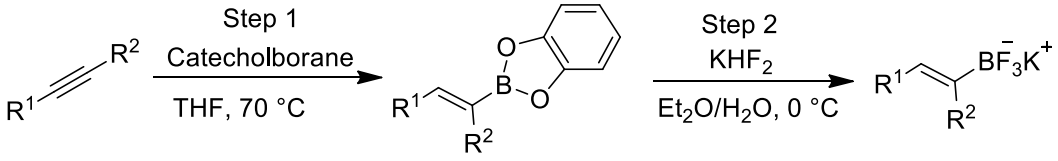
Supporting Information

1. General.

Toluene (ACS grade) and tetrahydrofuran (HPLC grade) was distilled over sodium/benzophenone under N_2 atmosphere. Dichloromethane (HPLC grade) and 1,2-dichloroethane (HPLC grade) were distilled over calcium hydride. Other commercially available solvents (ACS grade) and reagents were used without further purification. Reactions were monitored by thin layer chromatography (TLC) using Silicycle precoated silica gel plates. Flash column chromatography was performed over Silicycle silica gel (230-400 mesh). ^{1}H NMR and ^{13}C NMR spectra were recorded on Varian 400 MHz, 500 MHz, or 600 MHz spectrometers using residue solvent peaks as internal standards ($CHCl_3$, ^{1}H: 7.26 ppm; ^{13}C: 77.00 ppm. CH_2Cl_2, ^{1}H: 5.32 ppm; ^{13}C: 53.84 ppm. Acetone, ^{1}H: 2.05; ^{13}C: 206.68; DMSO, ^{1}H: 2.50; ^{13}C: 39.51). ^{19}F NMR spectra were recorded on Varian 400 MHz calibrated by trifluoroacetic acid peak (CF_3COOH, ^{19}F: -76.55 ppm). Infrared spectra were recorded with a Perkin Elmer FT-IR spectrum 2000 spectrometer and are reported in reciprocal centimeter (cm^{-1}). Mass spectra were recorded with HP 5970 GC/MS equipped with J&W DB 5 ms GC column (0.25 μm ID and 0.25 μm film thickness) using electron ionization and Xevo G2-XS QTof Quadrupole Time-of-Flight Mass Spectrometry using electron spray ionization. Chiral columns (IB or IC) were used for monitoring the chiral purities of **3h** or (*R*)-**3h** and their starting materials by using hexanes/IPA = 97 to 3 (v/v) as eluent at 1.0 mL/min. No effort was taken to improve the yields of the substrates.

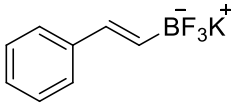
2. Synthesis of compounds 1:



General procedure A: step 1): In a sealed and flame-dried schlenk flask, the alkyne (1.0 equiv.) was heated with catecholborane (1.8 equiv. 1.0 M in THF) at 70 °C in THF overnight. Upon completion, the solvent was removed and the boron ester was obtained and directly used in the next step. Step 2): the boron ester was dissolved in Et_2O, and KHF_2 (3.5 equiv.) dissolved in H_2O

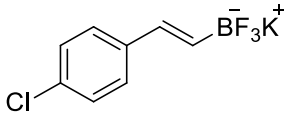
(4.5 M) was added dropwise at 0 ℃. The reaction was stirred at 0 ℃ for 3 hrs, and then the precipitation was filtered and washed with Et_2O twice. The solid was dissolved in hot acetone, and was precipitated after adding Et_2O slowly. The precipitation was filtered, washed with Et_2O, and dried under vacuum to get the target substrates as white solids.

Potassium (*E*)-trifluoro(styryl)borate ((*E*)-**1a**):



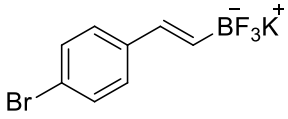
Compound (*E*)-**1a** was obtained according to the general procedure A (step 2) by using the commercially available (*E*)-2-phenylvinylboronic acid as starting material, yield 80%. Its spectral data was consistent with those described in the corresponding reference[1].

Potassium (*E*)-(4-chlorostyryl)trifluoroborate (**1b)**:



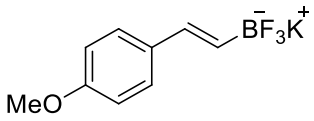
The starting material 1-chloro-4-ethynylbenzene was synthesized by following the known procedure[2], and then compound **1b** was obtained according to the general procedure A, yield 53%. Its spectral data was consistent with those described in the corresponding reference[3].

Potassium (*E*)-(4-bromostyryl)trifluoroborate (**1c**):



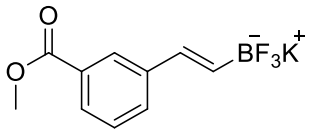
The starting material 1-bromo-4-ethynylbenzene was synthesized by following the known procedure[4], and then compound **1c** was obtained according to the general procedure A, yield 51%. Its spectral data was consistent with those described in the corresponding reference[5].

Potassium (*E*)-trifluoro(4-methoxystyryl)borate (**1d**):



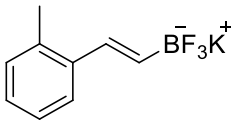
The starting material 1-ethynyl-4-methoxybenzene was synthesized by following the known procedure[4], and then compound **1d** was obtained according to the general procedure A, yield 64%. Its spectral data was consistent with those described in the corresponding reference[6].

Potassium (*E*)-trifluoro(3-(methoxycarbonyl)styryl)borate (**1e**):



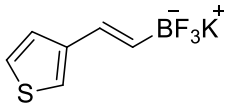
The starting material methyl 3-ethynylbenzoate was synthesized by following the known procedure[7], and then compound **1e** was obtained according to the general procedure A, yield 64%. ^{1}H NMR (400 MHz, $(CD_3)_2CO$) δ 7.99 (s, 1H), 7.74 (d, *J* = 6.0 Hz, 1H), 7.58 (s, 1H), 7.37 (s, 1H), 6.69 (d, *J* = 18.2 Hz, 1H), 6.45 (d, *J* = 18.4 Hz, 1H), 3.87 (s, 3H). ^{13}C NMR (126 MHz, $(CD_3)_2CO$) δ 167.90, 142.54, 134.24 (q, *J* = 4.4 Hz, 1H), 131.48, 131.29, 129.57, 127.88, 127.63, 52.56. ^{19}F NMR (376 MHz, $(CD_3)_2CO$) δ -139.95 (d, *J* = 49.2 Hz). **HRMS(ESI):** m/z calcd for $C_{10}H_9BF_3O_2$ $[M-K]^-$: 229.0653, found: 229.0647. IR (neat): 3012, 2964, 1709, 1633, 1599, 1457, 1924, 1098, 991 cm^{-1}.

Potassium (*E*)-trifluoro(2-methylstyryl)borate (**1f**):



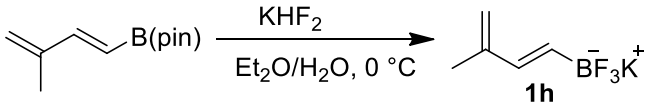
The starting material 1-ethynyl-2-methylbenzene was synthesized by following the known procedure[8], and then compound **1f** was obtained according to the general procedure A, yield 47%. Its spectral data was consistent with those described in the corresponding reference[9].

Potassium (*E*)-trifluoro(2-(thiophen-3-yl)vinyl)borate (**1g**):



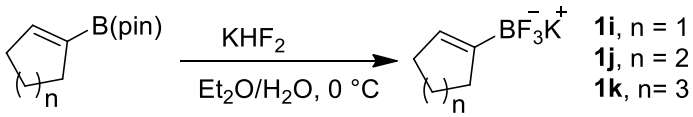
The starting material 3-ethynylthiophene was synthesized by following the known procedure[10], and then compound **1g** was obtained according to the general procedure A, yield 60%. ^{1}H NMR (400 MHz, $(CD_3)_2CO$) δ 7.28 (dd, *J* = 4.8, 3.0 Hz, 1H), 7.22 (d, *J* = 4.4 Hz, 1H), 7.02 (d, *J* = 2.3 Hz, 1H), 6.66 (d, *J* = 18.2 Hz, 1H), 6.10 (dq, *J* = 18.2, 3.7 Hz, 1H). ^{13}C NMR (101 MHz, $(CD_3)_2CO$) δ 145.87, 129.50 (q, *J* = 4.7 Hz), 126.54, 126.11, 119.96. ^{19}F NMR (376 MHz, DMSO-*d*$_6$) δ -136.04 (s). **HRMS(ESI):** m/z calcd for $C_6H_5BF_3S$ $[M-K]^-$: 117.0163, found: 117.0162. IR (neat): 3102, 3086, 2990, 2964, 1705, 1628, 1466, 1254, 1231, 1103, 973, 922, 839, 774 cm^{-1}.

Synthesis of potassium (*E*)-trifluoro(3-methylbuta-1,3-dien-1-yl)borate (**1h**)

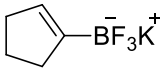


The (*E*)-4,4,5,5-tetramethyl-2-(3-methylbuta-1,3-dien-1-yl)-1,3,2-dioxaborolane was synthesized by following the previous known study[11]. and then compound **1h** was obtained according to the general procedure A, step 2, yield 56% . ^{1}H NMR (400 MHz, $(CD_3)_2CO$) δ 6.42 (d, *J* = 18.1 Hz, 1H), 5.67 (d, *J* = 18.1 Hz, 1H), 4.74 (s, 2H), 1.76 (s, 3H). ^{13}C NMR (101 MHz, $(CD_3)_2CO$) δ 146.00, 138.31 (q, *J* = 4.6 Hz), 112.66, 19.05. ^{19}F NMR (376 MHz, $(CD_3)_2CO$) δ -139.46 (q, *J* = 45.8 Hz). **HRMS(ESI):** m/z calcd for $C_5H_7BF_3$ $[M-K]^-$: 135.0598, found: 135.0602. IR (neat): 3081, 2988, 2947, 1709, 1628, 1599, 1434, 1368, 1236, 1105, 990, 962 cm^{-1}.

Synthesis of potassium potassium cyclo-en-1-yltrifluoroborate (**1i**-**k**)

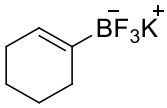


Potassium cyclopent-1-en-1-yltrifluoroborate (**1i**):



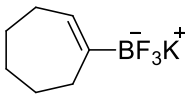
Compound **1i** was obtained according to the general procedure A (step 2) by using the commercially available 2-(cyclopent-1-en-1-yl)-4,4,5,5-tetramethyl-1,3,2-dioxaborolane as the starting material, yield 72%. ^{1}H NMR (500 MHz, DMSO-d_6) δ 5.31 (s, 1H), 2.12 (t, J = 7.3 Hz, 4H), 1.67 – 1.53 (m, 2H). ^{13}C NMR (126 MHz, DMSO-d_6) δ 126.41 – 126.30 (m), 35.53, 33.52, 23.77. ^{19}F NMR (376 MHz, $(CD_3)_2CO$) δ -140.29 (q, J = 52.0 Hz). **HRMS(ESI):** m/z calcd for $C_5H_7BF_3$ $[M-K]^-$: 135.0598, found: 135.0602. IR (neat): 3040, 2949, 2843, 1644, 1621, 1423, 1366, 1231, 983, 917, 842 cm^{-1}.

Potassium cyclohex-1-en-1-yltrifluoroborate (**1j**):



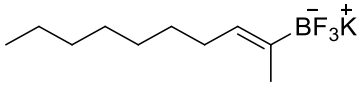
The 2-(cyclohex-1-en-1-yl)-4,4,5,5-tetramethyl-1,3,2-dioxaborolane was synthesized by following the known procedure[12], and then compound **1j** was obtained according to the procedure A (step 2), yield 42%. Its spectral data was consistent with those described in the corresponding reference[13].

Potassium cyclohept-1-en-1-yltrifluoroborate (**1k**):



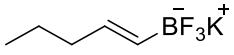
The 2-(cyclohept-1-en-1-yl)-4,4,5,5-tetramethyl-1,3,2-dioxaborolane was synthesized by following the known procedure[12], and then compound **1k** was obtained according to the general procedure A (step 2), yield 42%. ^{1}H NMR (400 MHz, $(CD_3)_2CO$) δ 5.87 (t, J = 6.1 Hz, 1H), 2.13 – 2.09 (m, 2H), 2.05 – 2.00 (m, 2H), 1.72 – 1.65 (m, 2H), 1.43 – 1.35 (m, 4H). ^{13}C NMR (101 MHz, $(CD_3)_2CO$) 130.35, 34.82, 31.57, 31.55, 30.79, 29.10. ^{19}F NMR (376 MHz, DMSO-d_6) δ -141.17 (s). **HRMS(ESI):** m/z calcd for $C_7H_{11}BF_3$ $[M-K]^-$: 163.0911, found: 163.0919. IR (neat): 3010, 2908, 2941, 1640, 1604, 1447, 971, 955, 893, 855, 806 cm^{-1}.

Potassium (*Z*)-dec-2-en-2-yltrifluoroborate (**1l**):



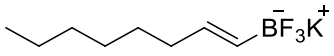
Compound **1l** was obtained according to the general procedure A by using the commercially available 2-decyne as starting material, yield 75%. ^{1}H NMR (500 MHz, $(CD_3)_2CO$) δ 5.46 (s, 1H), 1.94 (d, *J* = 5.9 Hz, 2H), 1.50 (s, 3H), 1.30 (s, 10H), 0.88 (t, *J* = 6.9 Hz, 3H). ^{13}C NMR (101 MHz, $(CD_3)_2CO$) δ 128.52, 33.23, 31.54, 30.89, 30.67, 28.99, 23.88, 15.27, 14.88. ^{19}F NMR (376 MHz, $(CD_3)_2CO$) δ -143.87 (d, *J* = 56.9 Hz). **HRMS(ESI):** m/z calcd for $C_{10}H_{19}BF_3$ $[M\text{-}K]^-$: 207.1537, found: 207.1530. IR (neat): 2957, 2923, 2855, 1710, 1641, 1467, 1365, 1229, 948, 752 cm^{-1}.

Potassium (*E*)-trifluoro(pent-1-en-1-yl)borate (**1m**):



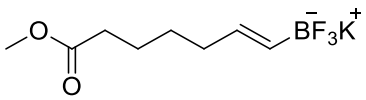
Compound **1m** was synthesized according to the general procedure A (step 2) by using the commercially available *(E)*-penten-1-ylboronic acid as starting material, yield 45%. Its spectral data was consistent with those described in the corresponding reference[6].

Potassium *(E)*-trifluoro(oct-1-en-1-yl)borate (**1n**):



Compound **1n** was obtained according to the general procedure A by using the commercially available 1-octyne as starting material, yield 65%. Its spectral data was consistent with those described in the corresponding reference[13].

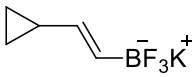
Potassium *(E)*-trifluoro(7-methoxy-7-oxohept-1-en-1-yl)borate (**1o**):



Compound **1o** was obtained according to the general procedure A by using the commercially available methyl 6-heptynoate, yield 41%. ^{1}H NMR (400 MHz, $(CD_3)_2CO$) δ 5.70 (dt, *J* = 17.0, 6.1 Hz, 1H), 5.38 (dd, *J* = 17.6, 3.7 Hz, 1H), 3.62 (s, 3H), 2.29 (t, *J* = 7.5 Hz,

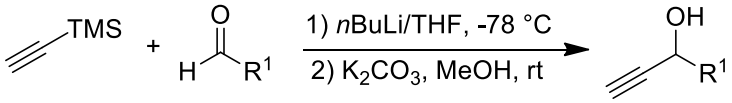
2H), 1.97 (dd, *J* = 13.8, 7.2 Hz, 2H), 1.59 (dt, *J* = 15.3, 7.5 Hz, 2H), 1.36 (dq, *J* = 15.0, 7.6 Hz, 2H). ^{13}C NMR (101 MHz, $(CD_3)_2CO$) δ 174.69, 135.95 (q, *J* = 4.8 Hz), 51.85, 36.53, 34.75, 30.18, 25.77. ^{19}F NMR (376 MHz, $(CD_3)_2CO$) δ -138.98 (s). **HRMS(ESI):** m/z calcd for $C_8H_{13}BF_3O_2$ $[M-K]^-$: 209.0966, found: 209.0971. IR (neat): 2990, 2949, 2856, 1745, 1644, 1467, 1230, 1166, 946, 924 cm^{-1}.

Potassium *(E)*-(2-cyclopropylvinyl)trifluoroborate (**1p**):



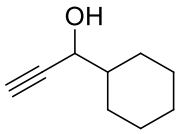
Compound **1p** was obtained according to the general procedure A by using the commercially available ethynylcyclopropane, yield 69%. Its spectral data was consistent with those described in the corresponding reference[14].

3. Synthesis of compounds 2.



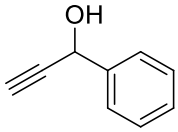
General procedure B: In a flame-dried Schlenk flask backfilled with N_2, trimethylsilylacetylene (1.1 equiv.) dissolved in THF was added and the mixture was cooled to -78 ºC. *n*BuLi (1.2 equiv. 2.5 M in hexaness) was added dropwise and the reaction was stirred for 30 min. After aldehyde (1.0 equiv.) was added dropwise, the reaction was elevated to room temperature slowly and stirred for another 3 hrs. Upon completion, the reaction was quenched using saturated NH_4Cl. The solvent was removed and the residue was extracted using EA, and washed with H_2O for three times. The EA layer was combined, dried, and concentrated. The residue was treated with K_2CO_3 (3.0 equiv.) in methanol overnight. After the reaction was completed, the solvent was removed, and the residue was dissolved in EA, washed with H_2O three times. The solvent was removed and the residue was purified by silica gel chromatography (hexanes/EA = 20:1 to 5 :1) to afford the propargylic alcohols.

1-Cyclohexylprop-2-yn-1-ol (**2a**):



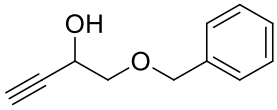
Compound **2a** was obtained according to the general procedure B by using the commercially available cyclohexanescarbaldehyde and ethynyltrimethylsilane as starting materials. Colorless oil, yield 78%, R_f = 0.80 (hexanes/EA = 4:1). Its spectral data was consistent with those described in the corresponding reference[15].

1-Phenylprop-2-yn-1-ol (**2b**):



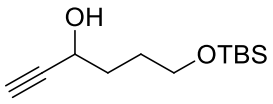
Compound **2b** was obtained according to the general procedure B by using commercially available benzaldehyde and ethynyltrimethylsilane as starting materials. Slight yellow oil, yield 83%, R_f = 0.2 (hexanes/EA = 8:1). Its spectral data was consistent with those described in the corresponding reference[16].

1-(Benzyloxy)but-3-yn-2-ol (**2c**):



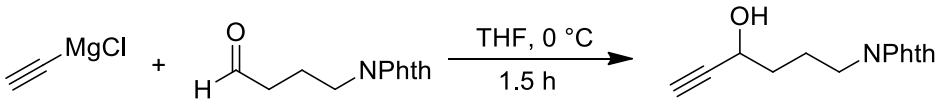
The 2-(benzyloxy)acetaldehyde was obtained by following the known procedure[17], and then compound **2c** was obtained according to the general procedure B. Slight yellow oil, yield 70%, R_f = 0.5 (hexanes/EA = 5:1). Its spectral data was consistent with those described in the corresponding reference.[18]

6-((*tert*-Butyldimethylsilyl)oxy)hex-1-yn-3-ol (**2d**):



4-((*tert*-Butyldimethylsilyl)oxy)butanal was obtained by following the known procedure[19], and then compound **2d** was obtained according to the general procedure B. colorless oil, yield 72%. R_f = 0.38 (hexaness/EA = 5:1). ^{1}H NMR (400 MHz, $CDCl_3$) δ 4.39 (d, *J* = 3.7 Hz, 1H), 3.71 – 3.56 (m, 2H), 2.40 (d, *J* = 1.9 Hz, 1H), 1.83 – 1.61 (m, 4H), 0.87 (s, 9H), 0.04 (s, 6H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 84.95, 72.46, 63.04, 61.66, 34.99, 28.27, 25.83, 18.21, -5.46, -5.49. **HRMS(EI):** m/z calcd for $C_8H_{15}O_2Si$ [M-*t*Bu]$^+$: 171.0841, found: 171.0842. IR (neat): 3351, 3312, 2956, 2930, 2859, 2130, 1472, 1464, 1256, 1098, 836, 776 cm^{-1}.

2-(4-Hydroxyhex-5-yn-1-yl)isoindoline-1,3-dione (**2e**):



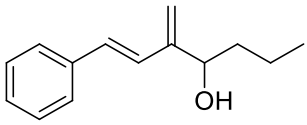
The 4-(1,3-dioxoisoindolin-2-yl)butanal was obtained by following the known procedure[20].

In a flame-dried Schlenk flask backfilled with N_2, ethynyl magnesium chloride (1.3 equiv., 0.6 M in THF/toluene) in THF was added and the flask was cooled to 0 ℃, and then aldehyde (1.0 equiv.) dissolved in THF was added dropwise at 0 ℃. The reaction was stirred at the same temperature for another 2 h. The reaction was quenched using saturated NH_4Cl and the solvent was removed. The residue was dissolved in DCM, washed with H_2O three times. The organic layer was dried and removed under the reduced pressure. The residue was purified by silica gel chromatography (hexanes/EA = 20:1 to 2:1) to afford the target compound as white solid with a yield of 57%. R_f = 0.38 (hexanes/EA = 1:1). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.84 – 7.79 (m, 2H), 7.72 – 7.67 (m, 2H), 4.43 (s, 1H), 3.73 (t, *J* = 6.9 Hz, 2H), 2.53 (s, 1H), 2.44 (d, *J* = 1.9 Hz, 1H), 1.95 – 1.80 (m, 2H), 1.80 – 1.69 (m, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 168.43, 133.91, 131.94, 123.19, 84.40, 73.18, 61.60, 37.46, 34.52, 24.27. **HRMS(ESI):** m/z calcd for $C_{14}H_{13}NO_3Na$ [M+Na]$^+$: 266.0788, found: 266.0797. IR (neat): 3360, 3257, 3031, 2956, 2935, 2864, 2112, 1767, 1704, 1612, 1469, 1435, 1402, 1046, 1028, 874, 721 cm^{-1}.

4. General procedure C: cross-coupling between potassium *E*-vinyltrifluoroborate salt and propargylic alcohols.

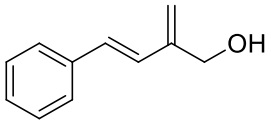
In a 10 mL vial, propargylic alcohols (0.3 mmol, 1.0 equiv.), potassium *E*-vinyltrifluoroborate salt (0.9 or 1.8 mmol, 3.0 or 6.0 equiv.), and gold catalyst (0.05 or 0.08 equiv.) were added successively. After the mixture was dissolved in DCM (1.5 mL) and H_2O (0.38 mL), $AgNTf_2$ (0.048 or 0.078 equiv.) was added and the reaction was stirred at room temperature for 24 h. The reaction was washed with 15% NaOH (2 mL) and H_2O (30 mL × 2) respectively. The organic layer was combined, dried, and removed. The residue was purified with silica gel chromatography (hexaness/EA = 30:1 – 2:1) to afford the target compounds as colorless oils or white solids.

(E)-3-Methylene-1-phenylhept-1-en-4-ol (**3a**)



Following the general procedure C, the target compound **3a** was obtained as a colorless oil in 71% yield. R_f = 0.43 (hexanes/EA = 5:1). ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.43 (d, *J* = 7.4 Hz, 2H), 7.33 (t, *J* = 7.6 Hz, 2H), 7.24 (t, *J* = 7.6 Hz, 1H), 6.78 (d, *J* = 16.5 Hz, 1H), 6.74 (d, *J* = 16.5 Hz, 1H), 5.29 (s, 1H), 5.28 (s, 1H), 4.53 (dt, *J* = 7.7, 3.9 Hz, 1H), 1.78 – 1.58 (m, 3H), 1.57 – 1.35 (m, 2H), 0.96 (t, *J* = 7.4 Hz, 3H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 149.00, 137.17, 128.93, 128.62, 127.93, 127.64, 126.44, 114.08, 72.07, 38.63, 19.06, 14.00. **HRMS(EI):** m/z calcd for $C_{14}H_{18}O$ $[M]^+$: 202.1358, found: 202.1361. IR (neat): 3303, 3028, 2958, 2933, 2872, 1602, 1494, 1449, 1378, 1068, 959, 895, 754 cm^{-1}.

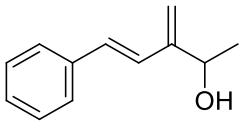
(E)-2-Methylene-4-phenylbut-3-en-1-ol (**3b**)



Following the general procedure C, the target compound **3b** was obtained as a cololess oil in 81% yield. R_f = 0.21 (hexanes/EA = 5:1). ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.43 (d, *J* = 7.4 Hz, 2H), 7.33 (t, *J* = 7.6 Hz, 2H), 7.25 (t, *J* = 7.6 Hz, 1H), 6.82 (d, *J* = 16.6 Hz, 1H), 6.67

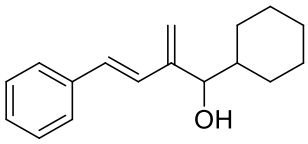
(d, *J* = 16.6 Hz, 1H), 5.35 (s, 1H), 5.28 (s, 1H), 4.46 (d, *J* = 4.7 Hz, 2H), 1.53 (s, 1H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 145.04, 137.01, 128.83, 128.62, 128.14, 127.71, 126.45, 116.19, 63.23. **HRMS(EI):** m/z calcd for $C_{11}H_{12}O$ $[M]^+$: 160.0888, found: 160.0888. IR (neat): 3224, 3026, 2853, 1605, 1449, 1195, 1071, 964, 901, 753 cm^{-1}.

(E)-3-Methylene-5-phenylpent-4-en-2-ol (**3c**)



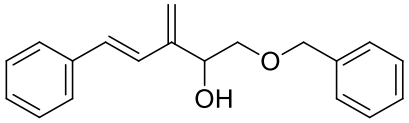
Following the general procedure C, the target compound **3c** was obtained as a cololess oil in 75% yield. R_f = 0.27 (hexanes/EA = 5:1). ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.43 (d, *J* = 7.4 Hz, 2H), 7.33 (t, *J* = 7.6 Hz, 2H), 7.24 (t, *J* = 7.4 Hz, 1H), 6.79 (d, *J* = 16.6 Hz, 1H), 6.73 (d, *J* = 16.6 Hz, 1H), 5.34 (s, 1H), 5.25 (s, 1H), 4.77 – 4.70 (m, 1H), 1.64 (s, 1H), 1.45 (d, *J* = 6.4 Hz, 3H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 150.05, 137.13, 128.91, 128.62, 128.03, 127.66, 126.43, 113.49, 67.78, 22.97. **HRMS(EI):** m/z calcd for $C_{12}H_{14}O$ $[M]^+$: 174.1045, found: 174.1053. IR (neat): 3357, 3028, 2925, 2854, 1602, 1495, 1449, 1285, 1073, 964, 855, 753 cm^{-1}.

(E)-1-Cyclohexyl-2-methylene-4-phenylbut-3-en-1-ol (**3d**)



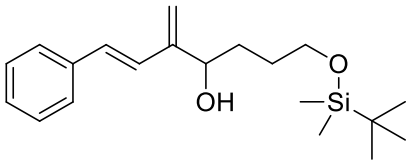
Following the general procedure C, the target compound **3d** was obtained as a colorless oil in 61%. R_f = 0.45 (hexanes/EA = 5:1). ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.44 (d, *J* = 7.6 Hz, 2H), 7.34 (t, *J* = 7.7 Hz, 2H), 7.25 (t, *J* = 7.2 Hz, 1H), 6.80 (d, *J* = 16.5 Hz, 1H), 6.76 (d, *J* = 16.5 Hz, 1H), 5.33 (s, 1H), 5.20 (s, 1H), 4.21 (d, *J* = 6.0 Hz, 1H), 1.96 (d, *J* = 12.7 Hz, 1H), 1.77 – 1.59 (m, 6H), 1.28 – 1.10 (m, 5H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 147.61, 137.20, 129.11, 128.57, 127.82, 127.57, 126.43, 114.91, 77.61, 41.88, 29.93, 27.97, 26.41, 26.26, 26.02. **HRMS(EI):** m/z calcd for $C_{17}H_{23}O$ $[M+H]^+$: 243.1749, found: 243.1748. IR (neat): 3392, 3027, 2925, 2852, 1637, 1493, 1450, 1265, 1027, 890, 755 cm^{-1}.

(E)-1-(Benzyloxy)-3-methylene-5-phenylpent-4-en-2-ol (**3e**)



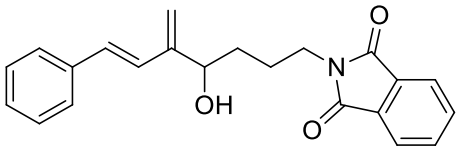
Following the general procedure C, the target compound **3e** was obtained as a white solid in 78% yield. R_f = 0.29 (hexanes/EA = 5:1). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.42 – 7.35 (m, 5H), 7.32 (t, *J* = 7.5 Hz, 3H), 7.26 – 7.22 (m, 2H), 6.77 (d, *J* = 16.6 Hz, 1H), 6.65 (d, *J* = 16.6 Hz, 1H), 5.45 (s, 1H), 5.36 (s, 1H), 4.81 (d, *J* = 8.5 Hz, 1H), 4.68 – 4.55 (m, 2H), 3.75 (dd, *J* = 9.9, 2.8 Hz, 1H), 3.47 (dd, *J* = 9.8, 8.6 Hz, 1H), 2.62 (d, *J* = 2.7 Hz, 1H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 144.49, 137.79, 136.99, 128.60, 128.54, 128.50, 128.14, 127.87, 127.79, 127.69, 126.42, 116.04, 74.34, 73.39, 70.47. **HRMS(EI):** m/z calcd for $C_{19}H_{20}O_2$ $[M]^+$: 280.1463, found: 280.1476. IR (neat): 3418, 3071, 3051, 3029, 2918, 2862, 1603, 1495, 1451, 1363, 1103, 964, 908, 754 cm^{-1}.

(E)-7-((*tert*-Butyldimethylsilyl)oxy)-3-methylene-1-phenylhept-1-en-4-ol (**3f**)



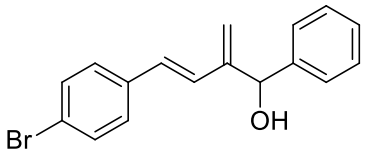
Following the general procedure C, the target compound **3f** was obtained as a colorless oil in 65%. R_f = 0.42 (hexanes/EA = 5:1). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.42 (d, *J* = 7.5 Hz, 2H), 7.32 (t, *J* = 7.6 Hz, 2H), 7.23 (t, *J* = 7.3 Hz, 1H), 6.78 (d, *J* = 16.5 Hz, 1H), 6.71 (d, *J* = 16.5 Hz, 1H), 5.35 (s, 1H), 5.29 (s, 1H), 4.60 – 4.52 (m, 1H), 3.70 (t, *J* = 5.6 Hz, 1H), 3.01 (s, 1H), 1.97 – 1.87 (m, 1H), 1.76 – 1.65 (m, 3H), 0.92 (s, 9H), 0.09 (s, 6H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 148.74, 137.25, 128.60, 128.55, 128.26, 127.50, 126.39, 114.29, 71.68, 63.44, 33.98, 29.13, 25.92, 18.31, -5.37. HRMS(EI): m/z calcd for $C_{20}H_{33}O_2Si[M+H]^+$: 333.2250, found: 333.2263. IR (neat): 3392, 3029, 2954, 2929,2885, 2857, 1639, 1472, 1463, 1389, 1256, 1097, 836, 776 cm^{-1}.

(E)-2-(4-Hydroxy-5-methylene-7-phenylhept-6-en-1-yl)isoindoline-1,3-dione (**3g**)



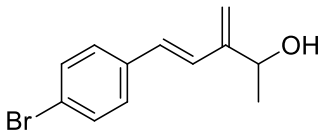
Following the general procedure C, the target compound **3g** was obtained as a white solid in 77% yield. R_f = 0.53 (hexanes/EA = 1:1). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.86 – 7.74 (m, 2H), 7.72 – 7.63 (m, 2H), 7.38 (d, *J* = 7.3 Hz, 2H), 7.30 (t, *J* = 7.5 Hz, 2H), 7.22 (t, *J* = 7.2 Hz, 1H), 6.73 (d, *J* = 16.8 Hz, 1H), 6.69 (d, *J* = 16.9 Hz, 1H), 5.29 (s, 1H), 5.27 (s, 1H), 4.58 (d, *J* = 6.9 Hz, 1H), 3.75 (t, *J* = 6.9 Hz, 2H), 2.00 (s, 1H), 1.92 – 1.63 (m, 4H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 168.45, 148.41, 137.00, 133.81, 132.00, 129.00, 128.53, 127.61, 127.59, 126.41, 123.12, 114.43, 71.62, 37.75, 33.10, 24.81. **HRMS(EI):** m/z calcd for $C_{22}H_{22}NO_3[M+H]^+$: 348.1600, found: 348.1608. IR (neat): 3457, 3027, 2931, 2850, 1770, 1708, 1614, 1494, 1467, 1438, 1398, 1371, 1043, 966, 897, 720 cm^{-1}.

(E)-4-(4-Bromophenyl)-2-methylene-1-phenylbut-3-en-1-ol (**3h**)



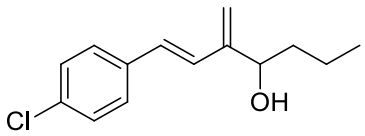
Following the general procedure C, the target compound **3h** was obtained as a white solid in 79% yield. R_f = 0.35 (hexanes/EA = 5:1). ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.46 – 7.43 (m, 2H), 7.41 – 7.35 (m, 4H), 7.32 – 7.28 (m, 1H), 7.20 – 7.16 (m, 2H), 6.71 (d, *J* = 16.5 Hz, 1H), 6.55 (d, *J* = 16.5 Hz, 1H), 5.57 (d, *J* = 3.7 Hz, 1H), 5.48 (s, 2H), 2.02 (d, *J* = 4.0 Hz, 1H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 147.16, 141.80, 135.99, 131.63, 128.82, 128.61, 128.33, 127.96, 127.90, 126.82, 121.39, 116.60, 74.43. **HRMS(EI):** m/z calcd for $C_{17}H_{16}BrO[M+H]^+$: 315.0385, found: 315.0385. IR (neat): 3384, 3032, 2918, 2850, 1602, 1487, 1453, 1038, 953, 861, 805, 757 cm^{-1}.

(E)-5-(4-Bromophenyl)-3-methylenepent-4-en-2-ol (**3i**)



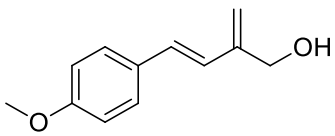
Following the general procedure C, the target compound **3i** was obtained as a white solid in 75% yield. R_f = 0.21 (hexanes/EA = 5:1). ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.44 (d, *J* = 8.5 Hz, 2H), 7.28 (d, *J* = 8.4 Hz, 2H), 6.76 (d, *J* = 16.5 Hz, 1H), 6.66 (d, *J* = 16.5 Hz, 1H), 5.37 (s, 1H), 5.26 (s, 1H), 4.70 (q, *J* = 6.4 Hz, 1H), 1.81 (s, 1H), 1.44 (d, *J* = 6.5 Hz, 3H). 13C NMR (126 MHz, $CDCl_3$) δ 149.73, 136.07, 131.68, 128.70, 127.86, 127.67, 121.34, 114.15, 67.70, 22.94. **HRMS(EI):** m/z calcd for $C_{12}H_{14}BrO$ $[M+H]^+$: 253.0228, found: 253.0217. IR (neat): 3375, 2972, 2925, 2855, 1700, 1612, 1588, 1488, 1402, 1072, 1010, 813 cm^{-1}.

(E)-1-(4-Chlorophenyl)-3-methylenehept-1-en-4-ol (**3j**)



Following the general procedure C, the target compound **3j** was obtained as a slight yellow oil in 64% yield. R_f = 0.35 (hexanes/EA = 5:1). ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.35 (d, *J* = 8.5 Hz, 2H), 7.29 (d, *J* = 8.5 Hz, 2H), 6.73 (d, *J* = 16.5 Hz, 1H), 6.69 (d, *J* = 16.5 Hz, 1H), 5.30 (s, 1H), 5.28 (s, 1H), 4.50 (s, 1H), 1.75 – 1.59 (m, 3H), 1.56 – 1.36 (m, 2H), 0.96 (t, *J* = 7.4 Hz, 3H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 148.74, 135.70, 133.20, 128.76, 128.51, 127.69, 127.59, 114.63, 72.10, 38.58, 19.05, 13.97. **HRMS(EI):** m/z calcd for $C_{14}H_{18}ClO$ $[M+H]^+$: 237.1046, found: 237.1051. IR (neat): 3388, 3030, 2960, 2929, 2873, 1706, 1611, 1593, 1491, 1465, 1096, 972, 814 cm^{-1}.

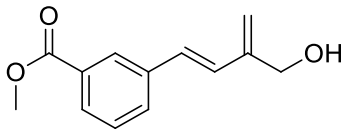
(E)-4-(4-Methoxyphenyl)-2-methylenebut-3-en-1-ol (**3k**)



Following the general procedure C, the target compound **3k** was obtained as a white solid in 76% yield. R_f = 0.11 (hexanes/EA = 5:1). ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.36 (d, *J* = 8.6 Hz, 2H), 6.86 (d, *J* = 8.7 Hz, 2H), 6.69 (d, *J* = 16.5 Hz, 1H), 6.62 (d, *J* = 16.6 Hz, 1H), 5.29 (s, 1H), 5.23 (s, 1H), 4.44 (s, 2H), 3.80 (d, *J* = 10.9 Hz, 3H), 1.60 (d, *J* = 14.3 Hz,

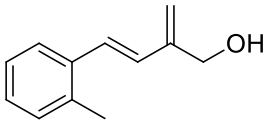
1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 159.29, 145.14, 129.74, 128.28, 127.64, 126.08, 115.19, 114.04, 63.26, 55. **HRMS(EI):** m/z calcd for $C_{13}H_{15}O_2[M+H]^+$: 191.1072, found: 191.1073. IR (neat): 3235, 2956, 2912, 2884, 2840, 1603, 1514, 1462, 1452, 1248, 1031, 956, 862 cm^{-1}.

(E)-Methyl 3-(3-(hydroxymethyl)buta-1,3-dien-1-yl)benzoate (**3l**)



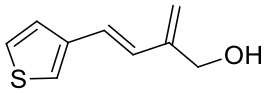
Following the general procedure C, the target compound **3l** was obtained as a white solid in 59% yield. R_f = 0.10 (hexanes/EA = 5:1). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.10 (s, 1H), 7.90 (d, *J* = 7.7 Hz, 1H), 7.59 (d, *J* = 7.8 Hz, 1H), 7.39 (t, *J* = 7.7 Hz, 1H), 6.88 (d, *J* = 16.6 Hz, 1H), 6.69 (d, *J* = 16.6 Hz, 1H), 5.39 (s, 1H), 5.32 (s, 1H), 4.46 (s, 2H), 3.97 – 3.90 (m, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 166.98, 144.75, 137.38, 130.78, 130.52, 129.34, 128.68, 128.60, 127.75, 127.40, 117.07, 63.12, 52.19. **HRMS(EI):** m/z calcd for $C_{13}H_{14}O_3$ $[M]^+$: 218.0943, found: 218.0941. IR (neat): 3375, 3032, 2953, 2925, 2854, 1721, 1604, 1586, 1444, 1291, 977, 752 cm^{-1}.

(E)-2-Methylene-4-(o-tolyl)but-3-en-1-ol (**3m**)



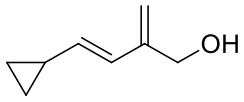
Following the general procedure C, the target compound **3m** was obtained as a colorless oil in 66% yield. R_f = 0.27 (hexanes/EA = 5:1). ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.52 – 7.49 (m, 1H), 7.22 – 7.13 (m, 3H), 6.90 (d, *J* = 16.4 Hz, 1H), 6.71 (d, *J* = 16.4 Hz, 1H), 5.36 (s, 1H), 5.29 (s, 1H), 4.48 (d, *J* = 4.3 Hz, 2H), 2.38 (s, 3H), 1.75 (t, *J* = 4.9 Hz, 1H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 145.30, 136.08, 135.72, 130.31, 129.39, 127.57, 126.54, 126.10, 125.15, 115.93, 63.20, 19.74. **HRMS(EI):** m/z calcd for $C_{12}H_{14}O$ $[M]^+$: 174.1045, found: 174.1041. IR (neat): 3332, 3056, 3020, 2925, 2858, 1631, 1600, 1484, 1461, 1061, 963, 890, 753 cm^{-1}.

(E)-2-Methylene-4-(thiophen-3-yl)but-3-en-1-ol (**3n**)



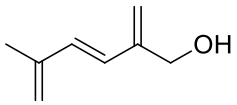
Following the general procedure C, the target compound **3n** was obtained as a white solid in 59% yield. R_f = 0.17 (hexanes/EA = 5:1). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.28 (dt, *J* = 10.4, 3.7 Hz, 2H), 7.22 – 7.19 (m, 1H), 6.70 (d, *J* = 16.6 Hz, 1H), 6.65 (d, *J* = 16.6 Hz, 1H), 5.31 (s, 1H), 5.24 (s, 1H), 4.42 (s, 2H), 1.68 (s, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 144.97, 139.79, 128.10, 126.14, 124.68, 123.10, 122.54, 115.72, 63.16. **HRMS(EI):** m/z calcd for $C_9H_{11}SO$ $[M+H]^+$: 167.0531, found: 167.0526. IR (neat): 3243, 3098, 2924, 2888, 1631, 1461, 1415, 1241, 1074, 960, 776 cm^{-1}.

(E)-4-Cyclopropyl-2-methylenebut-3-en-1-ol (**3o**)



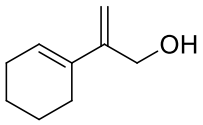
Following the general procedure C, the target compound **3o** was obtained as a white solid in 50% yield. R_f = 0.30 (hexanes/EA = 5:1). ^{1}H NMR (400 MHz, $CDCl_3$) δ 6.16 (d, *J* = 16.0 Hz, 1H), 5.30 (dd, *J* = 16.0, 8.9 Hz, 1H), 5.07 (s, 1H), 4.99 (s, 1H), 4.26 (s, 2H), 1.64 (s, 1H), 1.48 – 1.36 (m, 1H), 0.81 – 0.72 (m, 2H), 0.48 – 0.39 (m, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 144.87, 135.05, 126.94, 112.51, 63.32, 14.41, 7.25. **HRMS(EI):** m/z calcd for $C_8H_{12}O$ $[M]^+$: 124.0888, found: 124.0888. IR (neat): 3397, 3087, 3007, 2932, 2880, 1640, 1431, 1293, 1022, 977 cm^{-1}.

(E)-5-Methyl-2-methylenehexa-3,5-dien-1-ol (**3p**)



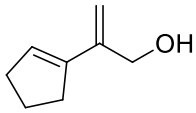
Following the general procedure C, the target compound **3p** was obtained as a white solid in 55% yield. R_f = 0.25 (hexanes/EA = 5:1). ^{1}H NMR (400 MHz, $CDCl_3$) δ 6.42 (d, *J* = 16.4 Hz, 1H), 6.24 (d, *J* = 16.4 Hz, 1H), 5.29 (s, 1H), 5.19 (s, 1H), 5.04 (s, 2H), 4.36 (s, 2H), 1.88 (s, 3H), 1.64 (s, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 145.03, 141.78, 131.73, 128.16, 117.72, 115.76, 63.14, 18.31. ^{19}F NMR (376 MHz, acetone) δ -141.69 (q, *J* = 47.8 Hz). HRMS(EI): m/z calcd for $C_8H_{12}O$ $[M]^+$: 124.0888, found: 124.0886. IR (neat): 3371, 3083, 2914, 2853, 1671, 1619, 1599, 1452, 1351, 1196, 1061, 961, 891 cm^{-1}.

