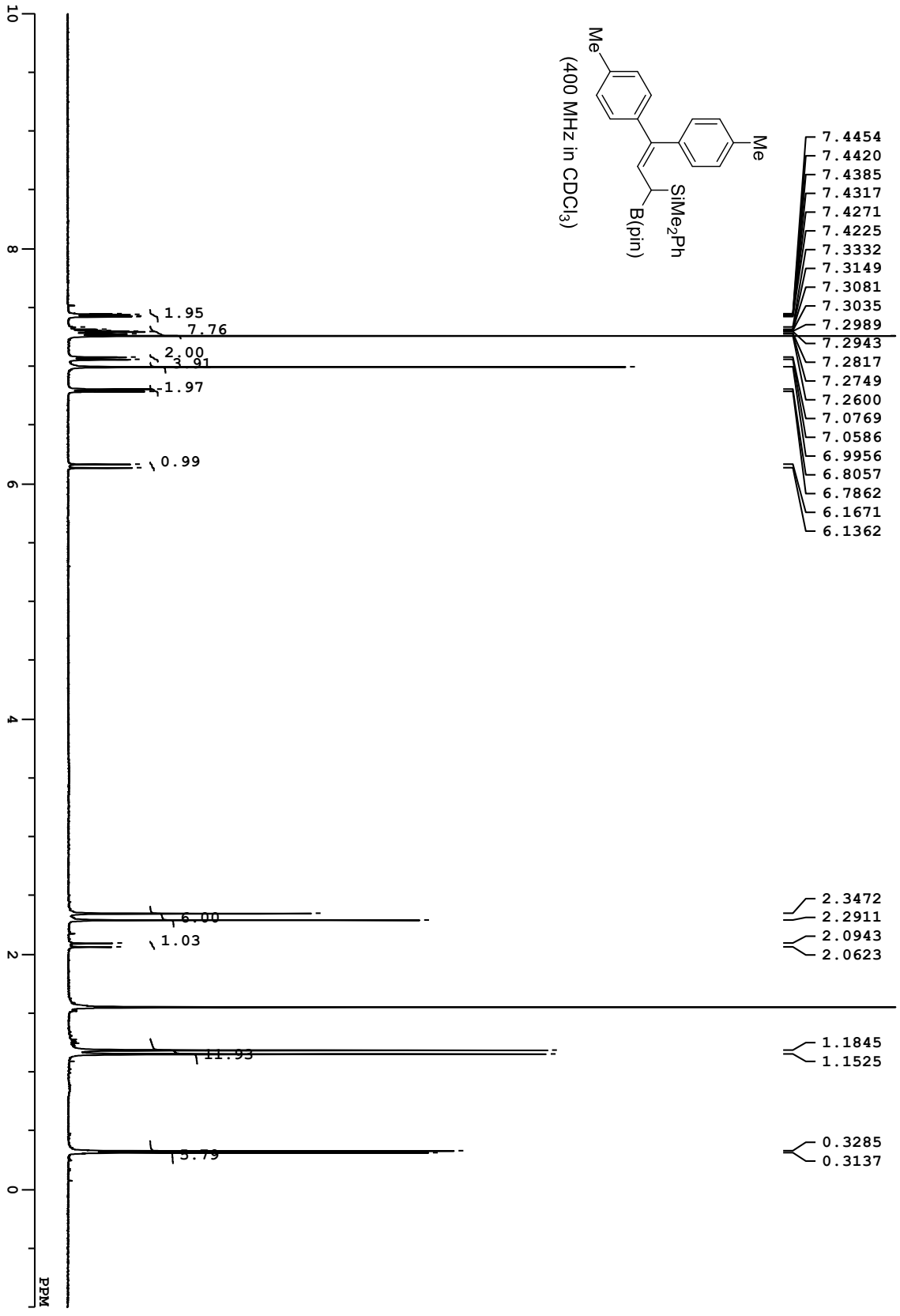
compound **3aa**



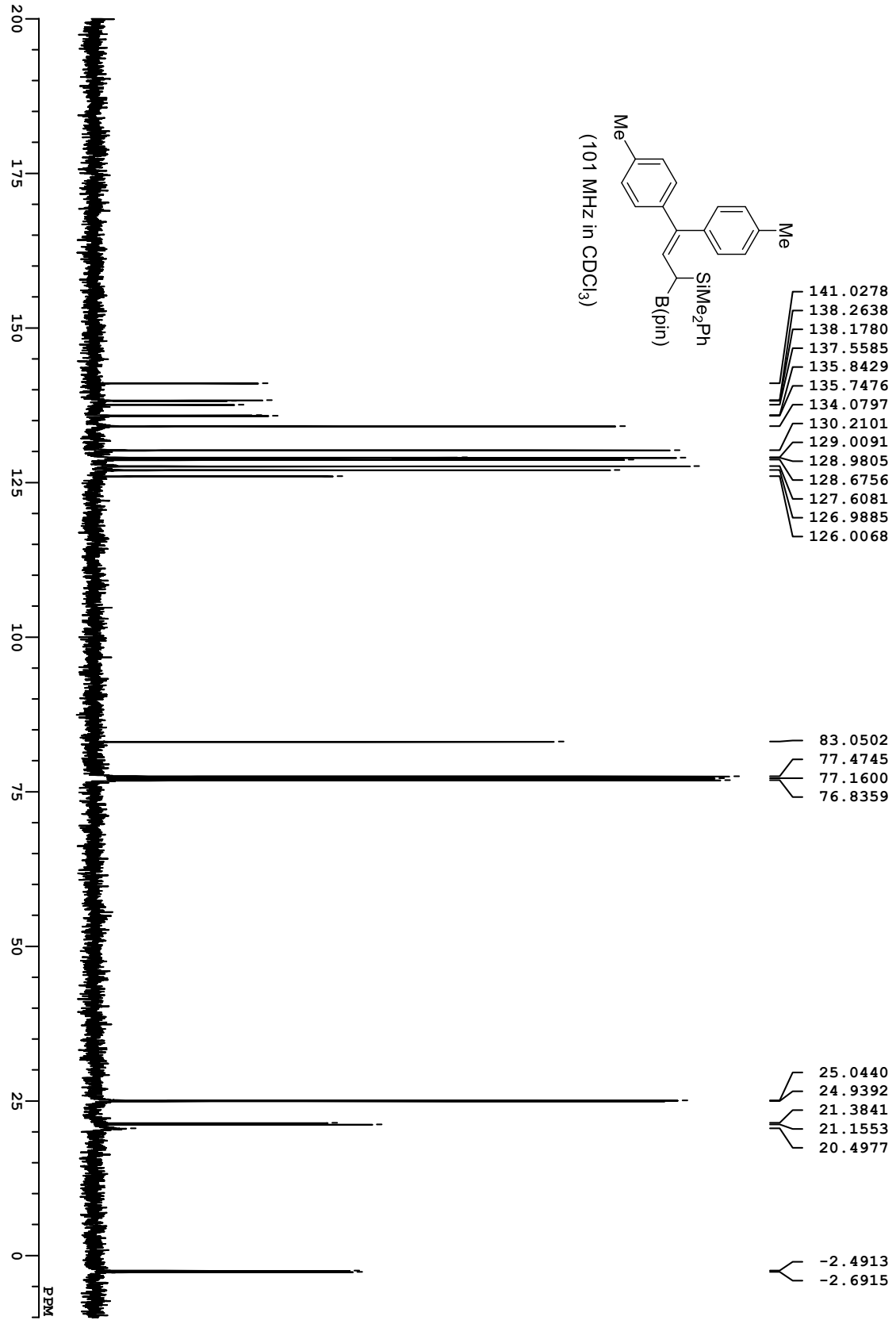
compound **3aa**



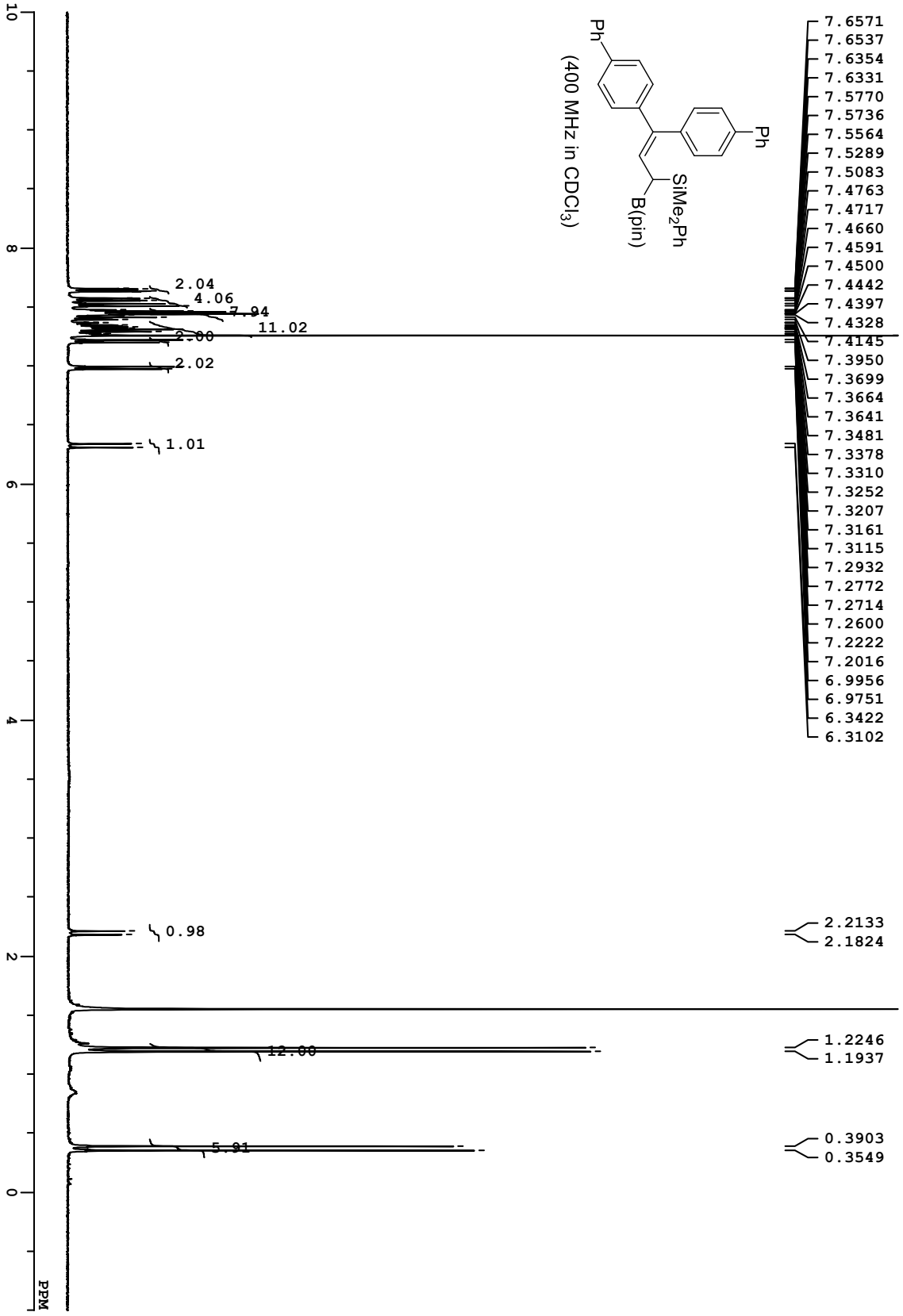
compound **3ba**



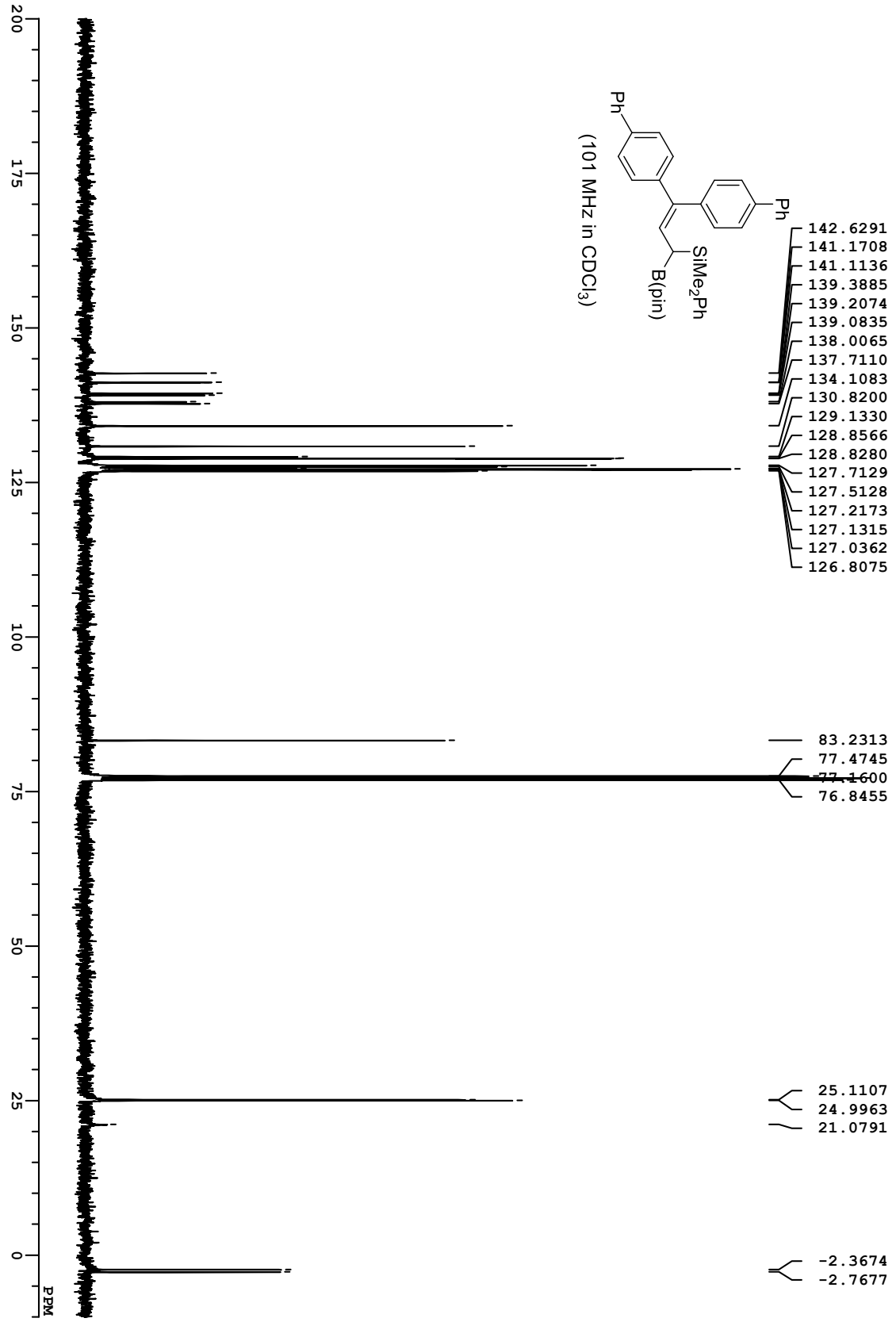
