Supporting Information for:

Formal Asymmetric Hydrobromination of Styrenes *via* Copper-Catalyzed 1,3-Halogen Migration

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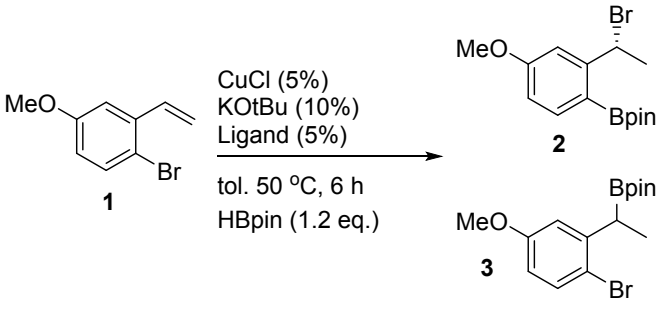
I. General Information

All glassware was either oven-dried overnight at 130 °C or flame-dried under a stream of dry nitrogen prior to use. Unless otherwise specified, reagents were used as obtained from the vendor without further purification. Tetrahydrofuran and diethyl ether were freshly distilled from purple Na/benzophenone ketyl. Dichloromethane, acetonitrile and toluene were dried over CaH_2 and freshly distilled prior to use. All other solvents were purified in accordance with "Purification of Laboratory Chemicals".[1] Air- and moisture-sensitive reactions were performed either in a Braun LabStar glovebox under an atmosphere of nitrogen or using standard Schlenk techniques under an atmosphere of nitrogen. Analytical thin layer chromatography (TLC) was performed utilizing pre-coated silica gel 60 F_{254} plates containing a fluorescent indicator, while preparative chromatography was performed using SilicaFlash P60 silica gel (230-400 mesh) via Still's method.[2] Unless otherwise stated, the mobile phases for column chromatography were mixtures of hexanes/ethyl acetate. Columns were typically run using a gradient method, beginning with 100% hexanes and gradually increasing the polarity using ethyl acetate. Various stains were used to visualize reaction products, including *p*-anisaldehyde, $KMnO_4$, ceric ammonium nitrate and phosphomolybdic acid in ethanol stain.

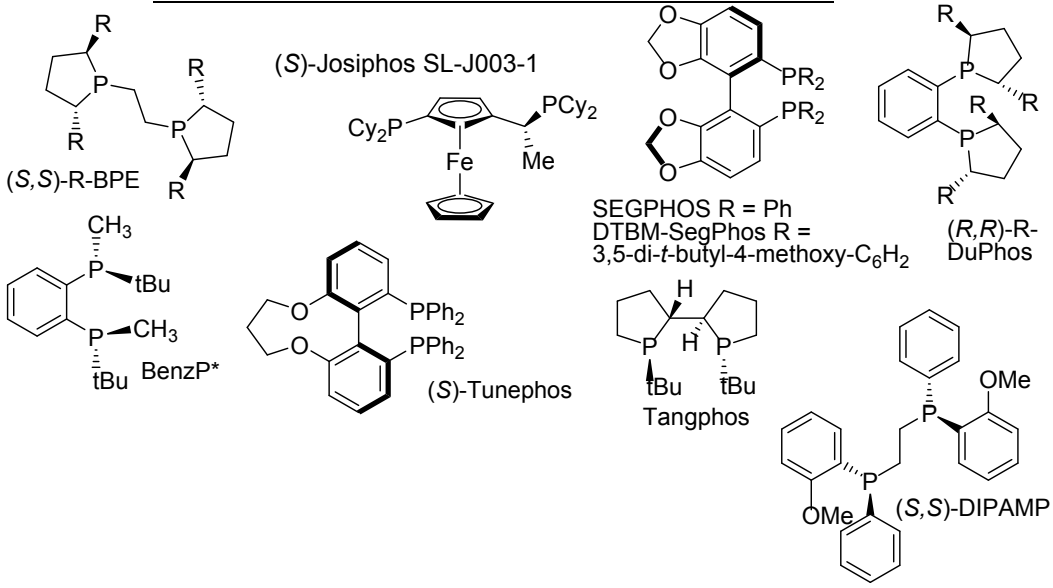
^1H NMR and ^{13}C NMR spectra were obtained using Bruker-300, Varian Inova-500, Varian Unity-500 or Varian Inova-600 NMR spectrometers. For ^1H NMR, chemical shifts are reported relative to residual protiated solvent peaks (δ 7.26, 2.49, 7.15 and 4.80 ppm for $CDCl_3$, $(CD_3)_2SO$, C_6D_6 and CD_3OD respectively). ^{13}C NMR spectra were measured at either 125 MHz or 150 MHz on the same instruments noted above for

recording ^{1}H NMR spectra. Chemical shifts were again reported in accordance to residual protiated solvent peaks (δ 77.0, 39.5, 128.0 and 49.0 ppm for $CDCl_3$, $(CD_3)_2SO$, C_6D_6, and CD_3OD, respectively). IR spectral data were obtained using a Bruker Vector 22 spectrometer using either a thin film or an ATR adapter. Melting points were obtained with a Mel-Temp II (Laboratory Devices, Inc.) melting point apparatus. High-pressure liquid chromatography (HPLC) analyses were performed at 224 and 254 nm using Shimadzu HPLC, Model LC-20AB. An AD-H column (4.6 μm diameter x 258 mm) at a temperature of 40 ºC was employed, using a flow rate of 1 mL/min and a gradient starting at 10% isopropanol in hexanes for 10 min and increasing to 30% isopropanol in hexanes. The eluent was then held at 30% isopropanol in hexanes until the run was completed. Accurate mass measurements were acquired at the University of Wisconsin, Madison using a Micromass LCT (electrospray ionization, time-of-flight analyzer or electron impact methods). The NMR and Mass Spectrometry facilities are funded by the NSF (CHE-9974839, CHE-9304546, CHE-9208463, CHE-9629688) and the University of Wisconsin, as well as the NIH (RR08389-01).

II. Ligand Optimization. In general, BINAP-derived ligands (entries 1-5) all gave the desired product in poor yield and poor to moderate *ee*. Ligands with larger R groups on phosphorous (entries 1, 2, and 4) tended to afford better *ee*'s than ligands with smaller R groups on phosphorous (entries 3 and 5). Tangphos produced a mixture of products with moderate mass balance (entry 6). The DIPAMP ligand gave poor yield and negligible *ee* (entry 7). A series of ligands with a defined bite angle enforced by a benzene ring gave poor to no yield of the desired product (entries 8-10). Me-DuPhos produced the desired product in poor yield and low *ee* (entry 8), while switching the R group to the bulkier



Entry	Ligand	1	2	3	*ee*
1	(*R*)-T-BINAP	23	17	0	54
2	(*R*)-DM-BINAP	18	33	0	66
3	(*R*)-SEGPHOS	12	29	0	30
4	(*R*)-DTBM-SegPhos	15	8	0	62
5	(*S*)-TunePhos	8	46	0	-41
6	(*S,S',R,R'*)Tangphos	22	17	31	n.d.
7	(*S,S*)-DIPAMP	20	17	0	6
8	(*R,R*)-Me-DuPhos	8	23	0	21
9	(*S,S*)-iPr-DuPhos	23	0	0	n.d.
10	(*R*)-BenzP*	36	21	0	-29
11	(*S*)-Josiphos SL-J003-1	0	82	0	37
12	(*S,S*)-Me-BPE	19	0	0	n.d.
13	(*R,R*)-iPr-BPE	13	17	0	-9
14	(*S,S*)-Ph-BPE	14	34	0	78

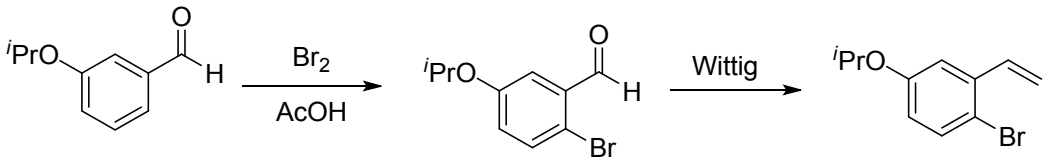


isopropyl shut down the reactivity completely (entry 9). Switching to a ligand chiral at phosphorous did not improve the yield or the *ee* (entry 10). The Josiphos SL-J003-1 ligand derivative produced the desired product in excellent yield, but poor *ee* (entry 11). However, more promising results were obtained by investigating a series of bis(phospholane) ligands (entries 12-14). The methyl derivative failed to catalyze the

desired 1,3-halogen migration (entry 12), but the isopropyl derivative gave the desired product in low yield and *ee* (entry 13). Finally, the phenyl derivative produced the product in low yield but good *ee* (entry 14). Taken together, this preliminary ligand screen indicates that an electron-rich, bulky, bidentate phosphine ligand is necessary to both promote the 1,3-halogen migration and obtain high *ee*. We continued optimization studies with the Ph-BPE ligand, as it most closely mimics the successful bis(1,2-bisdicyclohexyl)phosphine ligand that was successful in our initial racemic Cu-catalyzed 1,3-halogen migration reactions.[3]

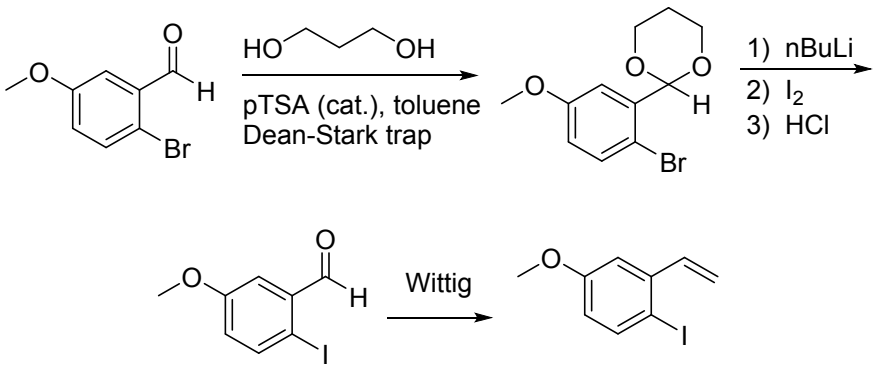
III. Preparation of substrates for the 1,3-halogen migration reaction.

Compounds **1**, **4c**, **4d**, and **4e** were all prepared according to previously reported procedures.[3]



Compound 4a. Acetic acid (12 mL), 3-isopropoxybenzaldehyde (1.6 mL, 10.1 mmol, 1.0 equiv), and bromine (1.5 mL, 29.3 mmol, 2.9 equiv) were added to a 50 mL round bottom flask and allowed to stir at ambient temperature for 2 h. The reaction was transferred to a separatory funnel, diluted with CH_2Cl_2 and the organic layer washed 3x with water, 1x with saturated $NaHSO_3$ and 1x with 1 M KOH. The organic layer was dried over Na_2SO_4 and concentrated *in vacuo*. The product 2-bromo-5-isopropoxybenzaldehyde was isolated in 94% yield and used without further purification.

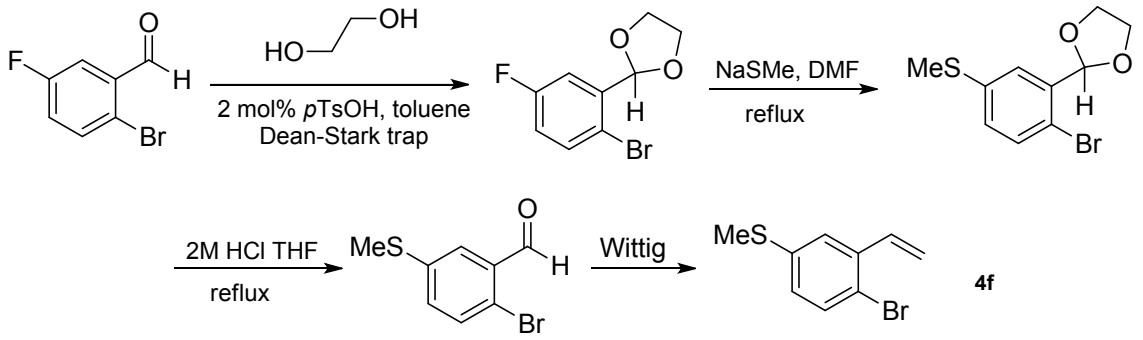
THF (40 mL) was added to a flame dried 200 mL round bottom flask under N_2 in an ice bath containing methyltriphenylphosphonium iodide (3.44 g, 8.5 mmol, 1.2 equiv). A solution of *n*BuLi (4.0 mL of a 2.27 M solution, 9.1 mmol, 1.32 equiv) was added in a dropwise fashion to the slurry and the reaction mixture allowed to stir for 30 min at 0 °C. An aliquot of 2-bromo-5-isopropoxybenzaldehyde (1.2 mL, 6.9 mmol, 1.0 equiv) was added slowly and the reaction mixture allowed to stir at rt for 3 h. Silica gel was added and the volatiles removed under reduced pressure. The resulting powder was loaded onto a plug of silica and flushed with ~200 mL of hexanes. The hexanes were removed *in vacuo* and the residue was purified by column chromatography using hexanes/EtOAc as the eluent. A gradient was employed using 0-2% in 0.5% increments. The 2-bromo-5-isopropoxystyrene **4a** was isolated as a clear, colorless oil in 50% yield. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.41 (d, *J* = 8.8 Hz, 1H), 7.07 (d, *J* = 3.0 Hz, 1H), 7.00 (dd, *J* = 17.4, 10.9 Hz, 1H), 6.69 (dd, *J* = 8.8, 3.0 Hz, 1H), 5.67 (d, *J* = 17.4 Hz, 1H), 5.35 (d, *J* = 10.9 Hz, 1H), 4.53 (hept, *J* = 6.3 Hz, 1H), 1.33 (d, *J* = 6.1 Hz, 6H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 157.24, 138.21, 135.87, 133.37, 116.91, 116.59, 114.24, 114.05, 70.27, 21.95. HRMS (EI) *m/z* calculated for $C_{11}H_{13}BrO$ $[M]^+$ 240.0146, found 240.0145.



Compound 4b. A 200 mL flask fitted with a Dean-Stark trap and reflux condenser was charged with 2-bromo-5-methoxybenzaldehyde (6.20 g, 28.8 mmol, 1.0 equiv), 1,3-propanediol (2.1 mL, 29.1 mmol, 1.01 equiv), *p*-toluenesulfonic acid (0.52 g, 2.7 mmol, 0.1 equiv) and 50 mL of toluene. The reaction mixture was heated to reflux for 1 h and cooled to rt. The mixture was washed with saturated $NaHCO_3$, the aqueous layer extracted 2x with portions of CH_2Cl_2 and the combined organic layers were dried with $NaSO_4$ and concentrated *in vacuo*. The acetal was isolated in quantitative yield and used without further purification.

A flame-dried 500 mL round bottom flask under N_2 was charged with THF (60 mL) and 2-bromo-5-methoxybenzaldehyde trimethylene glycol acetal (3.5 mL, 18.2 mmol, 1.0 equiv). The flask was placed in an acetone/CO_2 bath and *n*BuLi (9.0 mL of a 2.5 M solution, 22.5 mmol, 1.2 equiv) was added slowly. The reaction mixture was allowed to stir at -78 ^oC for 1 h and I_2 (10.15 g, 40.0 mmol, 2.2 equiv) added in a single portion. The reaction was allowed to warm slowly to rt and stirred overnight. A solution of 1 M HCl (~150 mL) was added to the flask and the reaction mixture refluxed under N_2 for 1 h. The cooled mixture was poured into a separatory funnel and diluted with CH_2Cl_2. The aqueous layer was extracted 1x with CH_2Cl_2 and the combined organic layers were washed with saturated $NaHSO_3$. The organic layer was dried with Na_2SO_4 and concentrated *in vacuo*. The crude material was of sufficient purity for subsequent reactions or could be purified by column chromatography with hexanes/EtOAc as the eluent. A 0-10% gradient of EtOAc was used in 2% increments. The product 2-iodo-5-methoxybenzaldehyde was isolated in 61% yield as a yellow solid. The aldehyde was used as the substrate for a Wittig olefination to prepare the styrene **4b** in a fashion similar

to that described for the synthesis of **4a**. The 2-iodo-5-methoxystyrene was purified by column chromatography using hexanes/EtOAc as the eluent. A gradient was employed using 0-2% EtOAc in 0.5% increments. The styrene **4b** was isolated as a clear, colorless oil in 47% yield. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.69 (d, J = 8.7 Hz, 1H), 7.07 (d, J = 3.1 Hz, 1H), 6.86 (dd, J = 17.2, 10.8 Hz, 1H), 6.59 (dd, J = 8.7, 3.1 Hz, 1H), 5.62 (dd, J = 17.3, 1.0 Hz, 1H), 5.32 (dd, J = 10.9, 1.0 Hz, 1H), 3.81 (s, 3H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 160.02, 141.52, 140.56, 139.82, 116.86, 115.72, 111.94, 88.39, 55.39. HRMS (EI) *m/z* calculated for C_9H_9IO $[M]^+$ 259.9693, found 259.9694.



Compound 4f. A 50 mL, two-neck round bottom flask equipped with a Dean-Stark apparatus was charged with 2.0 g (8.1 mmol, 1.0 equiv) 2-bromo-5-fluorobenzaldehyde dissolved in 12 mL toluene. Then 40.0 mg (0.195 mmol, 2 mol %) para-toluenesulfonic acid and 710 µl (786 mg, 12.7 mmol, 1.3 equiv) ethylene glycol was added. The reaction mixture was refluxed for 18 h. After cooling to room temperature, 10 mL of saturated $NaHCO_3$ was added and the mixture extracted three times with 25 mL portions of diethyl ether. The combined organic phases were dried over Na_2SO_4, filtered and evaporated under reduced pressure. The acetal was purified by column chromatography (R_f = 0.45, hexane/EtOAc [9:1]) and isolated in 90 % (2.4 g) yield as a colorless liquid. ^{1}H NMR

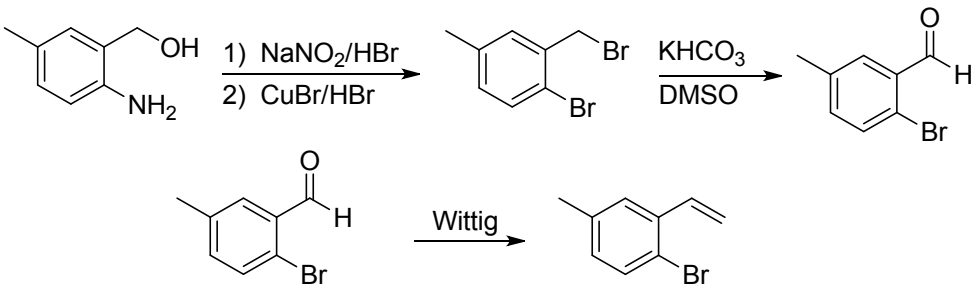
(500 MHz, $CDCl_3$) δ 7.52 (dd, *J* = 8.7 Hz, 5.1 Hz, 1H), 7.33 (dd, *J* = 9.2 Hz, 3.1 Hz, 1H), 6.96 (ddd, *J* = 11.0 Hz, 8.3 Hz, 3.1 Hz, 1H), 6.04 (d, *J* = 0.8 Hz, 1H), 4.22-4.03 (m, 4H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 162.0, 138.7, 134.3, 117.7, 116.8, 115.1, 102.0, 65.6. HRMS (EI) *m/z* calculated for $C_9H_8O_2BrF$ $[M + H]^+$ 245.9687, found 245.9687.

A 100 mL one-neck flask equipped with a condenser was charged with 625.0 mg (8.9 mmol, 1.1 equiv) of sodium thiomethoxide dissolved in 15 mL anhydrous DMF. An aliquot of 2.0 g (8.1 mmol, 1.0 equiv) of 2-(2-bromo-5-fluorophenyl)-1,3-dioxolane was added to this solution and the reaction mixture was stirred overnight (18 h) at 100 °C. The cooled reaction mixture was treated with 40 mL brine and extracted 4x with 50 mL portions of diethyl ether. The combined organic phases were dried over Na_2SO_4 and evaporated under reduced pressure. Column purification (R_f = 0.37, hexane/EtOAc [10:1]) gave 40 % (0.9 g) of 2-(2-bromo-5-(methylthio)phenyl)-1,3-dioxolane as a colorless oil. ^1H-NMR (500 MHz, $CDCl_3$) δ 7.48 (d, *J* = 2.2 Hz, 1H), 7.46 (d, *J* = 8.4 Hz, 1H), 7.26 (s, 1H), 7.10 (dd, *J* = 8.4, 2.3 Hz, 1H), 4.16 (dd, *J* = 8.8 Hz, 5.1 Hz, 2H), 4.07 (dd, *J* = 8.7 Hz, 5.1 Hz, 2H), 2.47 (d, *J* = 7.4 Hz, 3H). ^{13}C-NMR (125 MHz, $CDCl_3$) δ 138.41, 136.86, 133.17, 128.48, 125.68, 119.02, 102.35, 65.49, 15.87. HRMS (EI) *m/z* calculated for $C_{10}H_{11}O_2BrS$ $[M + H]^+$ 273.9658, found 273.9666.

A 50 mL one-neck round bottom flask was charged with 885.0 mg (3.2 mmol, 1.0 equiv) of 2-(2-bromo-5-(methylthio)phenyl)-1,3-dioxolane dissolved in 18 mL of THF. The solution was treated with 6 mL (12.1 mmol, 3.75 equiv) of 2 M hydrochloric acid and refluxed for 1.5 h. The reaction was monitored by SiO_2-TLC (R_f = 0.53, hexane/EtOAc [10:1]) until no starting material was detected. The reaction was quenched with 25 mL water and the mixture extracted twice with 25 mL portions of ethyl

acetate. The combined organic phases were dried over Na_2SO_4 and concentrated under evaporation to give 93% yield (689.0 mg) of the aldehyde as a colorless oil. The crude aldehyde was used in the subsequent Wittig reaction without further purification. ^{1}H-NMR (400 MHz, $CDCl_3$) δ = 10.33 (s, 1H), 7.73 (d, *J* = 2.5 Hz, 1H), 7.53 (d, *J* = 8.4 Hz, 1H), 7.31 (dd, *J* = 8.4 Hz, 2.5 Hz, 1H), 2.51 (s, 3H). HRMS (EI) *m/z* calculated for C_8H_7OBrS $[M + H]^+$ 229.9396, found 229.9391.

The aldehyde was employed in a Wittig olefination to prepare the styrene **4f** in a fashion similar to that described for the synthesis of **4a**. The 2-bromo-5-thiomethoxystyrene **4f** was purified by column chromatography using 10:1 hexanes/EtOAc as the eluent. The styrene **4f** was isolated as a clear, colorless oil in 70% yield. ^{1}H-NMR (300 MHz, $CDCl_3$) δ 7.45 (d, *J* = 8.4 Hz), 7.41 (d, *J* = 2.4 Hz), 7.08 – 6.94 (m), 7.08 – 6.93 (m), 5.70 (dd, *J* = 17.4, 0.9 Hz), 5.38 (dd, *J* = 11.0, 0.9 Hz), 2.49 (s). ^{13}C-NMR (100 MHz, $CDCl_3$) δ 138.1, 137.8, 135.5, 133.1, 127.3, 124.8, 120.0, 117.2. HRMS (EI) *m/z* calculated for $C_9H_{11}BrS$ $[M + H]^+$ 227.9603, found 227.9601.



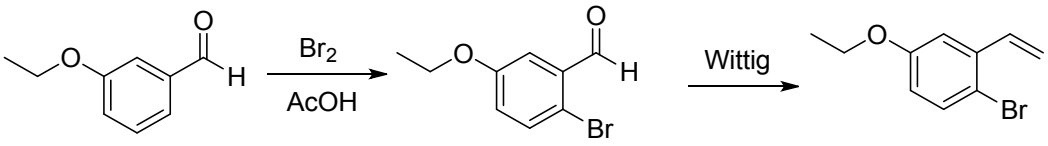
Compound 4g. The 2-amino-5-methylbenzyl alcohol (3.04 g, 22.2 mmol, 1.0 equiv) was dissolved in 20 mL of concentrated HBr and the mixture cooled to 0 °C. $NaNO_2$ (1.58 g, 23.0 mmol, 1.04 equiv) dissolved in 10 mL of H_2O was added dropwise. The solution was allowed to stir at rt for 1 h. Meanwhile, a 100 mL round bottom flask equipped with

a reflux condenser was charged with CuBr (1.68 g, 11.7 mmol, 0.53 equiv) was dissolved in 5 mL of conc. HBr and heated to 140 ^{o}C. The diazonium salt solution was added dropwise to the refluxing CuBr solution over 15-20 min. The heat was removed and the reaction was allowed to cool to rt slowly and stirred overnight. The reaction mixture was poured into CH_2Cl_2. The aqueous layer was extracted 3x with portions of CH_2Cl_2 and the combined organic layers were dried over Na_2SO_4 and concentrated *in vacuo*. The crude material was purified by column chromatography with hexanes as the eluent to give 2-bromo-5-methyl benzyl bromide in 41% yield as a clear, colorless oil.

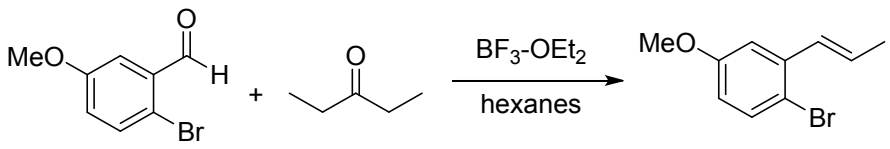
A 100 mL round bottom flask was charged with 2-bromo-5-methylbenzyl bromide (2.56 g, 9.69 mmol, 1.0 equiv) dissolved in 40 mL dry DMSO and $KHCO_3$ (4.91 g, 49.1 mmol, 5.1 equiv). The reaction mixture was heated under nitrogen at 80 ^{o}C overnight. The reaction mixture was allowed to cool to rt and then poured into water/CH_2Cl_2. The organic layer was washed two additional times with portions of water. The combined organic layers were dried over Na_2SO_4 and concentrated *in vacuo*. The 2-bromo-5-methylbenzaldehyde was purified with column chromatography using hexanes/EtOAc as the eluent. A gradient was employed using 0-8% EtOAc in 2% increments. The aldehyde was isolated as a clear colorless oil in 71% yield.

The aldehyde was used as the substrate for a Wittig olefination to prepare the styrene **4g** in a fashion similar to that described for the synthesis of **4a**. The 2-bromo-5-methylstyrene was purified by column chromatography using hexanes as the eluent. The styrene **4g** was isolated as a clear, colorless oil in 68% yield. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.41 (d, J = 8.1 Hz, 1H), 7.36 (d, J = 1.4 Hz, 1H), 7.03 (dd, J = 17.5, 10.9 Hz, 1H), 6.93 (dd, J = 8.1, 2.2 Hz, 1H), 5.68 (d, J = 17.4 Hz, 1H), 5.33 (d, J = 10.9 Hz, 1H),

2.31 (s, 3H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 137.25, 137.00, 135.83, 132.54, 130.03, 127.37, 120.32, 116.32, 20.96. HRMS (EI) *m/z* calculated for C_9H_9Br $[M]^+$ 195.9883, found 195.9883.

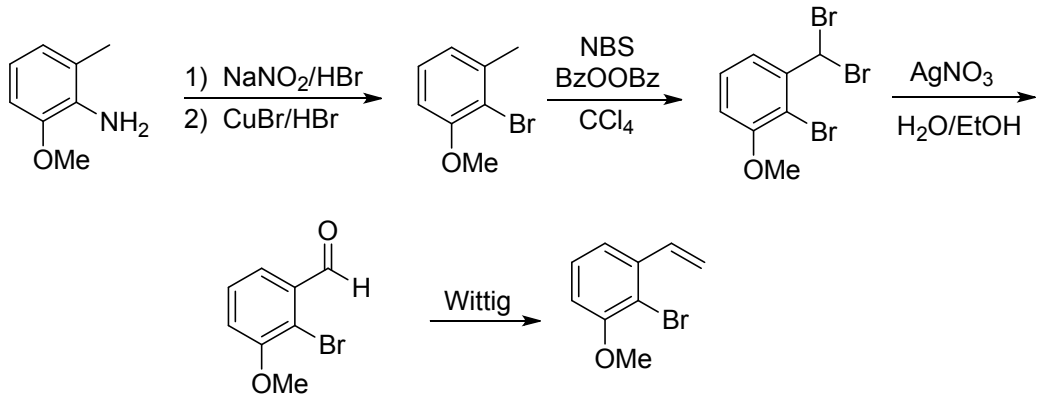


Compound 4h. Compound **4h** was synthesized and purified in a fashion similar to that described for **4a**. The 2-bromo-5-ethoxybenzaldehyde was isolated as a clear colorless oil in 91% yield and the styrene **4h** was isolated as a clear colorless oil in 45% yield. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.41 (d, *J* = 8.8 Hz, 1H), 7.07 (d, *J* = 3.0 Hz, 1H), 7.01 (dd, *J* = 17.4, 10.9 Hz, 1H), 6.69 (dd, *J* = 8.8, 3.0 Hz, 1H), 5.68 (dd, *J* = 17.4, 1.0 Hz, 1H), 5.35 (dd, *J* = 10.9, 1.0 Hz, 1H), 4.03 (q, *J* = 7.0 Hz, 2H), 1.42 (t, *J* = 7.0 Hz, 3H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 158.32, 138.12, 135.89, 133.36, 116.63, 115.71, 114.14, 112.60, 63.73, 14.77. HRMS (EI) *m/z* calculated for $C_{10}H_{11}BrO$ $[M]^+$ 225.9988, found 225.9992.



Compound 4i. A flame-dried 250 mL round bottom flask equipped with a reflux condenser under an atmosphere of N_2 was charged with 80 mL of hexanes and 2-pentanone (4.5 mL, 42.5 mmol, 0.98 equiv). Boron trifluoride diethyl etherate (5.5 mL, 44.6 mmol, 1.02 equiv) was added slowly, followed by 2-bromo-5-methoxybenzalde (9.36 g, 43.5 mmol, 1.0 equiv). The reaction was allowed to reflux for 1 h and then carefully quenched with water. The aqueous phase was extracted twice with hexanes and

the combined organic layers were dried with Na_2SO_4 and concentrated *in vacuo*. The crude material was purified using column chromatography with hexanes as the initial eluent. A mobile phase consisting of 99.5% hexanes/0.5% EtOAc was then employed until the material had fully eluted. The 2-bromo-5-methoxy-*trans*-β-methylstyrene **4i** was isolated as a clear, colorless oil in 27% yield. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.40 (d, J = 8.7 Hz, 1H), 7.00 (d, J = 3.0 Hz, 1H), 6.68 (dq, J = 15.7, 1.8 Hz, 1H), 6.65 (dd, J = 8.8, 3.1 Hz, 1H), 6.18 (dq, J = 15.6, 6.7 Hz, 1H), 3.79 (s, 3H), 1.92 (dd, J = 6.7, 1.8 Hz, 3H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 158.89, 138.39, 133.28, 129.94, 128.97, 114.30, 113.76, 111.91, 55.43, 18.64. HRMS (EI) *m/z* calculated for $C_{10}H_{11}BrO$ $[M]^+$ 225.9988, found 225.9990.

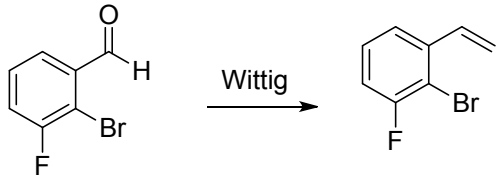


Compound 4j. The 2-bromo-3-methoxytoluene was prepared in similar fashion as described for the synthesis of **4g.** The crude material was purified by column chromatography with hexanes/EtOAc as the eluent. A gradient was employed using 0-3% EtOAc in 1% increments. The 2-bromo-3-methoxytoluene was isolated as a clear colorless oil which solidified upon standing in 47% yield.

A 500 mL round bottom flask was charged with 2-bromo-3-methoxytoluene (1.7 mL, 11.7 mmol, 1.0 equiv), NBS (5.32 g, 29.9 mmol, 2.56 equiv) and benzoyl peroxide (0.28

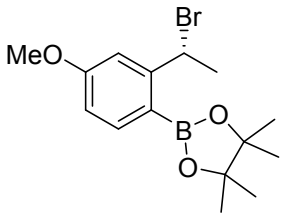
g, 1.15 mmol, 0.098 equiv) in 50 mL of carbon tetrachloride. The reaction was refluxed for 3 h under irradiation with a 300 W lamp. The reaction mixture was then filtered through pad of Celite and washed with CH_2Cl_2. The solvent was removed *in vacuo* and the residue dissolved in 50 mL 4:1 EtOH:H_2O. $AgNO_3$ (5.12 g, 30.1 mmol, 2.57 equiv) was added to the ethanol solution and the reaction mixture was refluxed for 1 h. The reaction was filtered through a pad of Celite and washed with EtOAc. The volume of the filtrate was reduced to about 20 mL and then added to a mixture of water and EtOAc. The aqueous layer was extracted 2x with portions of EtOAc and the combined organic layers were dried over Na_2SO_4 and concentrated *in vacuo*. The crude material was purified by column chromatography with hexanes/EtOAc as the eluent. A gradient was employed using 0-8% EtOAc in 2% increments. The 2-bromo-3-methoxybenzaldehyde was isolated a white solid in 82% yield over two steps.

The aldehyde was employed as the substrate for a Wittig olefination to prepare the styrene **4j** in a fashion similar to that described for the synthesis of **4a**. The 2-bromo-3-methoxystyrene was purified by column chromatography using hexanes/EtOAc as the eluent. A gradient was employed using 0-1% EtOAc in 0.5% increments. The styrene **4j** was isolated as a white solid in 64% yield. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.24 (t, J = 7.9 Hz, 1H), 7.17 (d, J = 6.5 Hz, 1H), 7.12 (dd, J = 17.5, 11.0 Hz, 1H), 6.82 (d, J = 7.8 Hz, 1H), 5.70 (dd, J = 17.4, 1.3 Hz, 1H), 5.37 (dd, J = 11.0, 1.2 Hz, 1H), 3.90 (s, 3H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 156.03, 139.20, 136.09, 127.78, 118.98, 116.99, 113.21, 110.74, 56.41. HRMS (EI) *m/z* calculated for C_9H_9BrO $[M]^+$ 211.9832, found 211.9835.



Compound 4k. The 2-bromo-3-fluorobenzaldehyde was used as the substrate for a Wittig olefination to prepare the styrene **4k** in a fashion similar to that described for the synthesis of **4a**. The 2-bromo-3-fluorostyrene was purified by column chromatography using hexanes as the eluent. The styrene **4k** was isolated as a clear colorless oil in 36% yield. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.34 (d, J = 7.9 Hz, 1H), 7.24 (td, J = 8.0, 5.5 Hz, 1H), 7.06 (dd, J = 17.7, 11.0 Hz, 1H), 7.03 (td, J = 8.5, 1.8 Hz, 1H), 5.74 (dd, J = 17.4, 0.9 Hz, 1H), 5.42 (d, J = 11.0 Hz, 1H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 160.20, 158.24, 139.75, 134.86, 134.83, 128.18, 128.12, 121.95, 121.93, 117.88, 115.19, 115.01, 110.59, 110.42. HRMS (EI) *m/z* calculated for C_8H_6BrF $[M]^+$ 199.9632, found 199.9633.

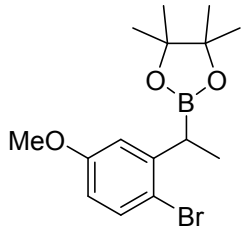
IV. General procedure for the asymmetric 1,3-halogen migration reaction.



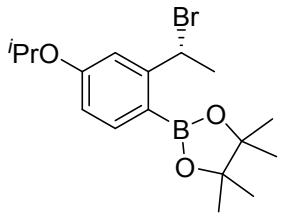
Compound 2. In a glovebox, CuCl (10.0 mg, 0.101 mmol, 0.10 equiv), NaO^{t}Bu (20.0 mg, 0.208 mmol, 0.21 equiv), (*S,S*)-Ph-BPE (51.0 mg, 0.101 mmol, 0.10 equiv) and 10 mL of dry, degassed toluene were added to a dry, 25 mL round bottom flask. The flask was fitted with a septum, removed from the glovebox and the reaction mixture stirred for 10 min. HBpin (0.18 mL, 1.24 mmol, 1.20 equiv) was added in one aliquot and the reaction was transferred to a cryo-bath set to 0 ^{o}C and stirred for a further 10 min. The 2-

bromo-5-methoxy-styrene (0.16 mL, 1.03 mmol, 1.0 equiv) was added and reaction was allowed to stir for 18 h at 0 °C. The mixture was filtered through a pad of Celite and the solids washed with Et_2O (3x10 mL). The volatiles were removed *in vacuo* and the residue purified by column chromatography using 8% EtOAc in hexanes as the eluent. The product **2** was isolated as a clear, colorless, viscous liquid in 72% yield and 96% *ee*. $[\alpha]_D^{24}$ -0.325 (c = 0.039 g/mL, CH_2Cl_2, *l* = 4.5 cm) All spectroscopic data were consistent with literature values.[3]

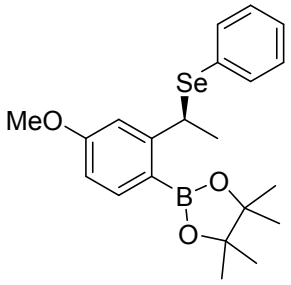
The following compounds were prepared in the same fashion as **2**, with exceptions noted as necessary.



Compound 3. Compound **3** was prepared in the same fashion as described for the preparation of **2**, except Xantphos was employed as the ligand in place of (*S,S*)-Ph-BPE and the reaction was conducted at 40 °C. An integrated ^{1}H NMR yield of 69% was obtained using 1,1,1,2-tetrachloroethane as an internal standard. ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.39 (d, *J* = 8.7 Hz, 1H), 6.83 (d, *J* = 3.0 Hz, 1H), 6.57 (dd, *J* = 8.7, 3.0 Hz, 1H), 3.77 (s, 3H), 2.73 (q, *J* = 7.5 Hz, 1H), 1.33 (d, *J* = 7.5 Hz, 3H), 1.24 (s, 12H). ^{13}C NMR (75 MHz, $CDCl_3$) δ 159.23, 145.80, 133.09, 115.66, 115.15, 112.26, 83.69, 55.50, 24.96, 24.90, 15.94. HRMS (ESI) *m/z* calculated for $C_{15}H_{26}BrNO$ $[M+NH_4]^+$ 357.1220, found 357.1217.

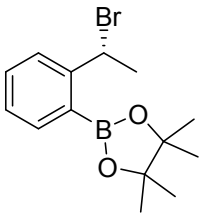


Compound 5a. Compound **5a** was prepared in the same fashion as described for compound **2**. The product was purified by column chromatography using 5% EtOAc in hexanes as the eluent. The product was isolated as a clear, colorless, viscous liquid in 53% yield and >99% ee. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.71 (d, *J* = 8.3 Hz, 1H), 7.19 (d, *J* = 2.2 Hz, 1H), 6.76 (dd, *J* = 8.3, 2.3 Hz, 1H), 6.24 (q, *J* = 6.8 Hz, 1H), 4.63 (hept, *J* = 6.0 Hz, 1H), 1.99 (d, *J* = 6.9 Hz, 3H), 1.35 (d, *J* = 5.9 Hz, 12H), 1.35 (s, 6H), 1.33 (s, 6H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 160.58, 151.72, 137.86, 114.41, 114.01, 83.53, 69.56, 48.53, 27.24, 25.01, 24.71, 21.98. HRMS (ESI) *m/z* calculated for $C_{17}H_{30}BrBNO_3$ $[M+NH_4]^+$ 385.1533, found 385.1533.



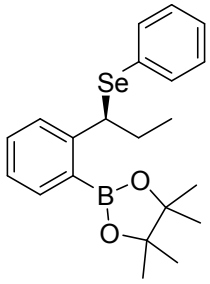
Compound 5b. Compound **5b** was prepared in the same fashion as described for compound **2** except the benzyl iodide was trapped with lithium phenylselenoate prior to isolation. Selenium (0.2199 g, 2.78 mmol, 2.81 equiv.) was added to a flame-dried conical flask under nitrogen and diluted with THF to prepare a 1 M solution.

Phenyllithium (1.7 mL of a 1.78 M solution, 3.03 mmol, 3.06 equiv.) was added to the selenium/THF mixture and the LiSePh solution allowed to form at ambient temperature for 30 min. The solution was transferred to the flask containing the benzyl bromide and the reaction mixture was allowed to stir at ambient temperature for 2 h. The mixture was filtered through a pad of Celite and the solids washed with Et_2O (3x10mL). The filtrate was concentrated *in vacuo* and the residue was purified by column chromatography using hexanes/EtOAc as the eluent in a 0-8% gradient in 2% increments. Compound **5b** was isolated as a pale yellow, viscous oil in 71% yield. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.72 (d, J = 8.3 Hz, 1H), 7.46 (dd, J = 8.1, 1.6 Hz, 2H), 7.25 – 7.17 (m, 3H), 6.88 (d, J = 2.4 Hz, 1H), 6.72 (dd, J = 8.3, 2.5 Hz, 1H), 5.55 (q, J = 7.0 Hz, 1H), 3.78 (s, 3H), 1.71 (d, J = 6.9 Hz, 3H), 1.32 (s, 12H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 161.86, 152.36, 137.93, 134.80, 130.38, 128.56, 127.28, 112.24, 111.33, 83.37, 55.06, 39.69, 24.91, 24.82, 22.36. HRMS (ESI) *m/z* calculated for $C_{21}H_{28}BO_3Se$ $[M+H]^+$ 432.1584, found 432.1588.

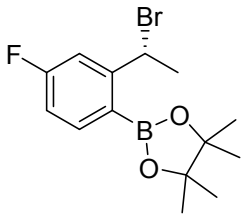


Compound 5c. Compound **5c** was prepared in the same manner as compound **2**. The crude material was purified by column chromatography using hexanes as the initial eluent. The eluent was then switched to 10% EtOAc/hexanes. The product was isolated as clear colorless, viscous oil in 28% yield. All spectroscopic data were consistent with literature values.[3]

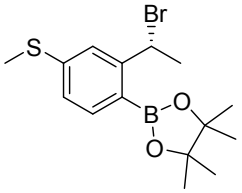
To determine enantiomeric excess, the product was trapped with 2-thionaphthalene as described for the sulfide of compound **6**. The sulfide was isolated in 84% *ee*. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.80 – 7.73 (m, 3H), 7.70 – 7.64 (m, 2H), 7.57 (dd, *J* = 7.7, 1.1 Hz, 1H), 7.46 – 7.36 (m, 4H), 7.21 (td, *J* = 7.4, 1.1 Hz, 1H), 5.57 (q, *J* = 6.9 Hz, 1H), 1.64 (d, *J* = 6.9 Hz, 3H), 1.33 (s, 6H), 1.32 (s, 6H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 149.41, 135.95, 133.66, 133.65, 131.98, 131.23, 129.33, 129.00, 127.85, 127.61, 127.23, 126.27, 126.22, 125.63, 83.72, 44.41, 24.90, 24.86, 22.47.



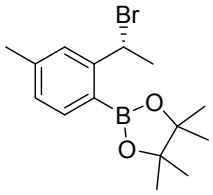
Compound 5d. Compound **5d** was prepared and purified in the same manner as compound **5b**. The product was isolated as a pale yellow, viscous oil in 40% yield and 89% *ee*. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.73 (d, *J* = 7.5 Hz, 1H), 7.43 (d, *J* = 6.9 Hz, 2H), 7.36 (d, *J* = 3.5 Hz, 2H), 7.23 – 7.14 (m, 4H), 5.32 (dd, *J* = 8.6, 6.7 Hz, 1H), 2.09 – 2.00 (m, 2H), 1.33 (s, 6H), 1.32 (s, 6H), 0.86 (t, *J* = 7.3 Hz, 6H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 148.96, 135.81, 134.72, 131.06, 130.42, 128.50, 127.13, 126.85, 125.77, 83.58, 47.40, 29.92, 24.95, 24.79, 13.07. HRMS (ESI) *m/z* calculated for $C_{21}H_{28}BSeO_2$ $[M+H]^+$ 399.1369, found 399.1374.



Compound 5e. Compound **5e** was prepared in the same fashion as described for compound **2**. The product was purified by column chromatography using 5% EtOAc in hexanes as the eluent. The product was isolated as a clear, colorless, viscous liquid in 38% yield and 81% *ee*. $[\alpha]_D^{24}$ -0.030 (c = 0.018 g/mL, CH_2Cl_2, *l* = 4.5 cm) All characterization data was consistent with literature values.[3]

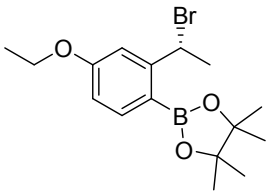


Compound 5f. Compound **5f** was prepared in the same fashion as described for compound **2**. An integrated ^{1}H NMR yield of 13% was obtained using 1,1,1,2-tetrachloroethane as an internal standard. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.68 (d, *J* = 7.9 Hz, 1H), 7.53 (d, *J* = 1.8 Hz, 1H), 7.10 (dd, *J* = 8.0, 1.9 Hz, 1H), 6.21 (q, *J* = 6.9 Hz, 1H), 2.51 (s, 3H), 2.00 (d, *J* = 6.9 Hz, 3H), 1.36 (s, 6H), 1.34 (s, 6H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 150.00, 142.97, 136.37, 124.36, 123.99, 83.81, 48.17, 27.12, 24.98, 24.87, 24.84, 24.72, 24.70, 24.64, 15.07. HRMS (ESI) *m/z* calculated for $C_{15}H_{26}BrBNO_2S$ $[M+NH_4]^+$ 373.1070, found 373.1060.



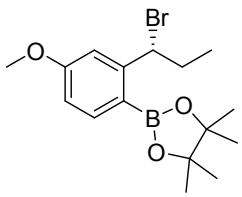
Compound 5g. Compound **5g** was prepared in the same fashion as described for compound **2**. The crude material was purified by column chromatography using hexanes as the initial eluent. The eluent was then switched to 10% EtOAc/hexanes. The product was isolated as a clear, colorless, viscous oil in 30% yield. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.67 (d, *J* = 7.6 Hz, 1H), 7.49 (s, 1H), 7.08 (d, *J* = 7.6 Hz, 1H), 6.25 (q, *J* = 6.9 Hz, 1H), 2.37 (s, 3H), 2.01 (d, *J* = 6.9 Hz, 3H), 1.36 (s, 6H), 1.34 (s, 6H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 149.48, 141.66, 136.05, 128.18, 127.18, 83.69, 48.80, 27.08, 24.98, 24.86, 24.68, 21.72. HRMS (ESI) *m/z* calculated for $C_{15}H_{26}BBrNO_2$ $[M+NH_4]^+$ 341.1271, found 341.1272.

To determine enantiomeric excess, the product was trapped with lithium phenylselenoate as described for compound **5b**. The selenide was isolated in 85% *ee*. $[\alpha]_D^{24}$ -0.077 (c = 0.025 g/mL, CH_2Cl_2, *l* = 4.5 cm) ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.66 (d, *J* = 7.6 Hz, 1H), 7.45 (dd, *J* = 7.9, 1.5 Hz, 2H), 7.25 – 7.18 (m, 3H), 7.16 (s, 1H), 7.01 (d, *J* = 7.5 Hz, 1H), 5.54 (q, *J* = 7.0 Hz, 1H), 2.31 (s, 3H), 1.72 (d, *J* = 7.0 Hz, 3H), 1.33 (s, 6H), 1.32 (s, 6H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 149.89, 141.07, 136.17, 134.68, 130.67, 128.55, 127.22, 127.07, 126.84, 83.49, 39.91, 24.90, 24.86, 22.40, 21.69. HRMS (EI) *m/z* calculated for $C_{21}H_{27}BO_2Se$ $[M]^+$ 416.1645, found 416.1642.



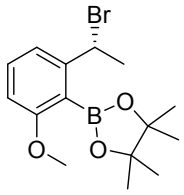
Compound 5h. Compound **5h** was prepared and purified in the same manner as compound **2**. The product was isolated as a clear, colorless, viscous oil in 57% yield. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.72 (d, *J* = 8.3 Hz, 1H), 7.21 (d, *J* = 2.4 Hz, 1H), 6.77 (dd, *J* = 8.4, 2.4 Hz, 1H), 6.25 (q, *J* = 6.8 Hz, 1H), 4.13 – 4.03 (m, 2H), 1.99 (d, *J* = 6.8 Hz, 3H), 1.43 (t, *J* = 7.0 Hz, 3H), 1.35 (s, 6H), 1.34 (s, 6H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 161.57, 151.65, 137.87, 113.20, 112.98, 83.54, 63.33, 48.48, 27.17, 24.99, 24.68, 14.74. HRMS (ESI) *m/z* calculated for $C_{16}H_{28}BBrNO_3$ $[M+NH_4]^+$ 371.1377, found 371.1369.

To determine enantiomeric excess, the product was trapped with 2-thionaphthalene as described for the sulfide of compound **6**. The sulfide was isolated in 89% *ee*. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.78 – 7.71 (m, 3H), 7.67 (d, *J* = 8.7 Hz, 2H), 7.45 – 7.38 (m, 3H), 7.13 (d, *J* = 2.4 Hz, 1H), 6.73 (dd, *J* = 8.3, 2.5 Hz, 1H), 5.61 (q, *J* = 6.9 Hz, 1H), 4.08 – 3.97 (m, 2H), 1.61 (d, *J* = 6.9 Hz, 3H), 1.38 (t, *J* = 7.0 Hz, 3H), 1.31 (s, 12H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 161.56, 151.93, 137.94, 133.86, 133.65, 131.90, 128.93, 128.77, 127.80, 127.58, 127.17, 126.18, 125.53, 112.77, 112.17, 83.39, 63.20, 44.15, 24.86, 24.84, 22.71, 14.73. HRMS (EI) *m/z* calculated for $C_{26}H_{32}BO_3S$ $[M+H]^+$ 434.2197, found 434.2195.



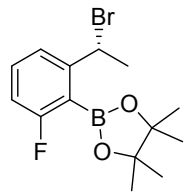
Compound 5i. Compound **5i** was prepared and purified in the same manner as compound **2**. The product was isolated as a clear, colorless, viscous oil in 50% yield. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.73 (d, *J* = 8.4 Hz, 1H), 7.19 (d, *J* = 2.4 Hz, 1H), 6.79 (dd, *J* = 8.4, 2.5 Hz, 1H), 6.00 (dd, *J* = 7.8, 6.7 Hz, 1H), 3.84 (s, 3H), 2.29 – 2.03 (m, 2H), 1.34 (s, 6H), 1.33 (s, 6H), 0.99 (t, *J* = 7.2 Hz, 3H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 162.21, 150.73, 137.73, 113.37, 112.70, 83.56, 56.15, 55.17, 34.21, 24.87, 24.84, 12.86. HRMS (ESI) *m/z* calculated for $C_{16}H_{28}BBrNO_3$ $[M+NH_4]^+$ 371.1377, found 371.1373.

To determine enantiomeric excess, the product was trapped with 2-thionaphthalene as described for the sulfide of compound **6**. The sulfide was isolated in 93% *ee*. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.77 – 7.70 (m, 3H), 7.67 – 7.62 (m, 2H), 7.46 – 7.35 (m, 3H), 7.15 (d, *J* = 2.5 Hz, 1H), 6.73 (dd, *J* = 8.4, 2.5 Hz, 1H), 5.44 (dd, *J* = 8.6, 6.0 Hz, 1H), 3.78 (s, 3H), 2.05 – 1.86 (m, 2H), 1.32 (s, 6H), 1.31 (s, 6H), 0.91 (t, *J* = 7.4 Hz, 3H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 162.24, 151.16, 137.74, 133.97, 133.63, 131.80, 128.77, 128.76, 127.73, 127.55, 127.12, 126.12, 125.44, 112.35, 111.81, 83.38, 55.05, 50.69, 30.62, 24.95, 24.79, 12.18. HRMS (EI) *m/z* calculated for $C_{26}H_{32}BO_3S$ $[M+H]^+$ 434.2197, found 434.2193.



Compound 5j. Compound **5j** was prepared and purified in the same manner as compound **2**. The product was isolated as a clear, colorless, viscous oil in 50% yield and 70% *ee*. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.32 (t, *J* = 8.0 Hz, 1H), 7.19 (d, *J* = 7.8 Hz, 1H), 6.74 (d, *J* = 8.3 Hz, 0H), 5.36 (q, *J* = 6.9 Hz, 1H), 3.78 (s, 3H), 2.03 (d, *J* = 6.9 Hz, 3H),

1.42 (s, 6H), 1.41 (s, 6H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 162.50, 148.01, 131.09, 118.45, 109.57, 84.15, 55.72, 48.81, 26.98, 24.88, 24.73. HRMS (ESI) *m/z* calculated for $C_{15}H_{26}BBrNO_3$ $[M+NH_4]^+$ 357.1120, found 357.1208.



Compound 5k. Compound **5k** was prepared in the same fashion as described for compound **2**. An integrated ^{1}H NMR yield of 65% was obtained using 1,1,1,2-tetrachloroethane as an internal standard. The crude material was purified by column chromatography using hexanes as the initial eluent. The eluent was then switched to 10% EtOAc/hexanes. The product was isolated as a clear, colorless, viscous oil in 41% yield. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.43 – 7.33 (m, 2H), 6.93 (ddd, *J* = 8.9, 7.5, 1.7 Hz, 1H), 5.76 (q, *J* = 6.9 Hz, 1H), 2.04 (d, *J* = 6.9 Hz, 3H), 1.43 (s, 6H), 1.40 (s, 6H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 166.94, 164.98, 149.87, 149.81, 132.12, 132.05, 121.77, 121.74, 114.76, 114.56, 84.36, 47.47, 47.45, 26.53, 24.92, 24.76. HRMS (ESI) *m/z* calculated for $C_{14}H_{23}BBrFNO_2$ $[M+NH_4]^+$ 345.1021, found 345.1020.

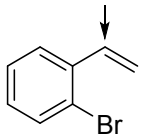
To determine enantiomeric excess, the product was trapped with 2-thionaphthalene as described for the sulfide of compound **6**. The sulfide was isolated in 81% *ee*. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.80 – 7.76 (m, 2H), 7.75 – 7.68 (m, 2H), 7.49 – 7.41 (m, 2H), 7.37 (dd, *J* = 8.5, 1.8 Hz, 1H), 7.33 – 7.25 (m, 2H), 6.90 (ddd, *J* = 9.0, 7.5, 1.7 Hz, 1H), 5.04 (q, *J* = 7.0 Hz, 1H), 1.68 (d, *J* = 7.0 Hz, 3H), 1.41 (s, 6H), 1.40 (s, 6H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 166.20 (d, J = 245 Hz), 150.12 (d, J = 7.5 Hz), 133.64, 132.71, 132.06,

131.71(d, J = 9.3 Hz), 129.52, 128.85, 128.03, 127.61, 127.30, 126.30, 125.81, 122.02 (d, J = 2.7 Hz), 113.66 (d, J = 24.5 Hz), 84.23, 45.53 (d, J = 1.9 Hz), 24.9 (d, J = 16 Hz), 22.54. HRMS (ESI) *m/z* calculated for $C_{24}H_{30}BFNO_2S$ $[M+NH_4]^+$ 408.1840, found 408.1834.

V. Computational Trend.

The tables below summarize the computational data used to create and test the trend. The geometries and absolute energies can be found below the summary tables. All structures were optimized in Gaussian 09[4] using B3LYP/6-311++G(2d,p) and the vibrational frequencies were checked to make sure the structure was at a minimum on the potential energy surface. A Natural Population Analysis was performed at the same level of theory and basis set. The volume was calculated using the volume(tight) key word.

Electron Density at the Olefin: To quantify the electron density at the olefin, we used the NPA charge at the α carbon of the olefin (indicated as 'Ole e den' in Tables 1 and 2 below; designated as 'α' in the manuscript) for a number of substituted styrenes. We believe that this is a reasonable assumption as this is the carbon that binds to the copper in the course of the reaction. The atomic charges at the β carbons of the various olefins did not appear to trend with the observed reactivity. In addition, the average electron density at the two carbons of the olefins were nearly the same for all the substrates that were initially optimized (H, 5-OMe, 5-F). Thus, this parameter does not appear to greatly impact the yield.



Electron Density at the Carbon Bearing Bromine: A more electron-rich sp^2 bromine-bearing carbon appeared to correlate with increased yield in the 1,3-halogen migration reaction, presumably because this facilitates the transposition of the bromine to the benzylic carbon. The importance of the electron density at this carbon is perhaps not surprising, as we hypothesize this carbon eventually binds to the copper catalyst during the course of the 1,3-halogen migration. To quantify the electron density at this carbon, we used the NPA charge (indicated as 'Br e den' in Tables 1 and 2 below; denoted as 'γ' in the manuscript) at the carbon bearing the bromine atom. Interestingly, it appears that this parameter has the largest impact on the yield of the reaction (except when the substrate is sterically congested).

Propensity to form Radicals: Atom Transfer Radical Polymerization (ATRP) is a major side reaction in this chemistry. It is well-known that a copper(I) salt can abstract the halide of a benzyl halide, resulting in a Cu(II) salt and a benzyl radical. The presence of this radical can initiate the polymerization of the remaining styrene substrate, simultaneously deactivating the catalyst and destroying the starting material. As would be expected, disfavoring this reaction is a prerequisite for high yields in the 1,3-halogen migration reaction. To quantify this empirical observation, the energy of the benzyl bromide (indicated as 'bn br e' in Tables 1 and 2 below), the energy of the benzyl radical (denoted as 'rad e'), and the energy of the radical bromine

(labeled as 'br rad e') was calculated. The ΔG (in kcal/mol) was calculated based upon these energies (dG) using the following formula: [(rad e + br rad e) – bn br e]*627.509. The ΔΔG relative to the substituted product was calculated by subtracting the ΔG for the substituted product from the ΔG for all of the substituted products (ddG, in Tables 1 and 2 below). The ΔΔG is the parameter used in generating an equation for the trend.

Sterics: Given the size of the Ph-BPE ligand, sterics are expected to play a significant role in the outcome of the reaction. However, sterics are traditionally difficult to parameterize. **A** values were initially investigated, as they are readily available for many groups. However, **A** values did not accurately reflect the steric effects that were present in many of our substrates. Fundamentally, **A** values quantify the steric interactions between a specific group and a proton, thus ignoring many of the potential steric interactions for many larger groups. A viable solution was to use the volumes of the groups bound to the aromatic ring as the steric parameter. The volumes of all substrates were calculated (in cm^3/mol) (molar V, in Tables 1 and 2 below) and the volume of 2-bromostyrene was subtracted from volume of the substituted styrene (indicated as 'dV' in Tables 1 and 2 below). This dV value was used as the steric parameter when generating the equation. There is an important assumption concerning this steric parameter that should be kept in mind in analyzing data from our equation. The steric parameter does not take into account where the steric bulk is located; thus, for substrates where the steric bulk is closer to the reactive site, the yield would be expected to be lower as the steric interactions would be exacerbated. For substrates containing long chains attached to the aromatic, the calculated volume would be quite large, but only the first few carbons in the

chain actually play a major role in affecting the yield. In these cases, the actual yield would probably be higher than that predicted by the model.