2-(Cyclohex-1-en-1-yl)prop-2-en-1-ol (**3q**)



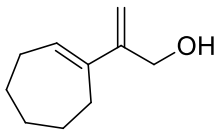
Following the general procedure C, the target compound **3q** was obtained as a colorless oil in 86% yield. R_f = 0.33 (hexanes/EA = 5:1). ^{1}H NMR (400 MHz, $CDCl_3$) δ 5.92 (s, 1H), 5.09 (s, 2H), 4.31 (s, 2H), 2.20 – 2.10 (m, 4H), 1.83 (s, 1H), 1.72 – 1.63 (m, 2H), 1.62 – 1.54 (m, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 147.22, 133.98, 124.98, 109.60, 64.15, 25.78, 25.70, 22.68, 22.06. **HRMS(EI):** m/z calcd for $C_9H_{14}O$ $[M]^+$: 138.1045, found: 138.1047. IR (neat): 3381, 2931, 2860, 1638, 1448, 1436, 1056, 1031, 895, 848 cm^{-1}.

2-(Cyclopent-1-en-1-yl)prop-2-en-1-ol (**3r**)



Following the general procedure C, the target compound **3r** was obtained as a colorless oil in 60% yield. R_f = 0.27 (hexanes/EA = 5:1). ^{1}H NMR (400 MHz, $CDCl_3$) δ 5.82 (s, 1H), 5.19 (s, 1H), 5.02 (s, 1H), 4.34 (s, 2H), 2.54 – 2.42 (m, 4H), 1.95 – 1.81 (m, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 143.41, 141.02, 127.12, 111.49, 64.16, 33.41, 32.67, 22.55. **HRMS(EI):** m/z calcd for $C_8H_{12}O$ $[M]^+$: 124.0888, found: 124.0889. IR (neat): 3349, 2953, 2877, 2850, 1670, 1438, 1298, 1042, 906, 843 cm^{-1}.

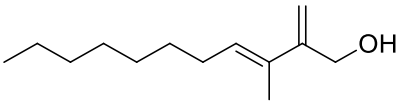
2-(Cyclohept-1-en-1-yl)prop-2-en-1-ol (**3s**)



Following the general procedure C, the target compound **3s** was obtained as a colorless oil in 78% yield. R_f = 0.29 (hexanes/EA = 5:1). ^{1}H NMR (400 MHz, $CDCl_3$) δ 6.00 (t, *J* = 6.8 Hz, 1H), 5.09 (s, 2H), 4.30 (d, *J* = 20.5 Hz, 2H), 2.38 – 2.34 (m, 2H), 2.21 (dd, *J* = 11.1, 6.6 Hz, 2H), 1.76 (dt, *J* = 15.0, 5.9 Hz, 3H), 1.54 – 1.43 (m, 4H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 148.76, 142.32, 129.31, 109.78, 64.41, 32.34, 29.80, 28.35, 26.53, 26.30. **HRMS(EI):** m/z calcd

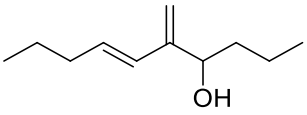
for $C_{10}H_{16}O$ $[M]^+$: 152.1201, found: 152.1195. IR (neat): 3346, 3040, 2922, 2851, 1632, 1605, 1447, 1282, 1041, 892, 850 cm^{-1}.

(E)-3-Methyl-2-methyleneundec-3-en-1-ol (**3t**)



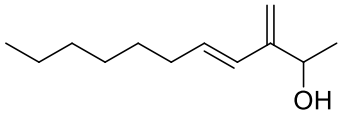
Following the general procedure C, the target compound **3t** was obtained as a colorless oil in 87% yield. R_f = 0.40 (hexanes/EA = 5:1). ^{1}H NMR (400 MHz, $CDCl_3$) δ 5.62 (t, *J* = 7.1 Hz, 1H), 5.12 (d, *J* = 9.6 Hz, 2H), 4.33 (s, 2H), 2.13 (q, *J* = 7.2 Hz, 2H), 1.80 (s, 3H), 1.68 (s, 1H), 1.45 – 1.34 (m, 2H), 1.33 – 1.23 (m, 8H), 0.88 (t, *J* = 6.8 Hz, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 148.31, 132.06, 128.45, 110.65, 64.29, 31.81, 29.54, 29.36, 29.17, 28.50, 22.63, 14.09, 14.05. **HRMS(EI):** m/z calcd for $C_{13}H_{24}O$ $[M]^+$: 196.1827, found: 196.1824. IR (neat): 3335, 2956, 2926, 2854, 1637, 1610, 1466, 1379, 1050, 895, 723 cm^{-1}.

(E)-5-Methylenedec-6-en-4-ol (**3u**)



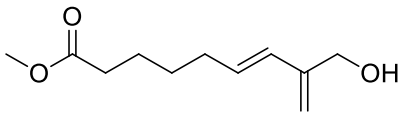
Following the general procedure C, the target compound **3u** was obtained as a colorless oil in 67% yield. R_f = 0.54 (hexanes/EA = 5:1). ^{1}H NMR (400 MHz, $CDCl_3$) δ 6.01 (d, *J* = 16.3 Hz, 1H), 5.82 (dt, *J* = 15.9, 6.9 Hz, 1H), 5.08 (s, 1H), 5.02 (s, 1H), 4.37 (s, 1H), 2.07 (q, *J* = 7.9 Hz, 2H), 1.69 – 1.56 (m, 3H), 1.52 – 1.35 (m, 4H), 0.93 (t, *J* = 5.6 Hz, 3H), 0.90 (t, *J* = 5.6 Hz, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 149.22, 131.12, 129.17, 111.35, 71.93, 38.53, 35.18, 22.43, 19.02, 13.99, 13.68. **HRMS(EI):** m/z calcd for $C_{11}H_{20}O$ $[M]^+$: 168.1514, found: 168.1513. IR (neat): 3359, 2960, 2932, 2873, 1649, 1608, 1465, 1379, 1029, 967, 896, 742 cm^{-1}.

(E)-3-Methyleneundec-4-en-2-ol (**3v**)



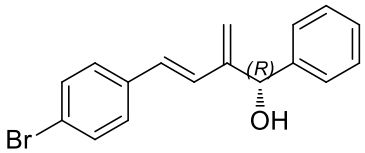
Following the general procedure C, the target compound **3v** was obtained as a colorless oil in 57% yield. R_f = 0.38 (hexanes/EA = 5:1). ^{1}H NMR (500 MHz, $CDCl_3$) δ 6.02 (d, *J* = 16.0 Hz, 1H), 5.82 (dt, *J* = 16.0, 6.9 Hz, 1H), 5.12 (s, 1H), 4.99 (s, 1H), 4.56 (q, *J* = 6.3 Hz, 1H), 2.12 – 2.07 (m, 2H), 1.60 (s, 1H), 1.40 (dd, *J* = 13.1, 7.5 Hz, 2H), 1.33 – 1.24 (m, 6H), 0.88 (t, *J* = 6.9 Hz, 3H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 150.30, 131.44, 129.10, 110.61, 67.77, 33.13, 31.69, 29.24, 28.87, 22.81, 22.59, 14.06. **HRMS(EI):** m/z calcd for $C_{12}H_{23}O[M+H]^+$: 183.1749, found: 183.1743. IR (neat): 3381, 2956, 2928, 2857, 1638, 1456, 1377, 1072, 906, 755 cm^{-1}.

(E)-Methyl 8-(hydroxymethyl)nona-6,8-dienoate (**3w**)



Following the general procedure C, the target compound **3w** was obtained as a white solid in 70% yield. R_f = 0.18 (hexanes/EA = 5:1). ^{1}H NMR (400 MHz, $CDCl_3$) δ 6.07 (d, *J* = 16.1 Hz, 1H), 5.74 (dt, *J* = 16.0, 6.9 Hz, 1H), 5.14 (s, 1H), 5.02 (s, 1H), 4.29 (s, 2H), 3.66 (s, 3H), 2.31 (t, *J* = 7.5 Hz, 2H), 2.15 – 2.07 (m, 2H), 1.68 – 1.58 (m, 3H), 1.48 – 1.37 (m, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 174.11, 145.03, 130.40, 129.78, 113.44, 63.21, 51.49, 33.86, 32.58, 28.62, 24.42. **HRMS(EI):** m/z calcd for $C_{11}H_{18}O_3[M]^+$: 198.1256, found: 198.1258. IR (neat): 3392, 2932, 2860, 1737, 1649, 1438, 1365, 1211, 1065, 967, 895, 745 cm^{-1}.

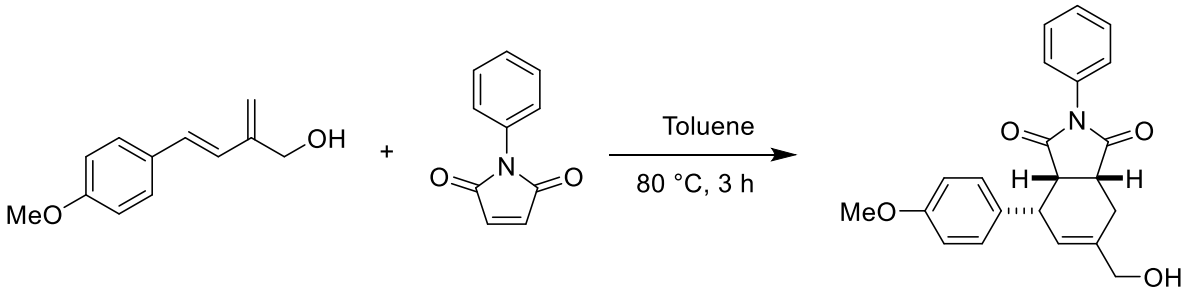
5. Synthesis of (R,*E*)-4-(4-Bromophenyl)-2-methylene-1-phenylbut-3-en-1-ol ((*R*)-3h).



Following the general procedure C, the target compound (*R*)-**3h** was obtained as a white solid 76%. R_f = 0.30 (hexanes/EA = 5:1). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.46 – 7.43 (m, 2H), 7.40 – 7.34 (m, 4H), 7.34 – 7.28 (m, 1H), 7.18 (d, *J* = 8.5 Hz, 2H), 6.72 (d, *J* = 16.5 Hz, 1H), 6.55 (d, *J* = 16.5 Hz, 1H), 5.56 (s, 1H), 5.48 (s, 2H), 2.20 (s, 1H). ^{13}C NMR (101

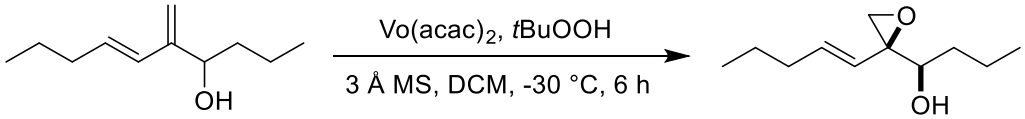
MHz, $CDCl_3$) δ 147.12, 141.77, 135.97, 131.62, 128.79, 128.61, 128.32, 127.96, 127.89, 126.82, 121.38, 116.63, 74.40. **HRMS(EI):** m/z calcd for $C_{17}H_{16}BrO[M+H]^+$: 315.0385, found: 315.0394. IR (neat): 3390, 3029, 2924, 2853, 1603, 1487, 1453, 1072, 962, 863, 810, 764 cm^{-1}. 95.6% *ee* (Chiralcel IC column, Hexane/^{i}PrOH = 97/3, 1.0 mL/min, λ = 280 nm, t_R(minor) = 11.63, t_R(major) = 13.99).

6. Diels-Alder reaction of compound 3k with N-phenylmaleimide.



Compound (1.0 equiv.) and N-phenylmaleimide (2.0 equiv.) were dissolved in toluene (2.0 mL) and heated at 80 ºC for 3 hrs. After the reaction was completed, the solvent was removed and the residue was purified directly using silica gel chromatography (hexanes/EA = 10:1 to 2:1). The product **4** was obtained as a white solid in 94% yield. R_f = 0.10 (hexanes/EA = 1:1). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.31 (dt, *J* = 15.0, 5.0 Hz, 3H), 7.09 (d, *J* = 8.6 Hz, 2H), 6.82 (d, *J* = 8.6 Hz, 2H), 6.72 (dd, *J* = 7.9, 1.4 Hz, 2H), 6.12 (d, *J* = 5.3 Hz, 1H), 4.19 (s, 2H), 3.92 (s, 1H), 3.76 (s, 3H), 3.46 – 3.34 (m, 2H), 2.95 (d, *J* = 17.3 Hz, 1H), 2.54 (dd, *J* = 17.4, 7.0 Hz, 1H), 1.89 (s, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 178.61, 176.37, 158.93, 138.42, 131.46, 130.20, 130.14, 128.82, 128.36, 126.18, 124.16, 113.88, 66.03, 55.27, 45.18, 40.44, 38.63, 22.88. **HRMS(EI):** m/z calcd for $C_{22}H_{22}NO_4$ $[M+H]^+$: 364.1543, found: 364.1556. IR (neat): 3047, 3062, 2925, 2854, 1755, 1708, 1609, 1513, 1501, 1456, 1386, 1251, 1178, 1031, 835, 737 cm^{-1}.

7. Selectively epoxidation of double bond in compound 3u.



In a flame-dried schlenk tube backfilled with N_2, $Va(acac)_2$ (3.8 mg, 0.014 mmol, 0.16 quiv.) and 3Å MS (20 mg) were added and followed with DCM (1.0 mL). Compound (15.0 mg, 0.09 mmol, 1.0 equiv.) dissolved in dried DCM (0.5 mL) was added, and after the mixture was cooled to -30 ^{o}C, ^{t}BuOOH (0.15 mL, 0.36 mmol, 4.0 equiv., 2.4 M in toluene) was added dropwise. After the reaction was completed (about 6 hrs), the reaction mixture was quenced using $Na_2S_2O_4$, and then dissolved in 20 mL DCM and washed using H_2O (10 mL × 3), dried using $MgSO_4$ and filtered through a pack of celite. After the solvent was removed using ice-H_2O bath under vacuum, the product **5** was obtained as a slight yellow oil with a quantitative yield. R_f = 0.24 (hexanes/EA = 5:1). ^{1}H NMR (400 MHz, CD_2Cl_2) δ 5.81 (dt, *J* = 15.6, 6.8 Hz, 1H), 5.58 (dt, *J* = 15.6, 1.3 Hz, 1H), 3.72 (dd, *J* = 8.2, 2.8 Hz, 1H), 2.95 (d, *J* = 5.3 Hz, 1H), 2.69 (d, *J* = 5.3 Hz, 1H), 2.03 (ddd, *J* = 14.5, 7.0, 1.3 Hz, 2H), 1.64 – 1.51 (m, 3H), 1.45 – 1.35 (m, 4H), 0.95 – 0.86 (m, 6H). ^{13}C NMR (101 MHz, CD_2Cl_2) δ 135.24, 125.95, 70.53, 61.07, 51.60, 35.67, 34.85, 22.52, 19.30, 14.26, 13.76. **HRMS(ESI):** m/z calcd for $C_{11}H_{20}O_2Na$ $[M+Na]^+$: 207.1356, found: 207.1367. IR (neat): 3351, 2960, 2932, 2874, 1706, 1586, 1530, 1458, 1380, 1364, 1246, 1197, 1026, 974, 847, 747 cm^{-1}.

Computational details.

Calculations were performed at the B3LYP[21] level of theory with differentiated basis set in gas phase and also in DCM as solvent with Polarizable Continuum Model (PCM)[22] as a single point calculation. The P, C, N, F, O, B and H atoms were described 6-31+G(d,p) basis set and Au atom with LANL2DZ[23],[24] relativistic effective core potential (ECP) basis set using Gaussian 09 software suite.[25] All of the degrees of conformational freedom were considered. Vibrational frequencies were computed at the same level of theory to verify that the optimized structures were

minima. For TS, IRC calculations were computed at the same level of theory in order to confirm the structures.

Pathway III, B(F)OH moiety, *in gas phase*

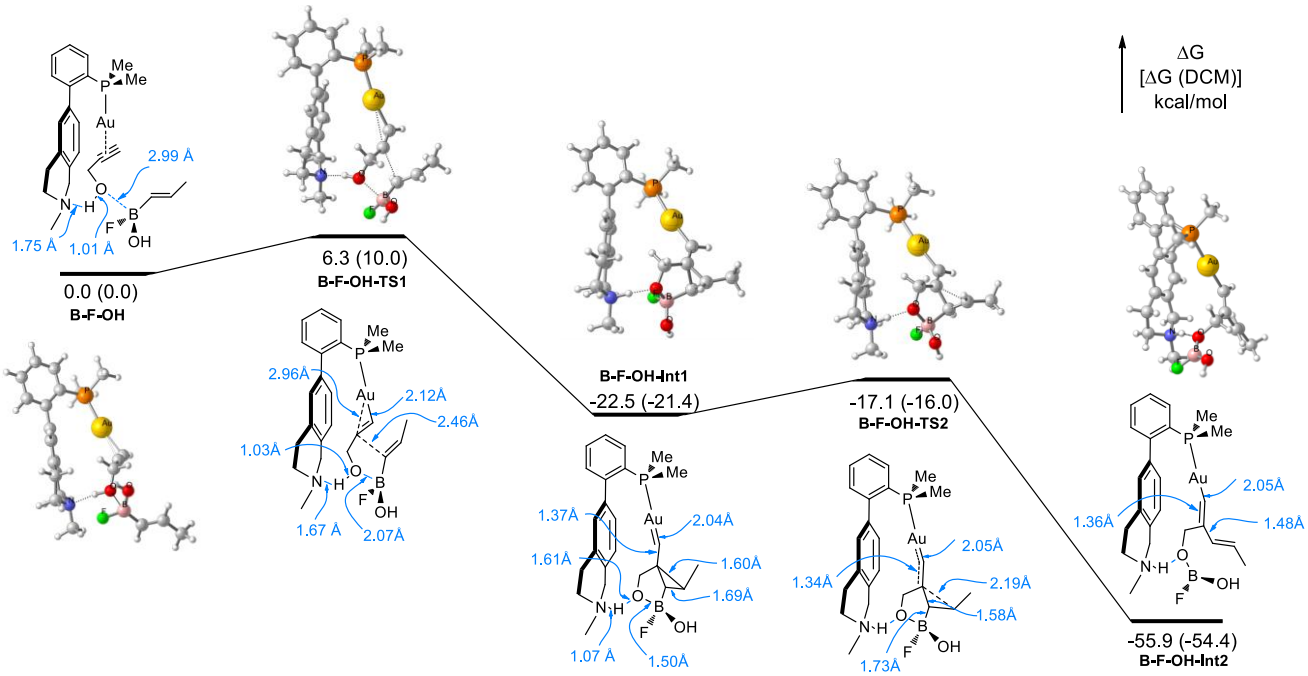
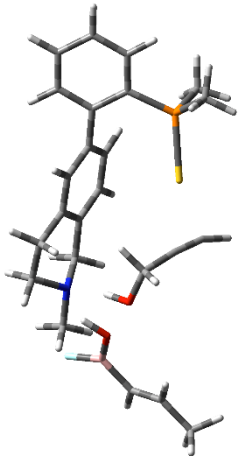


Figure 1. Reaction pathway modeled.

Cartesian coordinates and energies calculated for complex B-F-OH in gas phase.



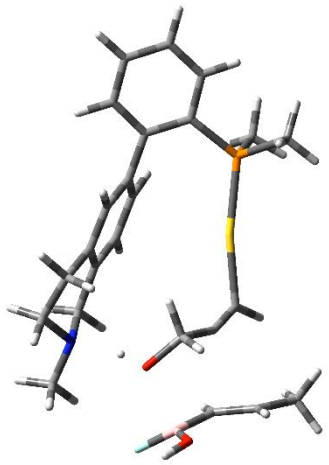
Energy = -1740.507147 (aU); Number of Imaginary Frequencies = 0

P	3.44955300	-1.27946400	0.04285200
C	4.04700200	0.29358600	0.78025800
C	5.26431800	0.22981200	1.48720800
C	5.80504000	1.35486700	2.10533500
C	5.12539600	2.57172900	2.03077100
C	3.92445600	2.65026400	1.32908800
C	3.36427600	1.53182400	0.68478300
H	5.80408900	-0.70749700	1.56917600
H	6.74512200	1.27701300	2.64220800
H	5.53158100	3.45762100	2.50922500
H	3.40726300	3.60180300	1.25332400
C	2.08417600	1.74122400	-0.05332900
C	1.99518000	1.58522300	-1.44787200
C	0.94920100	2.18389900	0.63949300
C	0.79028800	1.82715200	-2.10564500
H	2.87399100	1.30318100	-2.02031800
C	-0.26532700	2.43845900	-0.01324300
C	-0.35036600	2.23591600	-1.40096500

H	0.73503700	1.69914700	-3.18415400
C	3.96594000	-2.63231500	1.17809700
H	5.05301300	-2.69766500	1.26742600
H	3.52833200	-2.47549000	2.16680700
H	3.59216800	-3.57729800	0.77531700
C	4.45833500	-1.55623600	-1.47234900
H	5.52246800	-1.49342600	-1.22571100
H	4.23839100	-2.54501200	-1.88420000
H	4.22233200	-0.79941600	-2.22332100
C	-1.28404200	-1.60384400	-0.56088100
C	-2.14134100	-0.81953800	0.37147700
H	-1.50929700	-0.11556500	0.92921400
H	-2.56525100	-1.52331700	1.09917300
O	-3.19155700	-0.20312400	-0.31354700
H	-2.95311200	0.72519900	-0.62030000
C	-0.72639300	-2.29480800	-1.41501100
H	-0.55232700	-2.97556000	-2.22495800
Au	1.17359100	-1.51915200	-0.45874600
C	-1.47141200	2.90971500	0.77793400
H	-1.18681300	3.75102200	1.42102100
H	-1.79739400	2.10985800	1.45654900
C	-2.64569900	3.32404200	-0.11337400
H	-2.48605100	4.34091000	-0.51305400
H	-3.57041500	3.33810300	0.46857200
C	-1.65638800	2.46448800	-2.13193500
H	-1.64087900	3.45388100	-2.62753000
H	-1.77501000	1.71634800	-2.92347600
C	-4.07115700	2.58968100	-1.94489500

H	-4.16660800	1.85482900	-2.74928900
H	-4.90702700	2.45921000	-1.25406300
H	-4.12135000	3.59943300	-2.38272300
N	-2.80774900	2.36643700	-1.22311000
H	1.01132700	2.33145600	1.71559600
C	-6.44295100	-0.78898200	0.77357600
H	-6.88873100	-0.39128200	-0.13914800
C	-6.79018200	-2.03029100	1.16449200
H	-6.35651300	-2.42415200	2.08550100
B	-5.48379700	0.10732200	1.58123300
C	-7.74384400	-2.94121600	0.45311000
H	-8.13852400	-2.48666800	-0.46026100
H	-7.25424600	-3.88779400	0.18918500
H	-8.58786100	-3.20287000	1.10426400
F	-5.36253600	1.43189700	1.27395000
O	-4.77118900	-0.35208000	2.65415500
H	-4.33366900	0.35395800	3.14655300

Cartesian coordinates and energies calculated for TS B-F-OH-TS1 in gas phase.



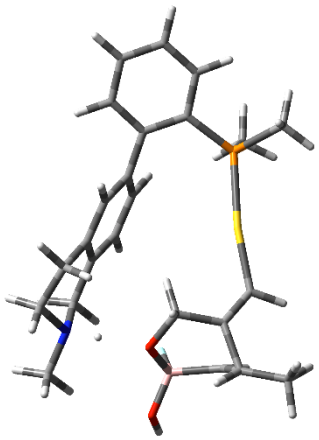
Energy = -1740.497046 (aU); Number of Imaginary Frequencies = 1(-171.2).

P	-3.15300200	-1.32135300	0.11839000
C	-4.01741200	0.25262300	-0.29219000
C	-5.35406700	0.14801100	-0.72395800
C	-6.09045200	1.27156200	-1.09301000
C	-5.49148700	2.53135600	-1.04327600
C	-4.17299800	2.65170100	-0.60965000
C	-3.41537400	1.53290200	-0.21708400
H	-5.83615000	-0.82203800	-0.78366700
H	-7.11951200	1.16016100	-1.41995300
H	-6.04998100	3.41682700	-1.33108100
H	-3.71486200	3.63412700	-0.54736200
C	-2.02457900	1.78163100	0.26226100
C	-1.63410600	1.48684600	1.58036200
C	-1.09119500	2.38886600	-0.58711000
C	-0.33508300	1.75596300	2.00472600
H	-2.35298000	1.06922300	2.27894900
C	0.21520500	2.67562300	-0.16661200
C	0.60348200	2.33277400	1.13829100

H	-0.04529400	1.51561700	3.02492500
C	-3.79368700	-2.57853800	-1.06634800
H	-4.86968100	-2.73692600	-0.96007300
H	-3.57260200	-2.26777200	-2.09028300
H	-3.28046200	-3.52363400	-0.87001000
C	-3.84601800	-1.85619500	1.74054900
H	-4.93931900	-1.86636900	1.70021100
H	-3.48165300	-2.85928100	1.97893600
H	-3.52614200	-1.17029100	2.52802900
C	2.11400000	-1.26253400	-0.39608200
C	2.50120600	-0.25589000	-1.41286700
H	1.57120800	0.27155600	-1.66920900
H	2.86269100	-0.75979800	-2.31496700
O	3.50774300	0.63533000	-1.00059400
H	3.20109500	1.38356400	-0.36335000
C	1.26813000	-1.90385000	0.30596800
H	1.44531800	-2.74207800	0.96922400
Au	-0.79505700	-1.42649400	0.15078800
C	1.19566200	3.33926100	-1.11473000
H	0.71490100	4.18961500	-1.61214000
H	1.47238500	2.63995200	-1.91489200
C	2.46266500	3.82053200	-0.40529700
H	2.26519000	4.75089500	0.15357000
H	3.24522500	4.03806700	-1.13744300
C	2.01029400	2.60172900	1.62765700
H	2.01484500	3.49924500	2.27301700
H	2.35585200	1.76674800	2.24720100
C	4.29698600	3.13813900	1.04237100

H	4.64661200	2.35798400	1.72221000
H	5.00770300	3.20838400	0.21632500
H	4.27344000	4.09815600	1.58011200
N	2.96497600	2.78022700	0.51815700
H	-1.38717200	2.64180300	-1.60284700
C	4.46419700	-1.62623900	0.23099000
H	4.30780800	-1.46133400	1.29845600
C	4.22829300	-2.87536500	-0.25670700
H	4.43514500	-3.05616500	-1.31240300
B	5.19198900	-0.50439600	-0.61470200
C	3.78941900	-4.06039300	0.53919200
H	3.56239500	-3.80472500	1.57854700
H	2.92390900	-4.55536700	0.08094200
H	4.59392400	-4.80808200	0.54698800
F	5.86809800	0.46920500	0.05960800
O	5.54884200	-0.81683000	-1.90258000
H	6.10192100	-0.14829300	-2.32538000

Cartesian coordinates and energies calculated for complex B-F-OH-Int1 in gas phase.



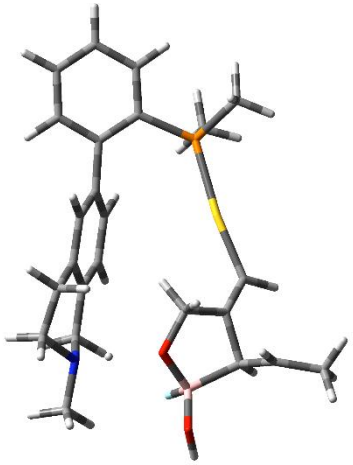
Energy = -1740.542943 (aU); Number of Imaginary Frequencies = 0

P	-3.06845600	-1.00737100	0.47709400
C	-3.79870100	0.59814200	-0.07667300
C	-5.16454900	0.59855400	-0.41996900
C	-5.80540300	1.74403500	-0.88907900
C	-5.07952900	2.92590200	-1.03229600
C	-3.72908700	2.94650100	-0.69085200
C	-3.06451700	1.80507600	-0.20421100
H	-5.74913900	-0.30985000	-0.33327000
H	-6.86012000	1.70694500	-1.14323500
H	-5.56045100	3.82793500	-1.39813100
H	-3.16988000	3.87321000	-0.77667400
C	-1.62602800	1.98284700	0.15768700
C	-1.15956800	1.79594400	1.47006000
C	-0.72219800	2.45794400	-0.80266600
C	0.16847400	2.06071000	1.79446700
H	-1.84395300	1.47577300	2.24845100
C	0.61386600	2.73780200	-0.48676600

C	1.06356600	2.53342400	0.82604100
H	0.51512300	1.89748100	2.81131100
C	-4.14487500	-2.31750400	-0.25243300
H	-5.16702800	-2.28427700	0.13325700
H	-4.16103000	-2.23015200	-1.34151900
H	-3.70884400	-3.28537800	0.00929900
C	-3.46140000	-1.14279400	2.27686800
H	-4.52273400	-0.94264800	2.45099000
H	-3.22285000	-2.15578200	2.61365800
H	-2.86433500	-0.43791300	2.85773600
C	2.17698100	-1.87462300	-0.78316300
C	2.23992100	-0.42366300	-1.23816300
H	1.32312800	0.08406200	-0.91565700
H	2.30855800	-0.36185400	-2.33265600
O	3.39722000	0.18747900	-0.67643700
H	3.39549100	1.75436500	-0.32564400
C	1.04324000	-2.46742600	-0.28375100
H	1.16465300	-3.51150500	0.00952900
Au	-0.80096400	-1.64785500	0.01280700
C	1.56631700	3.19332200	-1.57713900
H	1.11659500	4.00263600	-2.16288600
H	1.73473300	2.36767200	-2.28033900
C	2.91269700	3.68137300	-1.04257700
H	2.83820900	4.68161000	-0.60326700
H	3.66402800	3.70848000	-1.83490100
C	2.49615000	2.81329100	1.22392800
H	2.60672300	3.80676400	1.67560100
H	2.85006300	2.05535900	1.92531900

C	4.82834100	3.06147700	0.42073600
H	5.14961500	2.31907300	1.15093600
H	5.45675800	2.97467700	-0.46633900
H	4.88812500	4.07174500	0.83183000
N	3.41446900	2.76570300	0.03592200
H	-1.06589700	2.60689700	-1.82358500
C	3.50076500	-2.12071000	0.24537800
H	3.29562500	-2.78456200	1.08529800
C	3.51365100	-2.70273000	-1.07275300
H	4.06418300	-2.12885200	-1.82054600
B	3.95277600	-0.55611800	0.50023500
C	3.48275900	-4.19427200	-1.33092700
H	2.93969500	-4.74198400	-0.55573700
H	3.03625800	-4.42604100	-2.30253300
H	4.51138600	-4.57090300	-1.33549900
F	3.30674500	-0.11050400	1.71293100
O	5.35885300	-0.30064000	0.53392500
H	5.76065200	-0.58708500	1.36164900

Cartesian coordinates and energies calculated for TS B-F-OH-TS2 in gas phase.



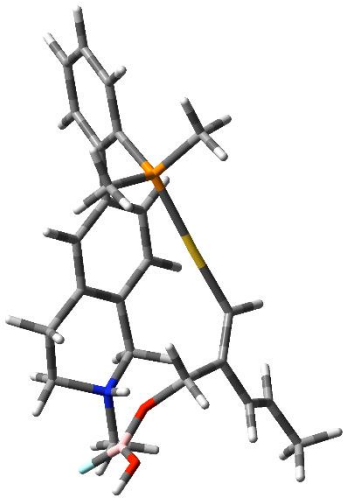
Energy = -1740.534404 (aU); Number of Imaginary Frequencies = 1(-131.9).

P	-3.14614300	-1.19379300	0.23461800
C	-3.92915200	0.43616900	-0.16065500
C	-5.29821100	0.41918400	-0.49082600
C	-5.98610200	1.57849200	-0.84321200
C	-5.30465700	2.79529700	-0.87821100
C	-3.95296000	2.83399400	-0.54454200
C	-3.24303700	1.67592000	-0.17296100
H	-5.84726400	-0.51615100	-0.48382700
H	-7.04178500	1.52720700	-1.09105900
H	-5.82210600	3.70945400	-1.15281900
H	-3.42888000	3.78504200	-0.54457200
C	-1.81027000	1.87203600	0.20242100
C	-1.33555600	1.59721100	1.49612200
C	-0.92415900	2.44579100	-0.71862700
C	-0.01597000	1.87936600	1.83968300
H	-2.00553400	1.18498200	2.24393900
C	0.40475700	2.73851400	-0.38468400
C	0.86357700	2.44851600	0.90894000

H	0.33518000	1.65329100	2.84321500
C	-3.99666600	-2.41032800	-0.86341100
H	-5.07049100	-2.47661100	-0.67169600
H	-3.83039800	-2.14289800	-1.90992500
H	-3.54898600	-3.39147700	-0.68310100
C	-3.80624600	-1.61999600	1.90674700
H	-4.89755200	-1.54515000	1.92499300
H	-3.50793800	-2.64181600	2.15772200
H	-3.39139300	-0.94424600	2.65830500
C	2.23057700	-1.57944800	-0.34853500
C	2.26683400	-0.35053000	-1.22256800
H	1.35009900	0.22842200	-1.07174500
H	2.32802100	-0.60852300	-2.29043300
O	3.41897900	0.40786000	-0.86441200
H	3.26911400	1.91657700	-0.30109600
C	1.16336800	-2.23502200	0.13437600
H	1.36928000	-3.15840900	0.67844300
Au	-0.79303000	-1.61478900	0.11479200
C	1.33916500	3.30913300	-1.43512900
H	0.84690100	4.11925200	-1.98417500
H	1.57328600	2.53588500	-2.17820400
C	2.64005800	3.85056000	-0.84798400
H	2.48664700	4.80010100	-0.32457900
H	3.39277100	4.00091600	-1.62503300
C	2.28611100	2.74682800	1.33258800
H	2.34897300	3.68376100	1.89974900
H	2.69015900	1.93834100	1.94592900
C	4.58897800	3.26247600	0.57704300

H	4.93411900	2.53543700	1.31135400
H	5.24058300	3.23020200	-0.29714400
H	4.57295600	4.26850400	1.00216100
N	3.20549800	2.88441800	0.15307700
H	-1.27608700	2.66440300	-1.72401400
C	3.71281200	-1.91264200	0.10150300
H	3.77709400	-2.33354200	1.10650600
C	3.92928600	-2.83513400	-0.92967300
H	3.86144000	-2.47073800	-1.95583400
B	4.36709200	-0.30815700	0.02336200
C	4.25092300	-4.27428800	-0.78403200
H	4.26859300	-4.60375200	0.25643200
H	3.55750500	-4.89577100	-1.36418900
H	5.24240100	-4.44429700	-1.23249800
O	5.68749400	-0.18360700	-0.46975100
H	6.35284200	-0.33018100	0.21160900
F	4.23838700	0.19113900	1.36626800

Cartesian coordinates and energies calculated for complex B-F-OH-Int2 in gas phase.



Energy = -1740.596171 (aU); Number of Imaginary Frequencies = 0

P	2.89448600	-1.21587700	0.64948100
C	3.97070000	0.24039200	0.25067700
C	5.35628200	0.11094000	0.46296900
C	6.24367900	1.14294700	0.16169600
C	5.75566800	2.33755100	-0.36980400
C	4.38576000	2.48812500	-0.57944100
C	3.47695500	1.46171600	-0.26924000
H	5.76086000	-0.81227800	0.86493200
H	7.30698400	1.01016500	0.33623000
H	6.43455400	3.14829900	-0.61613000
H	4.00103400	3.42067200	-0.98210400
C	2.02543000	1.73472600	-0.50836600
C	1.50750600	1.73967400	-1.81469400
C	1.16440500	2.03209400	0.55225600
C	0.15179900	1.96061000	-2.03145600
H	2.16323800	1.53185100	-2.65445000
C	-0.20046900	2.27460900	0.34469700
C	-0.71353300	2.20283400	-0.95644100

H	-0.24197800	1.91510500	-3.04385500
C	2.92858900	-1.29933200	2.49499100
H	3.95593100	-1.29923000	2.87126800
H	2.39695400	-0.44200100	2.91514600
H	2.42446100	-2.21419400	2.81946600
C	3.88989500	-2.68797300	0.15131600
H	4.83897100	-2.76125800	0.68840800
H	3.29633100	-3.58140200	0.36418800
H	4.08373100	-2.65340500	-0.92368100
C	-2.40432500	-1.52505900	-0.59461500
C	-2.59283000	-1.53305900	0.89695000
H	-1.63207400	-1.56875100	1.41226100
H	-3.21675600	-2.36952200	1.22582700
O	-3.27247700	-0.28986700	1.33024900
C	-1.16362800	-1.54414100	-1.14148000
H	-1.14669500	-1.65836100	-2.22876900
Au	0.68367300	-1.37293400	-0.27387100
C	-1.10968000	2.55505800	1.52523900
H	-0.64911200	3.28898400	2.19556800
H	-1.24761000	1.64009400	2.11518700
C	-2.47439400	3.09092700	1.10528400
H	-2.41509300	4.11151000	0.71485000
H	-3.18855900	3.06585000	1.93013100
C	-2.19011000	2.36088200	-1.24369600
H	-2.42192500	3.34130900	-1.67631300
H	-2.53485300	1.58849100	-1.93619600
C	-4.47265600	2.54638100	-0.29228700
H	-4.81624900	1.89075000	-1.09367700

H	-5.05464400	2.36632300	0.61131400
H	-4.55657800	3.59156200	-0.59527300
N	-3.03618100	2.23565200	-0.00451200
H	1.56090000	2.07201400	1.56403500
C	-3.86113800	-1.17254400	-2.63737800
H	-3.02829500	-0.71695100	-3.17668400
B	-4.13218000	-0.27411900	2.38213900
O	-4.44453200	-1.37252400	3.10524400
H	-5.07833500	-1.23238800	3.81969000
C	-5.13714000	-1.34108500	-3.41167400
H	-5.92754900	-1.78411300	-2.79774100
H	-5.50318500	-0.38458900	-3.80725200
H	-4.98188900	-1.99394500	-4.28044700
C	-3.66511500	-1.58763100	-1.37234500
H	-4.51988700	-2.02439000	-0.84933100
H	-3.00614100	1.24902700	0.33308500
F	-4.67374100	0.93922800	2.67465800

Energies for these structures computed as a single point in DCM using differentiated basis set (6-31+G(d,p) for C, H, O, N, F, P and B; def2-TZVP[26] for Au) were reported below.

Compound Name	Energy (aU)	ΔG and $\Delta G^{\neq}$
B-F-OH	-1740.889914	
B-F-OH-TS1	-1740.873925	$\Delta G^{\neq}$ = 10 kcal/mol
B-F-OH-Int1	-1740.924051	$\Delta G^{\text{B-F-OH/Int1}}$ = 21.4 kcal/mol
B-F-OH-TS2	-1740.915490	$\Delta G^{\neq}$ = 5.4 kcal/mol
B-F-OH-Int2	-1740.976708	$\Delta G^{\text{Int1/Int2}}$=33 kcal/mol

Pathway II, B(OH)F moiety, *in gas phase*.

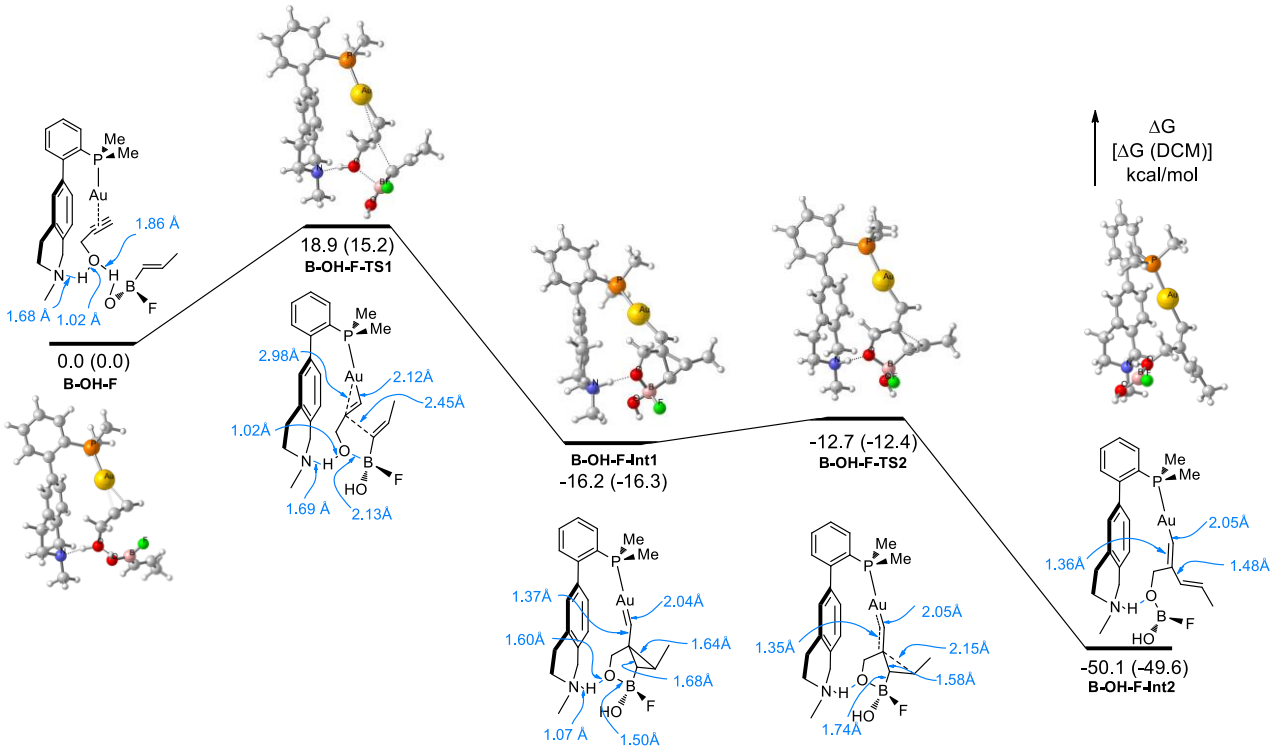
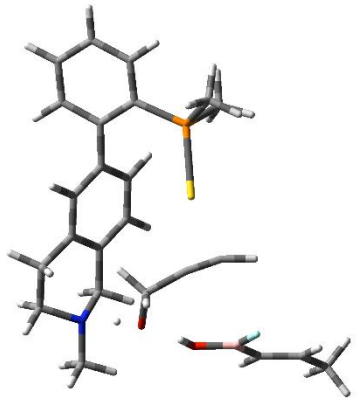


Figure 1. Reaction pathway modeled.

Cartesian coordinates and energies calculated for complex B-OH-F in gas phase.



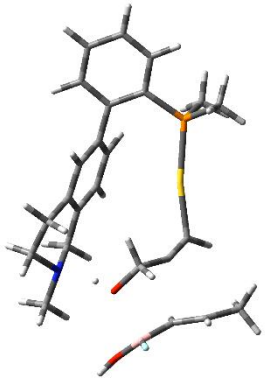
Energy = -1740.516494 (aU); Number of Imaginary Frequencies = 0

P	-2.83073900	-1.75962900	0.18883700
C	-3.95630300	-0.35889100	0.56882500
C	-5.33594200	-0.64498000	0.56923800
C	-6.28346100	0.34533400	0.81804200
C	-5.86073000	1.65218700	1.06499400
C	-4.49932100	1.94740000	1.07482400
C	-3.52145400	0.96293000	0.84044800
H	-5.68914800	-1.64998400	0.36583400
H	-7.33972800	0.09570200	0.81340600
H	-6.58597200	2.43666500	1.25814600
H	-4.17124800	2.95921000	1.29182200
C	-2.09456500	1.39392400	0.90330100
C	-1.19604600	0.86018700	1.84403300
C	-1.64327100	2.42464800	0.06696600
C	0.11585700	1.32604000	1.90836300
H	-1.53181600	0.10558300	2.54865800
C	-0.32954500	2.90968700	0.13153100

C	0.56649900	2.34006900	1.05192300
H	0.80019500	0.89932100	2.63759300
C	-3.73972100	-2.88080900	-0.95343100
H	-4.63328000	-3.30322000	-0.48730200
H	-4.02193900	-2.34118500	-1.86049900
H	-3.07047700	-3.70039000	-1.22783300
C	-2.66909400	-2.74676200	1.73480800
H	-3.66355000	-2.97998300	2.12688500
H	-2.13565600	-3.67690900	1.52013600
H	-2.11226200	-2.18643300	2.48806900
C	1.29543800	-0.54422000	-1.88281300
C	1.48642200	0.83191300	-2.40817100
H	0.59139700	1.43120000	-2.20569500
H	1.58560400	0.74403000	-3.49904100
O	2.65146700	1.40724900	-1.87145300
H	2.45273600	2.20240600	-1.26266700
C	1.37428300	-1.70859600	-1.49124400
H	1.73568100	-2.69770700	-1.28717600
Au	-0.72417100	-1.30615200	-0.73613200
C	0.11422500	4.02668200	-0.79542800
H	-0.60769400	4.85090100	-0.75556000
H	0.10048400	3.66920900	-1.83427400
C	1.51018100	4.56016400	-0.46080000
H	1.46164600	5.26350500	0.38790800
H	1.91732900	5.10854100	-1.31483400
C	2.00115200	2.81655000	1.12832800
H	2.11709900	3.52954100	1.96526200
H	2.66897300	1.97271500	1.32885200

C	3.82385000	3.90734200	-0.04300100
H	4.46979900	3.05709300	0.18895000
H	4.13033200	4.32738900	-1.00443100
H	3.94853400	4.67581300	0.73533800
N	2.42462700	3.44863300	-0.13497800
H	-2.33155300	2.85977100	-0.65439700
C	5.85428200	-1.34794500	1.25387200
H	6.22691700	-0.58047500	1.93387500
C	6.29853500	-2.61008600	1.41376900
H	5.93685800	-3.37921000	0.72865300
B	4.86902200	-0.93153900	0.14151100
O	4.45927200	0.35132800	-0.01455100
H	3.87091100	0.52392200	-0.77828000
C	7.27164400	-3.07512200	2.45369300
H	7.59055200	-2.25917500	3.10862100
H	6.83172500	-3.86857800	3.07170400
H	8.16181600	-3.51079500	1.98176700
F	4.36282600	-1.87503200	-0.71274700

Cartesian coordinates and energies calculated for TS B-OH-F-TS1 in gas phase.