compound **3ba**



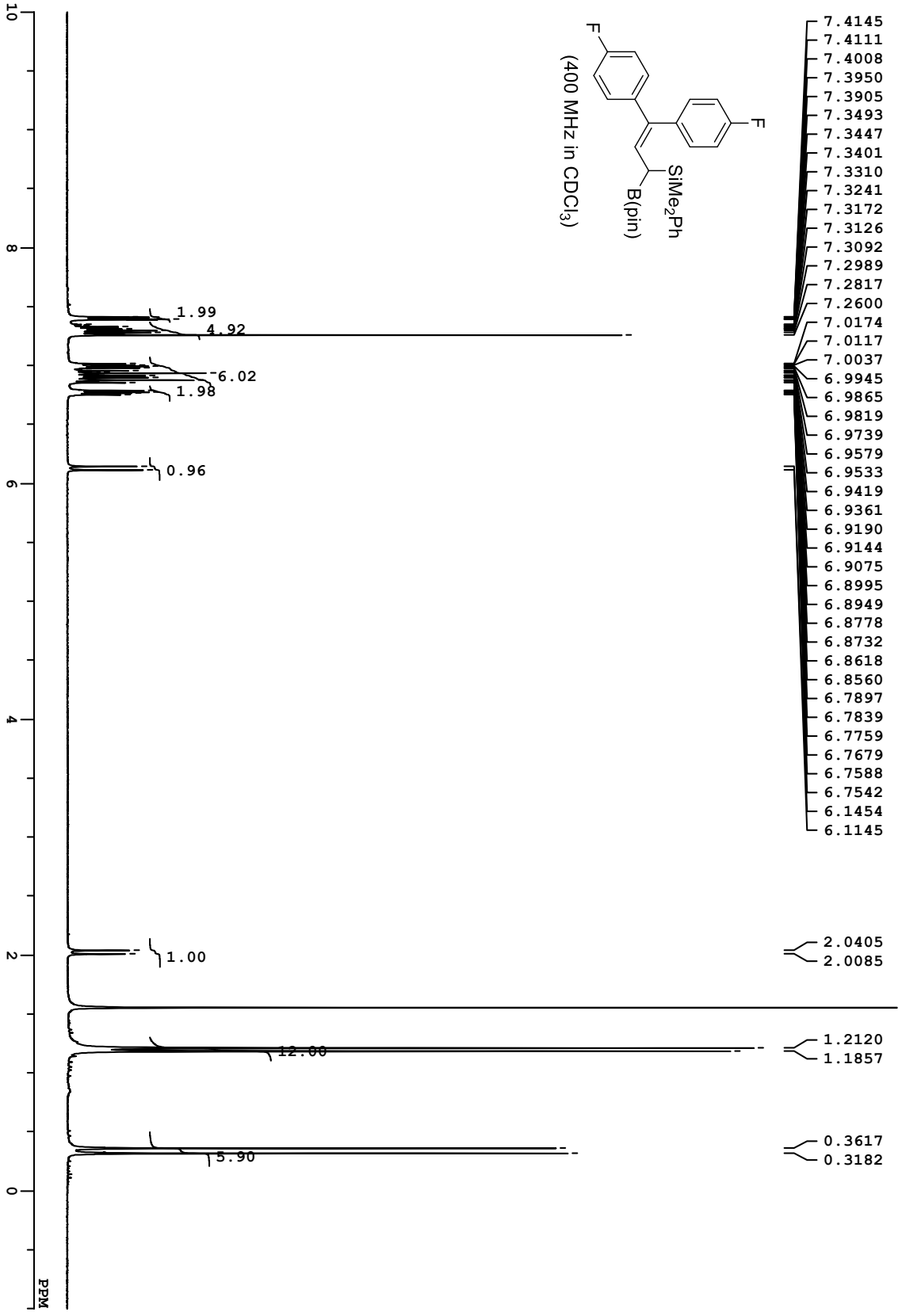
compound **3ca**



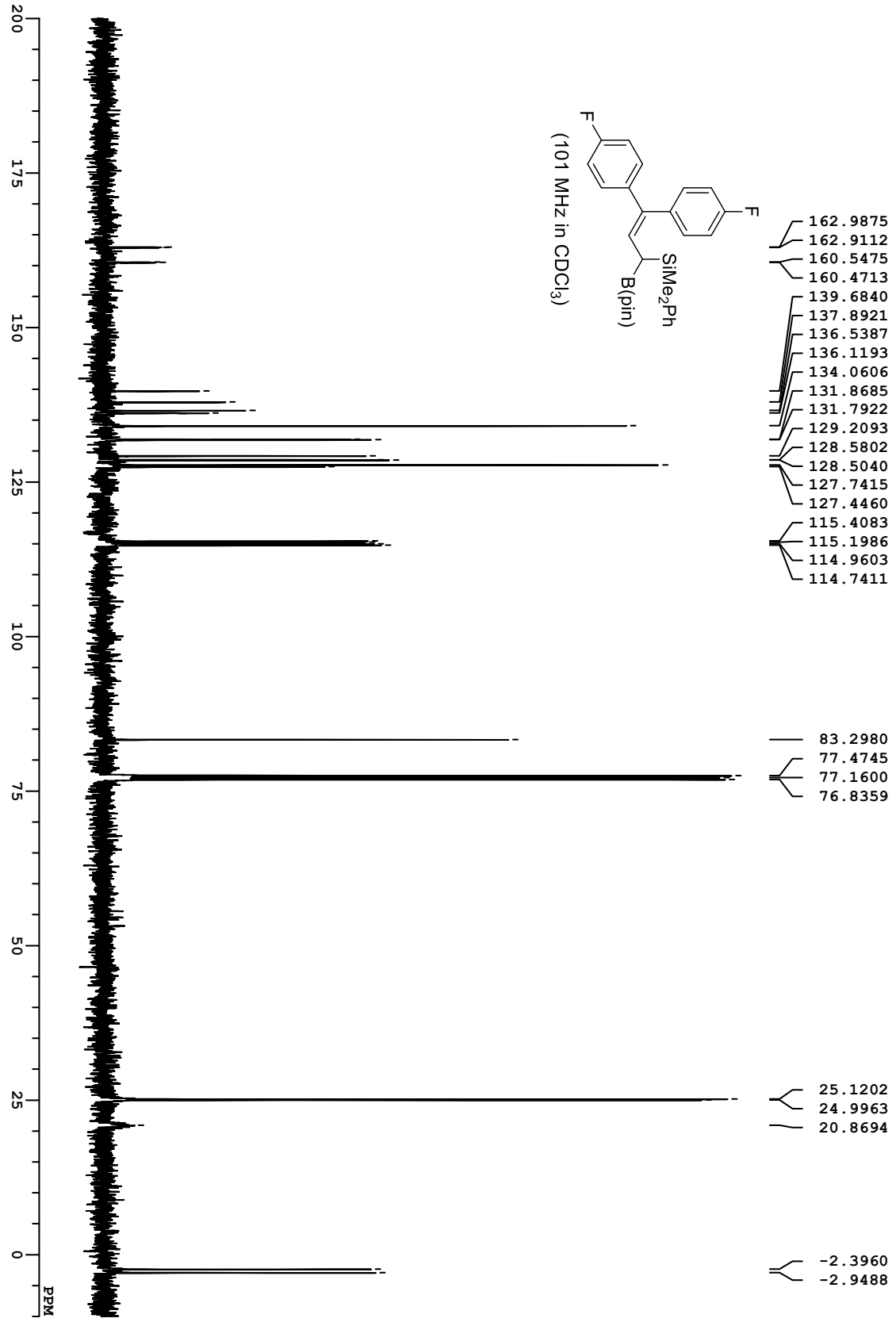
compound **3ca**



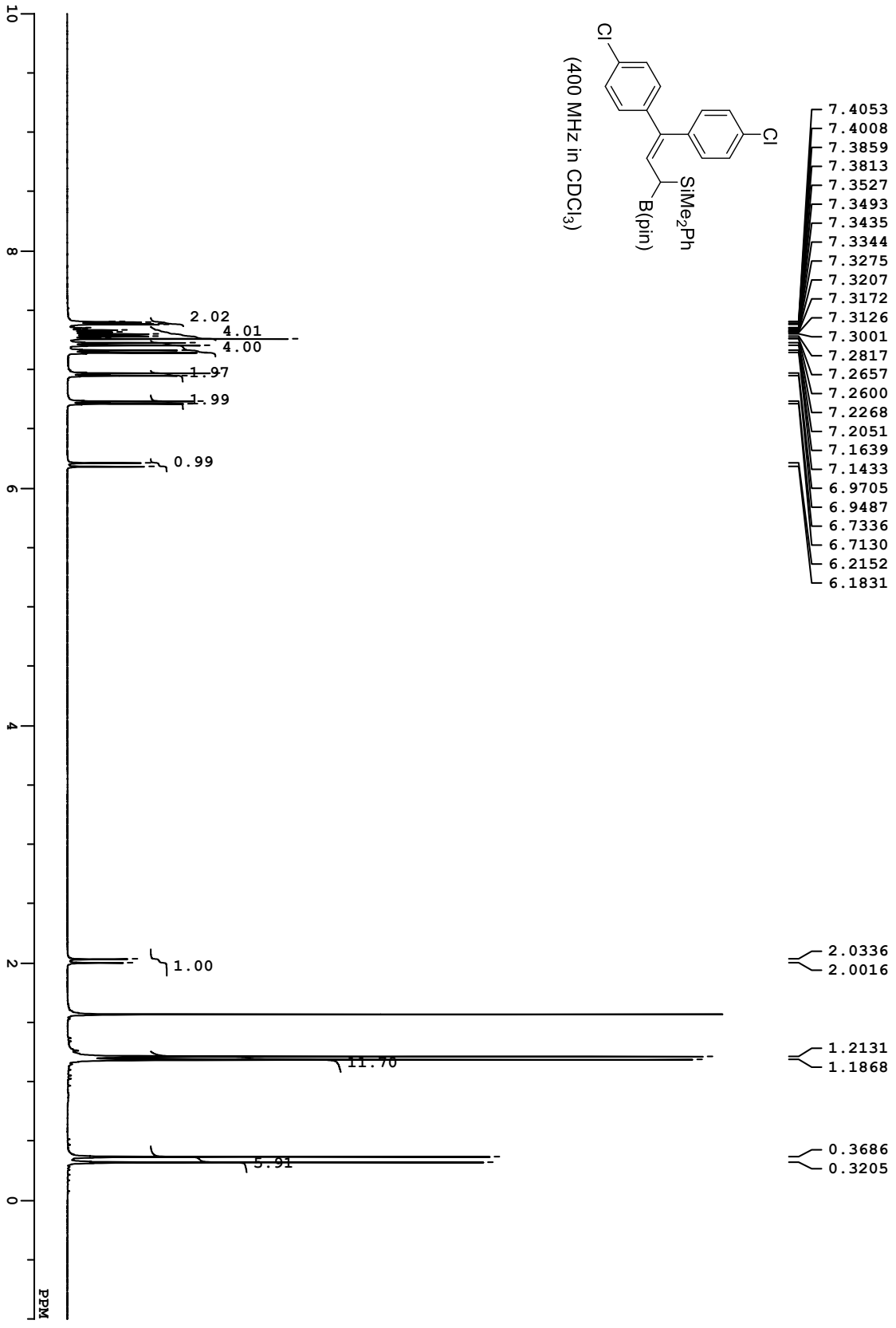
compound **3da**



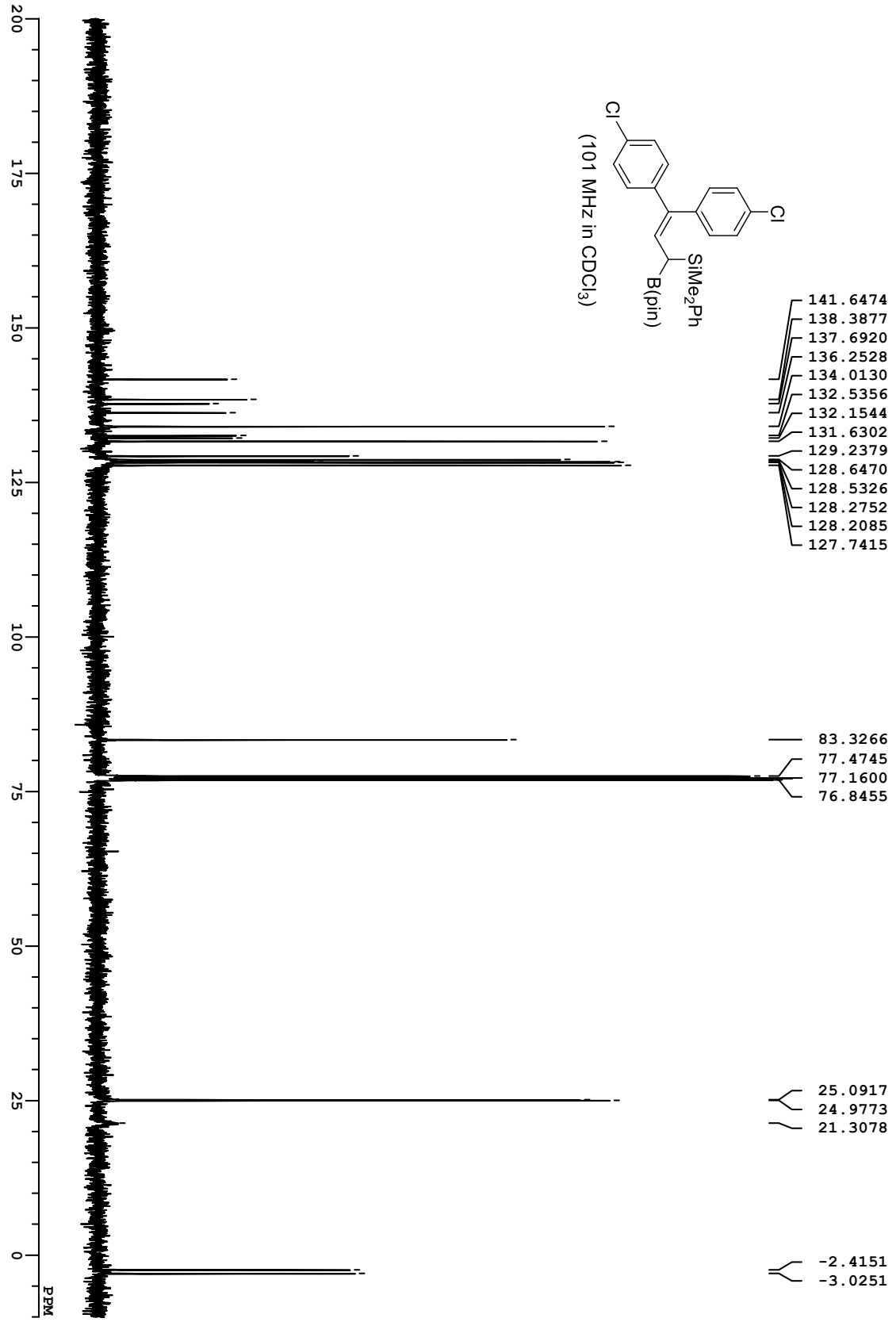