Creating the Trend Equation: The trend was modelled in Excel using the Solver add-on (See Figure 1). An initial equation was introduced into Excel that multiplied each of the parameters described above by a coefficient cell. The sums were then added together to generate a value that was designated as the predicted yield (denoted by 'pred. yield' in Tables 1 and 2 and Figure 1). A second equation was generated that calculated the difference between the predicted yield and the actual NMR yield ('dif' in Tables 1 and 2 and Figure 1). Solver was then allowed to change the coefficient cells such that the average of the differences was close to zero and none of the differences was greater than +/- 10%. The following equation resulted from these calculations:

pred. yield = -0.547(dV) + 227(Ole e den) + -1220(Br e den) + 18.5(ddG)

This equation was created in a double blind fashion. Ten substrates were used to generate the equation (see Table 1: Substrates in Model). An additional four substrates were randomly excluded in the development of the initial equation. These substrates were used as a preliminary test of the accuracy of the equation (Table 2: Substrates used to Test Model). All of the substrates outside the model were predicted within 12% yield. As many of the yields for the 1,3-halogen migration were measured by integrations of ^{1}H NMRs using an internal standard, a method that can give errors up to 10%, we felt this level of accuracy was sufficient for these initial studies.

Figure 1: Solver Parameters

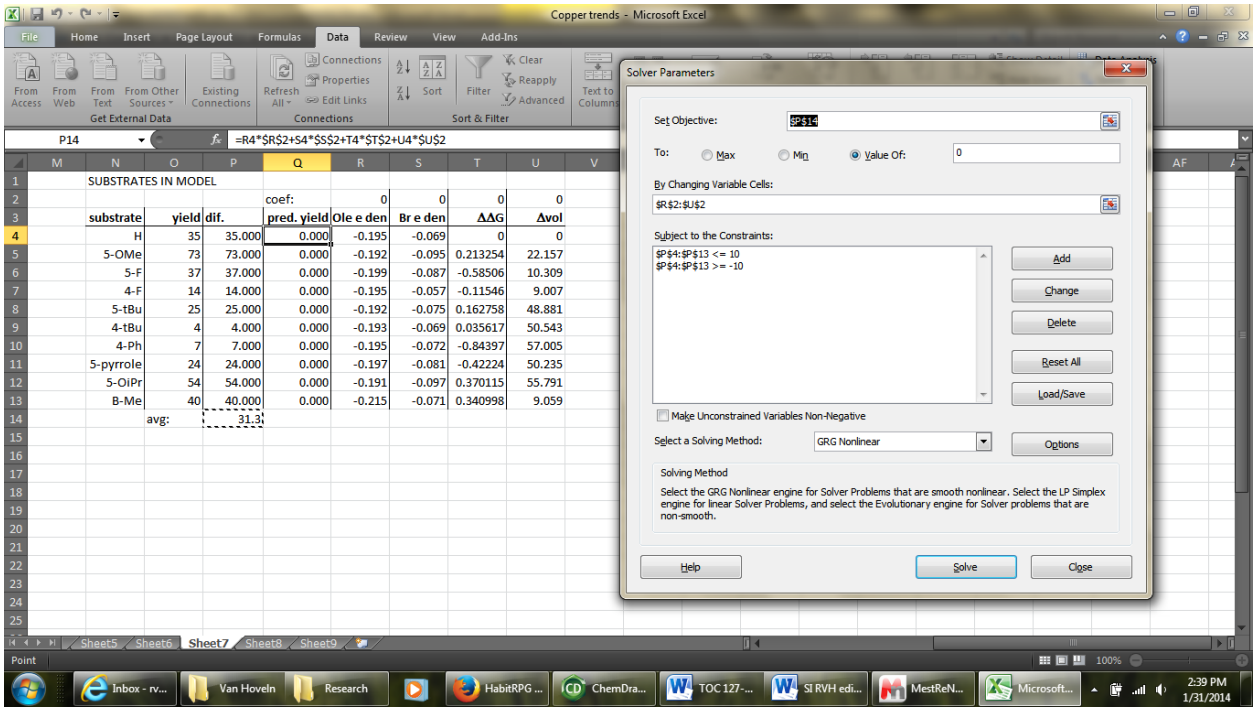


TABLE 1: SUBSTRATES IN MODEL

				coef:	227.1366	-1223.84					18.513		-0.5473
substrate	**ref. letter**	**yield**	**pred. yield**	**abs. diff.**	**Ole e den**	**Br e den**	**Bn rad. E.**	**Br rad. E.**	**rad. E.**	**ΔG**	**ΔΔG**	**Molar V.**	**Δvol**
H	A	35	40.2	5.2	-0.195	-0.069	-3295.32	-2574.1	-721.14	54.975	0.000	111.428	0
5-OMe	B	73	64.5	8.5	-0.192	-0.095	-3409.89	-2574.1	-835.70	55.188	0.213	133.585	22.157
5-F	C	37	44.8	7.8	-0.199	-0.087	-3394.60	-2574.1	-820.41	54.390	-0.585	121.737	10.309
4-F	D	14	18.4	4.4	-0.195	-0.057	-3394.60	-2574.1	-820.41	54.859	-0.115	120.435	9.007
5-tBu	E	25	24.4	0.6	-0.192	-0.075	-3452.62	-2574.1	-878.44	55.138	0.163	160.309	48.881
4-tBu	F	4	13.6	9.6	-0.193	-0.069	-3452.62	-2574.1	-878.44	55.010	0.036	161.971	50.543
4-Ph	G	7	-3.0	10.0	-0.195	-0.072	-3526.44	-2574.1	-952.26	54.131	-0.844	168.433	57.005
5-pyrrole	H	24	19.1	4.9	-0.197	-0.081	-3504.35	-2574.1	-930.17	54.553	-0.422	161.663	50.235
5-OiPr	J	54	51.6	2.4	-0.191	-0.097	-3488.54	-2574.1	-914.36	55.345	0.370	167.219	55.791
β-Me	K	40	39.4	0.6	-0.215	-0.071	-3334.65	-2574.1	-760.46	55.316	0.341	120.487	9.059

TABLE 2: SUBSTRATES TO TEST MODEL

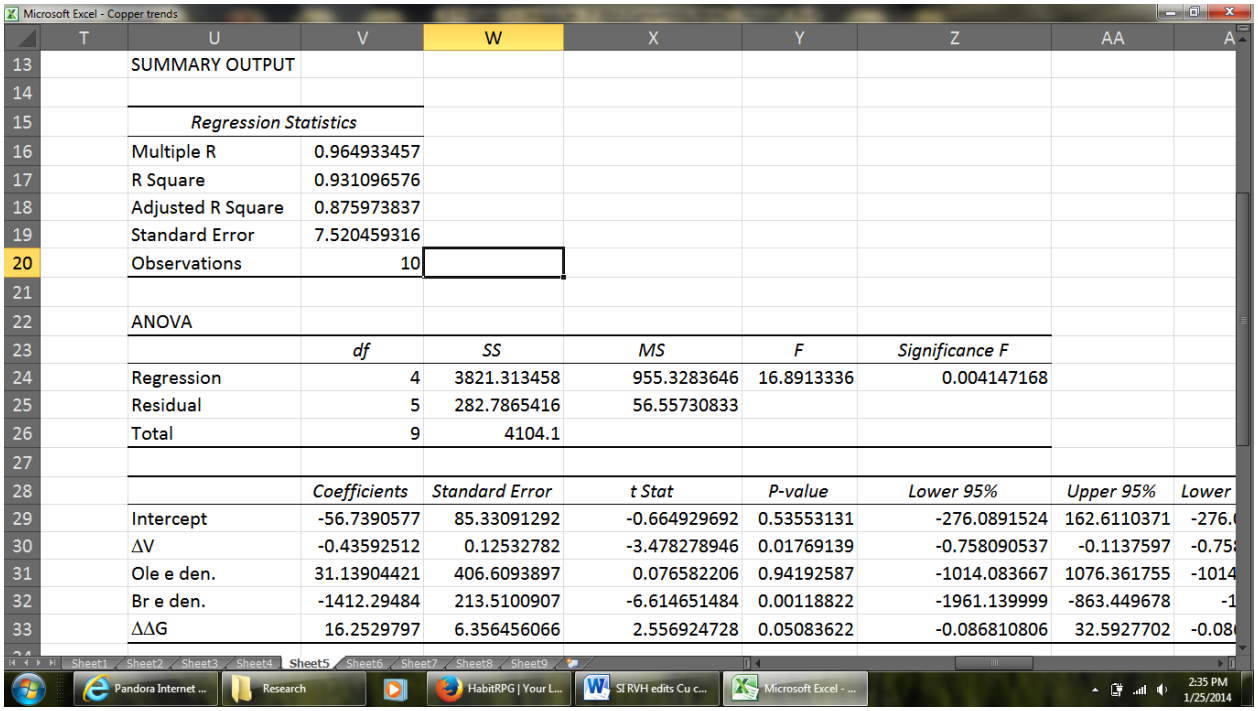
				coef:	227.1366	-1223.84					18.513		-0.5473
substrate	**ref. letter**	**yield**	**pred. yield**	**abs. diff.**	**Ole e den**	**Br e den**	**Bn rad. E.**	**Br rad. E.**	**rad. E.**	**ΔG**	**ΔΔG**	**Molar V.**	**Δvol**
5-OBz	L	8	7.5	0.5	-0.197	-0.086	-3715.05	-2574.1	-1140.9	54.252	-0.723	183.864	72.436
5-OTBS	M	21	9.7	11.3	-0.194	-0.095	-3897.32	-2574.1	-1323.1	55.236	0.261	234.378	122.95
5-Br	N	16	24.1	8.1	-0.199	-0.076	-5868.86	-2574.1	-3294.7	54.438	-0.537	136.627	25.199
6-F	P	9	21.3	12.3	-0.214	-0.057	-3394.59	-2574.1	-820.41	54.945	-0.030	110.091	-1.337

Refining the Equation: A regression analysis was performed on the parameters from Table 1, the results of which are shown in Figure 2. A strong linear correlation was observed ($R^2 = 0.93$), however the parameter that accounted for the electron density at the olefin had an error that was significantly higher than the coefficient itself. As such, this parameter was removed and another regression analysis was performed (Figure 3). Interestingly, the linear correlation was still present and the standard error for all other parameters decreased. The new equation without that does not take into account the electron density at the olefin is:

$$\textbf{predicted yield} = -0.4321(\Delta vol) - 1415(\text{Br e den}) + 16.22(\Delta\Delta G) - 63.16$$

The predicted yield was compared to actual yields and no one substrate deviated more than 10% (Table 3). Entries 1-10 represent the substrates whose parameters were used in the regression analysis and entries 11-14 represent the control group.

Figure 2: Regression Analysis of Parameters.



Microsoft Excel - Copper trends

	T	U	V	W	X	Y	Z	AA	A
13		SUMMARY OUTPUT							
14									
15		*Regression Statistics*							
16		Multiple R	0.964933457						
17		R Square	0.931096576						
18		Adjusted R Square	0.875973837						
19		Standard Error	7.520459316						
20		Observations	10						
21									
22		ANOVA							
23			*df*	*SS*	*MS*	*F*	*Significance F*		
24		Regression	4	3821.313458	955.3283646	16.8913336	0.004147168		
25		Residual	5	282.7865416	56.55730833				
26		Total	9	4104.1					
27									
28			*Coefficients*	*Standard Error*	*t Stat*	*P-value*	*Lower 95%*	*Upper 95%*	*Lower*
29		Intercept	-56.7390577	85.33091292	-0.664929692	0.53553131	-276.0891524	162.6110371	-276.(
30		ΔV	-0.43592512	0.12532782	-3.478278946	0.01769139	-0.758090537	-0.1137597	-0.75
31		Ole e den.	31.13904421	406.6093897	0.076582206	0.94192587	-1014.083667	1076.361755	-1014
32		Br e den.	-1412.29484	213.5100907	-6.614651484	0.00118822	-1961.139999	-863.449678	-1
33		ΔΔG	16.2529797	6.356456066	2.556924728	0.05083622	-0.086810806	32.5927702	-0.08(

Sheet1 Sheet2 Sheet3 Sheet4 Sheet5 Sheet6 Sheet7 Sheet8 Sheet9

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Figure 3: Regression Analysis without Olefin Electron Density.

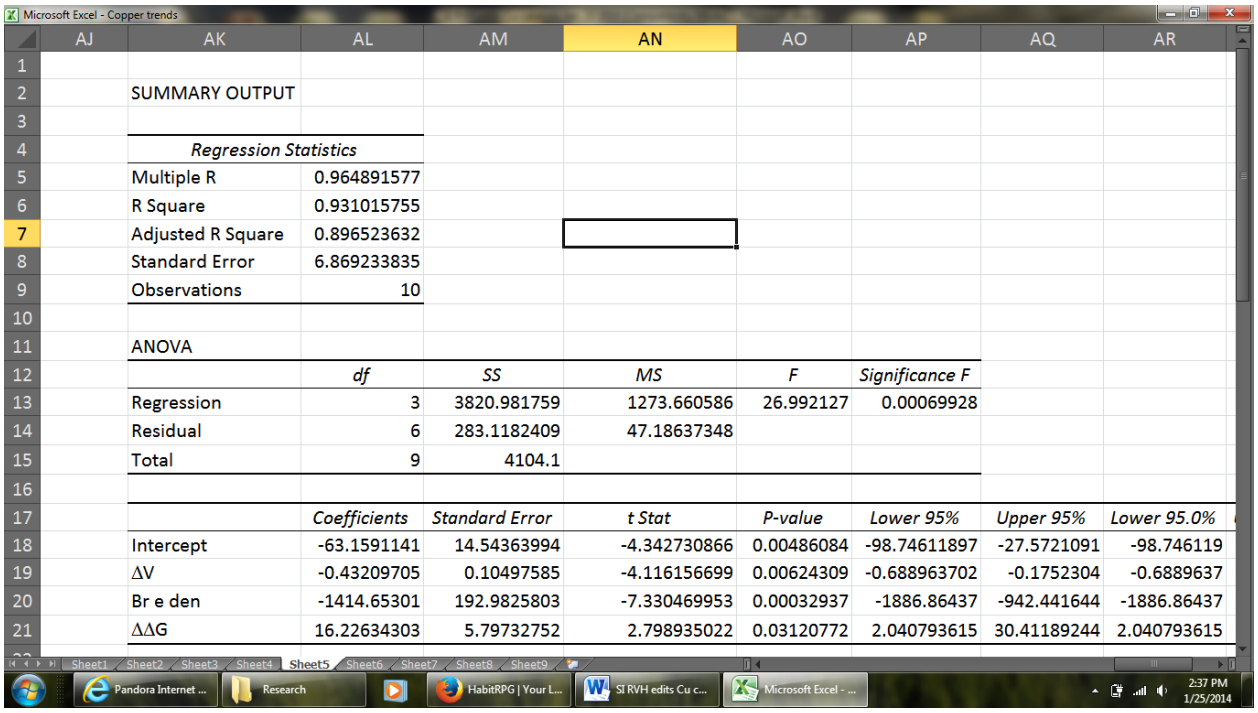


Table 3: Predicted vs. Actual Yield using Refined Equation.

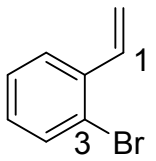
entry	substrate	ref. letter	pred. yield	actual yield	dif.
1	H	A	34.45	35	0.55
2	5-OMe	B	65.12	73	7.88
3	5-F	C	45.97	37	-8.97
4	4-F	D	11.71	14	2.29
5	5-tBu	E	24.46	25	0.54
6	4-tBu	F	13.19	4	-9.19
7	4-Ph	G	0.37	7	6.63
8	5-pyrrole	H	22.87	24	1.13
9	5-OiPr	J	55.96	54	-1.96
10	β-Me	K	38.90	40	1.10
11	5-OBz	L	15.48	8	-7.48
12	5-OTBS	M	22.34	21	-1.35
13	5-Br	N	24.75	16	-8.75
14	6-F	P	17.57	9	-8.57

Employing the Trend: A number of different substrates were optimized as potential candidates to be used in this methodology. Table 4 represents a summary of those substrates and their comparison of predicted vs. actual yield.

Table 4: Substrates Chosen for Testing the Predictive Model.

		int. = -63.16		coef:	-1415					16.22		-0.4321
Substrate	**ref. letter**	**yield**	**pred. yield**	**dif.**	**Br e den**	**Bn rad. E**	**Br rad. E**	**rad. E**	**ΔG**	**ΔΔG**	**Molar Vol.**	**Δvol.**
5-SMe	Q	13	10.44	2.56	-0.066	-3732.87	-2574.1	-1158.68	55.01623	0.041478	158.733	47.305
5-Me	R	30	36.51	-6.51	-0.075	-3334.65	-2574.1	-760.466	55.14445	0.169697	132.922	21.494
5-OEt	S	57	57.6	-0.6	-0.09408	-3449.21	-2574.1	-875.025	55.42837	0.453615	157.01	45.582
5-OMe-β-Me	T	50	62.66	-12.66	-0.09651	-3449.21	-2574.1	-875.022	55.18017	0.205421	143.922	32.494
3-OMe	U	50	110.4	-60.4	-0.118	-3409.88	-2574.1	-835.69	55.89818	0.923425	130.751	19.323
3-F	V	65	153.9	-88.9	-0.153	-3394.59	-2574.1	-820.405	55.01914	0.044386	111.626	0.198

GEOMETRIES, ENERGIES, VOLUMES AND NPA CHARGES.



Ref. Letter: A
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Volume: 111.428 cm**3/mol
NPA at C1: -0.19540
NPA at C3: -0.06883

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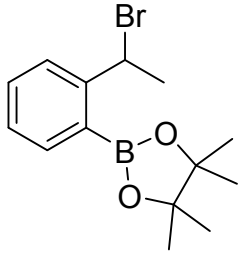
C	1.75176500	1.64009500	-0.08500400
C	0.83030600	2.69275400	-0.16721500
C	-0.52846800	2.33780700	-0.17606500
C	-0.94334200	1.01901300	-0.08830600
H	-2.00075200	0.78452300	-0.10277500
H	-1.26573200	3.12437000	-0.27796100
C	1.24485500	4.10075400	-0.26076100
C	0.53329900	5.14765700	0.15498200
H	-0.42904200	5.04196000	0.64239700
H	0.90881500	6.15564200	0.03275500
H	2.22198600	4.27698900	-0.69594300
Br	3.64585800	1.98511900	-0.05378000
H	2.09721000	-0.46879200	0.06721900
H	-0.31051400	-1.03582900	0.06186400



Ref. Letter: A
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C	-2.22012200	2.18403800	-2.05265400
C	-2.27300800	3.53303000	-2.44553700
C	-1.13642100	4.32354800	-2.51664000

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H 0.99909100 4.37297300 -2.24979400
H -1.21024700 5.35949000 -2.82593100
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B -3.58863800 1.42714100 -2.03902600
O -3.81907000 0.15136100 -1.58636000
C -5.17742100 -0.22734900 -1.96966900
C -5.86495600 1.17611300 -2.16428900
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H -7.37283400 1.19484400 -0.58746700
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H -1.78319000 -0.26194400 -1.17346500
Br 0.02037700 -0.89082400 -2.75962600
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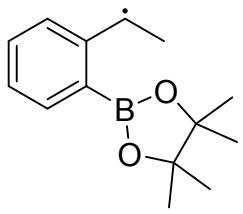

Ref. Letter: A
UB3LYP energy: -721.1363910

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O 3.95085100 -1.90911700 -0.05497000
C 5.37872400 -2.07055600 -0.29994400
C 5.59154500 -3.60454300 -0.01291700
O 4.27537300 -4.15384500 -0.29312200
C 5.89560400 -3.91304200 1.45558600
H 5.83744500 -4.99191100 1.60706300
H 6.89636400 -3.58031200 1.73746600
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H 7.60157100 -3.86190000 -0.78333200
H 6.66530500 -5.35430100 -0.65146100
H 6.32984000 -4.22473000 -1.96369700
C 5.62030900 -1.68408600 -1.76127500
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H 6.68124500 -1.72092000 -2.01596000
H 5.07652400 -2.33984600 -2.44269500
C 6.13613400 -1.12525500 0.62359900
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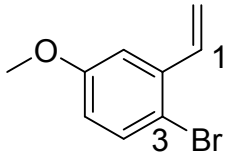
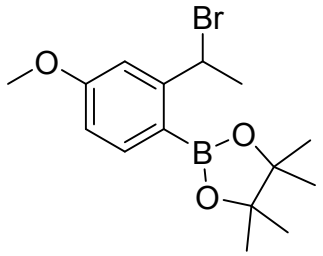
H 0.45724900 0.98854700 0.05162500
H -0.65845500 -0.01253200 -0.87747200



Ref. Letter: B
RB3LYP energy: -2997.835000
Volume: 133.585 cm**3/mol
NPA at C1: -0.19220
NPA at C3: -0.09534

C 0.00000000 0.00000000 0.00000000
O -0.86673900 -1.12328800 -0.07614900
C -2.21210900 -0.90724500 -0.07017500

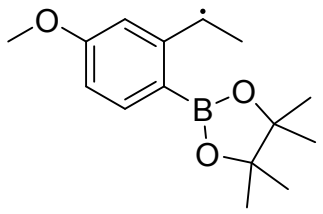
C -3.01155900 -2.05225400 -0.14491800
C -4.38743800 -1.92896000 -0.13014900
C -4.97815400 -0.67188900 -0.04410000
C -4.20813100 0.49165600 0.02382300
C -2.80890400 0.34320800 0.01820700
H -2.20439200 1.23314200 0.11193000
C -4.81255300 1.82956500 0.11475400
C -4.24940700 2.97070800 -0.28076800
H -3.27259200 3.00998700 -0.74902300
H -4.76850900 3.91325400 -0.16216500
H -5.81343000 1.86371800 0.52954700
Br -6.90170100 -0.60375300 -0.05895200
H -5.00921100 -2.81216700 -0.18771800
H -2.53854400 -3.02400600 -0.20433100
H -0.14666200 0.55363400 0.93221800
H 1.01031700 -0.40214400 -0.02542800
H -0.14462300 0.67218300 -0.85117600



Ref. Letter: B
RB3LYP energy: -3409.8858775

C 0.00000000 0.00000000 0.00000000
O 0.49171100 1.30044200 0.29563400
C 1.83674900 1.50672700 0.27139800
C 2.78469400 0.52542800 -0.01854400
C 4.12832400 0.87237300 -0.01428100
C 4.58251700 2.16761000 0.27341800
C 3.60212100 3.14750600 0.56659900
C 2.25584800 2.80423900 0.55946300
H 1.49286100 3.54700200 0.75362000
C 3.98800900 4.56142000 0.91166600
C 3.36235600 5.12624300 2.17470800
H 2.27374200 5.14740400 2.12785200
H 3.71722600 6.14036500 2.35830000
H 3.65347300 4.49745000 3.02237000
H 5.06330400 4.66796400 0.93868100
Br 3.51245800 5.78875300 -0.64270200
B 6.12539000 2.37470000 0.24128800
O 6.97455800 1.34695600 -0.09631000

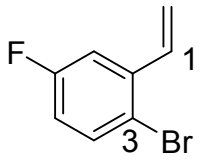
C 8.31335600 1.89419100 -0.25489100
C 8.23277400 3.22217300 0.58974600
O 6.80752000 3.53103400 0.53685800
C 9.00245200 4.40510100 0.01715500
H 8.86371700 5.27667400 0.65904700
H 10.0721110 4.18624300 -0.02647600
H 8.65781100 4.66515600 -0.98209000
C 8.58436100 3.02946700 2.06660900
H 8.31752100 3.93509300 2.61355300
H 8.03347900 2.19538400 2.50362400
H 9.65237800 2.85076300 2.20374200
C 8.51618100 2.13677700 -1.75260300
H 9.52367100 2.49785900 -1.96757800
H 8.36868900 1.19552700 -2.28418900
H 7.79766800 2.85972000 -2.14127800
C 9.31839600 0.86639900 0.24967000
H 10.3351070 1.26470500 0.20919800
H 9.10403000 0.55996200 1.27218900
H 9.27973500 -0.02152500 -0.38366400
H 4.86085800 0.10795700 -0.24327100
H 2.49345400 -0.48973800 -0.24869300
H 0.36661200 -0.73759100 0.72000500
H -1.08310300 0.06858100 0.07373100
H 0.27576600 -0.30912700 -1.01242000



Ref. Letter: B
UB3LYP energy: -835.69700677

C 0.00000000 0.00000000 0.00000000
O 0.65492500 1.25926300 -0.04416300
C 2.01974100 1.28335400 -0.04495300
C 2.82614200 0.14239400 0.00140900
C 4.21139100 0.30138000 -0.00621600
C 4.84150400 1.54302100 -0.05746600
C 4.00573100 2.71816700 -0.10547300
C 2.60155900 2.54208700 -0.09685500
H 1.93993800 3.39723100 -0.13200800
C 4.55027300 4.02140600 -0.16076600
C 3.73728800 5.27366400 -0.20987700
H 3.09046500 5.38160200 0.66986100

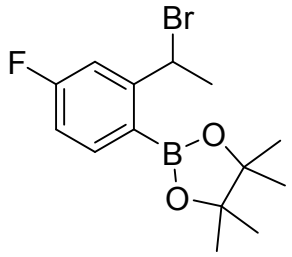
H 3.07452600 5.30288400 -1.08370900
H 4.37984400 6.15346700 -0.25505400
H 5.62581000 4.11743200 -0.16864500
B 6.39364000 1.52543000 -0.05346800
O 7.09557000 0.34472500 0.06854300
C 8.49653500 0.61611300 -0.20050000
C 8.59682900 2.16075500 0.08882400
O 7.23481400 2.60927300 -0.16943400
C 9.54037500 2.93285800 -0.82458900
H 9.52630300 3.99045100 -0.55520600
H 10.5661760 2.57167500 -0.71743300
H 9.24814800 2.84804900 -1.86994100
C 8.89659000 2.48918800 1.55363800
H 8.75052900 3.55885800 1.71142500
H 8.22571000 1.95420300 2.22726500
H 9.92635600 2.24169700 1.81858700
C 8.74439100 0.25379100 -1.66778300
H 9.79488900 0.37193200 -1.94073100
H 8.46564900 -0.78961500 -1.82285600
H 8.14003600 0.86675000 -2.33810200
C 9.34414700 -0.26897300 0.70493800
H 10.4075510 -0.05300100 0.57562000
H 9.08601000 -0.13776100 1.75442600
H 9.17979700 -1.31644600 0.44625300
H 4.82912100 -0.58815100 0.03011000
H 2.40090200 -0.85015000 0.04224000
H 0.24678000 -0.54773500 0.91449200
H -1.06579300 0.21875900 -0.01138200
H 0.25263000 -0.61286100 -0.87051500



Ref. Letter: C
RB3LYP energy: -2982.5458369
Volume: 121.737 cm**3/mol
NPA at C1: -0.19946
NPA at C3: -0.08679

C 0.00000000 0.00000000 0.00000000
C 1.38738900 0.04252500 -0.00528400
C 2.04969900 1.26069500 -0.08762500
C 1.35806300 2.47837200 -0.16353800
C -0.04385900 2.41406200 -0.16712000
C -0.68707800 1.19880000 -0.08058100

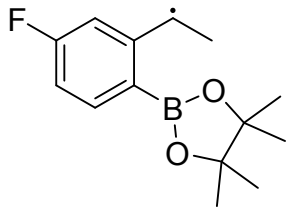
F	-2.03932200	1.17681500	-0.09101600
H	-0.63325200	3.31600500	-0.26214900
C	2.04751200	3.77437600	-0.25222600
C	1.54835300	4.94670100	0.13653500
H	0.56986700	5.04389300	0.59253400
H	2.12330500	5.85674600	0.02275500
H	3.05227100	3.74530800	-0.65730000
Br	3.97170500	1.21091200	-0.06144100
H	1.95534600	-0.87548400	0.05743000
H	-0.53795500	-0.93682300	0.05759700



Ref. Letter: C
RB3LYP energy: -3394.5971078

C	0.00000000	0.00000000	0.00000000
C	0.74452900	0.40950500	-1.25844000
C	0.65097800	1.86623400	-1.62599300
C	1.80161000	2.63281200	-1.91533300
C	1.62623800	3.99235800	-2.23036300
C	0.37884100	4.59467400	-2.26025400
C	-0.72116600	3.80613000	-1.97282700
C	-0.60963300	2.46774900	-1.66199500
H	-1.51022600	1.89861300	-1.47369500
F	-1.95209300	4.36561000	-2.00131200
H	0.24992400	5.64129400	-2.50354000
H	2.50154800	4.58713300	-2.45932400
B	3.27634500	2.11843700	-1.92990200
O	3.71384600	0.86946400	-1.56656800
C	5.17507700	0.88721100	-1.53860400
C	5.50709400	2.12356000	-2.45780100
O	4.30487400	2.93610700	-2.32669200
C	5.63545300	1.76460800	-3.94008000
H	4.78010700	1.18338700	-4.28725700
H	5.67553300	2.68592100	-4.52293700
H	6.54557400	1.19500800	-4.13650200
C	6.70275800	2.95704000	-2.01530700
H	7.62059300	2.36497700	-2.04411500
H	6.82651800	3.80223300	-2.69433500
H	6.57232100	3.35007100	-1.00845300

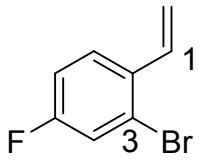
C 5.68116900 -0.45545100 -2.04839000
H 5.27521900 -0.69305100 -3.02993200
H 6.77205000 -0.45826300 -2.10985300
H 5.38110800 -1.24576900 -1.35831300
C 5.58076000 1.08406100 -0.07645000
H 6.66492300 1.05086900 0.04517500
H 5.21665100 2.03447900 0.31630400
H 5.14620900 0.28156700 0.52149400
H 1.77684200 0.09287900 -1.21063600
Br 0.05626000 -0.71208200 -2.80964700
H -1.07020200 0.19548900 -0.06518800
H 0.14163700 -1.06192400 0.20015100
H 0.39864400 0.56875300 0.84625800



Ref. Letter: C
UB3LYP energy: -820.40950926

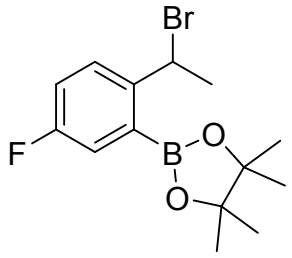
C 0.00000000 0.00000000 0.00000000
C 0.94755800 -1.15376700 -0.05255800
C 0.55288200 -2.50629300 -0.11407800
C 1.50785600 -3.58507400 -0.16460500
C 1.02799000 -4.89578600 -0.22428500
C -0.32931200 -5.20485400 -0.23650600
C -1.22778400 -4.14759500 -0.18657400
C -0.83161000 -2.83593500 -0.12719800
H -1.58945100 -2.06564200 -0.09006400
F -2.55428600 -4.42708000 -0.19651800
H -0.68863900 -6.22425700 -0.28241700
H 1.74554100 -5.70614500 -0.26250300
B 3.05623400 -3.42574200 -0.16163400
O 3.76451800 -2.25477000 -0.03094100
C 5.17126900 -2.54156800 -0.28669000
C 5.24763100 -4.09177500 -0.01718300
O 3.88412900 -4.51776800 -0.29128400
C 5.53269400 -4.44432300 1.44504400
H 4.86393600 -3.91093900 2.12216000
H 5.37078700 -5.51406100 1.58548200
H 6.56355800 -4.21505100 1.72172900
C 6.18902700 -4.86234800 -0.93428700
H 7.21886200 -4.51782900 -0.81240000

H 6.15682700 -5.92344500 -0.68122000
H 5.90752100 -4.75781300 -1.98077800
C 6.01531400 -1.67888400 0.64245500
H 5.73910200 -1.81905300 1.68615300
H 7.07699900 -1.91014000 0.52739100
H 5.87227500 -0.62586800 0.39385400
C 5.43780700 -2.16101700 -1.74502300
H 6.48978700 -2.28838900 -2.00730900
H 4.83424100 -2.75741600 -2.43063800
H 5.17437700 -1.11207100 -1.88895800
H 2.00580100 -0.93965100 -0.04024000
H 0.54063700 0.94605900 0.03319300
H -0.66468300 0.02958200 -0.87211800
H -0.65033400 -0.03917600 0.88272100



Ref. Letter: D
RB3LYP energy: -2982.5456217
Volume: 120.435 cm**3/mol
NPA at C1: -0.19547
NPA at C3: -0.05658

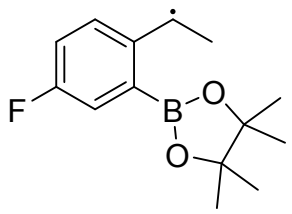
C 0.00000000 0.00000000 0.00000000
C -0.05156700 -1.26330100 -0.42014100
C -1.22775300 -2.14299800 -0.34908500
C -1.12278100 -3.53894600 -0.27552000
C -2.23607800 -4.36607200 -0.20896200
C -3.48758200 -3.78094900 -0.22087700
C -3.65869400 -2.41013600 -0.30196000
C -2.52805800 -1.61313800 -0.37049100
H -2.64724100 -0.54157900 -0.46614000
H -4.65473800 -1.98840600 -0.32600600
F -4.57506800 -4.57917400 -0.16020500
H -2.14115200 -5.44066300 -0.14586600
Br 0.59322200 -4.40190200 -0.23059200
H 0.84291700 -1.70557400 -0.84369200
H 0.90630300 0.58194500 -0.10795000
H -0.84027900 0.49199000 0.47631700



Ref. Letter: D
RB3LYP energy: -3394.5963625

C	0.00000000	0.00000000	0.00000000
C	0.78493000	0.44359200	-1.22173000
C	0.75294500	1.91466700	-1.52728000
C	1.93258100	2.63847200	-1.80789800
C	1.82809500	4.01379600	-2.07476000
C	0.59835600	4.63479300	-2.05570700
C	-0.56837200	3.94121000	-1.78781900
C	-0.47580100	2.58301800	-1.52846000
H	-1.38624100	2.02744100	-1.34347100
H	-1.52004600	4.45697900	-1.79172000
F	0.52465900	5.96250900	-2.31224800
H	2.71283400	4.59505100	-2.29958400
B	3.38628300	2.05823200	-1.85968500
O	3.77679300	0.79521700	-1.49773300
C	5.23880400	0.75123800	-1.50467800
C	5.60054300	1.96781200	-2.43937900
O	4.43537400	2.83044800	-2.28639400
C	5.67924000	1.59603600	-3.92181100
H	4.79222600	1.05020100	-4.24624800
H	5.74559000	2.51150500	-4.51136500
H	6.55936200	0.98666200	-4.13472700
C	6.83910200	2.75362300	-2.02954400
H	7.73072300	2.12393300	-2.07722800
H	6.98099400	3.59008700	-2.71569500
H	6.74914600	3.15576200	-1.02187400
C	5.67458900	-0.61427100	-2.01844200
H	5.23220800	-0.84091700	-2.98677900
H	6.76226100	-0.66269300	-2.10989600
H	5.36162700	-1.38730100	-1.31464700
C	5.68539900	0.93835800	-0.05341200
H	6.76976700	0.86139800	0.04428800
H	5.36923700	1.90483800	0.34163800
H	5.23179100	0.15742100	0.55871600
H	1.80249500	0.08272100	-1.16948900
Br	0.08805800	-0.58940000	-2.83807500
H	0.10200900	-1.07444300	0.15168200

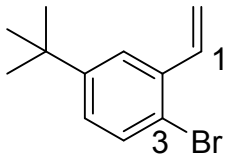
H 0.39893900 0.51428300 0.88034700
H -1.06179800 0.23340600 -0.07653100



Ref. Letter: D
UB3LYP energy: -820.40801555

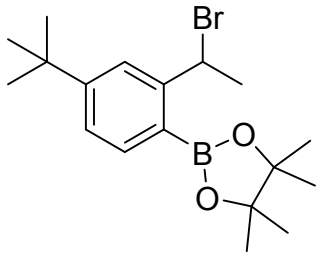
C 0.00000000 0.00000000 0.00000000
C -0.87469300 -1.21066900 0.06263700
C -0.39782900 -2.53491300 0.13634600
C -1.28425100 -3.67117700 0.18275600
C -0.73384200 -4.95361300 0.24055000
C 0.63633800 -5.13536000 0.26250800
C 1.52026200 -4.06540600 0.22305000
C 1.00504300 -2.78797900 0.15910100
H 1.69293800 -1.95347200 0.12538200
H 2.58761700 -4.24732700 0.24135300
F 1.13654700 -6.39442000 0.32344500
H -1.38003600 -5.82177600 0.27105200
B -2.84193600 -3.60949000 0.18294800
O -3.62135200 -2.47845600 0.19123800
C -5.00488500 -2.88422200 0.41982000
C -4.98628300 -4.39008400 -0.04104900
O -3.59660900 -4.75948900 0.18253500
C -5.25644000 -4.57210100 -1.53645100
H -4.62456500 -3.91743600 -2.13840400
H -5.03220000 -5.60372100 -1.81171700
H -6.30057200 -4.37068200 -1.78308800
C -5.87258900 -5.32717100 0.76942100
H -6.92365200 -5.04237300 0.67863500
H -5.76620000 -6.34560600 0.39202600
H -5.60118400 -5.32883000 1.82382300
C -5.91518700 -1.96810400 -0.38725000
H -5.64621600 -1.95846400 -1.44223500
H -6.95813400 -2.28069200 -0.29504800
H -5.83579700 -0.94767100 -0.00834200
C -5.27150300 -2.70859000 1.91610700
H -6.30945900 -2.93531400 2.16655700
H -4.62183100 -3.34877700 2.51448600
H -5.07126200 -1.67206200 2.19161500
H -1.94368100 -1.05893700 0.05080200
H -0.59942900 0.90834600 -0.06590300

H 0.64304300 0.09443500 0.88409200
H 0.66957400 -0.01588100 -0.86892600



Ref. Letter: E
RB3LYP energy: -3040.5750776
Volume: 160.309 cm**3/mol
NPA at C1: -0.19203
NPA at C3: -0.07463

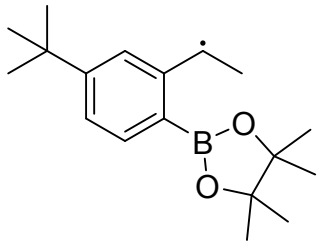
C 0.00000000 0.00000000 0.00000000
C -1.53541500 -0.06950600 0.00536000
C -2.18000700 -1.31103400 0.09060000
C -3.56168800 -1.40698100 0.08206000
C -4.33472900 -0.25745800 -0.00727700
C -3.74839000 1.00784100 -0.08514100
C -2.34252500 1.05836200 -0.08613900
H -1.88989700 2.03423800 -0.18622700
C -4.54438700 2.24115200 -0.17990800
C -4.15903400 3.45158000 0.22287300
H -4.80966300 4.30818100 0.10068300
H -3.20206100 3.63141600 0.69893400
H -5.53594400 2.12882100 -0.60370100
Br -6.24702800 -0.47761700 0.01443000
H -4.04062200 -2.37463200 0.14808100
H -1.60348800 -2.22530700 0.15736500
C 0.54547000 -0.63099700 1.30029800
H 1.63798000 -0.59243200 1.30907900
H 0.17979500 -0.09386800 2.17854500
H 0.24959600 -1.67658000 1.40131100
C 0.52112300 1.44390600 -0.08536500
H 1.61329800 1.43870700 -0.07926500
H 0.20050600 1.93975800 -1.00438400
H 0.19048700 2.04689100 0.76350700
C 0.54529500 -0.78162400 -1.21564600
H 0.17748600 -0.35492700 -2.15166500
H 1.63784700 -0.74340600 -1.23113000
H 0.25032000 -1.83211500 -1.18885200



Ref. Letter: E
RB3LYP energy: -3452.6245112

C	0.00000000	0.00000000	0.00000000
C	-0.52228100	-0.56856900	-1.30785400
C	-0.01176400	-1.93773400	-1.66833800
C	-0.89295100	-2.99946000	-1.94911500
C	-0.31728000	-4.24909500	-2.24158300
C	1.05072900	-4.44615800	-2.25626800
C	1.93448200	-3.39297500	-1.98382800
C	1.37088800	-2.15457900	-1.69440900
H	2.01694200	-1.30964800	-1.50248600
C	3.45180500	-3.63205500	-2.01499200
C	3.82202600	-4.69617600	-0.95800000
H	4.89885100	-4.88534500	-0.97304800
H	3.55048900	-4.36080100	0.04577500
H	3.31473700	-5.64490100	-1.14155600
C	4.25523900	-2.35617300	-1.71455800
H	5.32362500	-2.57980600	-1.75620400
H	4.05427200	-1.56733300	-2.44275000
H	4.04039100	-1.96483000	-0.71750300
C	3.86218500	-4.13898500	-3.41556900
H	3.61750000	-3.40234200	-4.18419600
H	4.93969800	-4.32121900	-3.44995300
H	3.35881100	-5.07191100	-3.67403500
H	1.43313600	-5.43270300	-2.48934600
H	-0.97351900	-5.08202500	-2.46319800
B	-2.45253300	-2.93899600	-1.96693300
O	-3.23779300	-1.85831500	-1.64614800
C	-4.62843900	-2.29989300	-1.59608900
C	-4.58783000	-3.61829900	-2.45887600
O	-3.20060100	-4.03597100	-2.31869700
C	-4.82621400	-3.37820400	-3.95170300
H	-4.18360600	-2.58547100	-4.33730200
H	-4.59442500	-4.29459200	-4.49645000
H	-5.86547800	-3.11264000	-4.15396400
C	-5.48257800	-4.74637400	-1.96127000
H	-6.53433900	-4.45214700	-1.99522100
H	-5.35669500	-5.61937700	-2.60381400

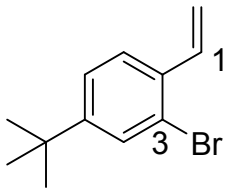
H -5.23460200 -5.03970800 -0.94257100
C -5.50499100 -1.18490000 -2.15138700
H -5.19172700 -0.88382100 -3.14945000
H -6.55115400 -1.49776700 -2.19166000
H -5.44028700 -0.31162300 -1.50012600
C -4.95657400 -2.54357400 -0.12142300
H -6.00101100 -2.83068500 0.01361500
H -4.32431300 -3.32354200 0.30526200
H -4.78093300 -1.62257500 0.43654500
H -1.60253400 -0.54185500 -1.32918700
Br -0.06929600 0.74482300 -2.80086700
H -0.42734200 0.98429600 0.19159300
H -0.29280000 -0.67045900 0.81454100
H   1.08625200 0.08840400 0.00964800



Ref. Letter: E
UB3LYP energy: -878.43572094

C   0.00000000 0.00000000 0.00000000
C -0.80495700 -1.25879400 0.05397400
C -0.26066600 -2.55829700 0.11277100
C -1.08974200 -3.73150700 0.16524300
C -0.45033400 -4.97243500 0.22114700
C   0.93151000 -5.10609400 0.22696000
C   1.76626400 -3.97436300 0.17472000
C   1.15493300 -2.73425200 0.12033400
H   1.76717500 -1.84562600 0.08054100
C   3.29277100 -4.15387300 0.17904200
C   3.72005500 -4.87131800 1.47856600
H   4.80376200 -5.01705900 1.49221000
H   3.44551200 -4.28214900 2.35675200
H   3.25073800 -5.85183000 1.57458100
C   4.04516700 -2.81531600 0.10327100
H   5.12207200 -2.99961000 0.10883400
H   3.80998300 -2.26679300 -0.81177900
H   3.81743600 -2.17183600 0.95615200
C   3.71114900 -5.00899100 -1.03775600
H   3.42227800 -4.52363000 -1.97302600
H   4.79573800 -5.14773800 -1.04764700
H   3.24899000 -5.99738500 -1.01851800

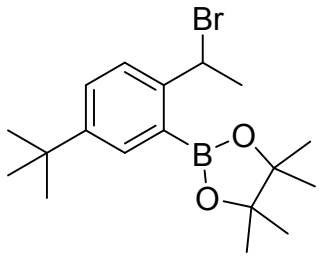
H 1.36031800 -6.09959200 0.27064000
H -1.06156900 -5.86645500 0.26143500
B -2.64417500 -3.75525900 0.16865300
O -3.48874400 -2.67477700 0.05343400
C -4.84968100 -3.12926600 0.30952900
C -4.74247300 -4.67374700 0.02089000
O -3.33965600 -4.93875600 0.28878700
C -4.98940700 -5.03831300 -1.44594100
H -4.38825500 -4.42320200 -2.11716800
H -4.70604400 -6.08053600 -1.60040800
H -6.04059500 -4.92503300 -1.71822800
C -5.58508400 -5.56234700 0.92750200
H -6.64960100 -5.35183700 0.79841900
H -5.41547100 -6.60913500 0.66957000
H -5.32721100 -5.42900600 1.97678400
C -5.79478400 -2.36144700 -0.60582800
H -5.50073200 -2.44587400 -1.65069800
H -6.81928100 -2.72663600 -0.49995900
H -5.78527400 -1.30364400 -0.33710000
C -5.15298200 -2.80133600 1.77364300
H -6.18181600 -3.05404100 2.03717700
H -4.48038600 -3.33251600 2.44855400
H -5.01269000 -1.73083600 1.93097300
H -1.88082100 -1.16390300 0.04626900
H -0.65040200 0.87422800 -0.04284500
H 0.64948900 0.11605900 0.87664200
H 0.65749600 0.03596900 -0.87755900



Ref. Letter: F
RB3LYP energy: -3040.5755169
Volume: 161.971 cm**3/mol
NPA at C1: -0.19292
NPA at C3: -0.06925

C 0.00000000 0.00000000 0.00000000
C 1.45568600 0.48855400 -0.05221800
C 2.50087600 -0.44015900 -0.02996600
C 3.82439600 -0.03502600 -0.07344000
C 4.19655000 1.31403300 -0.13566400
C 3.13916900 2.23152500 -0.17005800
C 1.81011700 1.83765300 -0.12492600

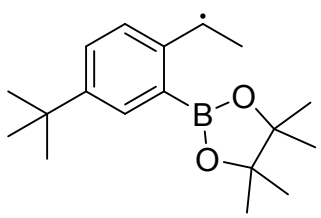
H 1.04749500 2.60310400 -0.16071100
H 3.37223700 3.28562100 -0.25804800
C 5.59763800 1.75560200 -0.18154300
C 6.05496000 2.93598400 0.23513000
H 7.10487900 3.18486400 0.14768600
H 5.41336300 3.68282500 0.68830900
H 6.30511400 1.03795100 -0.58141800
Br 5.16076200 -1.42406900 -0.01312100
H 2.28852200 -1.49878000 0.02599800
C -1.00348400 1.16356000 -0.05124300
H -0.88050300 1.84581100 0.79300000
H -0.91108600 1.74003500 -0.97452800
H -2.02125000 0.76956800 -0.00991200
C -0.27815600 -0.92888400 -1.20227300
H 0.37286100 -1.80481900 -1.20060500
H -1.31182900 -1.28368400 -1.17329300
H -0.12667300 -0.40168500 -2.14701900
C -0.23138600 -0.77952500 1.31355600
H 0.42483200 -1.64792000 1.39201500
H -0.04927700 -0.14325700 2.18273700
H -1.26350000 -1.13652100 1.36399800



Ref. Letter: F
RB3LYP energy: -3452.6241910

C 0.00000000 0.00000000 0.00000000
C -0.16306100 -0.89614700 -1.21491100
C 0.93705500 -1.89142100 -1.45057200
C 0.66845400 -3.25427100 -1.70817900
C 1.75535100 -4.11944800 -1.90094700
C 3.08884500 -3.71000000 -1.85054100
C 3.31871400 -2.35650100 -1.59830300
C 2.26558000 -1.47274600 -1.40472900
H 2.49039200 -0.42672600 -1.23583900
H 4.32764500 -1.96896900 -1.55501400
C 4.21886100 -4.72746400 -2.07277900
C 5.61110800 -4.08026800 -1.98863500
H 5.74717100 -3.30649600 -2.74787100
H 5.79444300 -3.63380000 -1.00838600

H 6.37882000 -4.83992500 -2.15231400
C 4.13419200 -5.83102300 -0.99534400
H 3.17999100 -6.35932900 -1.03184300
H 4.92954200 -6.56713900 -1.14184100
H 4.24402900 -5.40788100 0.00604600
C 4.06851300 -5.36634800 -3.47115400
H 3.11512600 -5.88628900 -3.57885000
H 4.12558000 -4.60742900 -4.25497200
H 4.86687900 -6.09348800 -3.64327700
H 1.52876100 -5.15914200 -2.10065300
B -0.74563300 -3.91474000 -1.80255100
O -1.95305200 -3.30665300 -1.56224600
C -2.99201000 -4.33249100 -1.56175500
C -2.30587900 -5.49700600 -2.37184700
O -0.89098600 -5.23710500 -2.14536900
C -2.53164600 -5.40584200 -3.88310100
H -2.29857400 -4.41012900 -4.26279100
H -1.87225000 -6.11903600 -4.37985100
H -3.56175100 -5.64778000 -4.15111400
C -2.62417200 -6.90260600 -1.87847600
H -3.69234300 -7.11332800 -1.97102300
H -2.08387100 -7.63221700 -2.48402600
H -2.32992900 -7.04298900 -0.83968900
C -4.24439100 -3.74725800 -2.20049600
H -4.04247200 -3.34876500 -3.19306200
H -5.02863000 -4.50406500 -2.27880200
H -4.62357700 -2.93290600 -1.58088900
C -3.26037300 -4.68164500 -0.09629000
H -4.06833600 -5.40913400 0.00003200
H -2.37002100 -5.08487200 0.38826600
H -3.55313000 -3.77450700 0.43464300
H -1.12789400 -1.38306900 -1.20216600
Br -0.35823900 0.29711700 -2.86199100
H -0.85304500 0.67110200 0.10001100
H 0.05478700 -0.62841900 0.89493200
H 0.90622900 0.60364400 -0.04488600

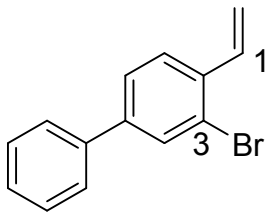


Ref. Letter: F
UB3LYP energy: -878.43560330

C 0.00000000 0.00000000 0.00000000

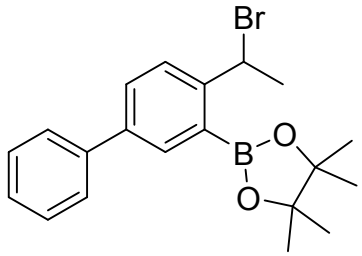
C	-0.37137300	-1.44811800	0.03225600
C	0.55808900	-2.50673800	0.06669900
C	0.16169000	-3.89190500	0.09384000
C	1.15362900	-4.87062700	0.12060600
C	2.52927200	-4.59731700	0.12890500
C	2.89790800	-3.24593800	0.10306400
C	1.95289700	-2.23893600	0.07234200
H	2.29308300	-1.21128300	0.05228900
H	3.94294500	-2.96495500	0.10633500
C	3.54573000	-5.74656900	0.16815300
C	4.99819700	-5.24153100	0.16259300
H	5.22494500	-4.66523300	-0.73752100
H	5.21471300	-4.61654000	1.03215600
H	5.68302300	-6.09226900	0.19036800
C	3.33106200	-6.57964500	1.45183400
H	2.32494800	-6.99991600	1.49707900
H	4.04258500	-7.40952400	1.49108800
H	3.47673600	-5.96507000	2.34345900
C	3.34805300	-6.65529800	-1.06594500
H	2.34438800	-7.08264200	-1.09717900
H	3.50139700	-6.09472200	-1.99120100
H	4.06320700	-7.48264300	-1.04714600
H	0.82541000	-5.90291500	0.13823900
B	-1.30645000	-4.41066000	0.10675300
O	-2.44997000	-3.64637400	0.08028800
C	-3.58914000	-4.51974000	0.33030900
C	-3.01729600	-5.93103400	-0.07235900
O	-1.59170700	-5.75809300	0.15248000
C	-3.19645300	-6.25721800	-1.55749400
H	-2.84198800	-5.44192200	-2.18985900
H	-2.61210800	-7.14734400	-1.79561500
H	-4.24149300	-6.45771300	-1.80126100
C	-3.50507900	-7.09503300	0.78122600
H	-4.58735900	-7.21636200	0.69120500
H	-3.03357700	-8.01850500	0.44063800
H	-3.25540400	-6.95716900	1.83200600
C	-4.76444300	-4.03128600	-0.50646800
H	-4.50678600	-3.96121200	-1.56191800
H	-5.62148600	-4.70055300	-0.39874400
H	-5.06780400	-3.03950300	-0.16636400
C	-3.91700400	-4.39766200	1.82043000
H	-4.80223700	-4.97889600	2.08562500
H	-3.08326200	-4.73099200	2.43997400
H	-4.11289700	-3.34995800	2.05350800
H	-1.42239000	-1.69600000	0.02951200
H	-0.89058300	0.62843900	-0.03332700
H	0.58104500	0.29965600	0.88130500

H 0.61375100 0.25216100 -0.87372300



Ref. Letter: G
RB3LYP energy: -3114.3939510
Volume: 168.433 cm**3/mol
NPA at C1: -0.19545
NPA at C3: -0.07227

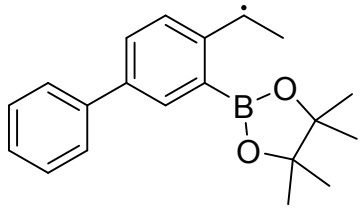
C 0.00000000 0.00000000 0.00000000
C -0.54464500 -1.10691700 -0.50506900
C -1.97507300 -1.44130100 -0.49793700
C -2.44728100 -2.75823600 -0.56935300
C -3.79905000 -3.06568400 -0.56144400
C -4.76110200 -2.05522600 -0.48485500
C -4.30938000 -0.73106000 -0.42261300
C -2.95784700 -0.44061800 -0.43381400
H -2.64009400 0.59416700 -0.40490300
H -5.02561200 0.07821000 -0.35266700
C -6.20689300 -2.38037200 -0.47866500
C -6.69278400 -3.49317600 0.21887900
C -8.04911600 -3.79417400 0.22633100
C -8.94970600 -2.99008100 -0.46488700
C -8.48140400 -1.88197800 -1.16348800
C -7.12530500 -1.58005200 -1.16949500
H -6.77099300 -0.72791300 -1.73703100
H -9.17305700 -1.25418400 -1.71284300
H -10.0072490 -3.22513600 -0.45926600
H -8.40419500 -4.65498900 0.78057200
H -6.00536800 -4.11403300 0.78095500
H -4.10735100 -4.09934200 -0.63759700
Br -1.22399500 -4.24321900 -0.66806200
H 0.10899600 -1.84607400 -0.95390900
H 1.06734200 0.16893300 -0.06375500
H -0.58340200 0.76176800 0.50411800



Ref. Letter: G
RB3LYP energy: -3526.4428746

C	0.00000000	0.00000000	0.00000000
C	0.12740800	-1.00209400	-1.13327100
C	1.47846200	-1.63290000	-1.31438100
C	1.62573400	-3.01997500	-1.53255300
C	2.92082300	-3.53524900	-1.68963900
C	4.06709700	-2.74162800	-1.63152900
C	3.89082200	-1.36980900	-1.41887600
C	2.62355000	-0.83332400	-1.26886900
H	2.52329900	0.23730400	-1.14138000
H	4.75183400	-0.71207400	-1.40031200
C	5.41941600	-3.32770000	-1.79412700
C	5.65533200	-4.34825600	-2.72362700
C	6.92259400	-4.89730100	-2.87555300
C	7.98334300	-4.43902100	-2.10063100
C	7.76463300	-3.42571300	-1.17291900
C	6.49725100	-2.87606500	-1.02248800
H	6.33564500	-2.10316000	-0.28046200
H	8.58176700	-3.06659600	-0.55818800
H	8.97153700	-4.86719200	-2.21912300
H	7.08369700	-5.68003600	-3.60762300
H	4.84281900	-4.69855900	-3.34871600
H	3.02958100	-4.60216800	-1.84018600
B	0.46665400	-4.06792000	-1.60783200
O	-0.83857500	-3.87175100	-1.23123800
C	-1.51776600	-5.16545500	-1.24979000
C	-0.59585500	-6.00723600	-2.21101800
O	0.69238400	-5.34354800	-2.06050300
C	-0.98128800	-5.88650300	-3.68738700
H	-1.09034200	-4.84395000	-3.98938500
H	-0.19146000	-6.33170400	-4.29416500
H	-1.91461200	-6.41025200	-3.90232900
C	-0.43177800	-7.47295700	-1.83073200
H	-1.39212800	-7.99277700	-1.86955600
H	0.24245800	-7.95885500	-2.53791100
H	-0.01279800	-7.58781200	-0.83247000
C	-2.94399100	-4.95189400	-1.73868800

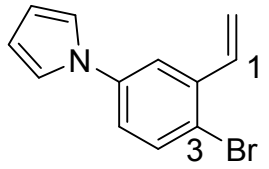
H -2.96928800 -4.44306700 -2.70061500
H -3.46722100 -5.90639500 -1.83313600
H -3.48934600 -4.33963000 -1.01846300
C -1.52458000 -5.67550100 0.19274800
H -2.06746800 -6.61838200 0.27947500
H -0.51171100 -5.82169800 0.57062500
H -2.01880700 -4.93725900 0.82606100
H -0.64316900 -1.75677900 -1.06025400
Br -0.40776500 -0.06876500 -2.87055900
H -1.02056400 0.37731400 0.06375100
H 0.24423700 -0.50113900 0.94223800
H 0.67041900 0.85112400 -0.11543300



Ref. Letter: G
UB3LYP energy: -952.25568862

C 0.00000000 0.00000000 0.00000000
C -0.07386700 -1.49163200 0.07771600
C 1.04305500 -2.34260400 0.12742300
C 0.92385200 -3.77832000 0.19629800
C 2.08555200 -4.54565100 0.22932300
C 3.37844700 -4.00057800 0.20966300
C 3.48138700 -2.59857200 0.14552900
C 2.36158900 -1.80159500 0.10316600
H 2.48945100 -0.72862300 0.03816200
H 4.46001800 -2.13518400 0.09929100
C 4.57869700 -4.86027400 0.25367000
C 4.58766400 -6.12552000 -0.35252400
C 5.71649300 -6.93332400 -0.31165400
C 6.86897300 -6.49963400 0.33662200
C 6.87819900 -5.24778800 0.94397600
C 5.74924500 -4.43975800 0.90273000
H 5.76674700 -3.47956000 1.40397100
H 7.76596800 -4.90173100 1.46061800
H 7.74956500 -7.13001500 0.36833700
H 5.69887600 -7.90279100 -0.79603900
H 3.70785800 -6.46983000 -0.88211200
H 1.97700700 -5.62085800 0.30022200
B -0.41585300 -4.57224400 0.25264400
O -1.68594700 -4.04526800 0.25214700
C -2.62601400 -5.12315600 0.53638100