Energy = -1740.495970 (aU); Number of Imaginary Frequencies = 1(-170.9).

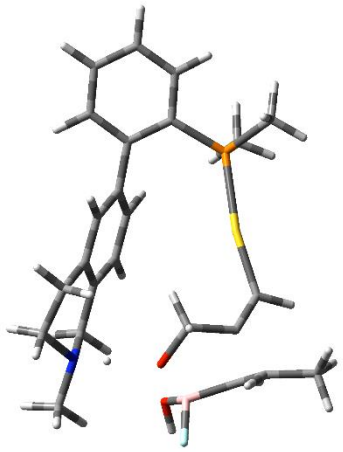
P	-3.14675700	-1.33153500	0.11537100
C	-4.02527700	0.23854200	-0.27953600
C	-5.36488500	0.12768100	-0.70042100
C	-6.11175000	1.24866400	-1.05591000
C	-5.52068500	2.51211500	-1.00304700
C	-4.19926600	2.63845300	-0.58019500
C	-3.43101700	1.52209000	-0.20163800
H	-5.84099300	-0.84525100	-0.76219500
H	-7.14280600	1.13260600	-1.37486000
H	-6.08750700	3.39566100	-1.28030500
H	-3.74678900	3.62337200	-0.51593100
C	-2.03702000	1.77624000	0.26547200
C	-1.63287200	1.48204800	1.57959200

C	-1.11433400	2.38774000	-0.59222100
C	-0.33107900	1.75693100	1.99197900
H	-2.34310900	1.06010800	2.28445400
C	0.19466900	2.67976600	-0.18387700
C	0.59685500	2.33841400	1.11716600
H	-0.03089100	1.51769200	3.00944400
C	-3.77901900	-2.58291000	-1.08005300
H	-4.85398500	-2.74909500	-0.97504500
H	-3.56030600	-2.26161400	-2.10125000
H	-3.25949000	-3.52628100	-0.89218500
C	-3.83524500	-1.88486500	1.73331100
H	-4.92840500	-1.90409600	1.69271700
H	-3.46234100	-2.88643500	1.96476500
H	-3.52152500	-1.20167500	2.52569700
C	2.13407400	-1.25457000	-0.39627500
C	2.51978100	-0.25196700	-1.42022000
H	1.58601900	0.27272100	-1.67053000
H	2.87037900	-0.75759000	-2.32553800
O	3.52800200	0.63943000	-1.01645400
H	3.21214200	1.39236500	-0.39927100
C	1.27650200	-1.87875900	0.31001200
H	1.45330300	-2.70832400	0.98441000
Au	-0.78711200	-1.41673500	0.14925900

C	1.16290600	3.34880500	-1.14019500
H	0.66970300	4.18892400	-1.64272600
H	1.44794500	2.64698300	-1.93534900
C	2.42458100	3.85054000	-0.43659300
H	2.21345700	4.77641600	0.12522100
H	3.19851800	4.08335500	-1.17320800
C	2.00601300	2.61672500	1.59527500
H	2.00611500	3.50829800	2.24915500
H	2.36604500	1.78011200	2.20448700
C	4.27752500	3.19083600	0.99728900
H	4.66662900	2.39089200	1.63124600
H	4.96668700	3.32559700	0.16031400
H	4.23701700	4.12608500	1.57669500
N	2.94914200	2.81576900	0.47967400
H	-1.42082200	2.64025200	-1.60492700
C	4.45814400	-1.64275100	0.26128900
H	4.30850300	-1.51421700	1.33409300
C	4.19084400	-2.86676700	-0.27402100
H	4.38980200	-3.01477200	-1.33647400
B	5.24185900	-0.52810200	-0.53736300
O	6.00333700	0.36701500	0.16176600
H	6.61979000	0.85527900	-0.39918000
C	3.73735700	-4.07436300	0.47926800

H	3.50603400	-3.85112400	1.52500400
H	2.87270600	-4.54934300	-0.00009900
H	4.53924700	-4.82489000	0.46910700
F	5.52970400	-0.78002500	-1.84687200

Cartesian coordinates and energies calculated for complex B-OH-F-Int1 in gas phase.



Energy = -1740.542306 (aU); Number of Imaginary Frequencies = 0

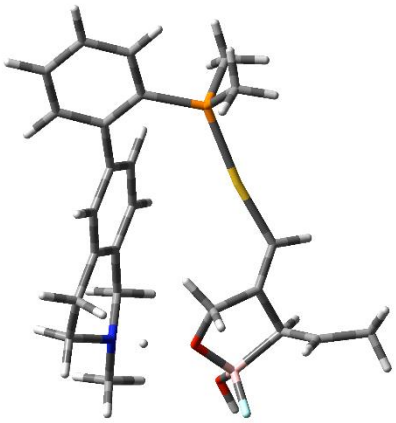
P	-3.10900300	-1.09323800	0.37718200
C	-3.87871700	0.51150500	-0.11417800
C	-5.24447400	0.49310700	-0.45676200
C	-5.91134500	1.64237800	-0.87704900
C	-5.21218100	2.84593400	-0.96966600
C	-3.86241100	2.88419300	-0.62697500
C	-3.17303400	1.73807200	-0.18839200
H	-5.80670500	-0.43264600	-0.40764000

H	-6.96506700	1.59271100	-1.13315900
H	-5.71426400	3.75100700	-1.29759600
H	-3.32425200	3.82608600	-0.67422700
C	-1.73816700	1.92370000	0.18124500
C	-1.27061200	1.70317700	1.48795400
C	-0.83871200	2.43085700	-0.76551800
C	0.05461500	1.97377900	1.82001400
H	-1.95155700	1.35024600	2.25574400
C	0.49497700	2.71285200	-0.44250500
C	0.94640900	2.48115100	0.86561400
H	0.39987300	1.79319600	2.83469900
C	-4.05925600	-2.39099200	-0.52748800
H	-5.11195600	-2.42118300	-0.23570500
H	-3.98515800	-2.22463500	-1.60501400
H	-3.60747400	-3.35914700	-0.29535100
C	-3.62263500	-1.36131300	2.13108600
H	-4.70597500	-1.25010900	2.23583100
H	-3.32980900	-2.36949600	2.43775900
H	-3.12647200	-0.64244400	2.78653700
C	2.24083600	-1.80891600	-0.64630200
C	2.32820400	-0.43390800	-1.29214400
H	1.37723600	0.08858300	-1.13846900
H	2.50401100	-0.52106300	-2.37411700

O	3.39427000	0.29317700	-0.69410000
H	3.33115800	1.83866800	-0.29023700
C	1.11079200	-2.33970900	-0.08145200
H	1.25231200	-3.32928500	0.35729900
Au	-0.77827400	-1.59166000	0.07592300
C	1.44029000	3.21474300	-1.51741700
H	0.96282600	4.00589400	-2.10577700
H	1.65923700	2.40187200	-2.22180100
C	2.75058000	3.75936700	-0.95480400
H	2.61433800	4.73916600	-0.48502400
H	3.50692900	3.85448000	-1.73715900
C	2.37075900	2.78084200	1.28070500
H	2.44352100	3.74616800	1.79676500
H	2.76319200	1.99397800	1.92947600
C	4.68279300	3.21141900	0.50419300
H	5.01836900	2.49291500	1.25080100
H	5.32969400	3.15234200	-0.37235200
H	4.68223400	4.22778000	0.90479300
N	3.29367100	2.83897400	0.09814500
H	-1.18462700	2.60698900	-1.78134300
C	3.64275200	-2.01620100	0.24909000
H	3.47724900	-2.55448900	1.18222100
C	3.53322500	-2.76779900	-0.96297200

H	3.99745400	-2.31745500	-1.84166500
B	4.25831500	-0.47680700	0.26320000
O	4.18224600	0.18563000	1.55217100
H	4.92993000	-0.06520500	2.10769200
C	3.41045800	-4.27287200	-1.02704000
H	2.95263000	-4.69485500	-0.12829600
H	2.84261100	-4.59990400	-1.90300300
H	4.41946800	-4.69337800	-1.10592000
F	5.59305200	-0.51761100	-0.20937600

Cartesian coordinates and energies calculated for TS B-OH-F-TS2 in gas phase.



Energy = -1740.536816 (aU); Number of Imaginary Frequencies = 1(-124.6).

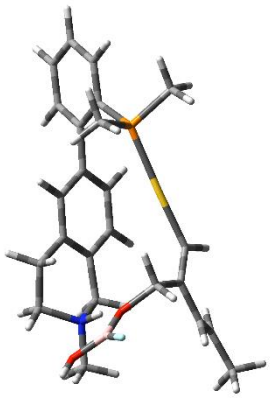
P	-3.14799600	-1.22860800	0.17067700
C	-3.95399400	0.39594600	-0.19515100

C	-5.31895700	0.36663000	-0.54063000
C	-6.01894100	1.52430500	-0.87381500
C	-5.35413100	2.75104600	-0.87317800
C	-4.00680200	2.80133600	-0.52323700
C	-3.28587800	1.64453800	-0.17020200
H	-5.85434100	-0.57667700	-0.56038500
H	-7.07101600	1.46467500	-1.13478600
H	-5.88149700	3.66379100	-1.13325000
H	-3.49546600	3.75898400	-0.49688800
C	-1.85933200	1.84761500	0.22598600
C	-1.40535700	1.58319700	1.52932400
C	-0.96035300	2.41561000	-0.68501600
C	-0.09221500	1.87179200	1.89199400
H	-2.08688800	1.17440900	2.26873200
C	0.36237100	2.71372000	-0.33210500
C	0.80101600	2.43544000	0.97073800
H	0.24121100	1.65815700	2.90443100
C	-3.92139500	-2.41982200	-1.00842500
H	-5.00312100	-2.50365800	-0.87869300
H	-3.70252700	-2.11551000	-2.03500800
H	-3.47124300	-3.40138600	-0.83651100
C	-3.86202000	-1.72798200	1.79932600
H	-4.95476900	-1.67890600	1.77931000

H	-3.54850700	-2.75016600	2.02929100
H	-3.49115700	-1.06715100	2.58653900
C	2.26544400	-1.52240600	-0.28749900
C	2.32450200	-0.34803400	-1.23581000
H	1.37651300	0.19666200	-1.22539800
H	2.52647300	-0.66777800	-2.26983900
O	3.38277400	0.48445700	-0.77204000
H	3.26837600	1.98144000	-0.17911100
C	1.18964100	-2.13370100	0.24113700
H	1.39991800	-3.00234500	0.86818200
Au	-0.77897900	-1.57406000	0.14178300
C	1.30837200	3.29117300	-1.36655000
H	0.80767600	4.07502800	-1.94513900
H	1.59144300	2.51301600	-2.08668600
C	2.56972000	3.88529400	-0.74893500
H	2.36448500	4.82947800	-0.23338500
H	3.33531300	4.06393200	-1.50705000
C	2.20988800	2.75985000	1.42234200
H	2.23454900	3.68462100	2.01188300
H	2.62295100	1.95442700	2.03509800
C	4.49632000	3.40734900	0.73658500
H	4.88606100	2.67016500	1.43661300
H	5.16208400	3.46289700	-0.12552400

H	4.39519300	4.39149400	1.19987300
N	3.15269500	2.94680300	0.26939800
H	-1.29749100	2.62934200	-1.69649300
C	3.74602900	-1.81720900	0.19237000
H	3.81225600	-2.05137800	1.25609100
C	3.85663300	-2.92491600	-0.66267500
H	3.82498000	-2.73269200	-1.73559900
B	4.51704200	-0.32008800	-0.25175000
O	5.07751500	0.35721400	0.87713000
H	6.01666000	0.15624800	0.96543400
C	4.04590800	-4.34220800	-0.26980900
H	5.04568500	-4.64837400	-0.61714100
H	3.98735000	-4.49665800	0.80928300
H	3.33888200	-5.00060200	-0.78757000
F	5.46934000	-0.59639100	-1.25729800

Cartesian coordinates and energies calculated for complex B-OH-F-Int2 in gas phase.



Energy = -1740.596431 (aU); Number of Imaginary Frequencies = 0

P	2.88543900	-1.21131100	0.66663200
C	3.97233900	0.23215600	0.25153400
C	5.35829900	0.09256500	0.45432400
C	6.25183400	1.11528700	0.13950100
C	5.76980400	2.31022500	-0.39656000
C	4.39968000	2.47064500	-0.59726600
C	3.48469700	1.45412900	-0.27302800
H	5.75850300	-0.83129200	0.85896300
H	7.31528100	0.97482000	0.30700800
H	6.45349100	3.11366100	-0.65333500
H	4.01962100	3.40369300	-1.00319500
C	2.03411400	1.73653600	-0.50475800
C	1.51515100	1.76346500	-1.81049700

C	1.17446700	2.01941400	0.56107100
C	0.16006100	1.99214400	-2.02273600
H	2.16955200	1.56617000	-2.65382400
C	-0.18989800	2.26893600	0.35851400
C	-0.70380500	2.22018600	-0.94345300
H	-0.23451100	1.96426800	-3.03548000
C	2.90154700	-1.26175100	2.51381500
H	3.92554300	-1.25812000	2.89910600
H	2.36927300	-0.39519600	2.91387700
H	2.39150800	-2.16903100	2.85017900
C	3.87528400	-2.69879100	0.20516700
H	4.81711300	-2.77153900	0.75492700
H	3.27173000	-3.58360000	0.42585600
H	4.08202700	-2.68419300	-0.86787800
C	-2.40401700	-1.52122100	-0.61278000
C	-2.59864800	-1.53804800	0.87798900
H	-1.63903300	-1.57464200	1.39546700
H	-3.22000600	-2.38062100	1.19688300
O	-3.28279500	-0.29967500	1.31617800
C	-1.16041700	-1.53638700	-1.15311900
H	-1.13793400	-1.64435100	-2.24088600
Au	0.68215500	-1.36858700	-0.27466400
C	-1.09837500	2.52939000	1.54429400

H	-0.63706100	3.25154100	2.22684600
H	-1.23545700	1.60433200	2.11852400
C	-2.46451600	3.07146500	1.13687200
H	-2.40781600	4.10056400	0.76903100
H	-3.17850900	3.02138200	1.96043800
C	-2.17985600	2.38892700	-1.22697000
H	-2.40865200	3.37906400	-1.63860700
H	-2.52686900	1.63293000	-1.93623300
C	-4.46271500	2.55698700	-0.27025100
H	-4.80450700	1.92560500	-1.09167300
H	-5.04069300	2.34485300	0.62896000
H	-4.54756000	3.61075200	-0.54179100
N	-3.02569800	2.24006400	0.00884300
H	1.57169600	2.04255700	1.57311200
C	-3.85111000	-1.15731700	-2.65972600
H	-3.01622200	-0.69646700	-3.19126600
B	-4.15273100	-0.28210100	2.35936600
O	-4.71096600	0.92160500	2.69466000
H	-5.32328700	0.86932700	3.44007500
C	-5.12290400	-1.32201100	-3.44152300
H	-5.91578700	-1.77055600	-2.83484100
H	-5.48812100	-0.36307300	-3.83184100
H	-4.96228700	-1.96829100	-4.31422600

C	-3.66107100	-1.58033700	-1.39651100
H	-4.51809300	-2.02154500	-0.88086000
H	-2.99749900	1.24800600	0.32796700
F	-4.46480700	-1.39309900	3.04654100

Energies for these structures computed as a single point in DCM using differentiated basis set (6-31+G(d,p) for C, H, O, N, F, P and B; def2-TZVP[26] for Au) were reported below.

Compound Name	Energy (aU)	ΔG and $\Delta G^{\neq}$
B-OH-F	-1740.897698	
B-OH-F-TS1	-1740.873480	$\Delta G^{\neq}$ = 15.2 kcal/mol
B-OH-F-Int1	-1740.923618	$\Delta G^{\text{CPX-PROD}}$ = 16.3 kcal/mol
B-OH-F-TS2	-1740.917418	$\Delta G^{\neq}$ = 3.9 kcal/mol
B-OH-F-Int2	-1740.976635	$\Delta G^{\text{PROD-PROD-REAL}}$ = 33.3 kcal/mol

Pathway I, $B(OH)_2$ moiety, *in gas phase*.

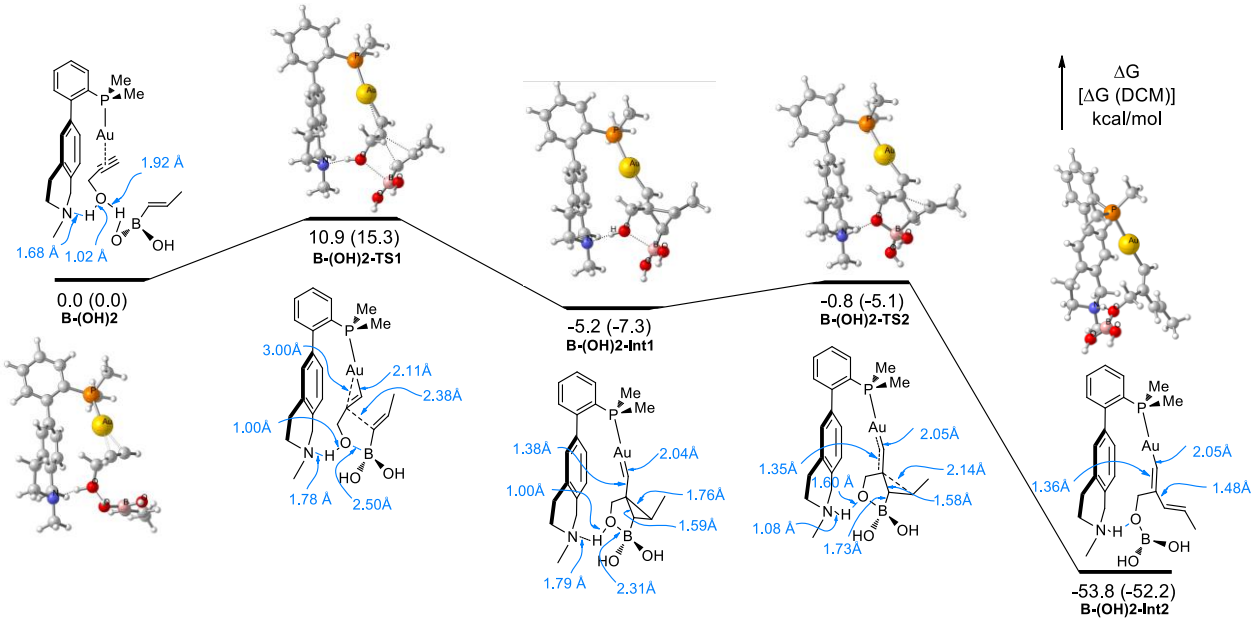
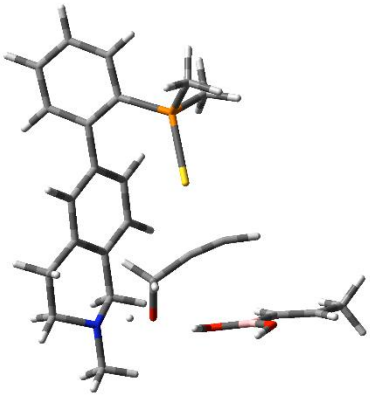


Figure 1. Reaction pathway modeled.

Cartesian coordinates and energies calculated for complex B-$(OH)_2$ in gas phase.



Energy = -1716.485291 (aU); Number of Imaginary Frequencies = 0

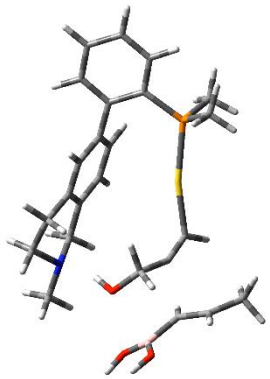
P -2.75253500 -1.71707800 0.02812200

C	-3.86669500	-0.34431700	0.52425300
C	-5.24670500	-0.62917500	0.52657500
C	-6.18837700	0.34213400	0.85814800
C	-5.75932100	1.62869300	1.18785000
C	-4.39743100	1.92171300	1.19681700
C	-3.42522000	0.95489400	0.88012800
H	-5.60442500	-1.61777700	0.25966700
H	-7.24504600	0.09424900	0.85324500
H	-6.48012200	2.39849200	1.44582400
H	-4.06406500	2.91599900	1.47747700
C	-1.99607200	1.37751100	0.95232200
C	-1.09219000	0.78816800	1.85427800
C	-1.54717300	2.44944800	0.16810800
C	0.22284400	1.24308000	1.93129600
H	-1.42605600	-0.00347300	2.51843900
C	-0.22945600	2.92236500	0.24582600
C	0.67097200	2.30012700	1.12674800
H	0.91282000	0.77311200	2.62759000
C	-3.66547700	-2.72165600	-1.21460400
H	-4.57005400	-3.16760400	-0.79401100
H	-3.93102200	-2.10069700	-2.07339100
H	-3.00686900	-3.52553200	-1.55369700

C	-2.60663300	-2.83692600	1.48217500
H	-3.60411800	-3.10182800	1.84557800
H	-2.07285000	-3.74554400	1.19031300
H	-2.05375800	-2.34509900	2.28472600
C	1.39067300	-0.40816900	-1.90806400
C	1.56512400	0.98523000	-2.39948800
H	0.68034500	1.57785000	-2.14172400
H	1.61964200	0.93367200	-3.49554100
O	2.75245600	1.54538000	-1.89366100
H	2.56576100	2.29262200	-1.22080500
C	1.49408600	-1.58262100	-1.55391900
H	1.85517500	-2.57385400	-1.35771900
Au	-0.63117800	-1.20906900	-0.82912700
C	0.21520100	4.08126900	-0.62795800
H	-0.50041800	4.90750700	-0.54232300
H	0.19109800	3.77600600	-1.68318000
C	1.61705600	4.58988700	-0.27889000
H	1.57819200	5.25167200	0.60301700
H	2.02063200	5.17723400	-1.10857500
C	2.10770600	2.76509000	1.22009900
H	2.22874600	3.43651900	2.08990500
H	2.77122100	1.90840500	1.37275600
C	3.92736800	3.91701300	0.10696800

H	4.57310600	3.06004500	0.31409300
H	4.24106600	4.37542700	-0.83453200
H	4.04653500	4.65334300	0.91647300
N	2.52967500	3.46036800	-0.01203800
H	-2.23994400	2.92648400	-0.52187800
C	4.96455600	-1.77220600	1.50792600
H	4.77669900	-1.22573500	2.43462600
C	5.49256300	-3.00771000	1.60107200
H	5.69809500	-3.55222300	0.67767100
B	4.64205600	-1.07304100	0.16013500
O	4.19607000	0.22840600	0.17954800
H	3.87675700	0.58574200	-0.66956100
O	4.77761700	-1.78758500	-1.01961700
H	4.74272400	-1.25699800	-1.82436100
C	5.85053200	-3.72060800	2.87075200
H	5.61533300	-3.12171600	3.75586600
H	5.31973600	-4.67876500	2.94586100
H	6.92140100	-3.96129600	2.89033200

Cartesian coordinates and energies calculated for TS B-$(OH)_2$-TS1 in gas phase.



Energy = -1716.467936 (aU); Number of Imaginary Frequencies = 1(-166.05).

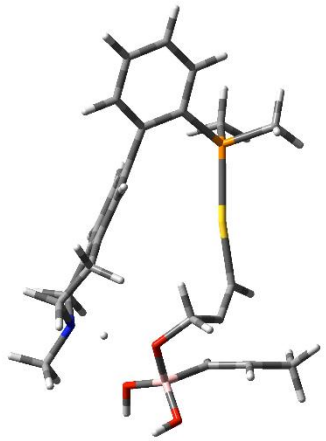
P	-3.04985000	-1.42602600	0.00214500
C	-4.05702800	0.09686500	-0.24244100
C	-5.40658400	-0.08867100	-0.60142000
C	-6.24676600	0.99273700	-0.85580500
C	-5.74190700	2.29130000	-0.76162800
C	-4.41216800	2.49030300	-0.39683100
C	-3.55107100	1.41270900	-0.11996200
H	-5.81615000	-1.08983600	-0.69308500
H	-7.28307200	0.82046000	-1.12925500
H	-6.38242400	3.14485700	-0.96178800
H	-4.02412500	3.49988000	-0.30099500
C	-2.15529400	1.73614800	0.29771600
C	-1.70548200	1.48398400	1.60524500
C	-1.28346300	2.36429300	-0.59870100

C	-0.40604700	1.82303100	1.97597400
H	-2.37732500	1.03954000	2.33395200
C	0.02504500	2.71217200	-0.23463600
C	0.47346600	2.42109100	1.06319700
H	-0.06836700	1.61819400	2.98924400
C	-3.52472100	-2.55561700	-1.37514000
H	-4.59521400	-2.77517500	-1.37911000
H	-3.24754400	-2.10306000	-2.33035000
H	-2.97259300	-3.49218200	-1.25925300
C	-3.75797300	-2.23270800	1.50153500
H	-4.84093400	-2.35025800	1.40113300
H	-3.29784600	-3.21538700	1.63668700
H	-3.54824900	-1.62233800	2.38316800
C	2.26307500	-1.19540700	-0.36254900
C	2.61322100	-0.28651400	-1.48618300
H	1.63934300	0.08105800	-1.84900800
H	3.07405500	-0.85650300	-2.29852600
O	3.49344700	0.75446500	-1.16126500
H	3.09299100	1.45790700	-0.56601500
C	1.37582600	-1.71444800	0.40354000
H	1.56531300	-2.45235200	1.17470200
Au	-0.69024800	-1.35526100	0.16110700
C	0.94518100	3.37932300	-1.23794200

H	0.41002100	4.17941600	-1.76262600
H	1.23998300	2.65266200	-2.00706700
C	2.20329500	3.95005500	-0.58251600
H	1.97064100	4.88630400	-0.04486100
H	2.94888200	4.18828100	-1.34651500
C	1.88414300	2.76412000	1.49231400
H	1.86819100	3.67414800	2.12210800
H	2.29045500	1.95869700	2.11441900
C	4.11867600	3.37268900	0.80449000
H	4.54308800	2.59599400	1.44591200
H	4.77546000	3.49897700	-0.06038500
H	4.08663900	4.32238500	1.36275400
N	2.78398300	2.96062200	0.34476700
H	-1.62810700	2.58329600	-1.60704000
C	4.48066000	-1.63586600	0.37133000
H	4.29349500	-1.48605500	1.43497000
C	4.17281800	-2.85378300	-0.16495900
H	4.41145200	-3.01693400	-1.21667500
B	5.42782700	-0.61308700	-0.37484300
O	6.01942400	0.34731700	0.40497900
H	6.69568400	0.88713500	-0.02050200
O	5.75966800	-0.92284900	-1.67171900
H	6.32186100	-0.29681600	-2.14148900

C	3.64669200	-4.03823800	0.57592500
H	3.38227700	-3.80380100	1.61094100
H	2.79033800	-4.49216400	0.06427100
H	4.43024600	-4.80809600	0.60223800

Cartesian coordinates and energies calculated for complex B-(OH)$_2$-int1 in gas phase.



Energy = -1716.493605 (aU); Number of Imaginary Frequencies = 0

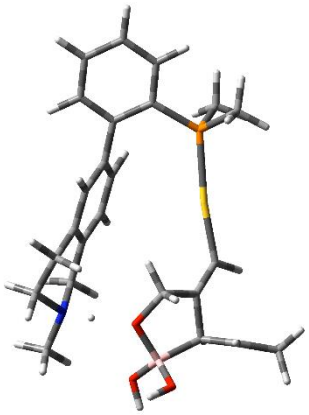
P	-3.04268200	-1.31197700	0.17386600
C	-3.96805300	0.21848400	-0.27600000
C	-5.30672000	0.06357100	-0.68505800
C	-6.07979500	1.15325200	-1.07986600
C	-5.51690600	2.43080800	-1.07771800
C	-4.19712300	2.60184700	-0.66629800
C	-3.40315500	1.51694000	-0.25008400
H	-5.76153600	-0.92138000	-0.70694200

H	-7.10937500	1.00256400	-1.38920100
H	-6.10448100	3.29058100	-1.38505600
H	-3.76607500	3.59811900	-0.64086200
C	-2.01338200	1.81762000	0.19997200
C	-1.59138200	1.56390700	1.51672700
C	-1.11256700	2.43013400	-0.67994200
C	-0.29484900	1.88697800	1.91289600
H	-2.28444700	1.13994300	2.23739500
C	0.19157300	2.76477100	-0.29045600
C	0.60984000	2.47336900	1.01761800
H	0.01836200	1.68312100	2.93422800
C	-3.63663600	-2.60850200	-0.99672600
H	-4.71009200	-2.79170400	-0.90642400
H	-3.40645700	-2.31222900	-2.02311900
H	-3.10447600	-3.53753700	-0.77482300
C	-3.76117400	-1.83993200	1.79022000
H	-4.85204500	-1.89169600	1.72685100
H	-3.36603000	-2.82359500	2.05909500
H	-3.48578300	-1.12756200	2.57144000
C	2.44069800	-1.39027000	-0.28476400
C	2.39425300	-0.26737600	-1.32307500
H	1.41596700	0.21929900	-1.25037600
H	2.49837600	-0.66891500	-2.33772900

O	3.45340000	0.65240200	-1.12456000
H	3.18622200	1.41861500	-0.53386100
C	1.34054500	-1.84237800	0.40804500
H	1.56633300	-2.63168400	1.12794800
Au	-0.64116800	-1.40332600	0.25577100
C	1.14143400	3.41064000	-1.28005600
H	0.63278500	4.22412700	-1.81047200
H	1.42686300	2.67675400	-2.04509100
C	2.40535300	3.95174400	-0.60956100
H	2.19261100	4.90162100	-0.08772000
H	3.16997000	4.15783100	-1.36413900
C	2.01508700	2.80346200	1.47349200
H	1.99943700	3.72768500	2.08236400
H	2.39468700	2.00612100	2.12226300
C	4.27627800	3.34858300	0.82370500
H	4.65667500	2.57978600	1.50131100
H	4.95882100	3.43227800	-0.02682800
H	4.25854000	4.31497500	1.35339500
N	2.94310300	2.96020900	0.34186800
H	-1.43106300	2.64477100	-1.69763600
C	3.91150400	-1.77181700	0.19951600
H	3.92721600	-2.04888800	1.25344600
C	3.42941600	-2.78040800	-0.70391100

H	3.61918700	-2.60774200	-1.76201600
B	5.06646800	-0.75489900	-0.25763600
O	5.58499000	0.04546900	0.73016000
H	6.40225900	0.50908100	0.51329800
O	5.65775400	-1.04598200	-1.46235100
H	6.32284300	-0.42781700	-1.78602000
C	3.11193400	-4.20376000	-0.34256000
H	2.91886300	-4.34491600	0.72287200
H	2.28192600	-4.61105400	-0.92553200
H	4.00618100	-4.79024800	-0.59350500

Cartesian coordinates and energies calculated for TS B-$(OH)_2$-TS2 in gas phase.



Energy = -1716.500687 (aU); Number of Imaginary Frequencies = 1(-107.61).

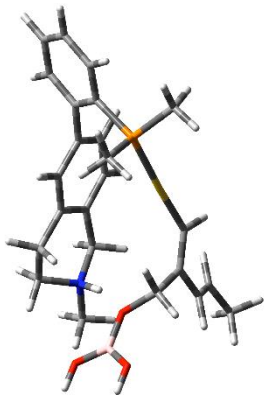
P	-3.13804900	-1.24852300	0.12092700
C	-3.96334900	0.37014900	-0.23042200
C	-5.32307800	0.32772000	-0.59417800

C	-6.03411200	1.48124400	-0.91836400
C	-5.38603500	2.71674900	-0.88974800
C	-4.04404900	2.77989200	-0.52153800
C	-3.31297600	1.62716900	-0.17718100
H	-5.84513800	-0.62250000	-0.63511300
H	-7.08187400	1.41199300	-1.19395200
H	-5.92264800	3.62620000	-1.14238100
H	-3.54566800	3.74357200	-0.47391900
C	-1.89351100	1.83567600	0.23974100
C	-1.45577700	1.55247100	1.54475600
C	-0.98307200	2.41226100	-0.65375200
C	-0.14329600	1.82165200	1.92272300
H	-2.14818400	1.13849600	2.27107200
C	0.33927700	2.69234900	-0.28458300
C	0.76459000	2.38484000	1.01565200
H	0.17933500	1.58886000	2.93446600
C	-3.85187400	-2.42168800	-1.11272000
H	-4.93631400	-2.52259700	-1.02347800
H	-3.60168600	-2.08931000	-2.12330500
H	-3.39395600	-3.40104000	-0.94882600
C	-3.89726600	-1.79932300	1.71217200
H	-4.98947400	-1.77162200	1.65586600
H	-3.57080600	-2.81997000	1.93066800

H	-3.56701800	-1.14876000	2.52575400
C	2.28944300	-1.45041900	-0.24545800
C	2.32862600	-0.32738400	-1.25909400
H	1.38255000	0.22109200	-1.25706000
H	2.50412400	-0.70966400	-2.27622700
O	3.40407100	0.52236200	-0.87150100
H	3.26268200	1.94216300	-0.13949800
C	1.21930500	-2.03969300	0.32294200
H	1.44177900	-2.86724800	0.99953600
Au	-0.76012600	-1.53767400	0.16946300
C	1.29977900	3.28305100	-1.29738900
H	0.80933900	4.08003200	-1.86683000
H	1.58992800	2.51704600	-2.02731000
C	2.55471900	3.86010700	-0.65135200
H	2.34332300	4.79021100	-0.11288600
H	3.32724700	4.05997000	-1.39699600
C	2.17559700	2.67422900	1.48246500
H	2.20722600	3.57448100	2.10850500
H	2.57348000	1.84167100	2.06872900
C	4.45999600	3.35804100	0.84829200
H	4.85603500	2.60304900	1.52485500
H	5.13779800	3.45336300	-0.00012100
H	4.33553600	4.32347200	1.34456000

N	3.13019600	2.89477500	0.34570000
H	-1.30909900	2.64371900	-1.66496500
C	3.77993300	-1.72165000	0.21501200
H	3.87301400	-1.85508300	1.29423600
C	3.82247800	-2.90784000	-0.53864500
H	3.79668100	-2.80032100	-1.62239400
B	4.57301600	-0.32638900	-0.43132300
O	5.26012600	0.44129700	0.58036700
H	6.17257800	0.14217200	0.66588200
O	5.38469400	-0.80972600	-1.52410000
H	5.76166600	-0.08727800	-2.04087100
C	3.95825900	-4.29170900	-0.02369400
H	3.85309100	-4.35781700	1.06116000
H	3.26603000	-4.98102900	-0.51896100
H	4.96988900	-4.63356400	-0.29691500

Cartesian coordinates and energies calculated for complex B-$(OH)_2$-Int2 in gas phase.



Energy = -1716.571007 (aU); Number of Imaginary Frequencies = 0

P	2.91010600	-1.21039300	0.63846300
C	3.97168600	0.26124400	0.25448800
C	5.35522900	0.14986700	0.48977900
C	6.23433200	1.19243900	0.20134700
C	5.73966700	2.38002300	-0.33995000
C	4.37150300	2.51300500	-0.57145100
C	3.47079900	1.47539400	-0.27476200
H	5.76447500	-0.76739700	0.90097100
H	7.29626500	1.07364100	0.39358000
H	6.41214300	3.19896500	-0.57669900
H	3.98132300	3.43998500	-0.98165400
C	2.01914300	1.73055800	-0.53371400
C	1.50940800	1.69432000	-1.84255100

C	1.14964900	2.05113800	0.51293300
C	0.15305900	1.89784400	-2.07288700
H	2.17175900	1.46844600	-2.67244600
C	-0.21596900	2.27612300	0.29094000
C	-0.72090200	2.16228400	-1.01013500
H	-0.23463200	1.81969000	-3.08565900
C	2.96988100	-1.32690300	2.48144200
H	4.00166300	-1.32963200	2.84534600
H	2.43999300	-0.47929600	2.92303700
H	2.47293500	-2.24929200	2.79545700
C	3.91522900	-2.66198400	0.09957000
H	4.87673800	-2.72797200	0.61511700
H	3.33920700	-3.56707200	0.31147800
H	4.08597700	-2.60891500	-0.97862400
C	-2.40168300	-1.52369100	-0.54906300
C	-2.58277500	-1.47620900	0.94451000
H	-1.61629100	-1.48134400	1.45170700
H	-3.18385300	-2.31686800	1.30362100
O	-3.28208000	-0.23875300	1.33557400
C	-1.16583500	-1.57160900	-1.10444800
H	-1.15710500	-1.72891900	-2.18647000
Au	0.68853000	-1.38011200	-0.25659100
C	-1.13420100	2.58373600	1.45713400

H	-0.68101500	3.33817900	2.10959900
H	-1.27221600	1.68447500	2.07039000
C	-2.49970900	3.09927300	1.01459700
H	-2.44458900	4.10921200	0.59638300
H	-3.21796100	3.08528900	1.83556200
C	-2.19779100	2.29572500	-1.30844400
H	-2.43467900	3.25730400	-1.77922900
H	-2.53150800	1.49550800	-1.97419000
C	-4.48484800	2.50472500	-0.37706000
H	-4.81651700	1.83170500	-1.16908200
H	-5.06765400	2.33139000	0.52718700
H	-4.57343800	3.54358200	-0.70052500
N	-3.04965700	2.20857800	-0.07161400
H	1.53971600	2.12159100	1.52558200
C	-3.86928000	-1.24380000	-2.59601000
H	-3.03791500	-0.81428800	-3.15848300
B	-4.12706300	-0.19683500	2.41474700
O	-4.68210400	1.04968100	2.65137000
H	-5.28346300	1.11286200	3.40144200
C	-5.15218700	-1.43344200	-3.35422900
H	-5.94068700	-1.84725300	-2.71772100
H	-5.51536300	-0.49017300	-3.78309800
H	-5.00843300	-2.11989700	-4.19881300

C	-3.66711200	-1.61000800	-1.31690800
H	-4.52136400	-2.01923300	-0.77136100
H	-3.02462800	1.23275200	0.30469000
O	-4.35095400	-1.32718700	3.14858200
H	-4.96407000	-1.27842500	3.88927000

Energies for these structures computed as a single point in DCM using differentiated basis set (6-31+G(d,p) for C, H, O, N, P and B; def2-TZVP[26] for Au) were reported below.

Compound Name	Energy (aU)	ΔG and $\Delta G^{\neq}$(for TSs)
B-$(OH)_2$	-1716.869283	
B-$(OH)_2$-TS1	-1716.844895	$\Delta G^{\neq}$ = 15.3 kcal/mol
B-$(OH)_2$-Int1	-1716.880957	$\Delta G^{CPX\text{-}INTERM}$ = 7.3 kcal/mol
B-$(OH)_2$-TS2	-1716.879067	$\Delta G^{\neq}$ = 1.18 kcal/mol
B-$(OH)_2$-Int2	-1716.952507	$\Delta G^{INTERM\text{-}PROD\text{-}REAL}$ = 44.9 kcal/mol

Pathway for L3, B(F)OH moiety, *in gas phase* and in DCM as a solvent.

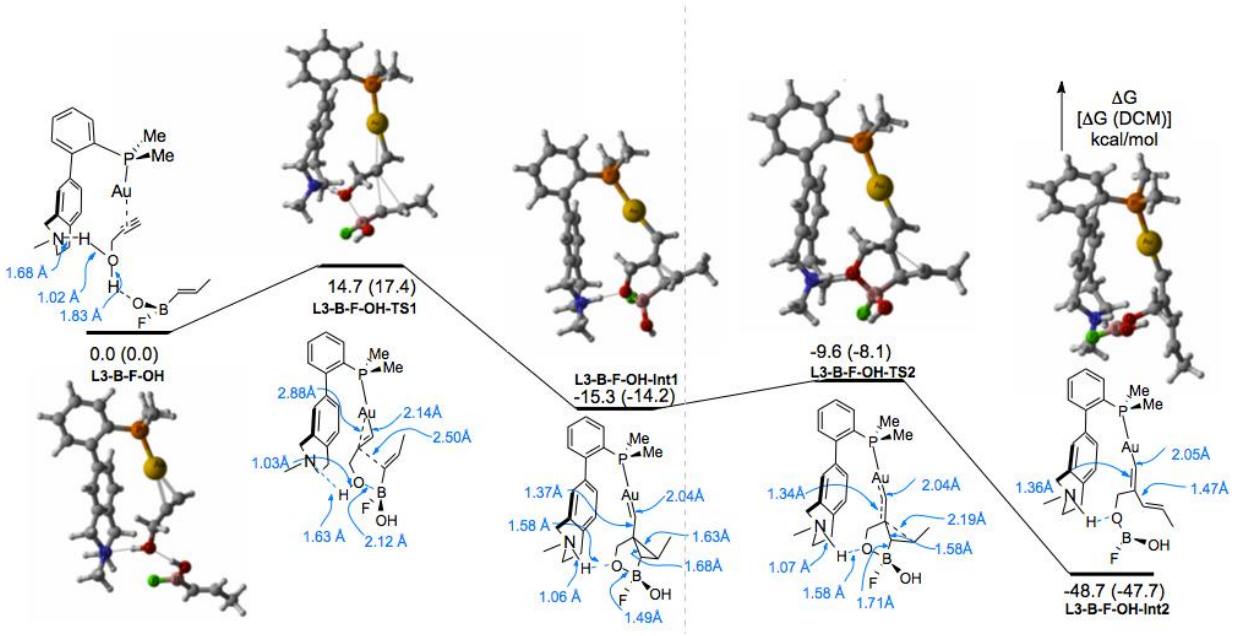
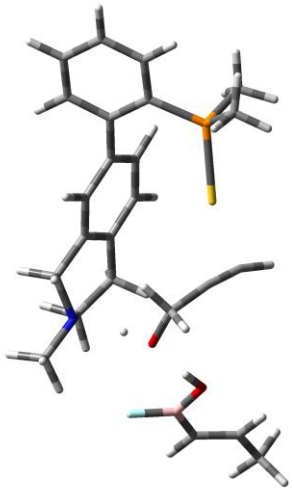


Figure 1. Reaction pathway modeled.

Cartesian coordinates and energies calculated for complex L3-B-F-OH in gas phase.



Energy = -1740.516199 (aU); Number of Imaginary Frequencies = 0.