compound **3da**



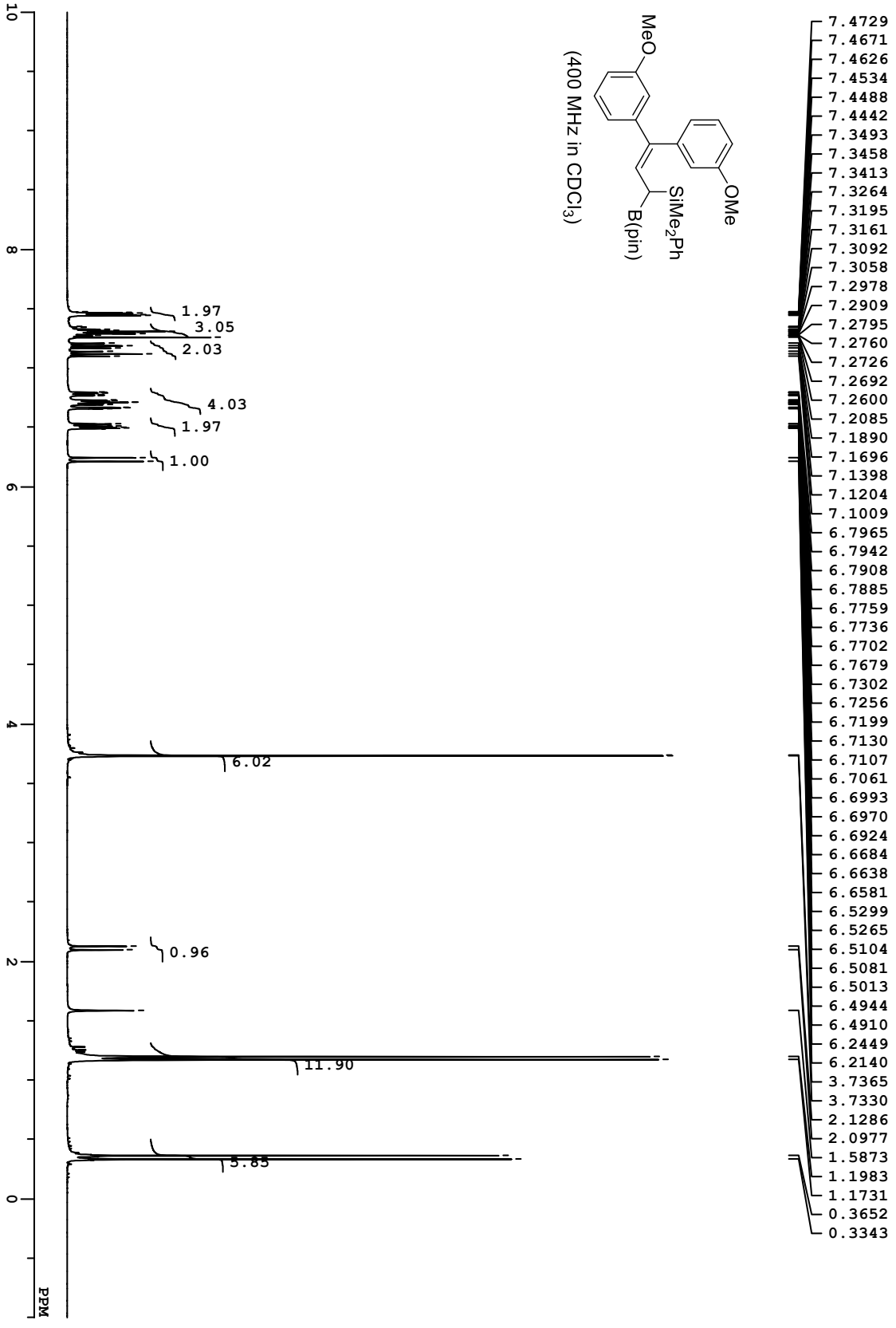
compound **3ea**



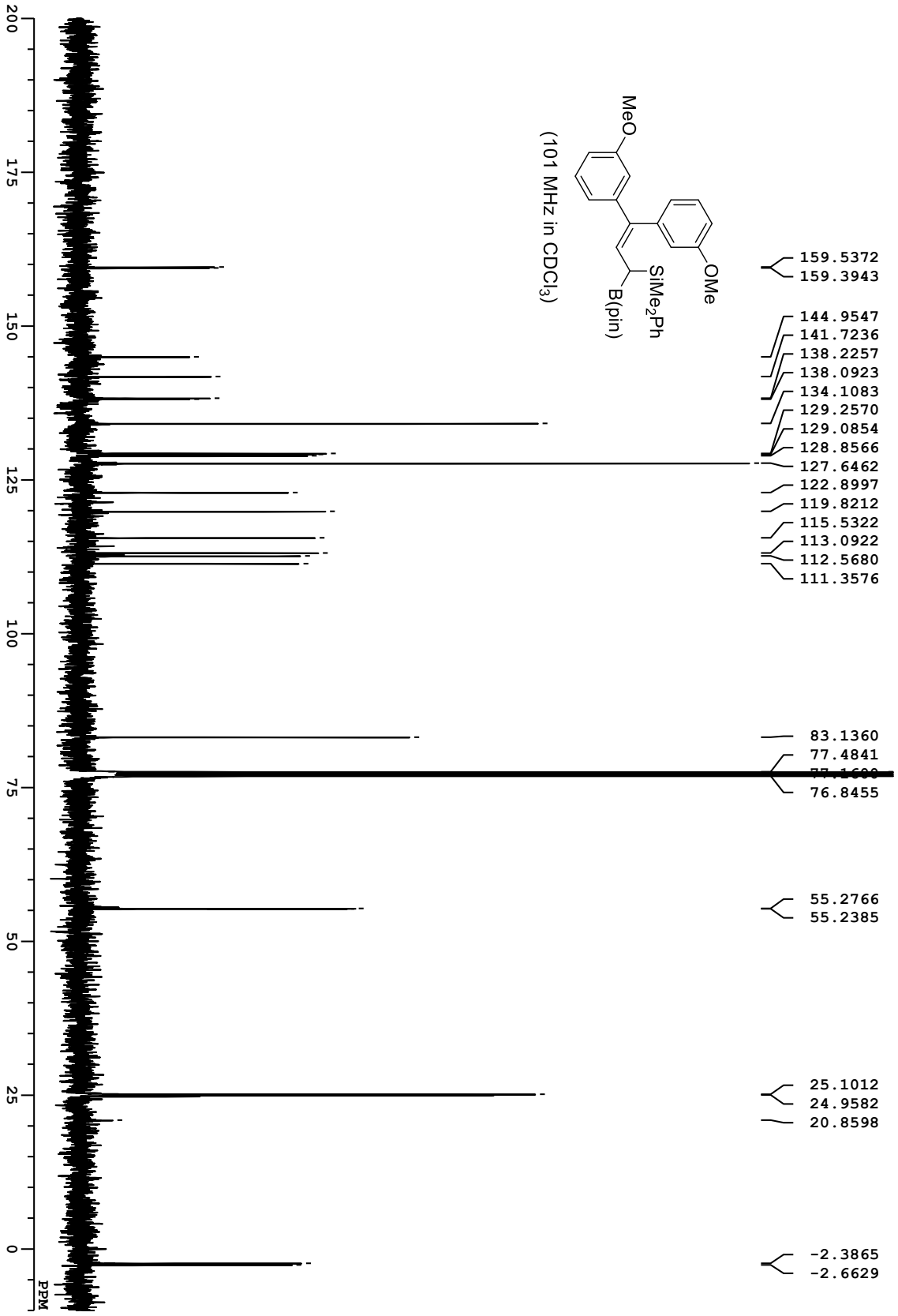
compound **3ea**



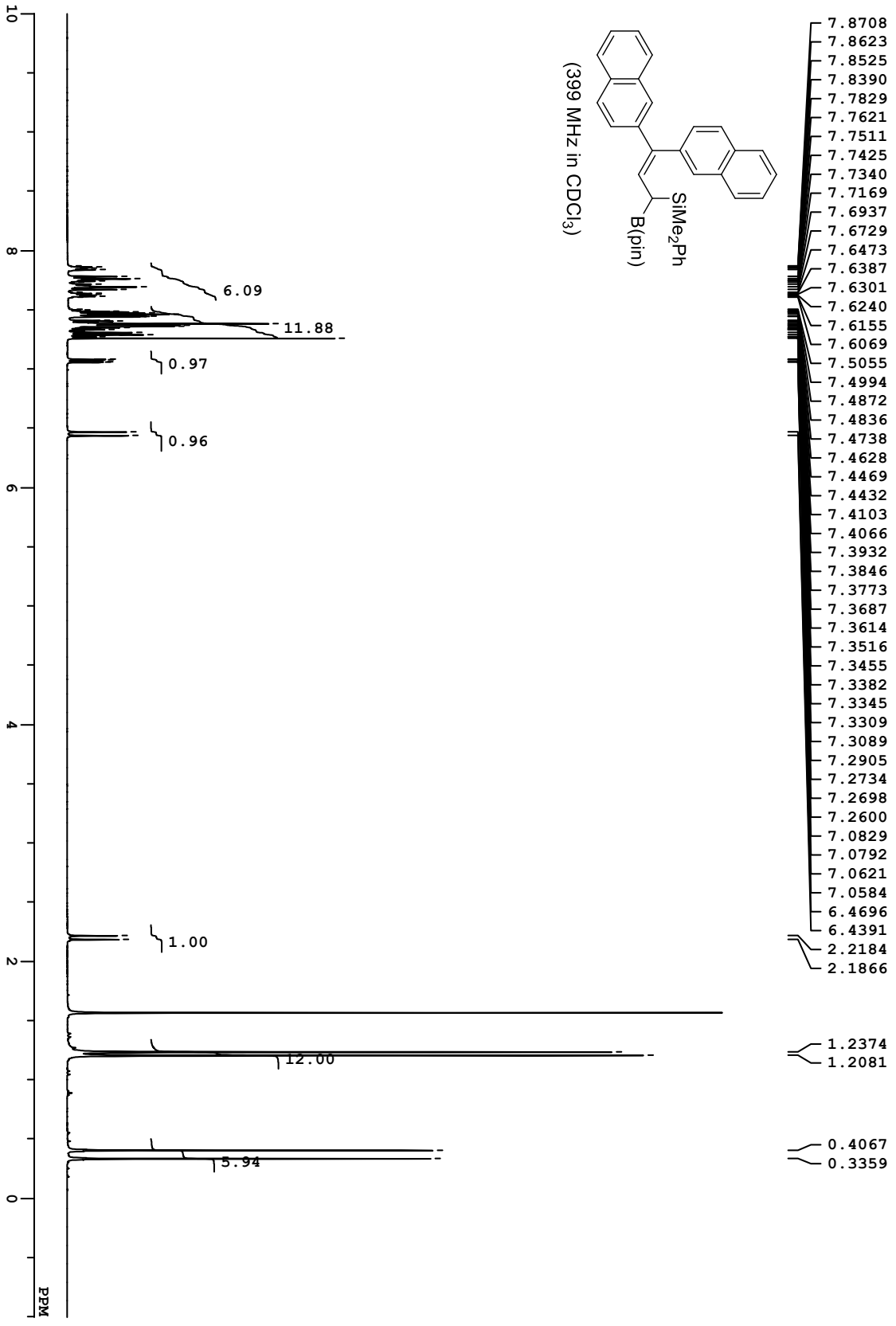
compound **3fa**



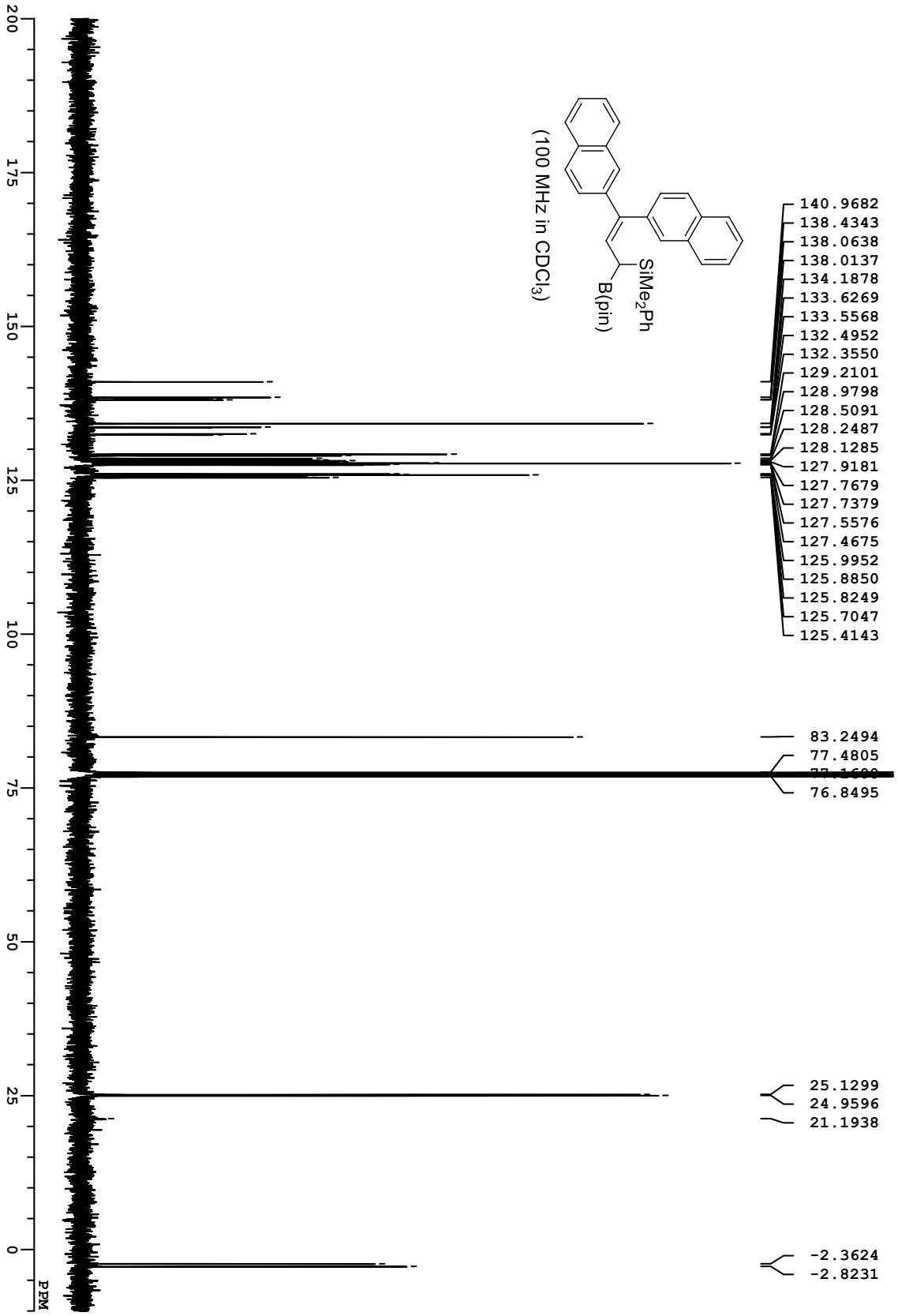