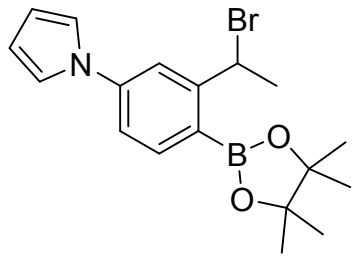
C -1.79985500 -6.39841900 0.12452100
O -0.43005400 -5.94765400 0.31113900
C -1.94553600 -6.76850900 -1.35402800
H -1.77652700 -5.90587900 -2.00024300
H -1.20019000 -7.52585200 -1.60146500
H -2.93422900 -7.17736800 -1.57125000
C -2.02767700 -7.62713400 0.99589100
H -3.06796400 -7.95683800 0.93876700
H -1.39560600 -8.44462300 0.64494300
H -1.77949100 -7.43364300 2.03809300
C -3.89510300 -4.88044600 -0.27060300
H -3.68339400 -4.77045900 -1.33290700
H -4.60251300 -5.70276700 -0.13822900
H -4.37699900 -3.96412200 0.07462100
C -2.93362300 -5.05325500 2.03412900
H -3.68105400 -5.79386300 2.32482600
H -2.03609700 -5.21137400 2.63365500
H -3.32488500 -4.06196800 2.26775400
H -1.05459100 -1.94362300 0.09571900
H -0.99855900 0.43739700 -0.02085300
H   0.53217000 0.43429800 0.85513900
H   0.52785100 0.34236700 -0.89868700



Ref. Letter: H
RB3LYP energy: -3092.3026437
Volume: 161.663 cm**3/mol
NPA at C1: -0.19699
NPA at C3: -0.08140

C   0.00000000 0.00000000 0.00000000
C   0.39739000 -1.16442200 -0.51054200
C -0.38618800 -2.40979600 -0.52098500
C   0.21555400 -3.67488600 -0.54361100
C -0.54102400 -4.83853100 -0.54665200
C -1.92520100 -4.77162200 -0.54145700
C -2.55742800 -3.52745000 -0.51730000
C -1.78685100 -2.37126300 -0.50731200
H -2.28055900 -1.40903800 -0.49103800
N -3.96917400 -3.44396000 -0.51925000
C -4.82713000 -4.30186000 0.14178800
C -6.11355300 -3.89352000 -0.09613000

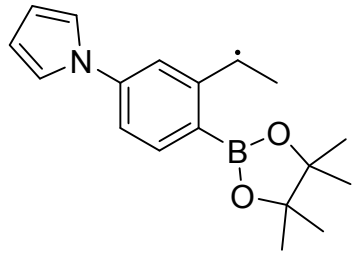
C -6.04762500 -2.74873100 -0.93858100
C -4.72292000 -2.49222000 -1.17895800
H -4.25238800 -1.74662700 -1.79658800
H -6.87794900 -2.18618400 -1.33429600
H -7.00287200 -4.35708600 0.29970100
H -4.44528600 -5.09851400 0.75699300
H -2.51055000 -5.68039400 -0.58699500
H -0.04802900 -5.80079500 -0.56829900
Br 2.12776500 -3.86903800 -0.54049400
H 1.38715500 -1.22970100 -0.94756000
H 0.64026000 0.87152500 -0.04830900
H -0.95580800 0.12577900 0.49549000



Ref. Letter: H
RB3LYP energy: -3504.3532618

C 0.00000000 0.00000000 0.00000000
C -0.57328700 -0.68462800 -1.22806100
C 0.00136100 -2.03817300 -1.55148900
C -0.83054100 -3.14722800 -1.81805200
C -0.20392800 -4.37281900 -2.10255200
C 1.17101400 -4.52132900 -2.11469400
C 1.98171300 -3.41440300 -1.85743300
C 1.38809700 -2.18599800 -1.58593000
H 2.02074900 -1.32012100 -1.44414900
N 3.38896900 -3.53796900 -1.87520200
C 4.11513900 -4.38144000 -2.69504800
C 5.44611800 -4.21314400 -2.41817500
C 5.54623500 -3.23785200 -1.38603600
C 4.27329600 -2.83824800 -1.07556400
H 3.91700200 -2.15147100 -0.32760700
H 6.44874400 -2.88018900 -0.91689200
H 6.25918200 -4.72221700 -2.91043700
H 3.62434600 -4.99171300 -3.43329200
H 1.61613900 -5.48988700 -2.30147800
H -0.82537800 -5.23638300 -2.30446500
B -2.39179800 -3.15847400 -1.82887100
O -3.22390300 -2.11410500 -1.51044600
C -4.59289900 -2.62094500 -1.45299700

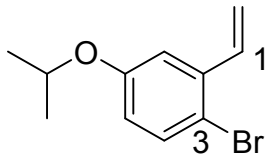
C -4.49318800 -3.94014200 -2.30972600
O -3.08654200 -4.29201500 -2.17102300
C -4.74479100 -3.71868200 -3.80311000
H -4.14319400 -2.89651000 -4.19315200
H -4.46820500 -4.62485700 -4.34399300
H -5.79624400 -3.50677400 -4.00522000
C -5.33380400 -5.10521300 -1.80381100
H -6.39732200 -4.85643900 -1.83145300
H -5.17475900 -5.97358500 -2.44521600
H -5.06710400 -5.38465900 -0.78594900
C -5.52373900 -1.55261500 -2.01111900
H -5.22557500 -1.23855400 -3.00978300
H -6.55230100 -1.91907700 -2.05129100
H -5.50433600 -0.67551400 -1.36208700
C -4.90293100 -2.87248900 0.02414200
H -5.93273800 -3.20561600 0.16534600
H -4.23451800 -3.62138500 0.45144800
H -4.76657300 -1.94194500 0.57717500
H -1.65153700 -0.73258500 -1.16902700
Br -0.31949700 0.54608700 -2.82870400
H -0.49651600 0.95462800 0.17348700
H -0.16683900 -0.64123700 0.87152300
H   1.07077500 0.18403000 -0.08588100



Ref. Letter: H
UB3LYP energy: -930.16540378

C   0.00000000 0.00000000 0.00000000
C -0.79049700 -1.26228800 0.11910700
C -0.22738700 -2.54931200 0.25419400
C -1.04022900 -3.73295600 0.36292700
C -0.39108200 -4.96378900 0.47942300
C   0.99229300 -5.09024400 0.50830300
C   1.78579200 -3.94178400 0.39770000
C   1.18550600 -2.70218400 0.26611000
H   1.81426800 -1.83137900 0.14368400
N   3.19749100 -4.05269200 0.42093600
C   3.93318100 -5.08352100 -0.13018400
C   5.26307400 -4.82912500 0.08416600

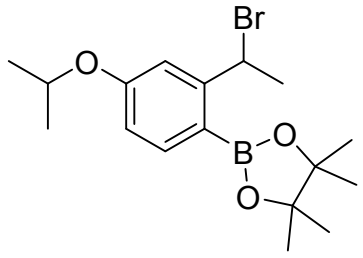
C 5.35061100 -3.60192900 0.79917200
C 4.07151200 -3.14631800 0.98807200
H 3.70413600 -2.28203700 1.51389500
H 6.24820400 -3.11685100 1.14806800
H 6.08222600 -5.44831700 -0.24488500
H 3.44850500 -5.88367500 -0.66239300
H 1.45336100 -6.05975700 0.64268400
H -0.99498100 -5.85863900 0.56918600
B -2.59566500 -3.77365200 0.37757800
O -3.45139800 -2.70512800 0.24894200
C -4.80418200 -3.16822600 0.53841600
C -4.68492700 -4.71760900 0.28149400
O -3.27371100 -4.96163400 0.53241400
C -4.95099500 -5.11649500 -1.17254900
H -4.36778600 -4.50972500 -1.86676500
H -4.65929300 -6.15883700 -1.30950700
H -6.00760000 -5.02002900 -1.42961600
C -5.50213600 -5.59468500 1.22165500
H -6.57066300 -5.39667400 1.10732100
H -5.32731600 -6.64511100 0.98285000
H -5.22716300 -5.43657400 2.26314700
C -5.77255200 -2.43065900 -0.37712300
H -5.49662000 -2.53616900 -1.42501200
H -6.79109800 -2.80351000 -0.24447000
H -5.76941400 -1.36702400 -0.13242400
C -5.08435600 -2.81089300 1.99981000
H -6.10553500 -3.06773900 2.28775200
H -4.39439200 -3.32014500 2.67403600
H -4.95247700 -1.73580700 2.13076200
H -1.86743000 -1.18488200 0.09974400
H -0.65905100 0.86349400 -0.09233500
H 0.64436300 0.16907400 0.87168600
H 0.66067000 -0.00524800 -0.87582900



Ref. Letter: J
RB3LYP energy: -3076.4930119
Volume: 167.219 cm**3/mol
NPA at C1: -0.19114
NPA at C3: -0.09718

C 0.00000000 0.00000000 0.00000000
O -0.94684300 -1.08796900 -0.01476900

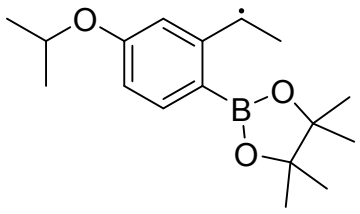
C	-2.28636900	-0.84927000	0.03637600
C	-3.09748100	-1.98967000	0.05354400
C	-4.47223200	-1.85930700	0.10090900
C	-5.05574500	-0.59716500	0.13005800
C	-4.27757300	0.56282100	0.10766200
C	-2.88005100	0.40719600	0.07158600
H	-2.27499900	1.30055200	0.10261600
C	-4.87270800	1.90792300	0.13928800
C	-4.32146800	3.01813300	-0.35001600
H	-3.36504800	3.02017000	-0.86016100
H	-4.83078300	3.97006100	-0.26977500
H	-5.85580000	1.97464500	0.59123700
Br	-6.97873500	-0.51665900	0.17034700
H	-5.09777000	-2.74174700	0.11274500
H	-2.63133000	-2.96639400	0.03523500
C	0.21293300	0.50998000	1.42135800
H	0.92100100	1.34208000	1.42079700
H	-0.71754200	0.85705200	1.87215600
H	0.61912100	-0.28704800	2.04796400
C	1.27415900	-0.55346300	-0.61847500
H	2.04333900	0.22074800	-0.65376100
H	1.65236600	-1.38947800	-0.02632800
H	1.08849900	-0.90601600	-1.63391100
H	-0.38272300	0.80351000	-0.63769000



Ref. Letter: J
RB3LYP energy: -3488.5440976

C	0.00000000	0.00000000	0.00000000
O	0.84721500	1.12843400	0.30088700
C	2.20065400	1.02592700	0.21734700
C	2.90999500	-0.14622500	-0.05343800
C	4.29585600	-0.09964700	-0.08862300
C	5.02951300	1.07458200	0.13531600
C	4.29241400	2.25353800	0.40476200
C	2.90417100	2.20959500	0.44034600
H	2.32694000	3.10747300	0.61941400
C	4.98428300	3.56329400	0.67247700
C	4.53136100	4.31038000	1.91427700

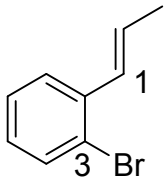
H	4.70221300	3.67376100	2.78851700
H	3.47250200	4.56639700	1.88446800
H	5.10319600	5.22993800	2.03891300
H	6.05750400	3.43491900	0.67536200
Br	4.74413700	4.79043700	-0.93708400
B	6.57828000	0.94022000	0.06238600
O	7.17521700	-0.25371700	-0.27098900
C	8.59540400	-0.01202900	-0.47457600
C	8.82804500	1.31353300	0.34318300
O	7.50386500	1.92536500	0.31556100
C	9.82285400	2.28975400	-0.27067000
H	9.89493700	3.18059600	0.35559600
H	10.8167490	1.84006400	-0.33269500
H	9.51837100	2.60351300	-1.26755600
C	9.16718900	1.07132500	1.81600100
H	9.11798900	2.02163200	2.34976900
H	8.45815700	0.38488900	2.28112800
H	10.1732780	0.66469300	1.93426800
C	8.80219400	0.15811800	-1.98197900
H	9.85716500	0.28742700	-2.23115800
H	8.43757600	-0.73629300	-2.48935600
H	8.24626500	1.01402600	-2.36711200
C	9.36948700	-1.22479000	0.02650200
H	10.4464360	-1.05411600	-0.04401500
H	9.12131800	-1.46407600	1.05925100
H	9.12525200	-2.09223600	-0.58900900
H	4.83807900	-1.01300800	-0.30151400
H	2.40551300	-1.08296200	-0.24204100
H	0.44072500	-0.89762200	0.44490700
C	-1.32668300	0.28679200	0.68533700
H	-2.02574900	-0.53421800	0.51297600
H	-1.18763200	0.40479100	1.76089300
H	-1.76785500	1.20499500	0.29171700
C	-0.14347900	-0.17489300	-1.50774500
H	-0.77493800	-1.03886100	-1.72841900
H	-0.60680400	0.71193600	-1.94555500
H	0.82285300	-0.32771300	-1.98964500



Ref. Letter: J
UB3LYP energy: -914.35497688

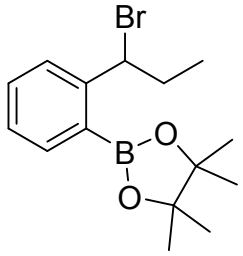
C	0.00000000	0.00000000	0.00000000
O	-0.85175800	1.15859600	0.08479200
C	-2.20868200	1.02709900	0.13461900
C	-2.90294300	-0.18482400	0.04377400
C	-4.29609500	-0.16615900	0.08258500
C	-5.04761200	1.00060700	0.20968700
C	-4.33109700	2.24825500	0.31172800
C	-2.91700300	2.21370100	0.26995800
H	-2.34451500	3.12884000	0.33957100
C	-4.99916100	3.48602300	0.45246700
C	-4.31186600	4.80770400	0.56625500
H	-3.69593000	5.03109500	-0.31393900
H	-3.63826700	4.85088800	1.43116900
H	-5.03670500	5.61529400	0.67331200
H	-6.07855400	3.47500700	0.47905500
B	-6.58992500	0.83016700	0.21374400
O	-7.17534700	-0.41104100	0.07412200
C	-8.59791300	-0.27759000	0.33549400
C	-8.84197900	1.25415800	0.06293100
O	-7.53240000	1.82617600	0.34283900
C	-9.86506400	1.92132900	0.97335800
H	-9.94263300	2.98051800	0.72147200
H	-10.8521680	1.47109900	0.84281500
H	-9.58265200	1.84413700	2.02202700
C	-9.15676300	1.56932800	-1.40157200
H	-9.11905800	2.65018300	-1.54559700
H	-8.42674200	1.11355800	-2.07191100
H	-10.1524890	1.22040100	-1.68167000
C	-8.82180700	-0.67719900	1.79676500
H	-9.88087800	-0.65857800	2.06147400
H	-8.44909800	-1.69194800	1.94475300
H	-8.28184700	-0.01747600	2.47757300
C	-9.35158300	-1.22788700	-0.58679700
H	-10.4315710	-1.11255700	-0.46587000
H	-9.09751500	-1.06152900	-1.63236000
H	-9.09322000	-2.25845500	-0.33710600
H	-4.82179700	-1.11094000	0.00906700
H	-2.38722800	-1.12902000	-0.05317200
H	-0.44748900	-0.71555600	-0.69692900
C	1.31467300	0.49508800	-0.58305800
H	2.01788500	-0.33391500	-0.68704600
H	1.15624100	0.94256800	-1.56526900
H	1.76139900	1.24749400	0.07055800
C	0.17421100	-0.64219200	1.37241300
H	0.80791800	-1.52928000	1.29711000
H	0.64845700	0.06300600	2.05872300

H -0.78287700 -0.94309800 1.80002500



Ref. Letter: K
RB3LYP energy: -2922.6066003
Volume: 120.487 cm**3/mol
NPA at C1: -0.21533
NPA at C3: -0.07125

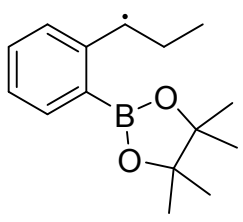
C   0.00000000 0.00000000 0.00000000
C -1.24048100 0.82499000 0.14016300
C -2.45081500 0.45172100 -0.28060300
C -3.67851400 1.25245300 -0.17201700
C -4.95086500 0.67184000 -0.07631100
C -6.10847900 1.43190000 0.02273800
C -6.02389100 2.81789200 0.02712800
C -4.77872100 3.43043000 -0.07451200
C -3.63420000 2.65687000 -0.17969300
H -2.67262800 3.14136700 -0.29497100
H -4.70135500 4.51087500 -0.08715300
H -6.92727800 3.41069500 0.10167100
H -7.06877500 0.94037300 0.09989100
Br -5.16111100 -1.24295100 -0.04541500
H -2.56288400 -0.53099600 -0.72673300
H -1.12112000 1.78469600 0.63765800
H -0.20325500 -0.95185500 -0.49351900
H   0.76046700 0.53097500 -0.58247000
H   0.44595800 -0.20852300 0.97795000



Ref. Letter: K
B3LYP energy: -3334.6495051

C   0.00000000 0.00000000 0.00000000
C   0.85076000 0.40104600 -1.20015100

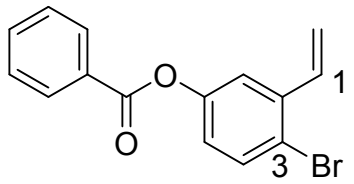
C	1.11904800	1.87577400	-1.33004200
C	2.43125400	2.37978800	-1.46730200
C	2.59833500	3.77371100	-1.55196600
C	1.52390200	4.64768500	-1.49861400
C	0.23586200	4.13756400	-1.36963700
C	0.04239300	2.76722000	-1.29049100
H	-0.96610600	2.37931200	-1.21883100
H	-0.61712200	4.80557700	-1.33803300
H	1.68612600	5.71709700	-1.56447200
H	3.60106900	4.16744200	-1.66411800
B	3.74435400	1.53419300	-1.54359800
O	3.86246300	0.17871100	-1.35881100
C	5.28376200	-0.15550600	-1.31330200
C	5.93697700	1.08105500	-2.03933700
O	4.95292100	2.12916000	-1.80840300
C	6.04907800	0.91008300	-3.55619900
H	6.32621700	1.86830300	-3.99797000
H	6.81291100	0.17683100	-3.82155100
H	5.10052900	0.59888300	-3.99579800
C	7.27182300	1.53810700	-1.46459300
H	8.02479600	0.75188700	-1.55860200
H	7.62524400	2.41046800	-2.01667700
H	7.18632400	1.81528300	-0.41520600
C	5.65809500	-0.26589700	0.16625800
H	5.01987500	-1.01537000	0.63667700
H	6.69744900	-0.57401100	0.29417300
H	5.51029200	0.68036900	0.68866200
C	5.48357300	-1.49614600	-2.00764600
H	5.07711400	-1.49178400	-3.01740200
H	6.54490500	-1.75092800	-2.05770800
H	4.97580100	-2.27980800	-1.44285800
H	1.77341500	-0.16353100	-1.21269500
Br	-0.03316100	-0.25560500	-2.91944900
H	-0.99677500	0.44008300	-0.07651000
C	-0.10505800	-1.50644600	0.22988100
H	0.88455400	-1.95924400	0.33367500
H	-0.66493000	-1.71441900	1.14430700
H	-0.61462200	-1.99972600	-0.59870000
H	0.47478800	0.46826500	0.87124800



Ref. Letter: K

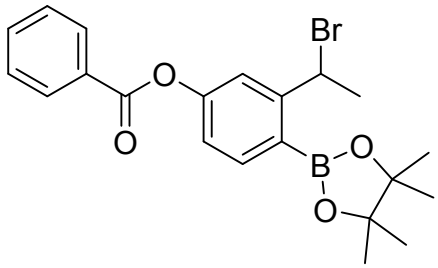
UB3LYP energy: -760.46043077

C	0.00000000	0.00000000	0.00000000
C	1.16299700	-0.93136800	0.13172500
C	1.10039700	-2.33589300	0.23320000
C	2.29017000	-3.14384500	0.36376600
C	2.14773200	-4.52989200	0.46740500
C	0.90647900	-5.15980700	0.44867200
C	-0.24794000	-4.38315800	0.32245700
C	-0.15524300	-3.01171100	0.21721500
H	-1.06554800	-2.43398000	0.12649100
H	-1.22290800	-4.85764000	0.30895600
H	0.83800200	-6.23777100	0.53134900
H	3.04287200	-5.13246600	0.56509700
B	3.75331700	-2.61051200	0.38888700
O	4.15743400	-1.29596600	0.34917600
C	5.60414000	-1.26842400	0.17315400
C	6.02691200	-2.69213500	0.69487600
O	4.82471400	-3.47369700	0.45770800
C	6.29124600	-2.73477800	2.20249700
H	6.37764000	-3.77676400	2.51420800
H	7.21845200	-2.22108500	2.46390000
H	5.47265600	-2.28211300	2.76399400
C	7.18297900	-3.33972700	-0.05694200
H	8.09175300	-2.74023600	0.03733000
H	7.38471700	-4.32596900	0.36451300
H	6.95601000	-3.46580600	-1.11426900
C	5.86021900	-1.06466600	-1.32236600
H	5.36306900	-0.14794400	-1.64308400
H	6.92615700	-0.96912100	-1.53789400
H	5.45886900	-1.89006300	-1.91196600
C	6.16435100	-0.09368300	0.96466600
H	5.86159100	-0.12971800	2.00983700
H	7.25591600	-0.07971800	0.91700900
H	5.79775600	0.84207800	0.53901700
H	2.13936600	-0.47102200	0.19580700
H	-0.85048400	-0.48425000	-0.48571100
C	-0.45782600	0.58641700	1.35191800
H	-0.79884000	-0.20334500	2.02464800
H	0.36109200	1.11346000	1.84681700
H	-1.27901800	1.29394700	1.20963000
H	0.29122100	0.82962100	-0.65348500



Ref. Letter: L
RB3LYP energy: -3303.0018388
Volume: 183.864 cm**3/mol
NPA at C1: -0.19734
NPA at C3: -0.08595

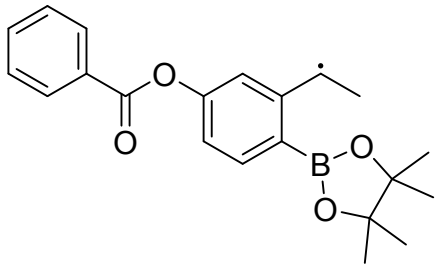
C	0.00000000	0.00000000	0.00000000
C	-0.99340100	-0.48532200	-0.83868000
C	-2.20953900	0.17462700	-0.94112700
C	-2.41868000	1.31934900	-0.17894400
C	-1.41995200	1.81044700	0.64472500
C	-0.18375200	1.16146700	0.76448600
C	0.86433900	1.69865400	1.64560000
C	0.66501700	2.47289500	2.71127500
H	-0.32345200	2.76222700	3.04889100
H	1.50166200	2.83469400	3.29514500
H	1.87920300	1.41398100	1.39363600
H	-1.59946700	2.73328000	1.18040600
O	-3.57185100	2.07544500	-0.28294500
C	-4.81829900	1.50686900	-0.48424600
O	-5.55507200	2.01883600	-1.27891500
C	-5.20390900	0.35090100	0.37386000
C	-4.63697900	0.12174900	1.62983400
C	-5.09275600	-0.92765000	2.41741500
C	-6.10277400	-1.76328100	1.95088400
C	-6.67146300	-1.53841400	0.69975400
C	-6.23277900	-0.47898700	-0.08123900
H	-6.67998600	-0.27646600	-1.04585700
H	-7.46168100	-2.18470300	0.33758300
H	-6.44992100	-2.58666500	2.56373600
H	-4.65810700	-1.09394200	3.39545900
H	-3.85264300	0.76798800	1.99893200
H	-2.97189600	-0.19008200	-1.61696500
H	-0.81656000	-1.37885300	-1.42160900
Br	1.63931200	-1.00103700	0.08598900



Ref. Letter: L
B3LYP energy: -3715.0525655

C 0.00000000 0.00000000 0.00000000
C -0.93809000 -0.84886100 -0.81658400
C -0.53441000 -2.09508400 -1.34646000
C -1.47571700 -2.81990000 -2.09711100
C -2.76475100 -2.36499700 -2.31884100
C -3.14188400 -1.14527900 -1.76745600
C -2.23758400 -0.39194200 -1.03597200
H -2.55692800 0.57330100 -0.66501700
O -4.38591500 -0.58619800 -1.98992300
C -5.52797800 -1.35673200 -2.12357400
O -6.28436300 -1.11150600 -3.02039200
C -5.79636000 -2.37945900 -1.07291300
C -5.25554500 -2.29699200 0.21225300
C -5.60085900 -3.23852300 1.17332900
C -6.47209100 -4.27538400 0.85401400
C -7.01423000 -4.36117200 -0.42592700
C -6.68747000 -3.41101700 -1.38253800
H -7.11677500 -3.45006000 -2.37534600
H -7.69673700 -5.16475400 -0.67451200
H -6.73244100 -5.01360400 1.60327300
H -5.18901400 -3.16322300 2.17233800
H -4.57948300 -1.49221600 0.46614800
H -3.45863400 -2.93804400 -2.92059800
H -1.17604200 -3.76831800 -2.52520300
B 0.86809400 -2.76168300 -1.18605800
O 1.17196400 -3.93412200 -1.83228800
C 2.59692600 -4.18900000 -1.66807600
C 2.94092500 -3.34163900 -0.38478100
O 1.90971200 -2.30713500 -0.41555500
C 4.30324700 -2.66164800 -0.40080900
H 4.43223800 -2.07986100 0.51339200
H 5.10444000 -3.40331200 -0.44345800
H 4.40740800 -1.98590600 -1.24773800
C 2.74958000 -4.10927300 0.92507800
H 2.81780500 -3.40795600 1.75812200
H 1.77195200 -4.59156300 0.96784400

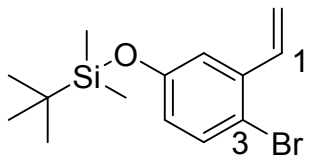
H	3.51901400	-4.87203700	1.05740300
C	3.28351700	-3.68078600	-2.93799400
H	4.35547000	-3.88597800	-2.92327800
H	2.84929600	-4.18934800	-3.79992300
H	3.13719500	-2.60803000	-3.07100400
C	2.80466100	-5.69140600	-1.52603900
H	3.85585800	-5.92160400	-1.33684800
H	2.20523500	-6.10821500	-0.71844200
H	2.51354600	-6.18776000	-2.45320900
C	-0.54354500	0.49297100	1.32967100
H	-1.43391500	1.11093100	1.21410300
H	0.20996000	1.07642800	1.85857100
H	-0.80624900	-0.37309800	1.94588900
H	0.94554600	-0.50442400	0.14038100
Br	0.56671600	1.61162400	-1.10167800



Ref. Letter: L
UB3LYP energy: -1140.8651860

C	0.00000000	0.00000000	0.00000000
O	-1.44657300	0.08525900	-0.12512600
B	-1.85514000	1.28892200	0.40310000
C	-3.31874700	1.78897300	0.23090300
C	-4.17209700	0.95449700	-0.49315400
C	-5.51040100	1.25538300	-0.72708300
C	-6.02392200	2.44044600	-0.20067500
C	-5.22414800	3.31043800	0.50892700
C	-3.85328100	3.02356500	0.74778400
C	-3.06155200	3.94101000	1.47087700
C	-3.55893300	5.23948400	2.01720500
H	-3.96239000	5.89120800	1.23271400
H	-2.75704000	5.78365400	2.51650600
H	-4.36632600	5.10016800	2.74721400
H	-2.02569400	3.68696600	1.63969100
H	-5.66661500	4.22722400	0.87462900
O	-7.32747900	2.84417600	-0.44493300
C	-8.38399600	1.95966700	-0.51059300
O	-9.20631800	2.11479200	-1.37061600
C	-8.50158200	0.92334900	0.55620600

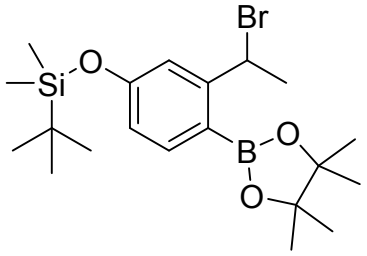
C -7.92695000 1.07049400 1.82077500
C -8.14152100 0.10708200 2.79846200
C -8.91479200 -1.01463800 2.51656900
C -9.48977400 -1.16559100 1.25720900
C -9.29410800 -0.19565100 0.28476300
H -9.75297400 -0.28592500 -0.69128600
H -10.0964420 -2.03570300 1.03729200
H -9.07306900 -1.76859700 3.27864500
H -7.70316400 0.23211600 3.78109700
H -7.32415700 1.93918900 2.04664700
H -6.13402500 0.59344200 -1.31371500
H -3.77178800 0.03272900 -0.89749400
O -0.83666000 1.93347800 1.06467000
C 0.29151700 1.01482400 1.16874300
C 1.57924000 1.81631000 1.02849800
H 1.67583000 2.50308300 1.87122000
H 2.44891900 1.15482800 1.03232300
H 1.59173600 2.40353900 0.11181200
C 0.21484000 0.38191200 2.56017400
H 0.22787000 1.17470200 3.30960700
H -0.70581000 -0.18901600 2.68866400
H 1.06289100 -0.27958000 2.74688200
C 0.58699100 0.43501500 -1.34534000
H 1.67486400 0.34543600 -1.35693300
H 0.18202400 -0.20624700 -2.12955000
H 0.32086800 1.46612800 -1.58235100
C 0.37574000 -1.44738700 0.29097800
H 1.45160900 -1.54356100 0.45621100
H -0.14749800 -1.83234200 1.16469700
H 0.10949800 -2.07156500 -0.56374000



Ref. Letter: M
RB3LYP energy: -3485.2702716
Volume: 234.378 cm**3/mol
NPA at C1: -0.19426
NPA at C3: -0.09471

Si 0.00000000 0.00000000 0.00000000
O 1.38324500 0.95967700 -0.03608300
C 2.71573000 0.70088900 -0.02472400
C 3.25800000 -0.58403100 -0.09847300
C 4.63619900 -0.75098500 -0.07267800

C 5.47560100 0.34753800 0.02269900
C 4.96528800 1.65206900 0.08967300
C 3.57311700 1.79272500 0.07336200
H 3.13318700 2.77720600 0.16303200
C 5.83720900 2.83305100 0.18961600
C 5.53073000 4.06307300 -0.22026000
H 4.59013100 4.29912700 -0.70433000
H 6.23207400 4.87832200 -0.09548300
H 6.81561400 2.65879200 0.62253400
Br 7.37149500 0.01237700 0.02442800
H 5.05672400 -1.74586700 -0.13102700
H 2.61947900 -1.45363700 -0.17154100
C 0.01306400 -1.07652100 1.53964100
H -0.91136500 -1.65576300 1.61213300
H 0.84214500 -1.78736000 1.53167200
H 0.10387000 -0.47440200 2.44629400
C -1.41028200 1.27905700 0.04124500
C -1.34902200 2.17129000 -1.21492100
H -2.14805000 2.92086100 -1.18137700
H -0.39787200 2.70312300 -1.28696100
H -1.48358500 1.59583700 -2.13457500
C -1.27862900 2.16981300 1.29269600
H -2.07845700 2.91914600 1.30481600
H -1.36132400 1.59328100 2.21771500
H -0.32508400 2.70173900 1.31183600
C -2.77089700 0.55411800 0.07947600
H -3.58557500 1.28674900 0.10290500
H -2.92852500 -0.07502000 -0.80075300
H -2.87809900 -0.07570600 0.96684800
C -0.08031100 -1.06722000 -1.54465300
H -1.03244500 -1.60224900 -1.59373100
H 0.01265900 -0.46404700 -2.45041100
H 0.71356500 -1.81692200 -1.56421900

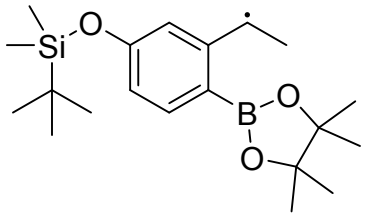


Ref. Letter: M
RB3LYP energy: -3897.3214523

Si 0.00000000 0.00000000 0.00000000
O 1.30175300 0.89684000 0.58274900

C	2.64808300	0.75115900	0.50161000
C	3.27827000	-0.46405400	0.22545600
C	4.66125000	-0.51371100	0.17269000
C	5.47185500	0.61147200	0.39586700
C	4.81878200	1.83386100	0.67759100
C	3.42809700	1.88316700	0.72433800
H	2.91483100	2.81757000	0.91055100
C	5.59845600	3.09409800	0.94047000
C	5.20509400	3.87095000	2.18414000
H	5.33850000	3.22517200	3.05811600
H	4.16592600	4.19832600	2.16068500
H	5.83863000	4.74984600	2.30355000
H	6.66087500	2.89499800	0.93630300
Br	5.42735200	4.33429000	-0.66914100
B	7.00869100	0.37432800	0.31661100
O	7.52247600	-0.83936700	-0.07610700
C	8.95874900	-0.68888800	-0.25693600
C	9.27528300	0.57078500	0.63380800
O	7.99844100	1.27715700	0.62659600
C	10.3453440	1.50424700	0.08332000
H	10.4694670	2.35460400	0.75597300
H	11.3067300	0.99008400	0.01009800
H	10.0789900	1.88875700	-0.89961100
C	9.57702300	0.22601200	2.09419800
H	9.59167900	1.14741100	2.67834100
H	8.81428400	-0.42993400	2.51637700
H	10.5490360	-0.25971300	2.19793100
C	9.19310300	-0.45266500	-1.75120200
H	10.2573520	-0.38688600	-1.98537100
H	8.77065400	-1.28937400	-2.30955300
H	8.70457600	0.46104000	-2.09249300
C	9.63865000	-1.97934000	0.18255700
H	10.7258100	-1.88379400	0.12798100
H	9.36340900	-2.25455800	1.19933100
H	9.33876100	-2.79263700	-0.48041600
H	5.14085200	-1.46005400	-0.04616000
H	2.69665900	-1.36086000	0.05787100
C	-0.15538900	-1.61144100	0.95645100
H	-1.08418900	-2.12568600	0.69549300
H	0.66665300	-2.29631600	0.73760100
H	-0.16104000	-1.43476700	2.03426000
C	-1.48729700	1.14433100	0.32719400
C	-1.30531200	2.47299000	-0.43304300
H	-2.14605800	3.14395400	-0.22213700
H	-0.38847700	2.98616300	-0.13584800
H	-1.27246800	2.32590500	-1.51578500
C	-1.59552600	1.44244800	1.83592600

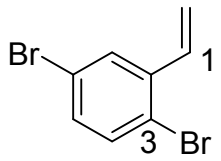
H -2.43661800 2.11954000 2.02541100
H -1.77034600 0.53664400 2.42276600
H -0.69139700 1.92144300 2.21779700
C -2.78723500 0.46553900 -0.14941600
H -3.64292200 1.12683700 0.02842800
H -2.76809700 0.24412400 -1.22014300
H -2.98620900 -0.46824200 0.38348500
C 0.24630300 -0.34486100 -1.82887000
H -0.60325400 -0.89911200 -2.23660500
H 0.35061300 0.58037100 -2.39948000
H 1.14298500 -0.94317400 -2.00452400



Ref. Letter: M
UB3LYP energy: -1323.1325047

Si 0.00000000 0.00000000 0.00000000
O 1.25816700 1.09889800 -0.18290100
C 2.61456200 1.00243800 -0.15346800
C 3.29705100 -0.21993700 -0.12268400
C 4.68817800 -0.21974200 -0.09998700
C 5.45306200 0.94751800 -0.10830600
C 4.75267300 2.20690600 -0.14488800
C 3.33489100 2.18616500 -0.16549100
H 2.77517300 3.11131700 -0.19290900
C 5.43632100 3.44284100 -0.16042100
C 4.76710600 4.77827300 -0.19667900
H 4.11069400 4.93635100 0.66811100
H 4.13803300 4.90225000 -1.08698200
H 5.50371200 5.58229400 -0.20101600
H 6.51581400 3.42067400 -0.14712600
B 6.99370600 0.76048300 -0.07034600
O 7.56023500 -0.49182700 0.04000100
C 8.99023900 -0.36831300 -0.18331700
C 9.24709500 1.15048400 0.14522500
O 7.95007000 1.74865500 -0.13961100
C 10.2949950 1.83465400 -0.72343500
H 10.3815880 2.88339000 -0.43377700
H 11.2737400 1.36699400 -0.59143700
H 10.0304490 1.79757700 -1.77889200
C 9.53848900 1.41266600 1.62506600

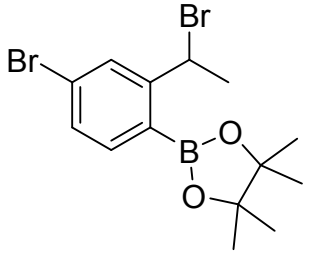
H 9.51418500 2.48867000 1.80421600
H 8.78971200 0.94654700 2.26704500
H 10.5235790 1.03951700 1.91144700
C 9.24251000 -0.72484700 -1.65122000
H 10.3075640 -0.71543100 -1.89125000
H 8.85770300 -1.72830000 -1.83944800
H 8.72858900 -0.03585300 -2.32311100
C 9.70972000 -1.35805600 0.72473100
H 10.7936050 -1.25138300 0.63505600
H 9.43083100 -1.22370000 1.76850500
H 9.44644600 -2.37654700 0.43401700
H 5.20311400 -1.17287100 -0.07493300
H 2.75590800 -1.15637100 -0.12086100
C 0.16726400 -0.90598400 1.63786300
H -0.68522500 -1.57101300 1.80066500
H 1.07048000 -1.51904500 1.66721700
H 0.21541100 -0.20926800 2.47750400
C -1.54465800 1.11748300 -0.03728000
C -1.61142800 1.87249700 -1.37944100
H -2.48202100 2.53869300 -1.39347500
H -0.72158600 2.48416800 -1.54255700
H -1.71095500 1.19057400 -2.22807000
C -1.47395600 2.14314400 1.11095400
H -2.34758900 2.80477500 1.07910000
H -1.46828600 1.66131600 2.09225400
H -0.58100000 2.76742200 1.03856200
C -2.81759700 0.26317300 0.12534200
H -3.70640900 0.90411100 0.10163700
H -2.92745400 -0.46985000 -0.67847800
H -2.83391000 -0.27583000 1.07647100
C -0.00234400 -1.22742600 -1.42451400
H -0.88802500 -1.86733200 -1.38290000
H -0.00219200 -0.71632800 -2.38981600
H 0.87262300 -1.88041400 -1.39759100



Ref. Letter: N
RB3LYP energy: -5456.8134754
Volume: 136.627 cm**3/mol
NPA at C1: -0.19909
NPA at C3: -0.07572

C 0.00000000 0.00000000 0.00000000

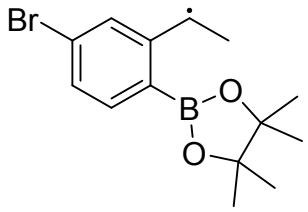
C 1.38644300 -0.07023100 -0.01013100
C 2.14500800 1.08883200 -0.10072000
C 1.55123800 2.35560700 -0.18049200
C 0.14793800 2.40214100 -0.18182400
C -0.60431300 1.24680900 -0.08590700
Br -2.51698400 1.36833300 -0.09461400
H -0.34522000 3.35869000 -0.28229500
C 2.33868700 3.59427500 -0.27798600
C 1.94457800 4.79696300 0.13726900
H 0.99086900 4.96330100 0.62468700
H 2.58490400 5.66109300 0.01482300
H 3.32591700 3.49055300 -0.71326500
Br 4.05539100 0.88958300 -0.08008000
H 1.87643300 -1.03205000 0.05622500
H -0.59206700 -0.90225900 0.06692200



Ref. Letter: N
RB3LYP energy: -5868.8643438

C 0.00000000 0.00000000 0.00000000
C 0.55086900 -0.53366000 -1.31087700
C 0.03202600 -1.88435900 -1.72870200
C 0.90383000 -2.94695400 -2.04828100
C 0.33134100 -4.18357700 -2.39298500
C -1.03900600 -4.38556700 -2.42927000
C -1.86935300 -3.31905600 -2.11410100
C -1.35125300 -2.08485400 -1.76924100
H -2.02221800 -1.26553000 -1.55099800
Br -3.77078400 -3.56045100 -2.16044500
H -1.45258400 -5.34764800 -2.69958300
H 0.98811800 -5.00809700 -2.64126500
B 2.46627200 -2.88960300 -2.06680100
O 3.20584600 -3.95688300 -2.50910100
C 4.60729800 -3.69782400 -2.20219800
C 4.63074200 -2.12922400 -2.05717500
O 3.25240600 -1.84088100 -1.66120500
C 4.86755400 -1.39541300 -3.37805900
H 4.66919300 -0.33259800 -3.23336500
H 5.89883200 -1.50862400 -3.71700800

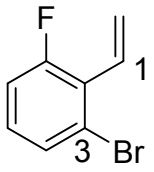
H 4.20183900 -1.75738600 -4.16266300
C 5.56151200 -1.58936000 -0.97986200
H 6.60040100 -1.84160400 -1.20515300
H 5.48152700 -0.50177600 -0.94016600
H 5.31345600 -1.98303000 0.00451600
C 4.91482900 -4.43624400 -0.89765300
H 4.68785400 -5.49504900 -1.03043900
H 5.96725400 -4.34357000 -0.62369400
H 4.30693600 -4.06156600 -0.07285700
C 5.45969700 -4.25538700 -3.33452600
H 5.15668300 -3.85802800 -4.30169700
H 6.51535000 -4.02270600 -3.17559900
H 5.35591300 -5.34117200 -3.36770000
H 1.63164600 -0.52769900 -1.30044900
Br 0.15737900 0.81842800 -2.77694100
H -1.08412900 0.11079000 -0.01728900
H 0.25730700 -0.70059400 0.80087900
H 0.44016900 0.96908500 0.23436600



Ref. Letter: N
UB3LYP energy: -3294.6766686

C 0.00000000 0.00000000 0.00000000
C 0.80977600 -1.25445900 -0.05185800
C 0.26714500 -2.55478400 -0.11131600
C 1.09360600 -3.73293700 -0.16209000
C 0.46634300 -4.97885500 -0.21633800
C -0.91761100 -5.13140900 -0.22528500
C -1.70325200 -3.98291600 -0.17718900
C -1.14752600 -2.72655500 -0.12148400
H -1.79282100 -1.86089300 -0.08470500
Br -3.61650100 -4.16471200 -0.18815200
H -1.37026000 -6.11218700 -0.26814800
H 1.08409000 -5.86805000 -0.25390200
B 2.65128900 -3.75134400 -0.16780700
O 3.34606600 -4.93321200 -0.28011100
C 4.75151400 -4.66206100 -0.02164000
C 4.85249300 -3.11903900 -0.32153300
O 3.48862100 -2.66688200 -0.06439600
C 5.14872000 -2.79951600 -1.78861100

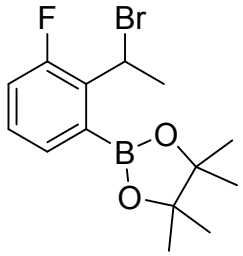
H 5.00494400 -1.73051900 -1.95255500
H 6.17735600 -3.05074500 -2.05386500
H 4.47591800 -3.33718700 -2.45817500
C 5.79656200 -2.34144200 0.58601000
H 6.82200500 -2.70342100 0.47922500
H 5.78241900 -1.28561100 0.31012200
H 5.50631500 -2.42015000 1.63233700
C 5.00612600 -5.01698900 1.44586500
H 4.72603700 -6.05881300 1.60830700
H 6.05850900 -4.90012200 1.71152700
H 4.40789700 -4.39896600 2.11704300
C 5.59050900 -5.55417400 -0.92765200
H 5.32559000 -5.42907100 -1.97613600
H 6.65498700 -5.33910300 -0.80685900
H 5.42638100 -6.59960800 -0.66116200
H 1.88566700 -1.16048800 -0.04328300
H -0.64430800 0.11321200 -0.88061500
H -0.66273600 0.02952300 0.87352400
H 0.64583000 0.87686400 0.04845400



Ref. Letter: P
RB3LYP energy: -2982.5437798
Volume: 110.091 cm**3/mol
NPA at C1: -0.21366
NPA at C3: -0.05664

C 0.00000000 0.00000000 0.00000000
C 0.89203900 -0.95883100 -0.25852000
C 0.71620100 -2.41442900 -0.18963100
C 1.81194000 -3.29867000 -0.15673000
C 1.67083100 -4.67783400 -0.11435300
C 0.40018700 -5.23753800 -0.10730700
C -0.71768100 -4.41553500 -0.14214300
C -0.53610200 -3.04806700 -0.17977200
F -1.65264700 -2.28677300 -0.22340200
H -1.72437300 -4.81194600 -0.14283300
H 0.28410500 -6.31342200 -0.07497000
H 2.54867500 -5.30775900 -0.08518800
Br 3.61567300 -2.62924200 -0.14847400
H 1.89050700 -0.65004700 -0.54230000
H 0.29566600 1.03785900 -0.09194000

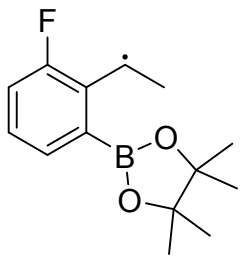
H -1.01518100 -0.19552300 0.31037300



Ref. Letter: P
RB3LYP energy: -3394.5938014

C   0.00000000 0.00000000 0.00000000
C -0.72923900 0.26203600 -1.30843300
C -0.81599900 1.69247700 -1.76055800
C -2.05559300 2.30251800 -2.07136800
C -2.07156100 3.65063700 -2.46230100
C -0.90840600 4.40045200 -2.55650900
C   0.31189100 3.80889400 -2.26077600
C   0.32834100 2.48286600 -1.87486300
F   1.53985100 1.93657300 -1.61304100
H   1.24741700 4.34960100 -2.32697700
H -0.94670300 5.43882300 -2.86252000
H -3.02305700 4.10867900 -2.69894800
B -3.45580900 1.59961800 -2.03440200
O -4.57655000 2.24545900 -2.49082600
C -5.74144300 1.44441800 -2.13616500
C -5.11191600 0.01494700 -1.93297600
O -3.73350100 0.33993900 -1.56809400
C -5.03909000 -0.81183600 -3.21795800
H -4.41382100 -1.68761300 -3.03964800
H -6.02813100 -1.15406300 -3.52816600
H -4.59508700 -0.24394300 -4.03655400
C -5.72257300 -0.81179600 -0.80960400
H -6.77578500 -1.01960100 -1.01263800
H -5.20037200 -1.76693000 -0.73386700
H -5.64632100 -0.30729600 0.15213500
C -6.31704700 2.04701200 -0.85250000
H -6.55295000 3.09709300 -1.03105000
H -7.23294800 1.53723900 -0.54831300
H -5.60217600 1.99655700 -0.02990800
C -6.75826200 1.54743900 -3.26558600
H -6.32384500 1.27386100 -4.22552500
H -7.61767700 0.90080200 -3.07341200
H -7.11925000 2.57465500 -3.33871700
H -1.72083900 -0.16401600 -1.26836700

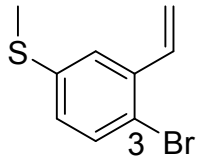
Br 0.10871400 -0.86564600 -2.77814500
H 1.04730900 0.28842600 -0.03796600
H -0.48968100 0.57585100 0.79246100
H -0.06469700 -1.05703700 0.25848800



Ref. Letter: P
UB3LYP energy: -820.40531767

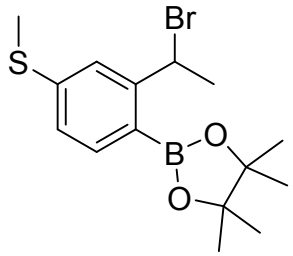
C 0.00000000 0.00000000 0.00000000
C 1.01114200 -1.10116900 -0.05798200
C 0.77544000 -2.48776100 -0.13015300
C 1.85979000 -3.44535300 -0.18142200
C 1.56886200 -4.80890500 -0.24968100
C 0.26523100 -5.29603400 -0.27317400
C -0.79791800 -4.39477400 -0.22510700
C -0.53069300 -3.05048400 -0.15636700
F -1.60305100 -2.21702100 -0.11031300
H -1.82969500 -4.72318300 -0.23915600
H 0.07372100 -6.36031700 -0.32718900
H 2.39400900 -5.50894600 -0.28630700
B 3.37831700 -3.08727400 -0.17143000
O 3.93555300 -1.83513000 -0.07114500
C 5.37008400 -1.95218400 -0.30948300
C 5.63362300 -3.47250600 0.00681900
O 4.33653200 -4.07081900 -0.26489500
C 5.94578900 -3.74289200 1.48105300
H 5.92599800 -4.82008000 1.65290200
H 6.93378200 -3.36936600 1.75651100
H 5.20492500 -3.28313800 2.13677200
C 6.67287200 -4.14717400 -0.87964100
H 7.65236000 -3.67916100 -0.75495900
H 6.76371200 -5.19791800 -0.59917600
H 6.39617900 -4.10240100 -1.93165800
C 5.60212100 -1.58472000 -1.77705200
H 5.21375800 -0.58080700 -1.95498300
H 6.66447800 -1.59060100 -2.02815000
H 5.08303500 -2.27102200 -2.44758000
C 6.09075800 -0.96433100 0.59849500
H 5.82342800 -1.10756100 1.64405800

H 7.17404600 -1.06533900 0.49739700
H 5.82039700 0.05489600 0.31716200
H 2.04813500 -0.80191400 -0.04173700
H -0.64684900 -0.07416500 0.88018200
H 0.50357300 0.96692000 0.03476100
H -0.66946100 -0.00177700 -0.86568500



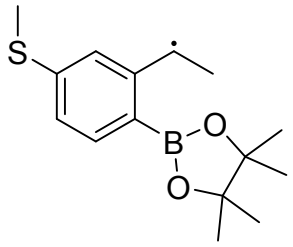
Ref. Letter: Q
RB3LYP energy: -3320.8154515
Volume: 158.733 cm**3/mol
NPA at C3: -0.06643

C 0.00000000 0.00000000 0.00000000
S 0.58223900 0.24951600 -1.72031500
C 2.35725200 0.11022800 -1.50053300
C 2.96991200 -1.14079600 -1.40744200
C 4.34820500 -1.22878700 -1.28149500
C 5.11702300 -0.07214500 -1.25912200
C 4.54240000 1.20134400 -1.35577900
C 3.14473600 1.25403900 -1.48339800
H 2.66771600 2.21875800 -1.59628800
C 5.34396100 2.43467000 -1.34298200
C 4.91997300 3.63143900 -0.93958900
H 5.57551800 4.49202300 -0.97849500
H 3.92348100 3.79589000 -0.54638200
H 6.36848700 2.33370200 -1.68240000
Br 7.01759100 -0.28989900 -1.06583200
H 4.82757300 -2.19555600 -1.20810000
H 2.37317200 -2.04307800 -1.45030400
H 0.38536200 0.78015600 0.65459300
H -1.08745000 0.06423500 -0.03916300
H 0.28788700 -0.98240100 0.37095400



Ref. Letter: Q
RB3LYP energy: -3732.8673367

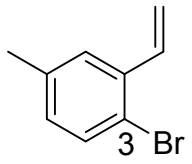
C	0.00000000	0.00000000	0.00000000
S	0.34319000	1.74640800	0.37488600
C	2.11447200	1.84773300	0.34771100
C	2.96705000	0.77682200	0.07563600
C	4.33788900	0.98031600	0.07676100
C	4.92142700	2.22763000	0.34910700
C	4.04705600	3.30433500	0.62636200
C	2.67045800	3.09860700	0.61784200
H	2.00867700	3.93628300	0.80438800
C	4.57251500	4.67518600	0.96288400
C	4.04074700	5.28072000	2.24997900
H	2.95655400	5.39129600	2.24101600
H	4.48463600	6.26042500	2.42668200
H	4.30731200	4.62294900	3.08355600
H	5.65335300	4.68198700	0.95704000
Br	4.16151000	5.95276000	-0.56724000
B	6.47926700	2.27652400	0.31802400
O	7.21676300	1.16710900	-0.01932100
C	8.60542100	1.57267300	-0.17901400
C	8.66263800	2.90526800	0.66077300
O	7.27517900	3.35695500	0.61286700
C	9.54430900	4.00304000	0.07988900
H	9.49436000	4.88707300	0.71779100
H	10.5868960	3.67912500	0.03458100
H	9.22441100	4.29149600	-0.91981500
C	8.99945700	2.68361800	2.13681900
H	8.83395600	3.61483500	2.68072800
H	8.36488900	1.91512500	2.58051400
H	10.0428430	2.39163200	2.26937700
C	8.83226200	1.78599600	-1.67764600
H	9.87180800	2.03912900	-1.89375900
H	8.58785800	0.86261200	-2.20480900
H	8.19277200	2.57761500	-2.07058700
C	9.49721000	0.44732400	0.32996500
H	10.5503750	0.73461100	0.28274200
H	9.25583800	0.17230900	1.35536100
H	9.36107000	-0.43537700	-0.29708600
H	4.98850200	0.14203200	-0.14123800
H	2.57754100	-0.20816900	-0.14086700
H	0.41854100	-0.65949700	0.75944100
H	-1.08584800	-0.08699600	0.01355800
H	0.36539500	-0.27400700	-0.98901900



Ref. Letter: Q
UB3LYP energy: -1158.6787399

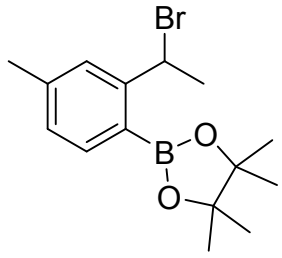
C	0.00000000	0.00000000	0.00000000
S	0.46883300	1.75663600	-0.06516900
C	2.24703700	1.72910000	-0.06656600
C	3.01665900	0.56190200	-0.02476100
C	4.40582800	0.66173900	-0.03146400
C	5.08470400	1.87885500	-0.07783700
C	4.29683900	3.08510300	-0.12173300
C	2.88403700	2.96218200	-0.11362200
H	2.27889600	3.85952100	-0.14581300
C	4.88933900	4.36652500	-0.17216200
C	4.12700300	5.65079100	-0.21697800
H	3.46939200	5.71238900	-1.09295800
H	4.80529300	6.50358200	-0.25569000
H	3.48293000	5.78137700	0.66157500
H	5.96783900	4.42111900	-0.17953500
B	6.63670800	1.80196300	-0.07115400
O	7.29170400	0.59535100	0.04709900
C	8.70404800	0.81501700	-0.21410300
C	8.86065800	2.35384900	0.08206400
O	7.51697400	2.85408200	-0.17964500
C	9.83574700	3.09389100	-0.82458200
H	9.85750300	4.15071500	-0.55277400
H	10.8474930	2.69645800	-0.71249700
H	9.54673900	3.02153700	-1.87175800
C	9.16668500	2.66456700	1.54930000
H	9.06535100	3.73883600	1.71073800
H	8.47082300	2.15562300	2.21772700
H	10.1837560	2.37249500	1.81747600
C	8.94518900	0.44936200	-1.68154700
H	10.0006710	0.52969300	-1.94881100
H	8.62885100	-0.58238700	-1.84228800
H	8.36744900	1.08698200	-2.35233100
C	9.51309800	-0.10459400	0.69202600
H	10.5844010	0.07236400	0.56882700
H	9.25472900	0.03215100	1.74074500
H	9.31139600	-1.14419700	0.42819800
H	4.98736100	-0.25211900	0.00178800

H 2.55485400 -0.41453600 0.01239300
H 0.35602500 -0.47450500 0.91373200
H -1.08954000 -0.00478600 -0.00060600
H 0.35727200 -0.54081400 -0.87559800



Ref. Letter: R
RB3LYP energy: -2922.6045069
Volume: 132.922 cm**3/mol
NPA at C3: -0.07525

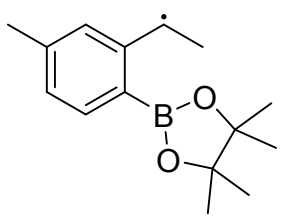
C 0.00000000 0.00000000 0.00000000
C 1.50764900 0.01723600 -0.00158300
C 2.23570100 -1.17307800 0.08235000
C 3.62188000 -1.15769700 0.07959100
C 4.29938100 0.05155800 -0.00342200
C 3.61816600 1.27090600 -0.08227000
C 2.21435500 1.20946200 -0.08917700
H 1.66532900 2.13807500 -0.19187400
C 4.31738900 2.56162600 -0.17419000
C 3.83653200 3.73781300 0.22710600
H 4.41839800 4.64288600 0.10759300
H 2.86642500 3.84168200 0.69922200
H 5.31619300 2.52707500 -0.59434100
Br 6.22335600 -0.01722800 0.02381200
H 4.17844100 -2.08306300 0.14289400
H 1.71684400 -2.12353100 0.14144100
H -0.38864700 -0.27859600 0.98394400
H -0.40970300 0.97861300 -0.25330800
H -0.38927800 -0.72510700 -0.71868800



Ref. Letter: R
RB3LYP energy: -3334.6543194

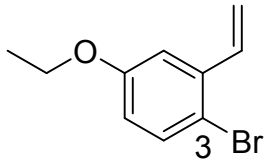
C 0.00000000 0.00000000 0.00000000

C	1.38004500	0.60207500	0.06111100
C	2.50824900	-0.16247600	-0.24936200
C	3.77105900	0.40031500	-0.19890600
C	3.97909200	1.74236000	0.16794100
C	2.84217800	2.51286000	0.48905900
C	1.57288700	1.92978800	0.42409400
H	0.70307700	2.53808100	0.64352400
C	2.96383800	3.94858400	0.92076200
C	2.21221100	4.32863800	2.18396000
H	2.38080900	5.37700100	2.43009700
H	2.58279900	3.71426400	3.01089200
H	1.13821800	4.16631800	2.09647200
H	4.00184400	4.24055500	0.99428800
Br	2.32526100	5.16178100	-0.59157400
B	5.46101800	2.23330500	0.16177400
O	5.93518500	3.42180000	0.66188200
C	7.32971700	3.56372500	0.25027400
C	7.74108500	2.06917400	-0.03231900
O	6.46302700	1.45623700	-0.36558100
C	8.27109700	1.33756000	1.20318400
H	8.34558800	0.27295900	0.97644400
H	9.26165400	1.69655200	1.48877100
H	7.60006700	1.45493000	2.05531300
C	8.69114800	1.87112600	-1.20645400
H	9.64296900	2.37628300	-1.02532300
H	8.89407600	0.80659200	-1.33511100
H	8.26749200	2.24772200	-2.13590400
C	8.09552000	4.24691700	1.37525600
H	7.71849000	5.26221400	1.50939500
H	7.98452800	3.71761700	2.32029300
H	9.15927600	4.31272100	1.13441800
C	7.32872900	4.44580500	-0.99974300
H	6.77481000	3.98220900	-1.81702400
H	6.84465400	5.39411200	-0.76243900
H	8.34402700	4.65527100	-1.34146600
H	4.63259800	-0.20566000	-0.45171600
H	2.39184900	-1.20188400	-0.53827000
H	-0.10072100	-0.82582300	0.71003700
H	-0.76861700	0.73812500	0.23232800
H	-0.20971500	-0.40312800	-0.99441700