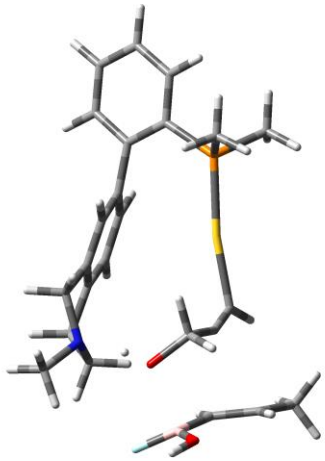
P	-3.34836900	-1.52421600	0.13634700
C	-4.23883300	0.08118900	0.18145600

C	-5.62700200	0.03889100	-0.05639900
C	-6.39482200	1.20101400	-0.07821800
C	-5.77765400	2.43549800	0.12994900
C	-4.40686000	2.49060400	0.37438300
C	-3.61262000	1.33039800	0.41811900
H	-6.12612400	-0.90752700	-0.23529300
H	-7.46281400	1.13955900	-0.26169900
H	-6.36116600	3.35085100	0.11130900
H	-3.93154700	3.44899400	0.55970000
C	-2.16165200	1.50595800	0.72229200
C	-1.58946000	1.01537300	1.90897500
C	-1.34924700	2.24601200	-0.14837700
C	-0.24004600	1.23356900	2.18392400
H	-2.20813400	0.49089300	2.63161200
C	0.00590000	2.47192700	0.12602100
C	0.57917200	1.94764000	1.29730100
H	0.18563700	0.85077000	3.10839700
C	-4.19349300	-2.56993500	-1.11884200
H	-5.22936000	-2.78107300	-0.84214100
H	-4.17144000	-2.07308600	-2.09164500
H	-3.65297500	-3.51695200	-1.19585700
C	-3.69429500	-2.36652600	1.73597600
H	-4.77382800	-2.39854700	1.91130200

H	-3.30045900	-3.38619600	1.70677800
H	-3.21654200	-1.82534200	2.55516000
C	1.22282700	-1.16568500	-1.09892800
C	1.55601500	-0.14126600	-2.12766700
H	0.69721000	0.52492700	-2.27284000
H	1.72467900	-0.67281800	-3.07285500
O	2.72298200	0.55689000	-1.78187300
H	2.51746900	1.44299200	-1.31686200
C	1.16267400	-2.05268900	-0.24782000
H	1.39685400	-2.84947600	0.43048200
Au	-1.04334900	-1.48707300	-0.27781700
C	0.83514000	3.31494500	-0.82237100
H	0.67012700	4.38561800	-0.59953300
H	0.50874100	3.15894700	-1.85700000
C	2.05794500	2.11913000	1.57554200
H	2.21558600	2.39770900	2.62376300
H	2.56063100	1.15323800	1.43696600
H	-1.78318200	2.64962500	-1.06089400
C	6.94965800	-0.77296700	0.79398600
H	7.49837500	-0.15975800	1.51068000
C	7.40010600	-2.01808900	0.54476400
H	6.85646700	-2.62878500	-0.17842600
B	5.70768600	-0.17366200	0.09852800

O	4.92959300	-0.85509100	-0.77482200
H	4.19981800	-0.32662700	-1.15788900
C	8.60304000	-2.65903700	1.16706300
H	9.09638500	-1.99405200	1.88188600
H	8.32589500	-3.58597800	1.68597100
H	9.33132700	-2.94384100	0.39660600
C	2.72202500	3.15832800	0.67097200
H	2.48730800	4.18012300	1.01535200
H	3.80614400	3.03279500	0.69970400
N	2.27027300	2.99643000	-0.72991000
C	3.05514900	3.85263000	-1.63730900
H	4.10805900	3.56679500	-1.58116200
H	2.71131300	3.71185500	-2.66594600
H	2.96107800	4.91795800	-1.37606700
F	5.35285000	1.12065200	0.38936900

Cartesian coordinates and energies calculated for TS L3-FOH-TS-I in gas phase.



Energy = -1740.492768 (aU); Number of Imaginary Frequencies = 1(-170.80).

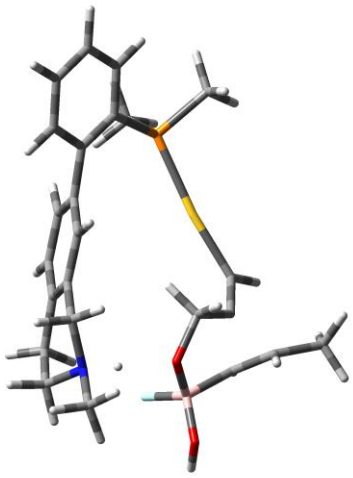
P	-3.14018500	-1.29014300	0.18193600
C	-3.88049700	0.22111300	-0.56000300
C	-5.09103100	0.07688900	-1.26496400
C	-5.69932400	1.16172200	-1.89430500
C	-5.09487800	2.41777500	-1.83578400
C	-3.89924500	2.57634800	-1.13700600
C	-3.27444900	1.50022500	-0.48209100
H	-5.57173100	-0.89213200	-1.33824300
H	-6.63332100	1.02125100	-2.42922900
H	-5.55376600	3.27179600	-2.32450400
H	-3.43975400	3.55810900	-1.07355300
C	-2.01229000	1.79722600	0.26085300
C	-1.94534900	1.71650200	1.66063300
C	-0.88409300	2.26306100	-0.43764700

C	-0.77812500	2.07033900	2.34429300
H	-2.82295900	1.41440100	2.22406700
C	0.27724600	2.63170800	0.24367900
C	0.33790300	2.53290300	1.64423200
H	-0.74867500	2.00647900	3.42900100
C	-3.79343500	-2.71882600	-0.77821700
H	-4.87695600	-2.82086500	-0.67550100
H	-3.53421300	-2.61385500	-1.83429900
H	-3.32174400	-3.62648100	-0.39263400
C	-3.90943400	-1.51553200	1.84031800
H	-4.99821300	-1.44532300	1.75850400
H	-3.63683400	-2.50024700	2.23053900
H	-3.55089600	-0.75375500	2.53375300
C	2.00381400	-1.30469000	-0.41603300
C	2.34668500	-0.47752900	-1.59231200
H	1.40220700	-0.02763300	-1.93215800
H	2.71672200	-1.12197300	-2.39712800
O	3.32428200	0.50217000	-1.35105000
H	3.02278700	1.32542400	-0.74904300
C	1.28831900	-1.87645300	0.45308500
H	1.51245600	-2.58938100	1.23512700
Au	-0.79472000	-1.42882600	0.26348700
C	1.47906100	3.22151100	-0.44864700

H	1.49213100	4.30889600	-0.26426000
H	1.42031800	3.08827600	-1.53395000
C	1.64295000	2.93774400	2.28013000
H	1.73220700	4.03345900	2.29236100
H	1.70098600	2.60691300	3.32176100
H	-0.92566500	2.34675900	-1.52128200
C	4.55192400	-1.40507000	0.11862800
H	4.43132000	-1.05391400	1.14602200
C	4.40412200	-2.73416300	-0.10772200
H	4.56670100	-3.10195000	-1.12207600
B	5.04251700	-0.37648100	-0.97949000
O	5.35238600	-0.88745700	-2.22317600
H	5.79757200	-0.25308600	-2.79799200
C	4.10171700	-3.77195800	0.92652000
H	3.93711900	-3.33453300	1.91628700
H	3.22924500	-4.37674300	0.64469200
H	4.94054900	-4.47584900	1.00516500
C	2.81255000	2.33015100	1.48680700
H	3.76715200	2.68400700	1.88437500
H	2.79298200	1.24138300	1.61147900
N	2.76881600	2.63289900	0.01769900
C	3.89033800	3.50334400	-0.40250100
H	4.83661200	3.00569700	-0.18553600

H	3.83037600	3.66871500	-1.48196900
H	3.85857300	4.47780100	0.10504000
F	5.69531100	0.75178600	-0.54151100

Cartesian coordinates and energies calculated for complex L3-FOH-INT in gas phase.



Energy = -1740.540558 (aU); Number of Imaginary Frequencies = 0.

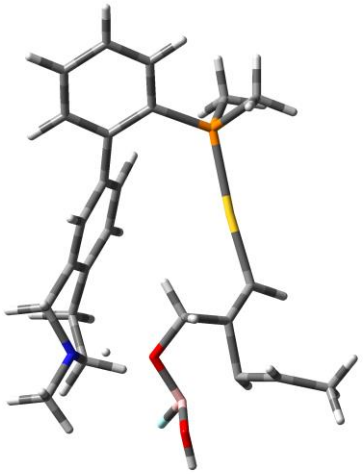
P	-3.14087000	-0.95126300	0.38614900
C	-3.73634600	0.65001100	-0.32321700
C	-5.03177800	0.66575700	-0.87506700
C	-5.56091100	1.80459500	-1.48041600
C	-4.78911200	2.96349600	-1.55356100
C	-3.50801100	2.96969800	-1.00596200
C	-2.95832900	1.83598100	-0.37852300
H	-5.64708700	-0.22583800	-0.84653300
H	-6.56461000	1.77983000	-1.89313400

H	-5.18280400	3.85993200	-2.02280500
H	-2.91902200	3.88144100	-1.03542500
C	-1.59458000	1.99724100	0.20789300
C	-1.35195600	1.82257400	1.58088000
C	-0.53157000	2.43569000	-0.59462000
C	-0.08781100	2.05216800	2.11654900
H	-2.16631300	1.54067000	2.23979400
C	0.73830800	2.68182500	-0.05646500
C	0.97680300	2.47985200	1.31122800
H	0.07797200	1.90349300	3.18044800
C	-4.13745900	-2.26131900	-0.44940000
H	-5.20351900	-2.18937800	-0.21939000
H	-3.99225700	-2.21452500	-1.53138200
H	-3.77245300	-3.22891600	-0.09444700
C	-3.79149600	-1.02048200	2.11357100
H	-4.85828600	-0.77838200	2.12683700
H	-3.64423500	-2.03193800	2.50319300
H	-3.25749800	-0.32243400	2.75998600
C	2.09909500	-1.89357600	-0.62341300
C	2.09620700	-0.50901000	-1.25243400
H	1.21726800	0.03516500	-0.88776200
H	2.03227100	-0.57414100	-2.34791600
O	3.29647100	0.16821500	-0.90242700

H	3.22915500	1.69734500	-0.50777100
C	1.01789000	-2.44213000	0.01360900
H	1.17816100	-3.43757900	0.43075700
Au	-0.84569900	-1.62932900	0.20059200
C	1.84371200	3.17568900	-0.96675600
H	1.84127500	4.26949100	-1.05225500
H	1.73814000	2.76145700	-1.97298400
C	2.35931000	2.63975400	1.90687500
H	2.31507400	3.26350800	2.80691900
H	2.72311100	1.65502400	2.21610900
C	4.29520800	3.24375000	-1.35241000
H	5.23423700	2.82031300	-0.99389000
H	4.10578200	2.88058700	-2.36326200
H	4.33568300	4.33532300	-1.34258000
H	-0.69760500	2.57628900	-1.66019000
C	3.59886800	-2.09336800	0.10992900
H	3.54385700	-2.65016000	1.04546000
C	3.36258300	-2.82317900	-1.09661200
H	3.71794800	-2.34910900	-2.01340900
B	4.16814200	-0.54099300	0.09387100
C	3.24950300	-4.32827700	-1.17505400
H	4.24710600	-4.73683800	-1.37263200
H	2.89661200	-4.77003500	-0.23928700

H	2.59111400	-4.64582500	-1.98886000
N	3.19505100	2.77310400	-0.45767600
C	3.38280600	3.25872400	0.95419700
H	3.30150100	4.35049200	0.91575900
H	4.39735800	2.99305400	1.25640800
O	5.52153200	-0.37041900	-0.32632100
H	6.14662300	-0.52306500	0.39107200
F	3.95144500	0.01541700	1.40595600

Cartesian coordinates and energies calculated for TS L3-FOH-TS-II in gas phase.



Energy = -1740.531399 (aU); Number of Imaginary Frequencies = 1(-103.69).

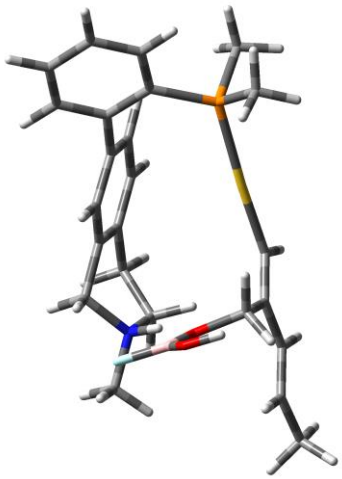
P	-3.11798300	-1.20750200	0.24135700
C	-3.79686700	0.32242700	-0.54410900
C	-5.02052300	0.21704700	-1.23202000
C	-5.58391700	1.30195200	-1.90230700
C	-4.91957000	2.52806800	-1.90295000
C	-3.71118200	2.65398100	-1.22052900

C	-3.13162100	1.57509400	-0.52719300
H	-5.54889400	-0.72910900	-1.26015200
H	-6.52985100	1.18434700	-2.42179900
H	-5.34121200	3.38361000	-2.42168900
H	-3.20777800	3.61595400	-1.19776900
C	-1.85773500	1.86291800	0.20041800
C	-1.76574000	1.76183200	1.59757700
C	-0.74629600	2.35753700	-0.50459900
C	-0.60070100	2.13126700	2.27444100
H	-2.62551600	1.42492900	2.16728500
C	0.41181100	2.74441700	0.17198300
C	0.49331200	2.63446900	1.56876900
H	-0.55602500	2.04621900	3.35688800
C	-3.85133300	-2.61182300	-0.70510300
H	-4.93890600	-2.66412800	-0.60787200
H	-3.58091100	-2.53562700	-1.76109600
H	-3.42326200	-3.53574900	-0.30674300
C	-3.97480000	-1.35317900	1.87159900
H	-5.05665500	-1.24824000	1.74706300
H	-3.75273400	-2.33575200	2.29804000
H	-3.61822800	-0.58939500	2.56498200
C	2.22537500	-1.45075400	-0.30025300
C	2.10831600	-0.50777400	-1.47947200

H	1.14146700	0.00368700	-1.47407400
H	2.21186900	-1.03875100	-2.43756200
O	3.16985400	0.43051500	-1.33423700
H	2.97723700	1.79070800	-0.54999500
C	1.24600900	-1.97013000	0.46239100
H	1.55930100	-2.66731800	1.24169300
Au	-0.75209500	-1.52683100	0.35284500
C	1.59414400	3.35584000	-0.53164100
H	1.65414400	4.43152100	-0.32647600
H	1.54663700	3.22042500	-1.61462600
C	1.79047100	3.07547800	2.19877500
H	1.85139500	4.17313500	2.21569200
H	1.86408200	2.74596500	3.23944800
C	4.06331400	3.55158200	-0.57455500
H	4.97813600	3.00335500	-0.35079400
H	3.96466400	3.67203400	-1.65505400
H	4.06730100	4.53057700	-0.08991100
H	-0.79781900	2.44461200	-1.58710000
C	3.76814900	-1.59834200	0.02962200
H	3.98896400	-1.55137700	1.09782500
C	3.86561400	-2.88364900	-0.53286900
H	3.69346000	-2.96523900	-1.60586000
B	4.41230100	-0.30028100	-0.88977600

C	4.21587100	-4.13993100	0.16450200
H	5.20284700	-4.44907800	-0.21787500
H	4.28037100	-4.02806200	1.24832500
H	3.53085200	-4.95367300	-0.10006100
N	2.90439600	2.75019700	-0.07257500
C	2.98551200	2.49830000	1.43031800
H	3.92826900	2.91815500	1.78326100
H	3.03402900	1.41569100	1.55405900
O	5.19031000	-0.85329600	-1.94336100
H	5.61246800	-0.18328900	-2.49362500
F	5.10625300	0.61050400	-0.04762300

Cartesian coordinates and energies calculated for complex L3-FOH-PROD in gas phase.



Energy = -1740.593797 (aU); Number of Imaginary Frequencies = 0.

P	2.95542000	-1.30301800	-0.00370400
C	3.69336300	0.33818900	0.43712400

C	4.91439300	0.34326900	1.13711800
C	5.51751600	1.52918100	1.55382300
C	4.89748800	2.74887000	1.28103700
C	3.69253400	2.76517100	0.58072400
C	3.07794800	1.57979500	0.13913800
H	5.40804200	-0.59282200	1.37491100
H	6.46016500	1.49640500	2.09136500
H	5.35083600	3.68151100	1.60267800
H	3.22002500	3.71472500	0.34656900
C	1.80916300	1.72376000	-0.63764800
C	1.74090200	1.38631300	-1.99849000
C	0.66633500	2.25948400	-0.02227000
C	0.55656500	1.54206300	-2.72288700
H	2.62529800	1.00387600	-2.49886200
C	-0.51349400	2.42579500	-0.74840300
C	-0.58089100	2.05742800	-2.10075100
H	0.52321700	1.25786800	-3.77110900
C	3.47830000	-2.43975200	1.35348000
H	4.56333500	-2.55620000	1.41555000
H	3.09787600	-2.07505900	2.31092100
H	3.03389500	-3.41915500	1.15597300
C	3.96012000	-1.89566600	-1.43617000
H	5.02951700	-1.84211500	-1.21146500

H	3.68681200	-2.93145700	-1.65734400
H	3.75080300	-1.28796100	-2.31935500
C	-2.48038000	-1.64343800	0.00783900
C	-2.31306500	-1.29294800	1.46211100
H	-1.27402000	-1.45241900	1.75973800
H	-2.98242400	-1.88859300	2.09427600
O	-2.63474400	0.12354700	1.68342700
H	-2.80768700	1.24480800	0.17293600
C	-1.39179300	-1.77656300	-0.79455500
H	-1.62400400	-2.06232000	-1.82574500
Au	0.59568300	-1.50602600	-0.38516600
C	-1.76728800	2.99390500	-0.14441400
H	-2.02345600	3.96687800	-0.57832600
H	-1.70681900	3.10252600	0.93933100
C	-1.92606100	2.21174400	-2.76398800
H	-2.14258600	3.27124700	-2.96018600
H	-1.95701800	1.70485100	-3.73294800
C	-4.23740900	2.70573600	0.03127200
H	-5.04188100	1.98020100	-0.09466100
H	-4.14157800	2.97345300	1.08359800
H	-4.43437600	3.59397500	-0.57162800
H	0.70265800	2.52908600	1.03018400
C	-3.84464200	-1.86576600	-0.50075700

H	-3.89288800	-2.20040900	-1.53850800
C	-5.00702200	-1.72313700	0.16694400
H	-4.99572000	-1.39398100	1.20654600
B	-2.55853300	0.69537700	2.92237900
C	-6.36264000	-2.02183300	-0.40679300
H	-7.03021200	-1.15252300	-0.34293700
H	-6.29901600	-2.32883500	-1.45534200
H	-6.85463200	-2.82856300	0.15156700
N	-2.95431000	2.08041000	-0.42678300
C	-3.03101200	1.60792000	-1.88434900
H	-4.02174300	1.87320400	-2.25653100
H	-2.94468800	0.52127900	-1.85082700
O	-2.28211900	0.10190200	4.10367500
H	-2.13334700	-0.85024400	4.09790100
F	-2.78005200	2.02973800	2.93993000

Energies for these structures computed as a single point in DCM using differentiated basis set (6-31+G(d,p) for C, H, O, N, F, P and B; def2-TZVP[26] for Au) were reported below.

Compound Name	Energy (aU)	ΔG and $\Delta G^{\neq}$(for TSs)
L3-CPX	-1740.899756	
L3-TS-I	-1740.872056	$\Delta G^{\neq}$ = 17.4 kcal/mol
L3-INTERM	-1740.922382	$\Delta G^{\text{CPX-INTERM}}$ = 14.2 kcal/mol
L3-TS-II	-1740.912621	$\Delta G^{\neq}$ = 6.1 kcal/mol
L3-FINAL-PROD	-1740.975827	$\Delta G^{\text{INTERM-PROD-REAL}}$ = 33.5 kcal/mol

Pathway for B-F-OH moiety and L4 *in gas phase* and in DCM as a solvent.

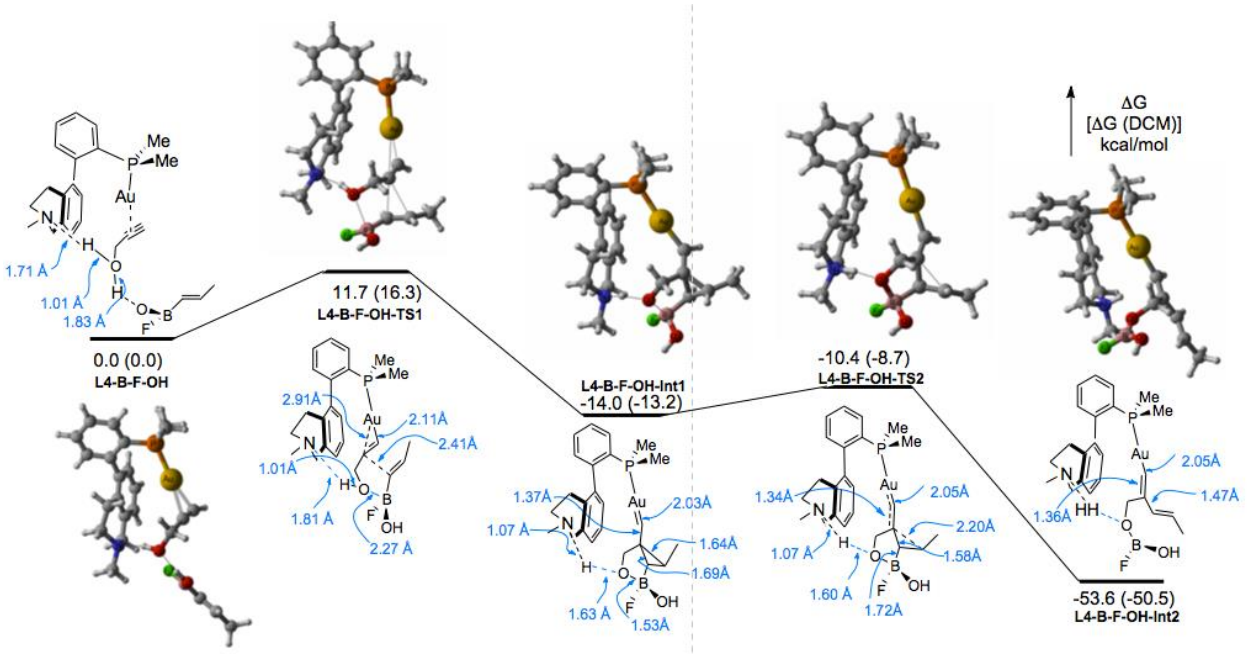
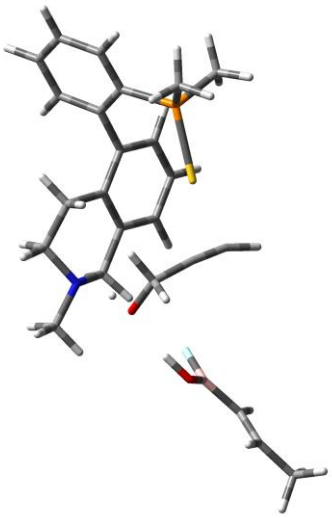


Figure 1. Reaction pathway modeled.

Cartesian coordinates and energies calculated for complex L4-B-F-OH in gas phase.



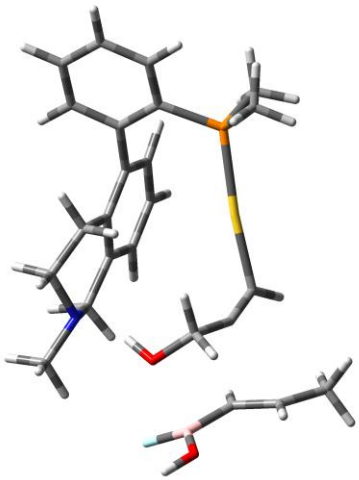
Energy = -1740.513948 (aU); Number of Imaginary Frequencies = 0

P	-3.12208000	-1.51075900	0.04688000
C	-3.90932200	0.14191100	-0.06458100
C	-5.19113800	0.21806100	-0.64462200

C	-5.87273000	1.43021800	-0.73144800
C	-5.27887400	2.59041900	-0.23189300
C	-4.01033200	2.52582900	0.34258200
C	-3.29903500	1.31693700	0.43707200
H	-5.67333200	-0.67075800	-1.03569800
H	-6.85970900	1.46354700	-1.18181500
H	-5.80186300	3.54047100	-0.28371300
H	-3.55447200	3.42660200	0.74339300
C	-1.95803000	1.35246200	1.10905300
C	-1.86223800	0.93356400	2.44376700
C	-0.82248000	1.89811100	0.46041300
C	-0.65208600	1.02478600	3.13572700
H	-2.75069600	0.57088200	2.95301500
C	0.38757400	2.00020200	1.16940500
C	0.46557800	1.55410400	2.49655500
H	-0.58966400	0.70250800	4.17072000
H	1.40798000	1.63820600	3.03194700
N	1.57215400	2.74034200	-0.91052300
C	2.69004400	3.57336400	-1.39554500
H	2.69896600	3.57339000	-2.48851400
H	2.60615700	4.61132900	-1.03903200
H	3.63625100	3.15836400	-1.03944500
C	0.27821000	3.28950500	-1.35350800
H	0.31507600	3.43264900	-2.43782700
H	0.11560600	4.28210300	-0.89812100
C	-3.88819300	-2.56875400	-1.24698500
H	-4.95673200	-2.71427800	-1.06765700
H	-3.74028900	-2.12736800	-2.23534700
H	-3.39608100	-3.54442200	-1.22212900
C	-3.67269100	-2.27797000	1.62571200

H	-4.76332900	-2.22818800	1.69789600
H	-3.35320100	-3.32364700	1.64964400
H	-3.22983600	-1.75276000	2.47323800
C	1.61131100	2.65793200	0.56225300
H	2.51375600	2.11085900	0.85016300
H	1.70343800	3.67508500	0.98605700
C	-0.87183000	2.35145200	-0.98816500
H	-1.81857400	2.85336100	-1.20727000
H	-0.84407200	1.47024200	-1.64641100
C	1.47592200	-1.41804200	-1.00748800
C	1.73174400	-0.63394200	-2.24449000
H	0.77571700	-0.36688100	-2.71462700
H	2.25810200	-1.29778000	-2.94149000
O	2.54480900	0.48236900	-2.00723700
H	2.04232900	1.25884200	-1.57991800
C	1.41849100	-2.06001500	0.04124700
H	1.67471700	-2.65001400	0.89950200
Au	-0.79662400	-1.58348500	-0.14233700
C	6.71705100	-0.31351500	0.88599000
H	6.86571600	-0.04986900	1.93442900
C	7.70723800	-0.96649300	0.24603100
H	7.56041100	-1.22439000	-0.80427400
B	5.39687000	0.08752700	0.19389900
O	5.10486900	-0.20454600	-1.09395800
H	4.23659800	0.11922600	-1.40925200
C	9.01934600	-1.37634500	0.84134200
H	9.09892500	-1.08963000	1.89402400
H	9.15924400	-2.46236400	0.76285600
H	9.85233200	-0.91922500	0.29155300
F	4.45633300	0.77614200	0.92429600

Cartesian coordinates and energies calculated for TS L4 L4-B-F-OH-TS-I in gas phase.



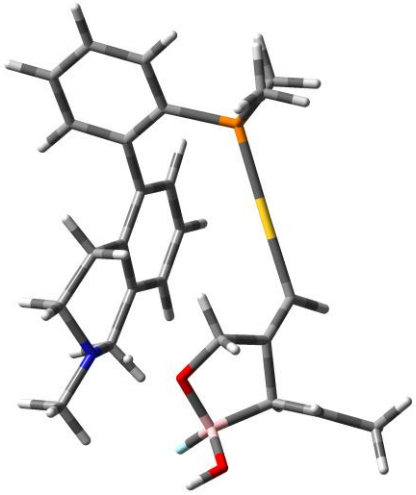
Energy = -1740.495316 (aU); Number of Imaginary Frequencies = 1(-188.43).

P	-2.82099000	-1.50973200	-0.24008000
C	-3.62367600	0.11551500	-0.55324700
C	-4.75718500	0.14651900	-1.38852000
C	-5.44115800	1.33484800	-1.63858300
C	-4.99953700	2.51972100	-1.04792100
C	-3.87734800	2.50186500	-0.22114300
C	-3.16675000	1.31706800	0.03997600
H	-5.12017400	-0.76240900	-1.85487500
H	-6.31264000	1.33062200	-2.28575300
H	-5.52750200	3.45188500	-1.22471300
H	-3.54087500	3.42125500	0.24952000
C	-1.99512400	1.41145500	0.97362700
C	-2.16602100	1.02905500	2.31126300
C	-0.76729400	1.98403100	0.55953200
C	-1.13284300	1.18670300	3.23779300
H	-3.12766100	0.64126300	2.63499100
C	0.26143000	2.15528200	1.50186900

C	0.07378000	1.74811700	2.83005800
H	-1.27794400	0.89150700	4.27253600
H	0.87488700	1.89096200	3.55153800
N	1.82242900	2.95259900	-0.30112900
C	2.94755800	3.87699500	-0.54330800
H	3.17033900	3.90541200	-1.61311900
H	2.71284500	4.89728300	-0.20216100
H	3.83512400	3.52094300	-0.01538400
C	0.61436700	3.40853600	-1.01339800
H	0.87080800	3.54815600	-2.06807000
H	0.29378700	4.39028000	-0.62206900
C	-3.29372100	-2.60848100	-1.63981600
H	-4.37161600	-2.78649500	-1.67493600
H	-2.96293500	-2.17746900	-2.58780900
H	-2.78851300	-3.56761800	-1.49926800
C	-3.70094900	-2.25098800	1.19882300
H	-4.78190800	-2.22946200	1.03116300
H	-3.37198200	-3.28638000	1.32529600
H	-3.46525200	-1.69499500	2.10780400
C	1.55698900	2.86096100	1.14624200
H	2.40487000	2.35115900	1.61712500
H	1.52326600	3.87771900	1.57978600
C	-0.52224400	2.39704900	-0.87979100
H	-1.42672600	2.82293800	-1.32312700
H	-0.28737700	1.50458100	-1.47831000
C	2.36586900	-1.18572600	-0.41091600
C	2.58195000	-0.37689700	-1.63707600
H	1.59068800	-0.27452100	-2.10350800
H	3.22020100	-0.91832400	-2.34187700
O	3.18203900	0.86750200	-1.39058900

H	2.55684000	1.52816200	-0.93954300
C	1.58461100	-1.75580800	0.42360100
H	1.84243800	-2.34051800	1.29775000
Au	-0.48848200	-1.54210500	0.06305800
C	4.57043700	-0.90016000	0.42212700
H	4.27433000	-0.68710600	1.44979600
C	4.66643200	-2.20950700	0.04921600
H	5.01094600	-2.42623400	-0.96301300
B	5.15809100	0.28124800	-0.44537900
O	5.78956200	-0.02285400	-1.61281200
H	6.18036600	0.73707600	-2.06265300
C	4.43678400	-3.39411800	0.92858500
H	4.04827100	-3.11654100	1.91255100
H	3.76829300	-4.12368400	0.45701900
H	5.39371300	-3.91133900	1.08211600
F	5.34195200	1.48447900	0.15320900

Cartesian coordinates and energies calculated for complex L4-B-F-OH-Int1 in gas phase.



Energy = -1740.536293 (aU); Number of Imaginary Frequencies = 0

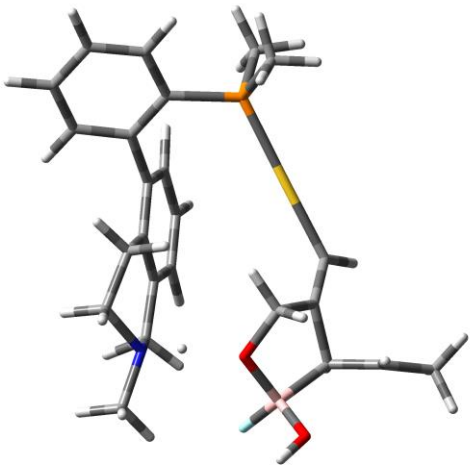
P	-2.75346100	-1.47781900	-0.08197600

C	-3.52634800	0.13250500	-0.53627300
C	-4.64671000	0.12180200	-1.38748100
C	-5.29587400	1.29938200	-1.75262400
C	-4.83411300	2.51929500	-1.26191700
C	-3.72580100	2.54587600	-0.41793600
C	-3.04958100	1.37198200	-0.04456100
H	-5.02642300	-0.81594700	-1.77743400
H	-6.15809100	1.25871400	-2.41129600
H	-5.33588700	3.44507800	-1.52746300
H	-3.37556200	3.49487000	-0.02078200
C	-1.89051300	1.52926200	0.89642000
C	-2.07525200	1.25035800	2.25645000
C	-0.66015100	2.07937300	0.46313700
C	-1.05849900	1.48351700	3.18383700
H	-3.03922000	0.88157900	2.59474900
C	0.34662000	2.33728300	1.40644400
C	0.14803400	2.02766500	2.75808400
H	-1.21654600	1.26087200	4.23466500
H	0.93702600	2.23053500	3.47820300
N	1.93723000	3.03831300	-0.43220000
C	3.06958400	3.96491000	-0.74795100
H	3.31325100	3.86097600	-1.80672800
H	2.76463000	4.99115900	-0.53002800
H	3.92807100	3.67583900	-0.14253300
C	0.71160900	3.37962800	-1.22730700
H	1.00633400	3.42338500	-2.27870400
H	0.39715100	4.38072900	-0.91315000
C	-3.31060400	-2.68970600	-1.35661200

H	-4.39516800	-2.83440600	-1.34815200
H	-2.99129500	-2.37057500	-2.35278300
H	-2.83279400	-3.64870400	-1.13447000
C	-3.64230300	-2.05346300	1.43117500
H	-4.72595200	-2.00296400	1.28275100
H	-3.35333900	-3.08899700	1.63856700
H	-3.36624700	-1.43870100	2.29059400
C	1.64421500	3.03132200	1.04035600
H	2.50381800	2.55569000	1.51745800
H	1.61300900	4.08100200	1.35849600
C	-0.39128600	2.35176000	-1.00496200
H	-1.29162400	2.71175700	-1.51072700
H	-0.12121200	1.41256500	-1.50822400
C	2.64789900	-1.52568300	-0.46262800
C	2.50223300	-0.52067500	-1.60245500
H	1.44288700	-0.37647300	-1.83873900
H	3.01377700	-0.87126100	-2.50957700
O	3.07184600	0.70672800	-1.16819900
H	2.27445400	2.06181600	-0.70631900
C	1.62289300	-1.97187100	0.32358500
H	1.92605200	-2.61354300	1.15271500
Au	-0.37446300	-1.63439900	0.13228900
C	4.03824100	-1.02586400	0.37520400
H	3.93017000	-1.10145100	1.45715800
C	4.12689700	-2.24431700	-0.36280200
H	4.54672300	-2.15377100	-1.36506000
B	4.32969800	0.43001300	-0.34896300
O	5.51296900	0.29301100	-1.13049900

H	5.84876300	1.13494000	-1.46896300
C	4.28951600	-3.61050800	0.26249800
H	3.88326000	-3.66144400	1.27704300
H	3.82889500	-4.39483500	-0.34622800
H	5.36260000	-3.82564500	0.33012900
F	4.38456500	1.50031600	0.60370400

Cartesian coordinates and energies calculated for TS L4-B-F-OH-TS-II in gas phase.



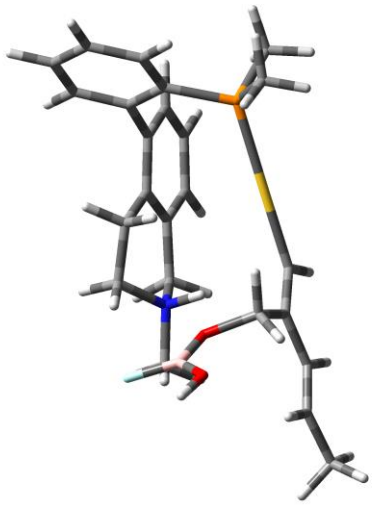
Energy = -1740.530522 (aU); Number of Imaginary Frequencies = 1(-105.25).

P	-2.85253900	-1.45602800	-0.22276000
C	-3.55594100	0.23060300	-0.50847800
C	-4.71501700	0.33765000	-1.30138000
C	-5.33088500	1.56495200	-1.54024200
C	-4.79521800	2.72313200	-0.97608400
C	-3.64822200	2.63509700	-0.18952900
C	-3.00411300	1.40778000	0.05496500
H	-5.15381000	-0.54879900	-1.74527400
H	-6.22394100	1.61122900	-2.15573300
H	-5.26978700	3.68613600	-1.13858700

H	-3.24310200	3.53302600	0.26923400
C	-1.80508100	1.45310100	0.95914700
C	-1.94352500	1.03283400	2.28818200
C	-0.58186700	2.03236700	0.53991700
C	-0.89164800	1.15814500	3.19767200
H	-2.89670000	0.63260400	2.61996300
C	0.46294000	2.17694500	1.46727000
C	0.30732800	1.73124000	2.78653600
H	-1.01434000	0.82455200	4.22327800
H	1.12493900	1.84446000	3.49412100
N	2.01055800	3.03698200	-0.34385600
C	3.14240800	3.98302400	-0.60026800
H	3.34042300	4.00121100	-1.67304000
H	2.86354100	4.98066400	-0.25381600
H	4.02302500	3.61724500	-0.07353600
C	0.76617300	3.46772000	-1.06269700
H	1.02728100	3.60341200	-2.11490900
H	0.48073700	4.44120500	-0.64952300
C	-3.40200100	-2.47438800	-1.65899200
H	-4.48925900	-2.57407200	-1.71458000
H	-3.02613900	-2.04545800	-2.59126500
H	-2.96819500	-3.47108000	-1.54097200
C	-3.84535800	-2.15152300	1.16964500
H	-4.91628900	-2.05384900	0.96835100
H	-3.59282300	-3.20912000	1.28926300
H	-3.60447800	-1.63241100	2.09942200
C	1.75952800	2.88864200	1.12820000
H	2.62445000	2.35928300	1.53490700

H	1.75200700	3.90065200	1.55123700
C	-0.35517500	2.44786600	-0.90170600
H	-1.26078700	2.87951900	-1.33551200
H	-0.13160200	1.55893600	-1.50658000
C	2.46999200	-1.25579300	-0.29165600
C	2.33863800	-0.41720200	-1.54209900
H	1.29001200	-0.18686700	-1.75072000
H	2.75588400	-0.92666100	-2.42358800
O	3.07561200	0.77379400	-1.28111100
H	2.33979800	2.08400600	-0.71772300
C	1.51325500	-1.89507600	0.40096800
H	1.83843900	-2.47635000	1.26547800
Au	-0.50205700	-1.67723500	0.09437400
C	3.94043000	-1.03457100	0.25895500
H	3.98015100	-0.92806700	1.34452400
C	4.43414600	-2.25638700	-0.22668800
H	4.43708000	-2.39342900	-1.30800400
B	4.36560200	0.39311500	-0.59411000
O	5.43647600	0.07440500	-1.47219300
H	5.75441000	0.83286200	-1.97569200
C	4.97624500	-3.37932900	0.56838500
H	4.88110000	-3.22948400	1.64530400
H	4.52593300	-4.33423900	0.27185100
H	6.04521100	-3.46721200	0.31420900
F	4.63739600	1.44189900	0.32751000

Cartesian coordinates and energies calculated for complex L4-FOH-PROD in gas phase.



Energy = -1740.599330 (aU); Number of Imaginary Frequencies = 0.

P	2.45695400	-1.62293700	-0.40655900
C	3.28555700	-0.60507100	0.90180300
C	3.97962300	-1.25073200	1.94073100
C	4.63429600	-0.52929000	2.94084700
C	4.61237200	0.86437200	2.91539800
C	3.92528500	1.52170300	1.89361600
C	3.25164100	0.81291500	0.88672500
H	4.01995900	-2.33291800	1.98095200
H	5.16182100	-1.05836400	3.72854800
H	5.12631500	1.43807200	3.68062500
H	3.91119900	2.60794800	1.86550300
C	2.54132900	1.60685100	-0.17069200
C	3.23075700	1.98460400	-1.32904700
C	1.20031500	2.01833500	0.00760800
C	2.59735100	2.71655600	-2.33655300
H	4.27439600	1.70416500	-1.43787700
C	0.55943800	2.71265400	-1.03011900
C	1.25606000	3.05765700	-2.19568000
H	3.14310000	3.00250400	-3.23013800

H	0.74650300	3.59388000	-2.99248600
N	-1.64168100	2.31293500	0.10189200
C	-3.05884200	2.77817300	0.24314800
H	-3.56773000	2.10587900	0.93111900
H	-3.05566100	3.80031200	0.62583100
H	-3.54112600	2.73944000	-0.73406200
C	-0.89515000	2.37068000	1.41211000
H	-1.52179800	1.89055200	2.16380900
H	-0.79343800	3.43300600	1.65514900
C	2.58822400	-3.37007000	0.16380700
H	3.62662500	-3.68996700	0.28807300
H	2.04290000	-3.51404500	1.09970300
H	2.11978700	-3.99625200	-0.60055700
C	3.60833200	-1.59828300	-1.84949000
H	4.62314100	-1.86393400	-1.53878500
H	3.25347400	-2.32289600	-2.58829100
H	3.61426400	-0.60988100	-2.31107800
C	-0.90003100	3.10344400	-0.93907700
H	-1.40547000	2.93199900	-1.89322100
H	-1.02838900	4.15931200	-0.67408400
C	0.45681900	1.67673700	1.28542100
H	1.05638100	1.95414000	2.15873600
H	0.31329100	0.59112100	1.34977400
C	-2.90185800	-0.81203300	-0.77502900
C	-2.86326800	-1.35654100	0.63565400
H	-1.90606000	-1.84871300	0.81903600
H	-3.66971900	-2.06869800	0.82655200
O	-2.97194200	-0.24988600	1.58139900
H	-1.67561300	1.31907400	-0.21109800
C	-1.75050800	-0.63781100	-1.48172800

H	-1.89425600	-0.25526700	-2.49799700
Au	0.18693000	-1.08370400	-0.96338000
C	-4.21303700	-0.49505800	-1.36545500
H	-4.17644300	-0.13881500	-2.39645900
C	-5.42315200	-0.62453100	-0.78777300
H	-5.49685800	-0.98837300	0.23687000
B	-3.52951000	-0.40115400	2.80776400
O	-4.07882000	-1.56591400	3.23431100
H	-4.45307400	-1.53742400	4.12353200
C	-6.72795700	-0.32483100	-1.46555600
H	-6.58128800	0.03651800	-2.48804000
H	-7.35972000	-1.22119100	-1.50927000
H	-7.30138500	0.42984200	-0.91168300
F	-3.51589800	0.69829600	3.60055700

Energies for these structures computed as a single point in DCM using differentiated basis set (6-31+G(d,p) for C, H, O, N, F, P and B; def2-TZVP[26] for Au) were reported below.