compound **3fa**



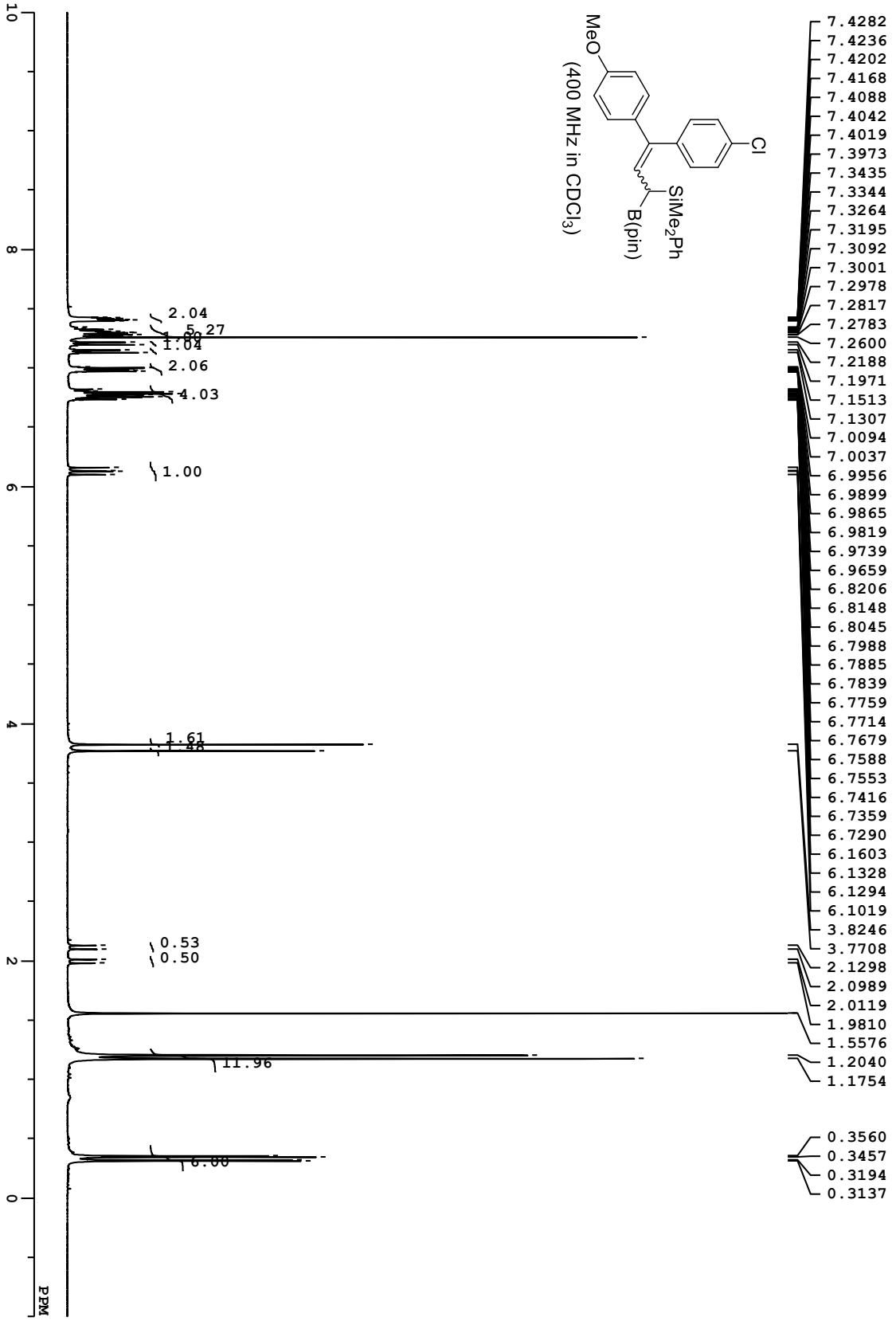
compound **3ga**



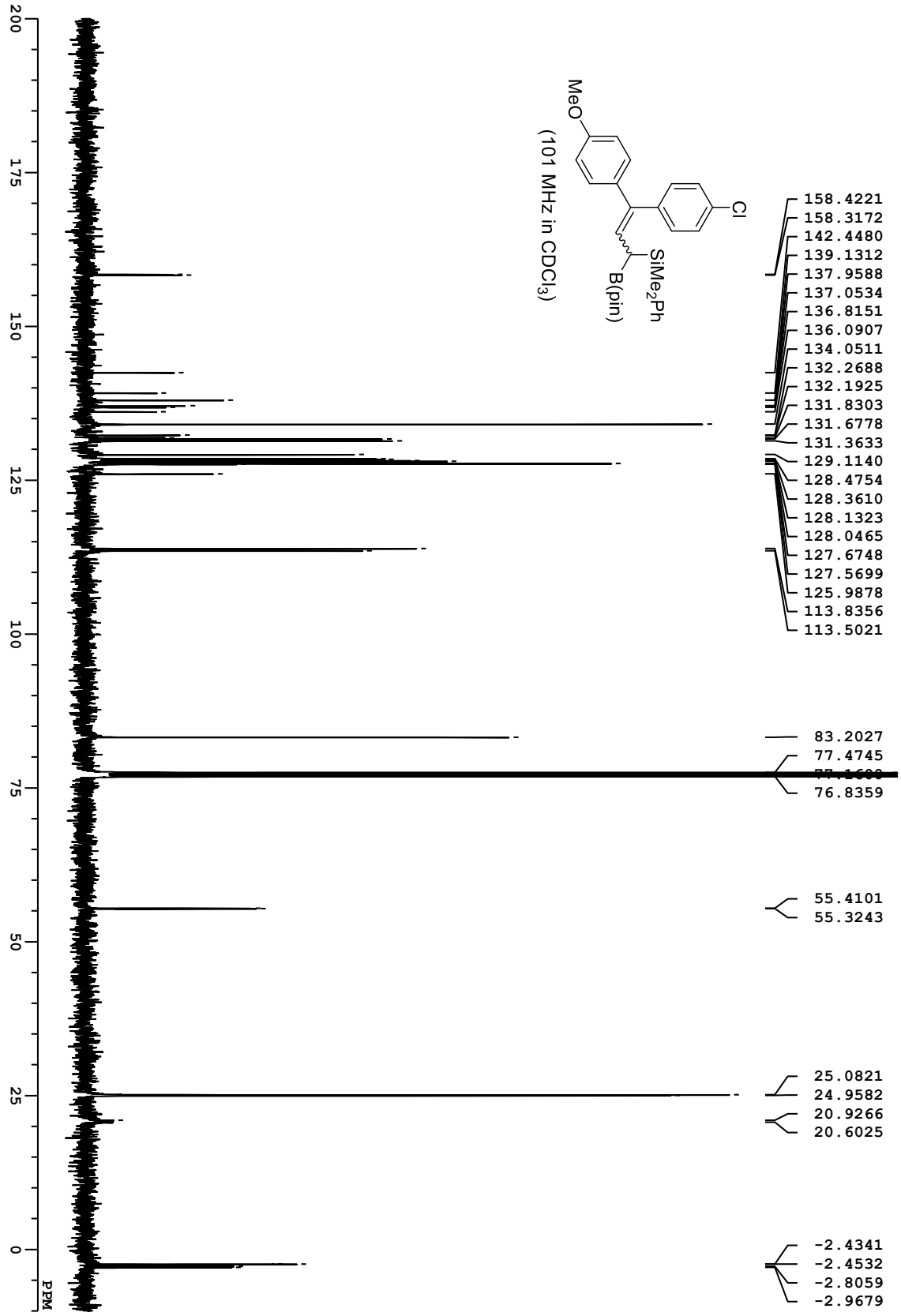
compound **3ga**



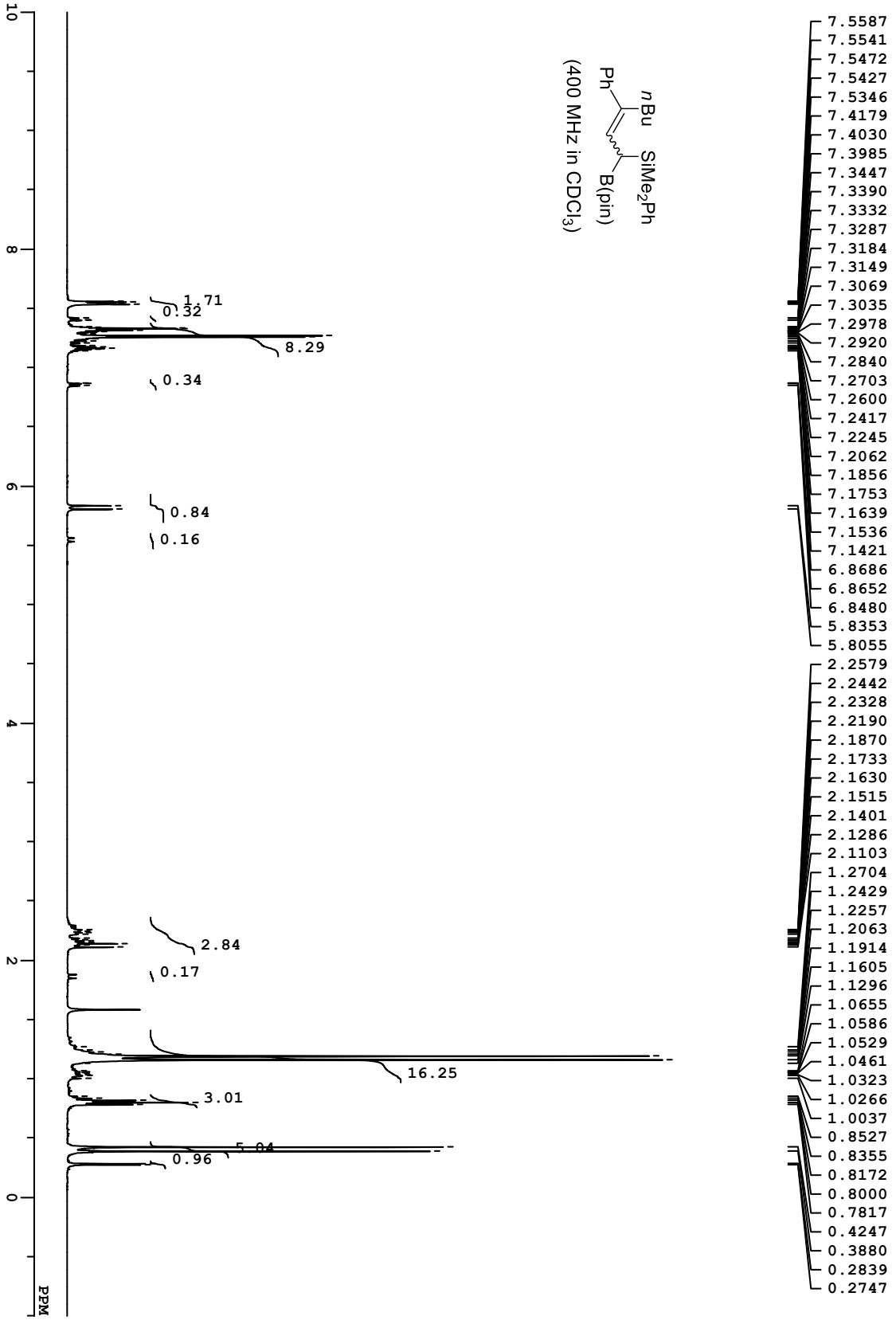
compound **3ha** (dr = 52/48)