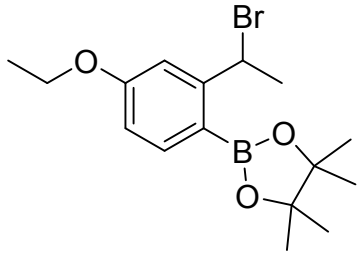
Ref. Letter: R
UB3LYP energy: -760.46551804

C	0.00000000	0.00000000	0.00000000
C	1.47640100	0.30441600	0.01368300
C	2.41556000	-0.73756900	-0.03378800
C	3.77595400	-0.45491600	-0.02177500
C	4.27506900	0.84929500	0.03709400
C	3.32738700	1.93196000	0.08661400
C	1.94062600	1.60493900	0.07231600
H	1.21635800	2.40973900	0.10979600
C	3.73183700	3.28117100	0.14819000
C	2.79638000	4.44620600	0.20015700
H	3.34862300	5.38581500	0.23495900
H	2.14386100	4.41529000	1.08167400
H	2.13332300	4.48556300	-0.67292400
H	4.79150600	3.48894200	0.16120300
B	5.82352800	0.99345000	0.03919200
O	6.54514500	2.15799400	0.16923200
C	7.94731000	1.85848200	-0.08877100
C	8.01006500	0.30796500	0.18136500
O	6.64401300	-0.10584900	-0.09132900
C	8.29403700	-0.04581700	1.64380200
H	8.12193900	-1.11385400	1.78535500
H	9.32736200	0.17403700	1.91930100
H	7.63077400	0.49442400	2.32088100
C	8.94464900	-0.47145700	-0.73557600
H	9.97770000	-0.13626700	-0.61432500
H	8.90274500	-1.53216300	-0.48207900
H	8.66352500	-0.36492500	-1.78199600
C	8.80160400	2.71417400	0.83782200
H	8.66788600	3.76824800	0.58832000
H	8.52547900	2.57790000	1.88208400
H	9.86096500	2.47280100	0.72148400
C	8.21530100	2.23535600	-1.54807100
H	7.60532900	1.64329900	-2.23177500
H	7.95994400	3.28625200	-1.69252300
H	9.26580300	2.09906700	-1.81214400
H	4.48289100	-1.27532300	-0.05933500
H	2.07739200	-1.76723700	-0.07952100
H	-0.27923100	-0.63401100	0.84629600
H	-0.59644800	0.91196100	0.05149600
H	-0.28269500	-0.53652100	-0.91025200



Ref. Letter: S
RB3LYP energy: -3037.1656602
Volume: 157.010 cm**3/mol
NPA at C3: -0.09408

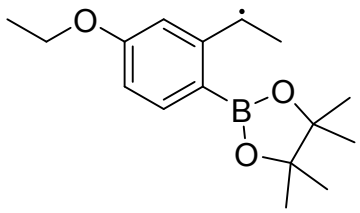
C	0.00000000	0.00000000	0.00000000
O	-0.85473800	-1.14362300	-0.07187500
C	-2.20384800	-0.95898900	-0.06468400
C	-2.97706500	-2.12245600	-0.13865700
C	-4.35554200	-2.03267700	-0.12326600
C	-4.97635700	-0.79037100	-0.03727700
C	-4.23423300	0.39118400	0.03029800
C	-2.83183600	0.27691100	0.02378900
H	-2.24971100	1.18145500	0.11723600
C	-4.87083600	1.71418400	0.12123900
C	-4.33484000	2.86911800	-0.27208200
H	-3.35832900	2.93258700	-0.73829000
H	-4.87691500	3.79865600	-0.15346000
H	-5.87299000	1.72389300	0.53426200
Br	-6.90131700	-0.76887200	-0.05122000
H	-4.95566800	-2.93078700	-0.18039600
H	-2.48120000	-3.08277100	-0.19826400
H	-0.20026000	0.54910200	0.92677800
C	1.43211300	-0.49072400	-0.03929900
H	2.11698300	0.35832800	0.01437200
H	1.63727000	-1.15349000	0.80294100
H	1.62924900	-1.03562000	-0.96393400
H	-0.20919500	0.66601900	-0.84456200



Ref. Letter: S
RB3LYP energy: -3449.2142778

C	0.00000000	0.00000000	0.00000000
O	-0.74852100	1.19195300	0.26727800

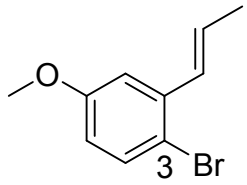
C	-2.10533000	1.18509500	0.16066900
C	-2.88470600	0.06660800	-0.13919300
C	-4.26370400	0.20570200	-0.19604200
C	-4.92030600	1.42423600	0.02945700
C	-4.11162500	2.54760500	0.32974300
C	-2.73011100	2.41049700	0.38943300
H	-2.09673900	3.26344000	0.59634700
C	-4.72110400	3.89494400	0.61020600
C	-4.21940200	4.60583200	1.85412800
H	-3.14778100	4.80073500	1.82103500
H	-4.42312900	3.97468400	2.72522700
H	-4.73633100	5.55613700	1.98746000
H	-5.80015000	3.83090500	0.61625900
Br	-4.41440200	5.11527500	-0.99392900
B	-6.47198800	1.40094800	-0.08959300
O	-7.13698500	0.27771800	-0.52362400
C	-8.56249700	0.48193400	-0.31396100
C	-8.66723600	2.05223200	-0.25572500
O	-7.33672600	2.42640500	0.21377700
C	-9.69487300	2.59949200	0.72598600
H	-9.66791400	3.69038500	0.71210000
H	-10.7029340	2.28445800	0.44591400
H	-9.49720100	2.26953200	1.74466800
C	-8.84849300	2.70392300	-1.62813000
H	-8.70751200	3.78109300	-1.52961400
H	-8.11523500	2.33437600	-2.34616000
H	-9.84860900	2.52312800	-2.02638900
C	-8.91776000	-0.20100400	1.00924100
H	-9.98854000	-0.14608500	1.21430000
H	-8.63373500	-1.25276500	0.95015300
H	-8.38028500	0.24737400	1.84610900
C	-9.31816400	-0.17456800	-1.46223300
H	-10.3915880	0.01166800	-1.37774400
H	-8.97609300	0.18868200	-2.42990600
H	-9.16047400	-1.25407100	-1.43194600
H	-4.86209300	-0.66636500	-0.43036900
H	-2.43874800	-0.89866600	-0.33230700
C	0.23059000	-0.22463200	-1.48639100
H	0.85883400	-1.10714300	-1.63308900
H	-0.70535000	-0.37963200	-2.02478900
H	0.73910200	0.63536600	-1.92544500
H	0.94944300	0.16285900	0.51097800
H	-0.48340800	-0.86028100	0.47132000



Ref. Letter: S
UB3LYP energy: -875.025023948

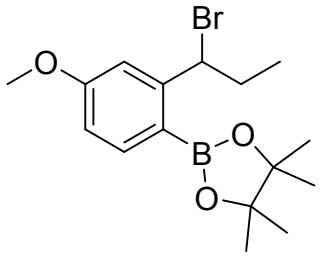
C	0.00000000	0.00000000	0.00000000
O	0.80741400	1.18071600	0.02483600
C	2.16753300	1.08139900	0.08933700
C	2.88377500	-0.12037200	0.07441600
C	4.27592800	-0.07322600	0.12439100
C	5.00350800	1.11325300	0.19805000
C	4.26334100	2.35115300	0.21326300
C	2.85060300	2.28756000	0.15750800
H	2.26044000	3.19402200	0.16236700
C	4.90715400	3.60798900	0.27401400
C	4.19497900	4.92129400	0.28694800
H	3.51159700	5.01359400	1.14024400
H	3.58477300	5.07002900	-0.61273500
H	4.90414300	5.74775200	0.34270500
H	5.98620600	3.61935300	0.31143300
B	6.54719500	0.97200900	0.27260400
O	7.15742300	-0.26472300	0.25361000
C	8.58990200	-0.06630800	0.11749600
C	8.77137400	1.40686500	0.64514500
O	7.46698900	1.99232800	0.37012900
C	9.83086100	2.23089600	-0.07559100
H	9.85398600	3.23945400	0.34113100
H	10.8219550	1.78977700	0.05598500
H	9.62345000	2.31158200	-1.14133200
C	8.98184600	1.48928300	2.15918000
H	8.90168100	2.53200000	2.47012300
H	8.22502500	0.91731600	2.69775400
H	9.96793900	1.12021600	2.44762400
C	8.92312000	-0.22442400	-1.36854100
H	9.99689900	-0.14630600	-1.54959800
H	8.59037900	-1.20891400	-1.70107400
H	8.41272900	0.52584600	-1.97417700
C	9.30629100	-1.13816900	0.92988900
H	10.3875580	-0.98076900	0.91429500
H	8.97021800	-1.15056800	1.96545100
H	9.10263500	-2.11946700	0.49767300
H	4.81990100	-1.01039800	0.11104600

H 2.38529100 -1.07782800 0.02798900
C -0.22580600 -0.58534500 1.38604400
H -0.90026300 -1.44331300 1.32044600
H 0.70699400 -0.91920900 1.84258700
H -0.68050900 0.15899900 2.04219600
H -0.94623100 0.33289100 -0.42845700
H 0.42856500 -0.73632700 -0.68568900



Ref. Letter: T
RB3LYP energy: -3037.16582354
Volume: 143.922 cm**3/mol
NPA at C3: -0.09651

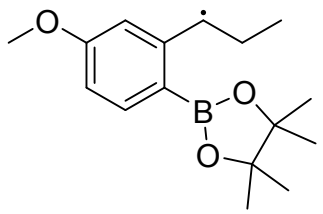
C 0.00000000 0.00000000 0.00000000
C 0.78368900 -1.26721000 0.14052500
C 0.36390800 -2.46697900 -0.26675900
C 1.11511100 -3.72581200 -0.15797800
C 0.48096100 -4.96825800 -0.07508300
C 1.20667300 -6.15098200 0.02534600
C 2.58788000 -6.12217000 0.04297800
C 3.25424800 -4.89622900 -0.04505600
C 2.52297500 -3.72072100 -0.15142600
H 3.02683500 -2.77182900 -0.26087600
O 4.61618500 -4.96166700 -0.03514300
C 5.35388300 -3.75093600 -0.11862100
H 6.40231500 -4.03842800 -0.08025800
H 5.15642300 -3.22713100 -1.05884200
H 5.12837200 -3.08867900 0.72278000
H 3.16535900 -7.03474200 0.11485200
H 0.68582900 -7.09649300 0.09313200
Br -1.43929000 -5.11411100 -0.05905500
H -0.62723300 -2.54633800 -0.70085600
H 1.75175400 -1.17633400 0.62786100
H 0.54829800 0.73715500 -0.59633900
H -0.96470100 -0.17483900 -0.47918800
H -0.18049000 0.46124200 0.97645400



Ref. Letter: T
RB3LYP energy: -3449.2106232

C	0.00000000	0.00000000	0.00000000
O	0.42611300	1.34827400	0.14410900
C	1.76109400	1.61264300	0.12097900
C	2.75839200	0.64683200	-0.01511500
C	4.08473400	1.05399700	-0.03169100
C	4.47397500	2.39625800	0.08763700
C	3.44454100	3.35917200	0.22811000
C	2.11492300	2.95519800	0.24041700
H	1.31587800	3.68138900	0.31633900
C	3.75804000	4.82261200	0.39664800
C	3.12021500	5.48362900	1.61344400
H	2.03143500	5.46094700	1.52996600
C	3.59969700	6.90766500	1.88807600
H	4.68665400	6.94287200	1.99957600
H	3.32340000	7.58307500	1.07746200
H	3.15691000	7.28771300	2.81139700
H	3.37446600	4.84333000	2.46733700
H	4.82694200	4.98952600	0.39231000
Br	3.19953100	5.81014800	-1.29743200
B	6.00614200	2.66966400	0.04402100
O	6.90526900	1.64667300	-0.14782600
C	8.21769800	2.22903200	-0.37932000
C	8.06982900	3.65545000	0.27373000
O	6.63175200	3.88597800	0.18400000
C	8.78364600	4.78289400	-0.46047200
H	8.60160000	5.72775000	0.05436400
H	9.86259400	4.61097200	-0.47747400
H	8.42958000	4.88464800	-1.48472000
C	8.42783400	3.68594100	1.76161100
H	8.12278300	4.64665100	2.17920500
H	7.91255200	2.89801300	2.31290400
H	9.50241500	3.57215400	1.91620600
C	8.42049900	2.27057900	-1.89641300
H	9.41109200	2.64684100	-2.15875200
H	8.32284100	1.25831700	-2.29149900
H	7.67083200	2.89588100	-2.38326400

C 9.26587100 1.32905100 0.26281400
H 10.2633880 1.76431400 0.16582000
H 9.06049800 1.15861600 1.31833000
H 9.27100800 0.36080400 -0.24058600
H 4.85572400 0.30146800 -0.14387500
H 2.51820700 -0.40248700 -0.11330500
H 0.37743200 -0.62659500 0.81345000
H -1.08674600 0.02640200 0.03970100
H 0.31794800 -0.41671400 -0.96013100



Ref. Letter: T
UB3LYP energy: -875.021764880

C 0.00000000 0.00000000 0.00000000
O 0.60668500 1.28323000 -0.04216400
C 1.96960000 1.35874000 -0.06015500
C 2.81865400 0.24829700 -0.04788200
C 4.19669700 0.45989200 -0.06731100
C 4.77883000 1.72554200 -0.09260700
C 3.89921500 2.86907700 -0.11155700
C 2.50268500 2.63937800 -0.09467800
H 1.80866400 3.46899800 -0.10801200
C 4.39452400 4.19255000 -0.15493200
C 3.54258800 5.42202900 -0.19368500
H 2.86299100 5.38125200 -1.05636100
C 4.35755100 6.71625400 -0.25364700
H 5.00783700 6.81188600 0.61950600
H 4.99152700 6.74000000 -1.14358600
H 3.70602200 7.59226800 -0.28339000
H 2.88146000 5.44975800 0.68398100
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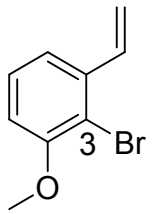

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Volume: 130.751 cm**3/mol
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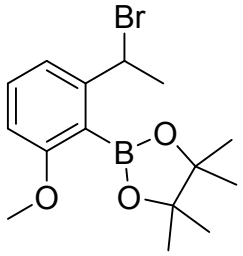

Ref. Letter: U
RB3LYP energy: -3409.8801241

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H 2.16630300 1.61396000 -0.23960500
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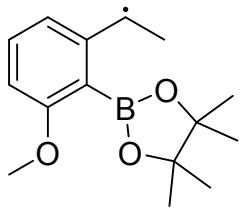

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UB3LYP energy: -835.690121648

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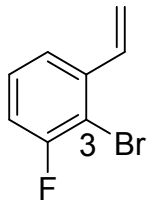

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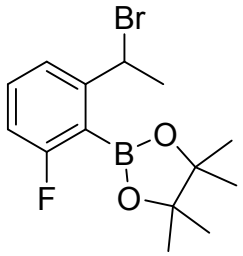

Ref. Letter: V
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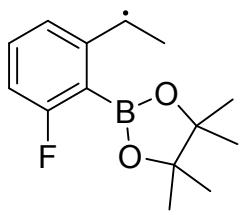

Ref. Letter: V
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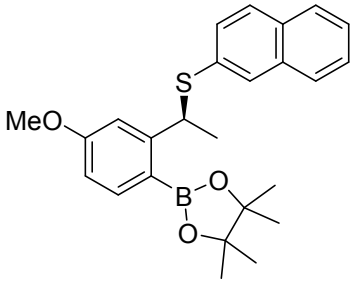
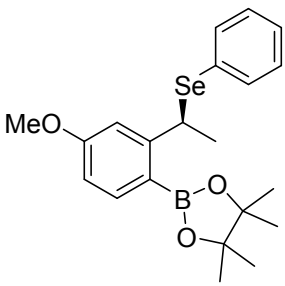
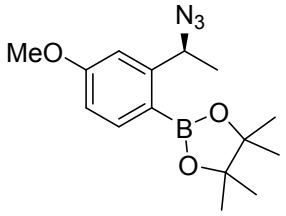
VI. Halogen Recycling



Compound 6. A solution of crude migration product **2** (21.7 mg, 0.06125 mmol, 1.0 equiv) in 300 μL DMF was treated with 2-naphthalenethiol (15.3 mg, 0.096 mmol, 1.57 equiv) and K_2CO_3 (22.0 mg, 0.159 mmol, 2.60 equiv). The yellow mixture was stirred at rt until judged complete by TLC (generally 1 h). The reaction was quenched by the addition of EtOAc (10 mL) and water (10 mL), the layers partitioned and the aqueous layer extracted with EtOAc (3x 10 mL). The organic layers were combined, washed with brine (10 mL), dried over Na_2SO_4 and concentrated *in vacuo*. The residue was purified by column chromatography (0 – 75% gradient, CH_2Cl_2/hexanes, 15% increments) and isolated as a clear oil (22.8 mg, 85%). ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.71 (m, 5H), 7.42 (m, 3H), 7.14 (d, *J* = 2.5 Hz, 1H), 6.74 (dd, *J* = 8.3, 2.5 Hz, 1H), 5.61 (q, *J* = 6.9 Hz, 1H), 3.78 (s, 3H), 1.62 (d, *J* = 6.9 Hz, 1H), 1.31 (s, 12H). ^{13}C NMR (75 MHz, $CDCl_3$) δ 162.43, 152.26, 138.20, 134.06, 133.90, 132.17, 129.24, 129.04, 128.06, 127.82, 127.41, 126.43, 125.79, 112.45, 111.97, 83.65, 55.30, 44.42, 25.10, 25.08, 22.97. HRMS (EI) *m/z* calculated for $C_{25}H_{30}BO_3S$ $[M+H]^+$ calculated 420.2040, found 420.2050.

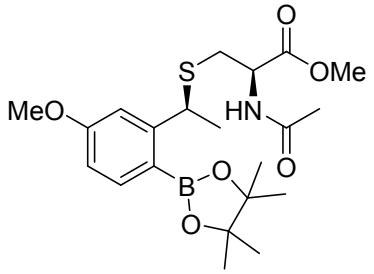


Compound 7. Compound **7** was prepared from compound **1** in the same fashion as Compound **5b.** The product was isolated in 70% yield and 83% *ee* in one pot and over two steps. $[\alpha]_D^{24}$ -0.199 (c = 0.075 g/mL, CH_2Cl_2, *l* = 4.5 cm)



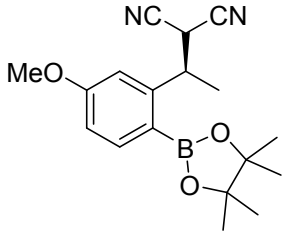
Compound 8. In a glovebox, a dry 25 mL round bottom flask was charged with CuCl (10 mg, 0.101 mmol, 10%), NaOtBu (20 mg, 0.208 mmol, 20%), (*S,S*)-Ph-BPE (51 mg, 0.101, 10%) and dry, degassed toluene (10 mL). The flask was equipped with a septum and removed from the glovebox and the reaction was allowed to stir for 10 min. HBpin (0.18 mL, 1.24 mmol, 1.20 equiv) was added in one aliquot and the reaction was transferred to a cryo-bath set to 0 ^oC and stirred for a further 10 min and then 2-bromo-5-methoxystyrene (0.16 mL, 1.03 mmol, 1.0 equiv) was added. The reaction was allowed to stir for 18 hours at 0 ^oC. The reaction was filtered through a pad of celite and washed with Et_2O (2x10 mL). The solvent was removed *in vacuo*. The crude material was dissolved in 2 mL dry DMSO and then NaN_3 (0.1997 g; 3.07 mmol, 2.98 equiv) was added and the reaction was allowed to stir at 40 ^oC for 1 hour. The reaction was poured into water and diethyl ether and then filtered through a pad of silica. The organic layer was then dried with Na_2SO_4 and concentrated *in vacuo.* The residue was purified by column chromatography using hexanes/CH_2Cl_2 as the eluent. A gradient was employed using 0-50% in 10% increments. Compound **8** was isolated in 47% yield and 85% *ee*. $[\alpha]_D^{24}$ -0.955 (c = 0.060 g/mL, CH_2Cl_2, *l* = 4.5 cm) ^1H NMR (500 MHz, $CDCl_3$) δ 7.79 (d, *J* = 8.4 Hz, 1H), 7.02 (d, *J* = 2.5 Hz, 1H), 6.81 (dd, *J* = 8.3, 2.5 Hz, 1H), 5.56 (q, *J* = 6.7 Hz, 1H), 3.84 (s, 3H), 1.47 (d, *J* = 6.7 Hz, 3H), 1.34 (s, 6H), 1.33 (s, 6H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 162.36, 150.09,

138.20, 112.27, 111.03, 83.57, 58.88, 55.17, 24.89, 24.78, 22.44. HRMS (ESI) *m/z* calculated for $C_{15}H_{26}BN_4O_3$ $[M+NH_4]^+$ 320.2129, found 320.2117.



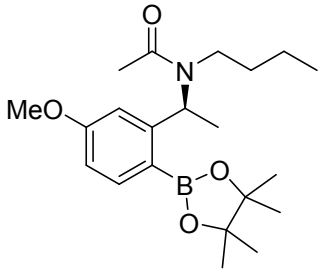
Compound 9. In a glovebox, A dry 25 ml round bottom flask was charged with (10 mg, 0.101 mmol, 10%), NaOtBu (20 mg, 0.208 mmol, 20%), (*S,S*)-Ph-BPE (51 mg, 0.101, 10%) and dry, degassed toluene (10 mL). The flask was fitted with a septum, removed from the glovebox and mixture was allowed to stir for 10 min. HBpin (0.18 mL, 1.24 mmol, 1.20 equiv) was added in one aliquot and the reaction was transferred to a cryo-bath set to 0 °C and stirred for a further 10 min and then 2-bromo-5-methoxystyrene (0.16 mL, 1.03 mmol, 1.0 equiv) was added. The reaction was allowed to stir for 18 hours at 0 °C. The reaction was filtered through a pad of celite and washed with Et_2O (2x10 mL). The solvent was removed *in vacuo*. The crude material was dissolved in 5 mL dry DMSO and then *N*-acetyl cysteine methyl ester (0.2383 g; 1.34 mmol, 1.30 equiv) and K_2CO_3 (0.3328 g, 2.41 mmol, 2.34 equiv) was added and the reaction was allowed to stir at 40 °C for 3 hours. The reaction was poured into water and diethyl ether. The organic layer was washed once with water and then dried with Na_2SO_4 and concentrated *in vacuo.* The residue was purified by column chromatography using hexanes/EtOAc as the eluent. A gradient was employed using 10-50% in 10% increments. Compound **9** was isolated in 46% yield, >99% *ee*, and 95:5 d.r. $[\alpha]_D^{24}$ -1.363 (c = 0.062 g/mL, CH_2Cl_2, *l* = 4.5 cm) ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.72 (d, *J* = 8.3 Hz, 1H), 7.10 (d, *J* = 2.5 Hz, 1H), 6.76 (dd, *J* = 8.3, 2.5 Hz, 1H), 6.11 (d, *J* = 7.5 Hz, 1H), 4.96 (q, *J* = 7.0 Hz, 1H), 4.71 (td, *J* = 7.1, 4.3 Hz, 1H), 3.83 (s, 3H), 3.64 (s, 3H), 2.83 (dd, *J* = 13.3, 4.3 Hz, 1H), 2.70 (dd, *J* = 13.3, 6.7 Hz, 1H), 1.98 (s, 3H), 1.50 (d, *J* = 7.0 Hz, 3H), 1.35 (s, 6H), 1.34 (s, 6H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 171.30, 169.80, 162.20,

152.38, 137.66, 112.32, 111.63, 83.62, 55.10, 52.39, 51.58, 41.50, 32.71, 24.92, 24.72, 23.03, 22.95. HRMS (EI) *m/z* calculated for $C_{21}H_{33}BNO_6S$ $[M+H]^+$ 437.2153, found 437.2153.



Compound 10. In a glovebox, a dry 25 mL round bottom flask was charged with CuCl (10 mg, 0.101 mmol, 10%), NaOtBu (20 mg, 0.208 mmol, 20%), (*S,S*)-Ph-BPE (51 mg, 0.101, 10%) and dry, degassed toluene (10 mL). The flask was equipped with a septum and removed from the glovebox and the reaction was allowed to stir for 10 min. HBpin (0.18 mL, 1.24 mmol, 1.20 equiv) was added in one aliquot and the reaction was transferred to a cryo-bath set to 0 °C and stirred for a further 10 min and then 2-bromo-5-methoxystyrene (0.16 mL, 1.03 mmol, 1.0 equiv) was added. The reaction was allowed to stir for 18 hours at 0 °C and then allowed to warm to ambient temperature. A solution of lithium malononitrile was prepared by treating diisopropylamine (0.42 mL, 3.00 mmol, 2.91 equiv) with nBuLi (1.2 mL of a 2.5 M solution, 3.00 mmol, 2.91 equiv) in 12 mL of dry THF. The lithium diisopropylamide was allowed to stir at 0 °C for 15 min and then malononitrile (0.19 ml, 3.02 mmol, 2.93 equiv) was added. The solution was allowed to stir for a further 15 min at 0 °C and then it added to the reaction flask. The reaction was allowed to stir for 18 hours at ambient temperature. The reaction was filtered through a pad of celite and washed with Et_2O (2x10 mL). The solvent was removed *in vacuo*. The residue was purified by column chromatography using hexanes/EtOAc as the eluent. A gradient was employed using 0-10% in 2% increments. Compound **10** was isolated in 46% yield and 80% *ee*. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.83 (d, J = 8.3 Hz, 1H), 6.96 (d, J = 2.4 Hz, 1H), 6.84 (dd, J = 8.4, 2.4 Hz, 1H), 4.27 (qd, J = 7.1, 4.1 Hz, 1H), 4.20 (d, J = 4.2 Hz, 1H), 1.65 (d, J = 7.1 Hz, 3H), 1.36 (s, 6H), 1.36 (s, 6H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 162.44, 146.94, 139.10, 112.98,

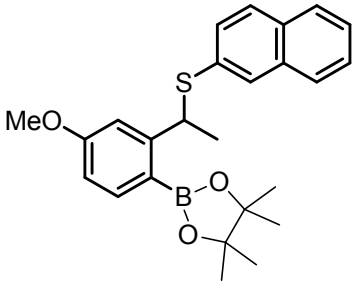
112.93, 112.22, 111.71, 84.06, 55.23, 38.41, 31.63, 24.95, 24.79, 15.53. HRMS (EI) *m/z* calculated for $C_{18}H_{27}BN_3O_3$ $[M+NH_4]^+$ 343.2177, found 343.2165.



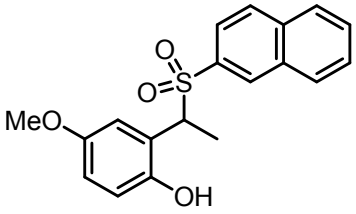
Compound 11. In a glovebox, A dry 25 ml round bottom flask was charged with (5 mg, 0.0506 mmol, 10%), NaOtBu (10 mg, 0.104 mmol, 20%), (*S,S*)-Ph-BPE (26 mg, 0.0513, 10%) and dry, degassed toluene (5 mL). The flask was fitted with a septum, removed from the glovebox and mixture was allowed to stir for 10 min. HBpin (0.10 mL, 0.689 mmol, 1.34 equiv) was added in one aliquot and the reaction was transferred to a cryo-bath set to 0 ^oC and stirred for a further 10 min and then 2-bromo-5-methoxystyrene (0.08 mL, 0.514 mmol, 1.0 equiv) was added. The reaction was allowed to stir for 18 hours at 0 ^oC. The reaction was filtered through a pad of celite and washed with Et_2O (2x10 mL). The solvent was removed *in vacuo*. The crude material was dissolved in 2.5 mL dry DMF and then *n*-butylamine (0.15 mL, 1.52 mmol, 2.96 equiv) and K_2CO_3 (0.3249 g, 2.35 mmol, 4.55 equiv) was added and the reaction was allowed to stir for 1 hour. Then, acetic anhydride (0.24 mL, 2.54 mmol, 4.94 equiv) was added and the reaction was allowed to stir for another hour. The reaction was poured into water and diethyl ether. The organic layer was washed once with water and then dried with Na_2SO_4 and concentrated *in vacuo.* The residue was purified by column chromatography using hexanes/EtOAc as the eluent. A gradient was employed using 10-50% in 10% increments. Compound **11** was isolated as a mixture of rotamers in a 3:1 ratio in 46% yield and 85% *ee*. $[\alpha]_D^{24}$ -0.114 (c = 0.036 g/mL, CH_2Cl_2, *l* = 4.5 cm) ^1H NMR (500 MHz, $CDCl_3$) δ 7.83 (d, *J* = 8.2 Hz, 1H), 6.85 (d, *J* = 2.4 Hz, 1H), 6.79 (dd, *J* = 8.3, 2.5 Hz, 1H), 5.67 (q, *J* = 6.9 Hz, 1H), 3.83 (s, 3H), 3.36 (ddd, *J* = 13.3, 10.9, 5.0 Hz, 1H), 3.12 (ddd, *J* = 13.2, 10.7, 5.2 Hz, 1H), 2.16 (s, 3H), 1.65 (broad s, 2H), 1.53 (d, *J* =

6.7 Hz, 3H), 1.32 (d, J = 1.3 Hz, 12H), 1.16 (hex, J = 7.2 Hz, 2H), 0.77 (t, J = 7.3 Hz, 3H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 171.69, 162.25, 150.55, 138.75, 112.69, 110.78, 83.56, 75.03, 55.16, 55.05, 43.09, 31.55, 24.87, 24.86, 24.75, 24.71, 24.68, 22.35, 20.39, 20.37, 13.69. HRMS (EI) *m/z* calculated for $C_{21}H_{35}BNO_4$ $[M+H]^+$ 375.2690, found 375.2694.

VII. Determination of absolute stereochemistry *via* X-ray diffraction.



Sulfide precursor of Compound 6. A solution of crude migration product **2** (21.7 mg, 0.061 mmol, 1.0 equiv) in 300 μL DMF was treated with 2-naphthalenethiol (15.3 mg, 0.096 mmol, 1.6 equiv) and K_2CO_3 (22.0 mg, 0.159 mmol, 2.6 equiv). The yellow mixture was stirred at rt until judged complete by TLC (generally 1 h). The reaction was quenched by the addition of EtOAc (10 mL) and water (10 mL), the layers partitioned and the aqueous layer extracted with EtOAc (3x 10 mL). The organic layers were combined, washed with brine (10 mL), dried over Na_2SO_4 and concentrated *in vacuo*. The residue was purified by column chromatography (0 – 75% gradient, CH_2Cl_2/hexanes, 15% increments) and isolated as a clear oil (22.8 mg, 85%). ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.71 (m, 5H), 7.42 (m, 3H), 7.14 (d, J = 2.5 Hz, 1H), 6.74 (dd, J = 8.3, 2.5 Hz, 1H), 5.61 (q, J = 6.9 Hz, 1H), 3.78 (s, 3H), 1.62 (d, J = 6.9 Hz, 1H), 1.31 (s, 12H). ^{13}C NMR (75 MHz, $CDCl_3$) δ 162.43, 152.26, 138.20, 134.06, 133.90, 132.17, 129.24, 129.04, 128.06, 127.82, 127.41, 126.43, 125.79, 112.45, 111.97, 83.65, 55.30, 44.42, 25.10, 25.08, 22.97. HRMS (EI) *m/z* calculated for $C_{25}H_{30}BO_3S$ $[M+H]^+$ calculated 420.2040, found 420.2050.



Compound 12. A stirred solution of the sulfide synthesized above (22.8 mg, 0.052 mmol, 1.0 equiv) in CH_2Cl_2 (0.65 mL) at 0 °C was treated with *m*CPBA (44.0 mg, 0.255 mmol, 4.9 equiv). The reaction mixture was stirred at 0 °C until complete as judged by TLC (generally 1-1.5 h), then quenched with saturated sodium thiosulfate (2 mL) and saturated sodium bicarbonate (2 mL). The biphasic mixture was separated and the aqueous layers extracted with CH_2Cl_2 (3 x 10 mL). The combined organics were dried over Na_2SO_4 and concentrated *in vacuo*. The residue was purified by column chromatography (0-50% EtOAc/hexane gradient, 10% increments) and isolated as a white solid (16 mg, 90%). ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.26 (d, *J* = 1.7 Hz, 1H), 7.89 (m, 3H), 7.62 (m, 3H), 6.86 (d, *J* = 8.8 Hz, 1H), 6.76 (dd, *J* = 8.8, 3.0 Hz, 1H), 6.45 (d, *J* = 3.0 Hz, 1H), 6.40 (s, 1H), 4.82 (q, *J* = 7.2 Hz, 1H), 3.56 (s, 3H), 1.69 (d, *J* = 7.2 Hz, 3H). ^{13}C NMR (75 MHz, $CDCl_3$) δ 154.33, 149.11, 135.58, 133.06, 132.10, 131.55, 129.64, 126.92, 129.04, 128.14, 127.85, 123.98, 122.31, 119.79, 115.98, 114.72, 55.92, 13.86. HRMS (ESI) *m/z* calculated for $C_{19}H_{22}O_4N$ $[M+NH_4]^+$ calculated 360.1265, found 360.1269.

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Structure Report 2014
X-RAY
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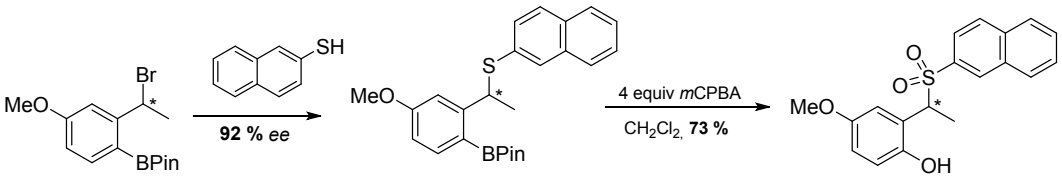
XI. Crystallographic Experimental Section

CCDC-no. 985120

Crystal Structure of Compound 12



12

Preparation of Crystals of 12. A sample consisting of 16.0 mg of the enantiopure 12 was dissolved in deuterated chloroform and crystallized at 7 °C slowly overnight. The air-stable crystals were selected using a microscope to choose the best sample for X-ray crystallography.

Data Collection: A colorless crystal with approximate dimensions 0.110 x 0.205 x 0.785 mm^3 (block) was selected under oil under ambient conditions and attached to the tip of a X-ray capillary (MiTeGenMicroMount©). The crystal was mounted in a stream of cold nitrogen at 100.0(15) K and centered in the X-ray beam by using a video camera. The crystal evaluation and data collection were performed on a three-circle Bruker Quazar SMART APEXII diffractometer with copper radiation K_α(α = 1.54184 Å) and the diffractometer to crystal distance of 4.96 cm. The initial cell constants were obtained from three series of ω scans at different starting angles. Each series consisted of 12 frames collected at intervals of 0.5° in 6° range about ω with the exposure time of 10 seconds per frame. The reflections were successfully indexed by an automated indexing routine built in the APEXII program suite. The final cell constants were calculated from a set of 9893 strong from the actual data collection.

The data were collected by using the full sphere data collection routine to survey the reciprocal space to the extent of a full sphere to a high-resolution of 1.54 Å. A total of 25291 reflection data were harvested by collecting 6 sets of frames with 0.6° scans in ω and φ with exposure times of 5/10 sec per frame. These highly redundant datasets were corrected for Lorentz and polarization effects. The absorption correction was based on fitting a function to the empirical transmission surface as sampled by multiple equivalent measurements. [5,6]

Structure Solution and Refinement: The systematic absences in the diffraction data were consistent for the orthorhomic space groups $P2_12_12_1$. The E-statistics strongly suggested the chiral space group that yielded chemically reasonable and computationally stable results of refinement. [7,8] The systematic absences in the diffraction data were uniquely consistent for the space group $P2_12_12_1$. A successful solution by the direct methods by using SHELX-2013 provided most non-hydrogen atoms from the E-map. Using Olex2, all non-hydrogen atoms were refined with anisotropic displacement coefficients. All hydrogen atoms were included in the structure factor calculation at idealized positions and were allowed to ride on the neighboring atoms with relative isotropic displacement coefficients.

Table 1. Crystal data collection and structure solution refinement for compound 12 [Schomaker34]

Parameter	Compound 12	Parameter	Compound 12
empiric formula	$C_{19}H_{37}O_4S$	$\rho_{calc.}$ [g · cm^{-1}]	1.27
MW [g · mol^{-1}]	342.41	crystal size [mm]	0.158 x 0.437 x 0.437
X-ray lab code	Schomaker34	T [K]	100.0(15)
a [Å]	5.5066(1)	radiation type / λ [nm]	Mo K_α / 0.71072
b [Å]	14.1867(2)	μ [mm^{-1}]	0.227
c [Å]	20.9510(4)	F(000)	945.3
α [°]	90.000(0)°	Reflections collected	25180
β [°]	90.000(0)	Independent reflections	3198 [R_{int} = 0.0534]
γ [°]	90.000(0)°	Data/restraints/parameters	3198/0/221
V [Å^3]	1633(2)	GooF on F^2	0.446
Z	4	Largest diff. peak/hole [eÅ^{-3}]	0.49 / -0.27
crystal system	orthorhombic	Flack *x* parameter	0.0143(160)
crystal color	colorless	Final R_1[a]/ wR_2[b] all data	0.0282/ 0.0757
space group	$P2_12_12_1$	Final R_1[a]/ wR_2[b] I>2s(I)	0.0278/ 0.0731

[a] $R_1 = \sum | F_o | - | F_c | / | F_o |$;[b] $wR_2 = [\sum\{w(F_o^2 - F_o^2)^2\} / \sum\{w(F_o^2)^2\}]^{1/2}$

The final least-squares refinement of 221 parameters against 3198 data resulted in R = 0.0278 (based on F^2 for I>2s) and wR2 = 0.0757 (based on F^2 for all data), respectively. The final structure was visualized using Interactive Molecular Graphics. [9]

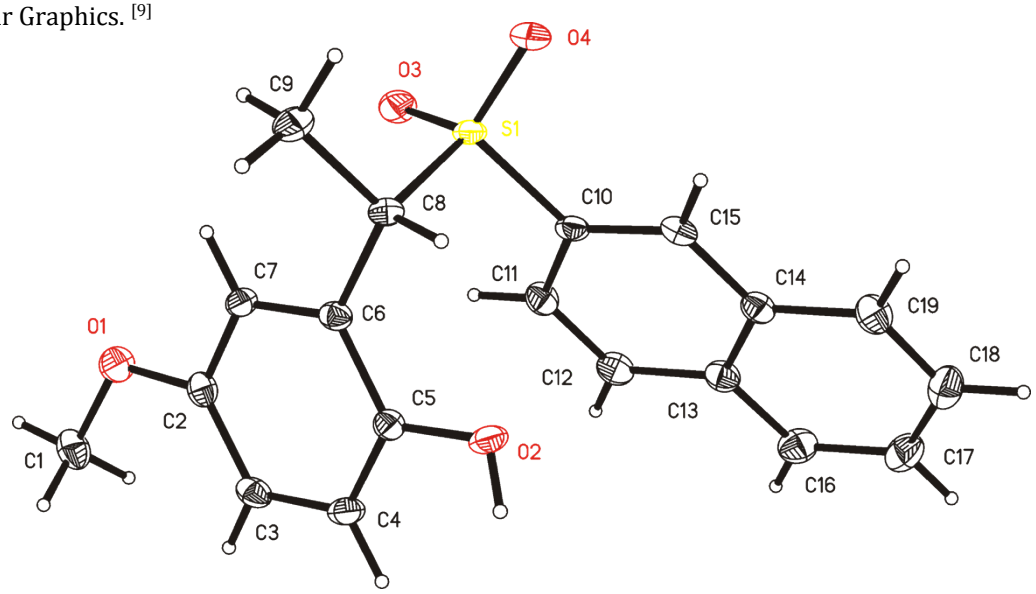


Figure 1. Thermal-ellipsoid of compound 12 [Schomaker34] are set with 50 % probability.

Table 2. Fractional Atomic Coordinates (×10^4) and Equivalent Isotropic Displacement Parameters (Å^2×10^3) for compound 12 [Schomaker34]. U_{eq} is defined as 1/3 of of the trace of the orthogonalised U_{IJ} tensor.

Atom	*x*	*y*	*z*	U(eq)
C2	4283(3)	3034.9(11)	6049.8(7)	15.9(3)
C3	4794(3)	3957.7(10)	6233.7(7)	16.7(3)
C4	6733(3)	4130.6(10)	6643.7(7)	17.5(3)
C5	8168(3)	3398(1)	6869.9(7)	14.5(3)
C6	7643(3)	2470.2(9)	6691.2(6)	13.6(3)
C7	5694(3)	2303.8(10)	6281.8(7)	14.6(3)
C9	9702(3)	865.0(11)	6493.6(7)	19.3(3)
C8	9100(3)	1662.3(10)	6962.5(7)	13.6(3)
C10	7036(3)	2093.9(10)	8169.9(7)	14.3(3)
C11	5054(3)	2721.2(11)	8095.7(7)	16.9(3)
C12	4828(3)	3456.9(11)	8511.3(7)	19.0(3)
C13	6512(3)	3595.2(10)	9015.2(7)	17.3(3)
C14	8497(3)	2958.7(10)	9081.1(7)	15.9(3)
C15	8724(3)	2202.4(10)	8643.9(7)	15.4(3)
C16	6280(3)	4344.4(11)	9459.0(8)	22.1(3)
C17	7943(3)	4457.6(12)	9941.1(8)	24.3(4)
C18	9918(3)	3826.5(13)	10002.5(8)	24.2(3)
C19	10190(3)	3095.4(11)	9584.6(7)	20.0(3)
C1	1058(3)	3517.7(12)	5365.1(8)	22.9(3)
O1	2409(2)	2777.5(7)	5652.9(5)	20.7(2)
O2	10082(2)	3546.1(8)	7277.0(5)	18.8(2)
O3	5010(2)	885.1(7)	7391.3(5)	19.7(2)
O4	8886(2)	446.8(7)	7919.9(5)	20.0(2)
S1	7383.6(6)	1159.9(2)	7617.45(16)	14.0(1)

Table 3. Anisotropic Displacement Parameters ($Å^2 \times 10^3$) for compound 12 [Schomaker34]. The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+...+2hka\times b\times U_{12}]$

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
C2	15.7(7)	19.1(7)	12.9(6)	0.5(5)	2.1(6)	0.6(6)
C3	18.8(7)	14.0(7)	17.4(6)	3.2(6)	2.7(6)	5.2(6)
C4	22.6(7)	10.7(6)	19.1(7)	-0.1(6)	3.6(6)	-1.4(6)
C5	16.6(7)	13.9(6)	13.0(6)	0.8(5)	1.7(5)	-1.6(6)
C6	14.9(7)	11.9(6)	13.9(6)	1.2(5)	3.1(6)	0.6(6)
C7	17.4(7)	11.5(6)	15.0(6)	-1.3(6)	0.8(6)	-0.8(5)
C9	21.5(8)	14.2(7)	22.2(7)	-3.6(6)	1.2(6)	3.3(6)
C8	13.3(6)	10.4(6)	16.9(6)	0.7(6)	0.9(5)	-1.4(5)
C10	17.3(7)	10.0(6)	15.6(6)	2.7(5)	2.1(5)	-1.7(5)
C11	13.9(7)	18.5(7)	18.2(7)	2.3(6)	-1.4(6)	1.2(6)
C12	16.4(7)	17.9(7)	22.8(7)	2.5(6)	0.2(6)	4.7(6)
C13	17.8(7)	16.8(7)	17.2(7)	2.6(6)	2.9(6)	0.2(6)
C14	15.5(7)	16.1(7)	16.1(7)	3.8(6)	1.2(6)	-0.7(6)
C15	15.2(7)	13.4(7)	17.5(7)	4.4(6)	1.5(6)	2.4(6)
C16	21.2(8)	18.2(8)	26.7(8)	-2.2(6)	1.0(7)	2.9(7)
C17	28.2(9)	21.2(7)	23.6(8)	-6.9(6)	1.5(7)	-1.2(7)
C18	22.7(8)	28.1(8)	21.8(7)	-3.0(7)	-2.7(6)	-4.3(7)
C19	17.0(7)	22.9(8)	20.2(7)	1.7(6)	-0.6(6)	2.9(7)
C1	22.6(8)	27.2(8)	18.8(7)	3.6(6)	-3.7(6)	4.3(7)
O1	19.9(5)	20.0(5)	22.1(5)	0.1(4)	-6.2(5)	2.1(5)
O2	22.1(5)	10.3(5)	24.0(5)	0.0(4)	-5.3(5)	-3.5(4)
O3	19.2(5)	16.7(5)	23.2(5)	2.2(4)	-2.2(5)	-6.6(4)
O4	25.6(6)	11.0(5)	23.4(6)	2.2(4)	-2.3(5)	2.8(4)

S1	16.59(17)	8.40(16)	17.01(17)	1.47(12)	-0.90(14)	-0.80(13)

Table 4. Bond Lengths for compound 12 [Schomaker34].

Atom	Atom	Length/Å	Atom	Atom	Length/Å
C2	C3	1.393(2)	C10	S1	1.7699(15)
C2	C7	1.384(2)	C11	C12	1.365(2)
C2	O1	1.3745(19)	C12	C13	1.419(2)
C3	C4	1.392(2)	C13	C14	1.425(2)
C4	C5	1.389(2)	C13	C16	1.418(2)
C5	C6	1.399(2)	C14	C15	1.416(2)
C5	O2	1.3719(18)	C14	C19	1.421(2)
C6	C7	1.394(2)	C16	C17	1.373(2)
C6	C8	1.5102(19)	C17	C18	1.415(3)
C9	C8	1.5345(19)	C18	C19	1.366(2)
C8	S1	1.8123(15)	C1	O1	1.4211(19)
C10	C11	1.417(2)	O3	S1	1.4439(11)
C10	C15	1.369(2)	O4	S1	1.4525(11)

Table 5. Bond Angles for compound 12 [Schomaker34].

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
C7	C2	C3	119.57(14)	C11	C12	C13	121.37(14)
O1	C2	C3	124.64(14)	C12	C13	C14	119.08(14)
O1	C2	C7	115.78(13)	C16	C13	C12	122.18(15)
C4	C3	C2	119.40(14)	C16	C13	C14	118.74(14)
C5	C4	C3	121.00(14)	C15	C14	C13	119.02(14)
C4	C5	C6	119.69(14)	C15	C14	C19	121.73(14)
O2	C5	C4	122.31(13)	C19	C14	C13	119.25(14)
O2	C5	C6	117.99(13)	C10	C15	C14	119.64(13)
C5	C6	C8	120.24(13)	C17	C16	C13	120.66(15)
C7	C6	C5	118.89(13)	C16	C17	C18	120.39(15)
C7	C6	C8	120.81(13)	C19	C18	C17	120.43(15)
C2	C7	C6	121.43(13)	C18	C19	C14	120.53(15)
C6	C8	C9	115.67(12)	C2	O1	C1	116.96(12)
C6	C8	S1	107.83(10)	C10	S1	C8	104.90(6)
C9	C8	S1	107.91(10)	O3	S1	C8	109.26(7)
C11	C10	S1	118.81(11)	O3	S1	C10	108.60(7)
C15	C10	C11	122.14(14)	O3	S1	O4	118.08(7)
C15	C10	S1	119.02(11)	O4	S1	C8	107.89(7)
C12	C11	C10	118.74(14)	O4	S1	C10	107.32(7)

Table 6. Torsion Angles compound 12 [Schomaker34].

A	B	C	D	Angle/°	A	B	C	D	Angle/°
C2	C3	C4	C5	0.2(2)	C11	C12	C13	C14	0.9(2)
C3	C2	C7	C6	-0.8(2)	C11	C12	C13	C16	-178.74(15)
C3	C2	O1	C1	6.3(2)	C12	C13	C14	C15	-0.4(2)
C3	C4	C5	C6	-0.9(2)	C12	C13	C14	C19	179.93(14)
C3	C4	C5	O2	-179.63(13)	C12	C13	C16	C17	180.00(15)
C4	C5	C6	C7	0.7(2)	C13	C14	C15	C10	-0.3(2)
C4	C5	C6	C8	-176.58(13)	C13	C14	C19	C18	0.2(2)

C5	C6	C7	C2	0.1(2)	C13	C16	C17	C18	0.0(3)
C5	C6	C8	C9	-140.67(14)	C14	C13	C16	C17	0.3(2)
C5	C6	C8	S1	98.46(14)	C15	C10	C11	C12	0.0(2)
C6	C8	S1	C10	-60.13(11)	C15	C10	S1	C8	-91.77(12)
C6	C8	S1	O3	56.14(11)	C15	C10	S1	O3	151.50(11)
C6	C8	S1	O4	-174.31(9)	C15	C10	S1	O4	22.81(14)
C7	C2	C3	C4	0.6(2)	C15	C14	C19	C18	-179.50(15)
C7	C2	O1	C1	-174.85(13)	C16	C13	C14	C15	179.26(14)
C7	C6	C8	C9	42.10(19)	C16	C13	C14	C19	-0.4(2)
C7	C6	C8	S1	-78.77(15)	C16	C17	C18	C19	-0.2(3)
C9	C8	S1	C10	174.27(10)	C17	C18	C19	C14	0.2(3)
C9	C8	S1	O3	-69.47(12)	C19	C14	C15	C10	179.39(14)
C9	C8	S1	O4	60.09(11)	O1	C2	C3	C4	179.42(13)
C8	C6	C7	C2	177.39(13)	O1	C2	C7	C6	-179.70(13)
C10	C11	C12	C13	-0.7(2)	O2	C5	C6	C7	179.50(13)
C11	C10	C15	C14	0.5(2)	O2	C5	C6	C8	2.2(2)
C11	C10	S1	C8	86.46(12)	S1	C10	C11	C12	-178.16(12)
C11	C10	S1	O3	-30.27(13)	S1	C10	C15	C14	178.65(11)
C11	C10	S1	O4	-158.96(11)					

Table 7. Hydrogen Atom Coordinates ($Å \times 10^4$) and Isotropic Displacement Parameters ($Å^2 \times 10^3$) for compound 12

Atom	***x***	***y***	***z***	**U(eq)**
H20	10430(40)	4104(15)	7261(9)	17(5)
H3	3848	4454	6084	20
H4	7073	4746	6768	21
H7	5335	1688	6162	18
H9C	10630	388	6709	29
H9A	10630	1113	6144	29
H9B	8223	595	6335	29
H8	10626	1914	7132	16
H11	3929	2633	7770	20
H12	3543	3876	8463	23
H15	10012	1782	8679	18
H16	4988	4763	9423	26
H17	7770	4952	10229	29
H18	11039	3910	10330	29
H19	11492	2684	9630	24
H1A	-193	3254	5101	34
H1C	2121	3898	5109	34
H1B	335	3901	5691	34

X. References.

1) Armarego, W.L.F.; Chai, C.L.L. *Purification of Laboratory Chemicals* 6th ed., Elsevier: Burlington, MA, 2009.Still, W. C.; Kahn, M.; Mitra, A. *J. Org. Chem.* **1978**, *43*, 2923.

2) R. D. Grigg, R. Van Hoveln, J. M. Schomaker, *J. Am. Chem. Soc.* **2012**, *134,* 16131-16134.

3) Gaussian 09, Revision D.01, M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima,Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, T. Keith, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, N. Rega, J. M. Millam, M. Klene, J. E. Knox, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, O. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski, and D. J. Fox, Gaussian, Inc., Wallingford CT, 2013.

4) BRUKER-AXS. (2007-2013), APEX2 (Ver. 2013.2-0), SADABS (2012-1).

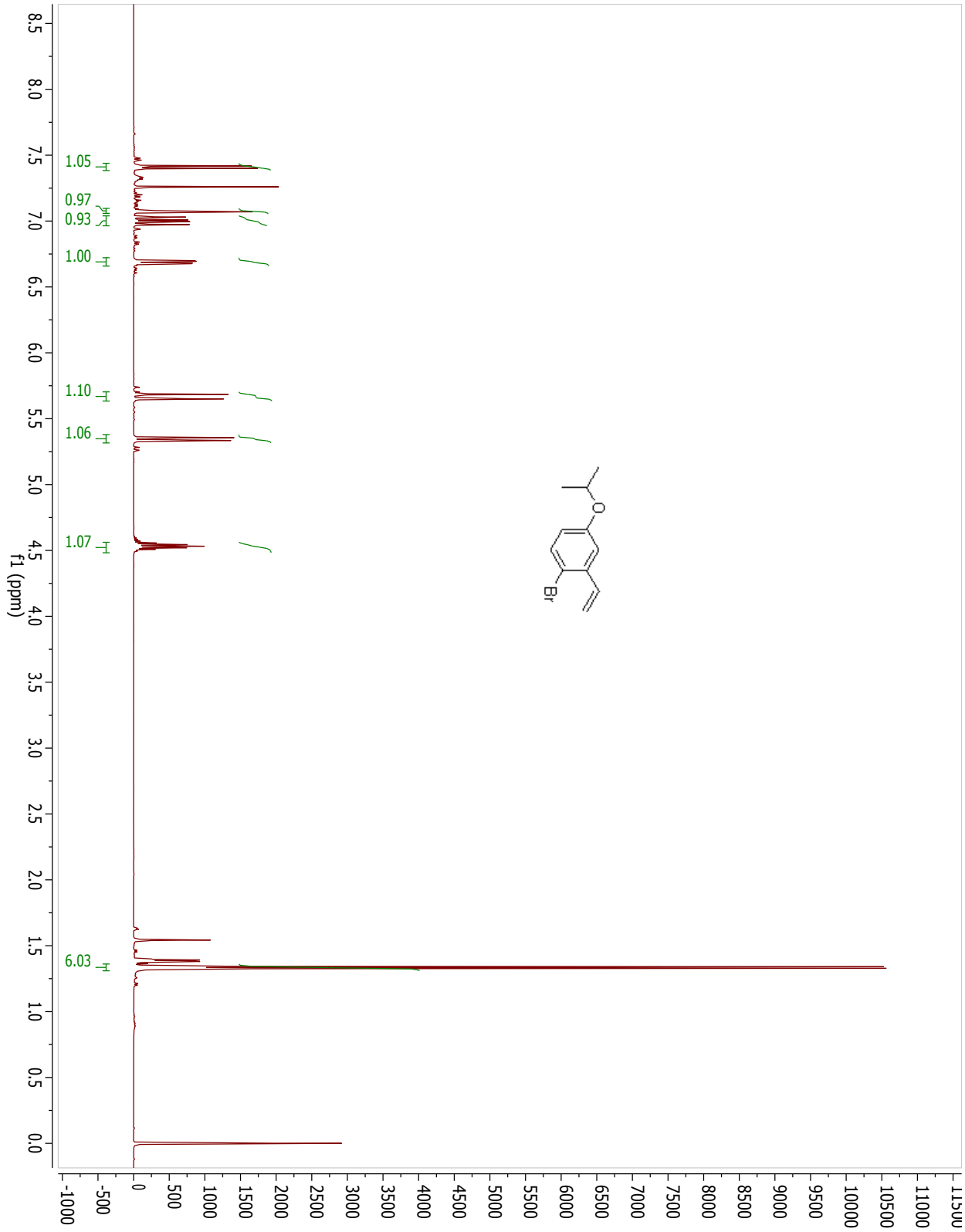
5) SAINT+ (Ver. 8.30C) Software Reference Manuals, BRUKER-AXS, Madison, Wisconsin, USA.

6) G. M. Sheldrick, *Acta Cryst.*, **2008**, *A64*, 112-122.

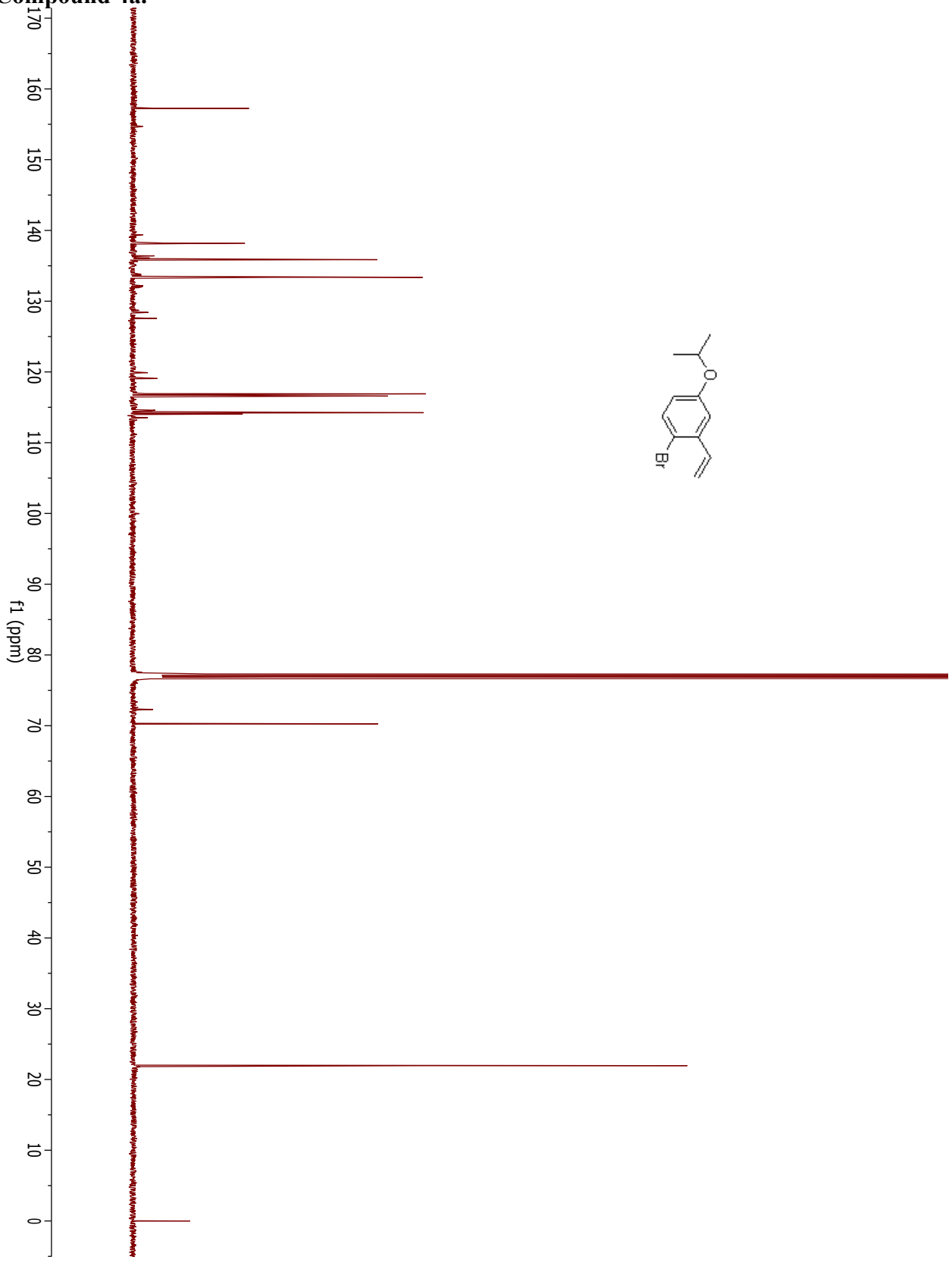
7) O. V. Dolomanov, L. J. Bourhis, R. J. Gildea, J. A. L. Howard, H. Puschmann, *J. Appl. Cryst.* **2009**, *42*, 339-341.