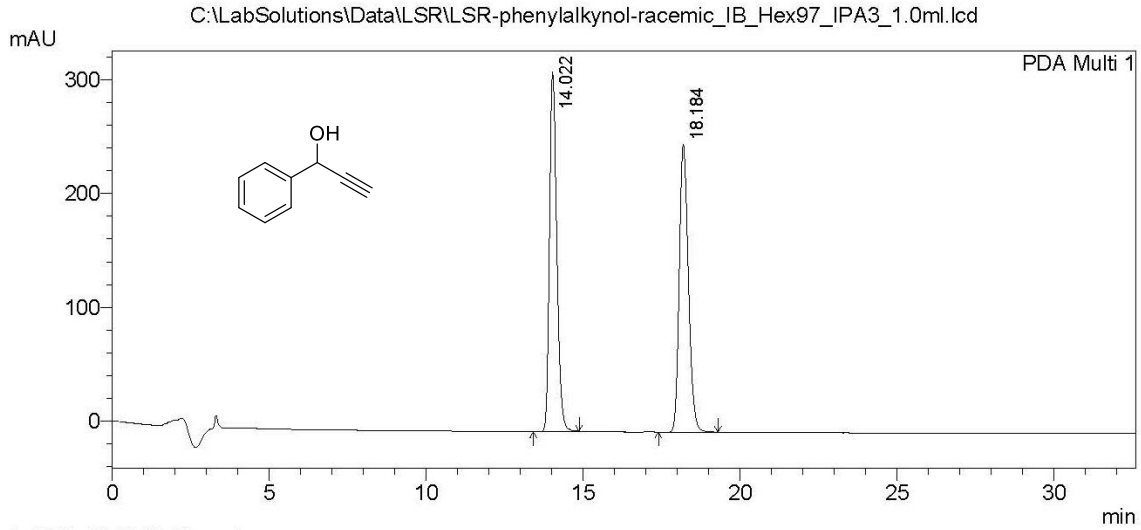
Compound Name	Energy (aU)	ΔG and $\Delta G^{\neq}$(for TSs)
L4-CPX	-1740.898343	
L4-TS-I	-1740.872386	$\Delta G^{\neq}$ = 16.3 kcal/mol
L4-INTERM	-1740.919389	$\Delta G^{\text{CPX-INTERM}}$ = 13.2 kcal/mol
L4-TS-II	-1740.912245	$\Delta G^{\neq}$ = 4.5 kcal/mol
L4-FINAL-PROD	-1740.978763	$\Delta G^{\text{INTERM-PROD-REAL}}$ = 37.3 kcal/mol

8. References:

[1] A. J. J. Lennox, G. C. Lloyd-Jones, *Angew Chem Int Edit* **2012**, *51*, 9385-9388.
[2] E. Najahi, A. Valentin, P. L. Fabre, K. Reybier, F. Nepveu, *Eur J Med Chem* **2014**, *78*, 269-274.
[3] S. R. Dubbaka, M. Salla, R. Bolisetti, S. Nizalapur, *Rsc Adv* **2014**, *4*, 6496-6499.
[4] H. Ueda, M. Yamaguchi, H. Kameya, K. Sugimoto, H. Tokuyama, **2014**, *16*, 4948-4951.
[5] A. T. Parsons, T. D. Senecal, S. L. Buchwald, *Angew Chem Int Edit* **2012**, *51*, 2947-2950.
[6] K. Brak, J. A. Ellman, *J Am Chem Soc* **2009**, *131*, 3850-+.
[7] Y. S. Feng, C. Q. Xie, W. L. Qiao, H. J. Xu, *Org Lett* **2013**, *15*, 936-939.
[8] C. X. Xu, W. Y. Du, Y. Zeng, B. Dai, H. Guo, *Org Lett* **2014**, *16*, 948-951.
[9] Y. Yasu, T. Koike, M. Akita, *Chem Commun* **2013**, *49*, 2037-2039.
[10] Z. P. Chen, W. Zhang, C. A. Palma, A. L. Rizzini, B. L. Liu, A. Abbas, N. Richter, L. Martini, X. Y. Wang, N. Cavani, H. Lu, N. Mishra, C. Coletti, R. Berger, F. Klappenberger, M. Klaui, A. Candini, M. Affronte, C. W. Zhou, V. De Renzi, U. del Pennino, J. V. Barth, H. J. Rader, A. Narita, X. L. Feng, K. Mullen, *J Am Chem Soc* **2016**, *138*, 15488-15496.
[11] A. Cannillo, S. Norsikian, P. Retailleau, M. E. T. H. Dau, B. I. Iorga, J. M. Beau, *Chem-Eur J* **2013**, *19*, 9127-9131.
[12] J. Takagi, K. Takahashi, T. Ishiyama, N. Miyaura, *J Am Chem Soc* **2002**, *124*, 8001-8006.
[13] B. Gopula, C. W. Chiang, W. Z. Lee, T. S. Kuo, P. Y. Wu, J. P. Henschke, H. L. Wu, *Org Lett* **2014**, *16*, 632-635.
[14] V. Bagutski, A. Ros, V. K. Aggarwal, *Tetrahedron* **2009**, *65*, 9956-9960.
[15] L. J. Cheng, C. J. Cordier, *Angew Chem Int Edit* **2015**, *54*, 13734-13738.
[16] L. W. Ye, W. M. He, L. M. Zhang, *J Am Chem Soc* **2010**, *132*, 8550-+.
[17] N. Maulucci, I. Izzo, G. Bifulco, A. Aliberti, C. De Cola, D. Comegna, C. Gaeta, A. Napolitano, C. Pizza, C. Tedesco, D. Flot, F. De Riccardis, *Chem Commun* **2008**, 3927-3929.
[18] J. M. Aurrecoechea, E. Perez, M. Solay, *J Org Chem* **2001**, *66*, 564-569.
[19] K. Asano, S. Matsubara, *J Am Chem Soc* **2011**, *133*, 16711-16713.
[20] M. Spallarossa, Q. Wang, R. Riva, J. P. Zhu, *Org Lett* **2016**, *18*, 1622-1625.
[21] (a) A. D. Becke, *J. Chem. Phys.* **1993**, *98*, 5648-5652; (b) C. Lee, W. Yang, R. G. Parr, *Phys. Rev. B* **1988**, *37*, 785-789.
[22] J. Tomasi, B. Mennucci, R. Cammi, *Chem. Rev.* **2005**, *105*, 2999-3094.
[23] P. J. Hay, W. R. Wadt, *J. Chem. Phys.* **1985**, *82*, 270-283.
[24] W. R. Wadt, P. J. Hay, *J. Chem. Phys.* **1985**, *82*, 284-298.
[25] M. J. T. Frisch, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Scalmani, G..; Barone, V.; Mennucci, B.; Petersson, G.. A.; Nakatsuji, H.; Caricato, M.; Li, X.; Hratchian, H. P.; Izmaylov, A. F.; Bloino, J.; Zheng, G..; Sonnenberg, J. L.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Vreven, T.;. Montgomery, A. Jr.; Peralta, J. E.; Ogliaro, F.; Bearpark, M.; Heyd, J. J.; Brothers, E.; Kudin, K. N.; Staroverov, V. N.; Kobayashi, R.; Normand, J.; Raghavachari, K.; Rendell, A.; Burant, J. C.; Iyengar, S. S.; Tomasi, J.; Cossi, M.; Rega, N.; Millam, J. M.; Klene, M.; Knox, J. E.; Cross, J. B.; Bakken, V.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Martin, R. L.; Morokuma, K.; Zakrzewski, V. G.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Dapprich, S.; Daniels, A. D.; Farkas, O.; Foresman, J. B.; Ortiz, J. V.; Cioslowski J.; Fox, D. J., Gaussian, Inc., Wallingford, CT, **2009**.
[26] a) F. Weigend and R. Ahlrichs, "*Balanced basis sets of split valence, triple zeta valence and quadruple zeta valence quality for H to Rn: Design and assessment of accuracy*," *Phys. Chem. Chem. Phys.*, *7*, **2005**, 3297-3305. (b) F. Weigend, "*Accurate Coulomb-fitting basis sets for H to Rn*," *Phys. Chem. Chem. Phys.*, *8*, **2006**, 1057-1065

10. Chiral HPLC analysis.

<Chromatogram>



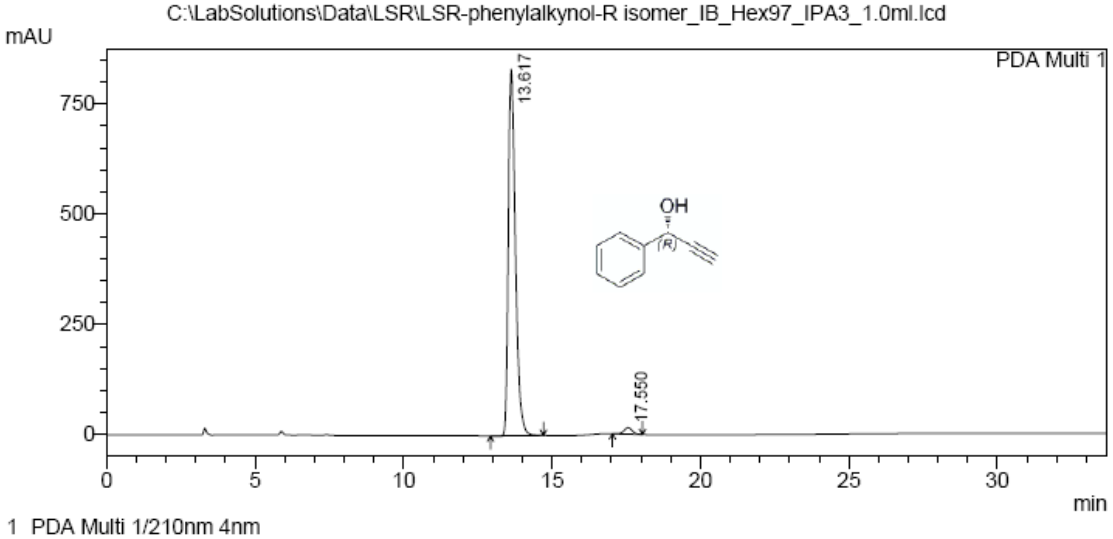
1 PDA Multi 1/210nm 4nm

PeakTable

PDA Ch1 210nm 4nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	14.022	5100869	315702	49.885	55.530
2	18.184	5124310	252825	50.115	44.470
Total		10225179	568527	100.000	100.000

<Chromatogram>



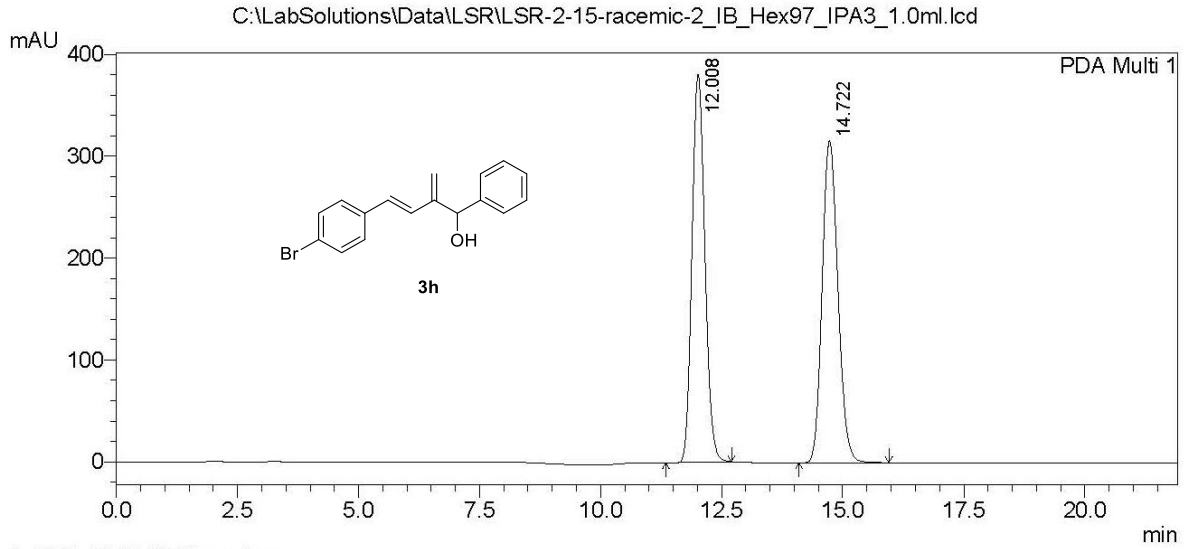
1 PDA Multi 1/210nm 4nm

PeakTable

PDA Ch1 210nm 4nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	13.617	13806858	830934	98.023	98.252
2	17.550	278435	14780	1.977	1.748
Total		14085293	845714	100.000	100.000

<Chromatogram>

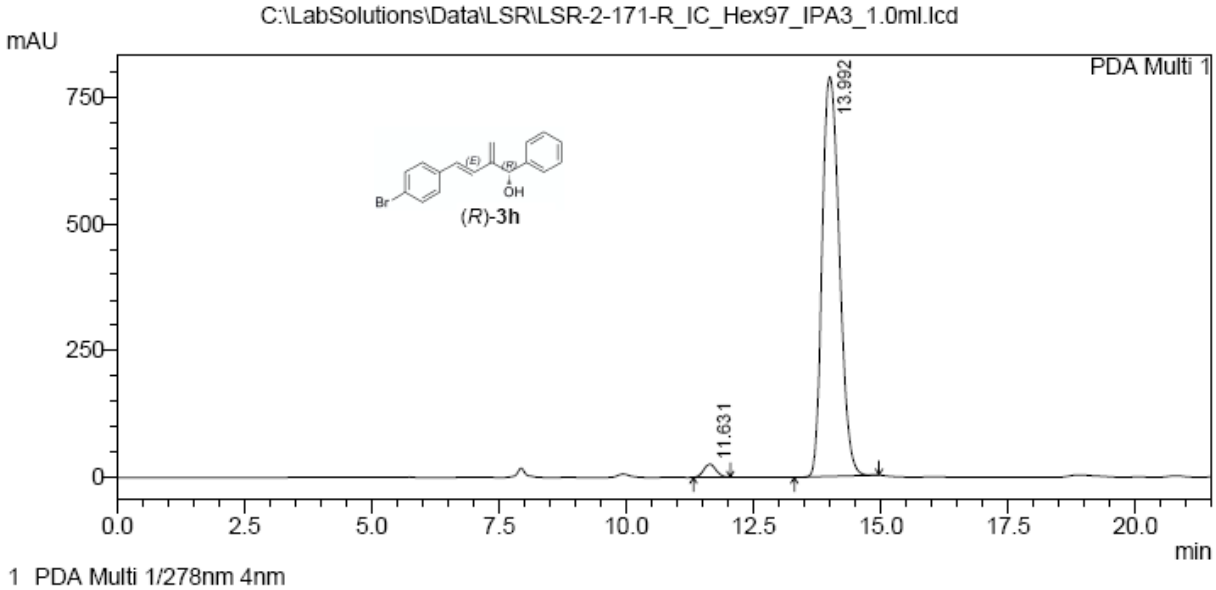


PeakTable

PDA Ch1 280nm 4nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	12.008	7028704	380142	49.621	54.605
2	14.722	7135957	316021	50.379	45.395
Total		14164661	696163	100.000	100.000

<Chromatogram>

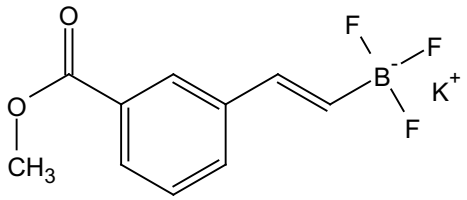


PeakTable

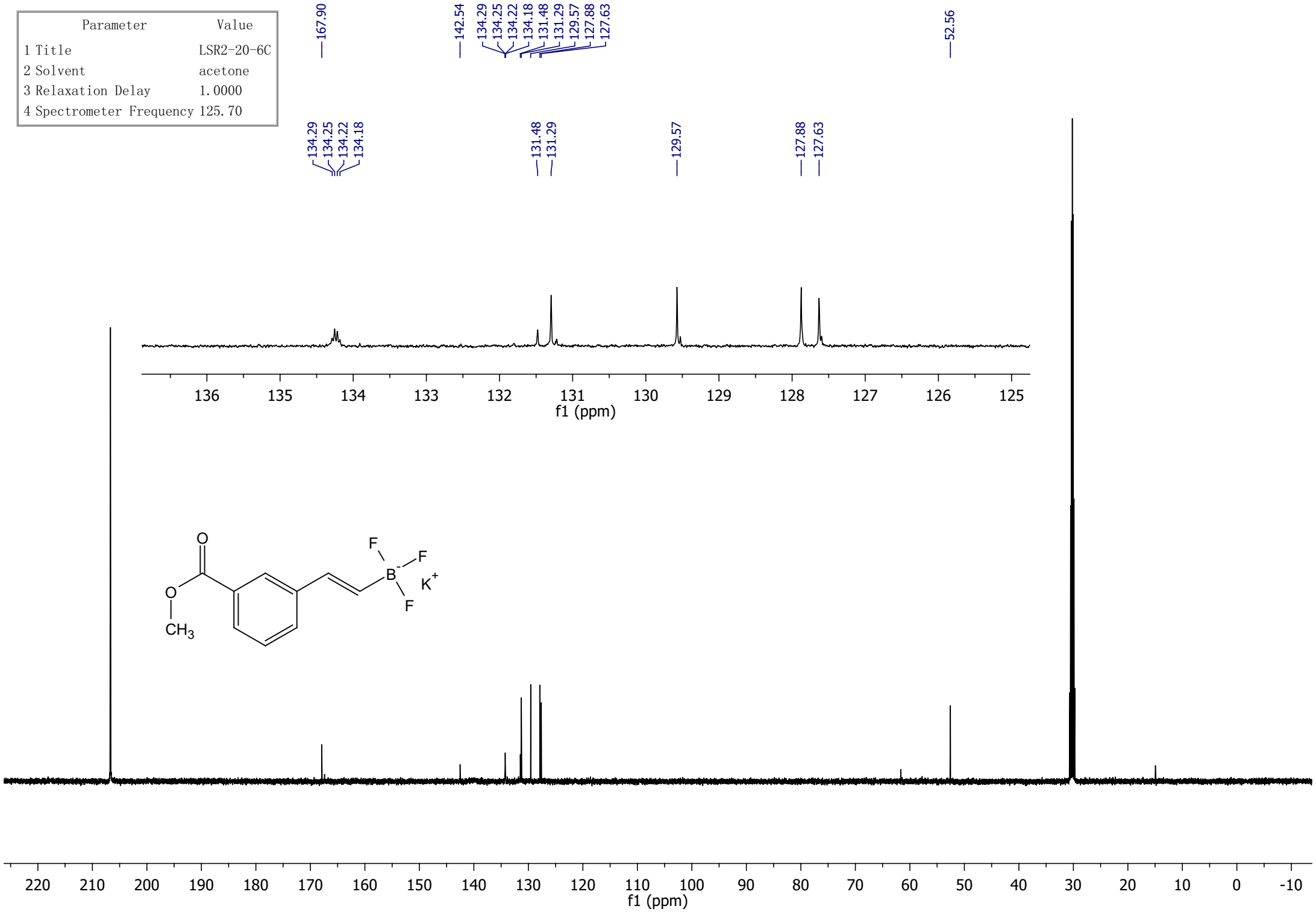
PDA Ch1 278nm 4nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	11.631	440702	26145	2.320	3.212
2	13.992	18556004	787768	97.680	96.788
Total		18996706	813913	100.000	100.000

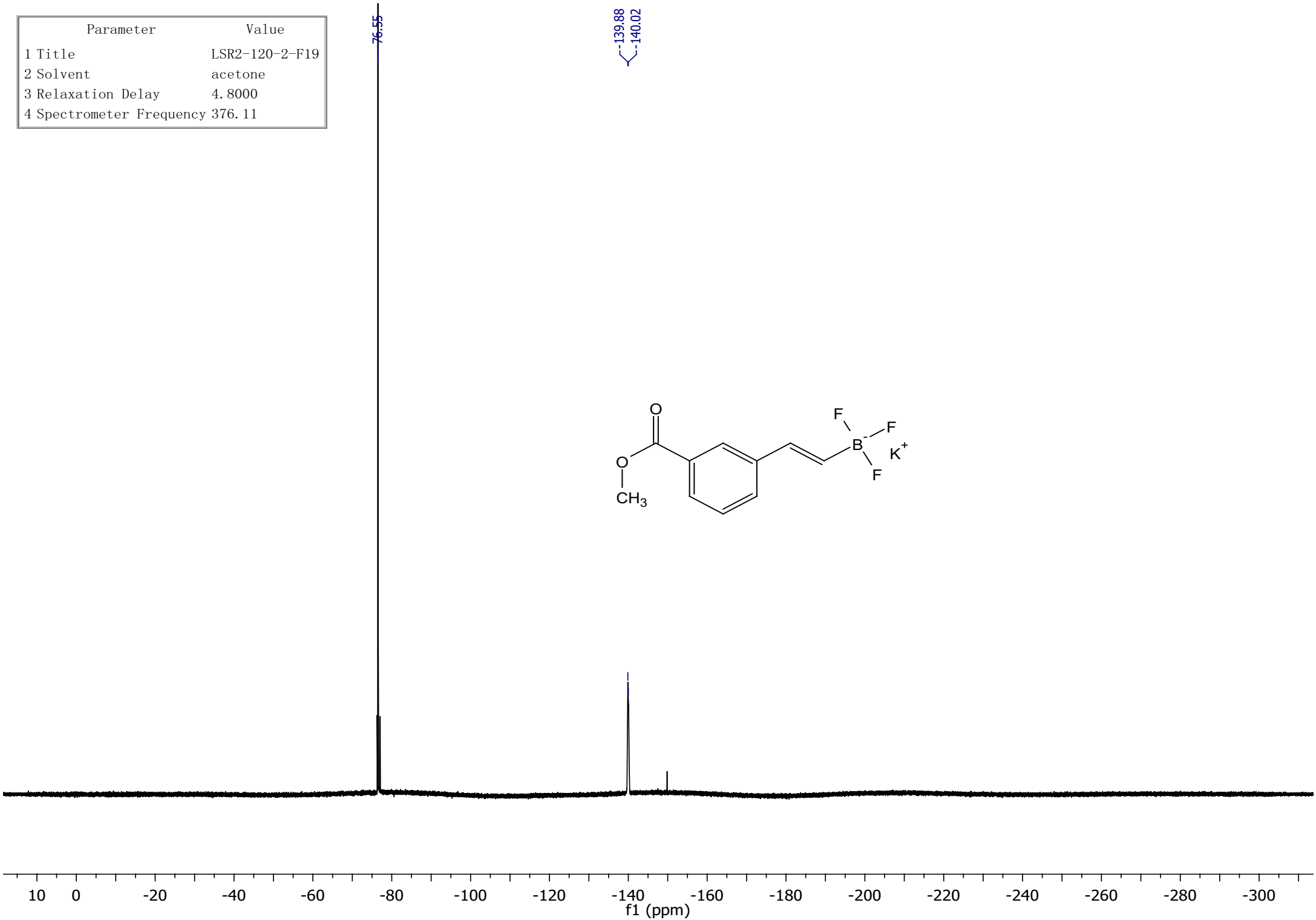
Parameter	Value
1 Title	LSR2-56-ST1
2 Solvent	acetone
3 Relaxation Delay	4.8000
4 Spectrometer Frequency	399.78



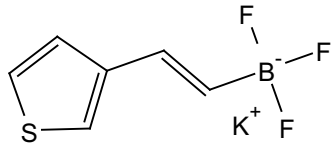
Parameter	Value
1 Title	LSR2-20-6C
2 Solvent	acetone
3 Relaxation Delay	1.0000
4 Spectrometer Frequency	125.70

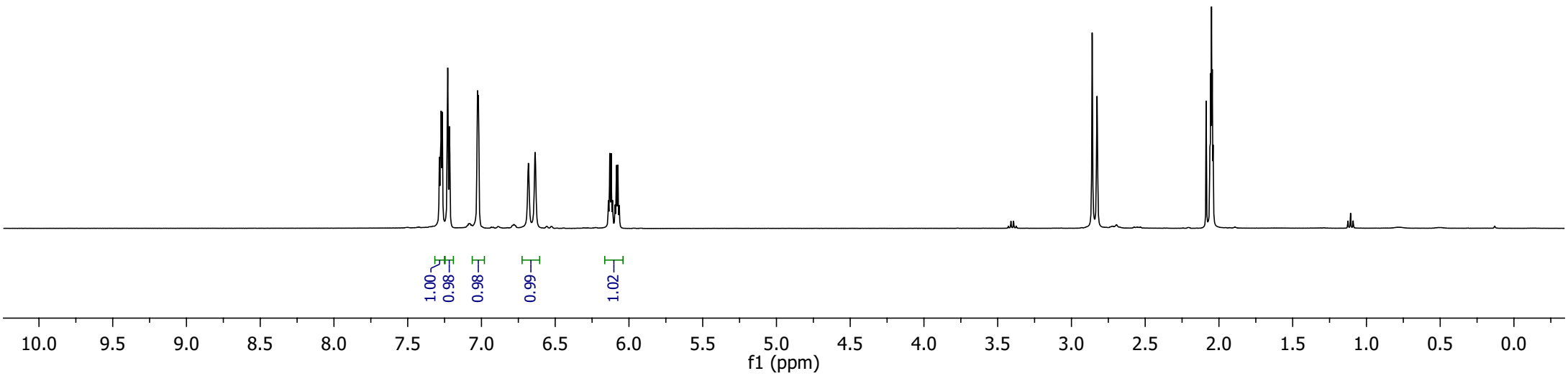


Parameter	Value
1 Title	LSR2-120-2-F19
2 Solvent	acetone
3 Relaxation Delay	4.8000
4 Spectrometer Frequency	376.11



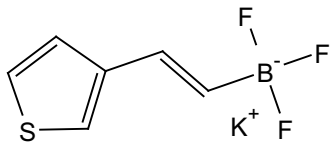
Parameter	Value
1 Title	LSR2-129-ST2
2 Solvent	acetone
3 Relaxation Delay	4.8000
4 Spectrometer Frequency	399.78



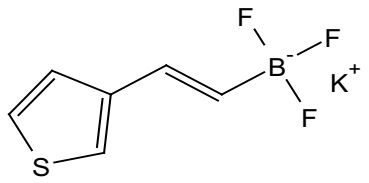


Parameter	Value
1 Title	LSR2-129-ST2-C
2 Solvent	acetone
3 Relaxation Delay	1.0000
4 Spectrometer Frequency	100.54

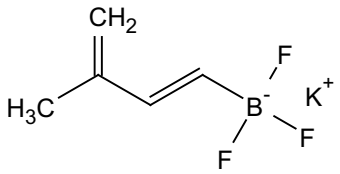
145.87
129.57
129.52
129.48
129.43
126.54
126.11
119.96

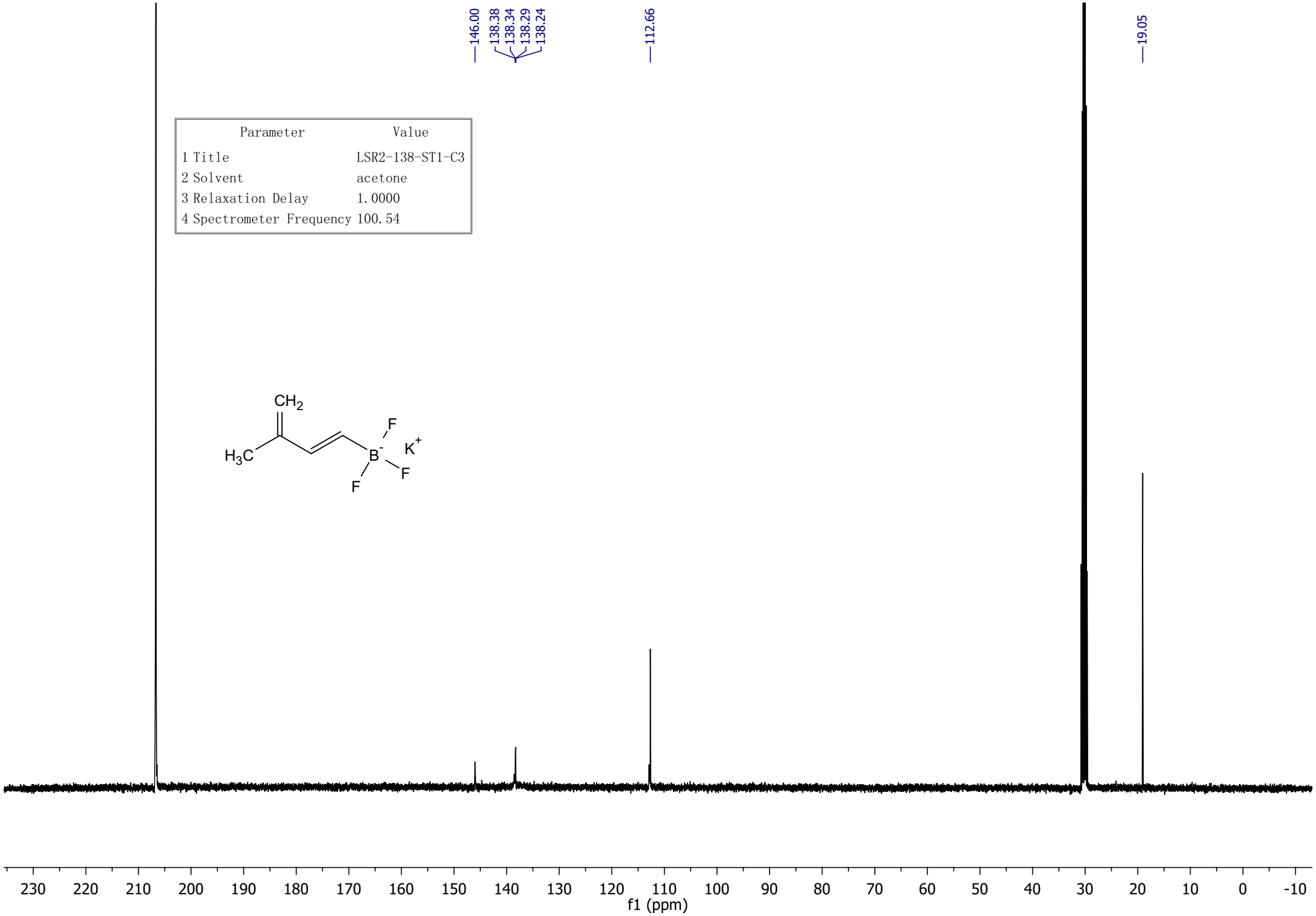


Parameter	Value
1 Title	LSR2-129-F19
2 Solvent	dmso
3 Relaxation Delay	4.8000
4 Spectrometer Frequency	376.11



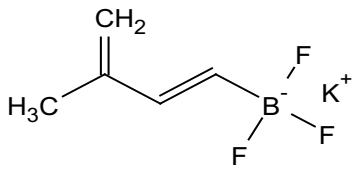
Parameter	Value
1 Title	LSR2-138-ST1
2 Solvent	acetone
3 Relaxation Delay	4.8000
4 Spectrometer Frequency	399.78

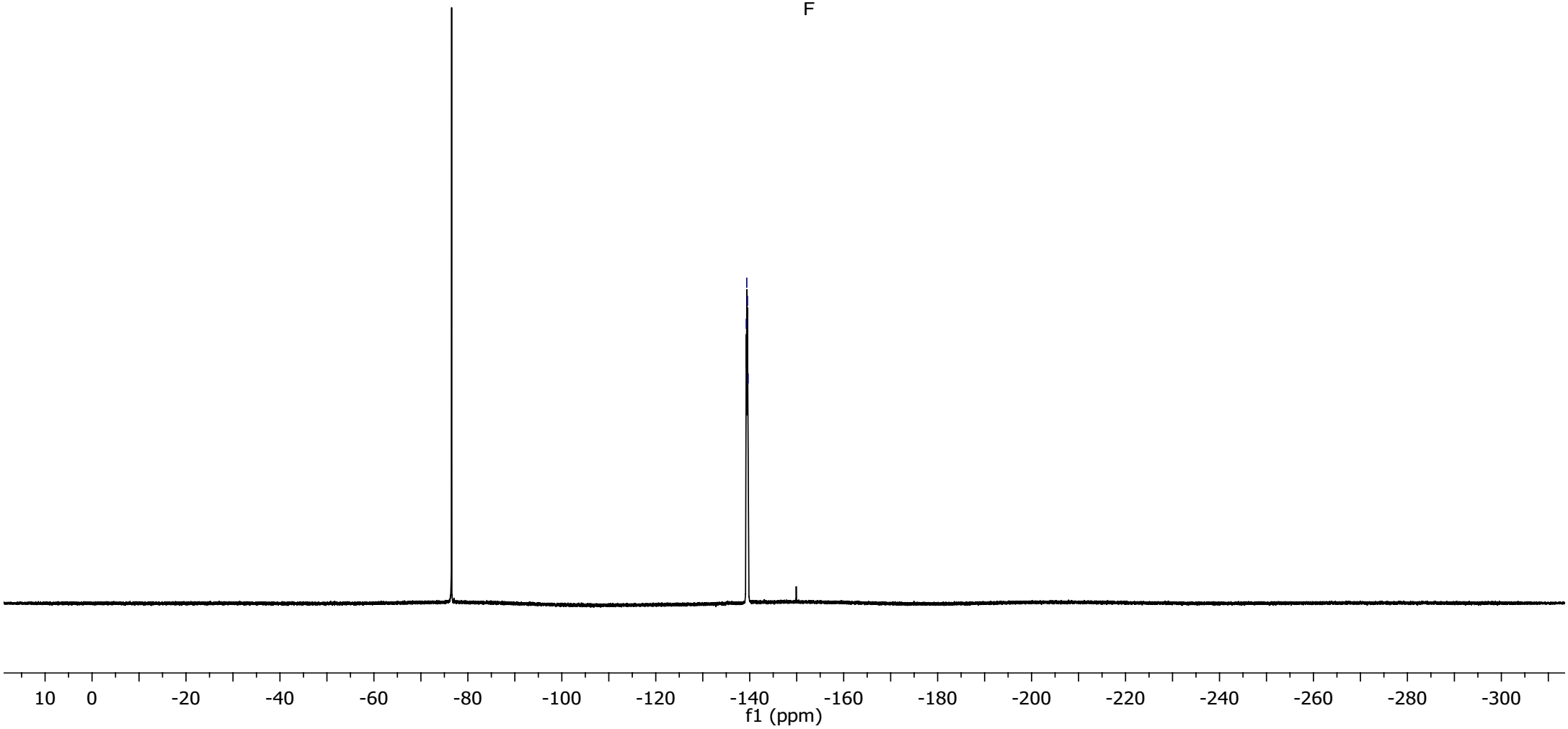



146.00
138.38
138.34
138.29
138.24
112.66
19.05
Parameter Value
1 Title LSR2-138-ST1-C3
2 Solvent acetone
3 Relaxation Delay 1.0000
4 Spectrometer Frequency 100.54
CH2
H3C
B-
F
F
F
K+
230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

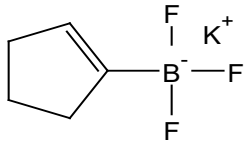
Parameter	Value
1 Title	LSR2-138-F19-2
2 Solvent	acetone
3 Relaxation Delay	4.8000
4 Spectrometer Frequency	376.11

-139.26
-139.37
-139.53
-139.66

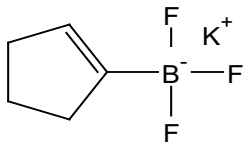




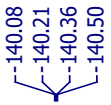
Parameter	Value
1 Title	LSR2-162-TM1
2 Solvent	dmso
3 Relaxation Delay	4.8000
4 Spectrometer Frequency	499.86

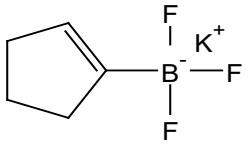


Parameter	Value
1 Title	LSR2-162-TM1-C
2 Solvent	dmso
3 Relaxation Delay	1.0000
4 Spectrometer Frequency	125.70

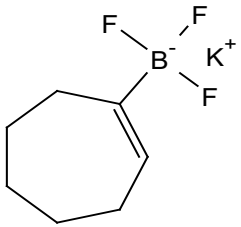


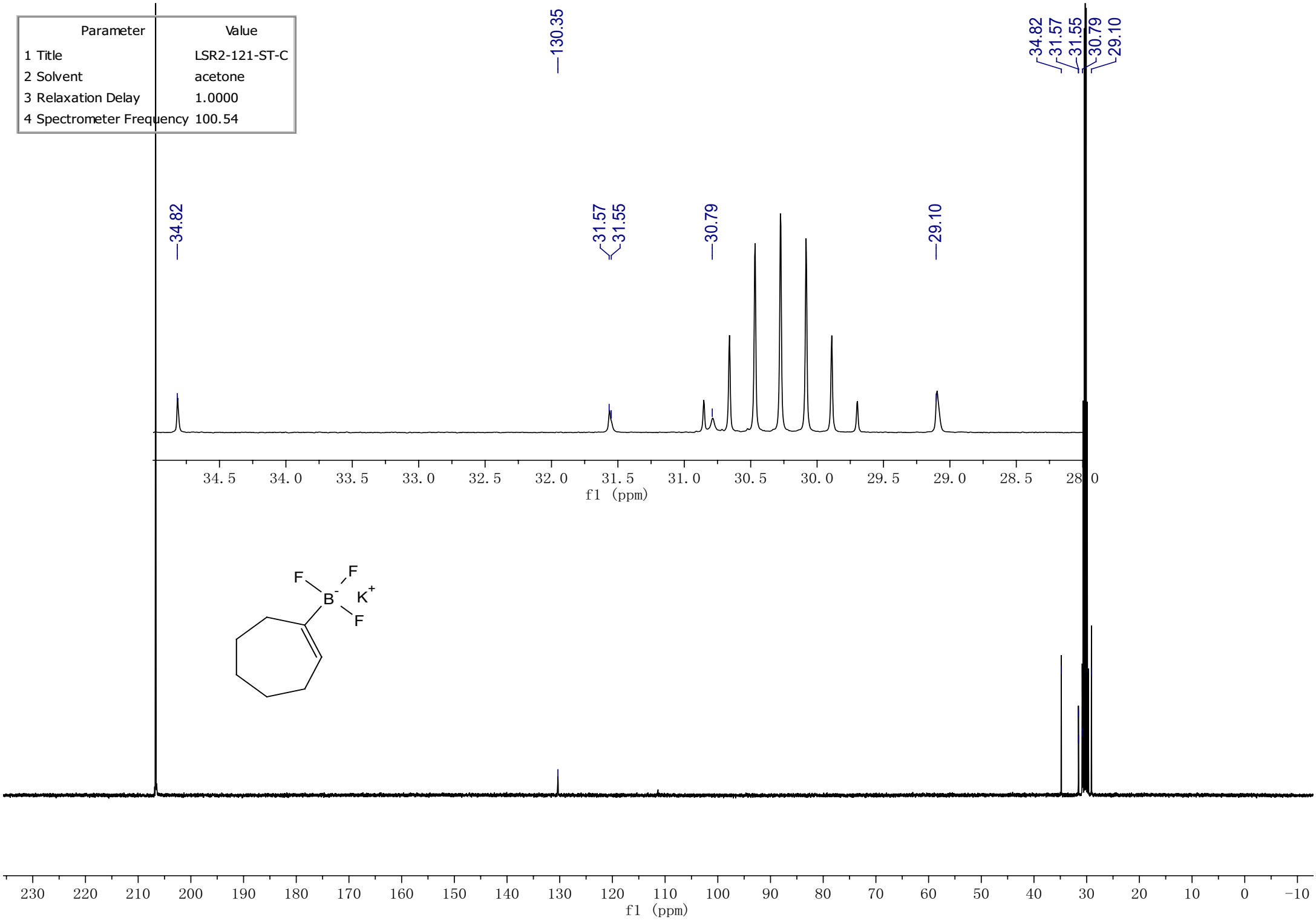
Parameter	Value
1 Title	LSR2-162-F19
2 Solvent	acetone
3 Relaxation Delay	4.8000
4 Spectrometer Frequency	376.11



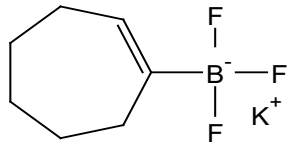


Parameter	Value
1 Title	LSR2-121-ST
2 Solvent	acetone
3 Relaxation Delay	4.8000
4 Spectrometer Frequency	399.78

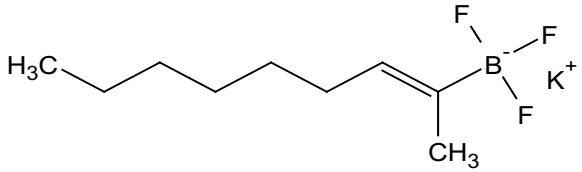


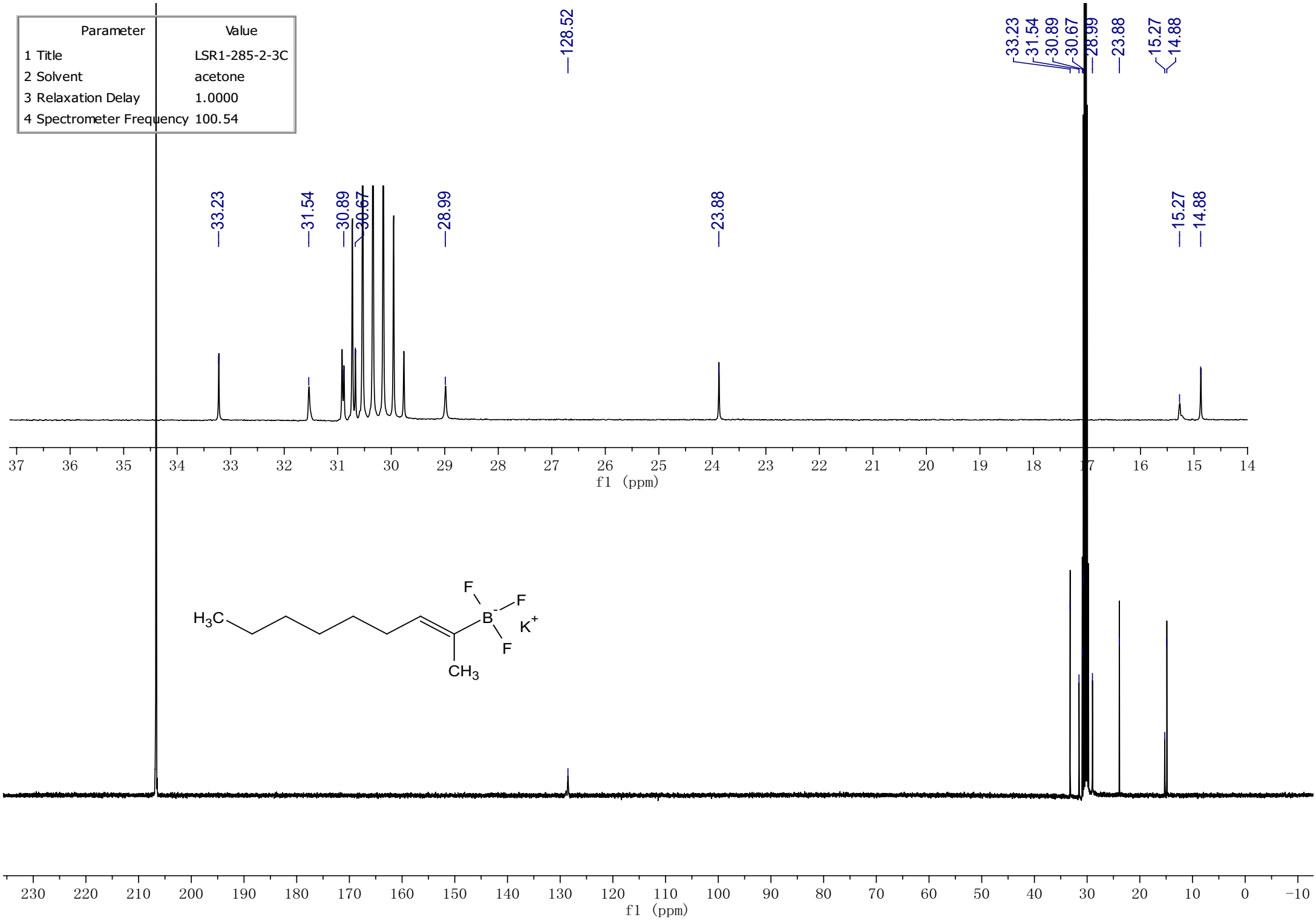

Parameter
Value
1 Title
LSR2-121-ST-C
2 Solvent
acetone
3 Relaxation Delay
1.0000
4 Spectrometer Frequency
100.54
130.35
34.82
31.57
31.55
30.79
29.10
f1 (ppm)
F
F
B
K+
F

Parameter	Value
1 Title	LSR2-121-F19
2 Solvent	dmso
3 Relaxation Delay	4.8000
4 Spectrometer Frequency	376.11