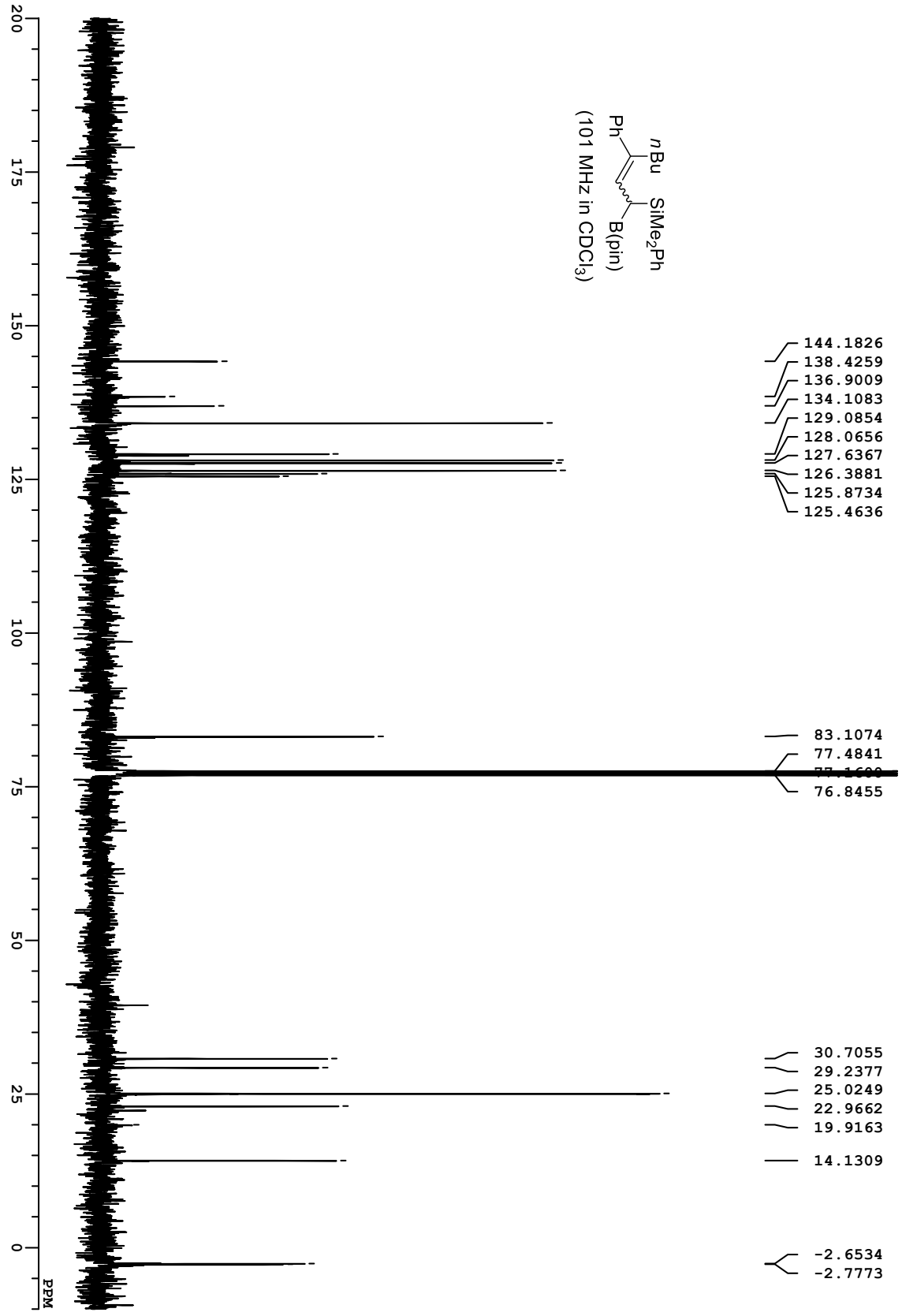
compound **3ha** (dr = 52/48)



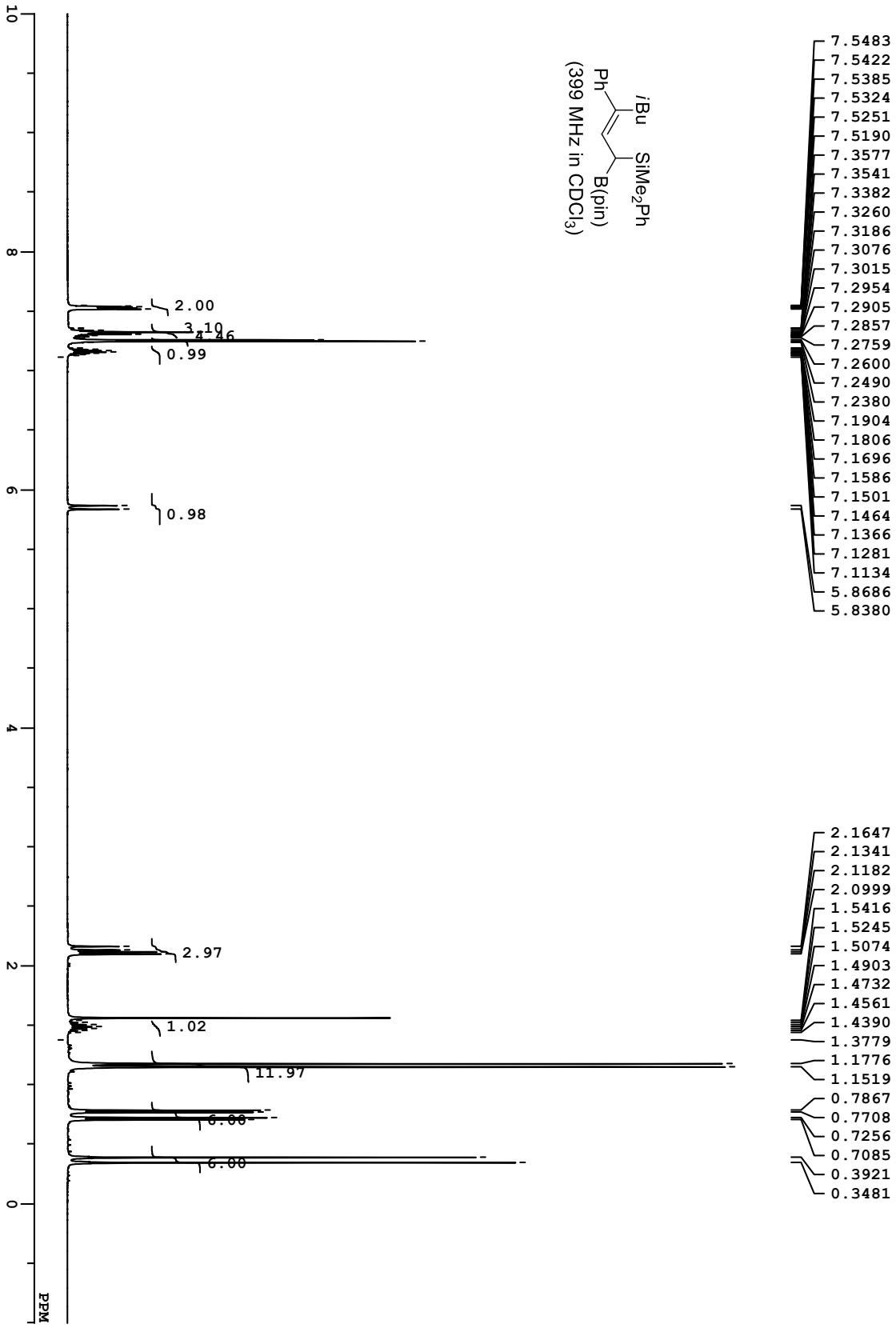
compound **3ia** (dr = 84/16)



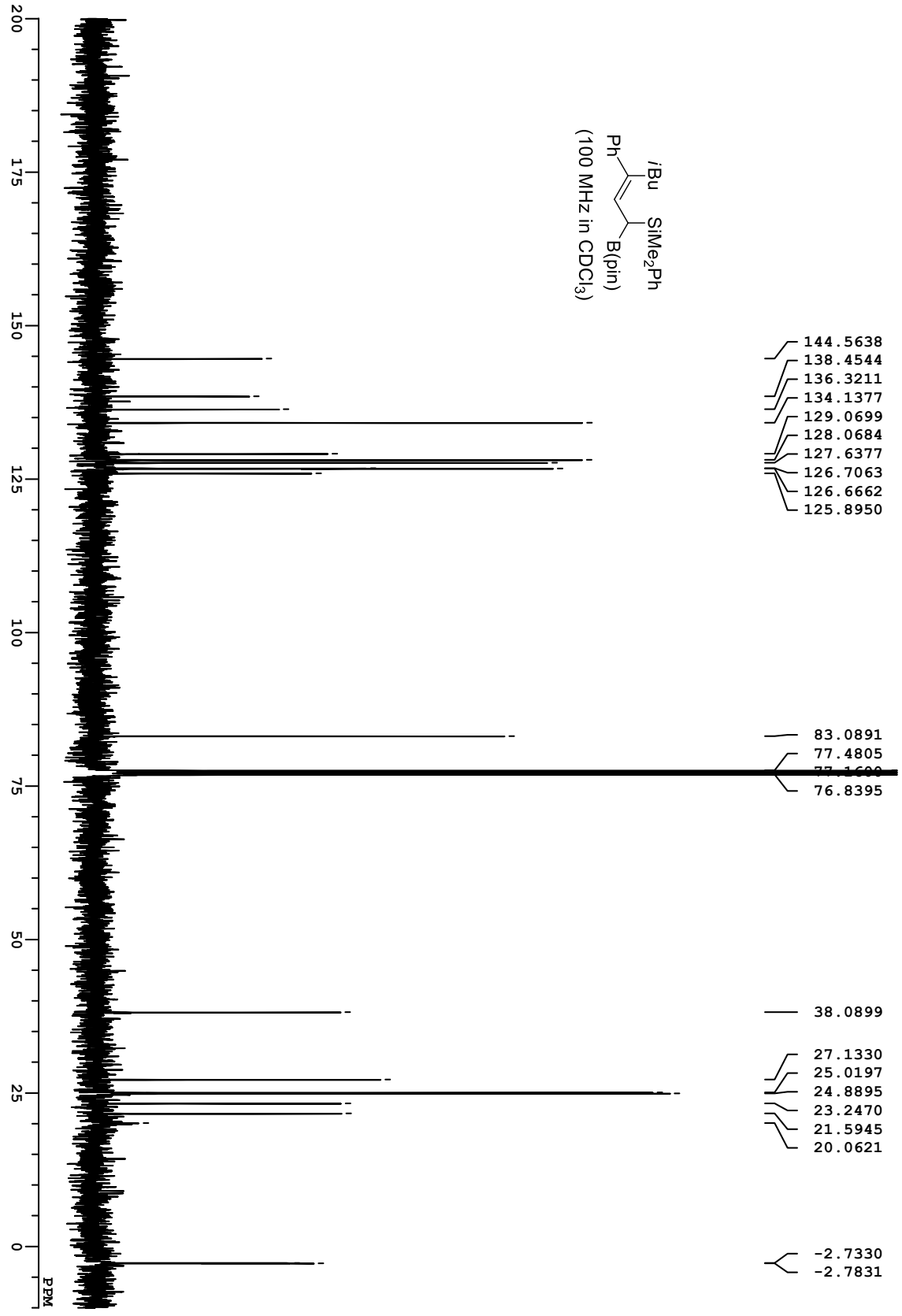
compound **3ia** (dr = 84/16)