8) XP – X-Ray Crystal Structure Visualization BRUKER, AXS, **1998**, V5.1

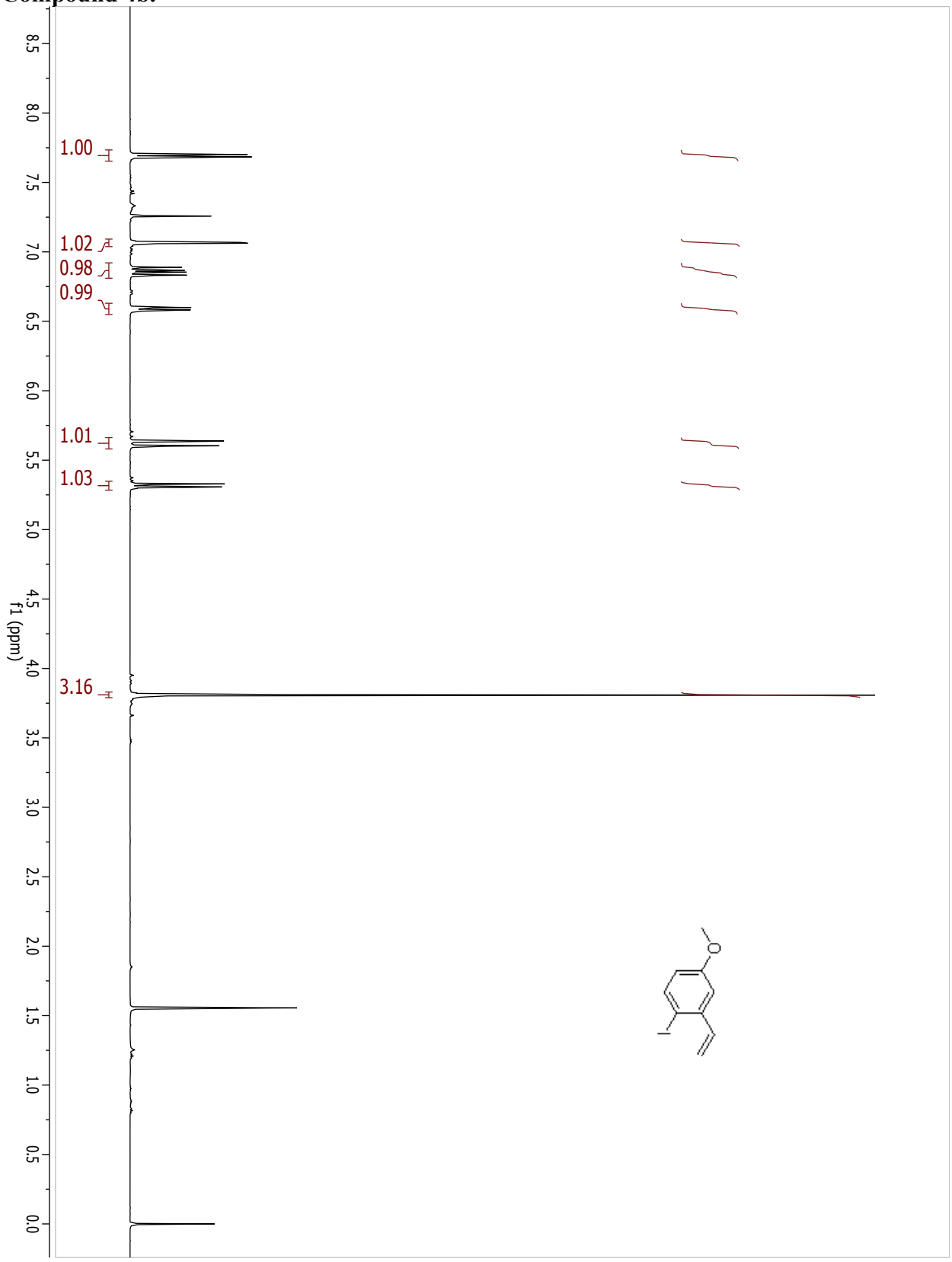
XI. NMR Spectra.
Compound 4a.



Compound 4a.


170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)
O
Br

Compound 4b.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1.01
1.03
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f1 (ppm)
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7.5
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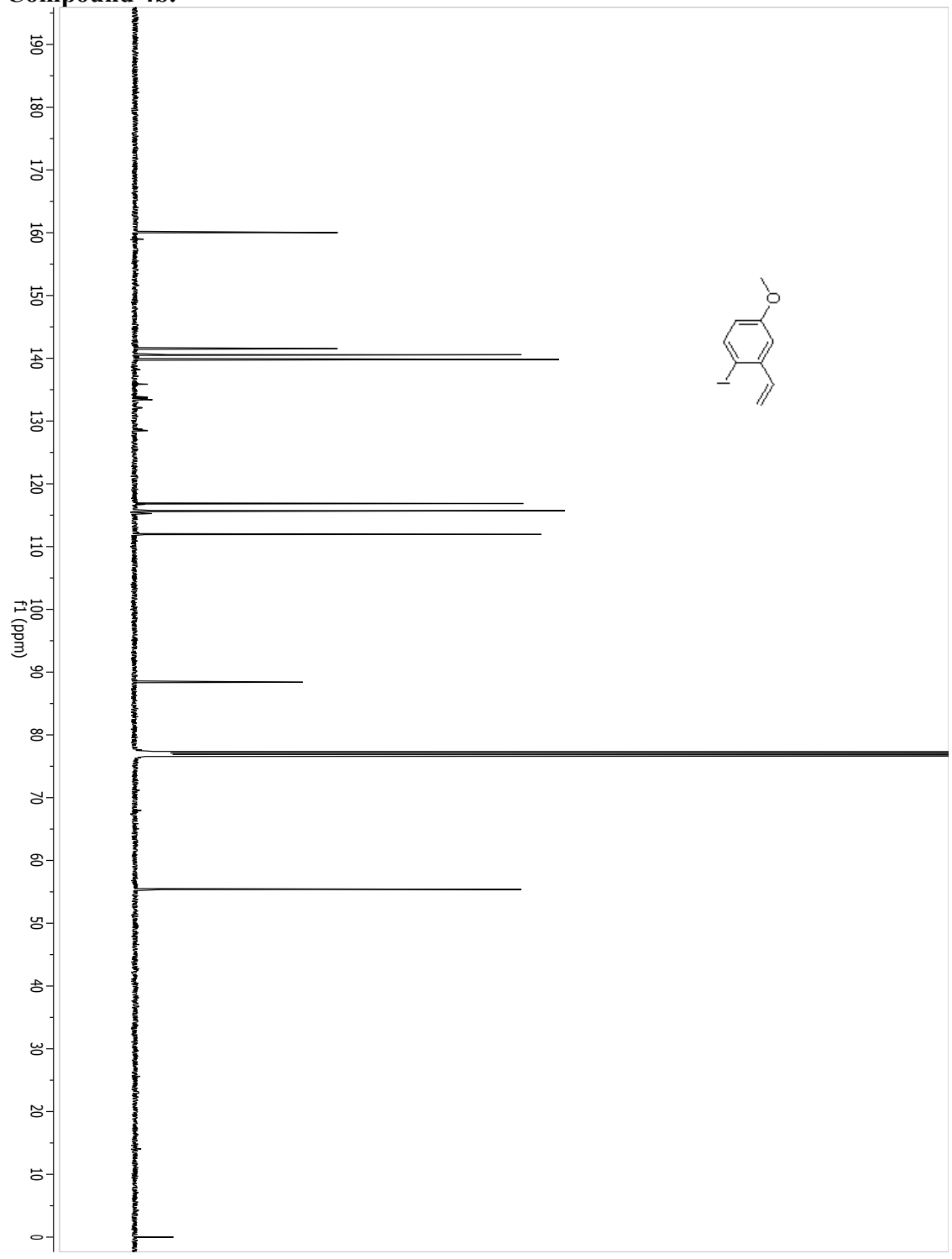
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
O
I

Compound 4b.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170
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80
70
60
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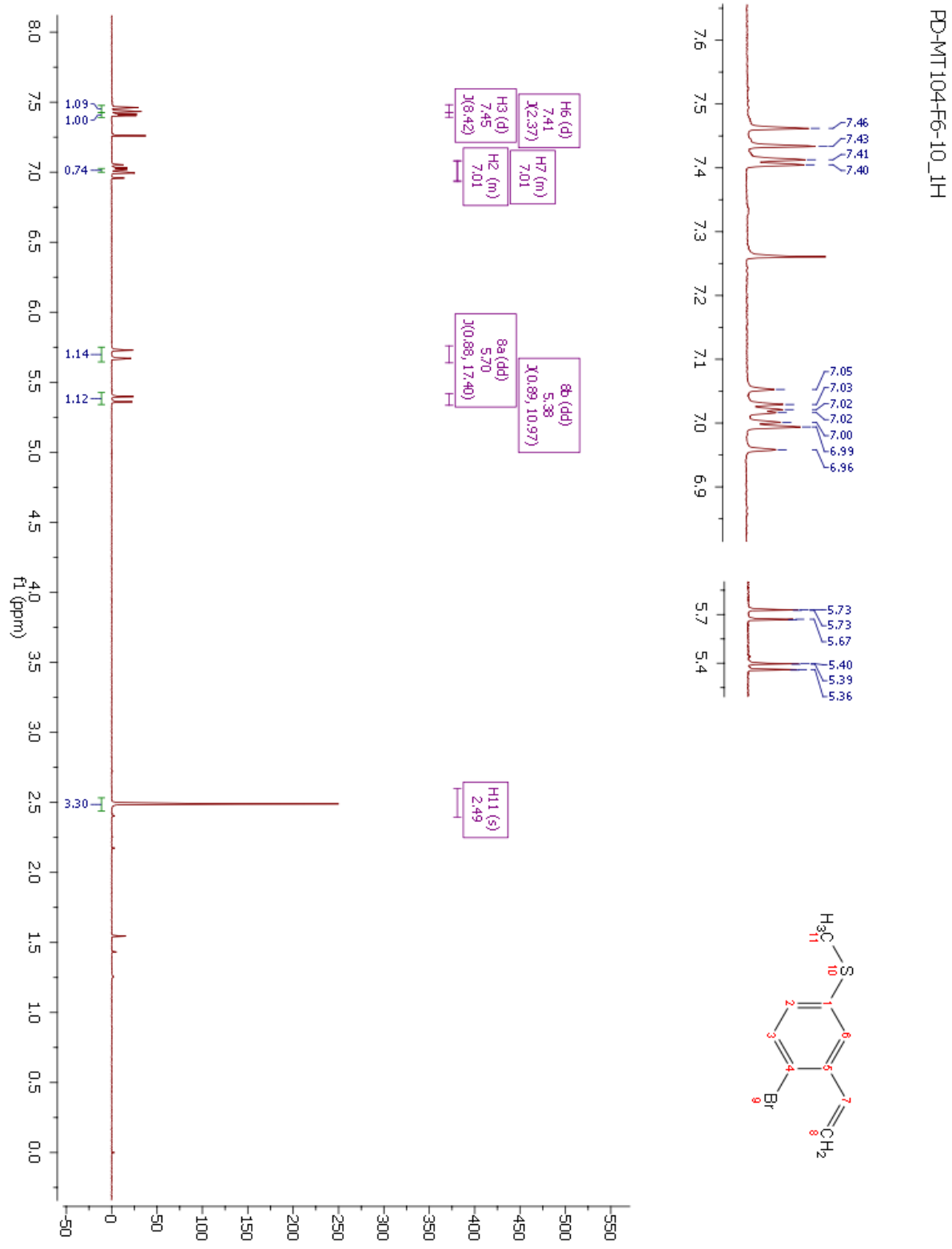
40
30
20
10
0
O

Compound 4f.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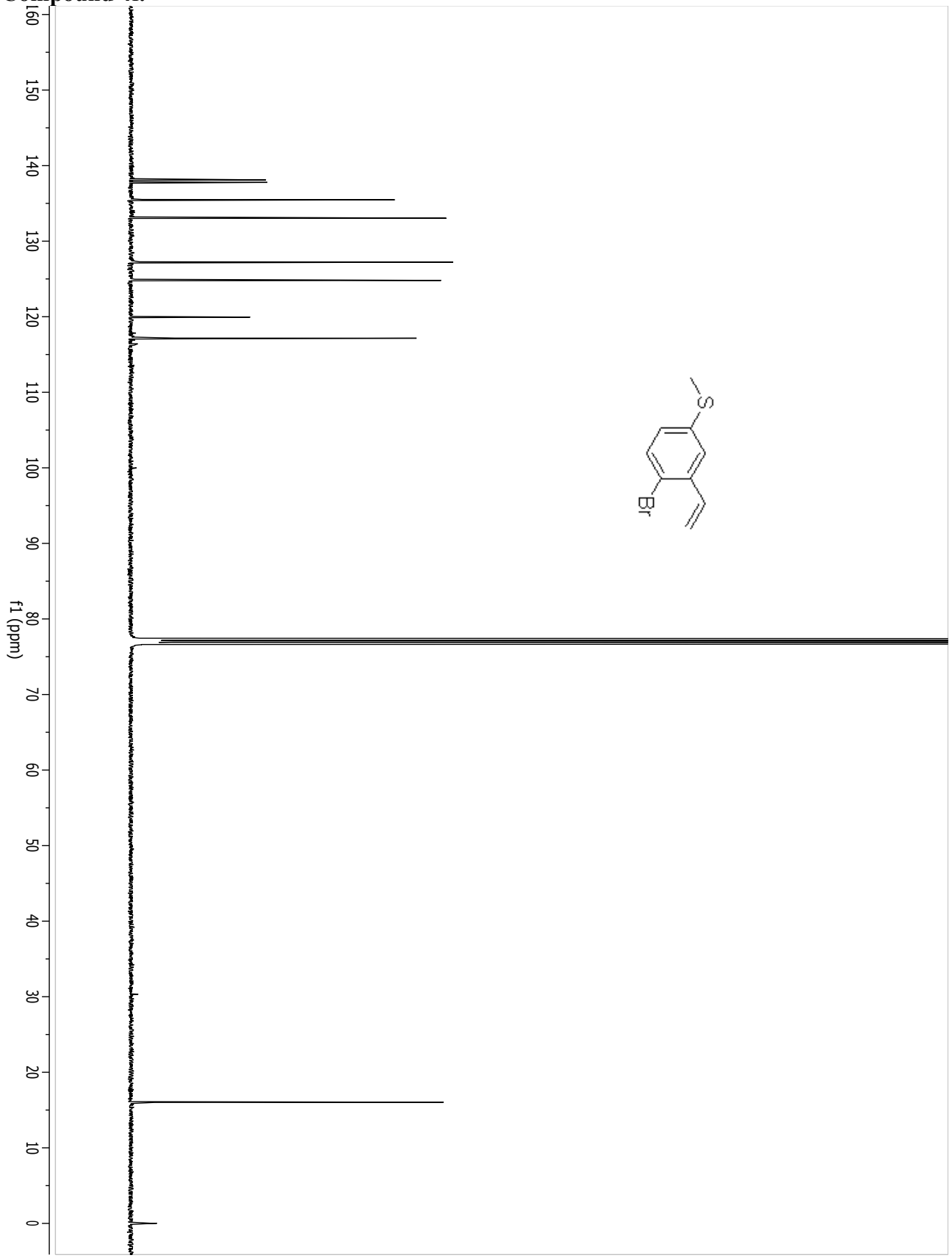
7.41
7.40
7.05
7.03
7.02
7.02
7.00
6.99
6.96
5.73
5.73
5.67
5.40
5.39
5.36
H6 (d)
7.41
J(2.37)
H3 (d)
7.45
J(8.42)
H7 (m)
7.01
H2 (m)
7.01
8a (dd)
5.70
J(0.88, 17.40)
8b (dd)
5.38
J(0.89, 10.97)
H11 (s)
2.49
1.09
1.00
0.74
1.14
1.12
3.30
f1 (ppm)

Compound 4f.



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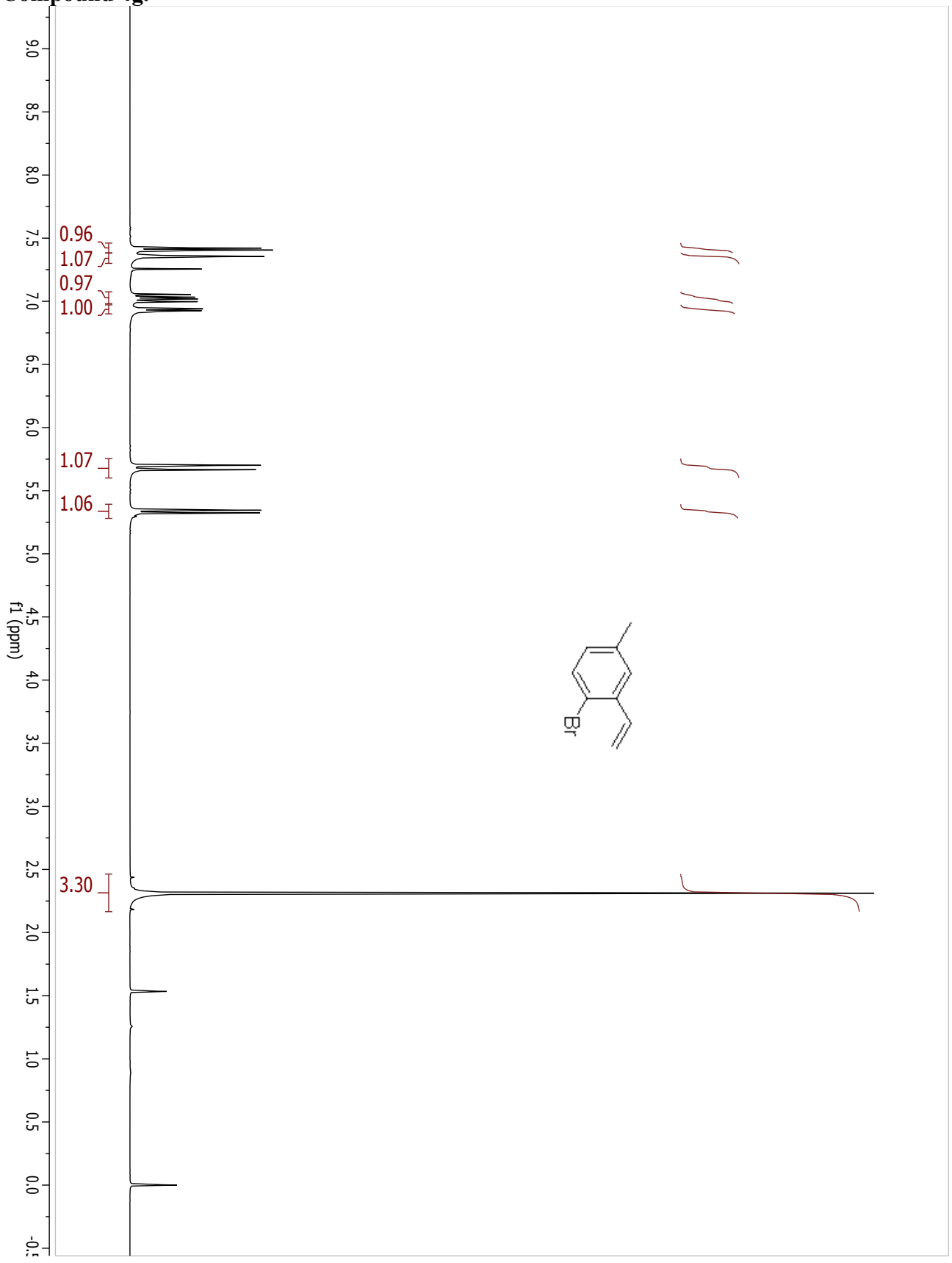
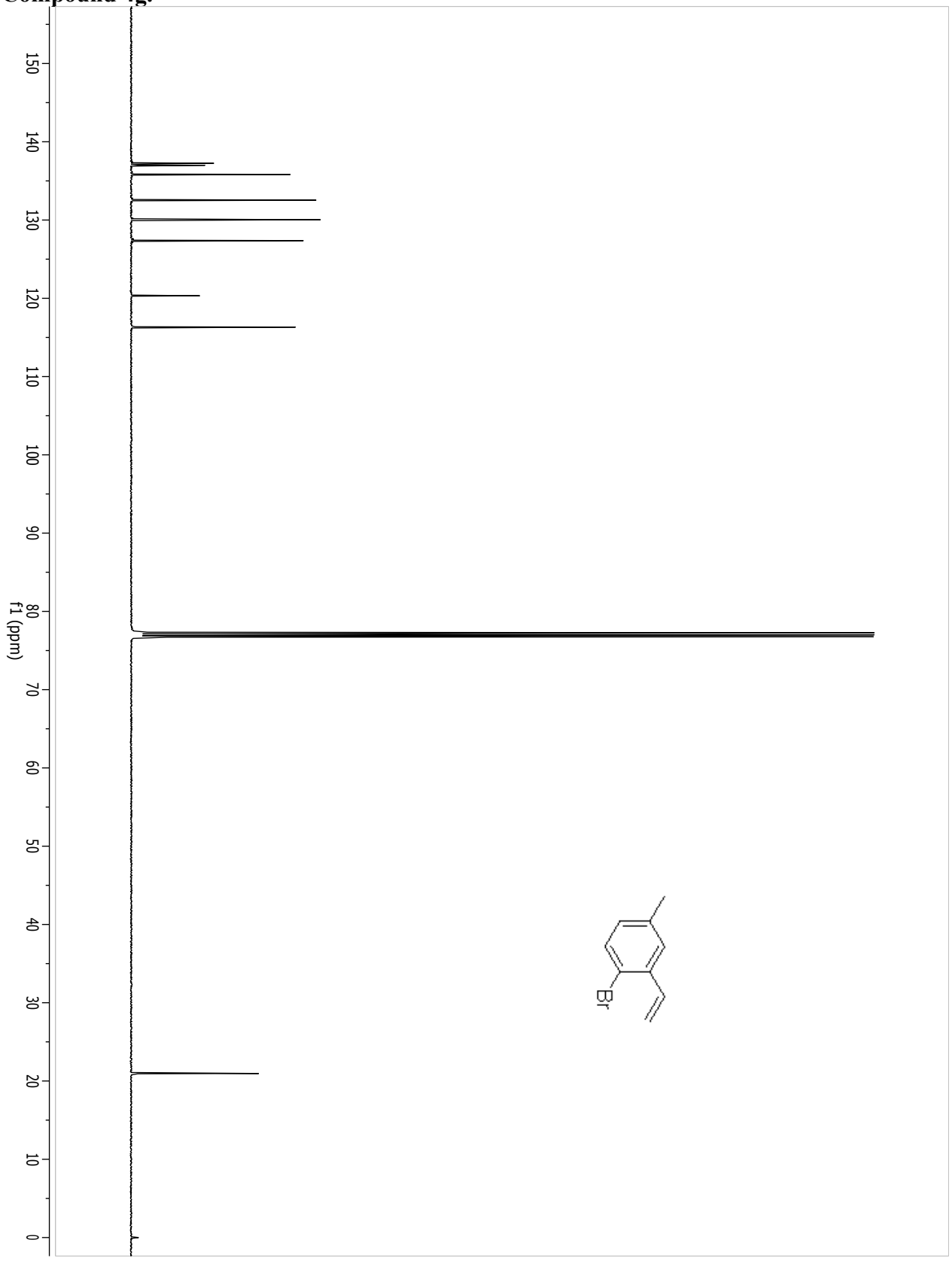
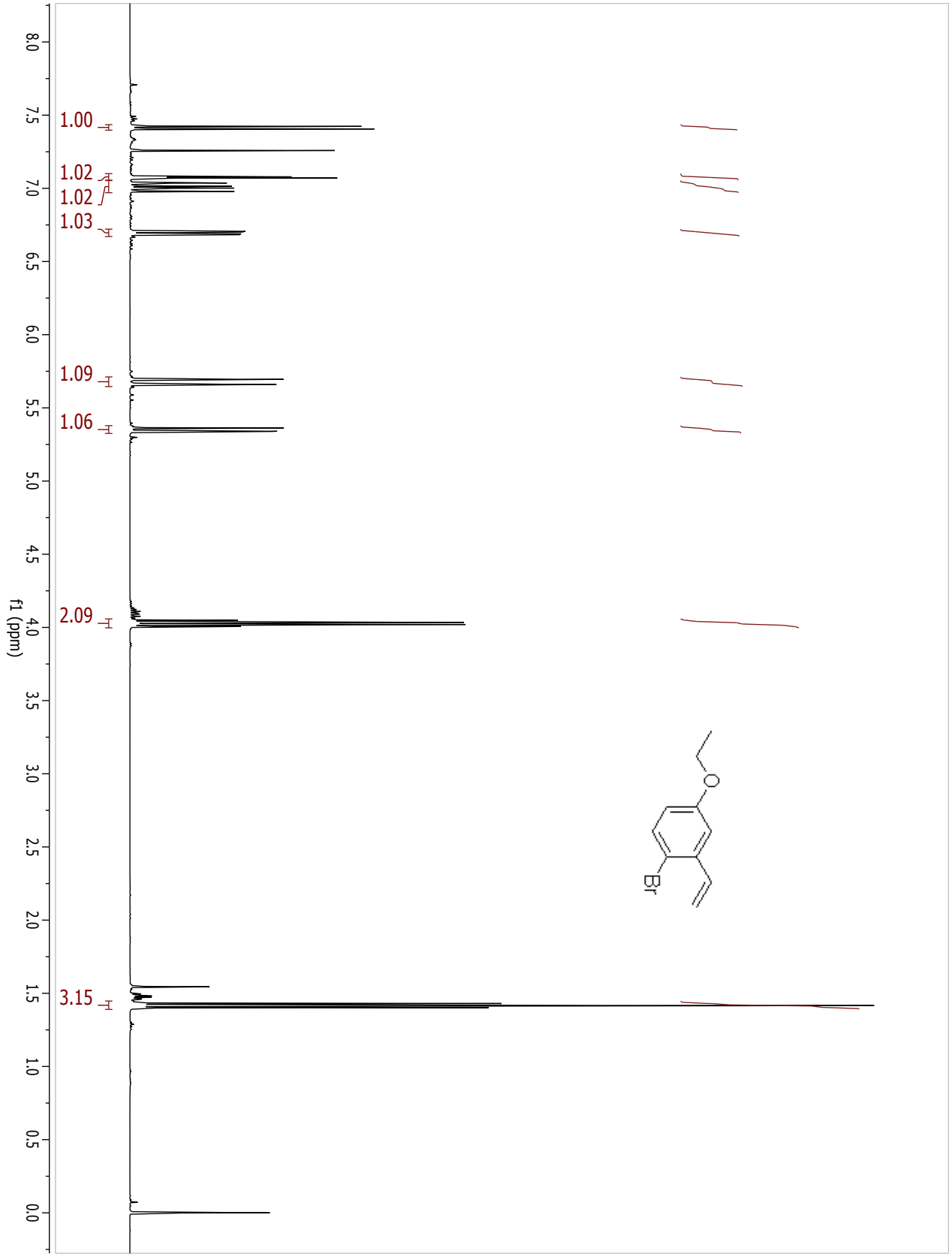


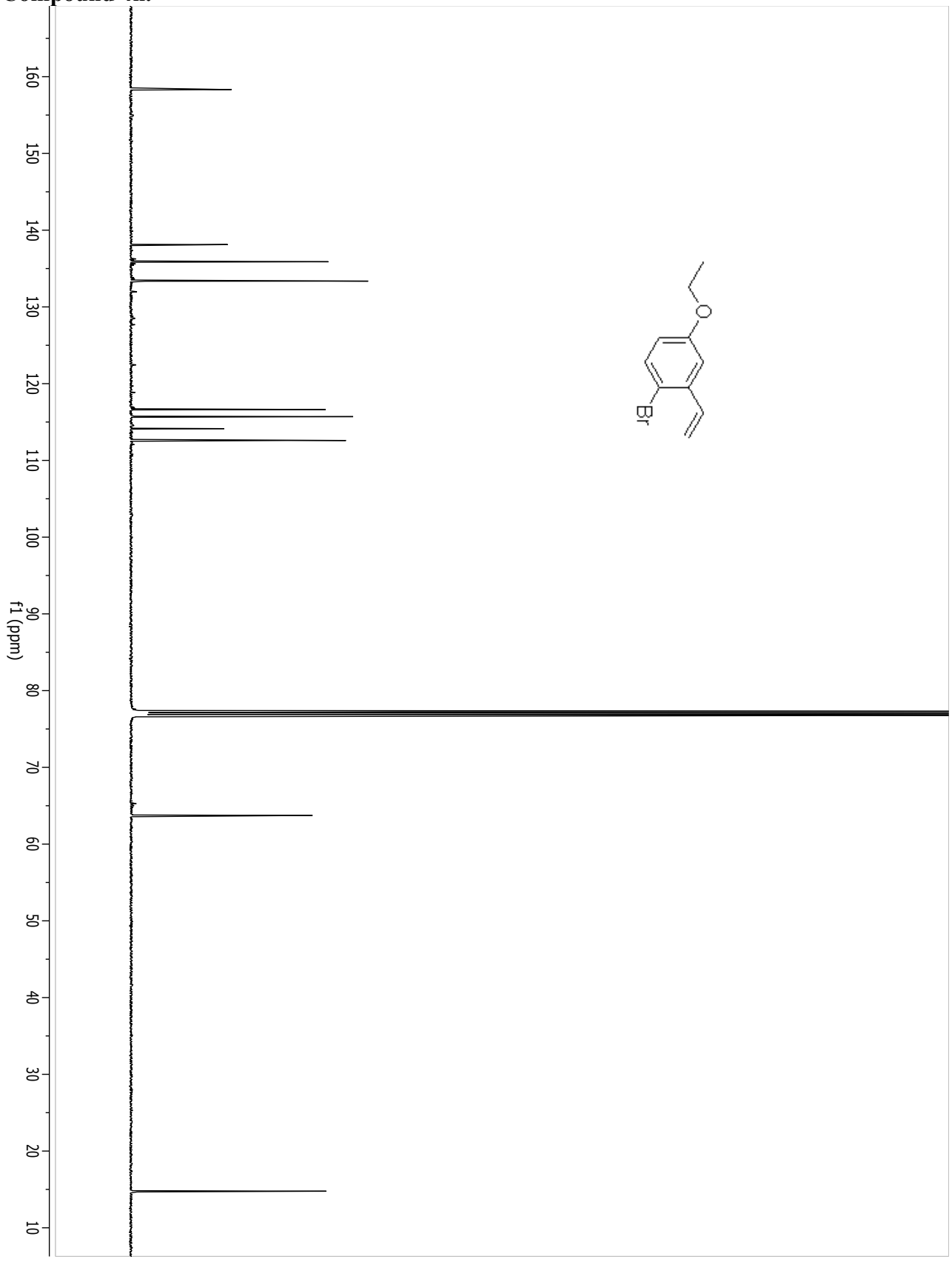
Compound 4g.



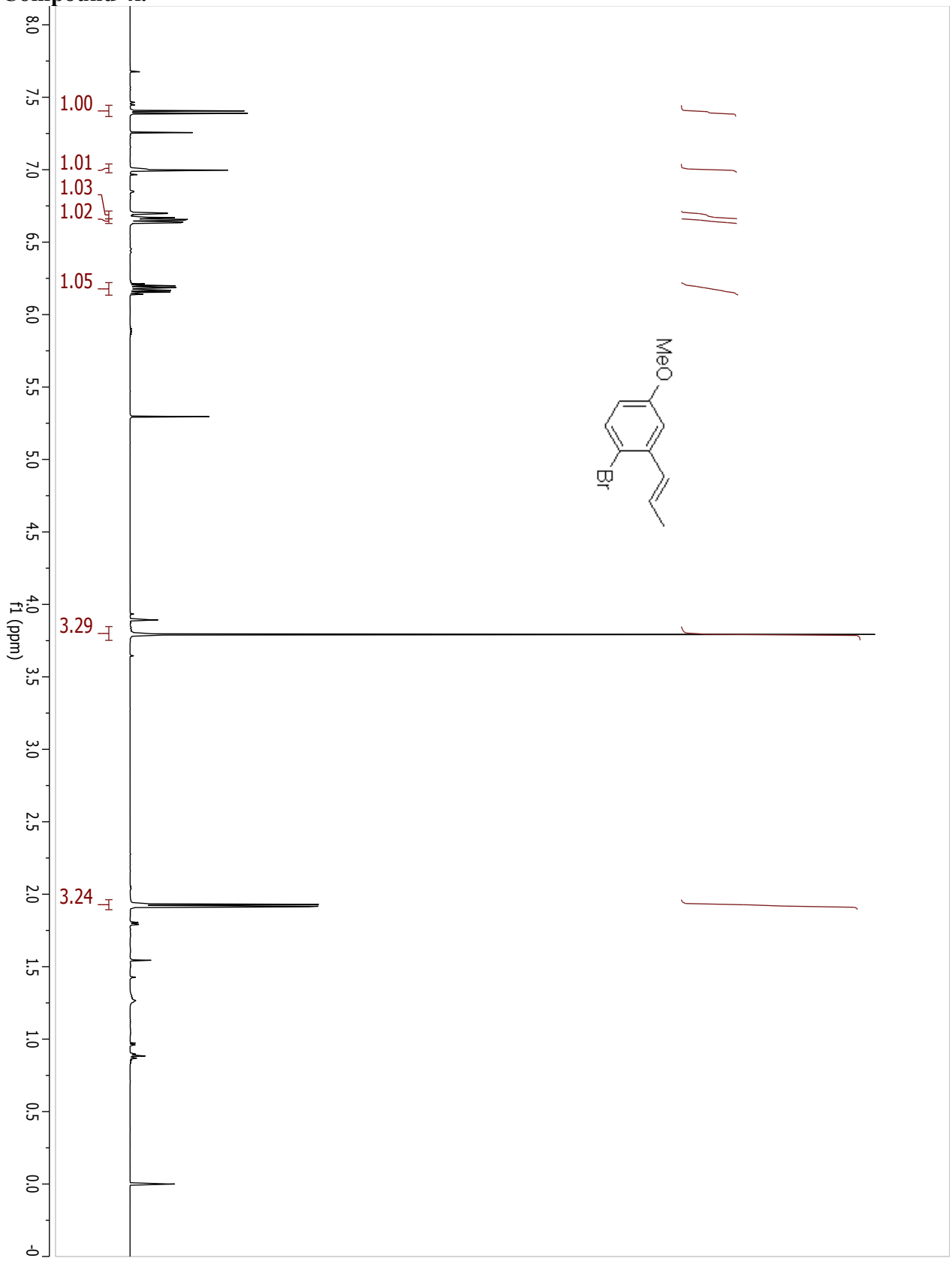
Compound 4h.



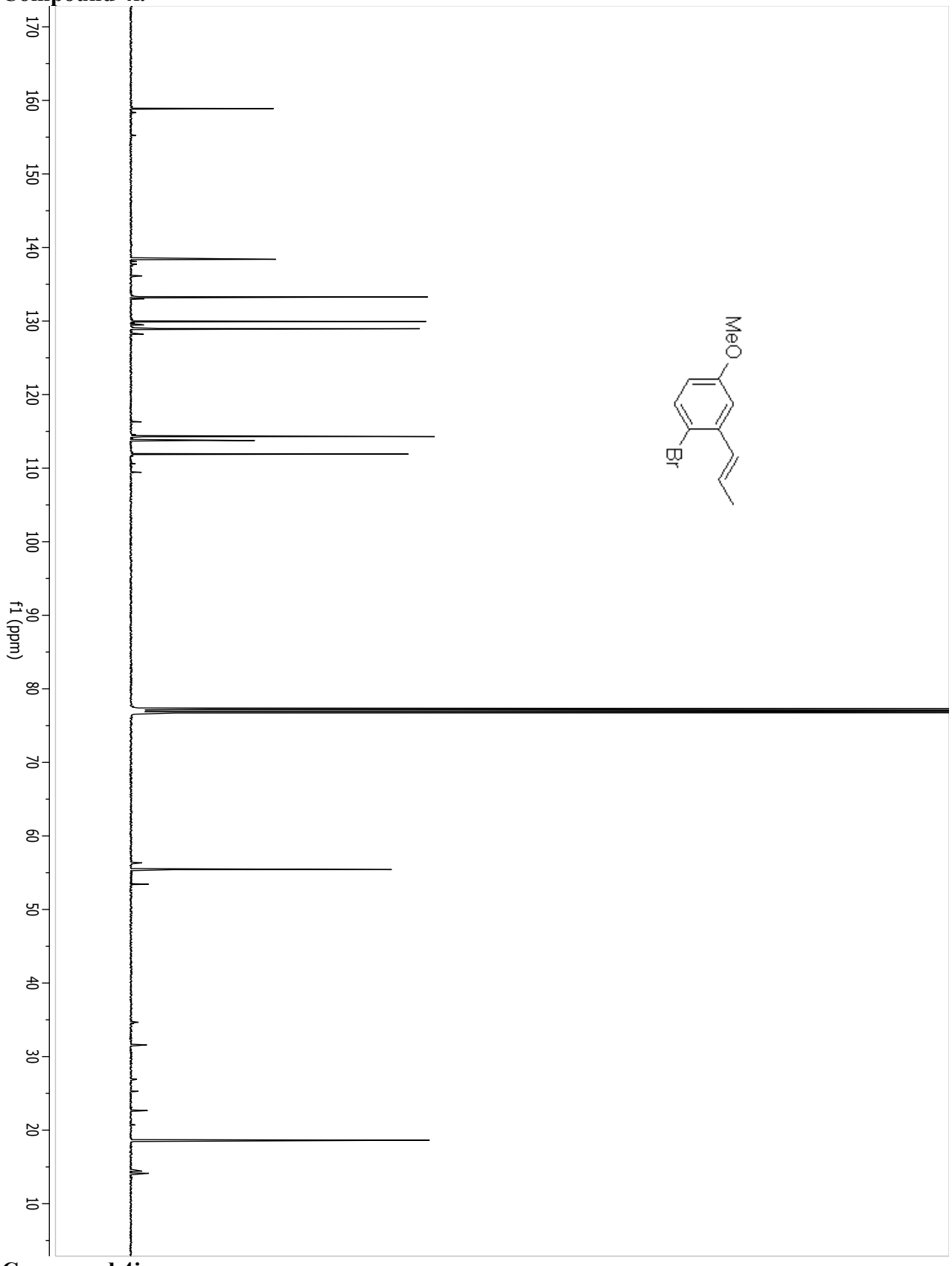
Compound 4h.



Compound 4i.



Compound 4i.



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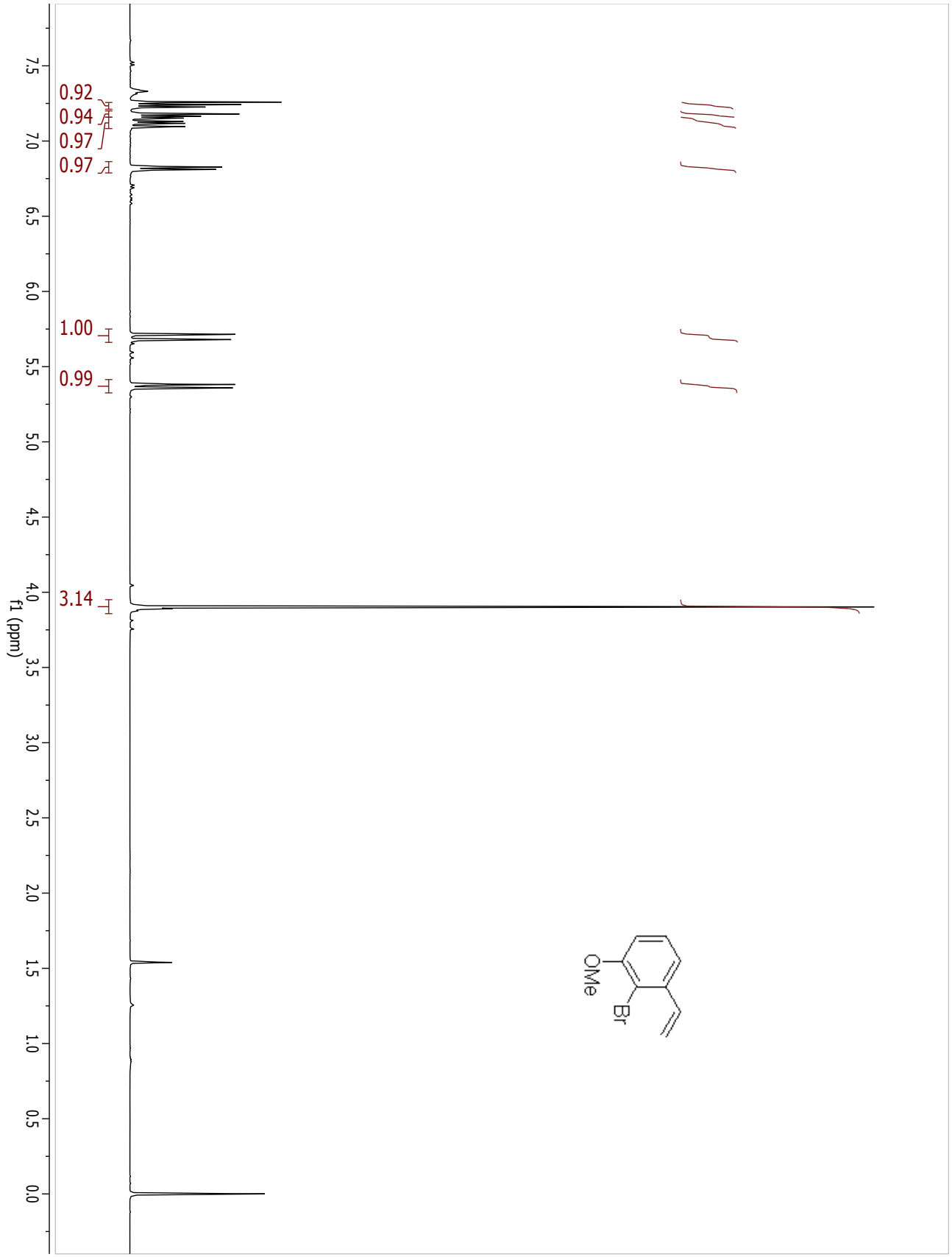

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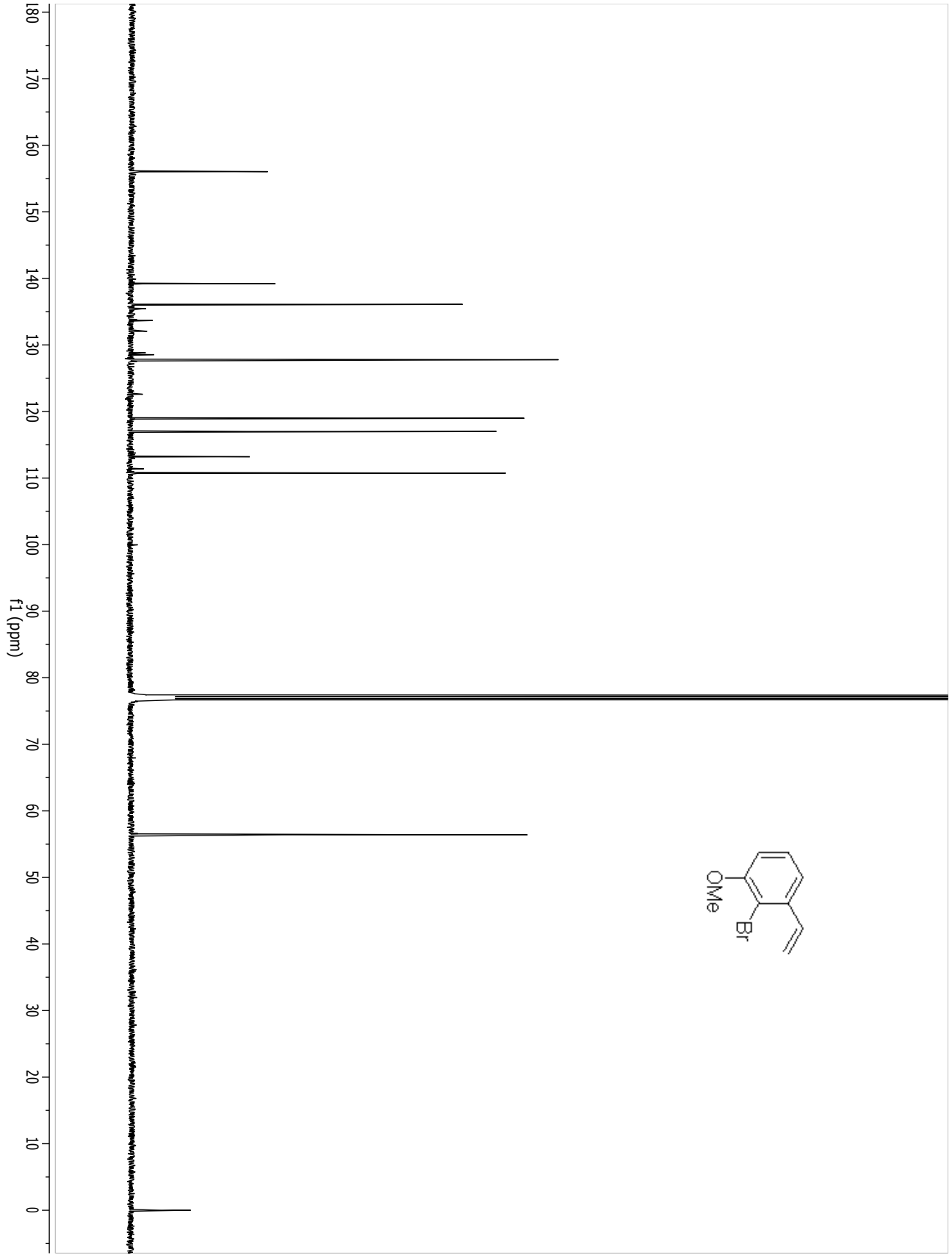
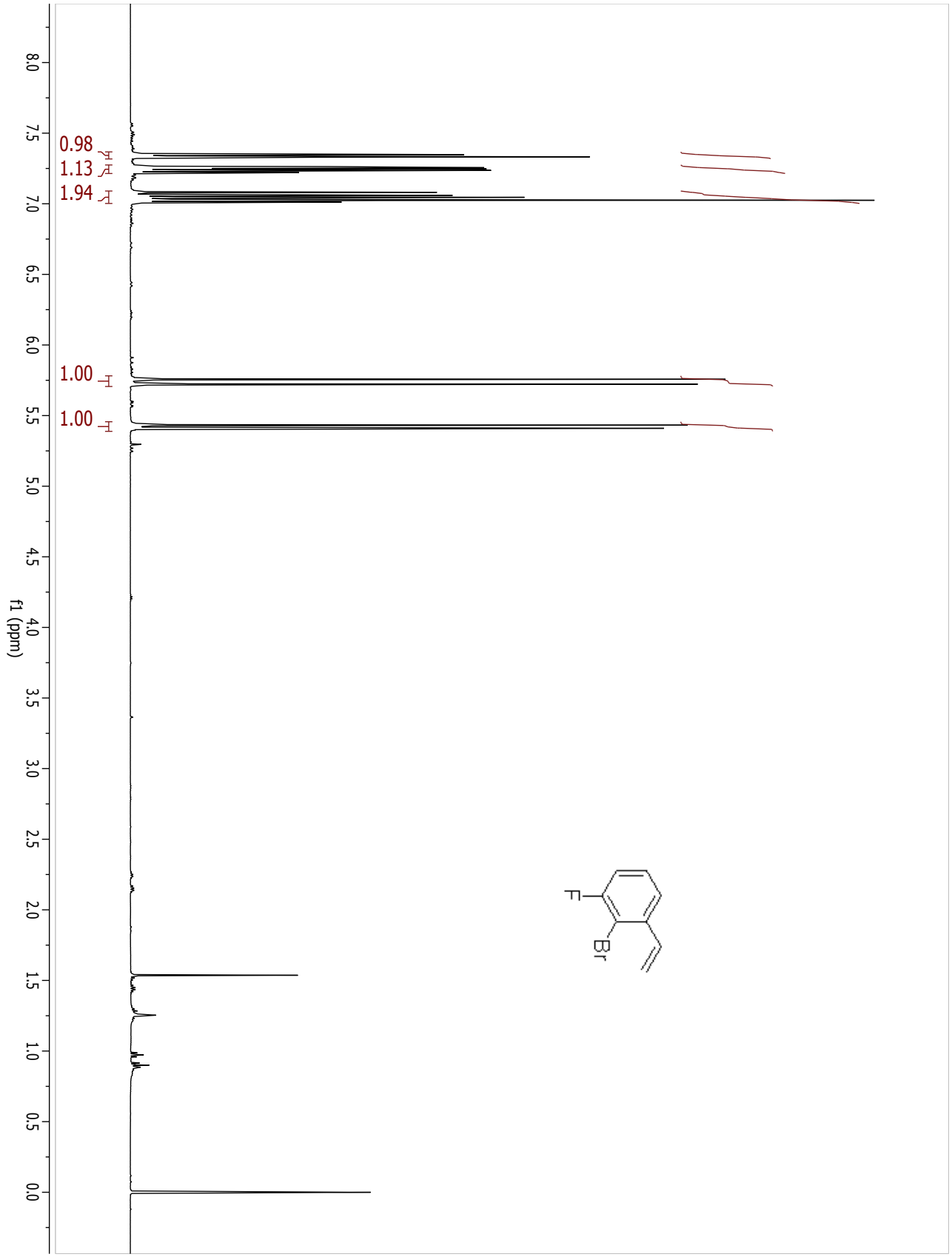

f1 (ppm)
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
OMe
Br

Compound 4k.



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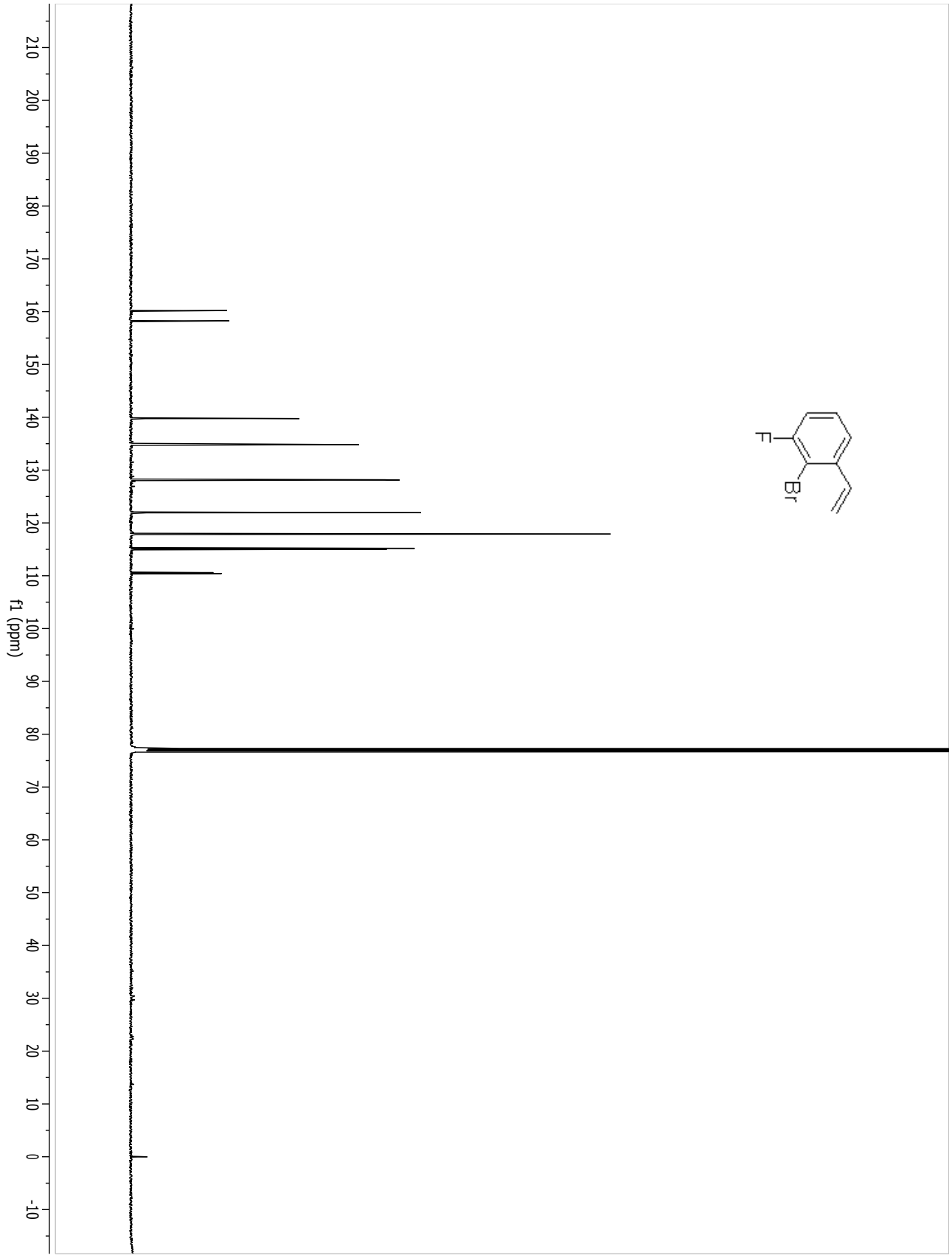
F
Br
f1 (ppm)
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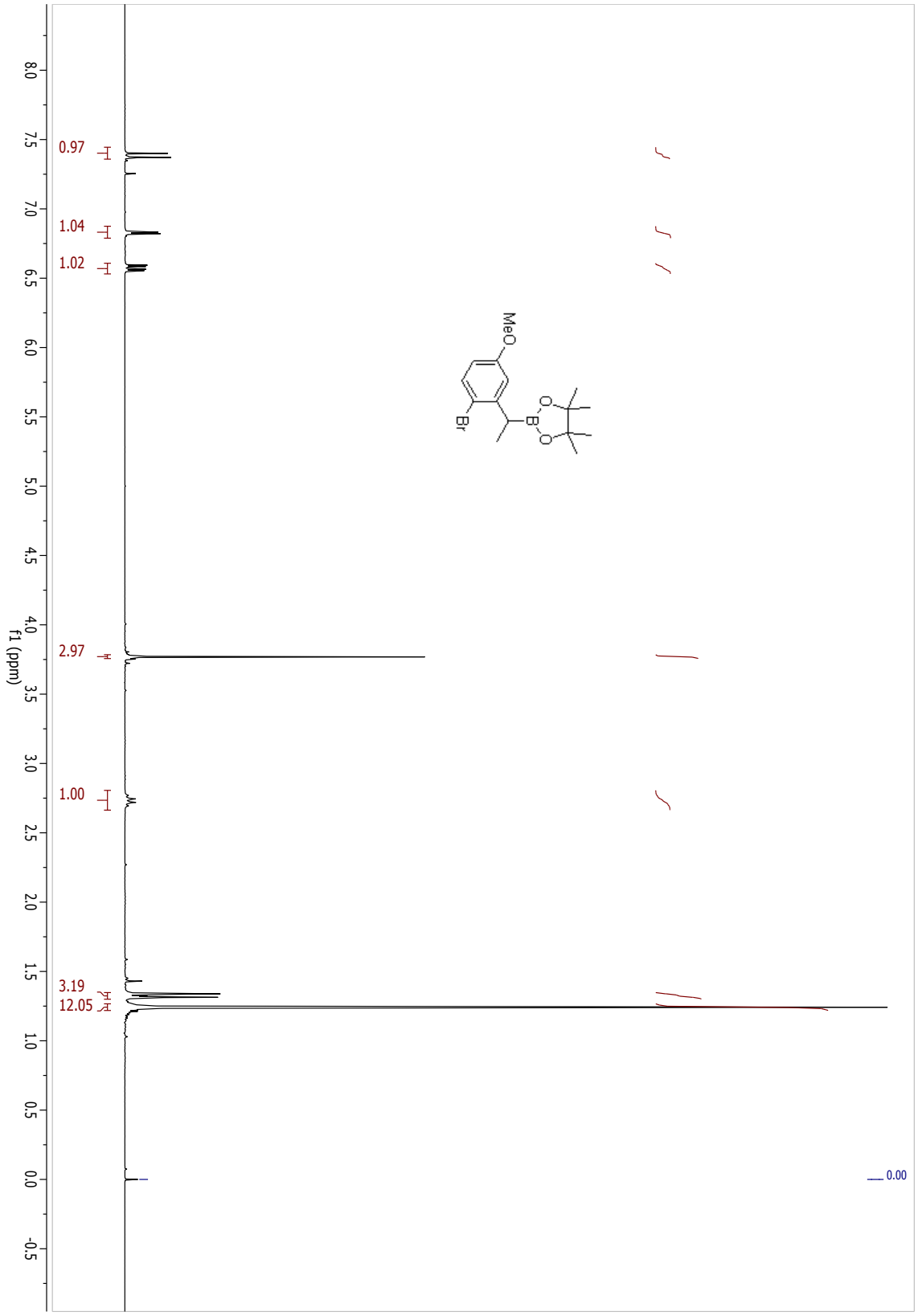
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10

Compound 3.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f1 (ppm)
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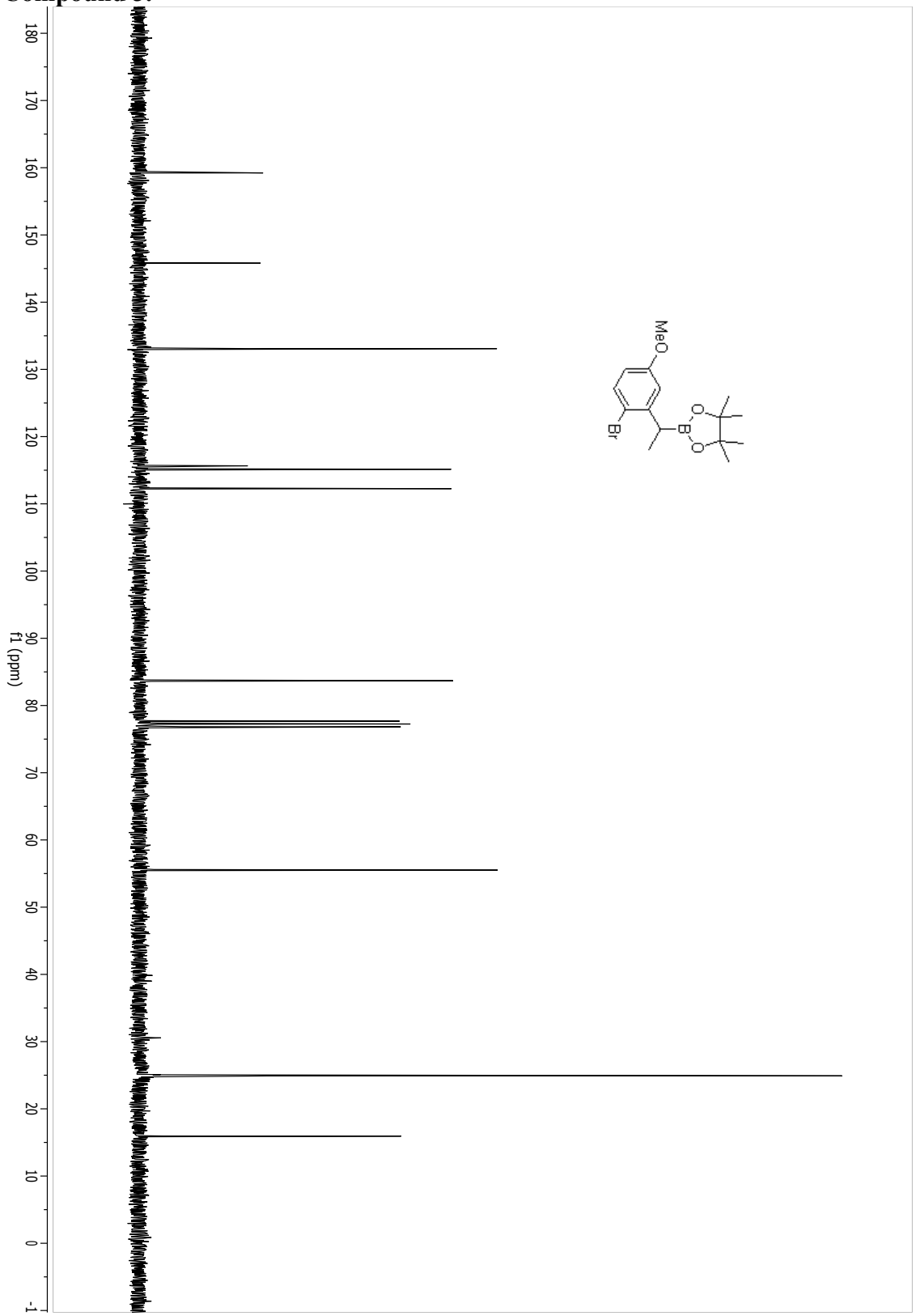
Br
B
O
O

Compound 3.