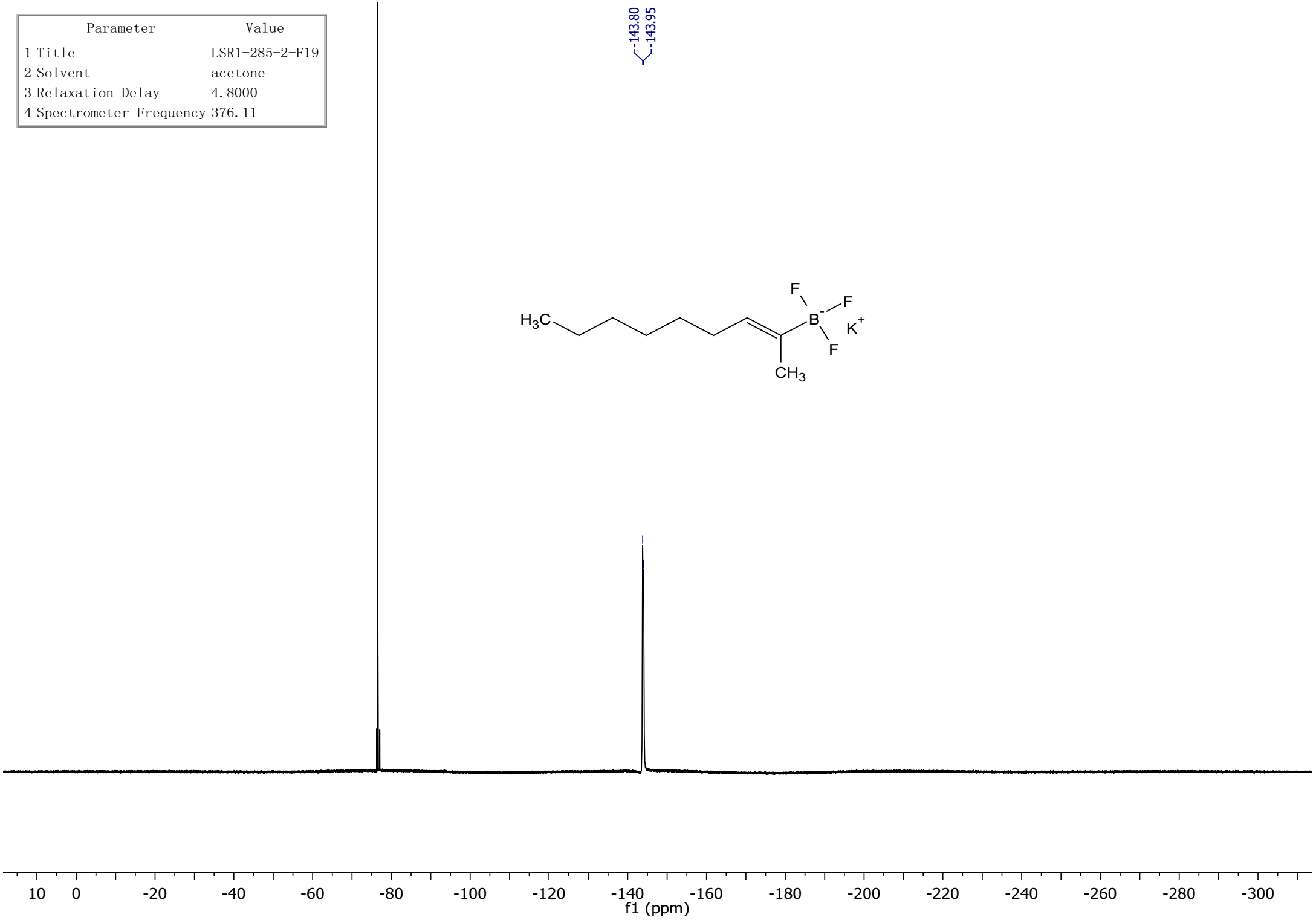


Parameter	Value
1 Title	LSR1-285-2-2
2 Solvent	acetone
3 Relaxation Delay	4.8000
4 Spectrometer Frequency	499.86

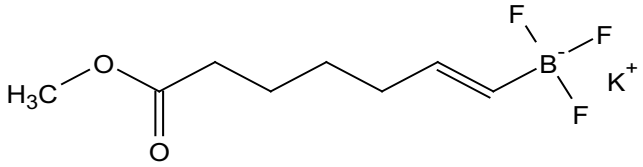



Parameter
Value
1 Title
LSR1-285-2-3C
2 Solvent
acetone
3 Relaxation Delay
1.0000
4 Spectrometer Frequency
100.54
128.52
33.23
31.54
30.89
30.67
28.99
23.88
15.27
14.88
f1 (ppm)
F
F
B
K+
F
H3C
CH3

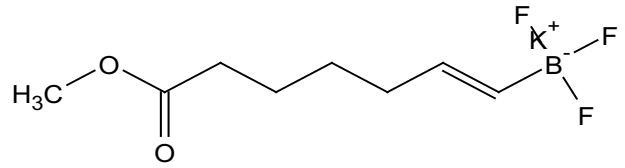
Parameter	Value
1 Title	LSR1-285-2-F19
2 Solvent	acetone
3 Relaxation Delay	4.8000
4 Spectrometer Frequency	376.11



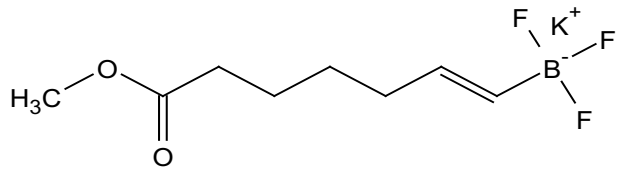
Parameter	Value
1 Title	LSR2-122-ST
2 Solvent	acetone
3 Relaxation Delay	4.8000
4 Spectrometer Frequency	399.78



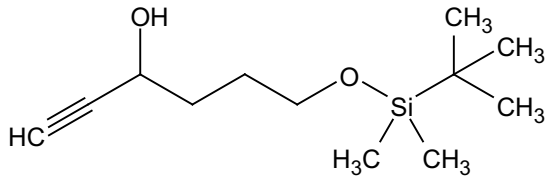
Parameter	Value
1 Title	LSR2-122-ST-C
2 Solvent	acetone
3 Relaxation Delay	1.0000
4 Spectrometer Frequency	100.54



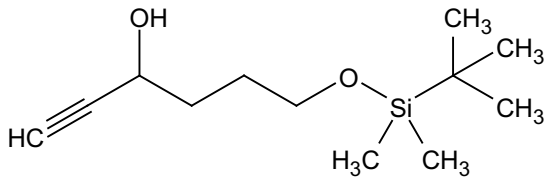
Parameter	Value
1 Title	LSR2-122-F19-2
2 Solvent	acetone
3 Relaxation Delay	4.8000
4 Spectrometer Frequency	376.11



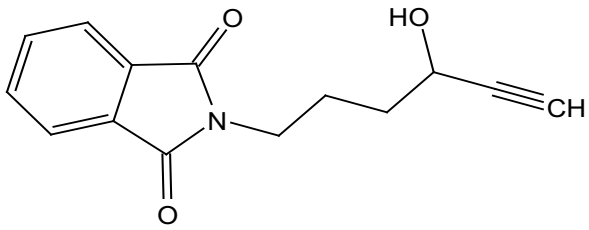
Parameter	Value
1 Title	cxp1-218p-H
2 Solvent	cdcl3
3 Relaxation Delay	10.0000
4 Spectrometer Frequency	399.78

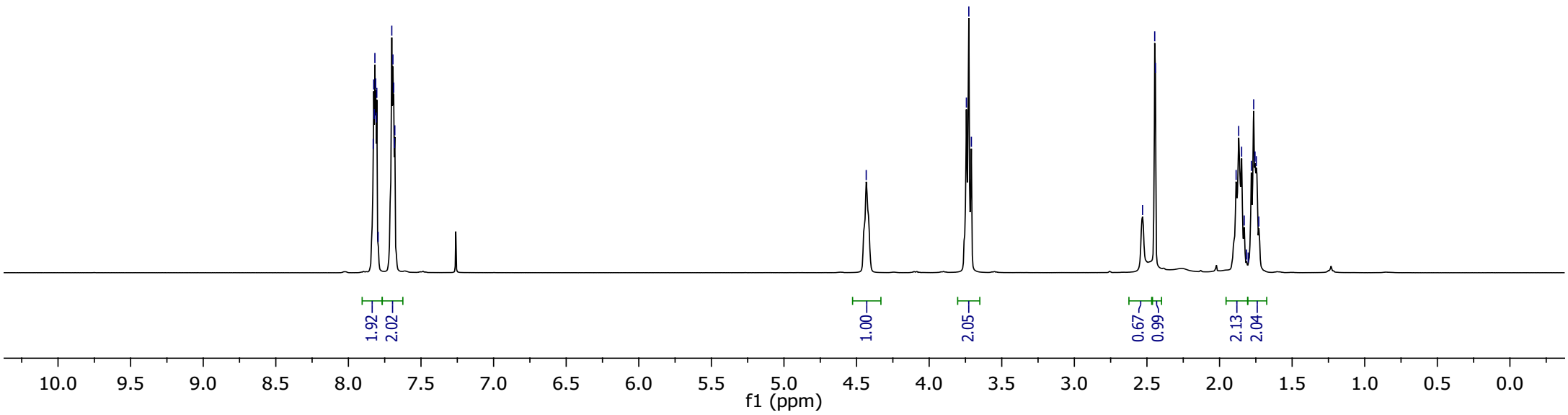


Parameter	Value
1 Title	cxp1-218p-C13
2 Solvent	cdcl3
3 Relaxation Delay	1.0000
4 Spectrometer Frequency	100.53



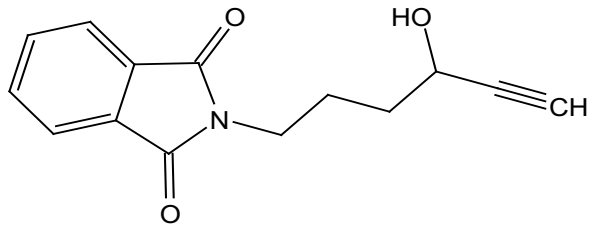
Parameter	Value
1 Title	LSR2-155-ST1
2 Solvent	cdcl3
3 Relaxation Delay	4.8000
4 Spectrometer Frequency	399.78

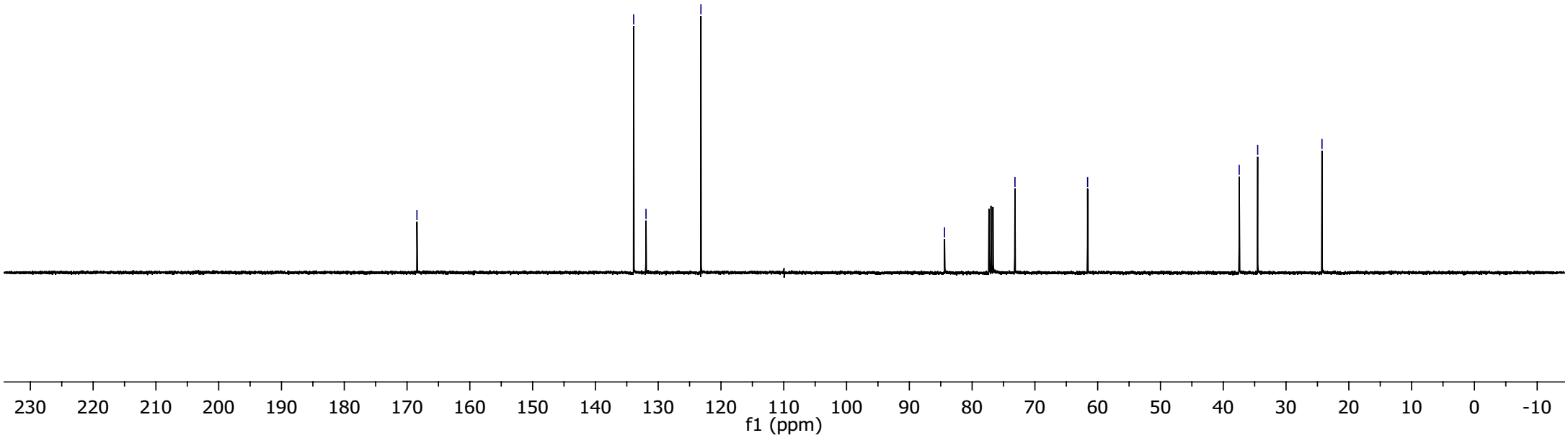




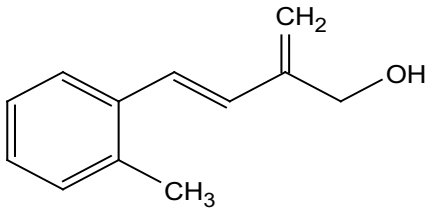
Parameter	Value
1 Title	LSR2-155-ST1-C
2 Solvent	cdcl3
3 Relaxation Delay	1.0000
4 Spectrometer Frequency	100.53

168.43
133.91
131.94
123.19
84.40
73.18
61.60
37.46
34.52
24.27

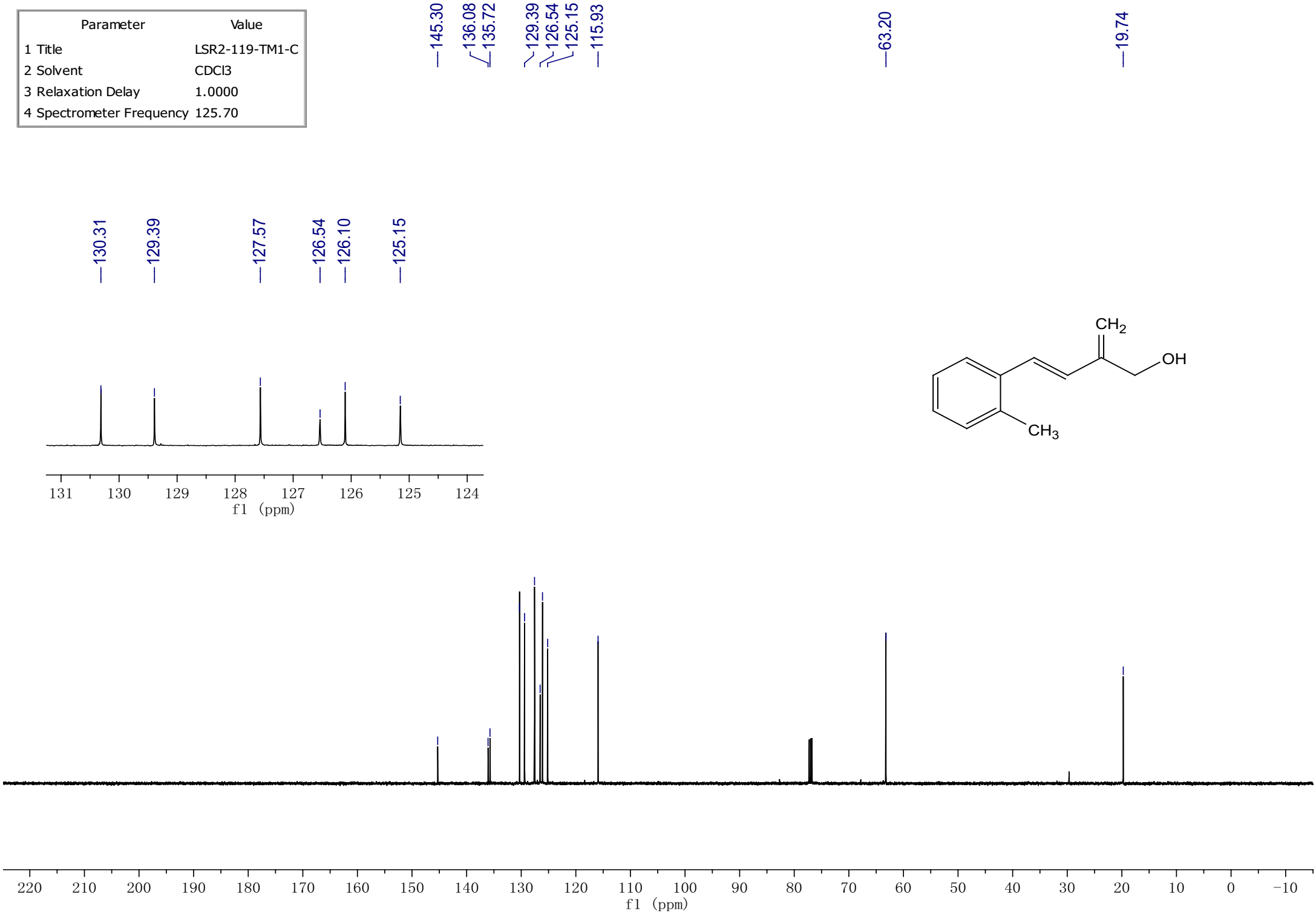




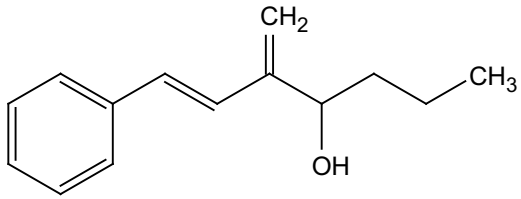
Parameter	Value
1 Title	LSR2-119-TM1
2 Solvent	CDCl3
3 Relaxation Delay	4.8000
4 Spectrometer Frequency	499.86



Parameter	Value
1 Title	LSR2-119-TM1-C
2 Solvent	CDCl3
3 Relaxation Delay	1.0000
4 Spectrometer Frequency	125.70

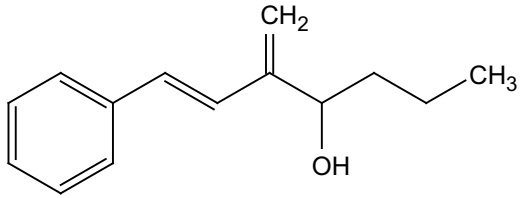


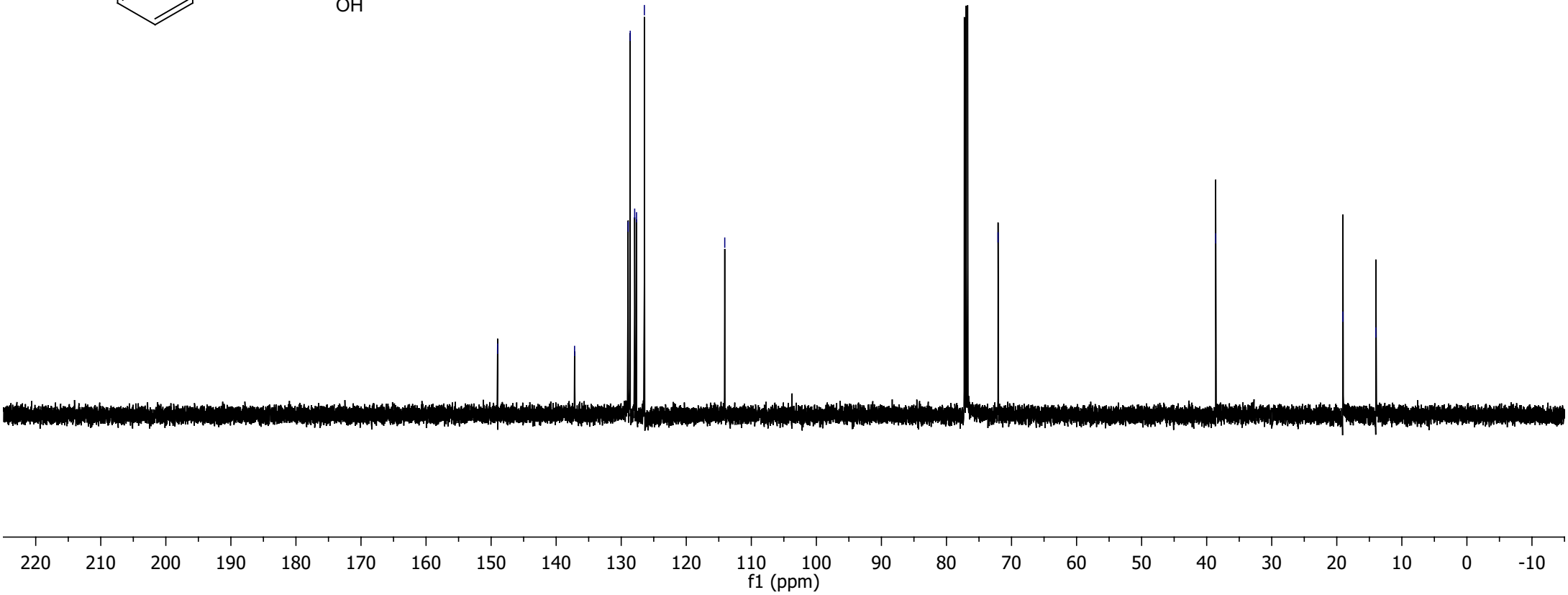
Parameter	Value
1 Title	LSR1-233-1
2 Solvent	CDCl3
3 Relaxation Delay	4.8000
4 Spectrometer Frequency	499.86



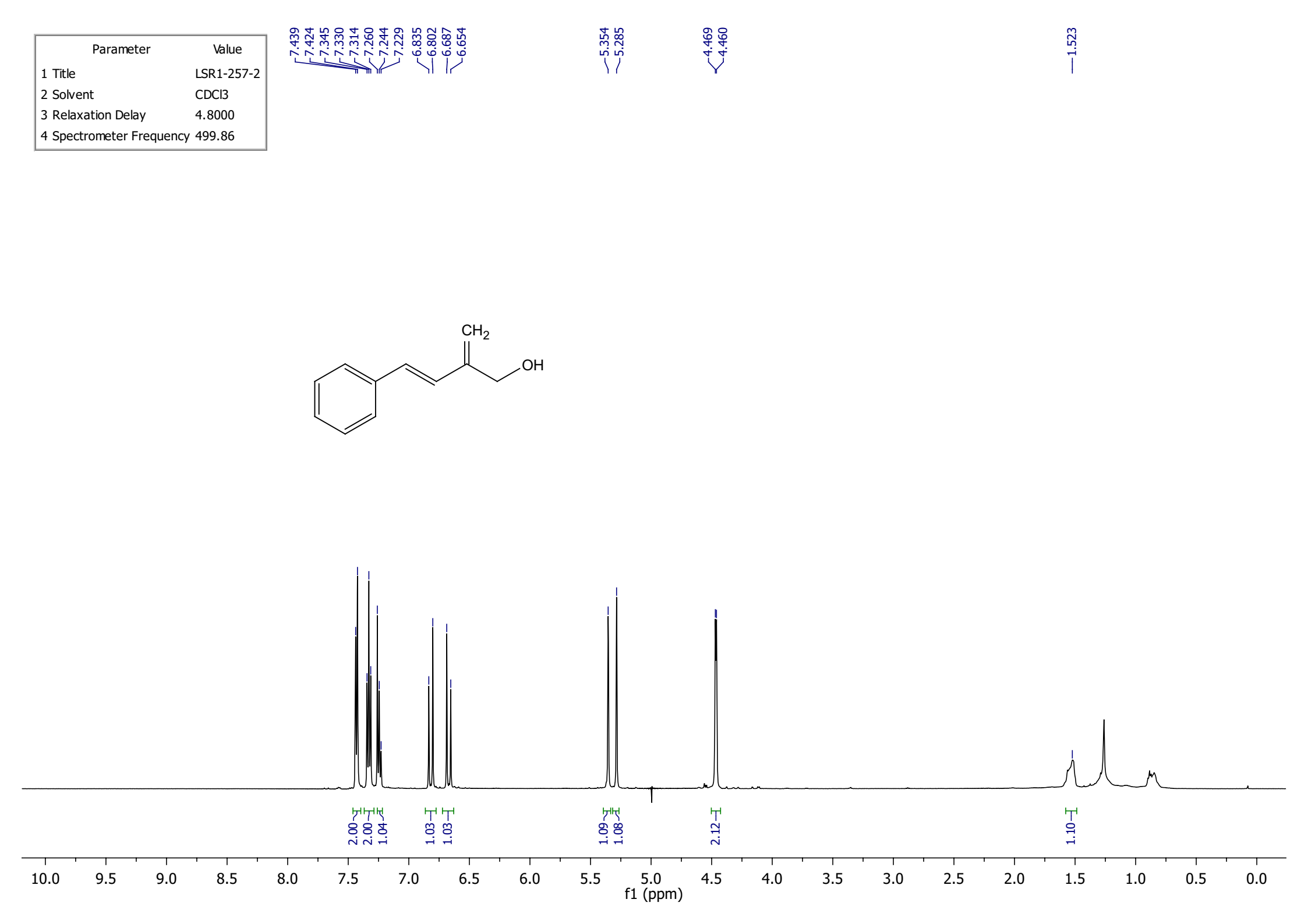
Parameter	Value
1 Title	LSR1-233-1C
2 Solvent	CDCl3
3 Relaxation Delay	1.0000
4 Spectrometer Frequency	125.70

149.00
137.17
128.93
128.62
127.93
127.64
126.44
114.08
72.07
38.63
19.06
14.00

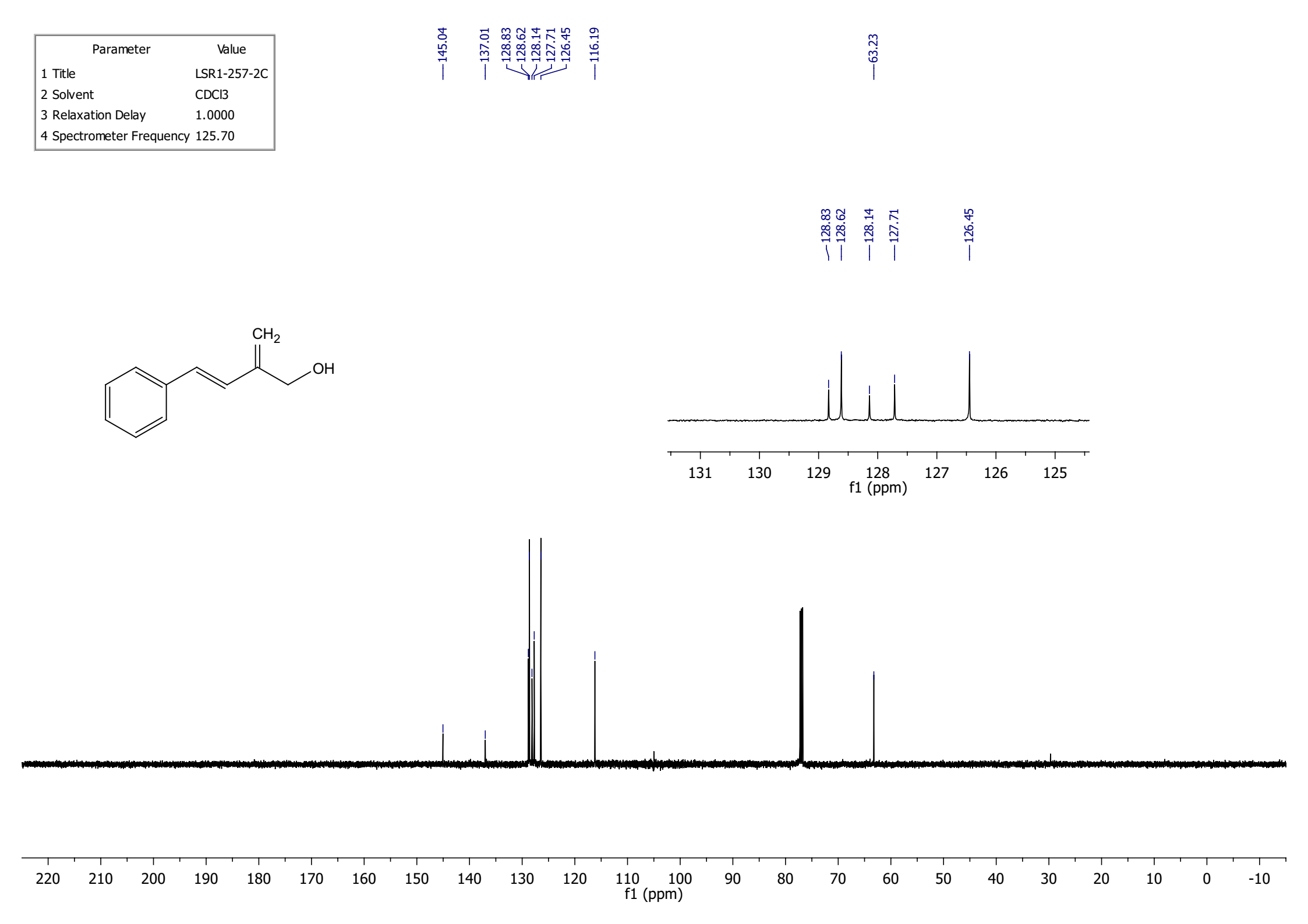




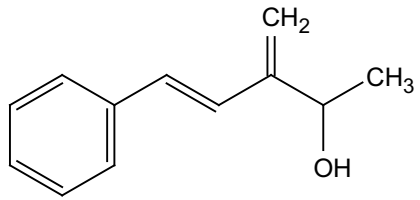
Parameter	Value
1 Title	LSR1-257-2
2 Solvent	CDCl3
3 Relaxation Delay	4.8000
4 Spectrometer Frequency	499.86



Parameter	Value
1 Title	LSR1-257-2C
2 Solvent	CDCl3
3 Relaxation Delay	1.0000
4 Spectrometer Frequency	125.70

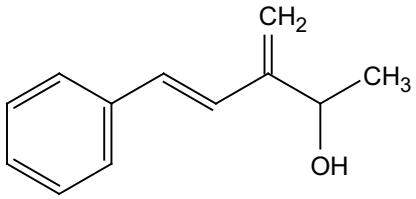


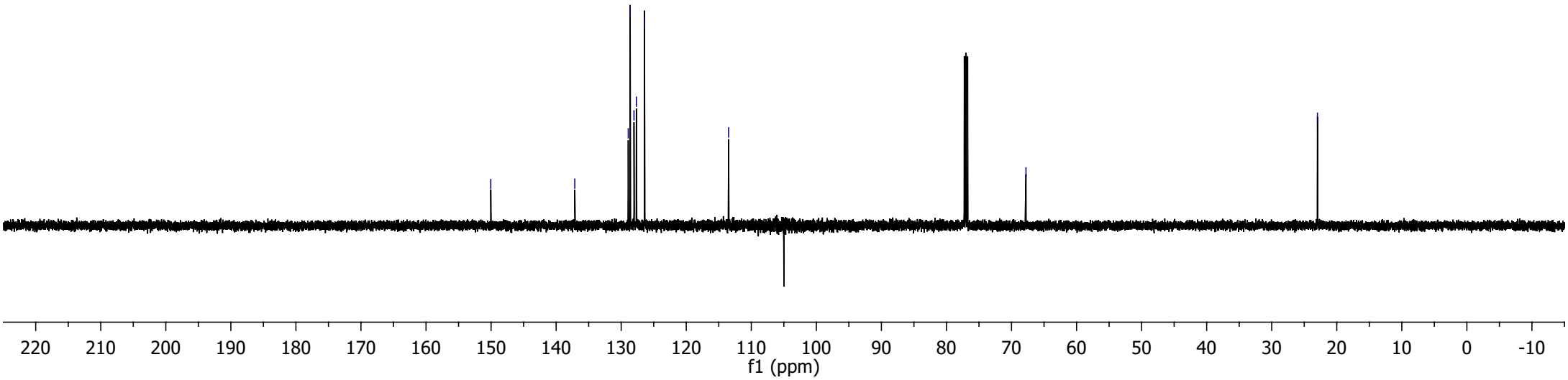
Parameter	Value
1 Title	LSR1-253-1
2 Solvent	CDCl3
3 Relaxation Delay	4.8000
4 Spectrometer Frequency	499.86



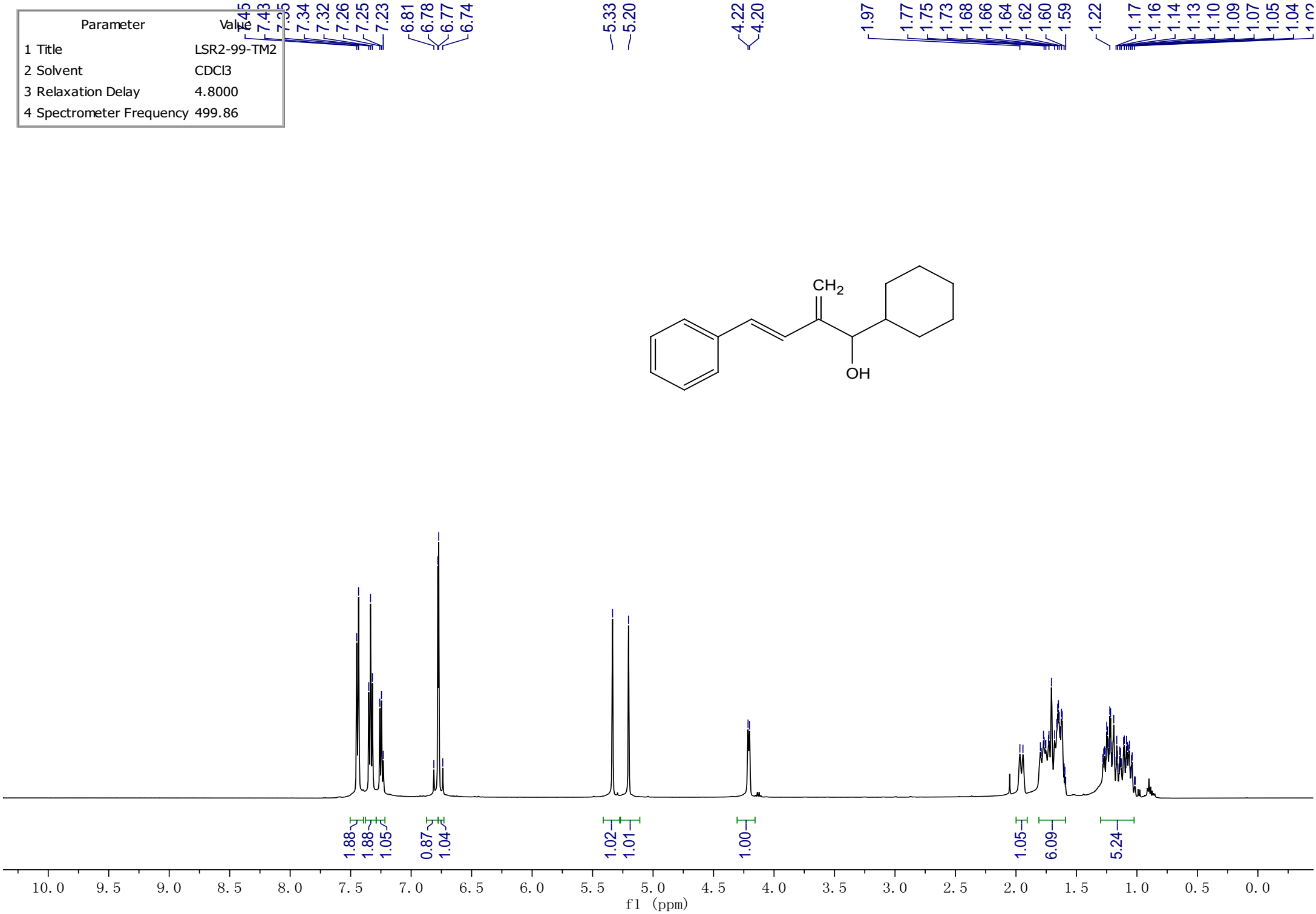
Parameter	Value
1 Title	LSR1-253-1C
2 Solvent	CDCl3
3 Relaxation Delay	1.0000
4 Spectrometer Frequency	125.70

150.05
137.13
128.91
128.62
128.03
127.66
126.43
113.49
67.78
22.97





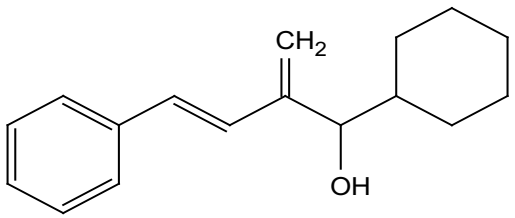
Parameter	Value
1 Title	LSR2-99-TM2
2 Solvent	CDCl3
3 Relaxation Delay	4.8000
4 Spectrometer Frequency	499.86

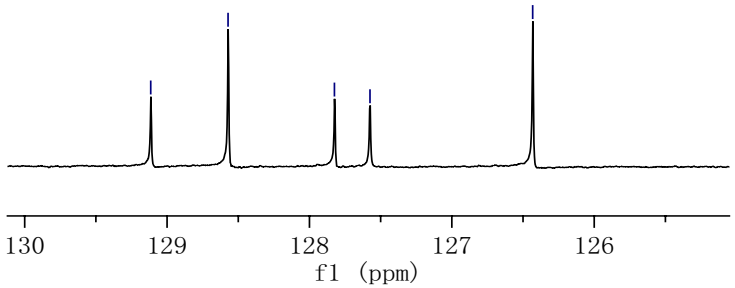


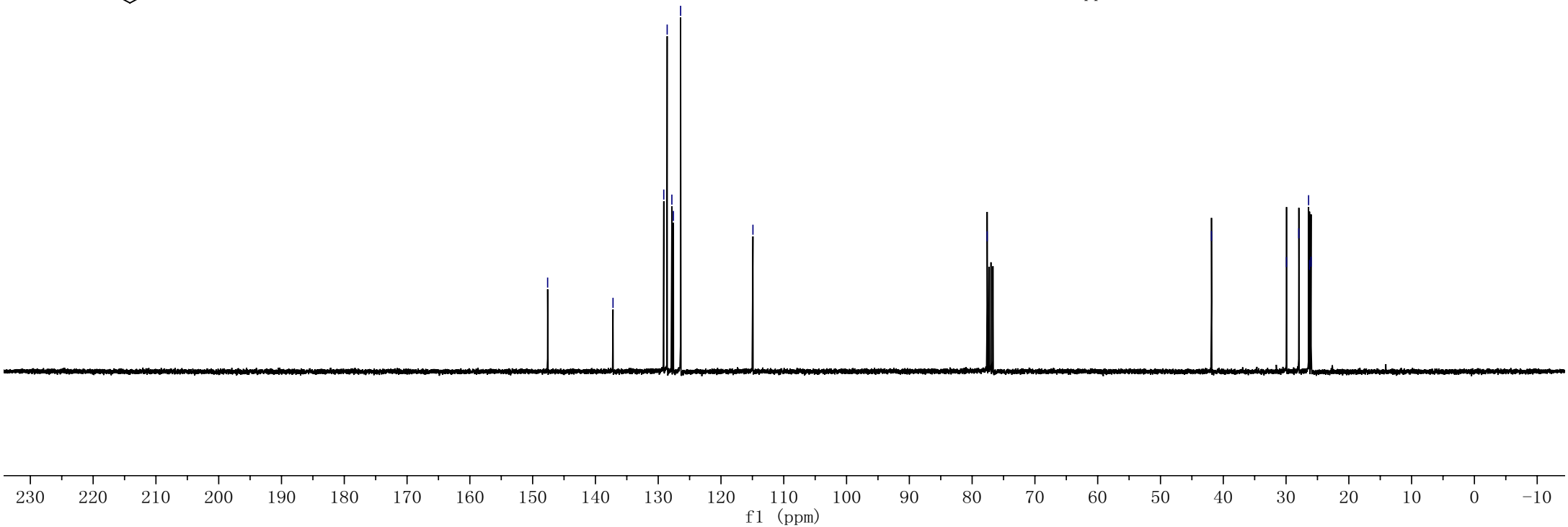
Parameter	Value
1 Title	LSR2-99-TM2-C
2 Solvent	cdcl3
3 Relaxation Delay	1.0000
4 Spectrometer Frequency	100.53

147.61
137.20
128.57
127.82
127.57
126.43
114.91
77.61
41.88
29.93
27.97
26.41
26.26
26.02

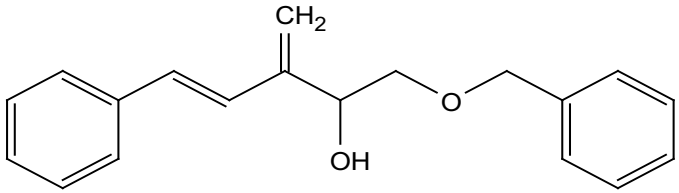
129.11
128.57
127.82
127.57
126.43



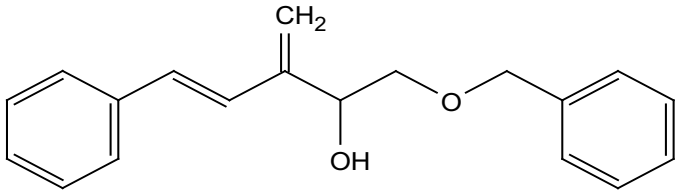




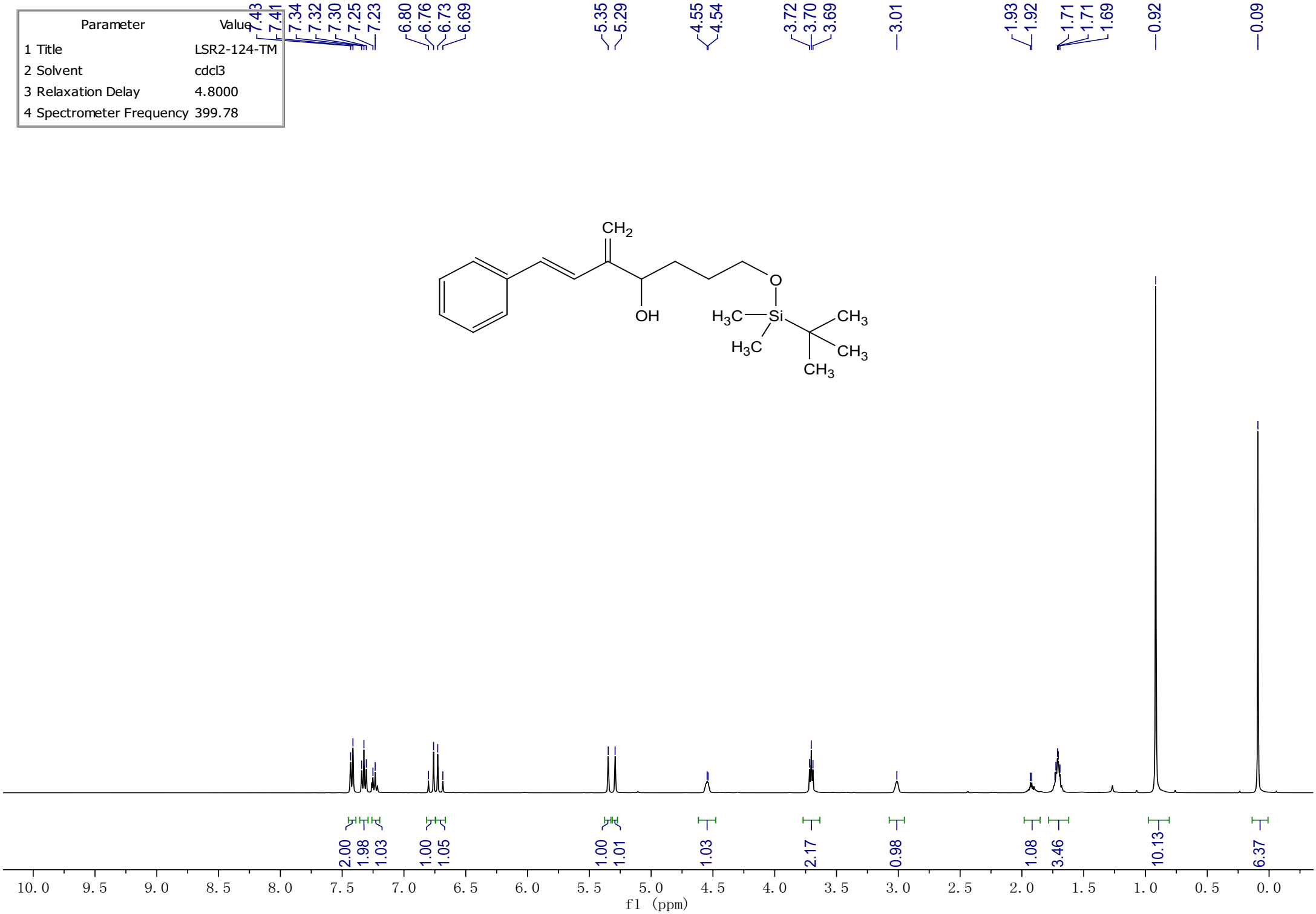
Parameter	Value
1 Title	LSR2-130-TM1
2 Solvent	cdcl3
3 Relaxation Delay	4.8000
4 Spectrometer Frequency	399.78



Parameter	Value
1 Title	LSR2-106-TM1-C
2 Solvent	cdcl3
3 Relaxation Delay	1.0000
4 Spectrometer Frequency	150.79