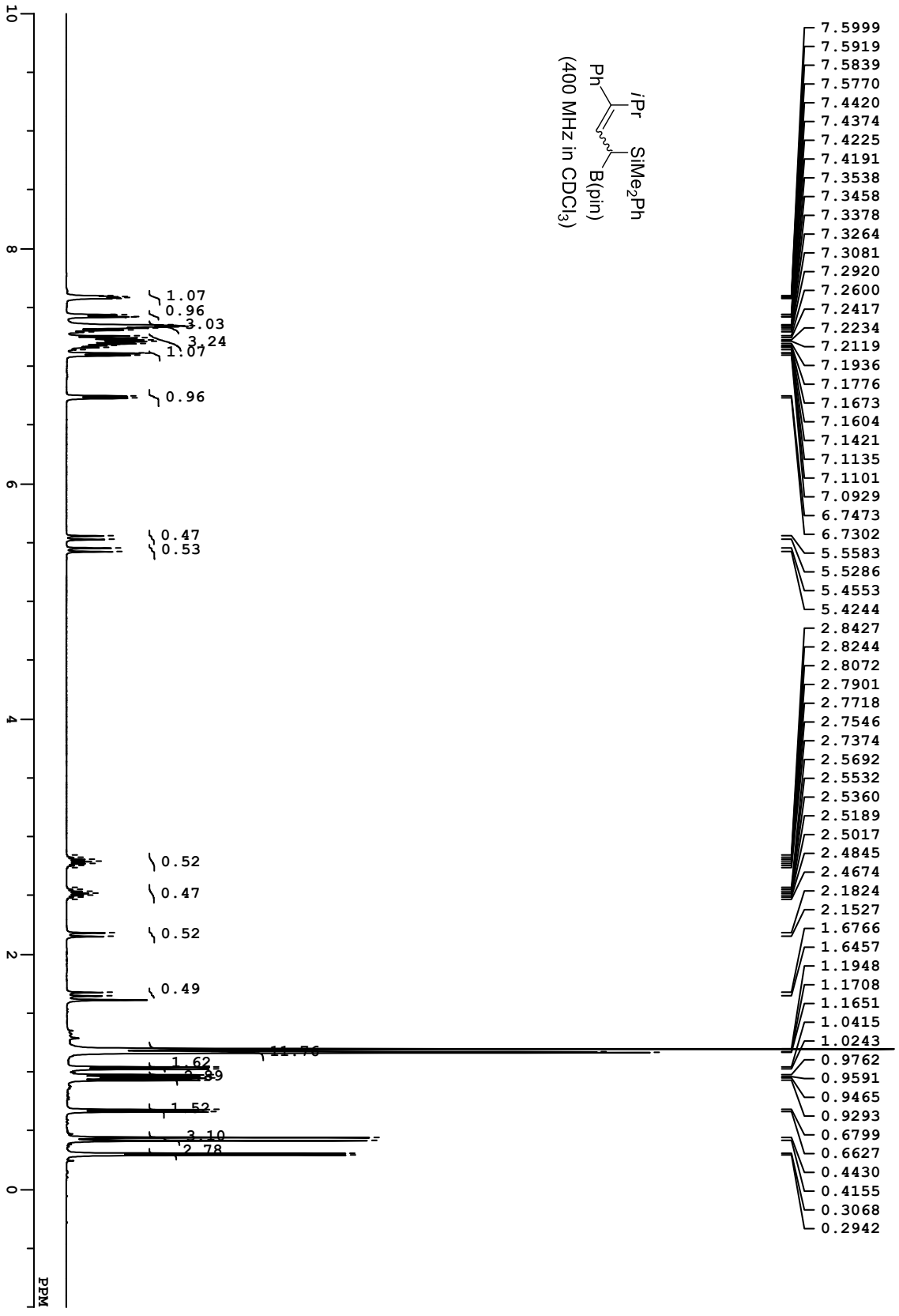
compound (*E*)-**3ja**



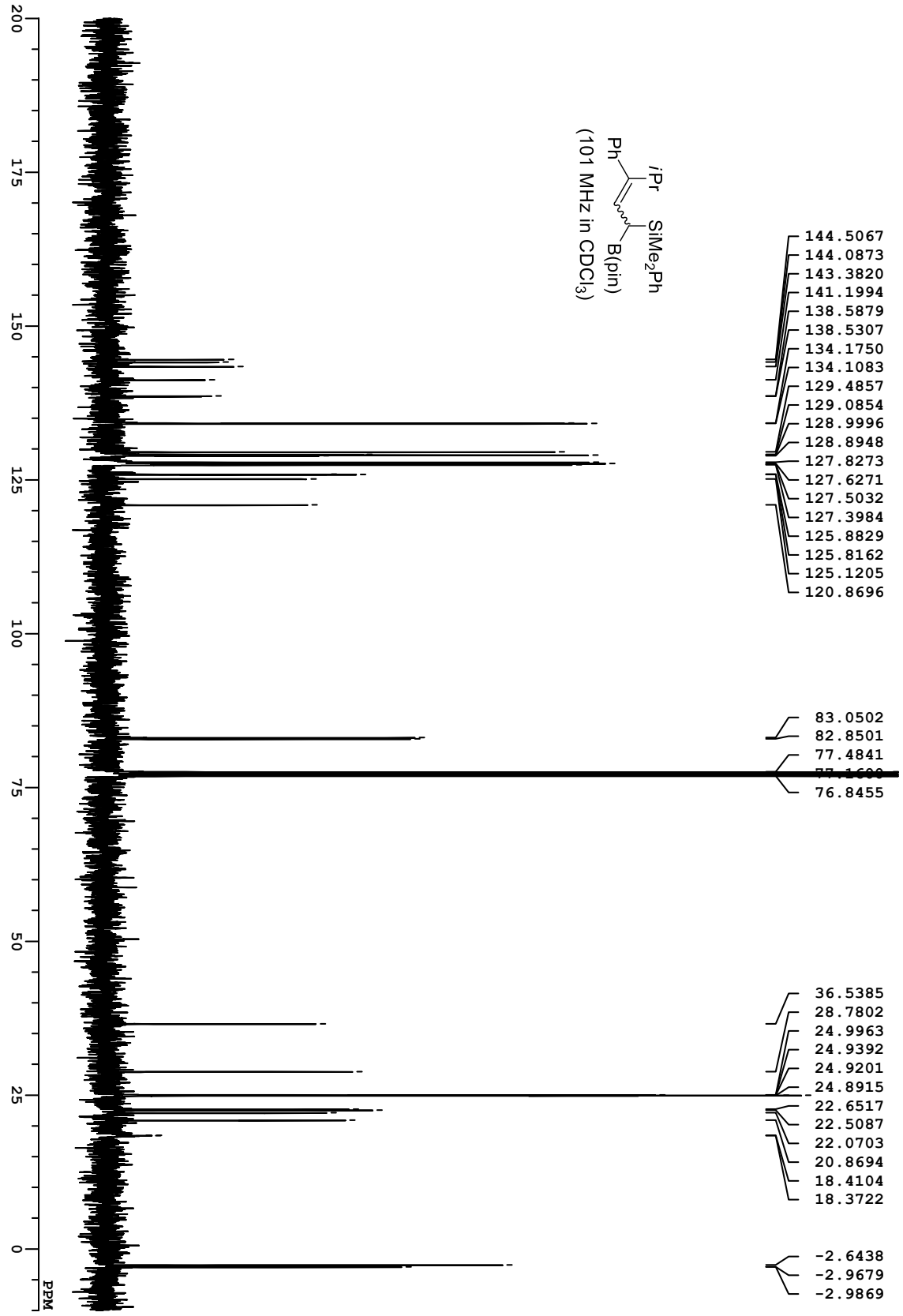
compound (*E*)-**3ja**



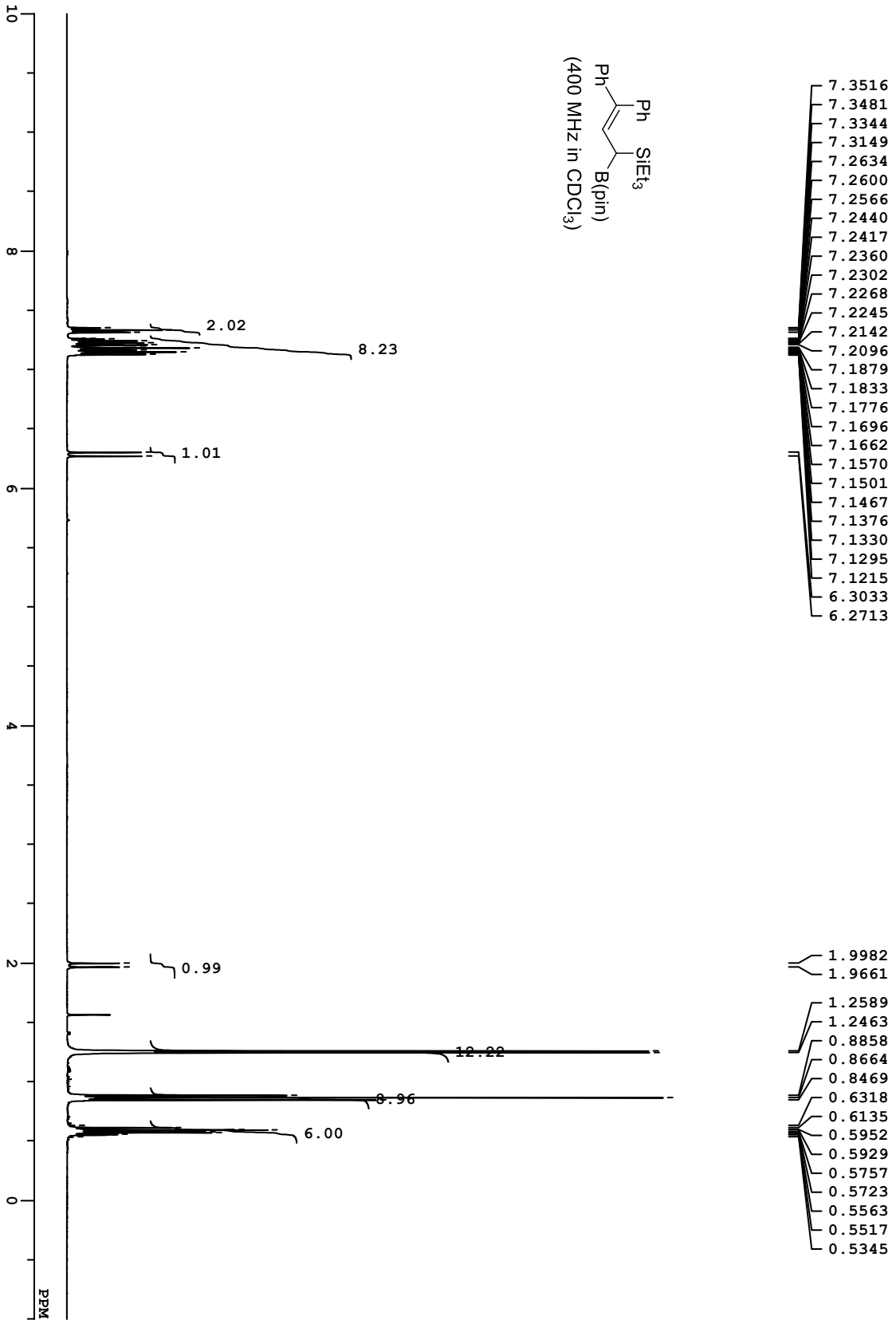
compound **3ka** (dr = 53/47)



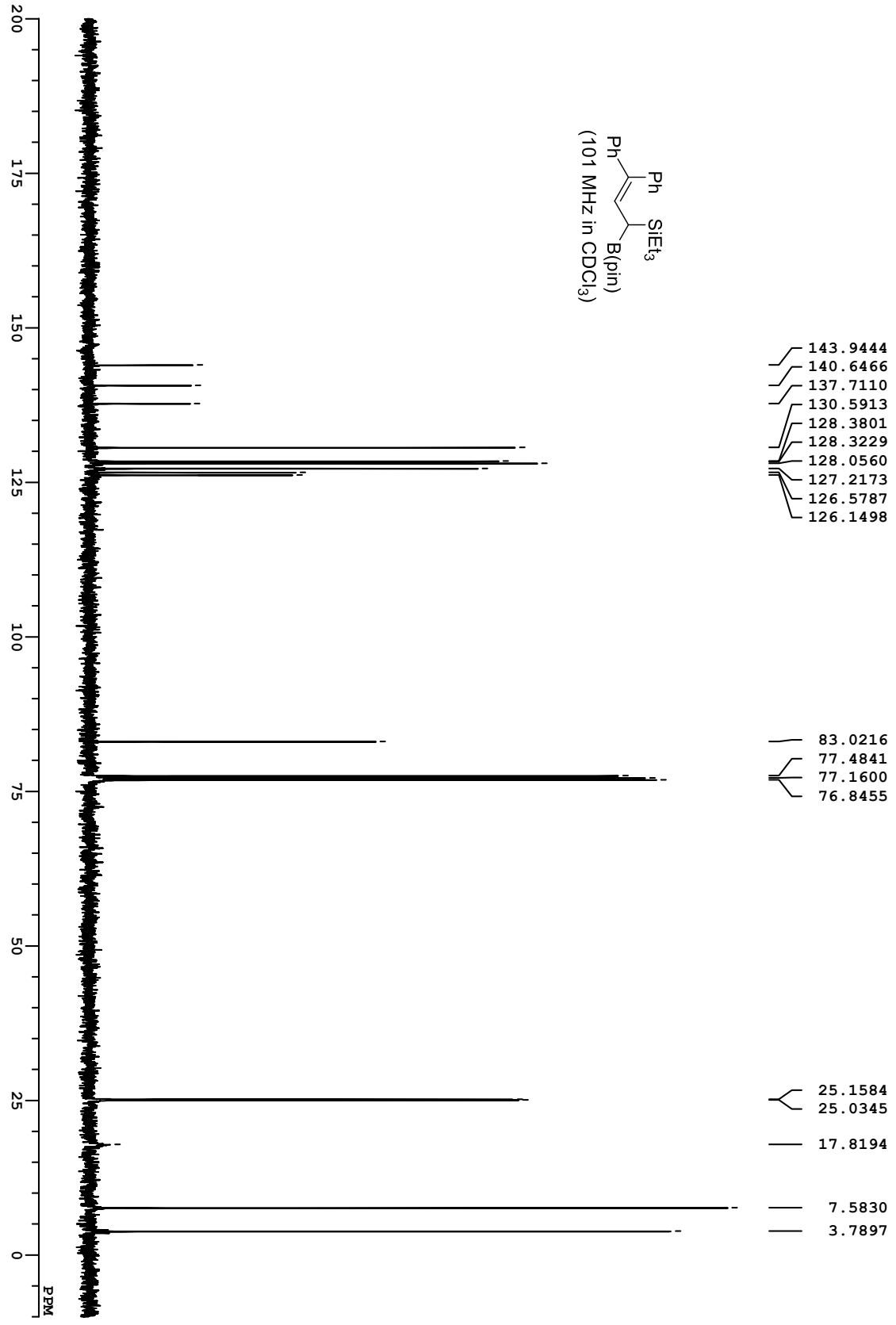
compound **3ka** (dr = 53/47)