MeO
Br
O
B
O
f1 (ppm)
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170
160
150
140
130
120
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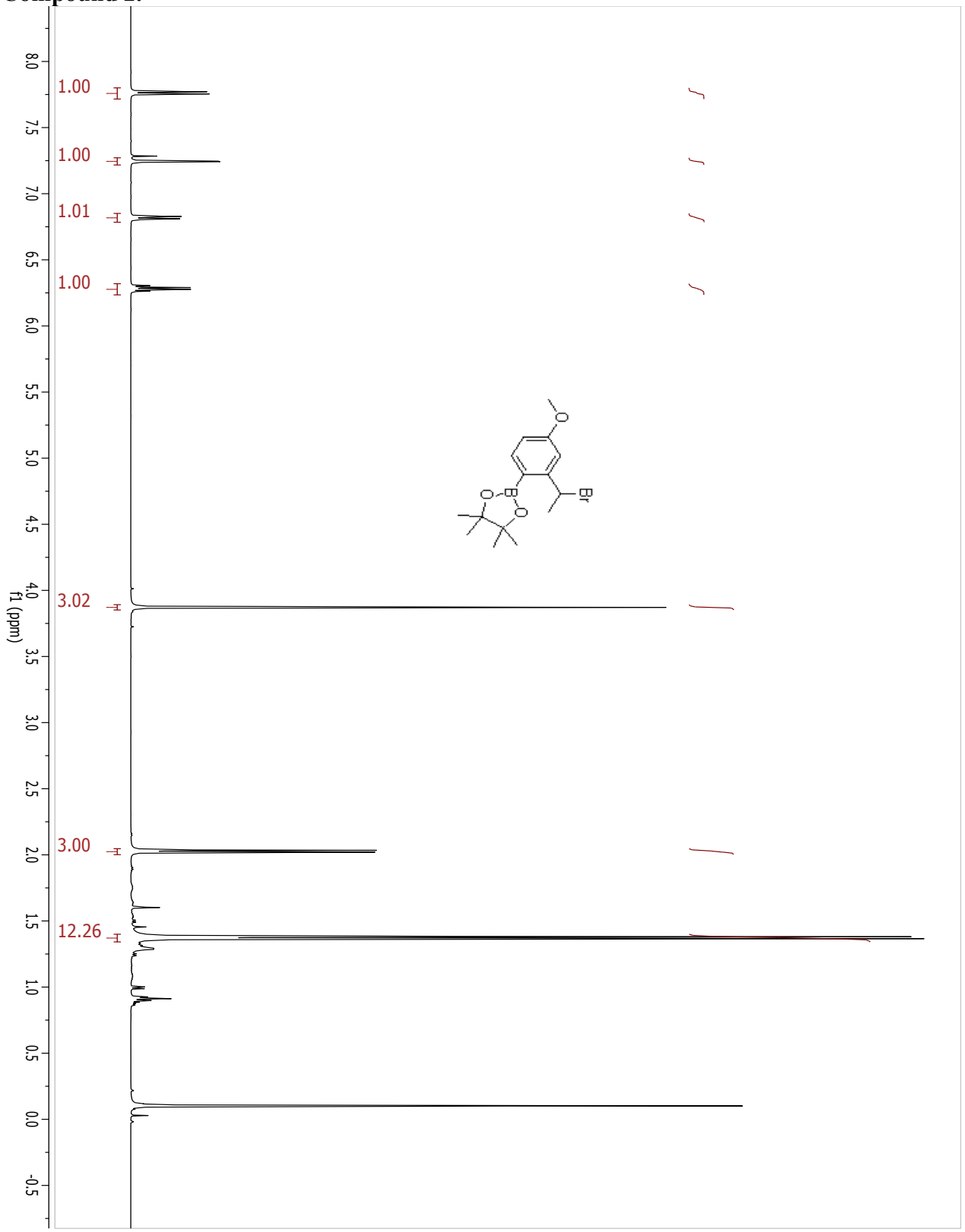
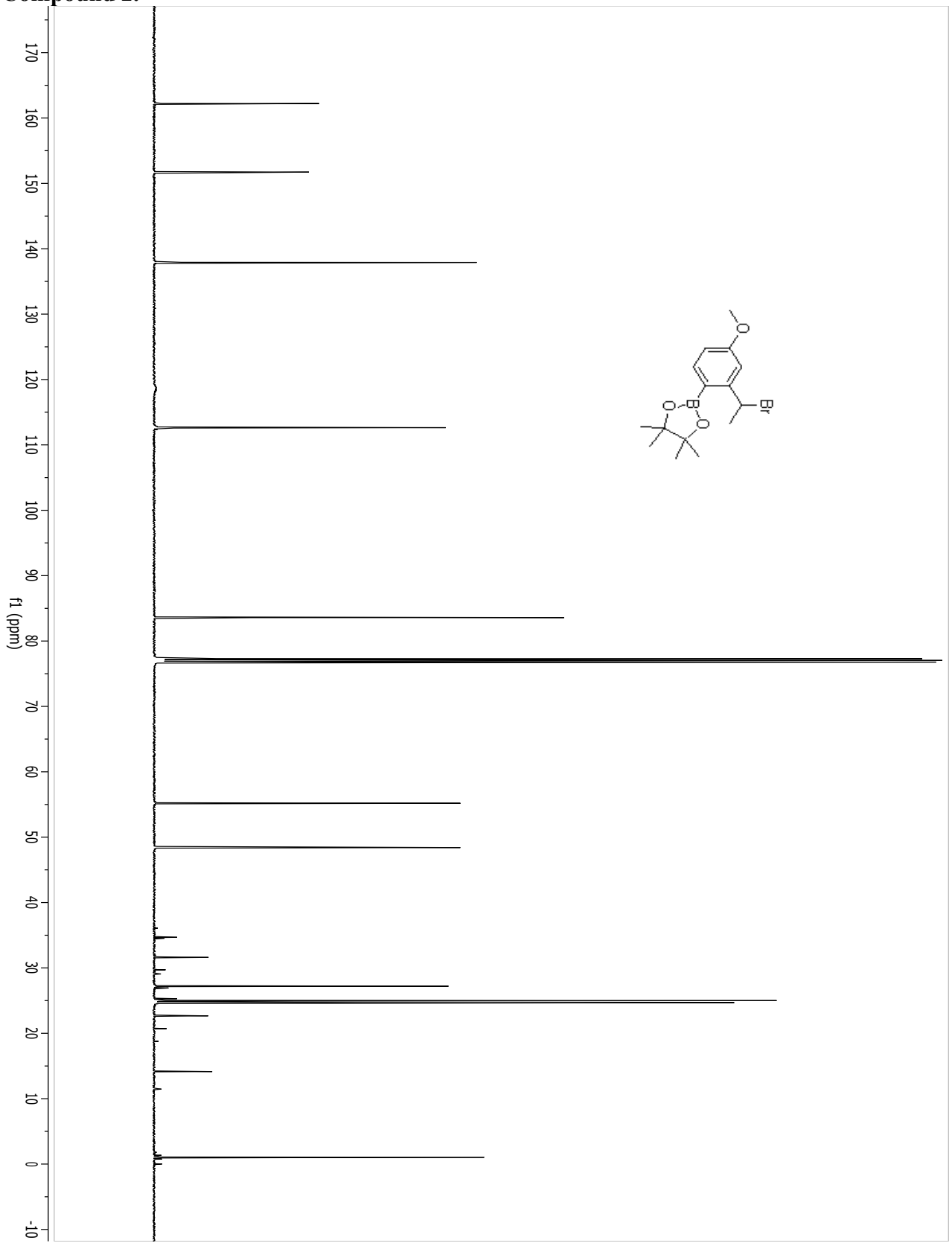
90
80
70
60
50
40
30
20
10
0
-1

Compound 2.



Compound 2.


f1 (ppm)
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150
140
130
120
110
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80
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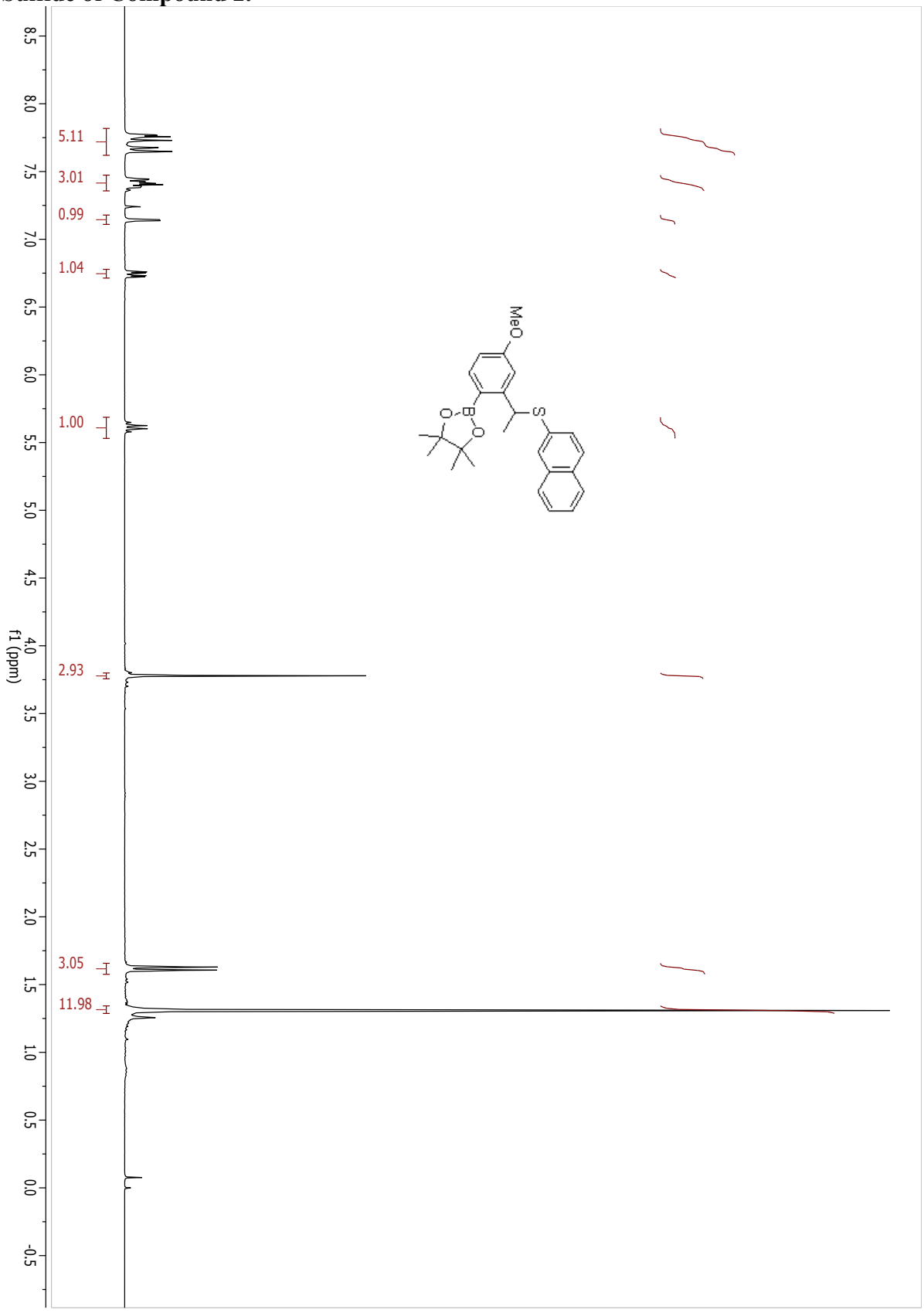
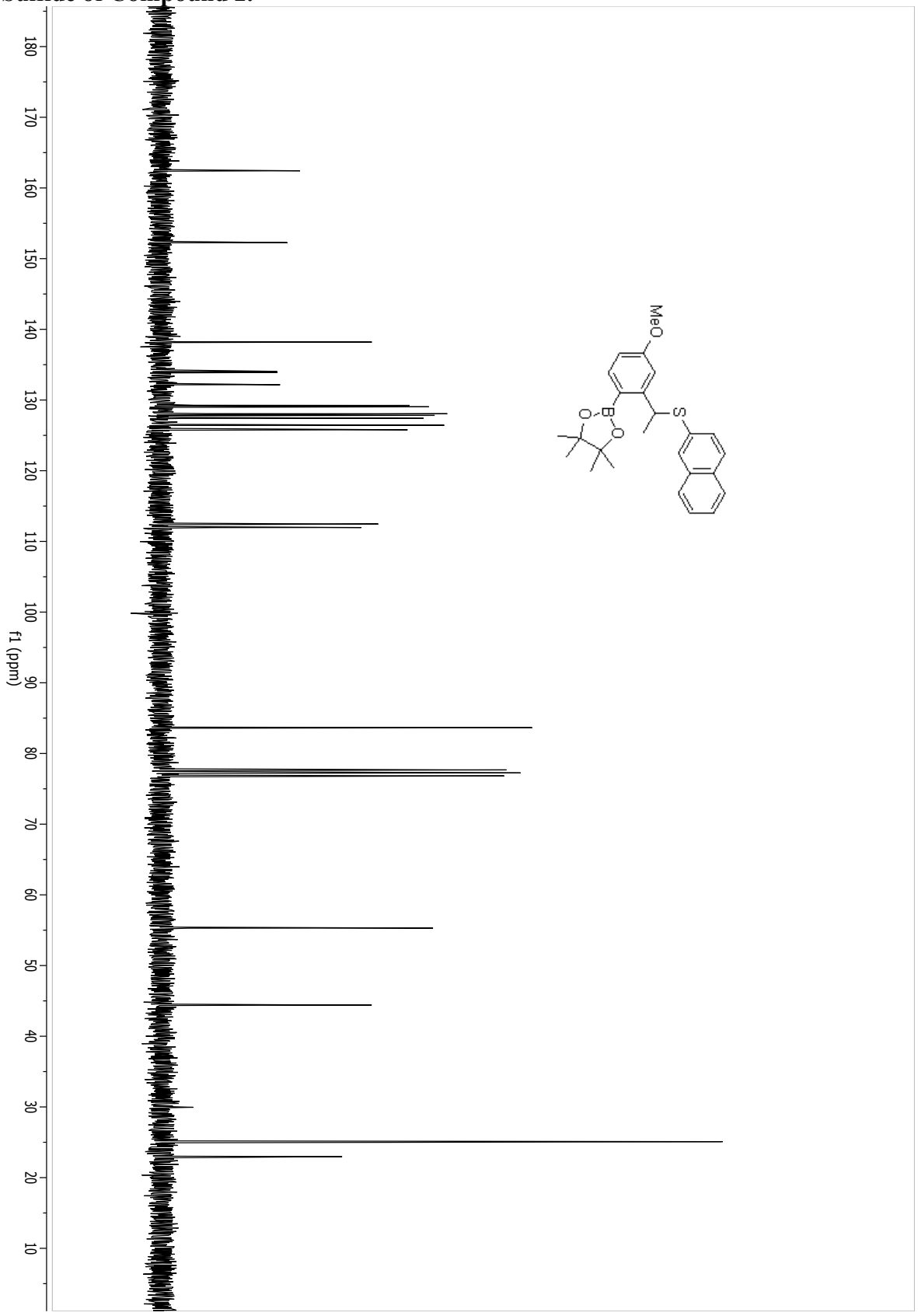
50
40
30
20
10
0
-10
O
B
O
Br

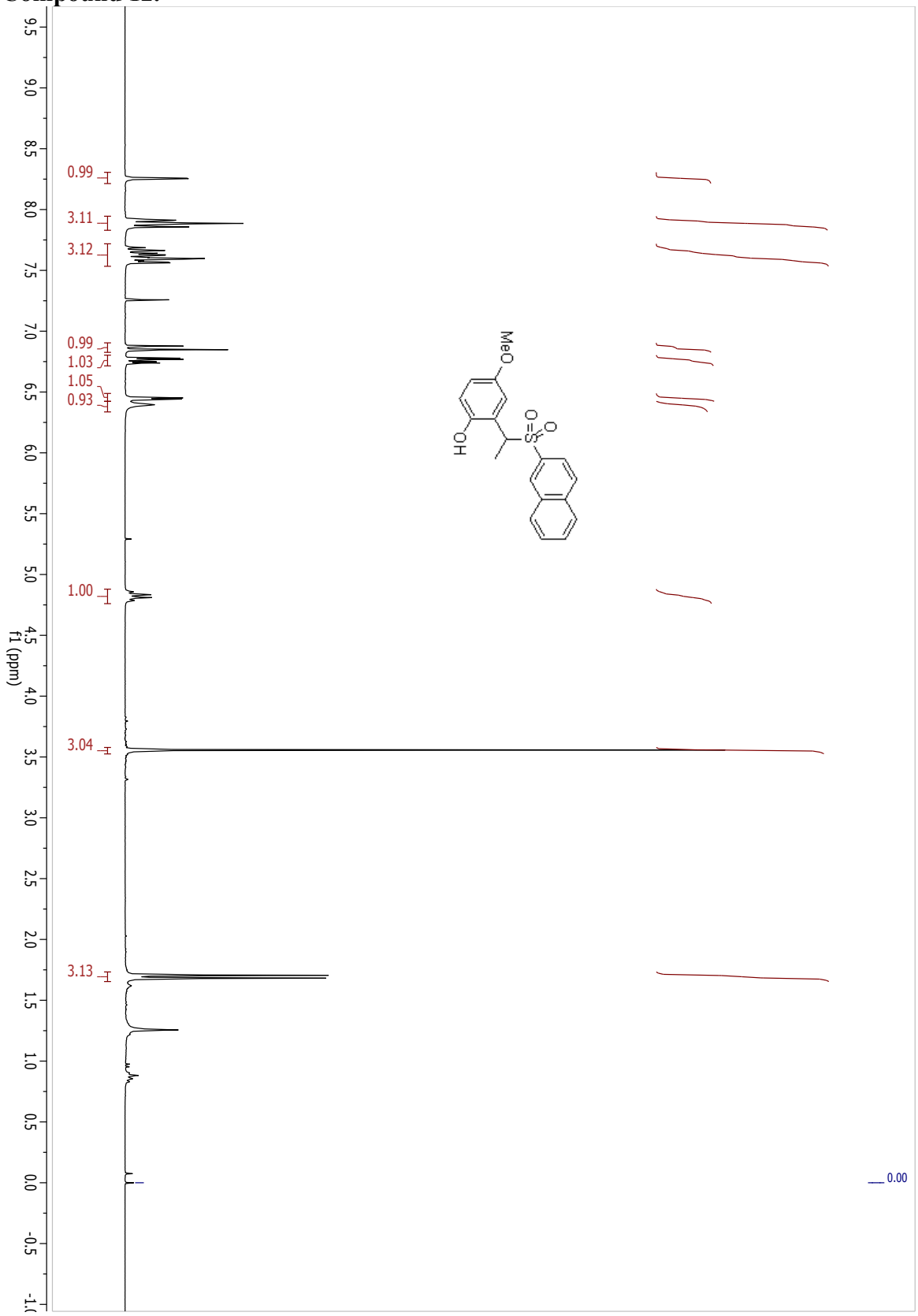
Sulfide of Compound 2.



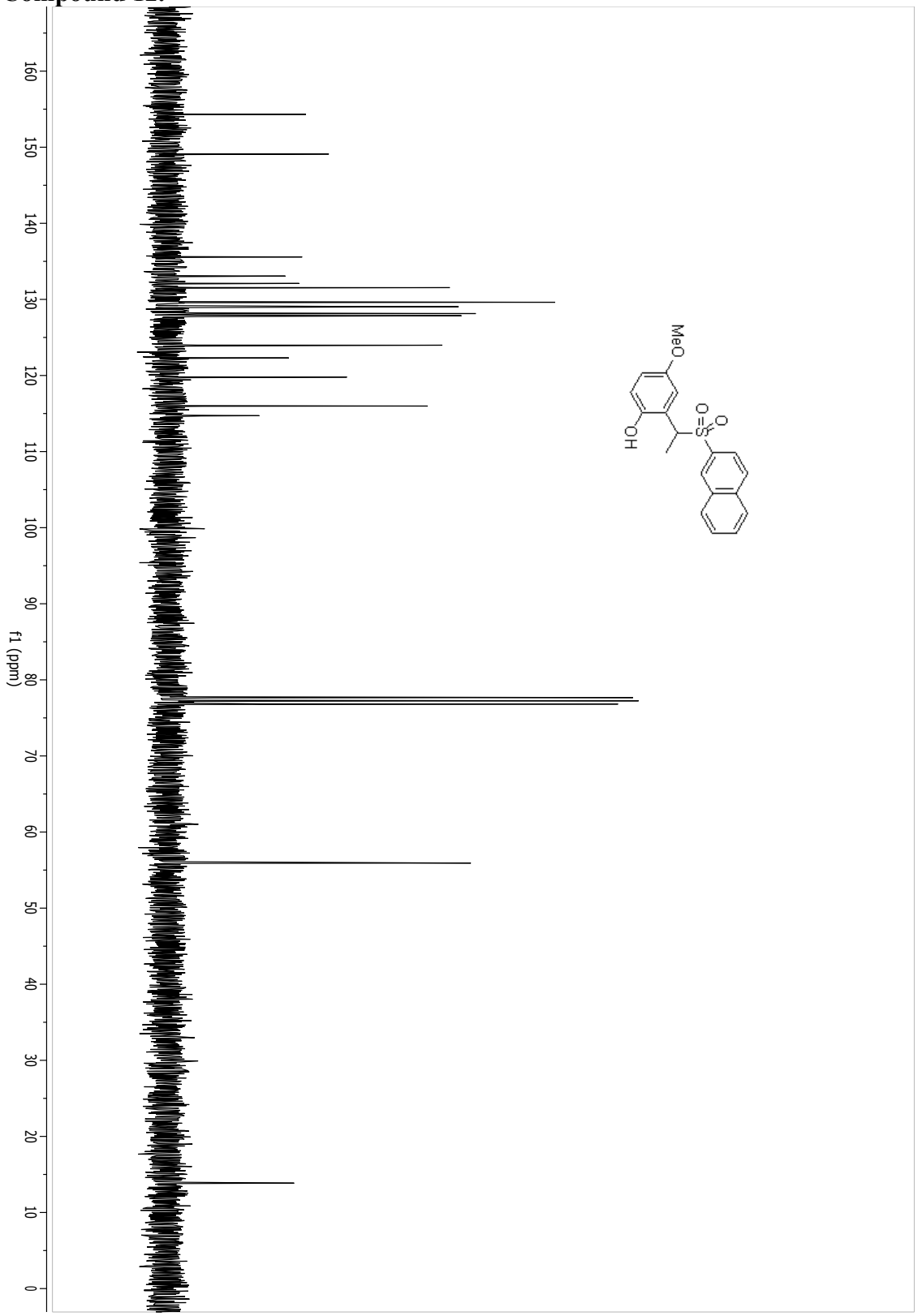
Sulfide of Compound 2.



Compound 12.



Compound 12.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150
140
130
120
110
100
90
80
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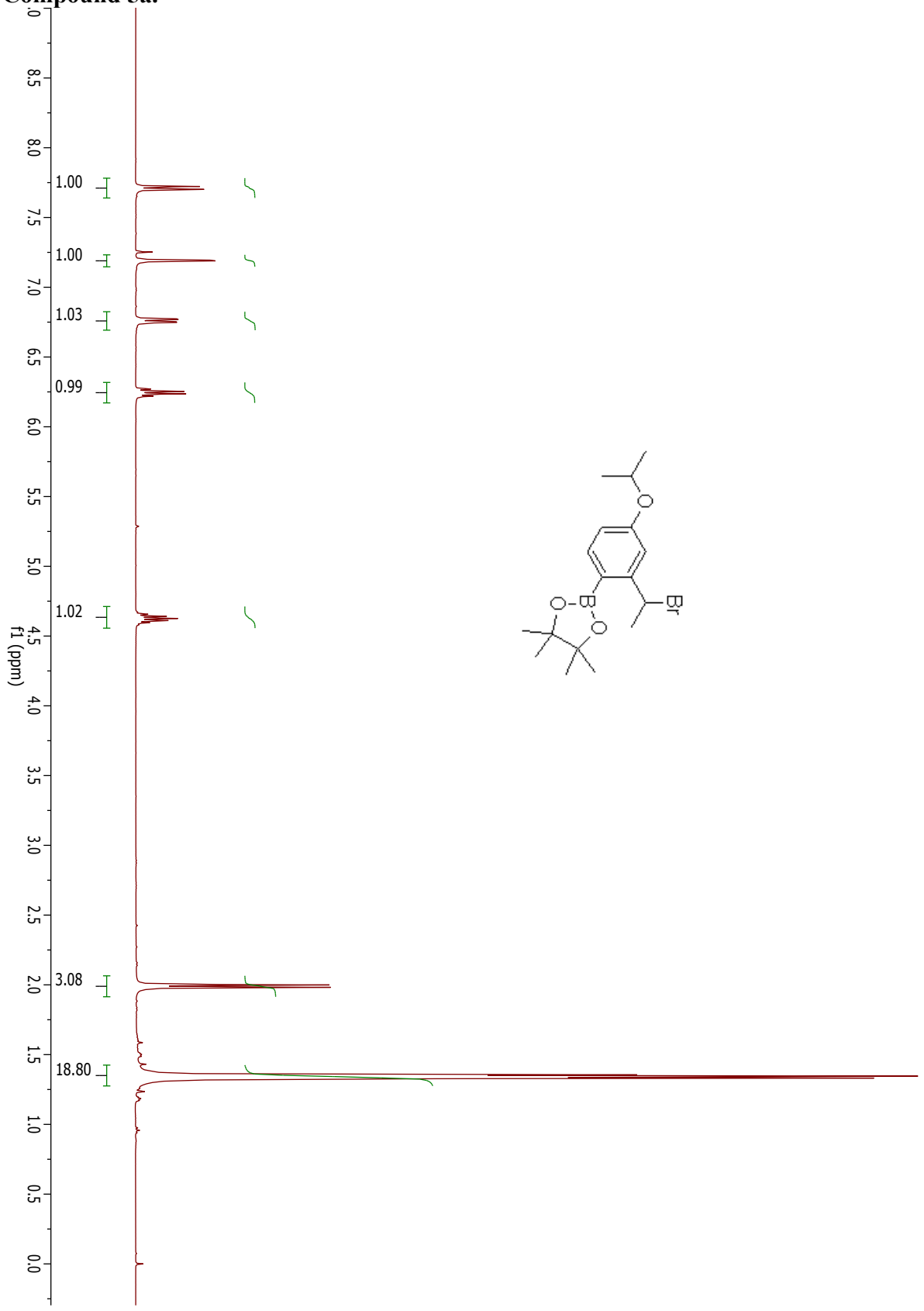
50
40
30
20
10
0
MeO
OH
O=S
O

Compound 5a.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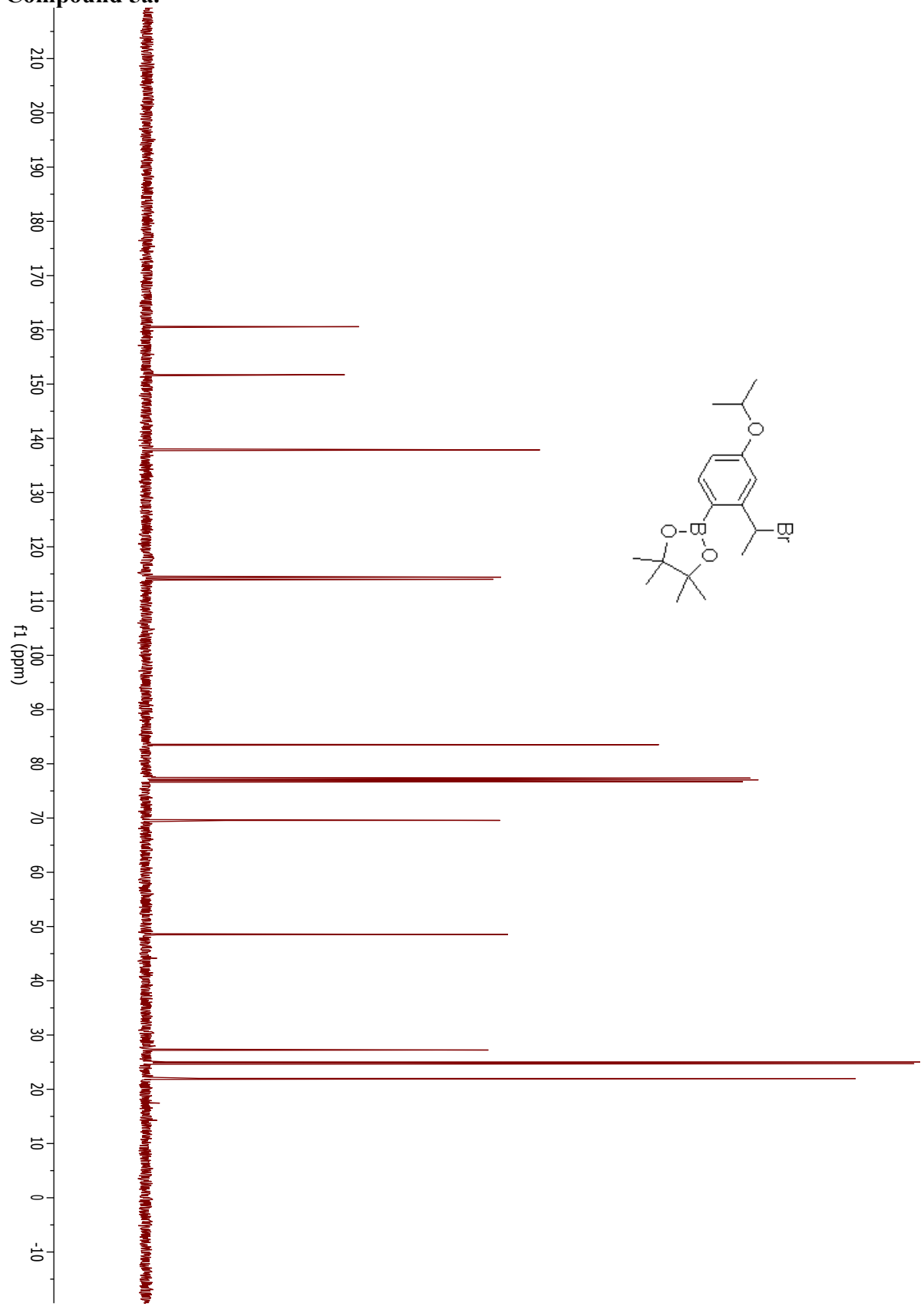
1.02
3.08
18.80
f1 (ppm)
Br

Compound 5a.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120
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90
80
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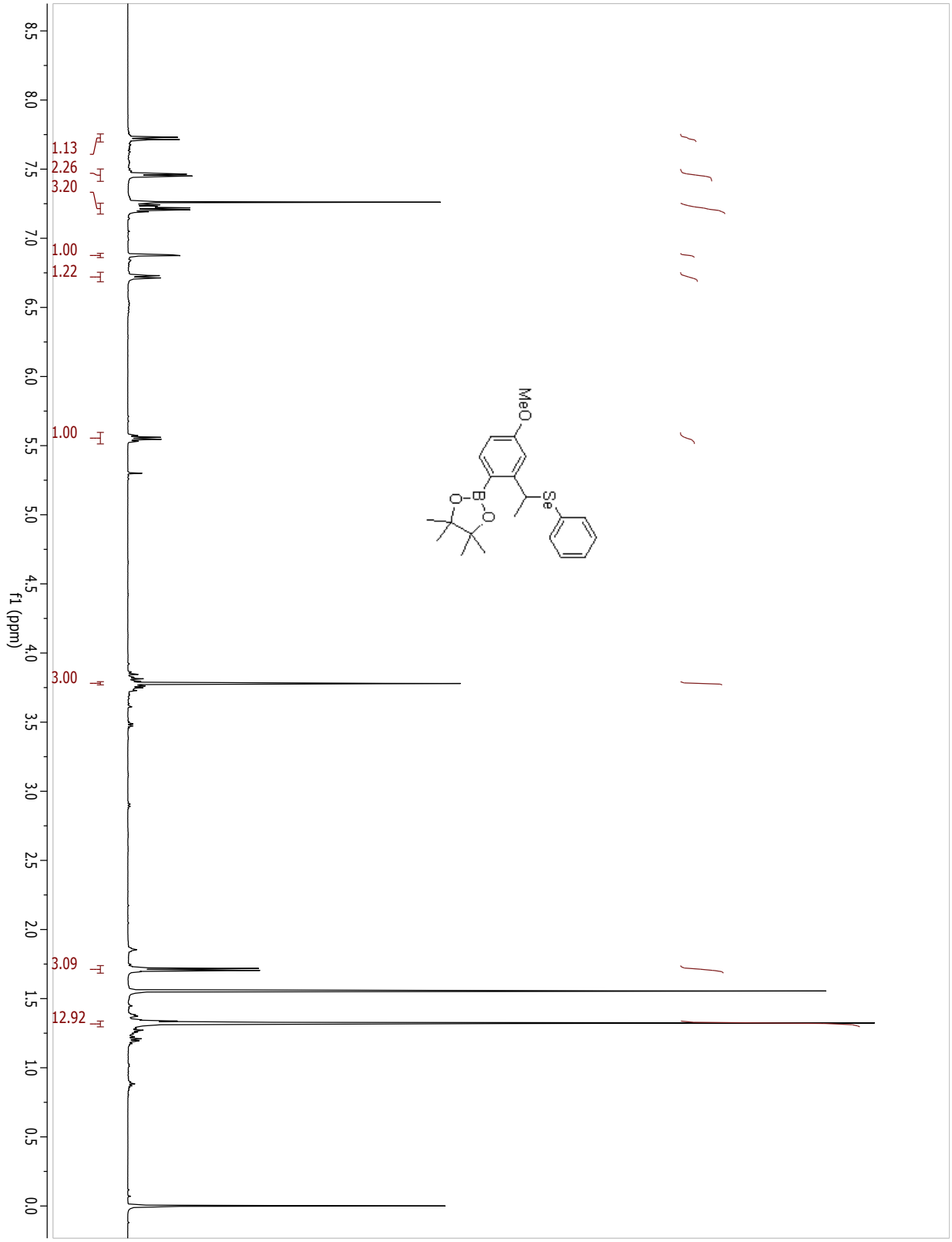
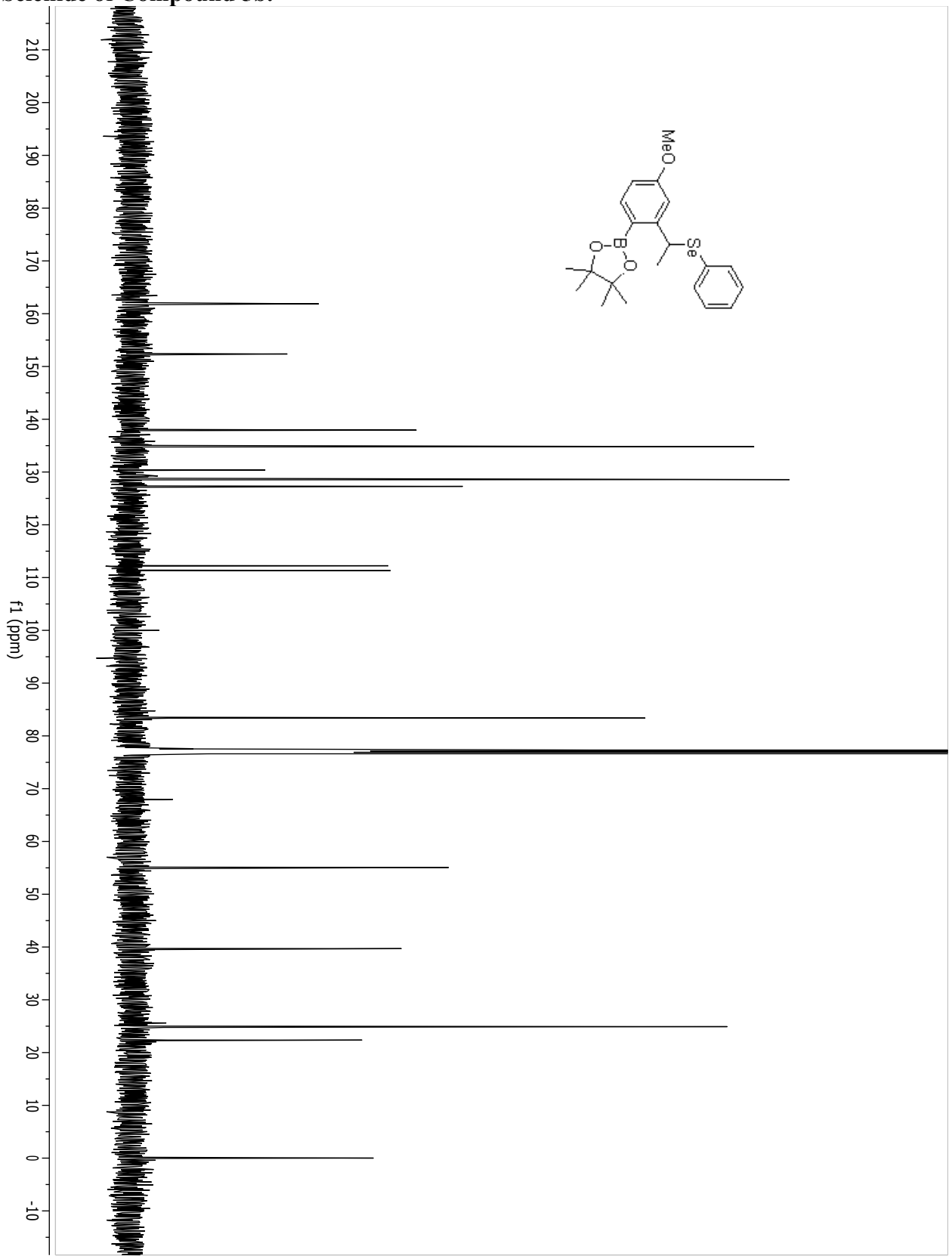
60
50
40
30
20
10
0
-10
O
B
O
O
Br

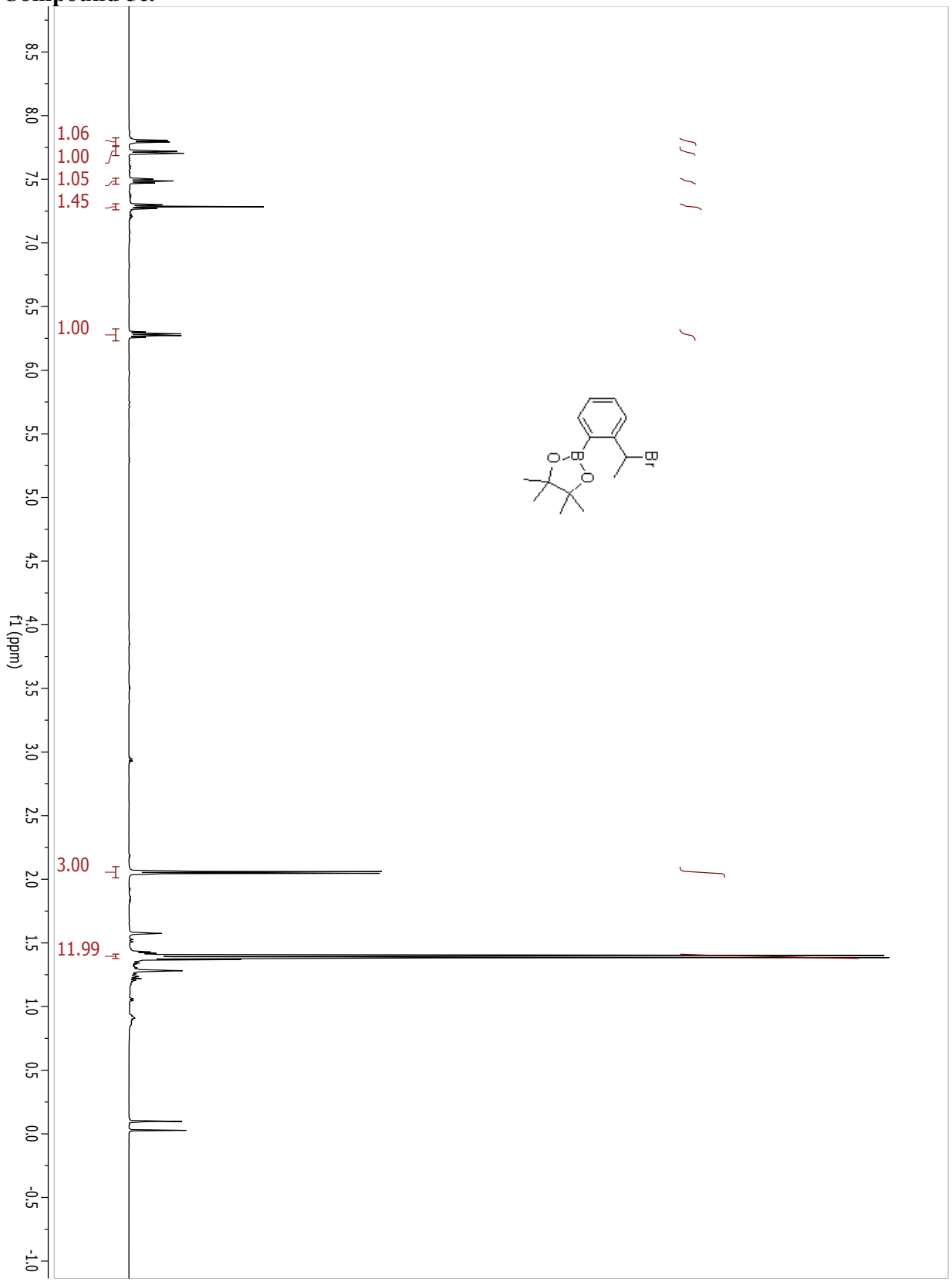
Selenide of Compound 5b.



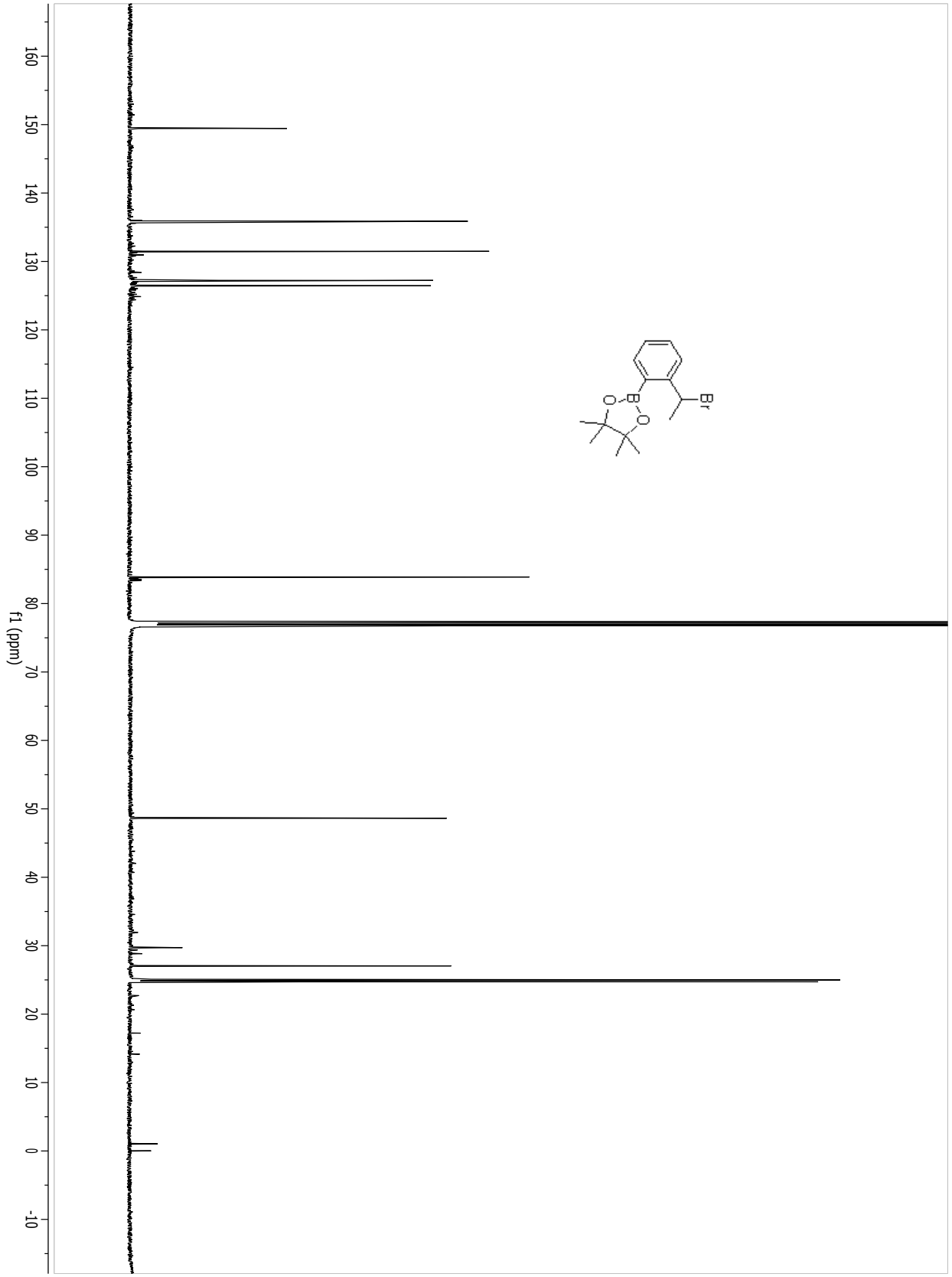
Selenide of Compound 5b.



Compound 5c.



Compound 5c.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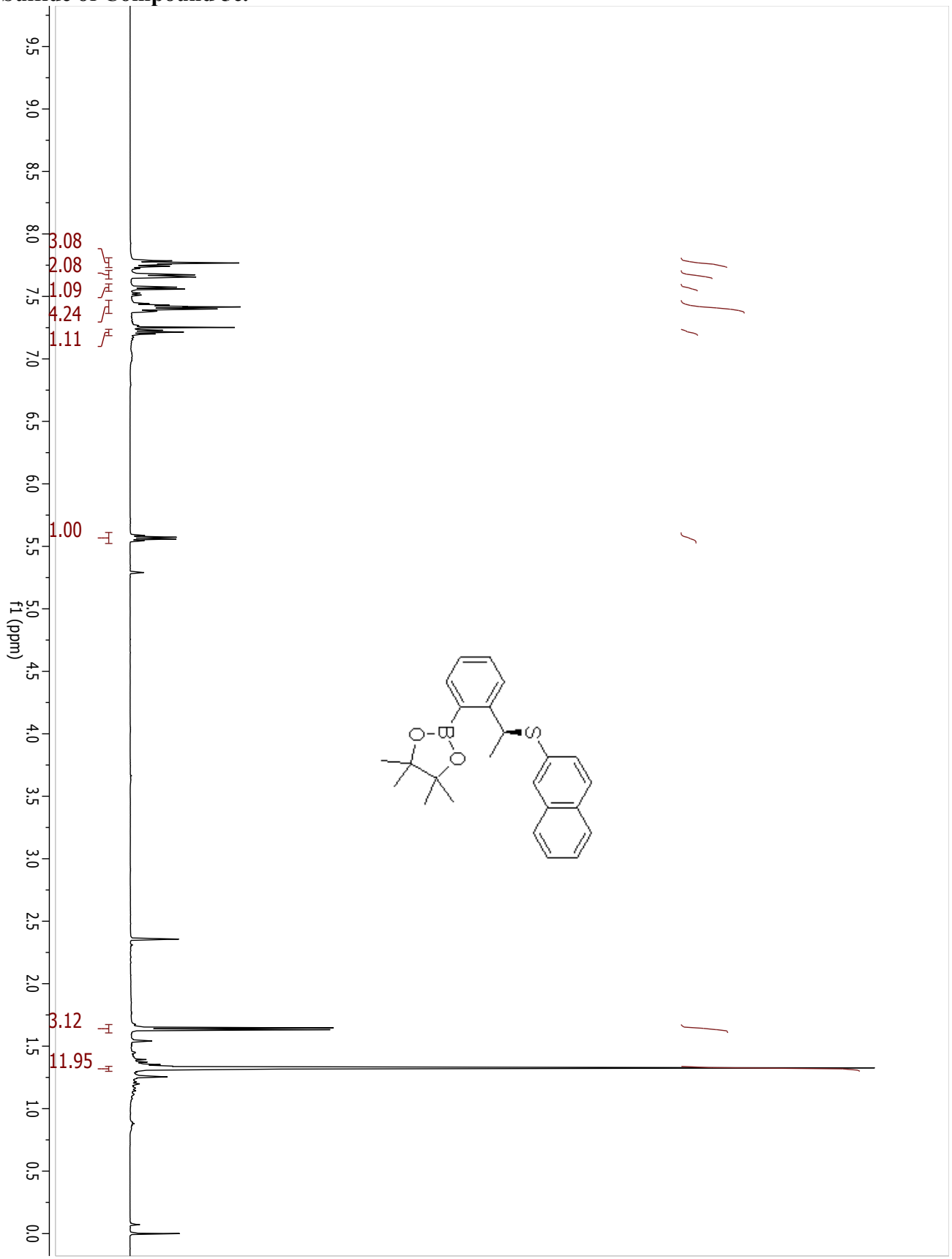
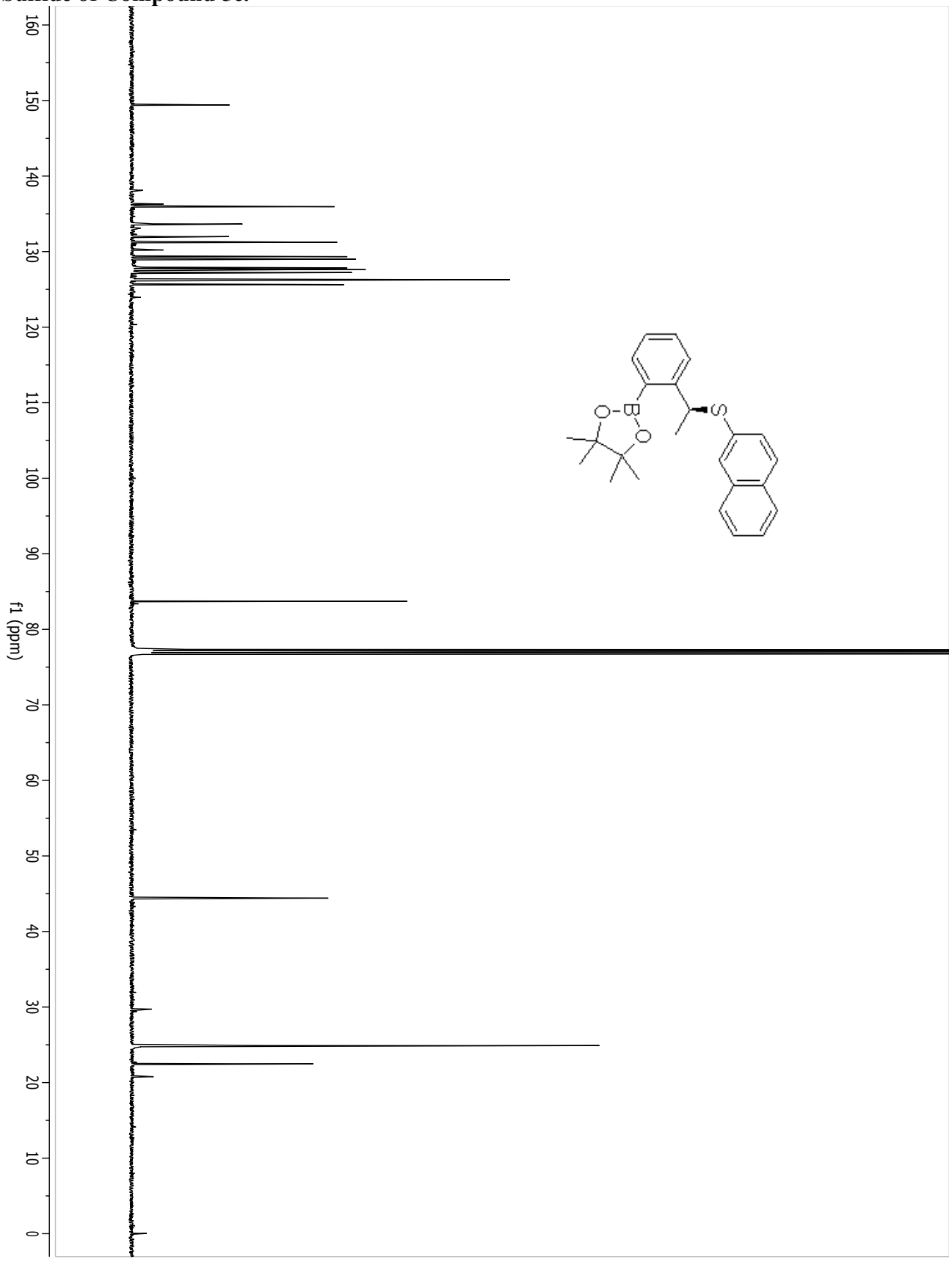
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)
B
O
O
Br

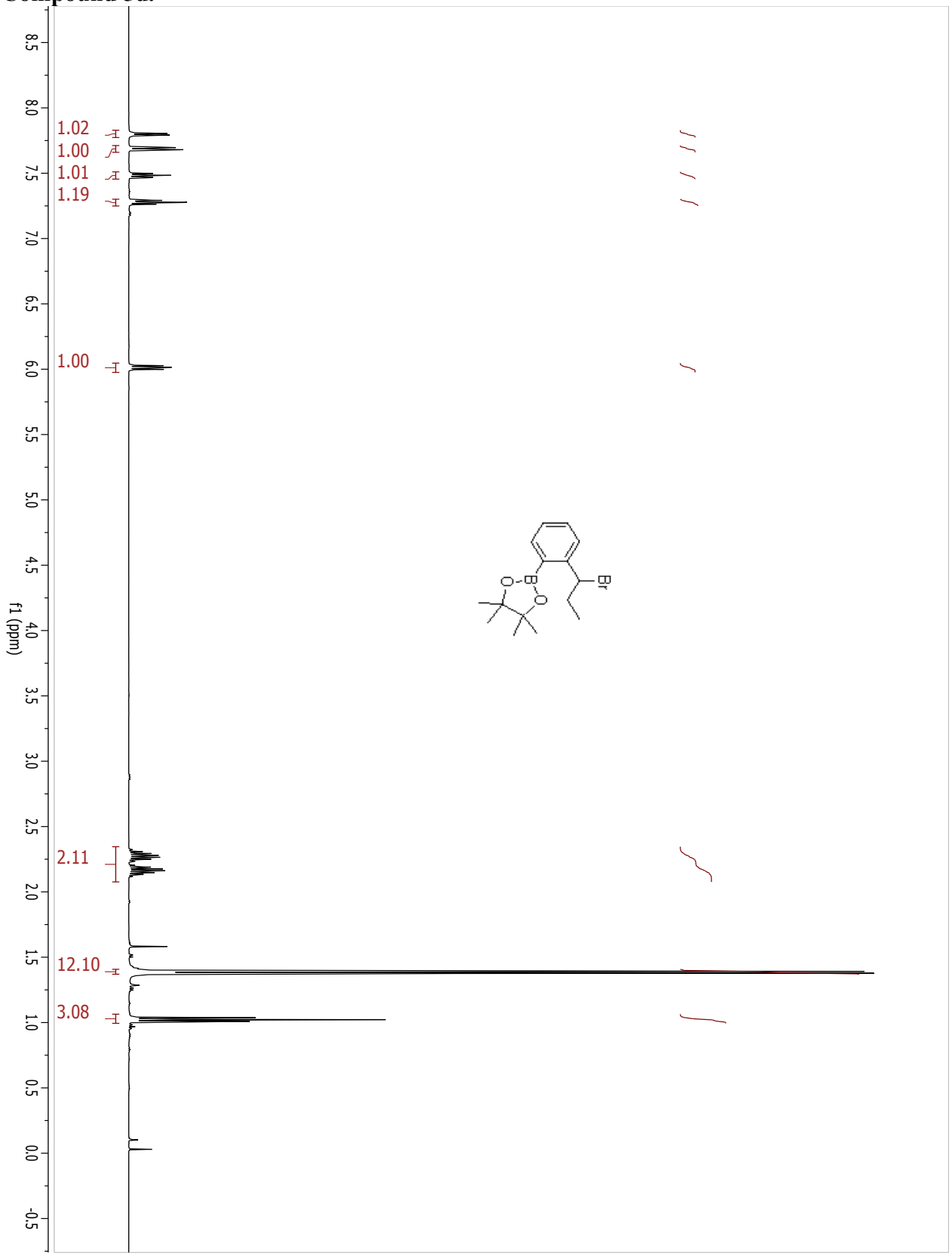
Sulfide of Compound 5c.