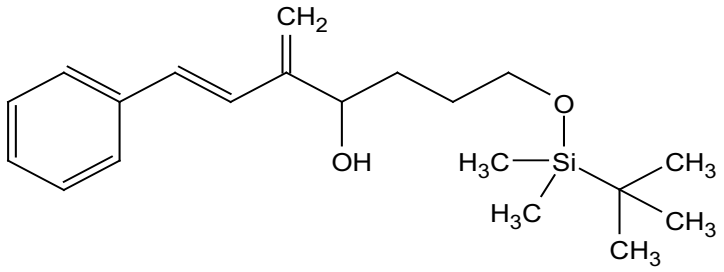


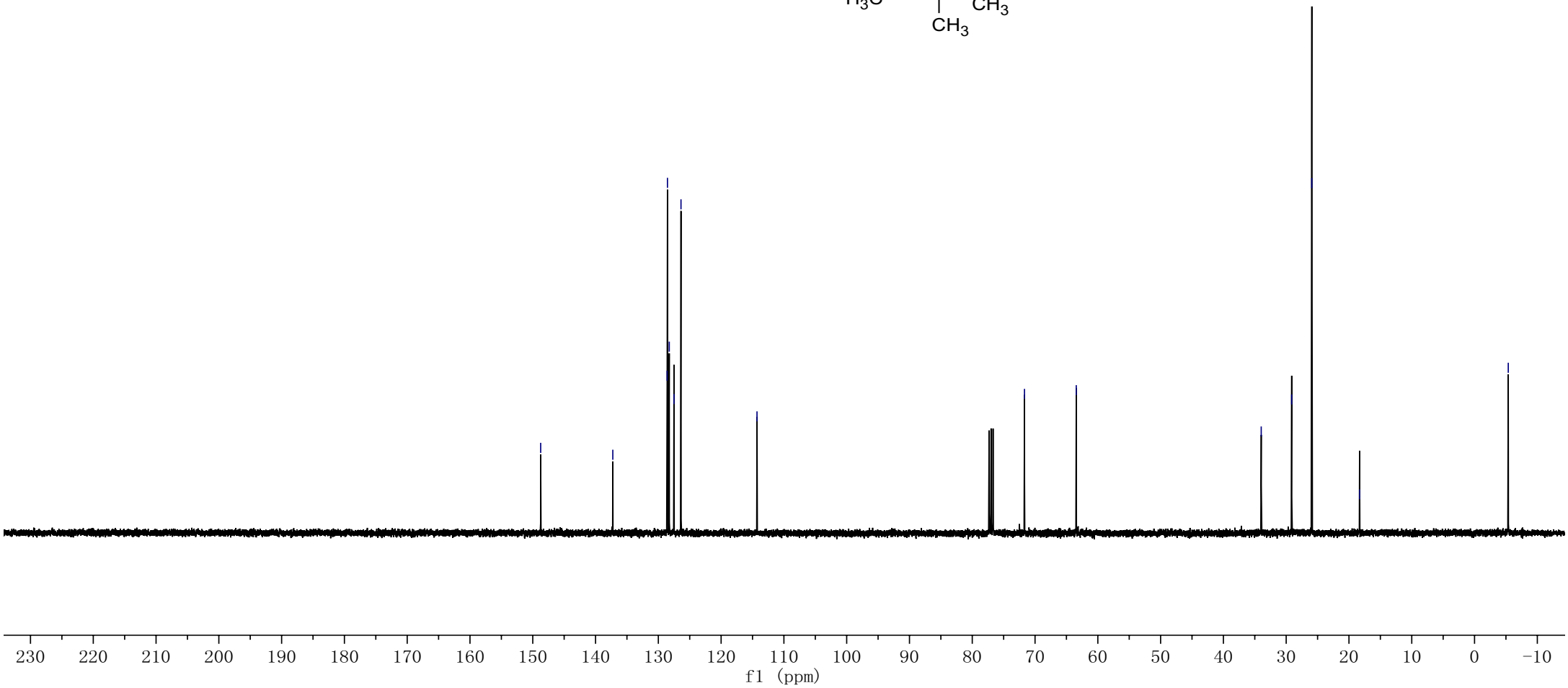
Parameter	Value
1 Title	LSR2-124-TM
2 Solvent	cdcl3
3 Relaxation Delay	4.8000
4 Spectrometer Frequency	399.78



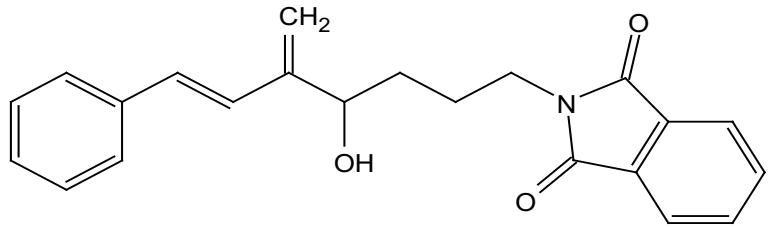
Parameter	Value
1 Title	LSR2-124-TM-C
2 Solvent	cdcl3
3 Relaxation Delay	1.0000
4 Spectrometer Frequency	100.53

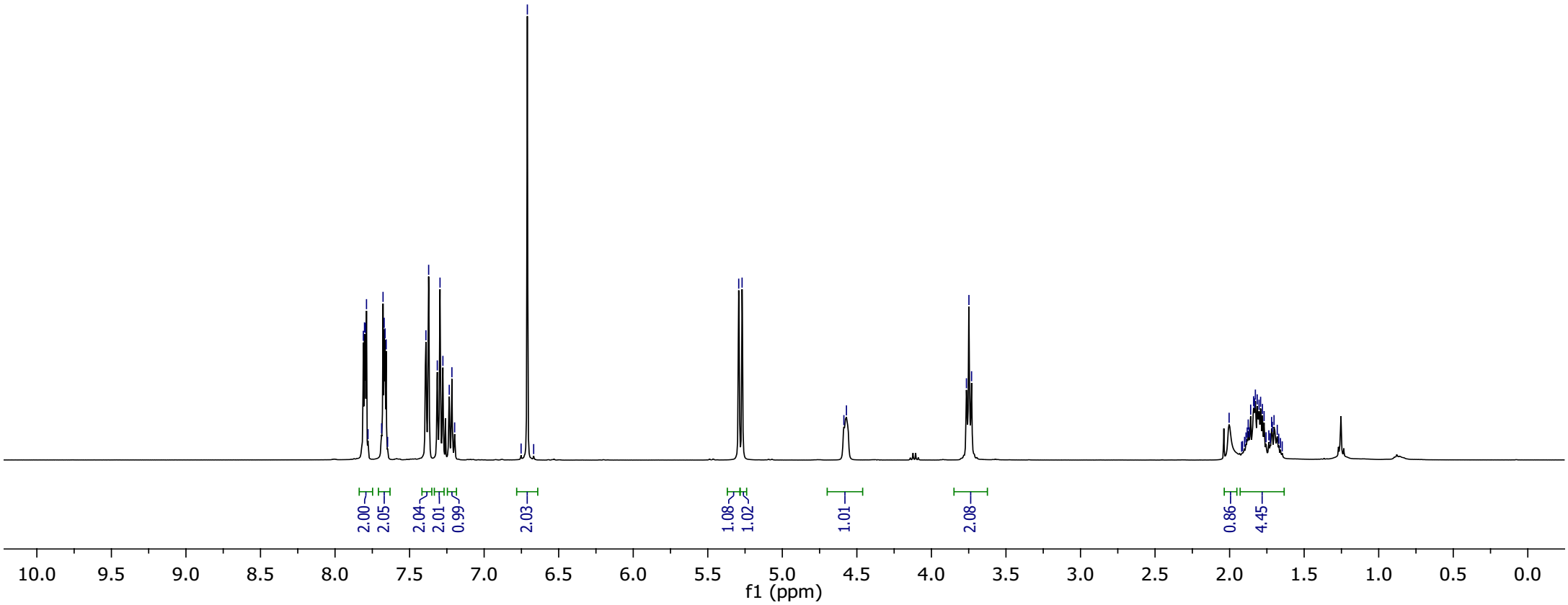
148.74
137.25
128.55
128.26
127.50
126.39
114.29
71.68
63.44
33.98
29.13
25.92
18.31
-5.37



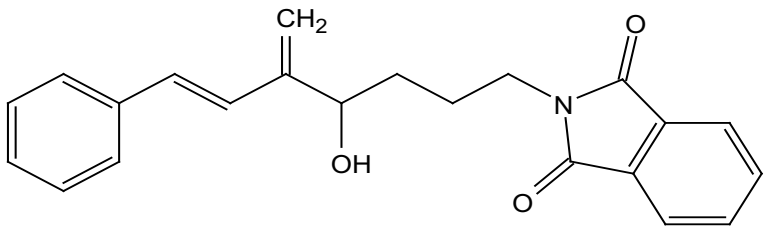


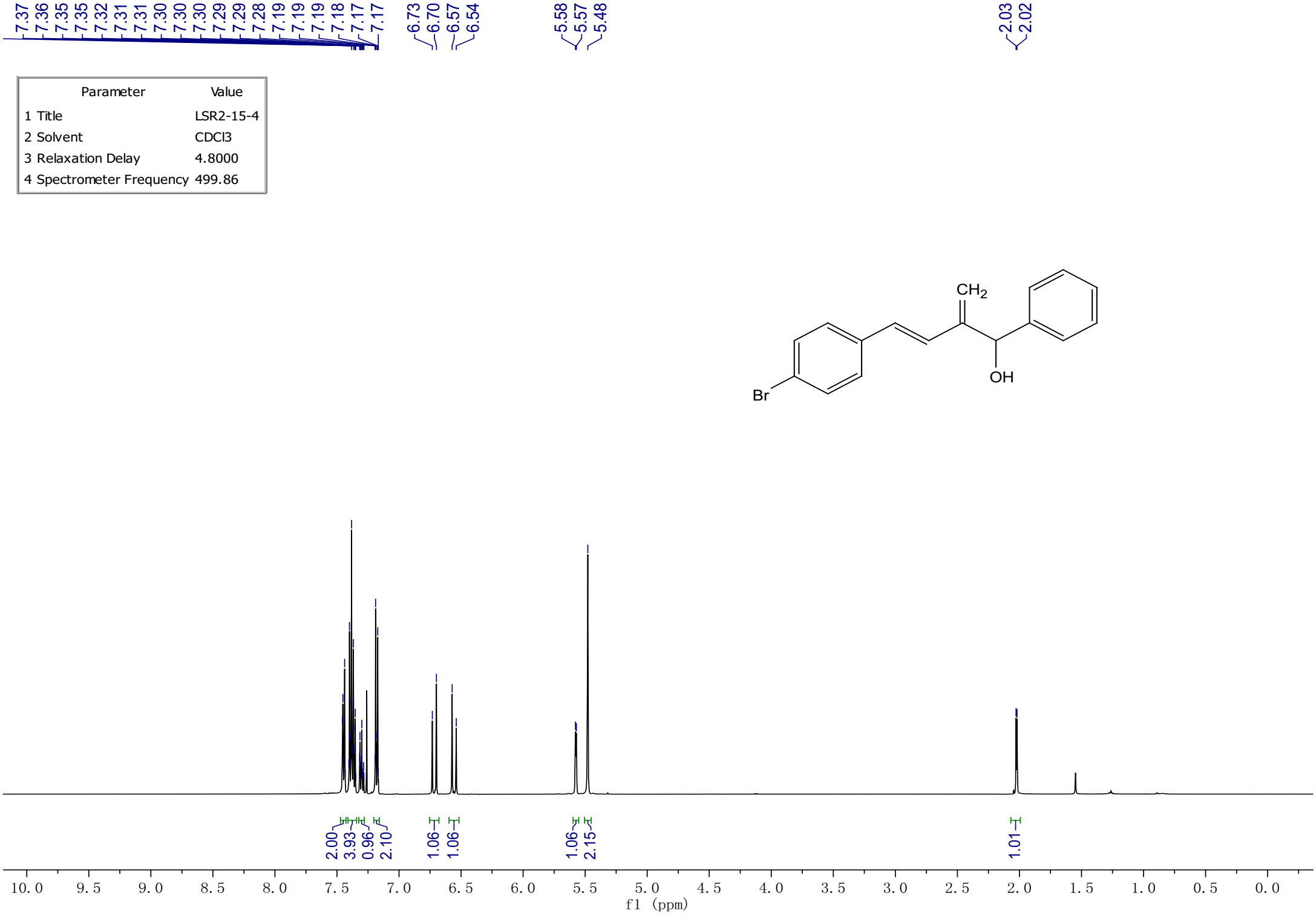
Parameter	Value
1 Title	LSR2-158-TM1
2 Solvent	cdcl3
3 Relaxation Delay	4.8000
4 Spectrometer Frequency	399.78





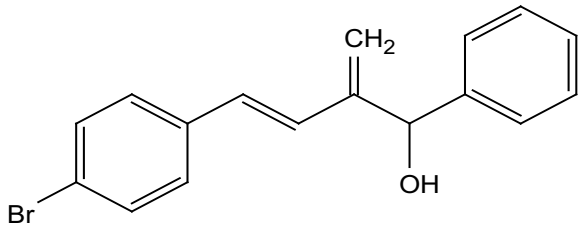
Parameter	Value
1 Title	LSR2-158-TM1-C
2 Solvent	cdcl3
3 Relaxation Delay	1.0000
4 Spectrometer Frequency	100.53

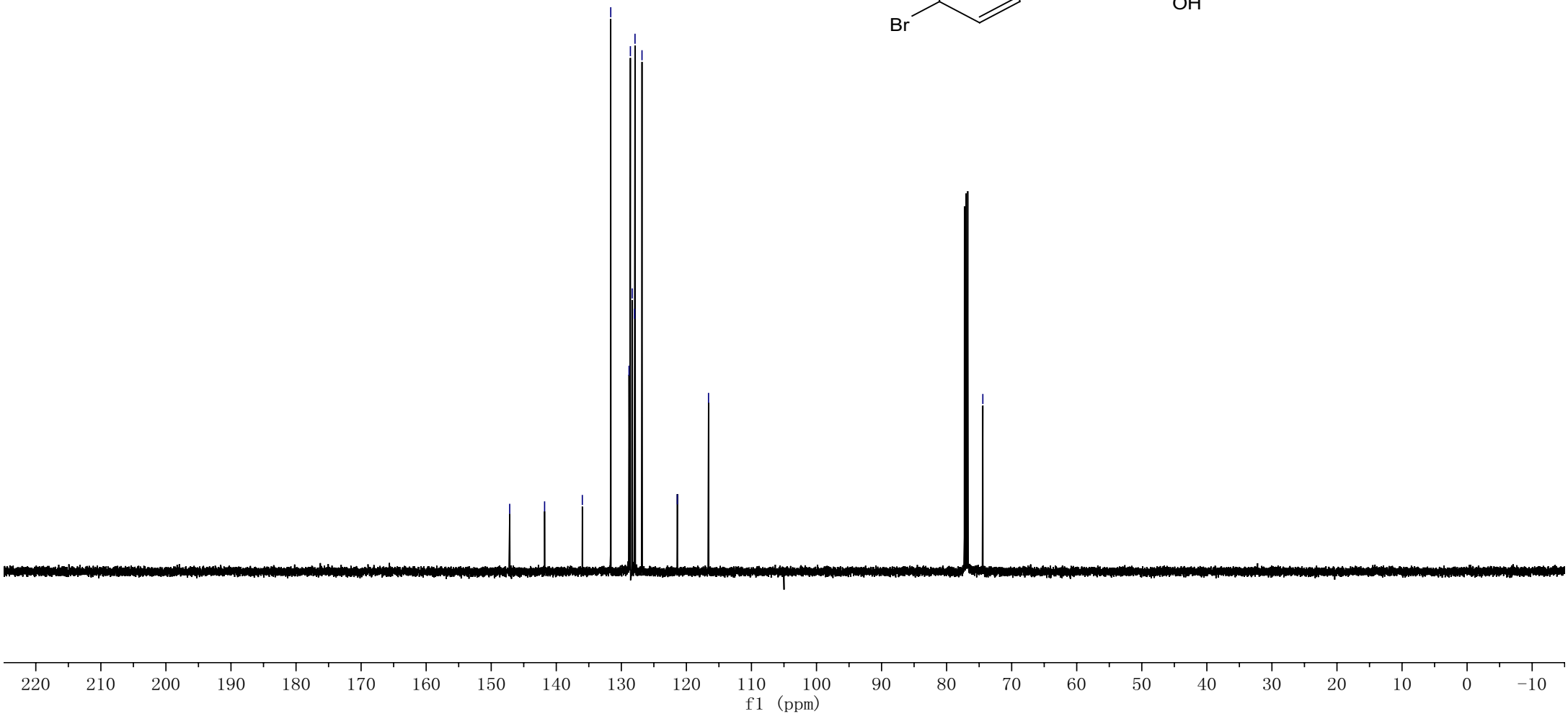



7.37
7.36
7.35
7.35
7.32
7.31
7.31
7.30
7.30
7.30
7.29
7.29
7.28
7.19
7.19
7.19
7.18
7.17
7.17
6.73
6.70
6.57
6.54
5.58
5.57
5.48
2.03
2.02
Parameter Value
1 Title LSR2-15-4
2 Solvent CDCl3
3 Relaxation Delay 4.8000
4 Spectrometer Frequency 499.86
CH2
OH
Br
2.00
3.93
0.96
2.10
1.06
1.06
1.06
2.15
1.01
10.0
9.5
9.0
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
f1 (ppm)

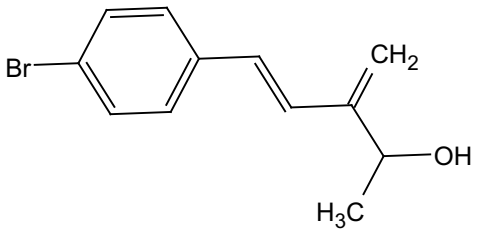
Parameter	Value
1 Title	LSR2-15-4C
2 Solvent	CDCl3
3 Relaxation Delay	1.0000
4 Spectrometer Frequency	125.70

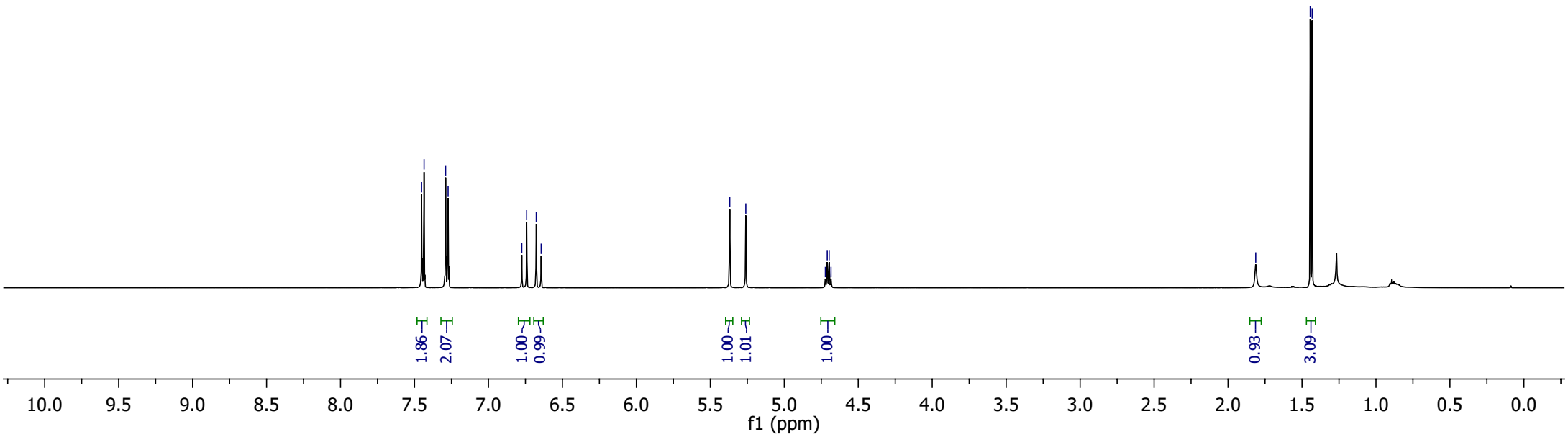
147.16
141.80
135.99
131.63
126.82
121.39
116.60
74.43





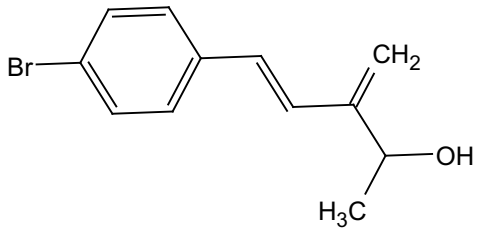
Parameter	Value
1 Title	LSR2-3-2
2 Solvent	CDCl3
3 Relaxation Delay	4.8000
4 Spectrometer Frequency	499.86

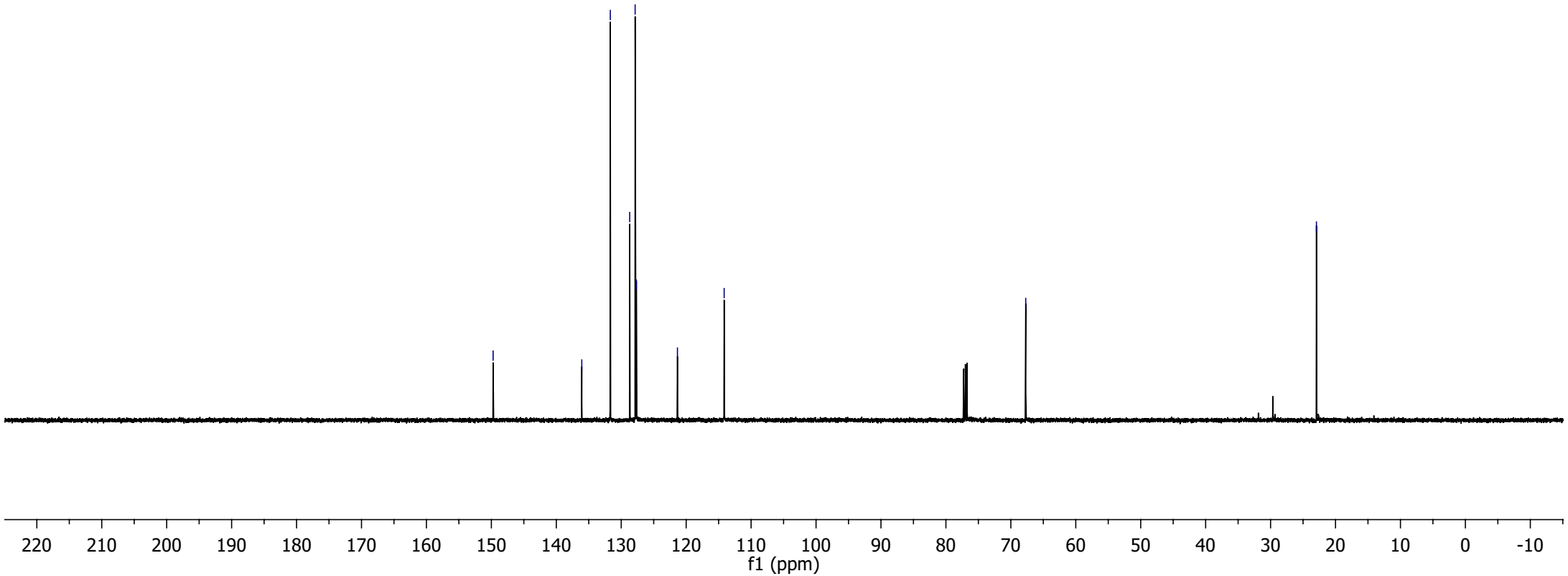




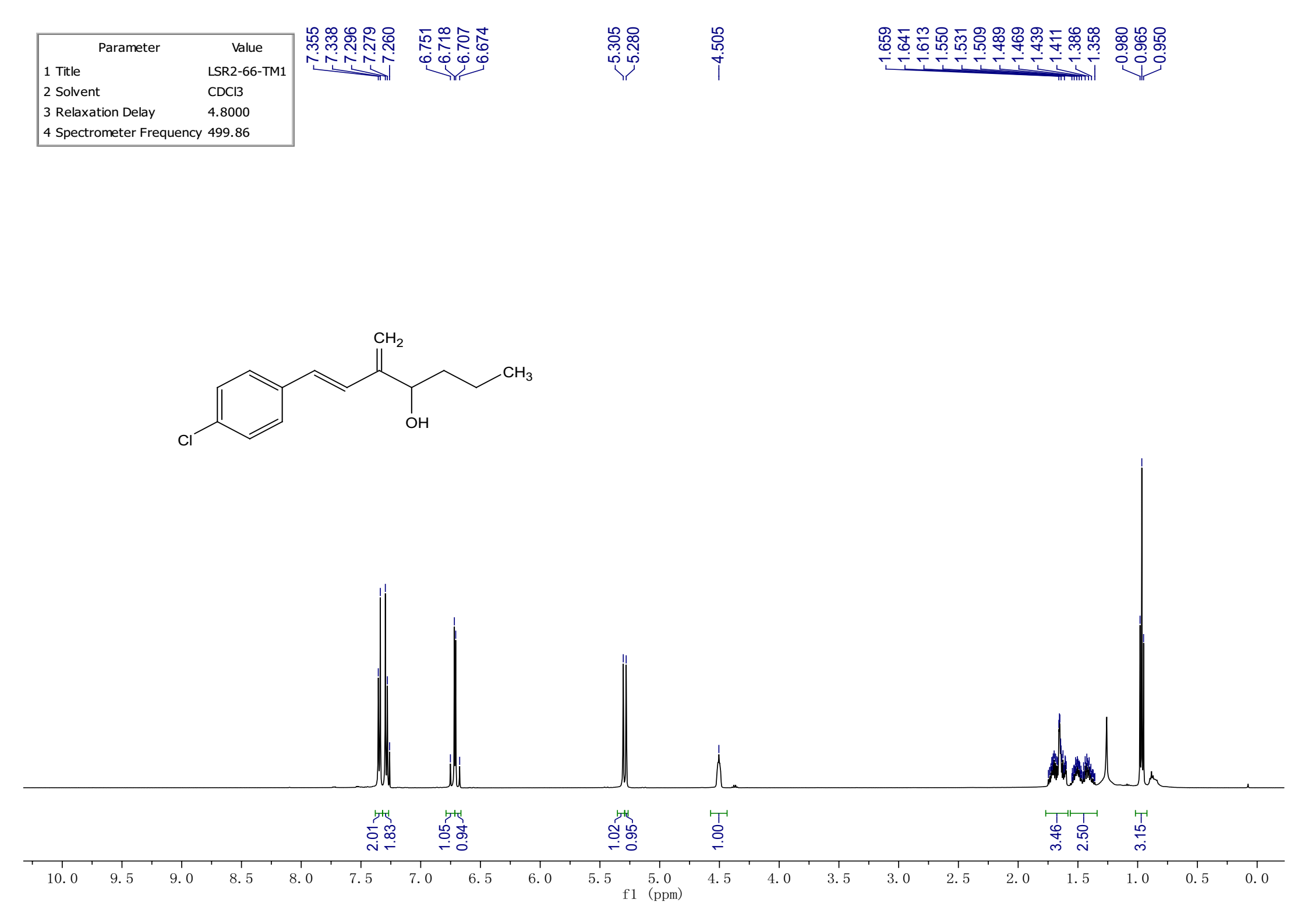
Parameter	Value
1 Title	LSR2-3-2C
2 Solvent	CDCl3
3 Relaxation Delay	1.0000
4 Spectrometer Frequency	125.70

149.73
136.07
131.68
127.86
127.67
121.34
114.15
67.70
22.94



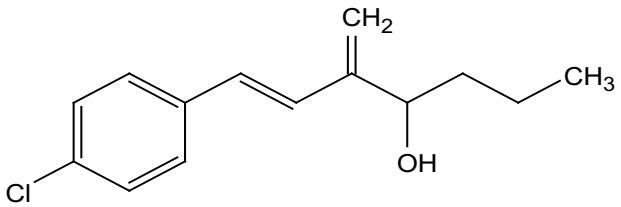


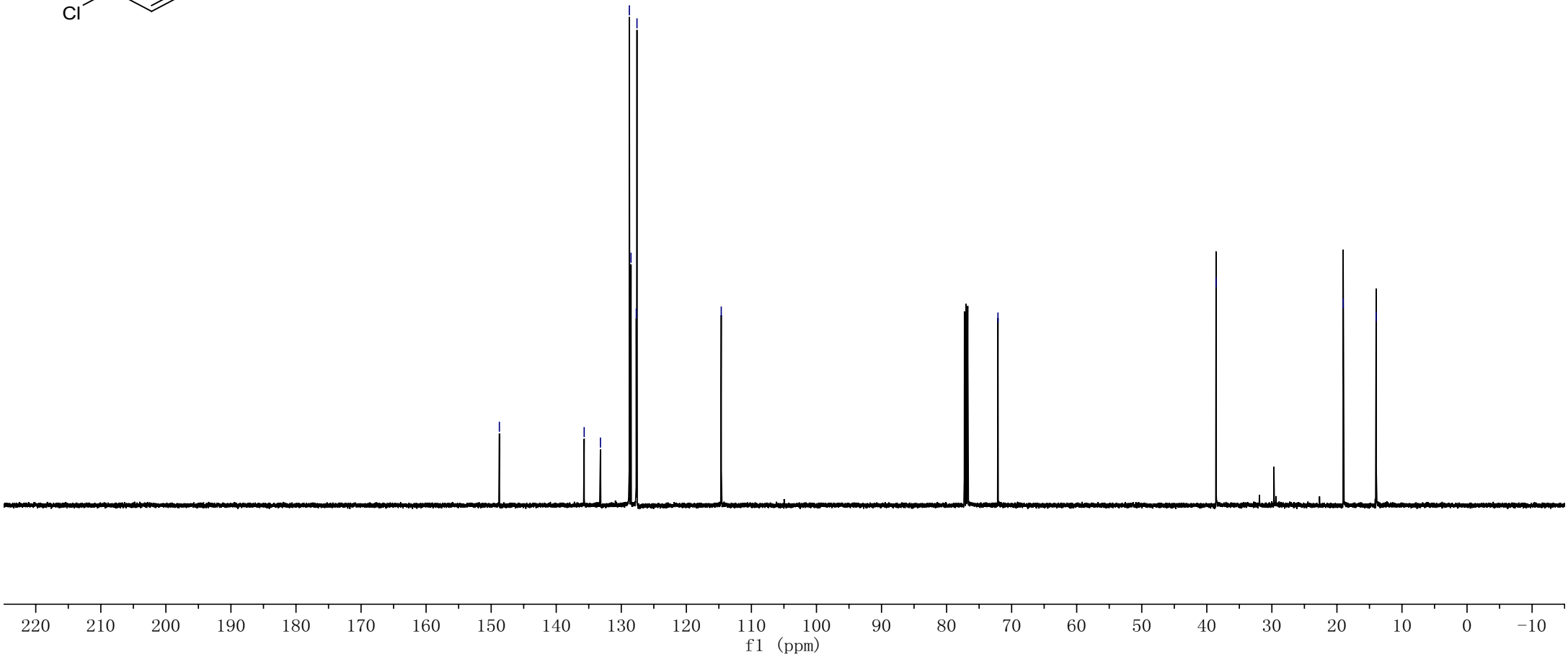
Parameter	Value
1 Title	LSR2-66-TM1
2 Solvent	CDCl3
3 Relaxation Delay	4.8000
4 Spectrometer Frequency	499.86



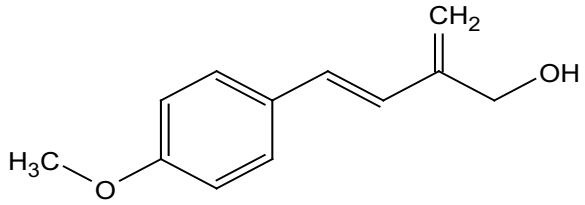
Parameter	Value
1 Title	LSR2-66-TM1-C
2 Solvent	CDCl3
3 Relaxation Delay	1.0000
4 Spectrometer Frequency	125.70

148.74
135.70
133.20
128.78
127.69
127.59
114.63
72.10
38.58
19.05
13.97



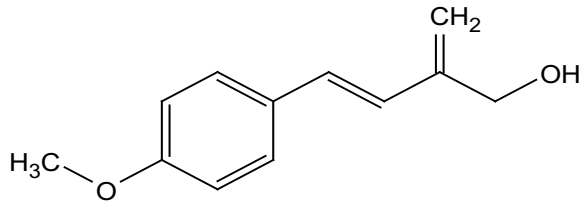


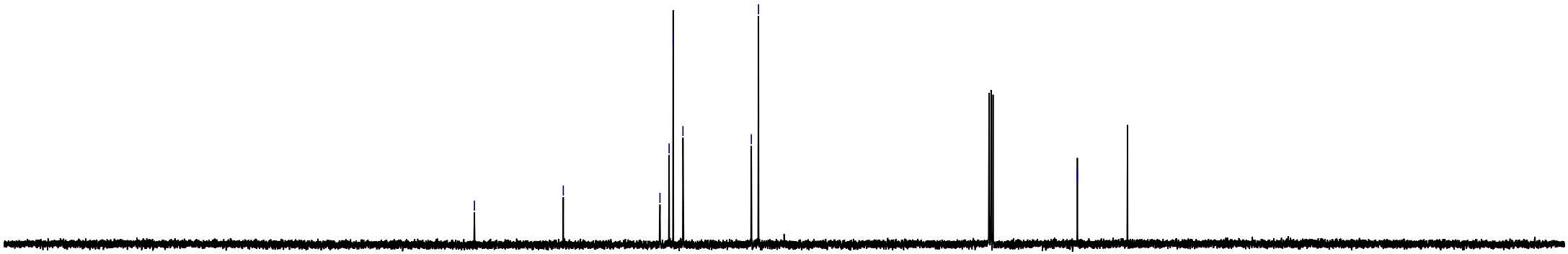
Parameter	Value
1 Title	LSR2-98-TM2
2 Solvent	CDCl3
3 Relaxation Delay	4.8000
4 Spectrometer Frequency	499.86

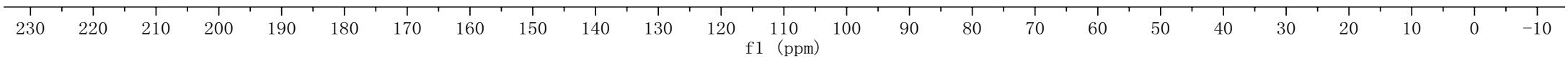


Parameter	Value
1 Title	LSR2-98-TM-C
2 Solvent	cdcl3
3 Relaxation Delay	1.0000
4 Spectrometer Frequency	100.53

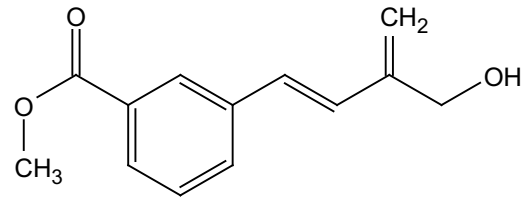
159.29
145.14
129.74
128.28
127.64
126.08
115.19
114.04
63.26
55.27







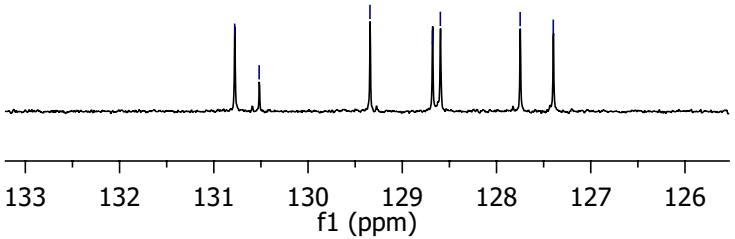
Parameter	Value
1 Title	LSR2-109-TM1
2 Solvent	cdcl3
3 Relaxation Delay	4.8000
4 Spectrometer Frequency	399.78

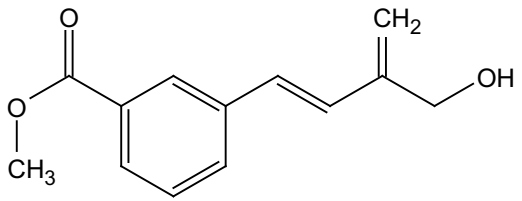


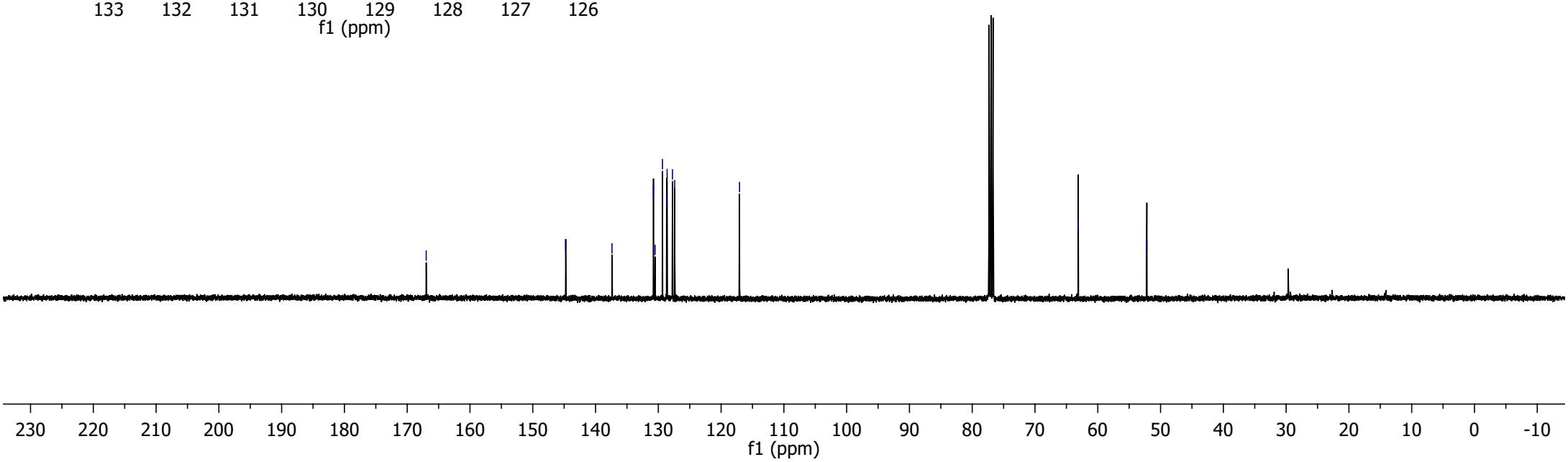
Parameter	Value
1 Title	LSR2-109-TM1-C
2 Solvent	cdcl3
3 Relaxation Delay	1.0000
4 Spectrometer Frequency	100.53

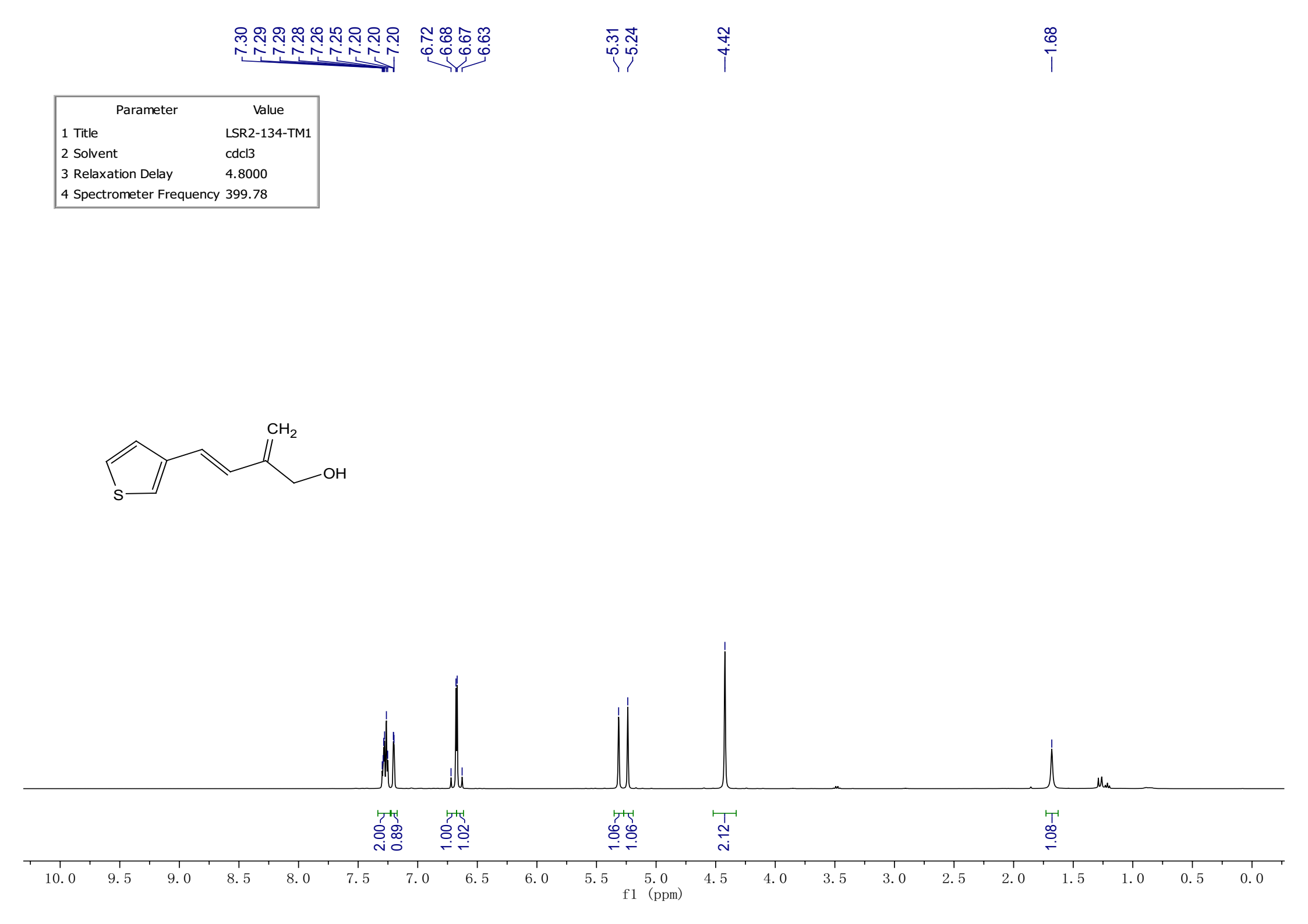
166.98
144.75
137.38
129.34
128.68
128.60
127.75
127.40
117.07
63.12
52.19

130.78
130.52
129.34
128.68
128.60
127.75
127.40

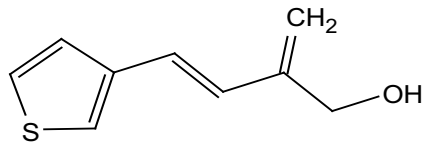




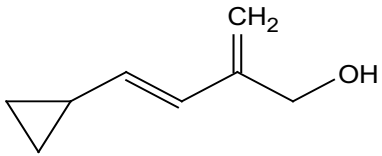



7.30
7.29
7.29
7.28
7.26
7.25
7.20
7.20
7.20
6.72
6.68
6.67
6.63
5.31
5.24
4.42
1.68
Parameter Value
1 Title LSR2-134-TM1
2 Solvent cdcl3
3 Relaxation Delay 4.8000
4 Spectrometer Frequency 399.78
CH2
OH
S
2.00
0.89
1.00
1.02
1.06
1.06
2.12
1.08
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

Parameter	Value
1 Title	LSR2-134-TM1-C
2 Solvent	cdcl3
3 Relaxation Delay	1.0000
4 Spectrometer Frequency	100.53

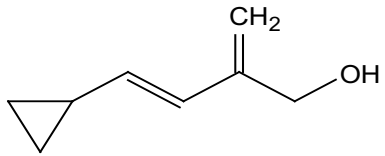


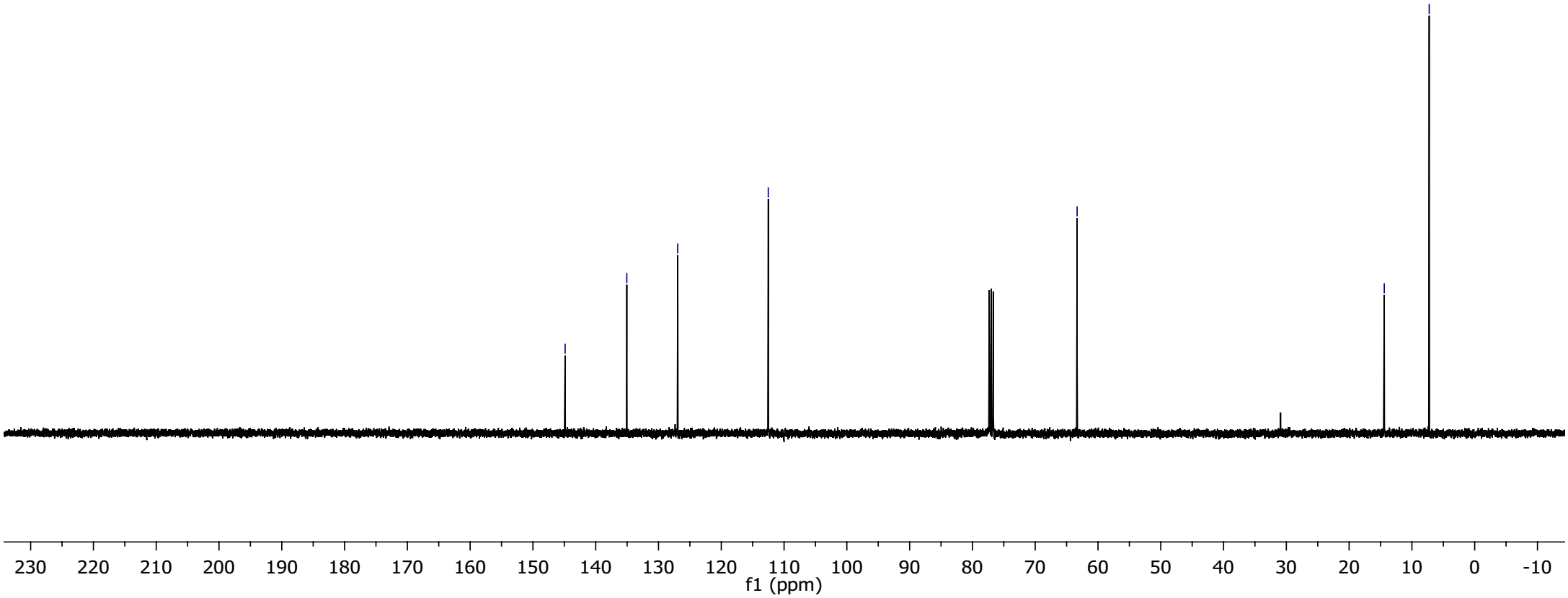
Parameter	Value
1 Title	LSR2-163-TM1
2 Solvent	cdcl3
3 Relaxation Delay	4.8000
4 Spectrometer Frequency	399.78