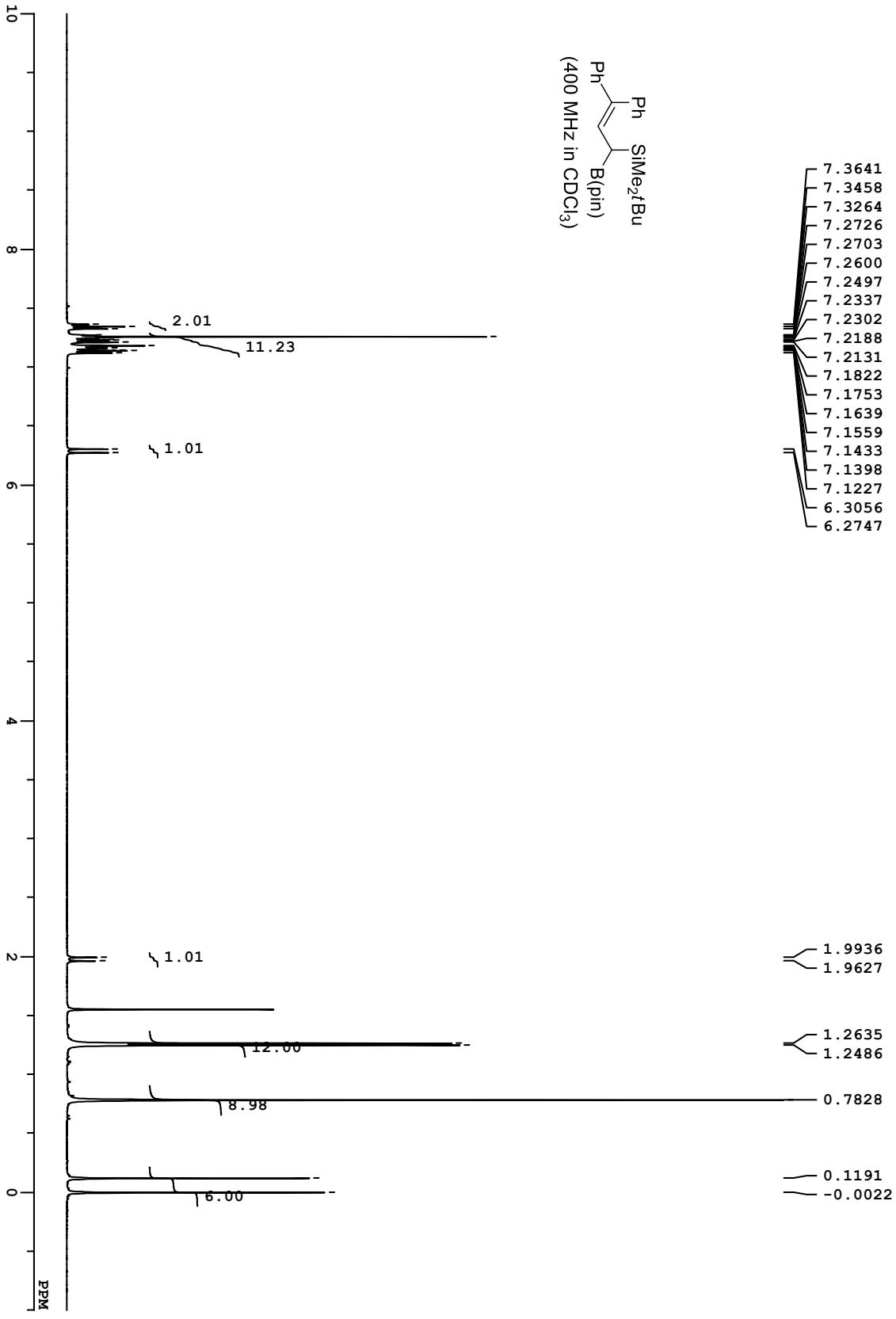
compound **3ab**



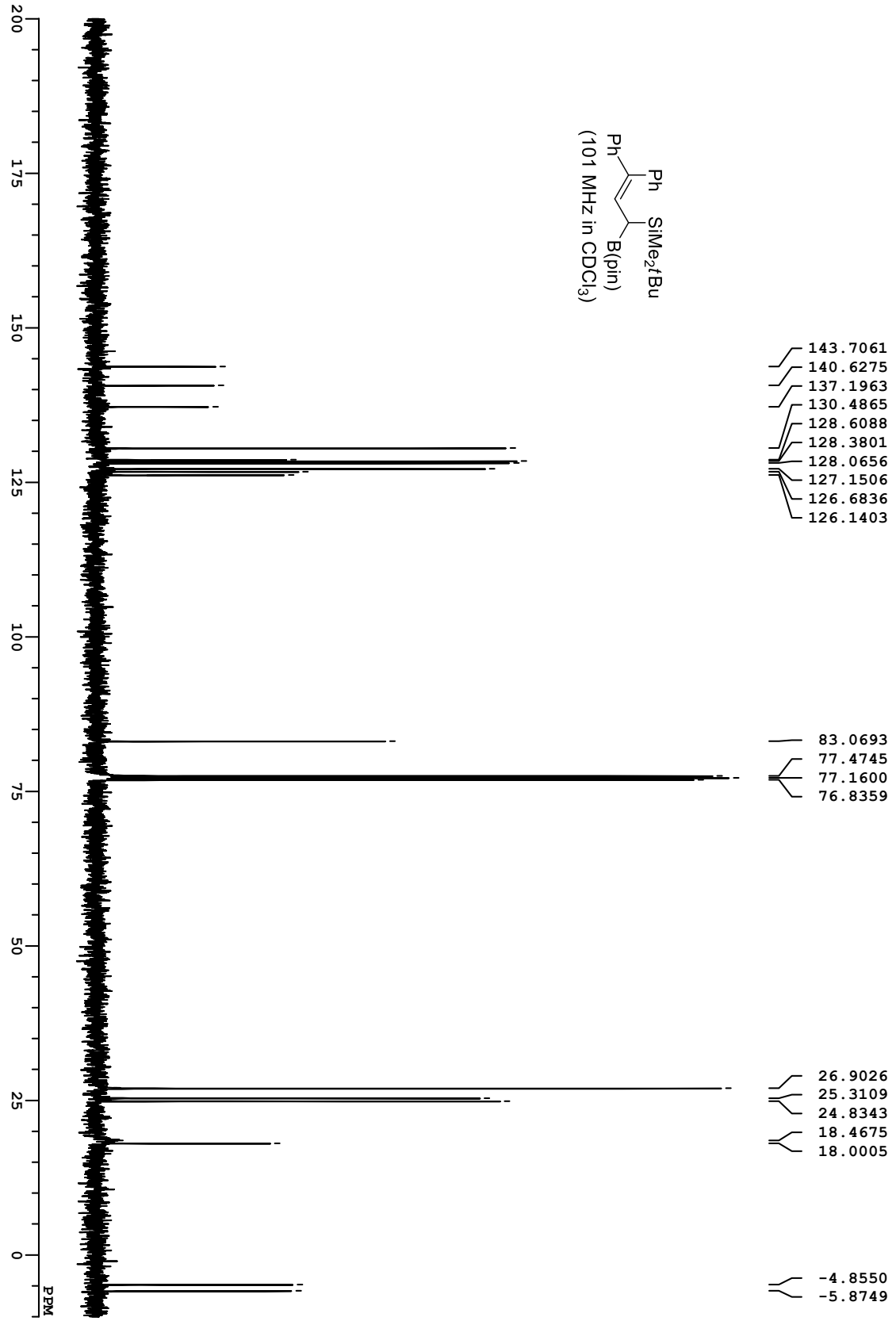
compound **3ab**



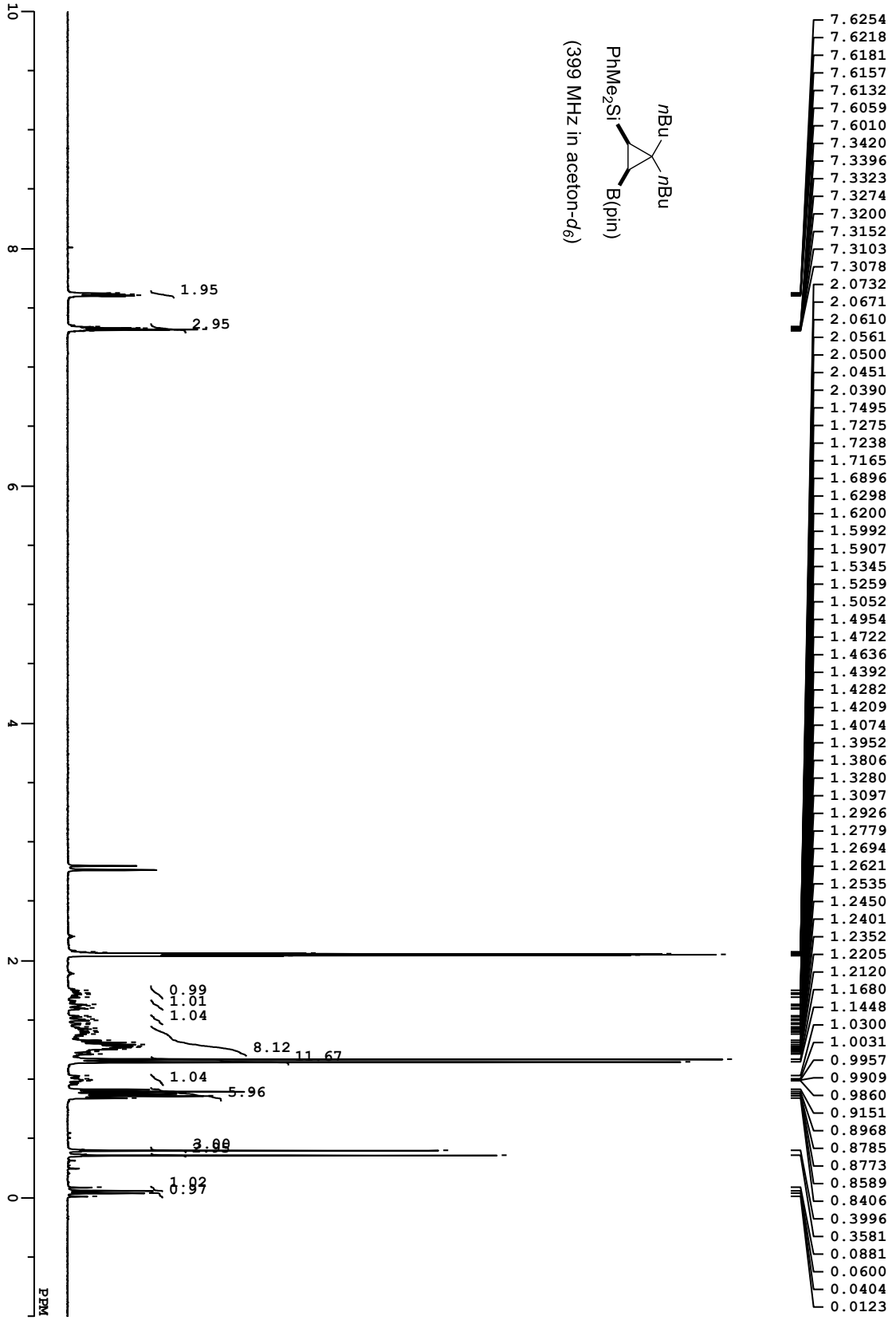
compound **3ac**



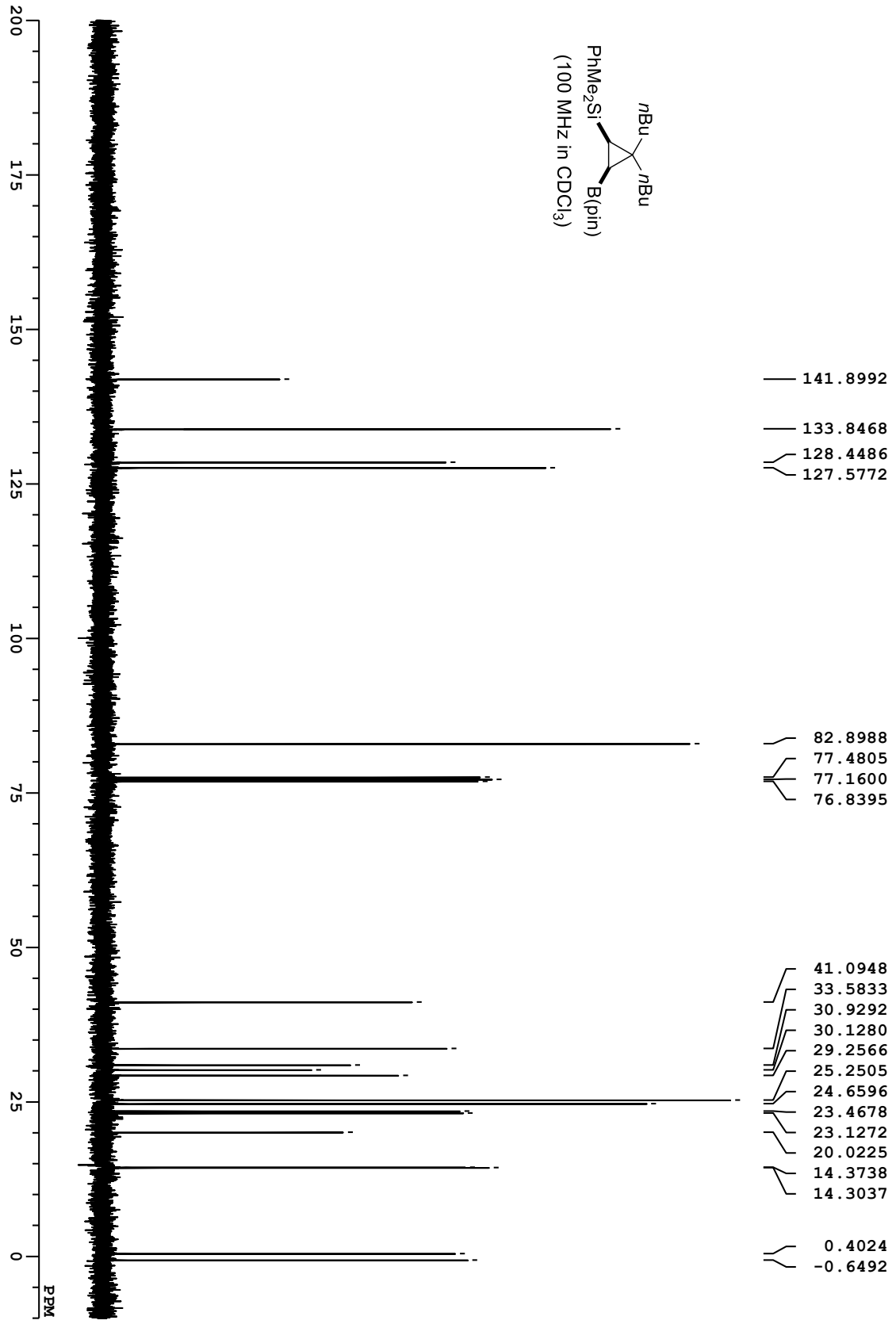
compound **3ac**



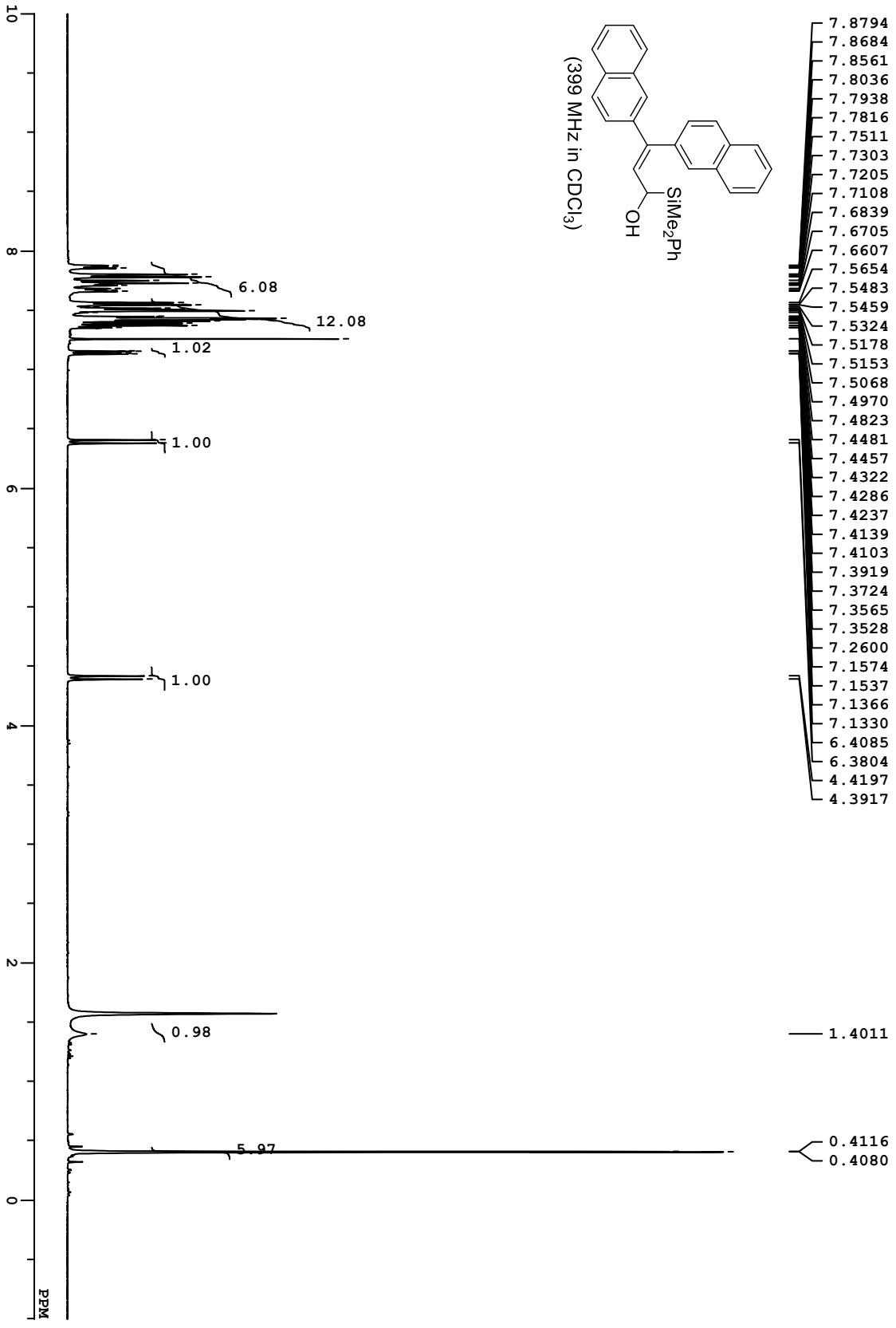
compound **5la**



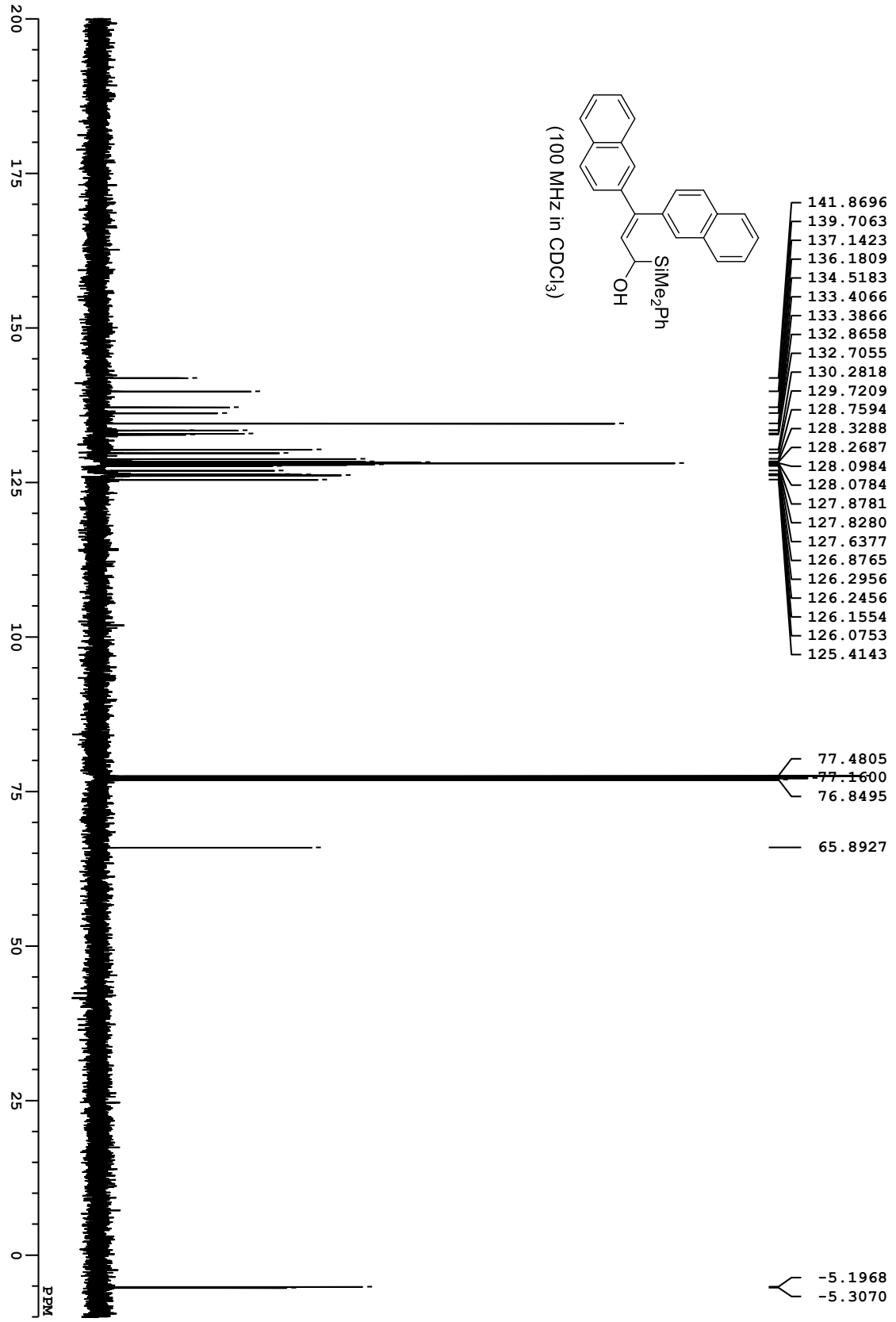
compound **5la**



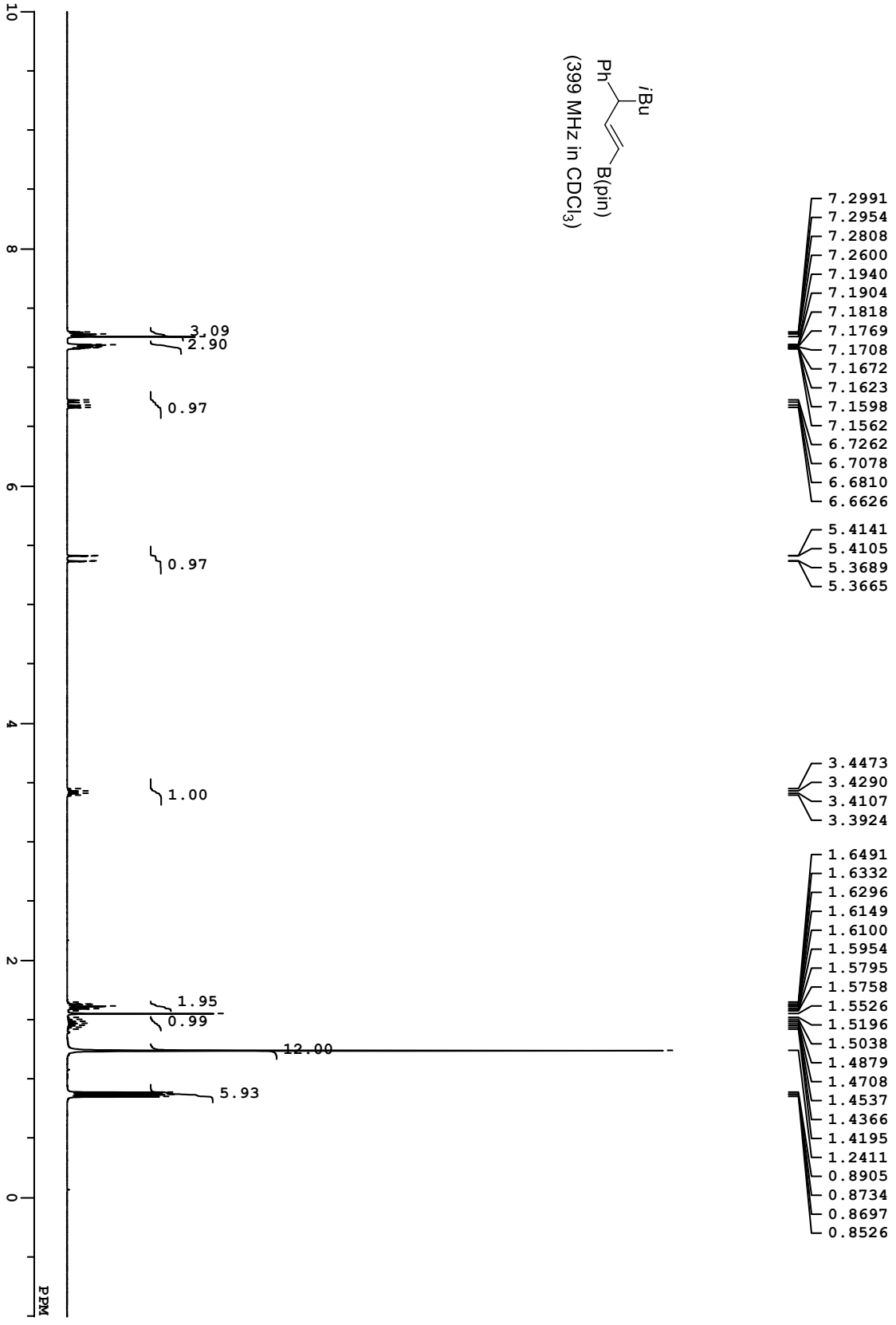
compound **6**


(399 MHz in CDCl3)
SiMe2Ph
OH
7.8794
7.8684
7.8561
7.8036
7.7938
7.7816
7.7511
7.7303
7.7205
7.7108
7.6839
7.6705
7.6607
7.5654
7.5483
7.5459
7.5324
7.5178
7.5153
7.5068
7.4970
7.4823
7.4481
7.4457
7.4322
7.4286
7.4237
7.4139
7.4103
7.3919
7.3724
7.3565
7.3528
7.2600
7.1574
7.1537
7.1366
7.1330
6.4085
6.3804
4.4197
4.3917
1.4011
0.4116
0.4080
6.08
12.08
1.02
1.00
1.00
0.98
5.97
10
8
6
4
2
0
PPM

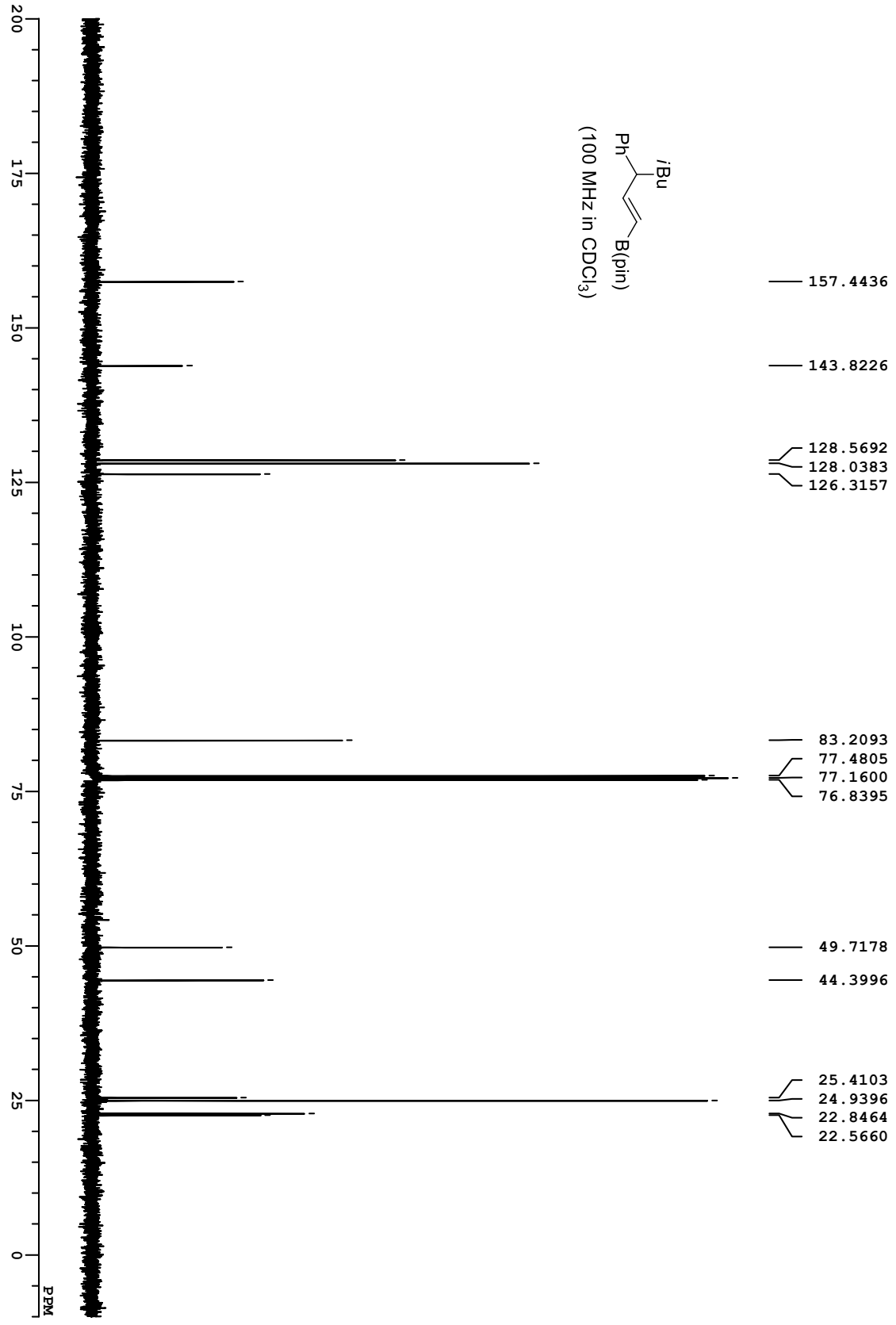
compound **6**


(100 MHz in $CDCl_3$)
OH
$SiMe_2Ph$
141.8696
139.7063
137.1423
136.1809
134.5183
133.4066