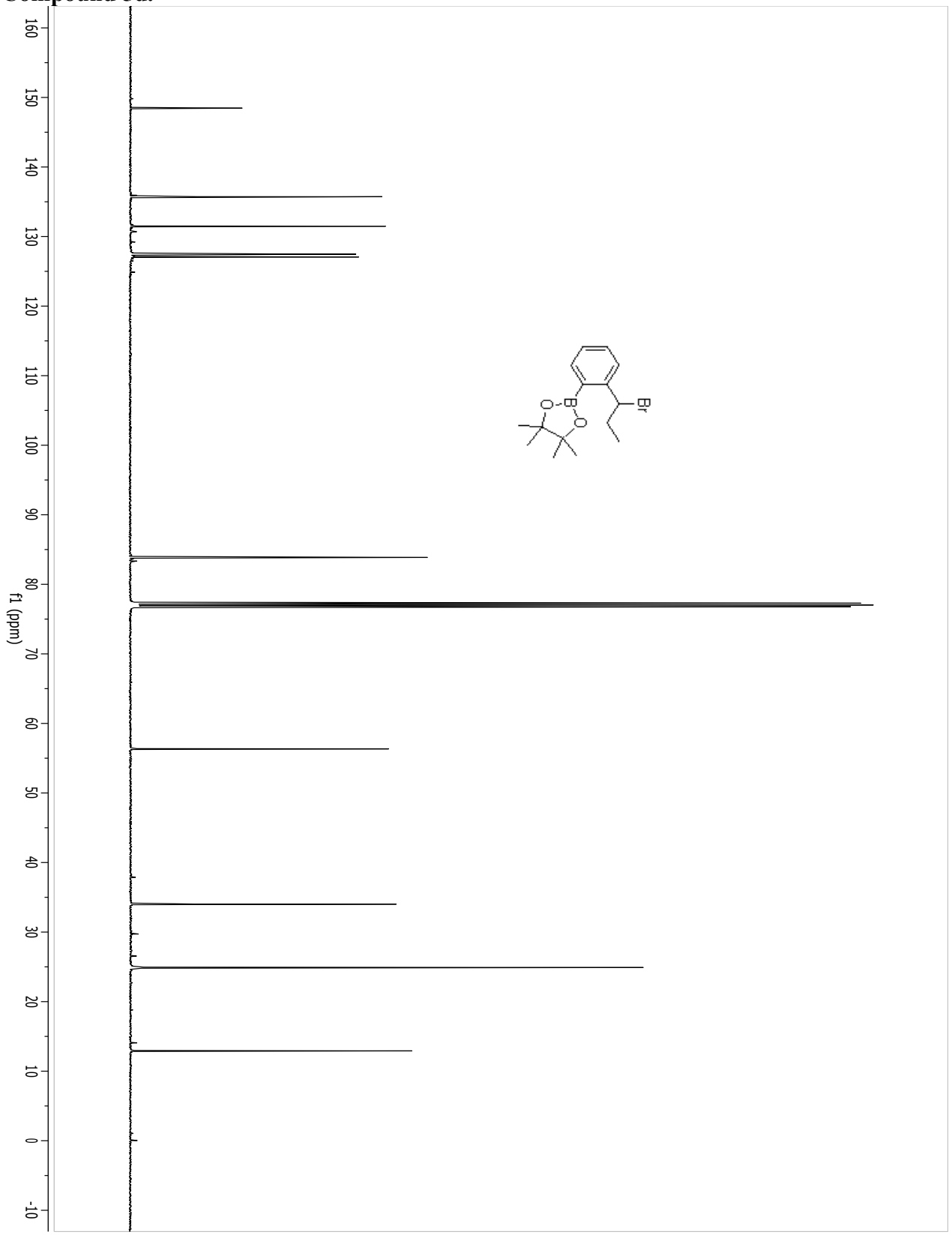
Sulfide of Compound 5c.



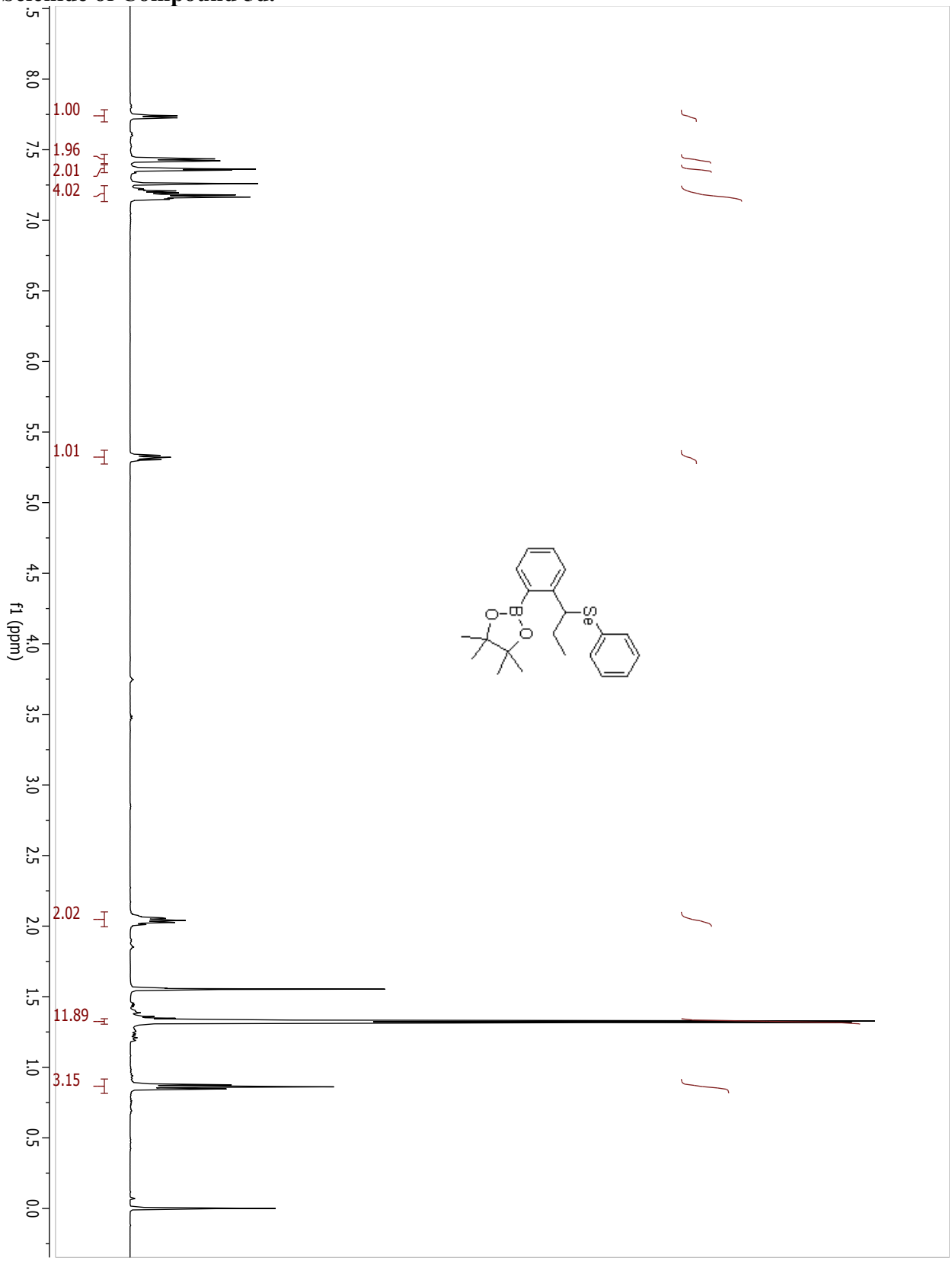
Compound 5d.



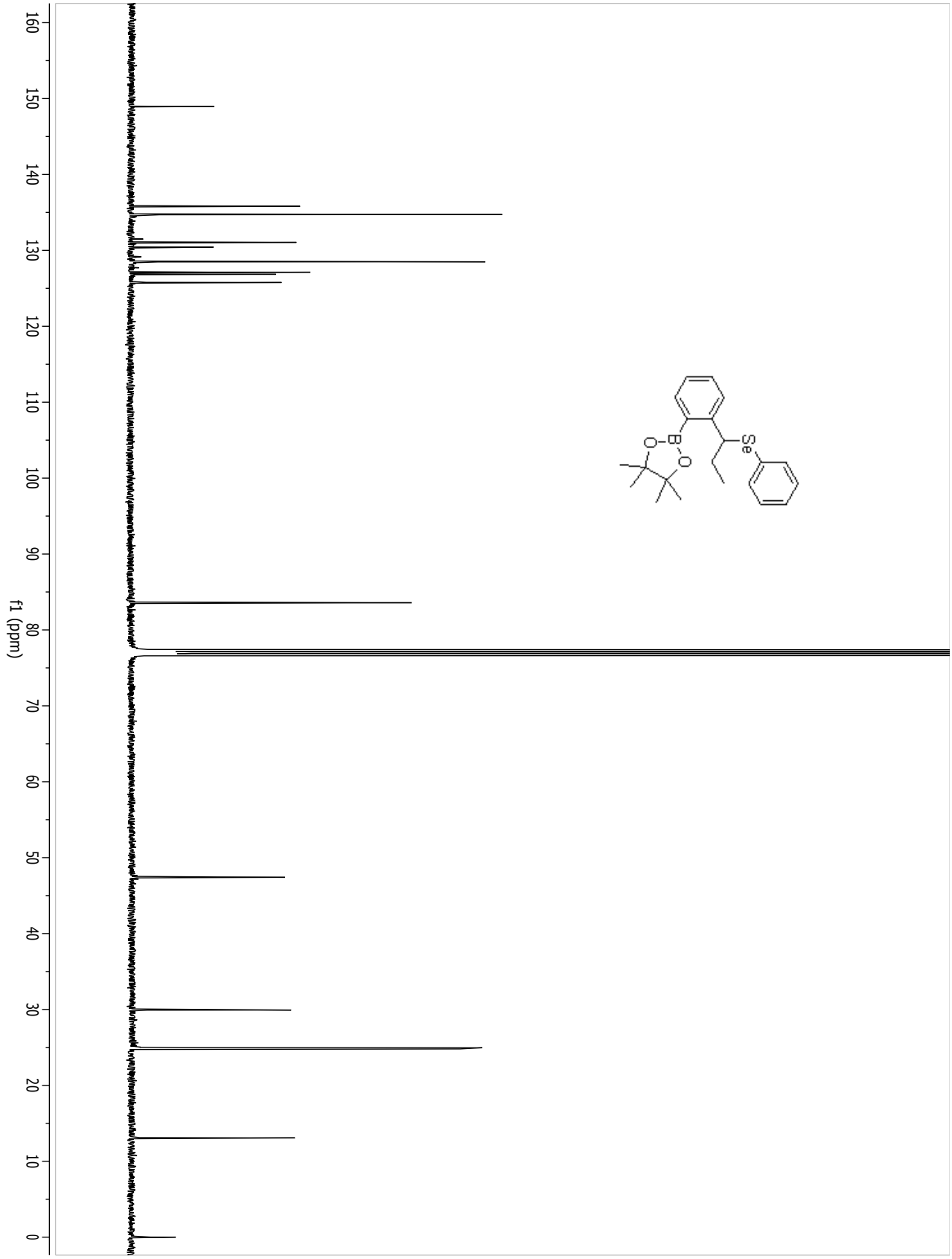
Compound 5d.


160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)
B
O
O
Br

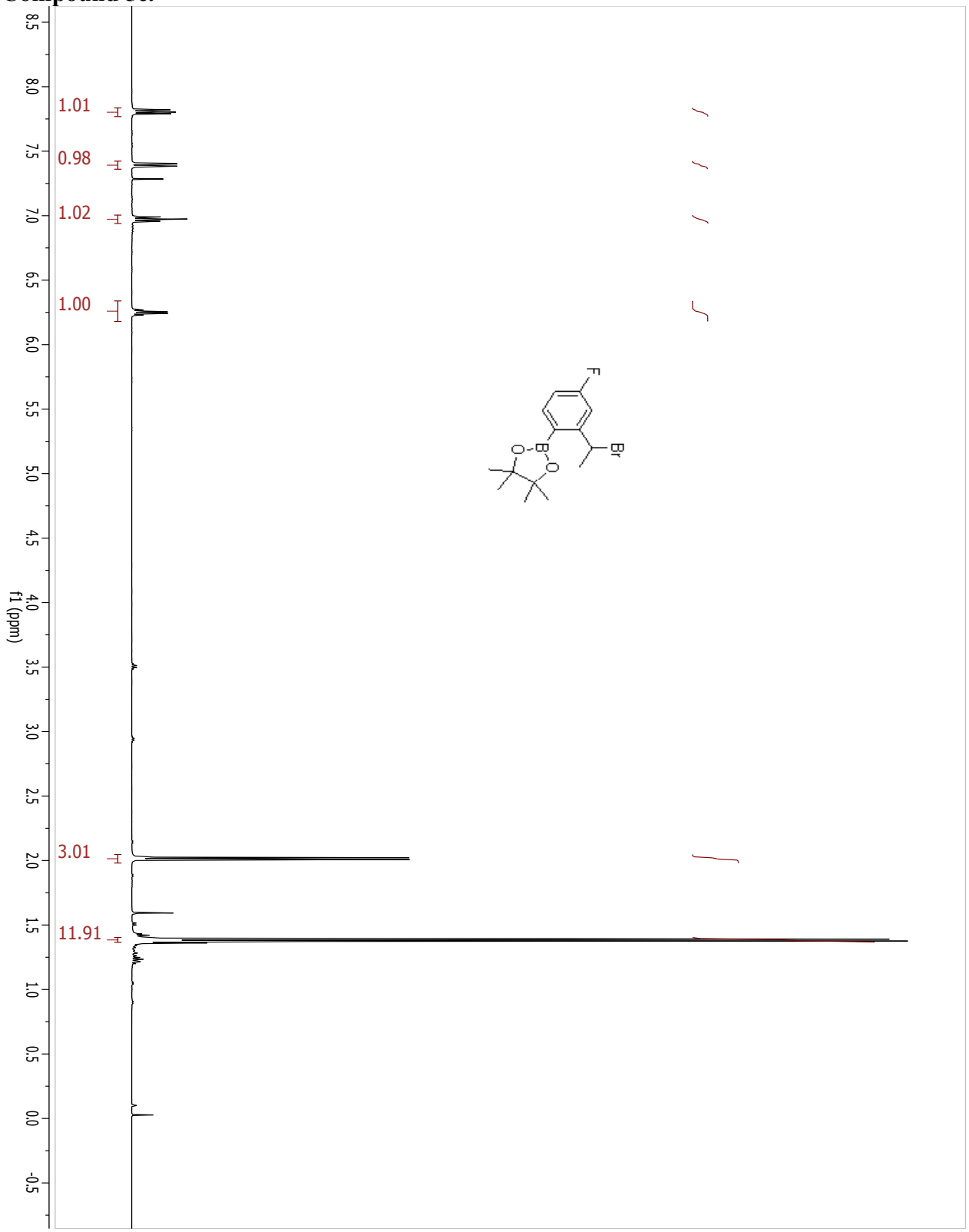
Selenide of Compound 5d.



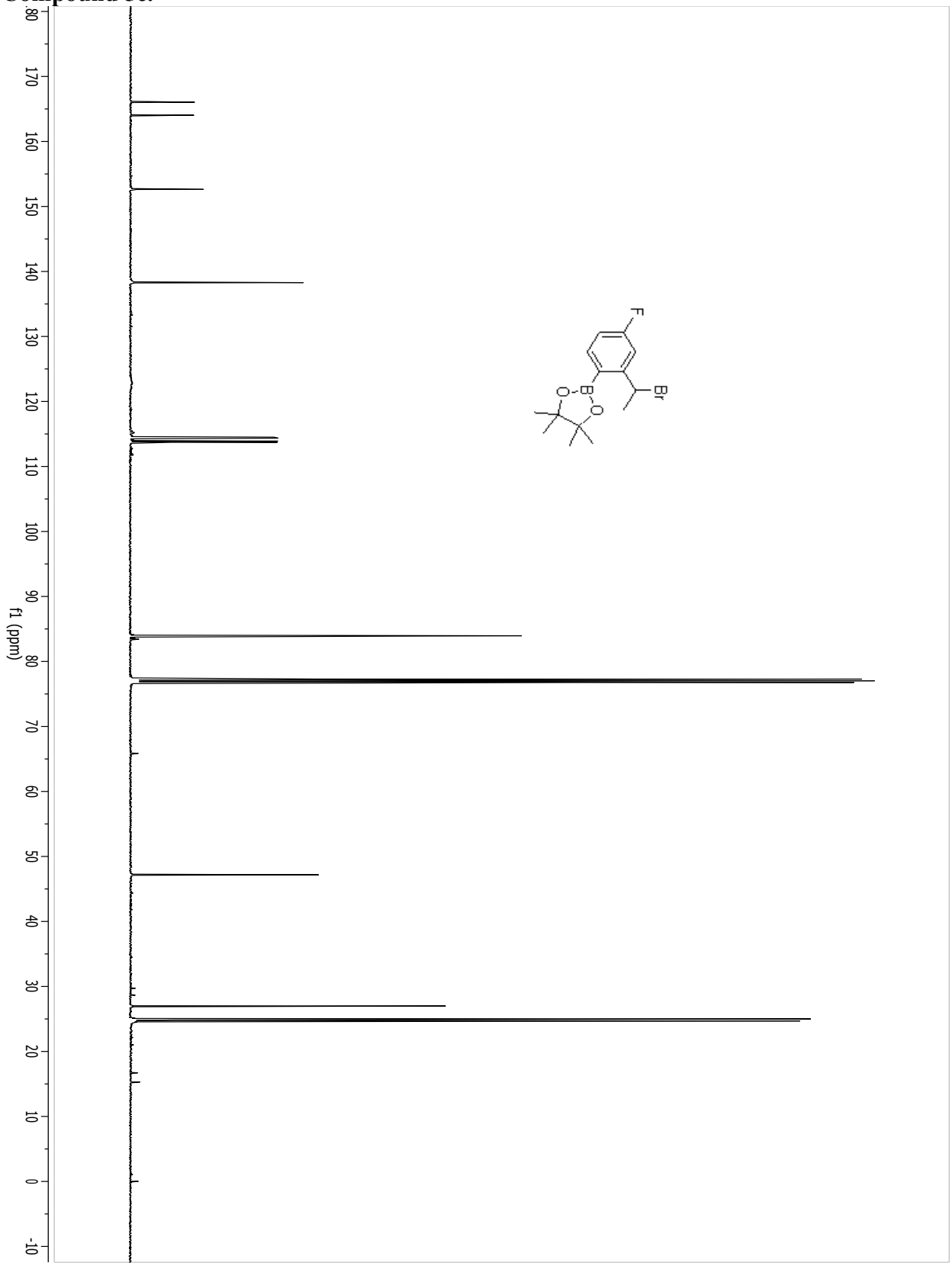
Selenide of Compound 5d.



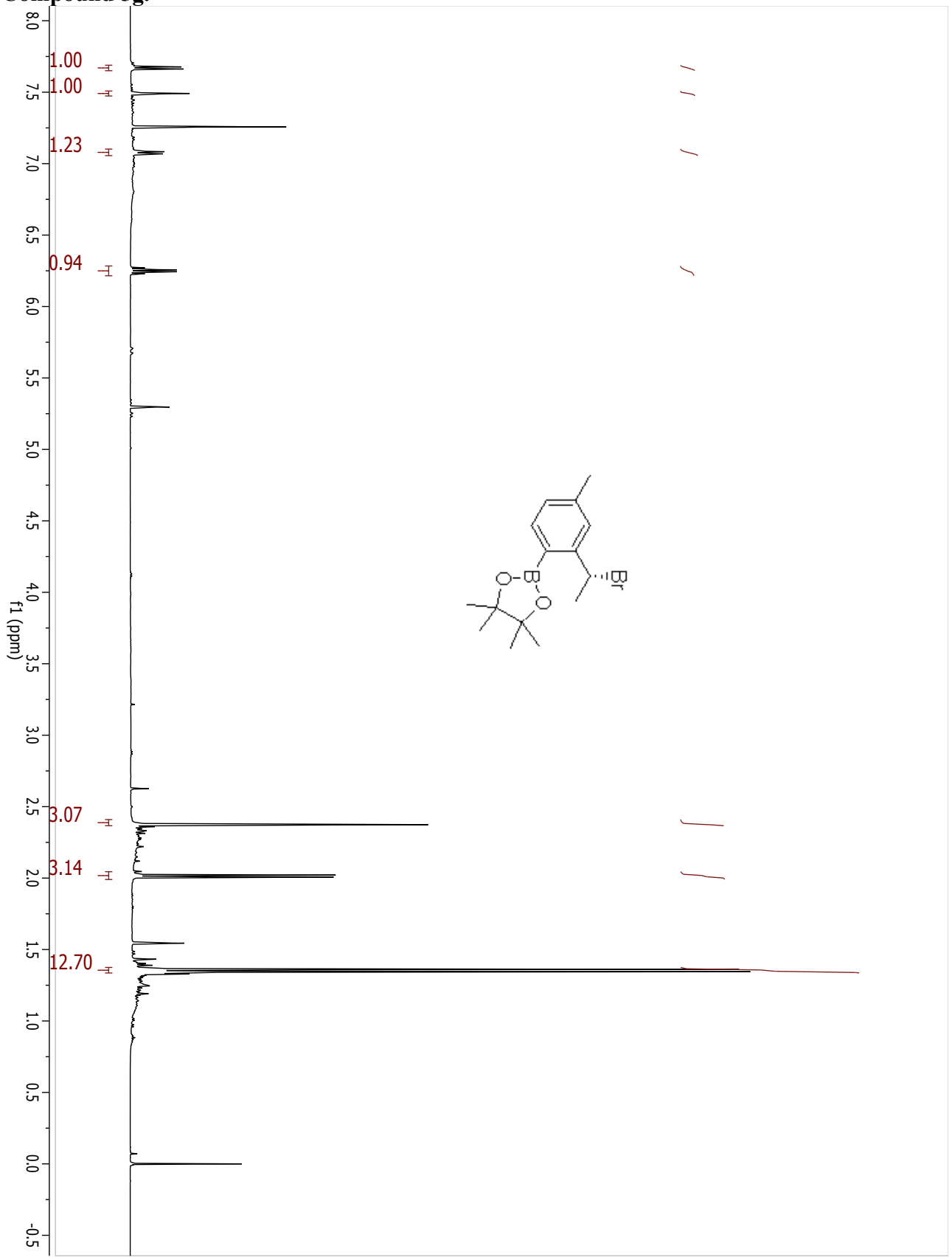
Compound 5e.



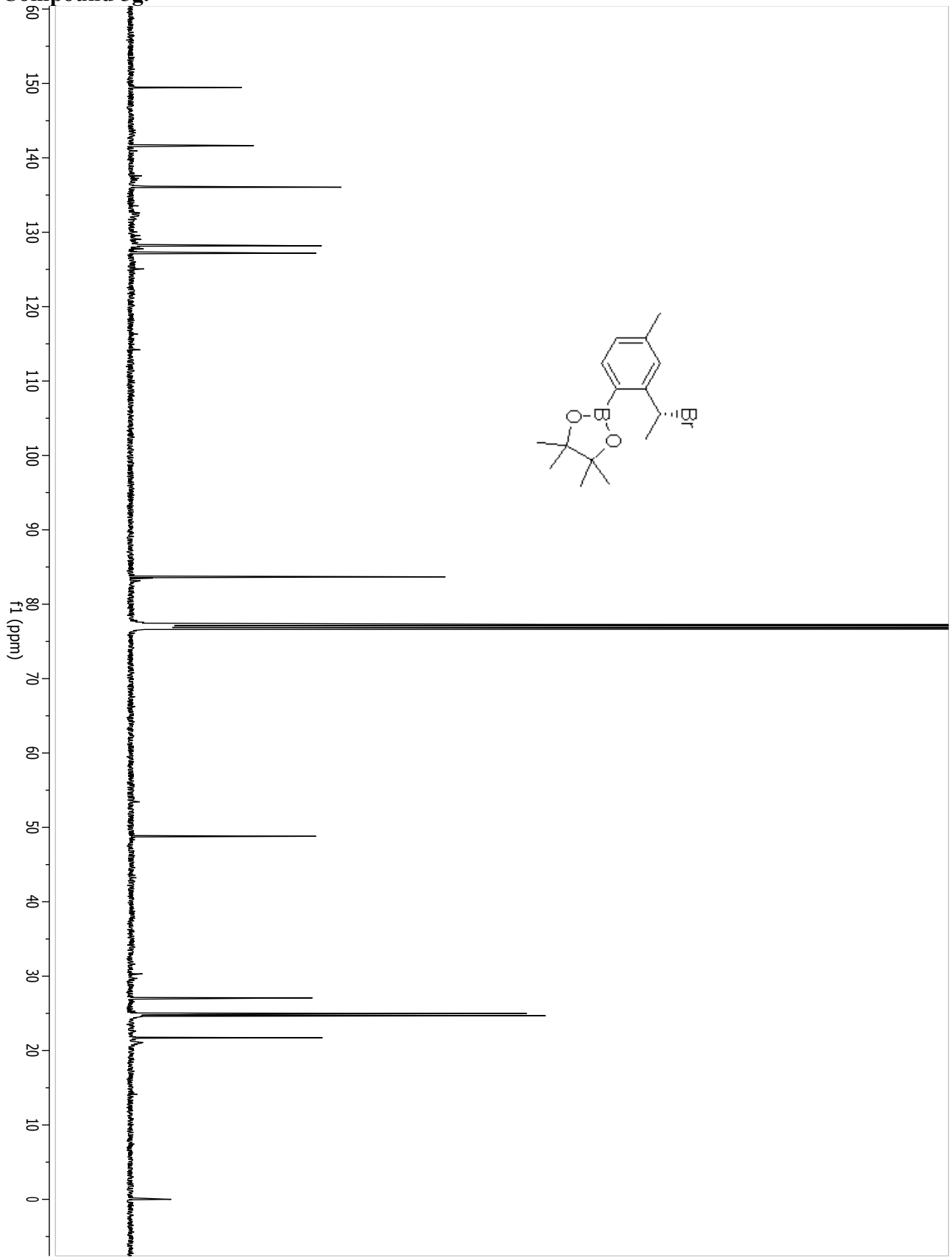
Compound 5e.


F
B
O
O
Br
f1 (ppm)
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10

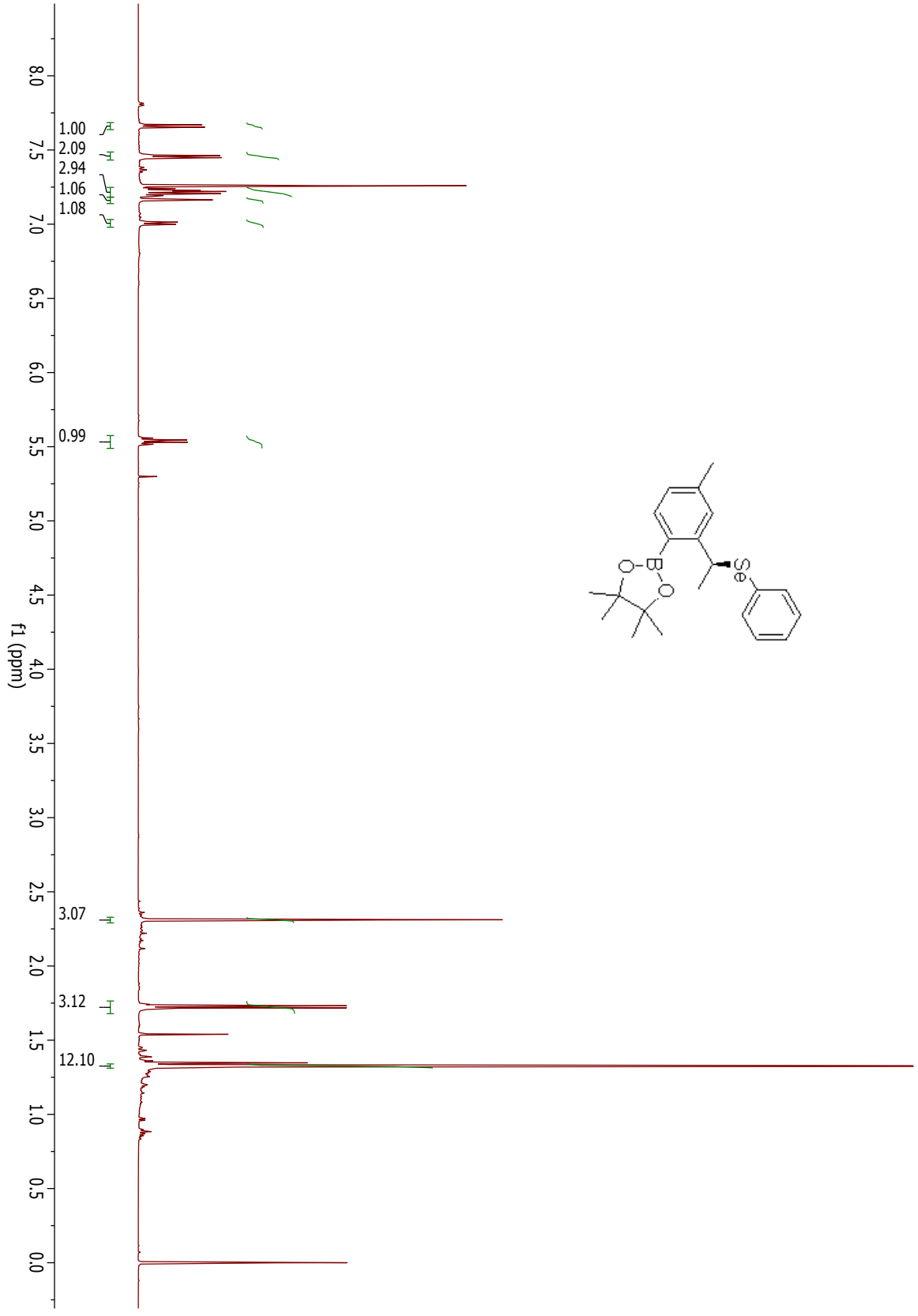
Compound 5g.



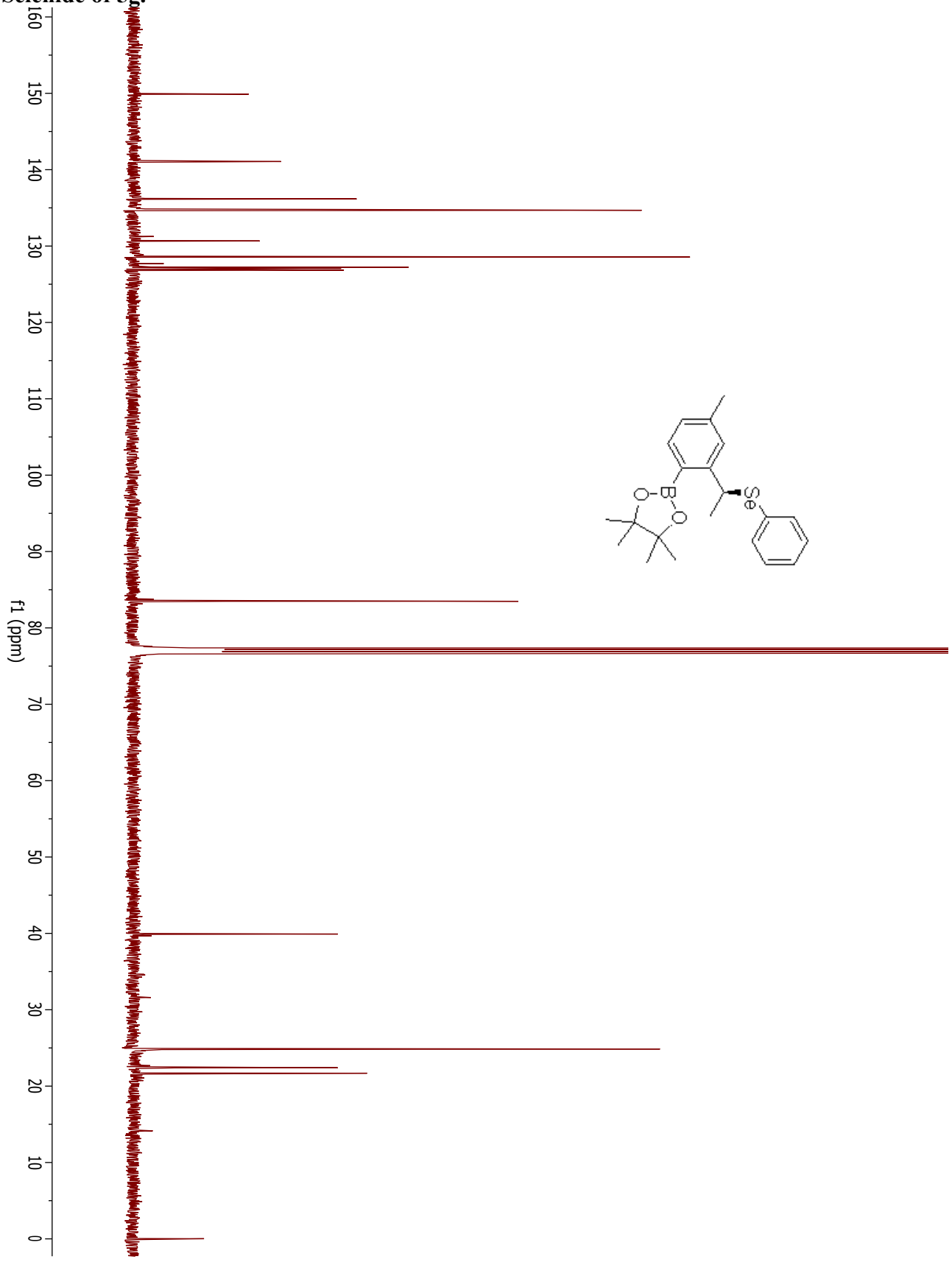
Compound 5g.



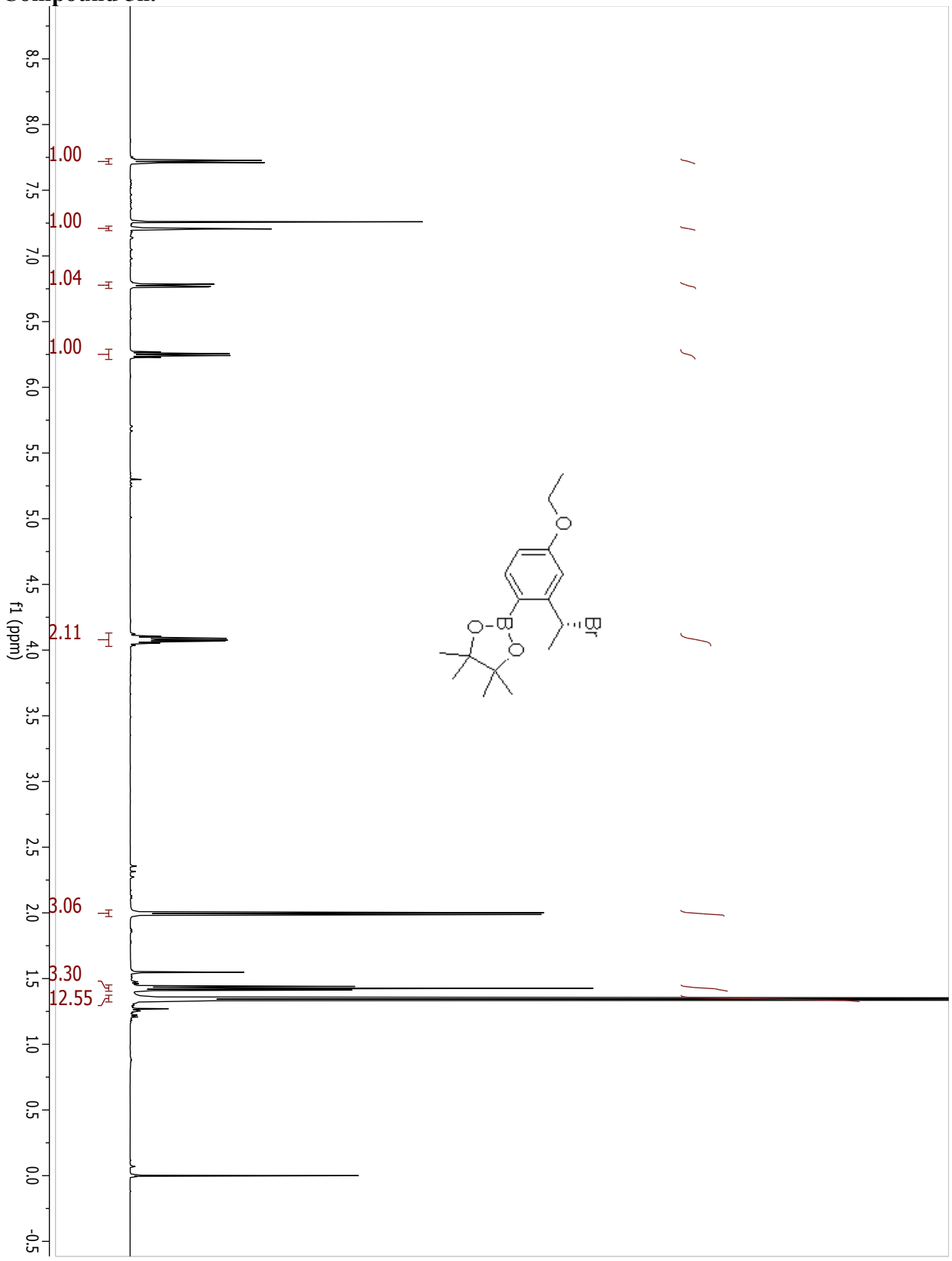
Selenide of 5g.



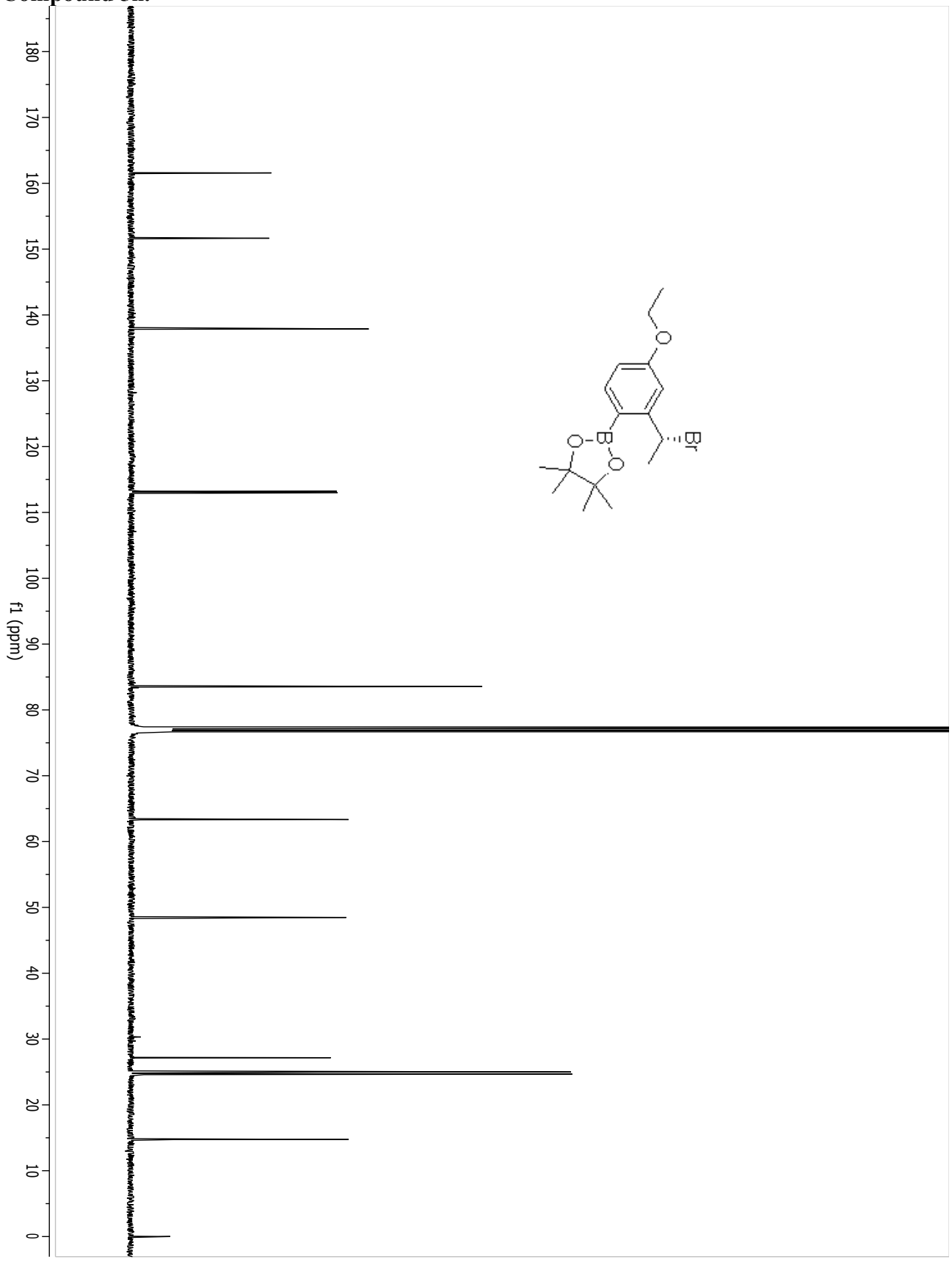
Selenide of 5g.



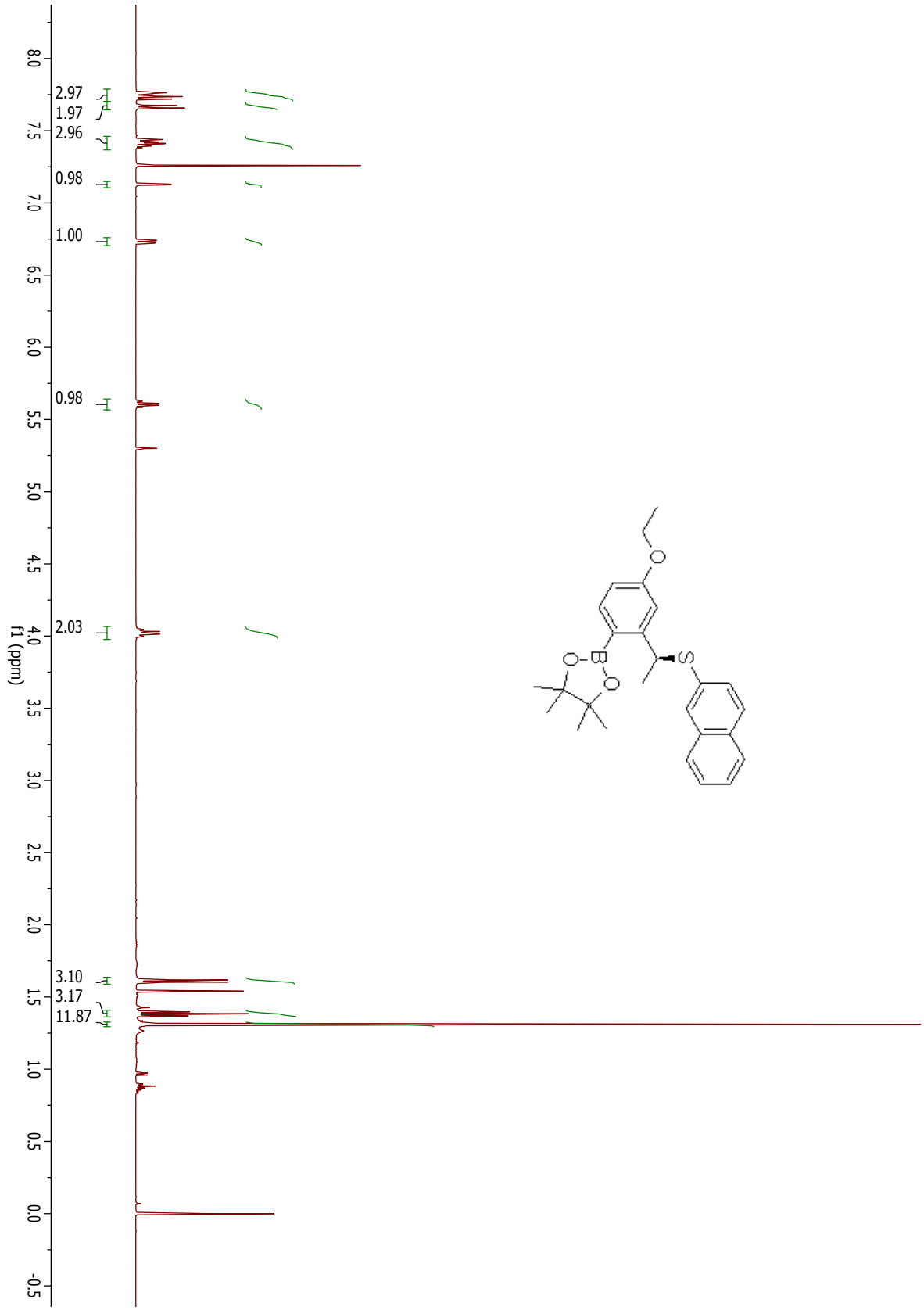
Compound 5h.



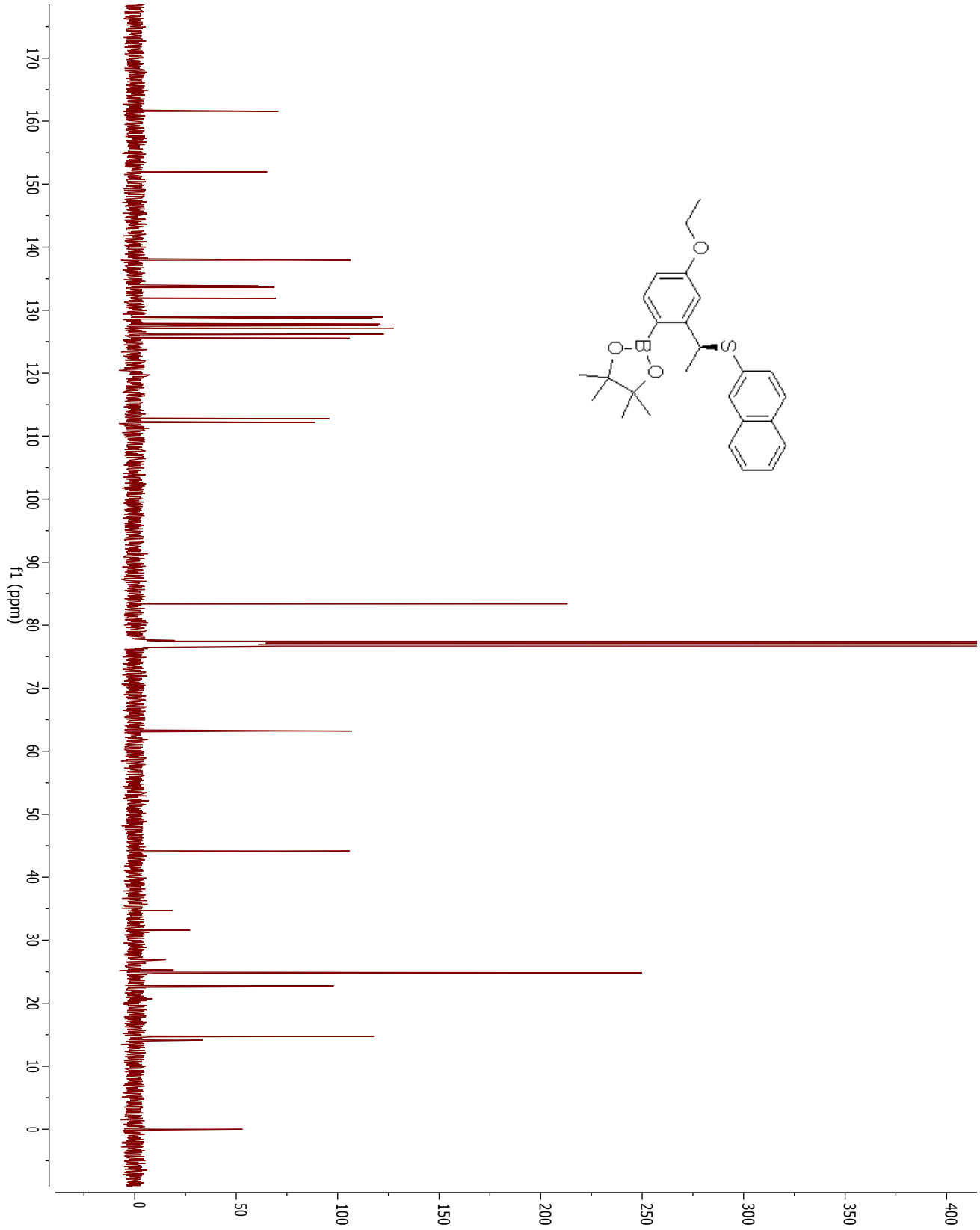
Compound 5h.


f1 (ppm)
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
O
B
O
O
Br

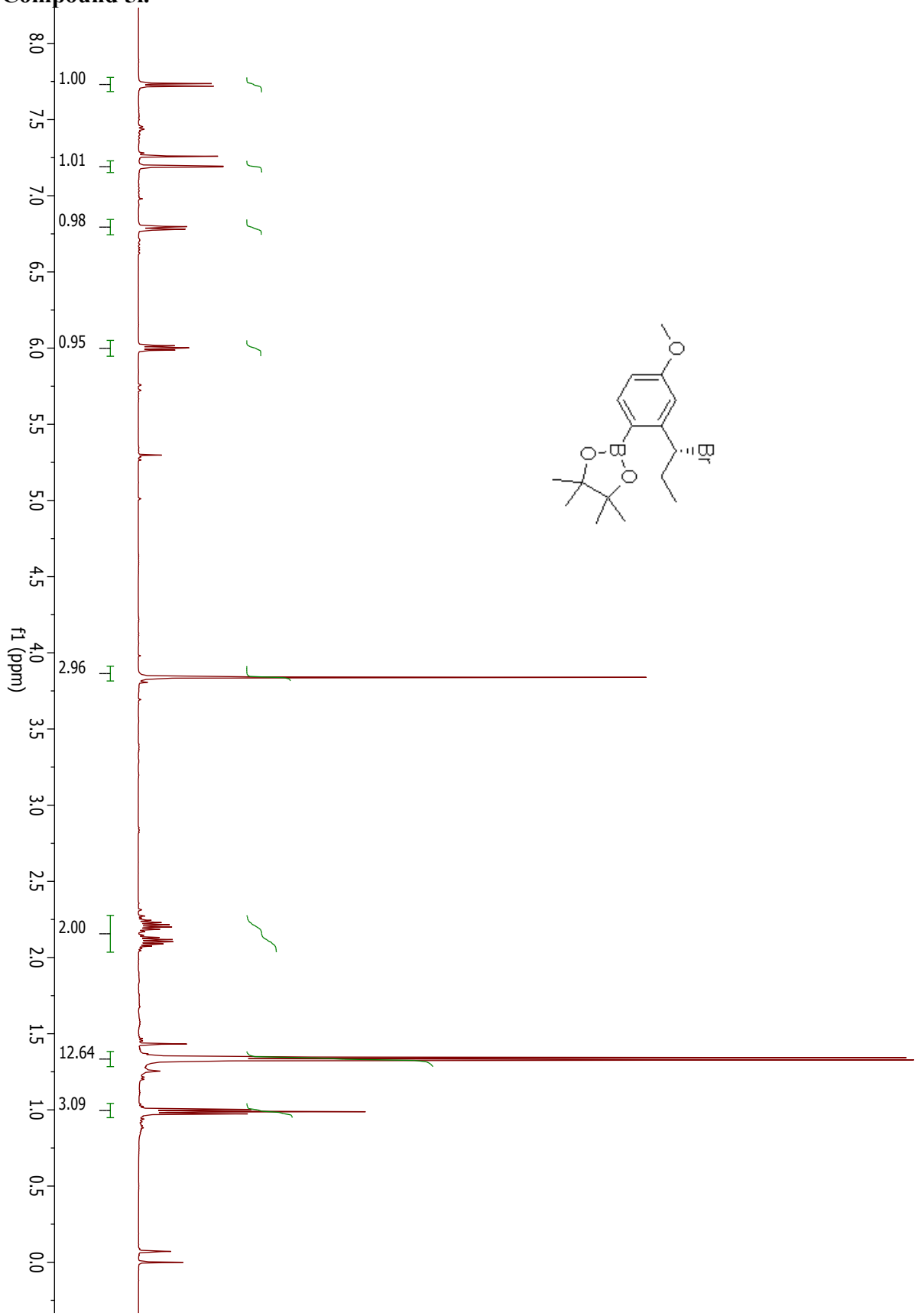
Sulfide for 5h.



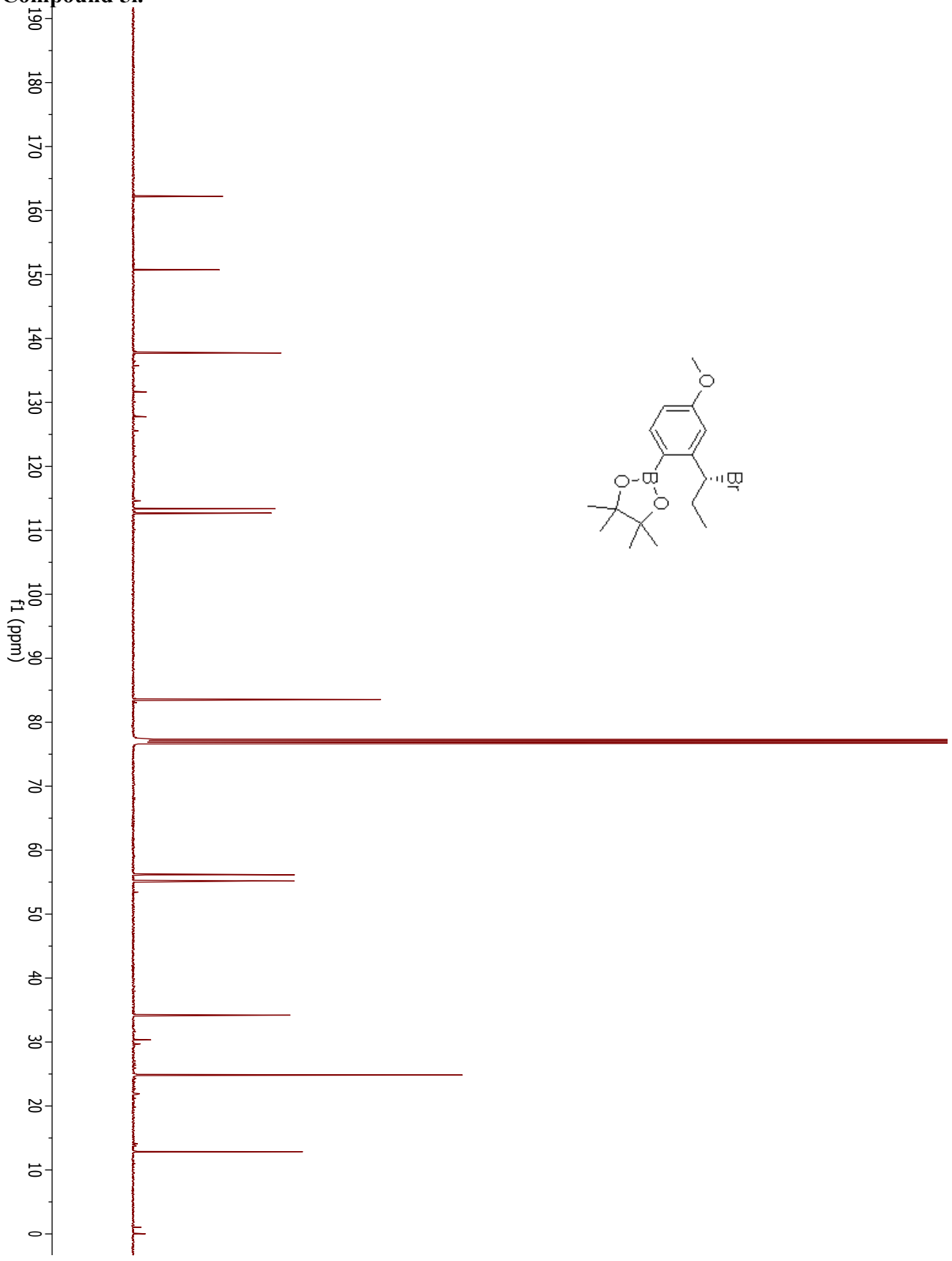
Sulfide for 5h.



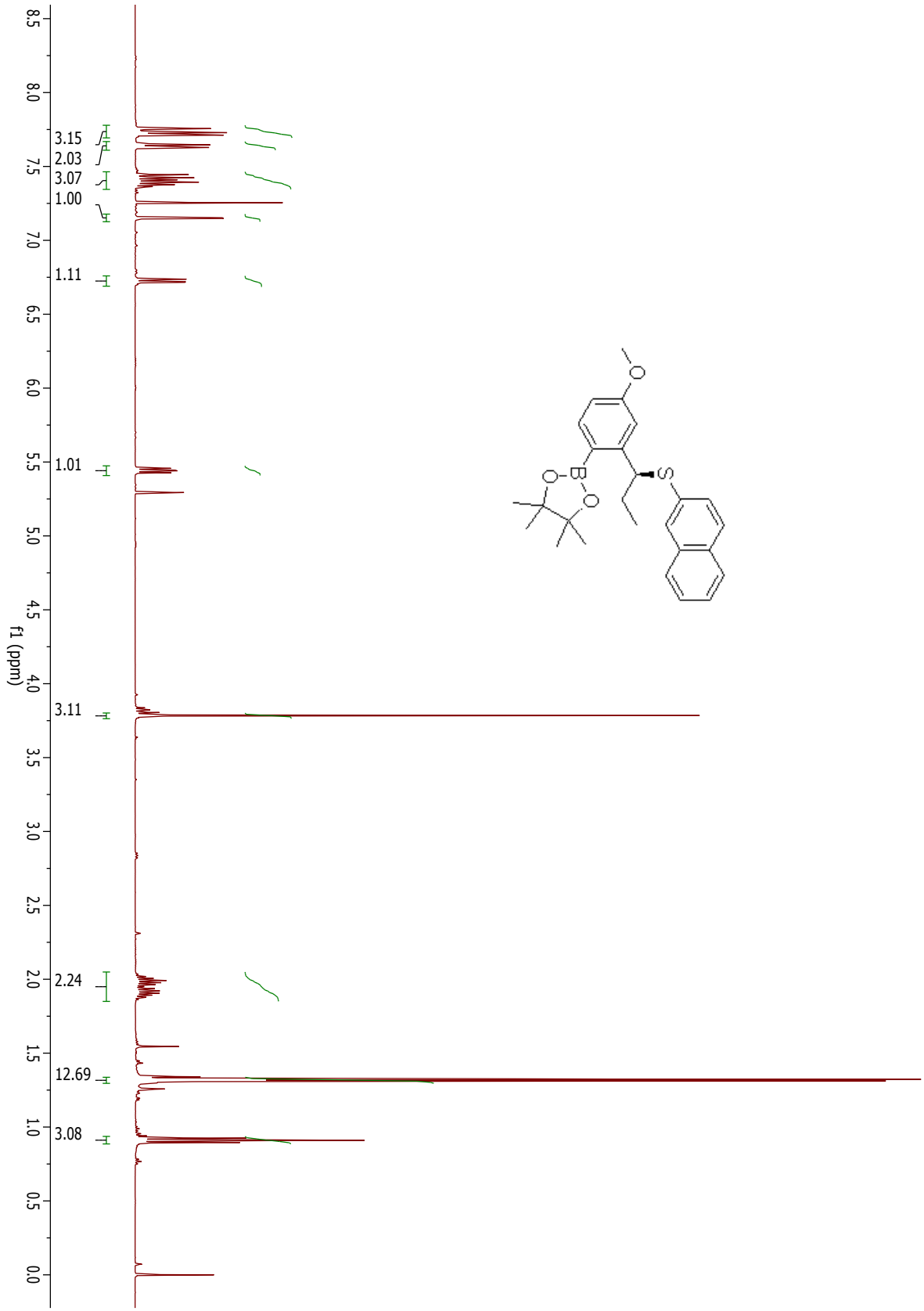
Compound 5i.