133.3866
132.8658
132.7055
130.2818
129.7209
128.7594
128.3288
128.2687
128.0984
128.0784
127.8781
127.8280
127.6377
126.8765
126.2956
126.2456
126.1554
126.0753
125.4143
77.4805
77.1600
76.8495
65.8927
-5.1968
-5.3070
200
175
150
125
100
75
50
25
0
PPM

compound **7**


Ph
iBu
B(pin)
(399 MHz in CDCl3)
7.2991
7.2954
7.2808
7.2600
7.1940
7.1904
7.1818
7.1769
7.1708
7.1672
7.1623
7.1598
7.1562
6.7262
6.7078
6.6810
6.6626
5.4141
5.4105
5.3689
5.3665
3.4473
3.4290
3.4107
3.3924
1.6491
1.6332
1.6296
1.6149
1.6100
1.5954
1.5795
1.5758
1.5526
1.5196
1.5038
1.4879
1.4708
1.4537
1.4366
1.4195
1.2411
0.8905
0.8734
0.8697
0.8526
3.09
2.90
0.97
0.97
1.00
1.95
0.99
12.00
5.93
10
8
6
4
2
0
PPM

compound **7**


(100 MHz in CDCl3)
Ph
iBu
B(pin)
157.4436
143.8226
128.5692
128.0383
126.3157
83.2093
77.4805
77.1600
76.8395
49.7178
44.3996
25.4103
24.9396
22.8464
22.5660
200
175
150
125
100
75
50
25
0
PPM

VII. References

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