8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)
1.00
1.01
0.98
0.95
2.96
2.00
12.64
3.09
O
B
O
O
Br

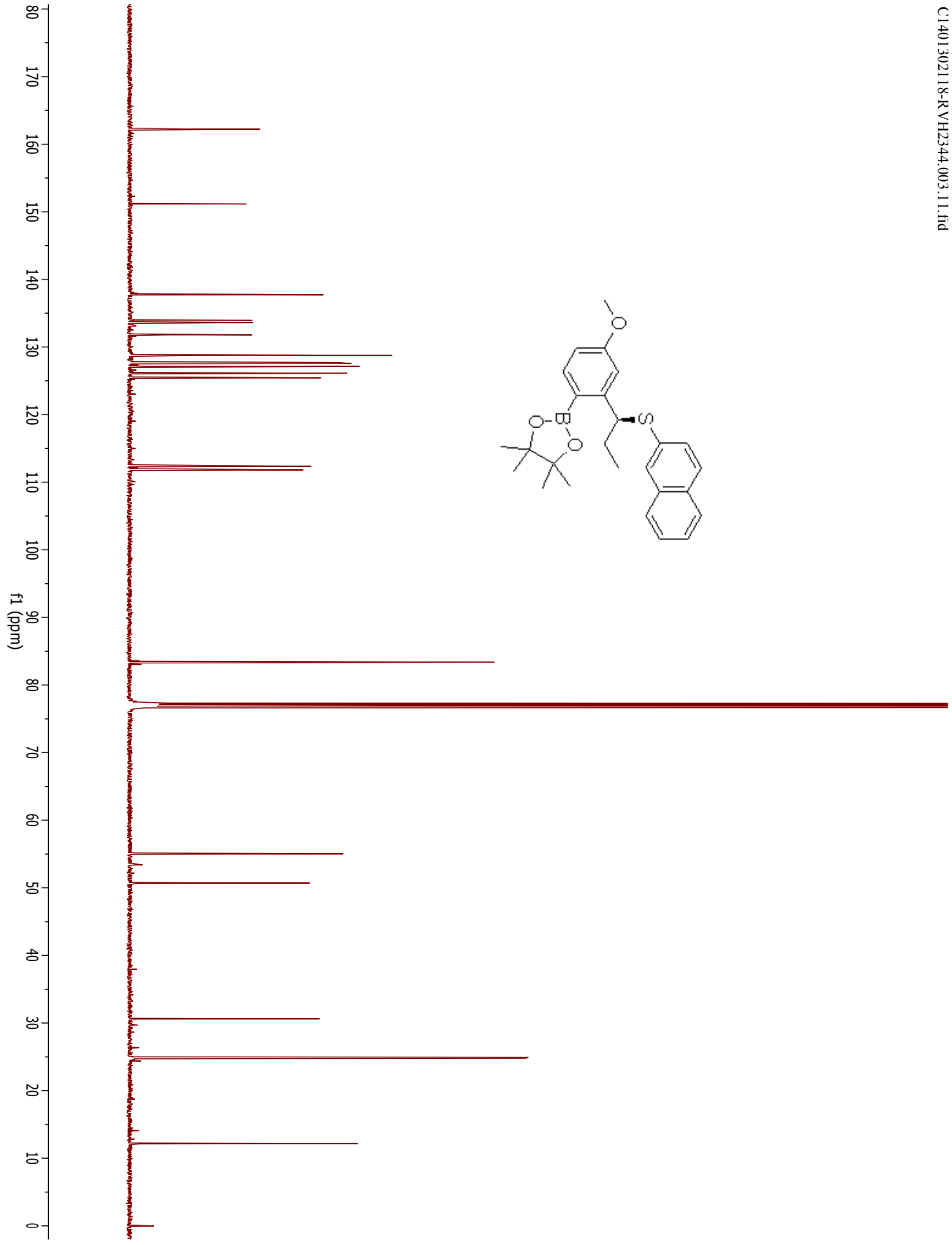
Compound 5i.


f1 (ppm)
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
O
B
O
O
Br

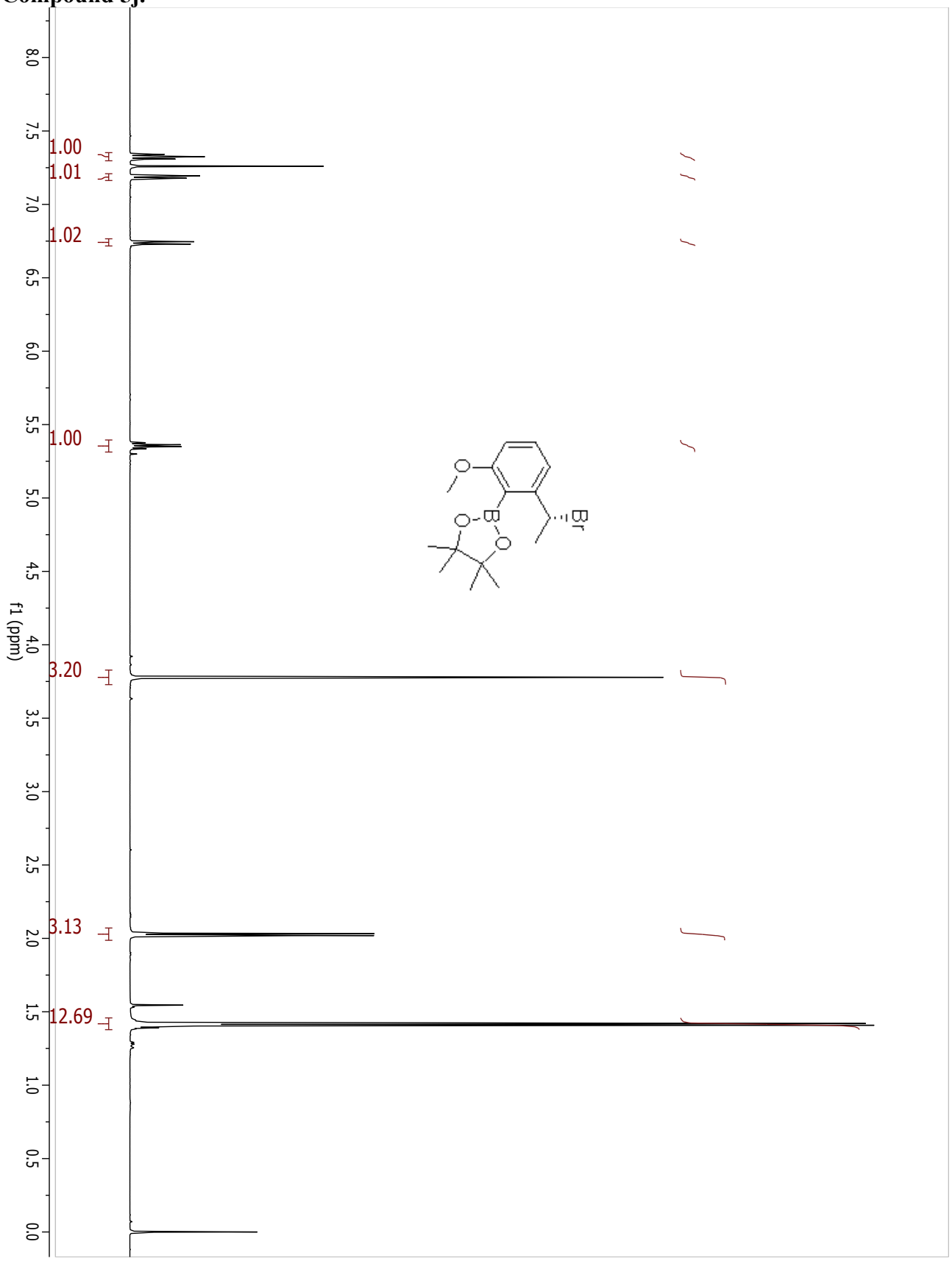
Sulfide of 5i.



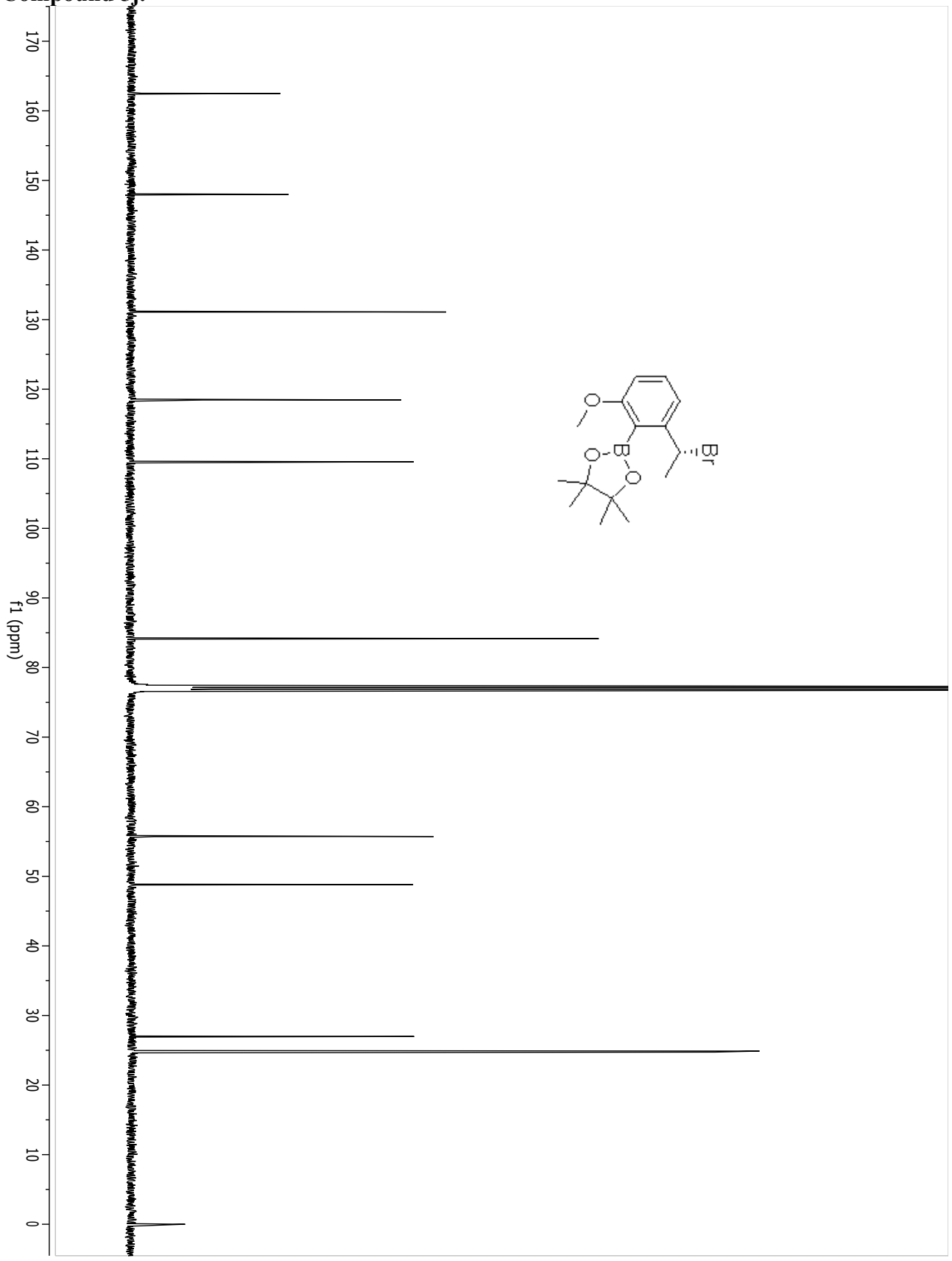
Sulfide of 5i.



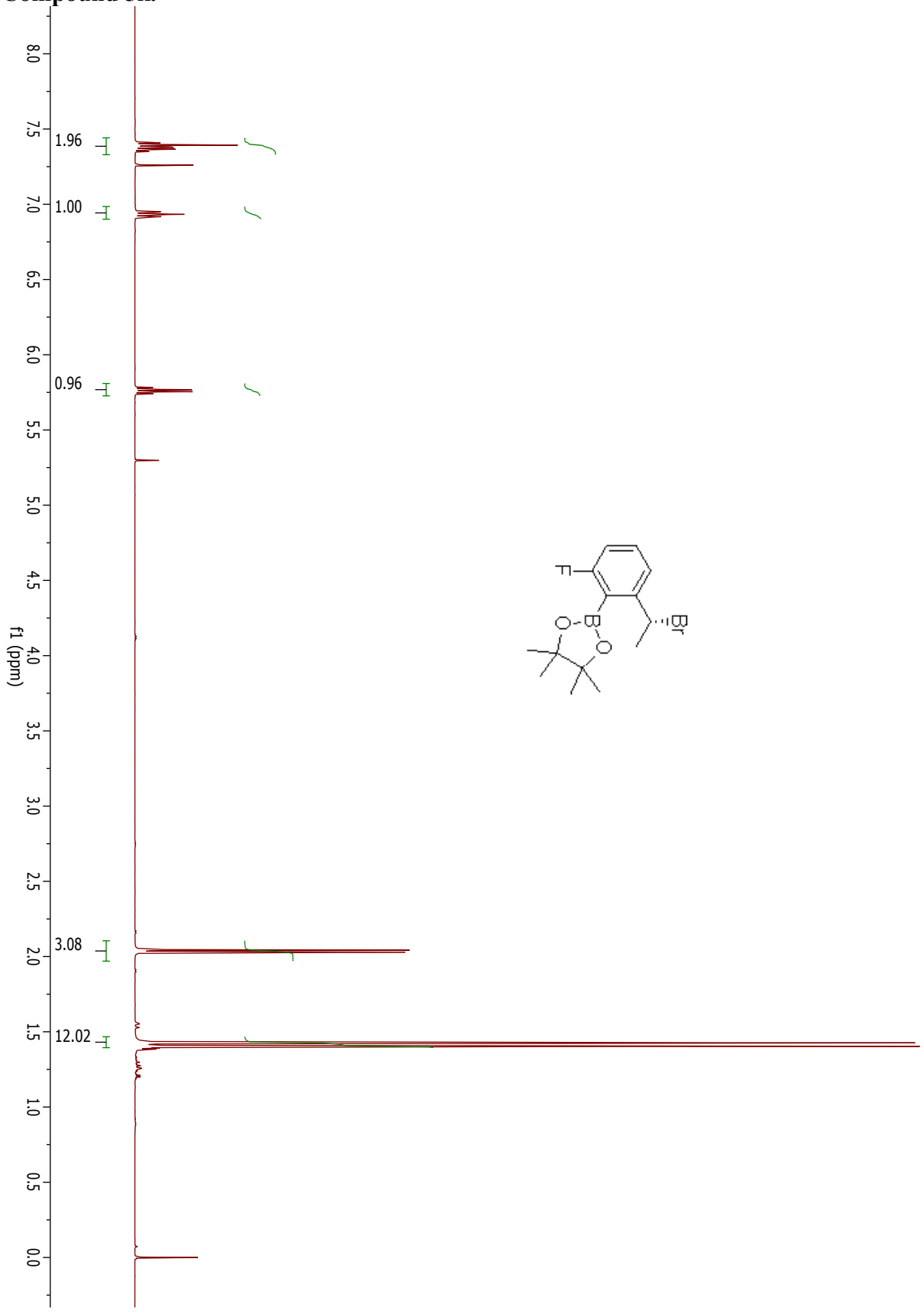
Compound 5j.



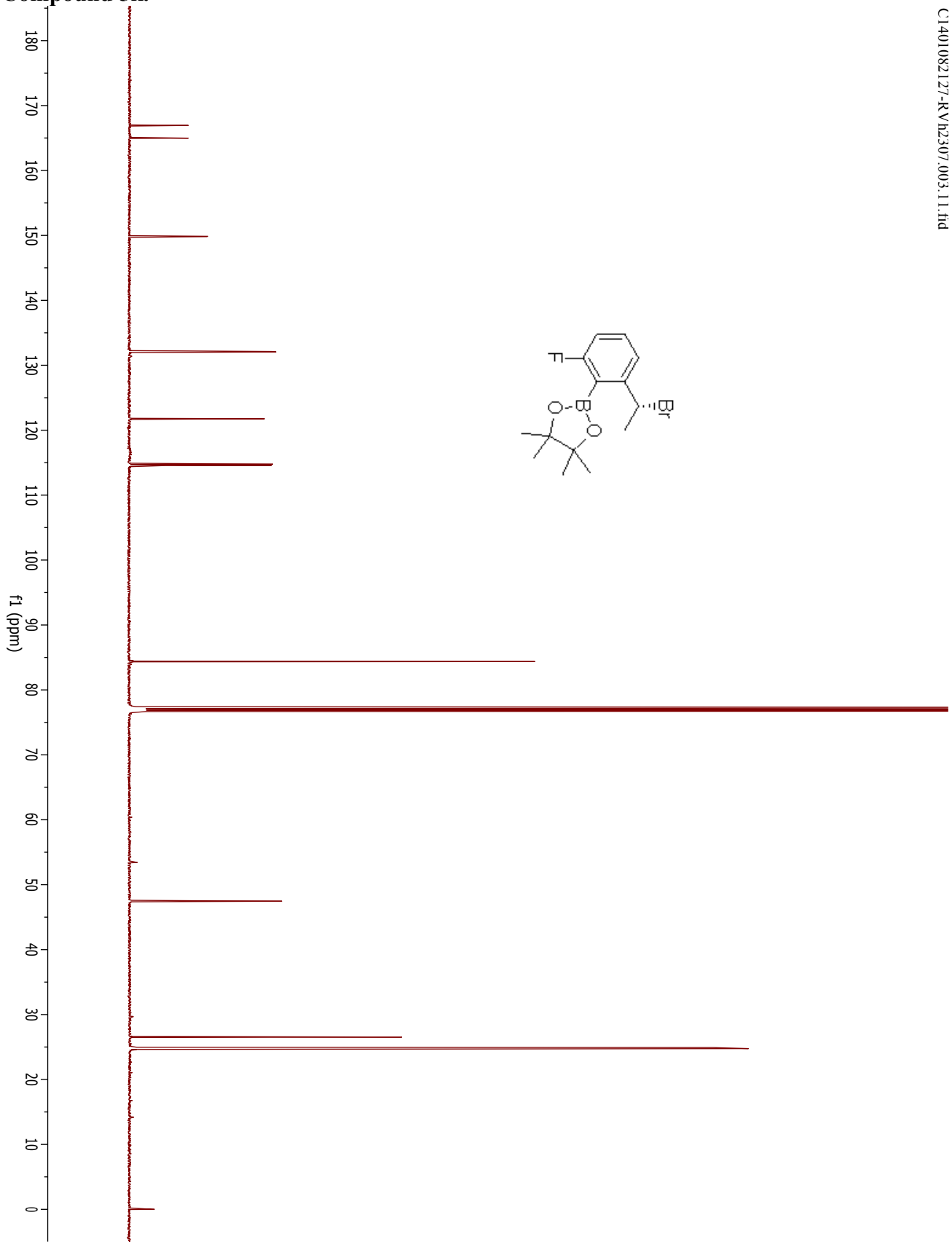
Compound 5j.


f1 (ppm)
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
O
B
O
O
Br

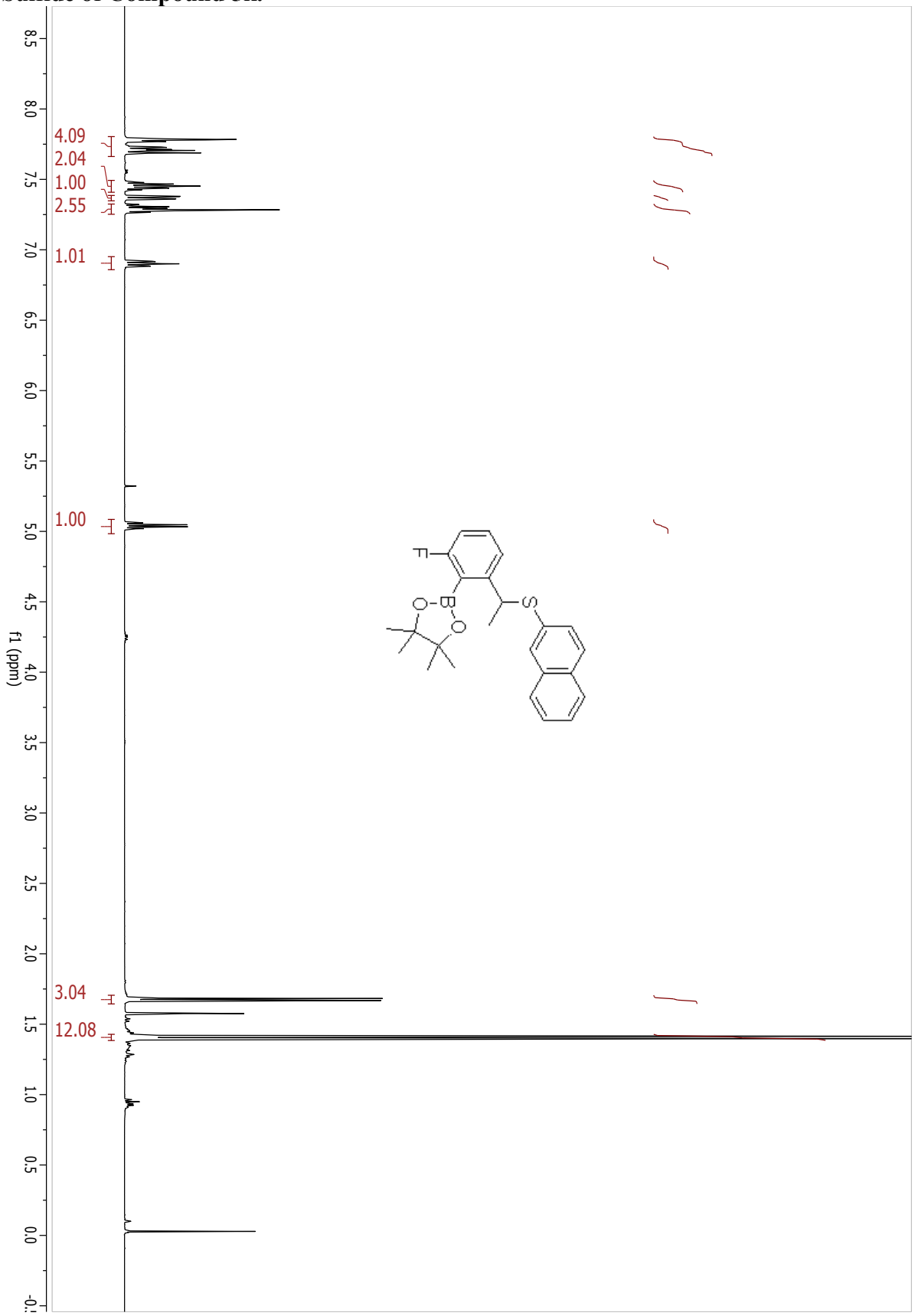
Compound 5k.


C1401082127-RVb2307.003.10.fid
1.96
1.00
0.96
3.08
12.02
f1 (ppm)
F
B
O
O
Br

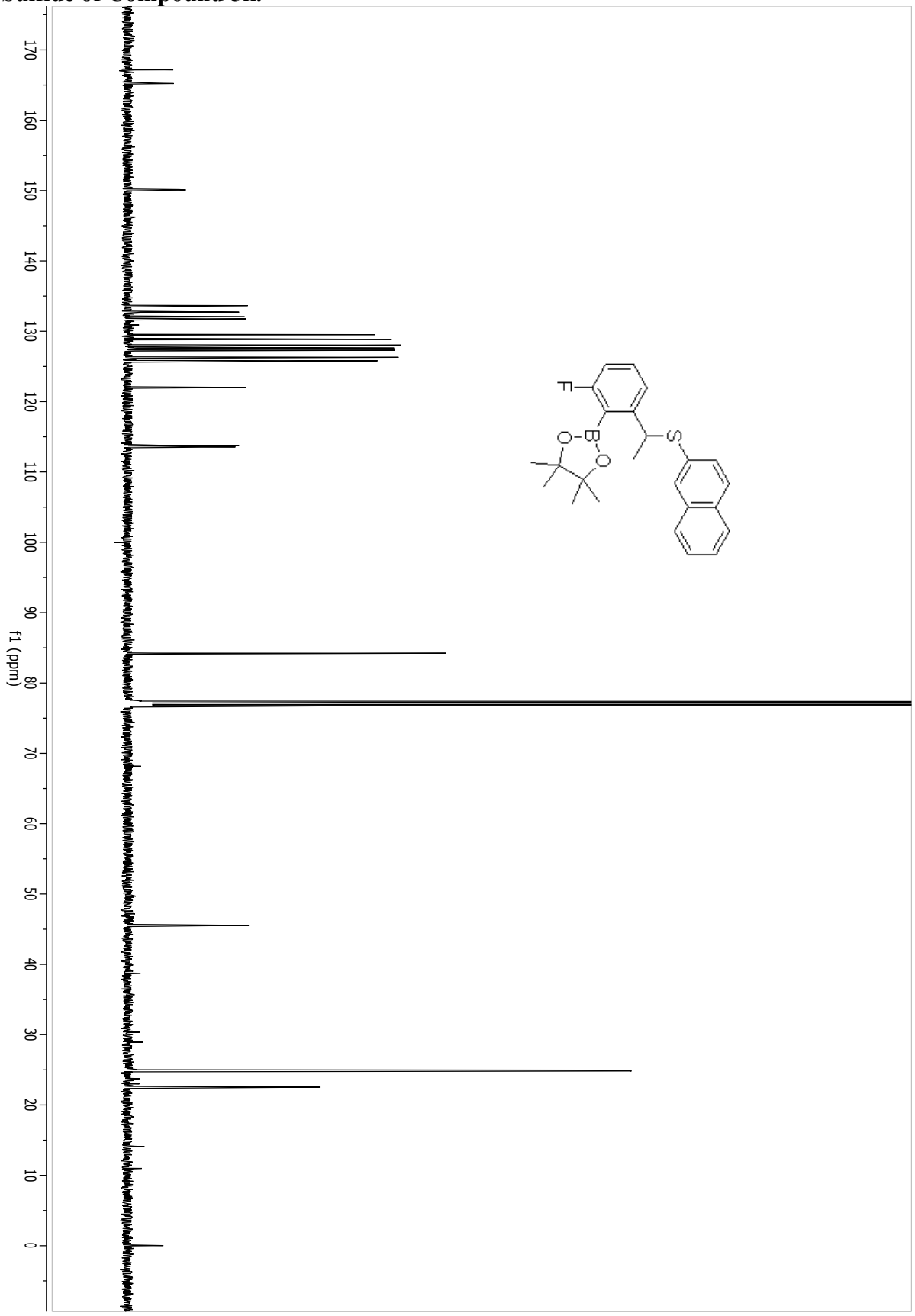
Compound 5k.


C140108212 7-RVh2307.003.11.fid
F
B
O
O
Br
f1 (ppm)
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0

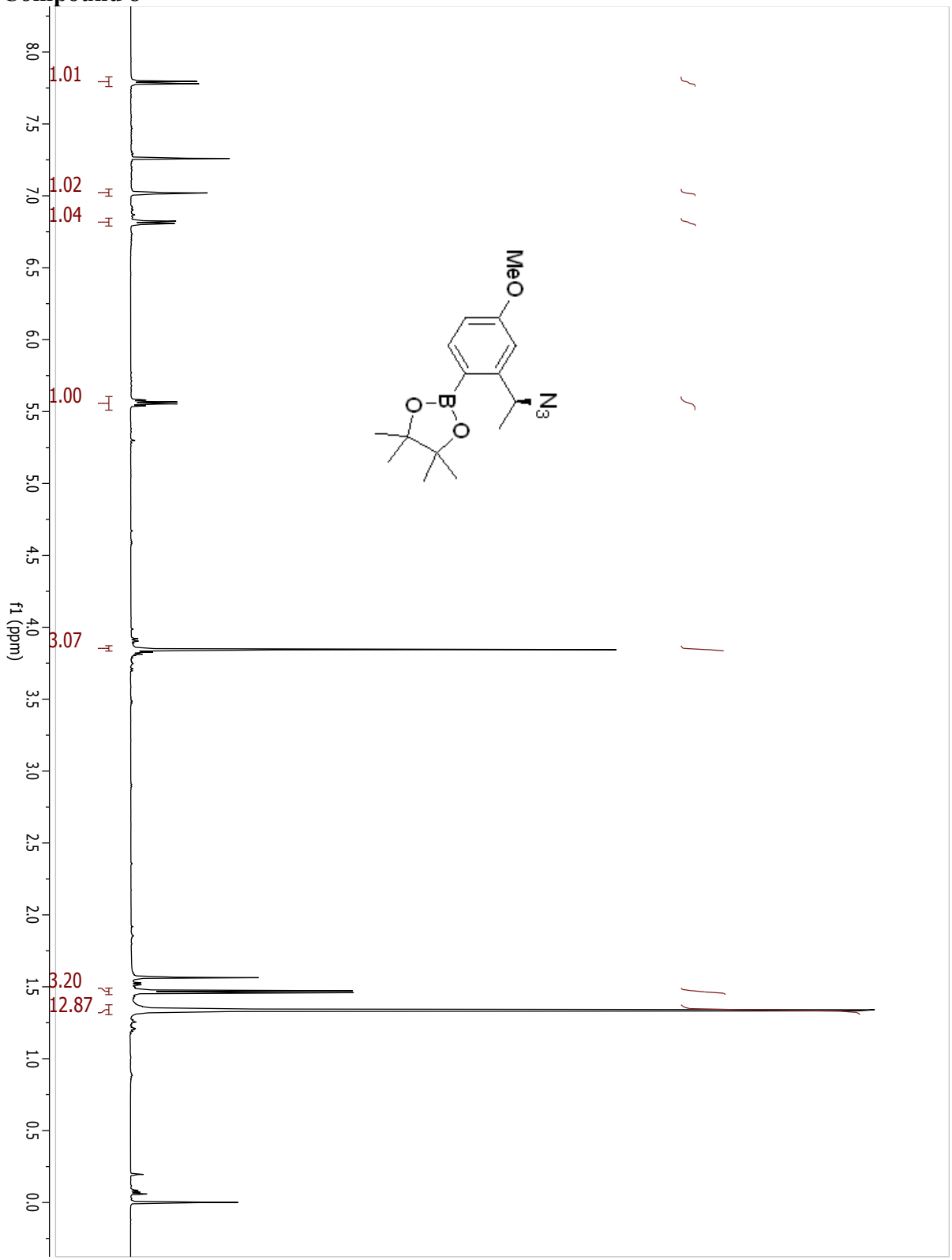
Sulfide of Compound 5k.



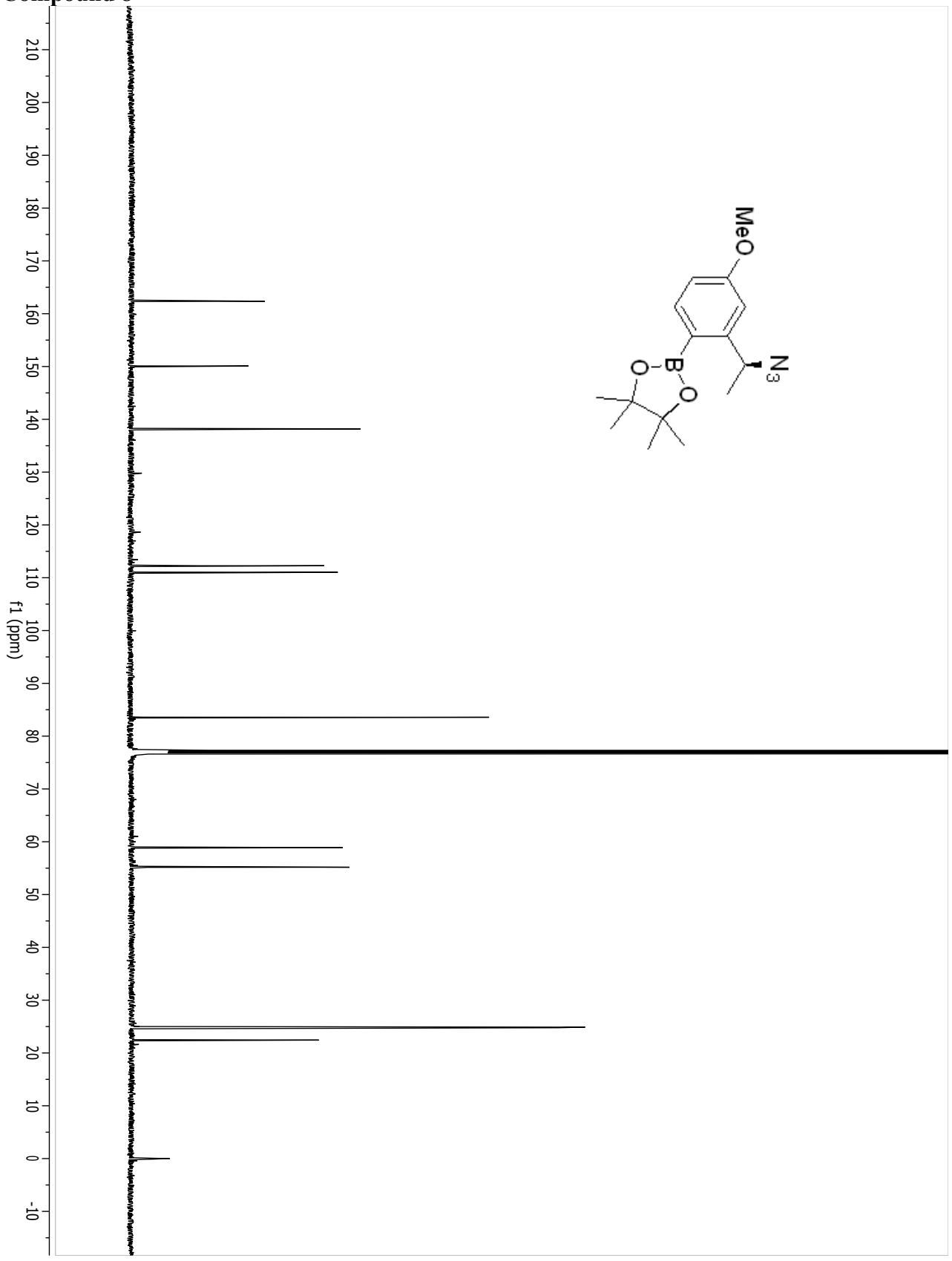
Sulfide of Compound 5k.



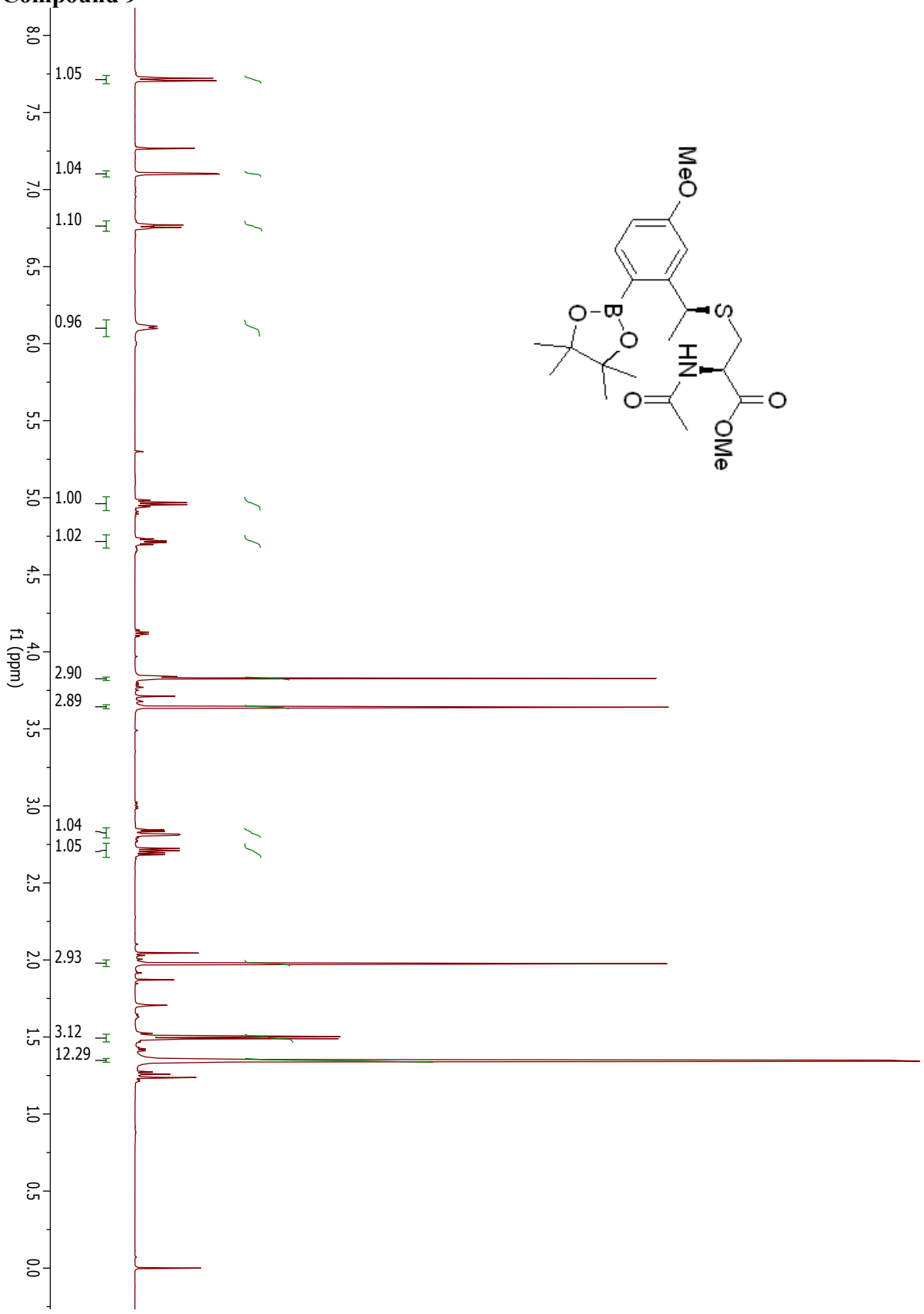
Compound 8



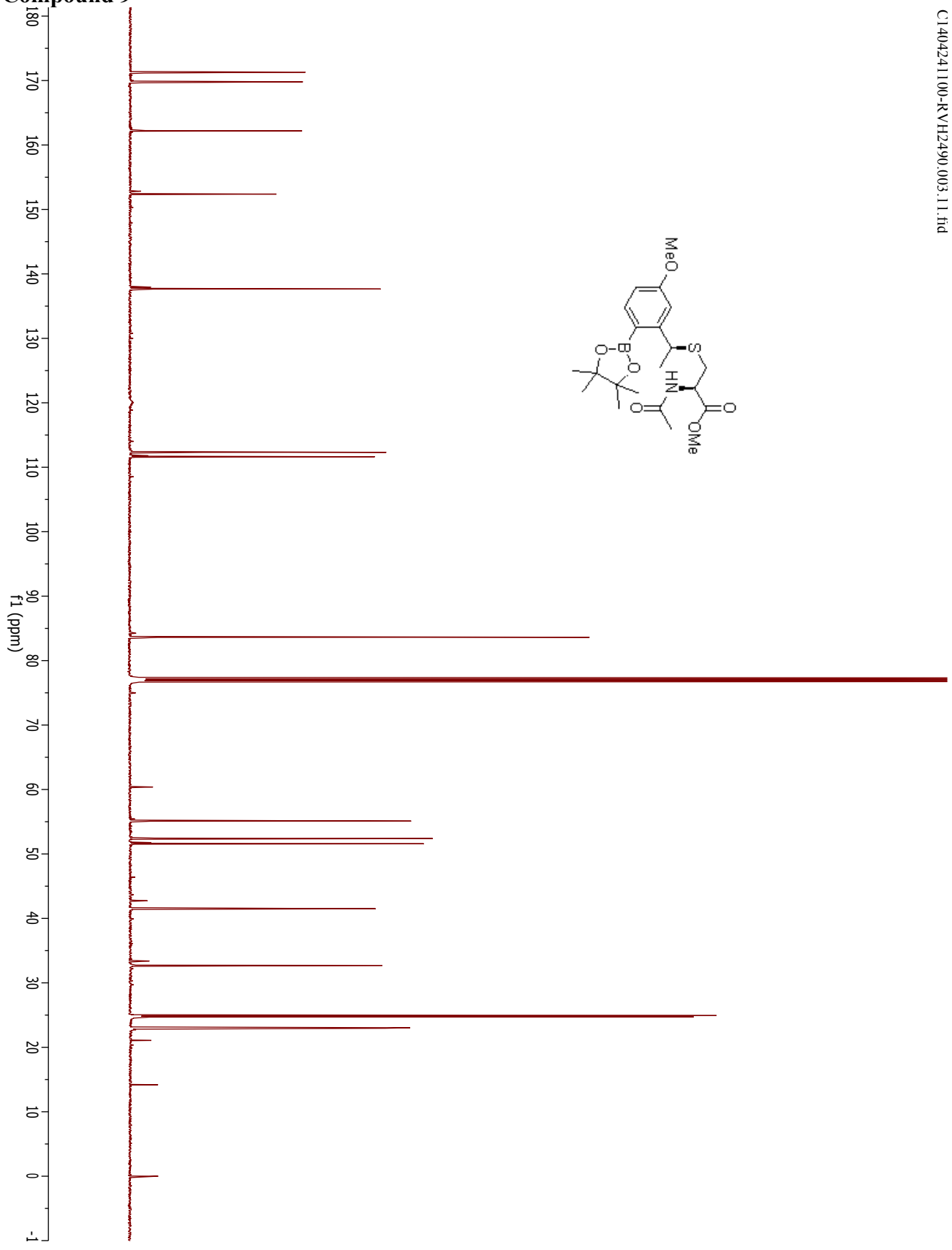
Compound 8


MeO
N3
B
O
O
f1 (ppm)
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10

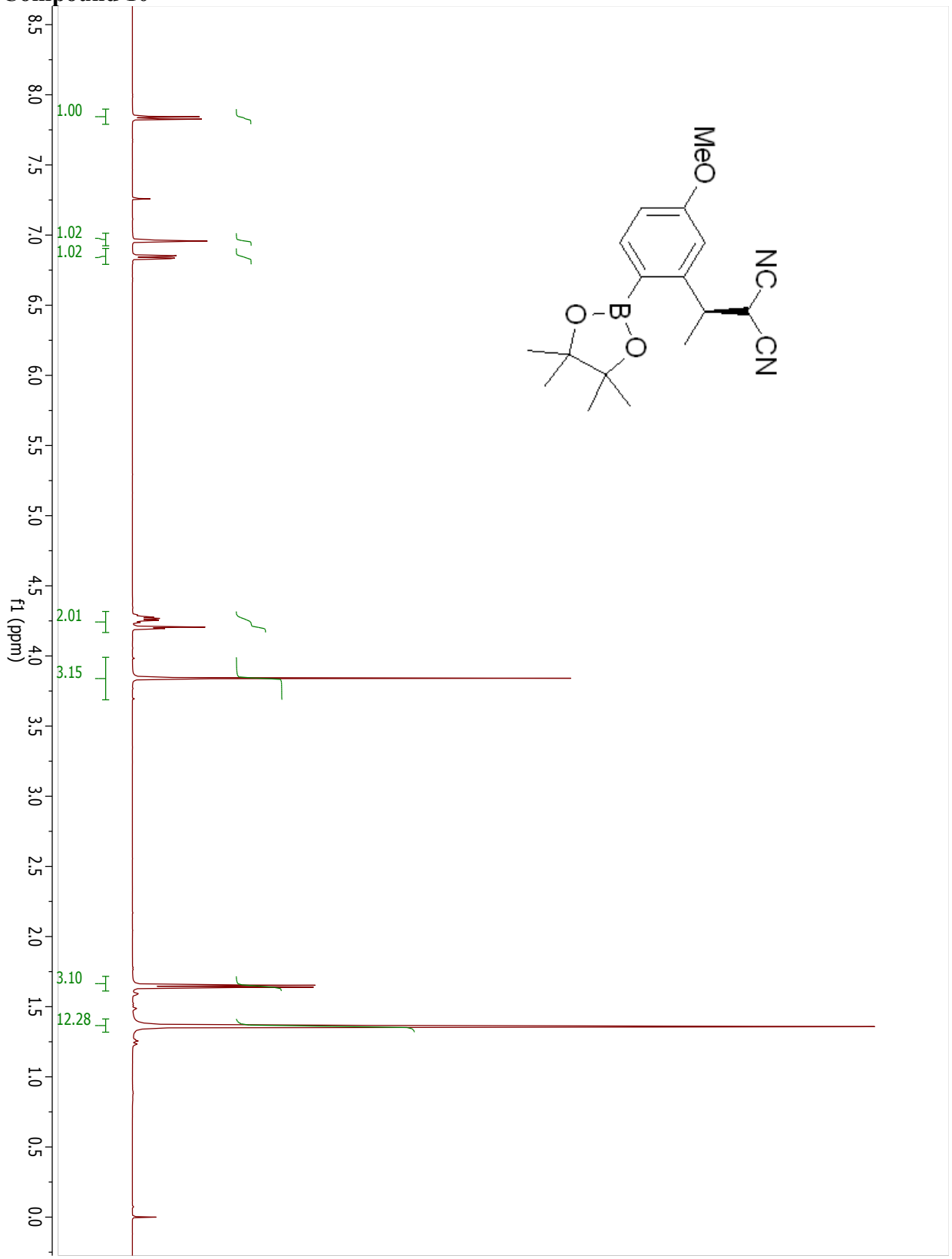
Compound 9


C1404241100-RVH2490.003.10.fid
MeO
B
O
O
S
HN
O
O
O
OMe
f1 (ppm)
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
1.05
1.04
1.10
0.96
1.00
1.02
2.90
2.89
1.04
1.05
2.93
3.12
12.29

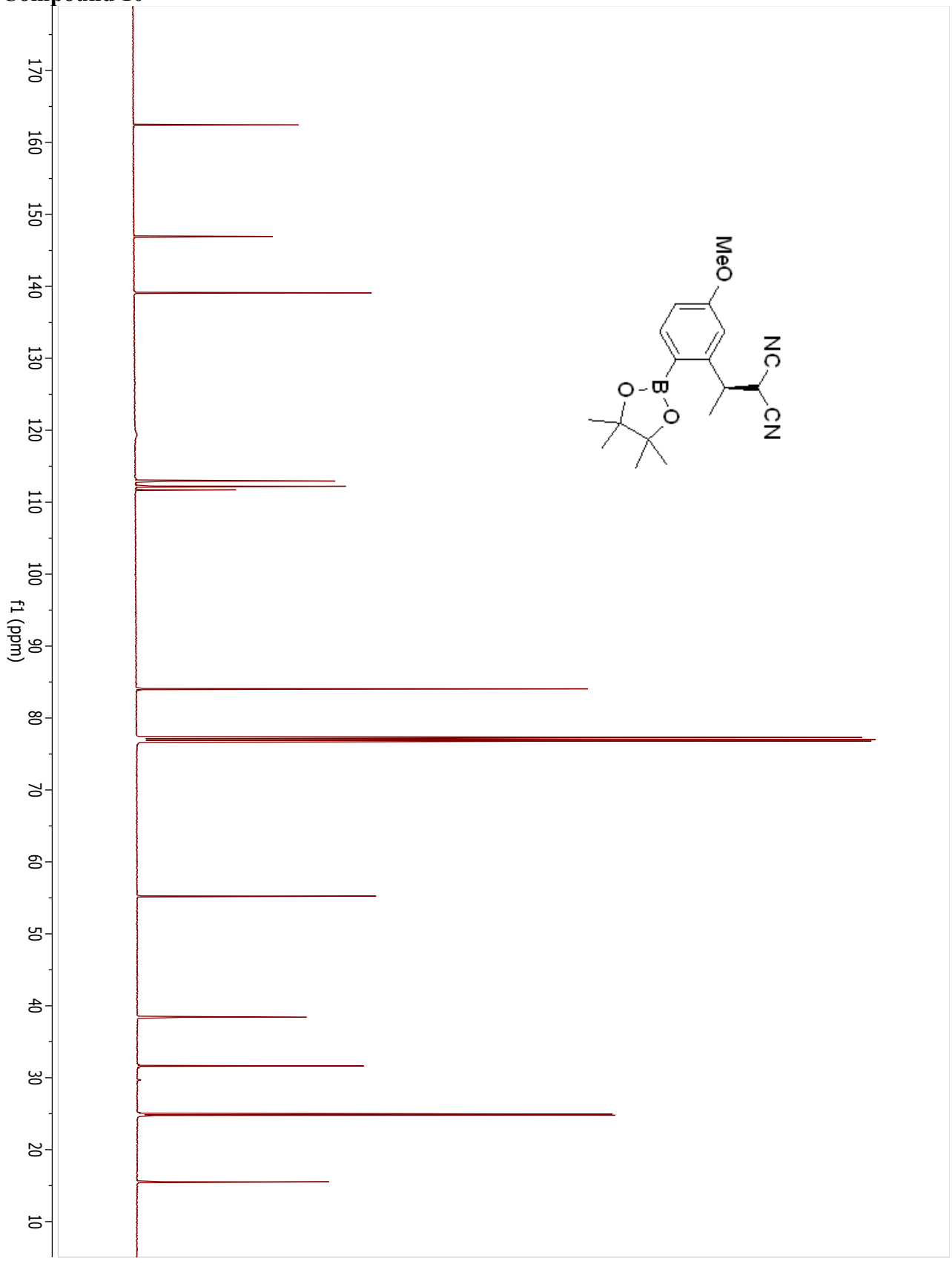
Compound 9


C140424100-RVH2490.003.11.fid
MeO
B
O
O
S
HN
O
O
OMe
f1 (ppm)
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-1

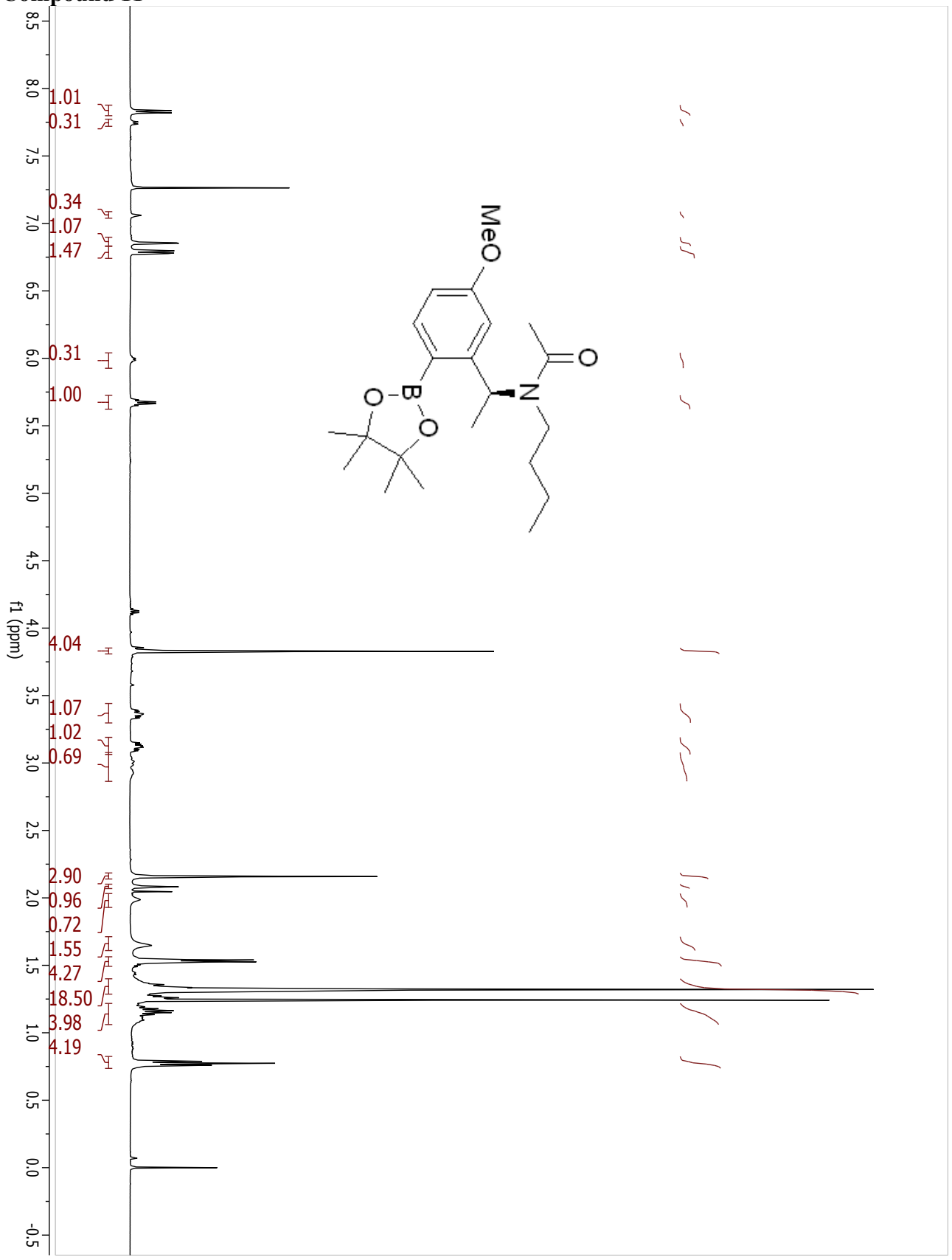
Compound 10



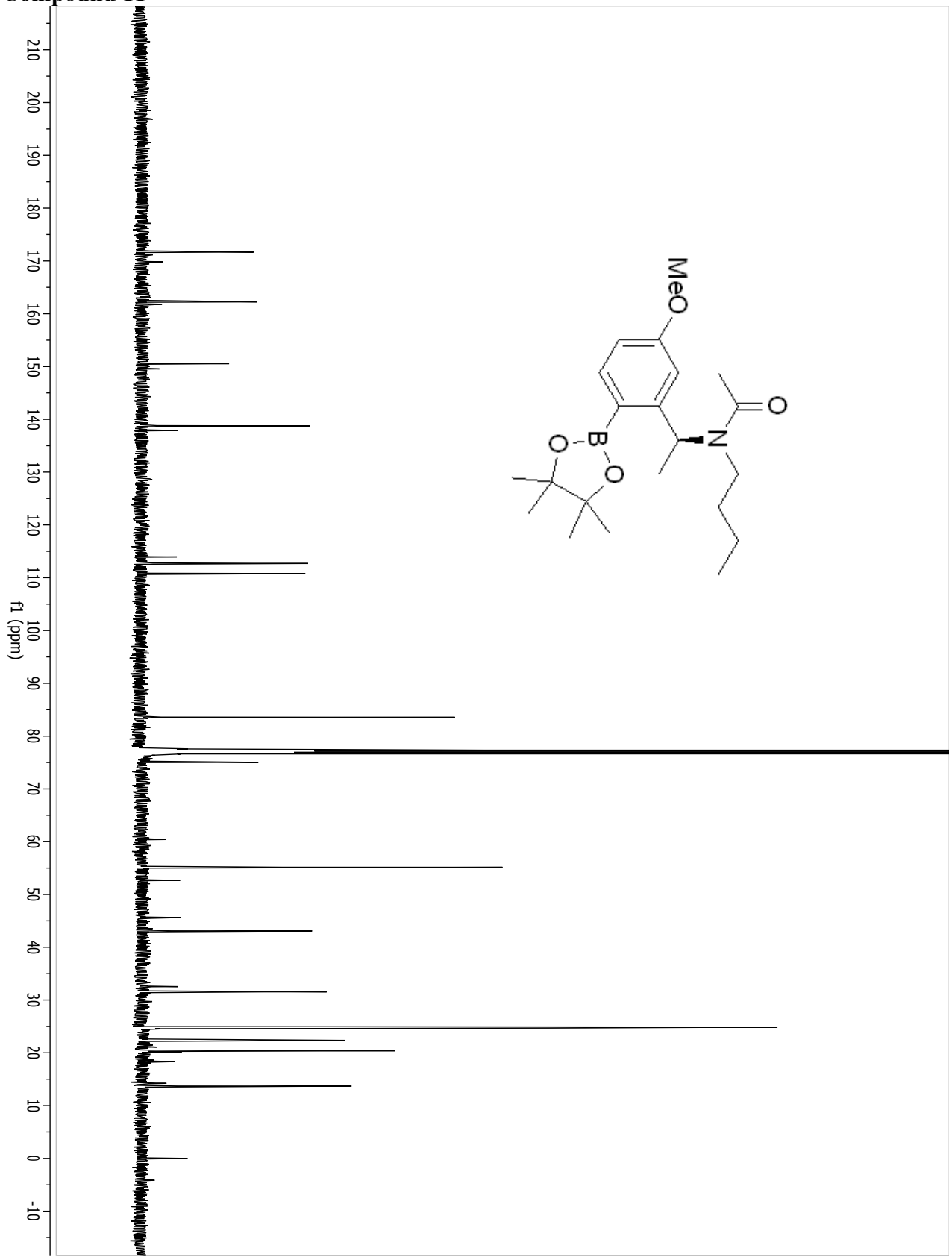
Compound 10


MeO
NC
CN
B
O
O
f1 (ppm)
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10

Compound 11


MeO
O
N
O
B
O
O
f1 (ppm)
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
1.01
0.31
0.34
1.07
1.47
0.31
1.00
4.04
1.07
1.02
0.69
2.90
0.96
0.72
1.55
4.27
18.50
3.98
4.19

Compound 11


MeO
O
N
B
O
O
f1 (ppm)
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10