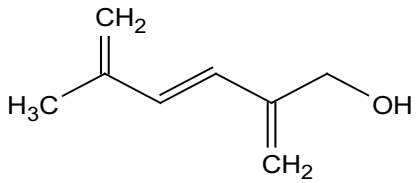
Parameter	Value
1 Title	LSR2-149-TM1-C
2 Solvent	cdcl3
3 Relaxation Delay	1.0000
4 Spectrometer Frequency	100.53

144.87
135.05
126.94
112.51
63.32
14.41
7.25



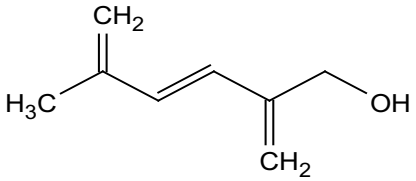


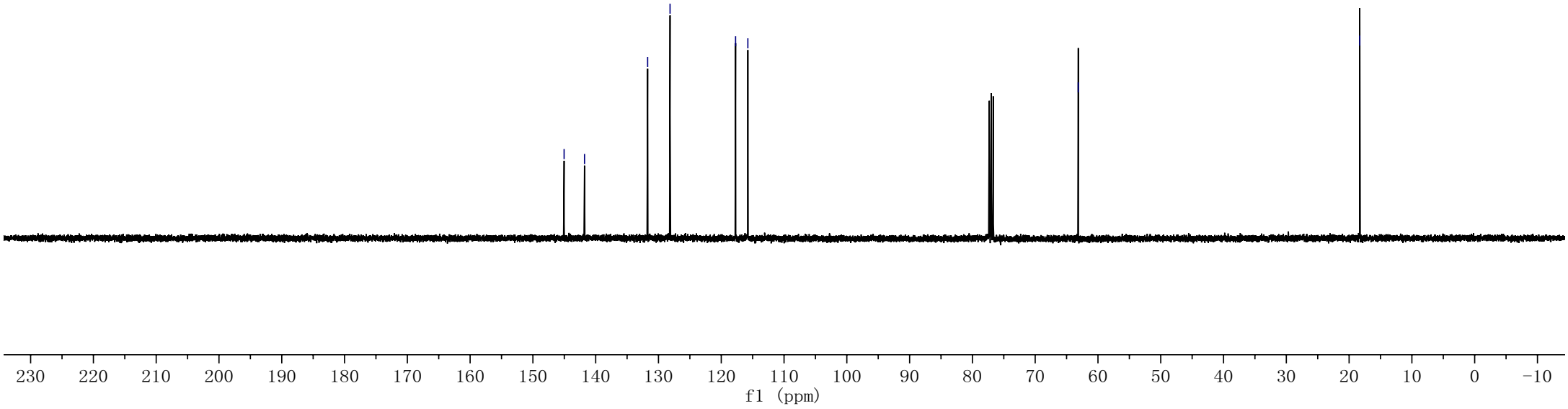
Parameter	Value
1 Title	LSR2-146-TM1
2 Solvent	cdcl3
3 Relaxation Delay	4.8000
4 Spectrometer Frequency	399.78



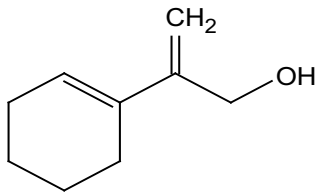
Parameter	Value
1 Title	LSR2-146-TM1-C
2 Solvent	cdcl3
3 Relaxation Delay	1.0000
4 Spectrometer Frequency	100.53

145.03
141.78
131.73
128.16
117.72
115.76
63.14
18.31



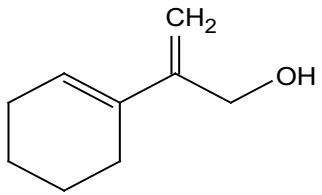


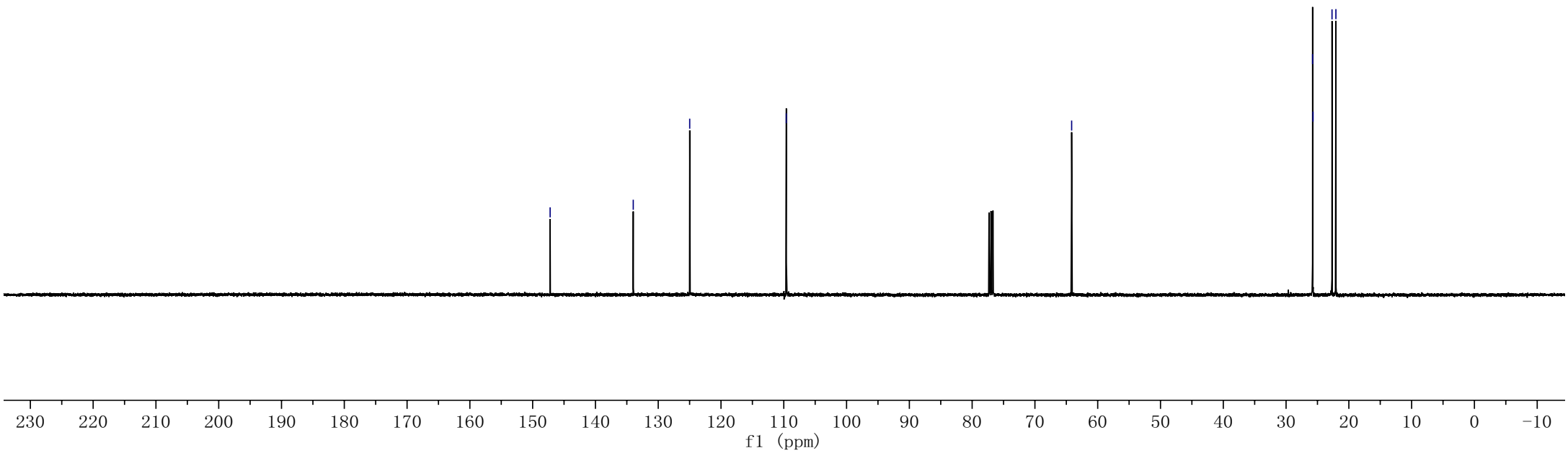
Parameter	Value
1 Title	LSR2-145-TM1
2 Solvent	cdcl3
3 Relaxation Delay	4.8000
4 Spectrometer Frequency	399.78



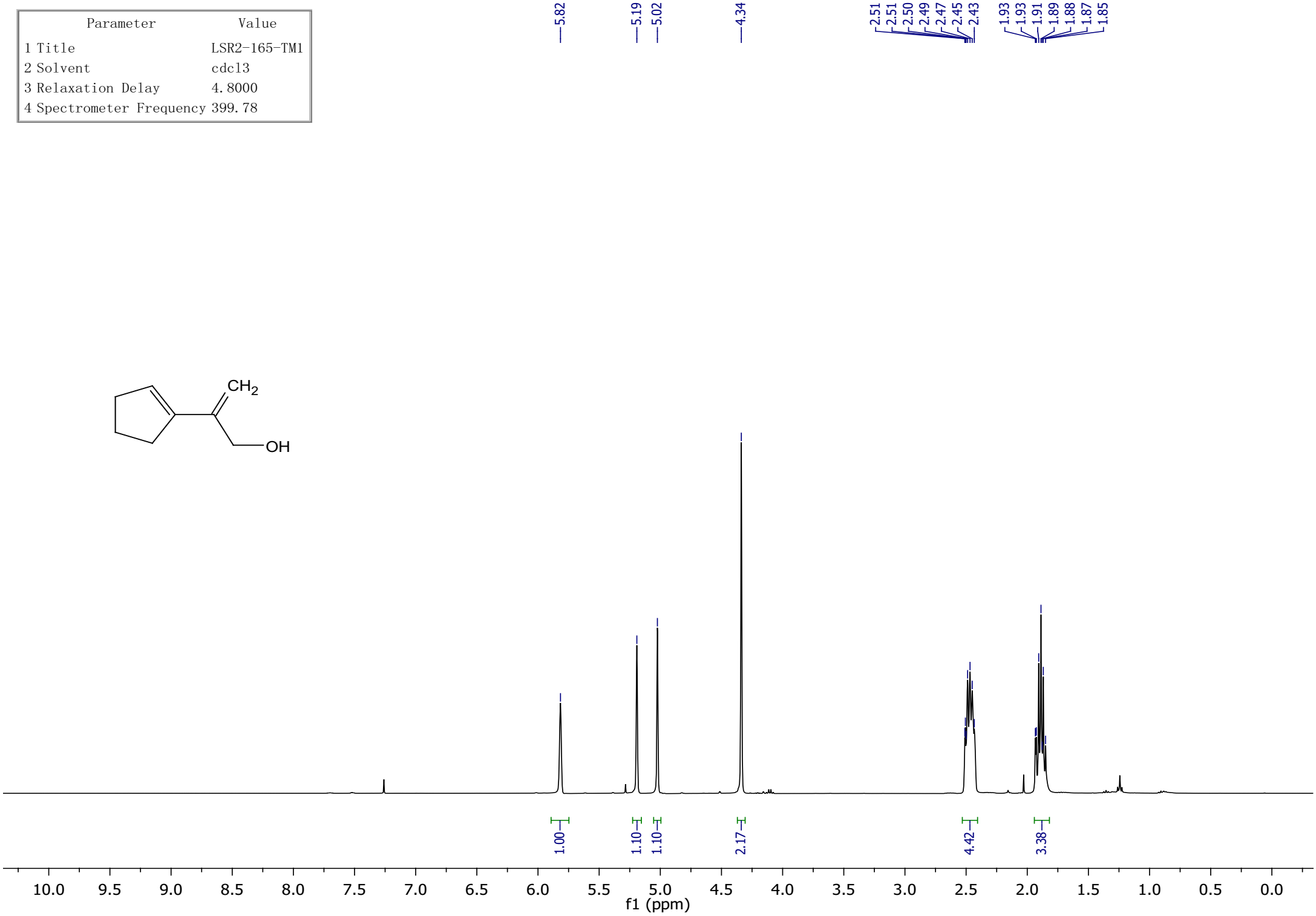
Parameter	Value
1 Title	LSR2-145-TM1-C
2 Solvent	cdcl3
3 Relaxation Delay	1.0000
4 Spectrometer Frequency	100.53

147.22
133.98
124.98
109.60
64.15
25.78
25.70
22.68
22.06

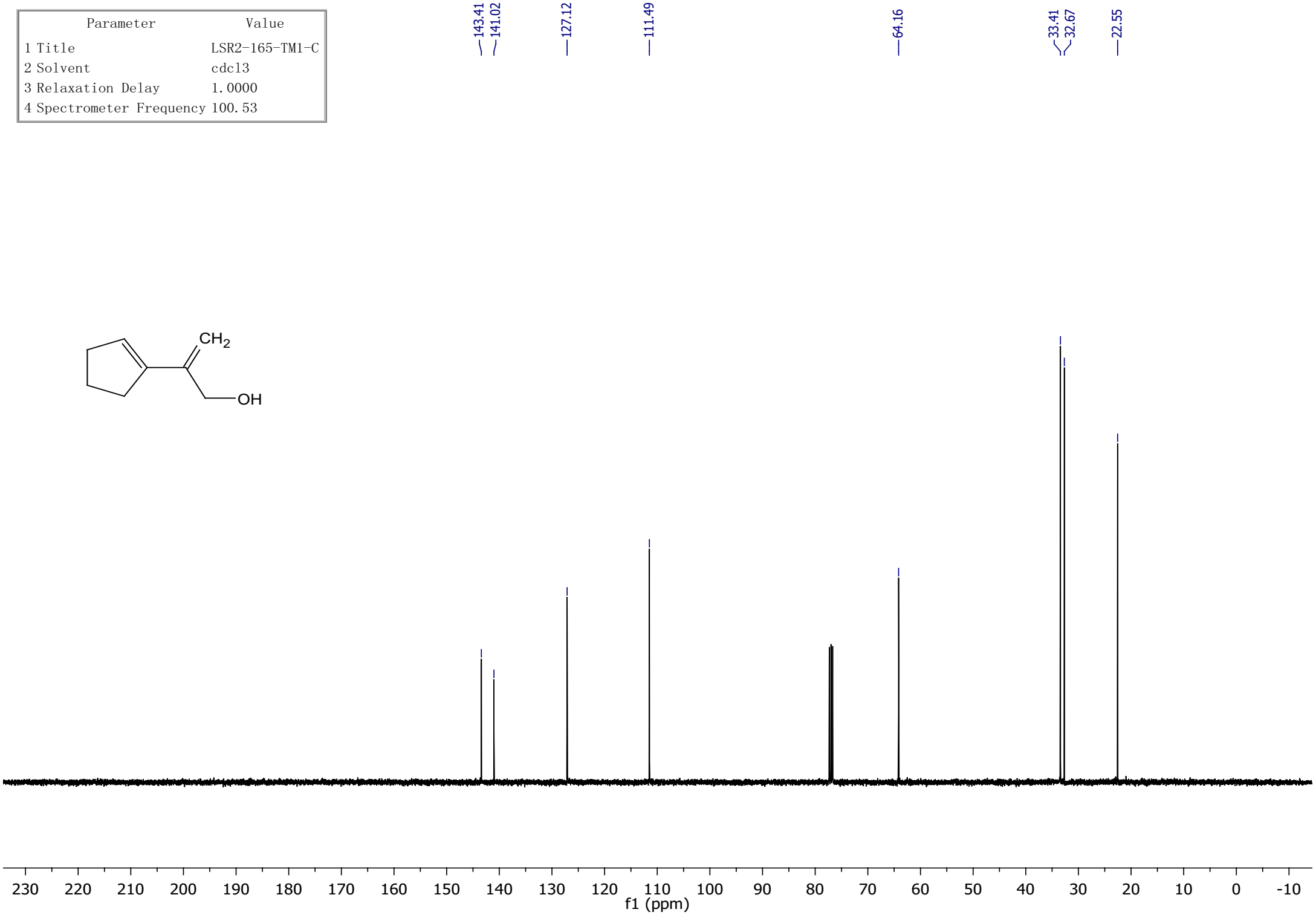




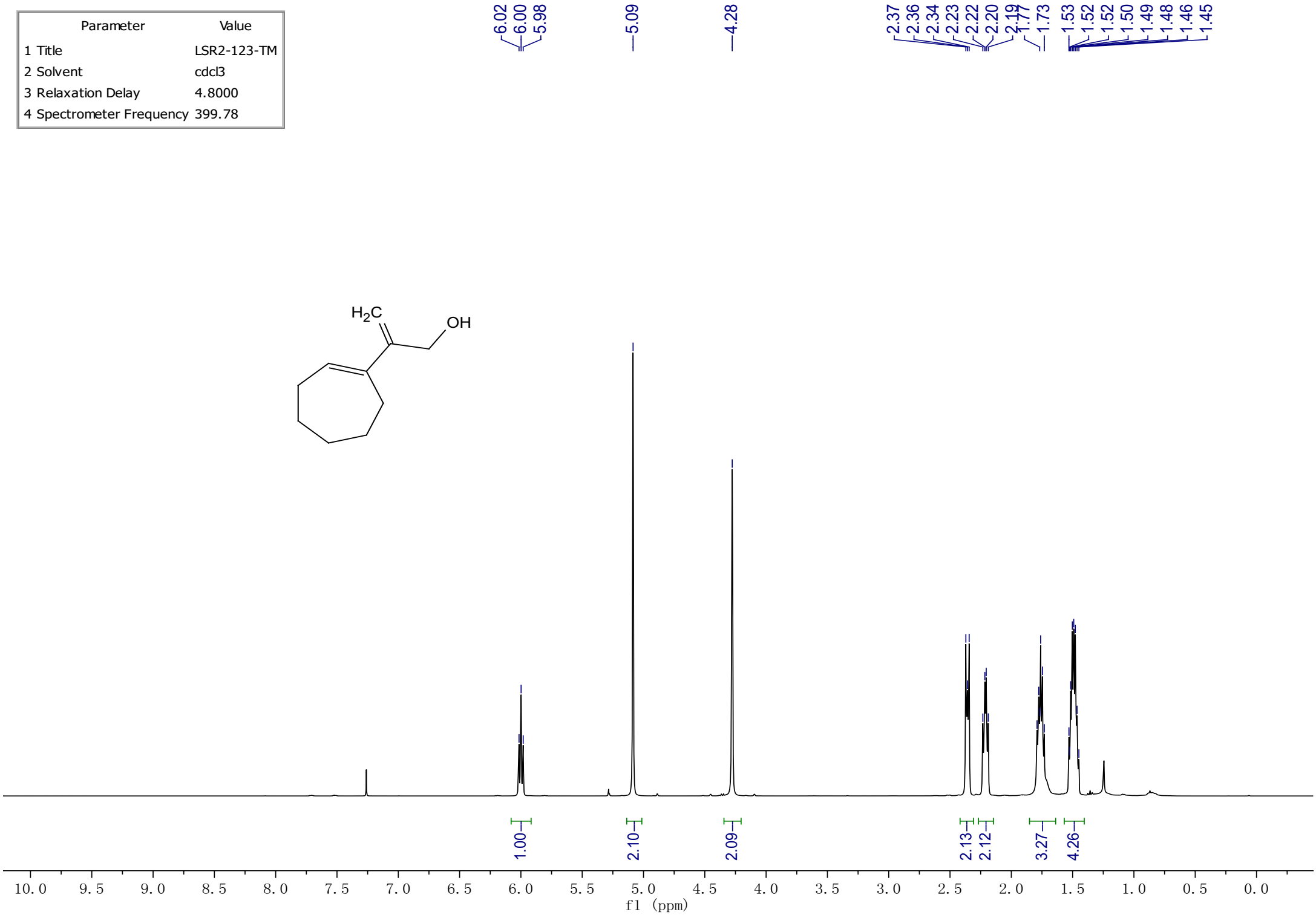
Parameter	Value
1 Title	LSR2-165-TM1
2 Solvent	cdcl3
3 Relaxation Delay	4.8000
4 Spectrometer Frequency	399.78



Parameter	Value
1 Title	LSR2-165-TM1-C
2 Solvent	cdcl3
3 Relaxation Delay	1.0000
4 Spectrometer Frequency	100.53

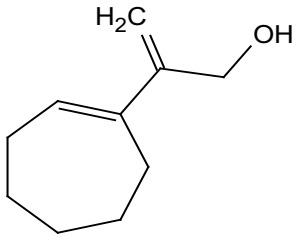


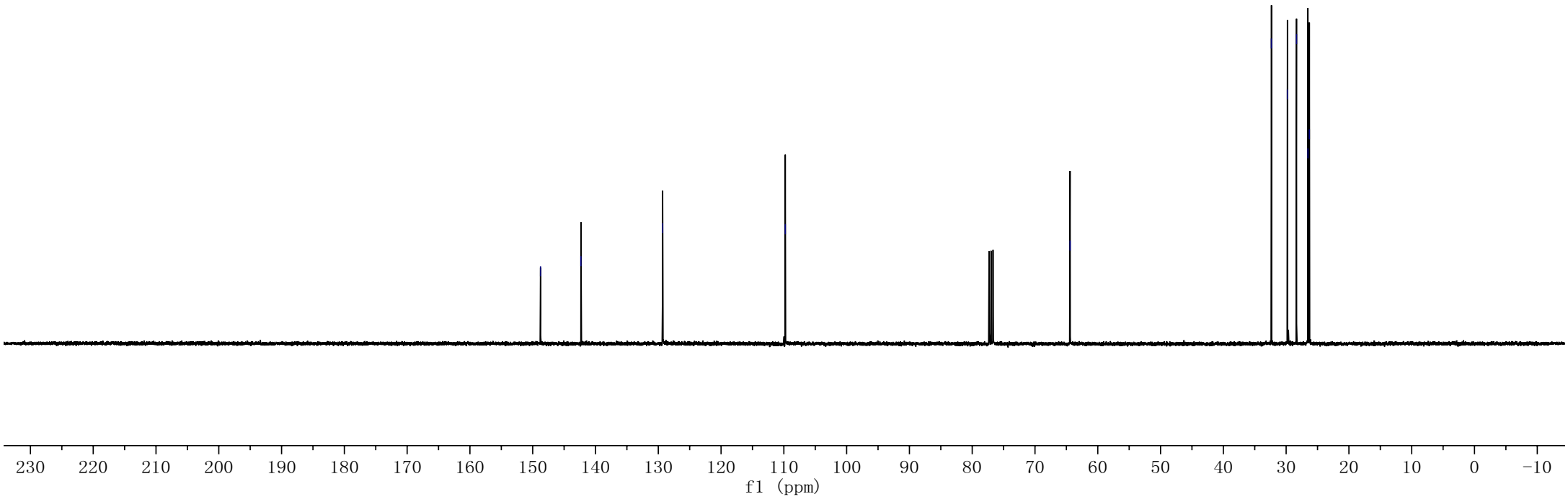
Parameter	Value
1 Title	LSR2-123-TM
2 Solvent	cdcl3
3 Relaxation Delay	4.8000
4 Spectrometer Frequency	399.78



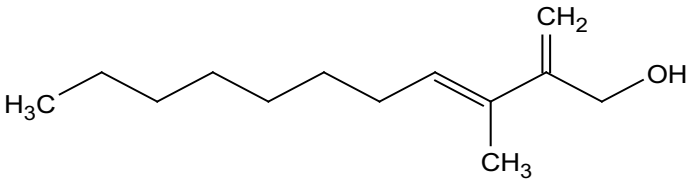
Parameter	Value
1 Title	LSR2-123-TM-C
2 Solvent	cdcl3
3 Relaxation Delay	1.0000
4 Spectrometer Frequency	100.53

148.76
142.32
129.31
109.78
64.41
32.34
29.80
28.35
26.53
26.30



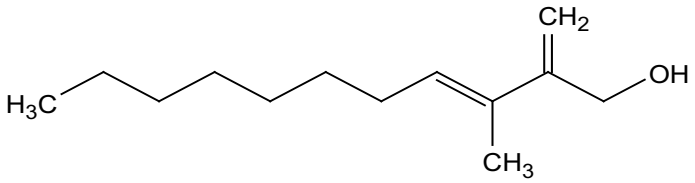


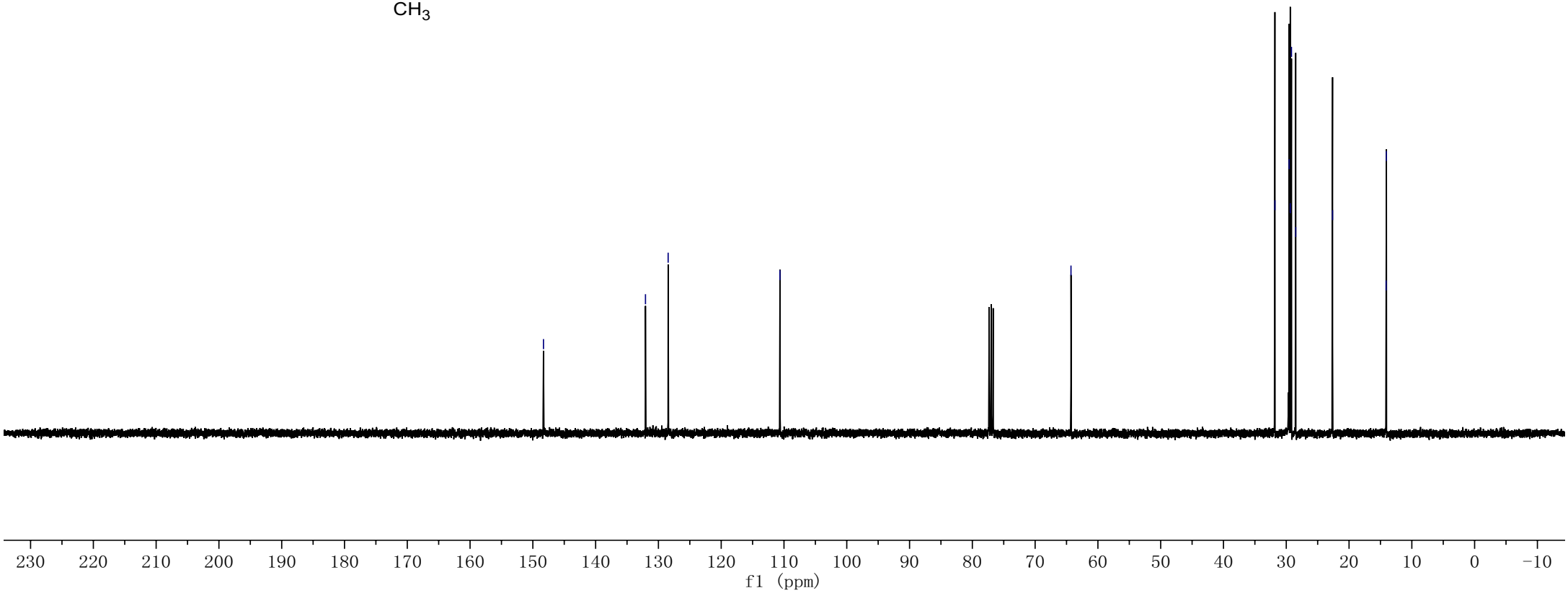
Parameter	Value
1 Title	LSR2-73-TM1
2 Solvent	cdcl3
3 Relaxation Delay	4.8000
4 Spectrometer Frequency	399.78



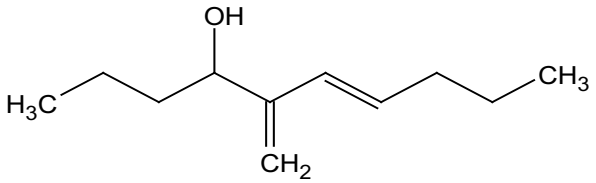
Parameter	Value
1 Title	LSR2-73-TM1-C
2 Solvent	cdcl3
3 Relaxation Delay	1.0000
4 Spectrometer Frequency	100.53

148.31
132.06
128.45
110.65
64.29
31.81
29.54
29.36
29.17
28.50
22.63
14.09
14.05



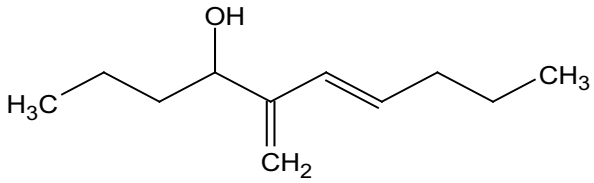


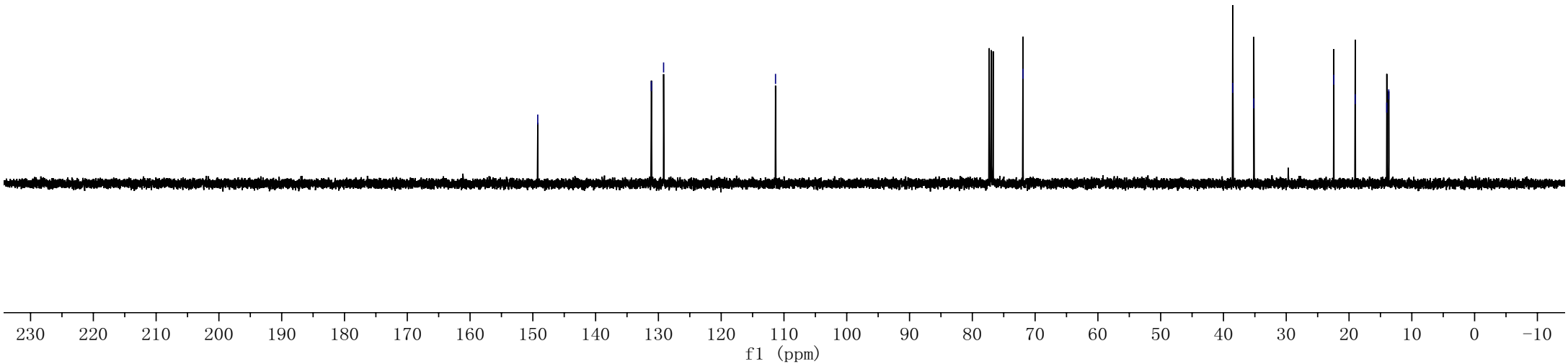
Parameter	Value
1 Title	LSR1-282-1-3
2 Solvent	cdcl3
3 Relaxation Delay	4.8000
4 Spectrometer Frequency	399.78



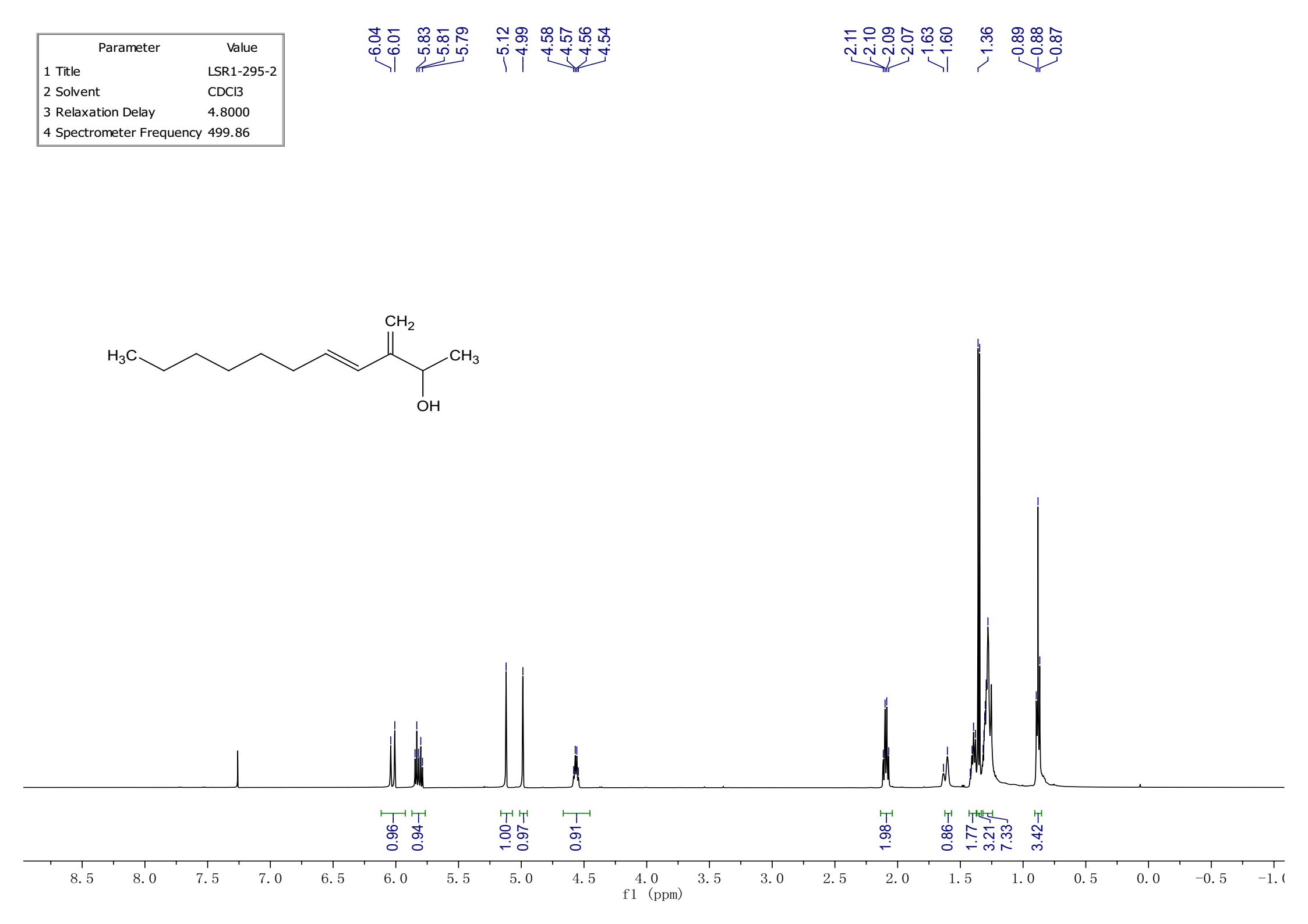
Parameter	Value
1 Title	LSR1-282-1-3C
2 Solvent	cdcl3
3 Relaxation Delay	1.0000
4 Spectrometer Frequency	100.53

149.22
131.12
129.17
111.35
71.93
38.53
35.18
22.43
19.02
13.99
13.68



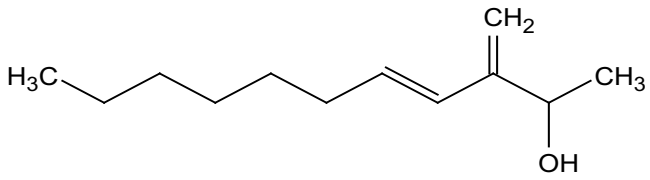


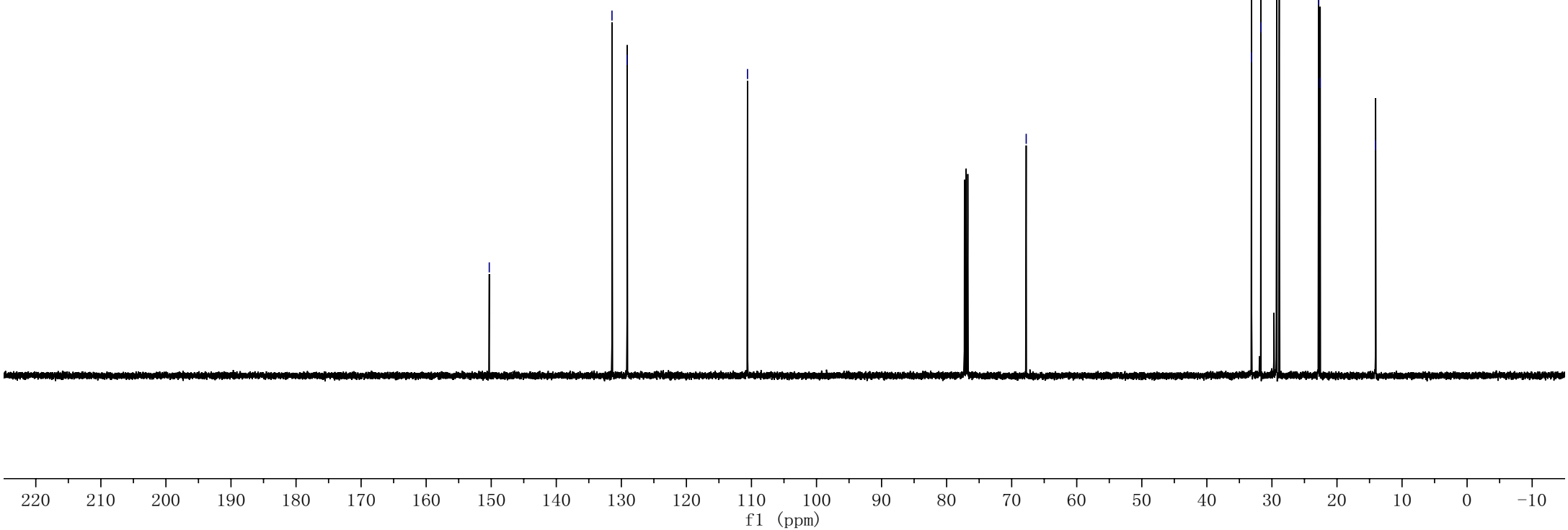
Parameter	Value
1 Title	LSR1-295-2
2 Solvent	CDCl3
3 Relaxation Delay	4.8000
4 Spectrometer Frequency	499.86



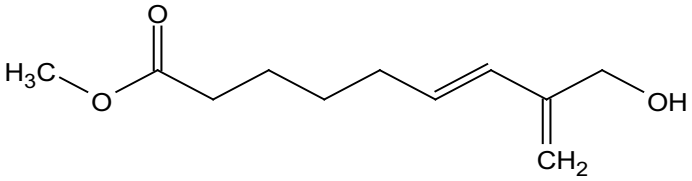
Parameter	Value
1 Title	LSR1-295-2C
2 Solvent	CDCl3
3 Relaxation Delay	1.0000
4 Spectrometer Frequency	125.70

150.30
131.44
129.10
110.61
67.77
33.13
31.69
29.24
28.87
22.81
22.59
14.06



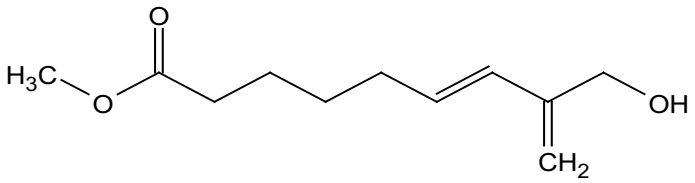


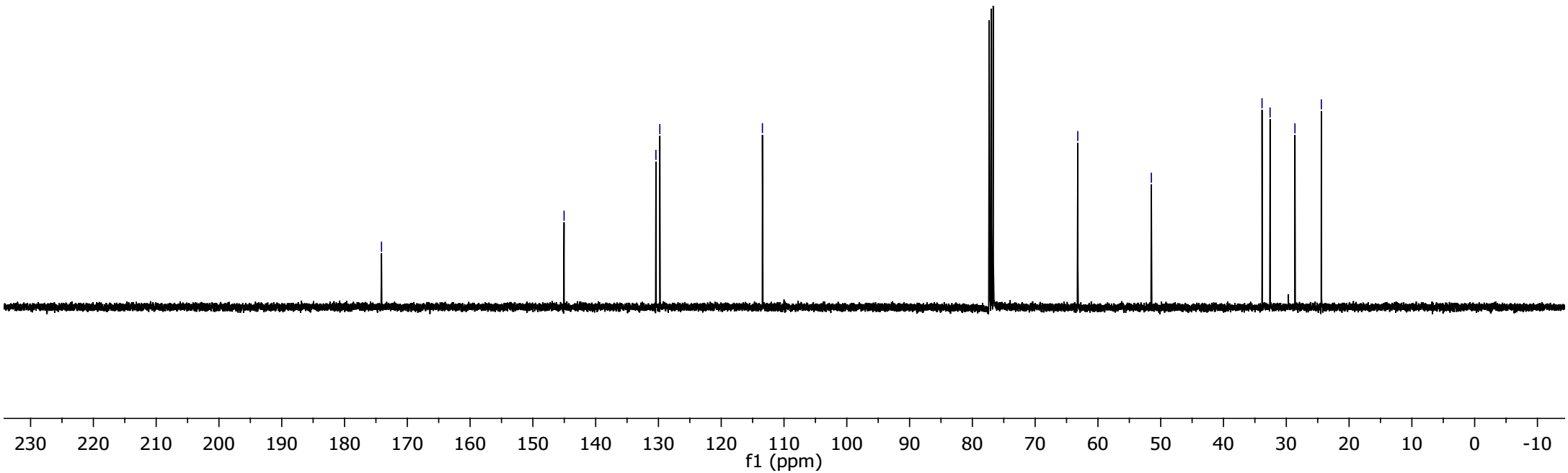
Parameter	Value
1 Title	LSR2-135-TM3
2 Solvent	cdcl3
3 Relaxation Delay	4.8000
4 Spectrometer Frequency	399.78



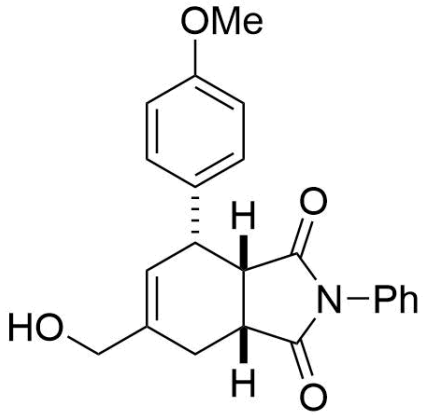
Parameter	Value
1 Title	LSR2-135-TM3-C
2 Solvent	cdcl3
3 Relaxation Delay	1.0000
4 Spectrometer Frequency	100.53

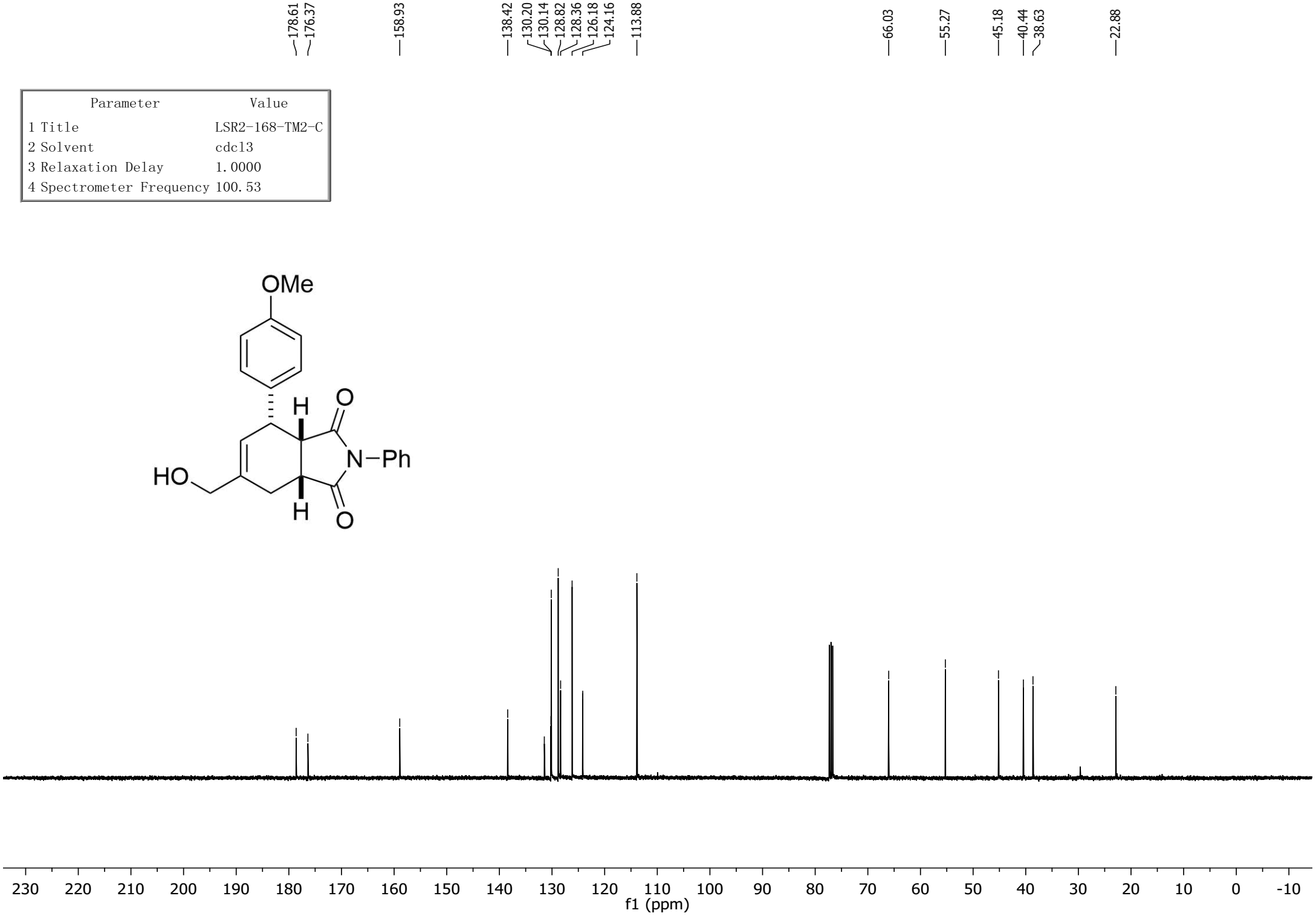
174.11
145.03
130.40
129.78
113.44
63.21
51.49
33.86
32.58
28.62
24.42

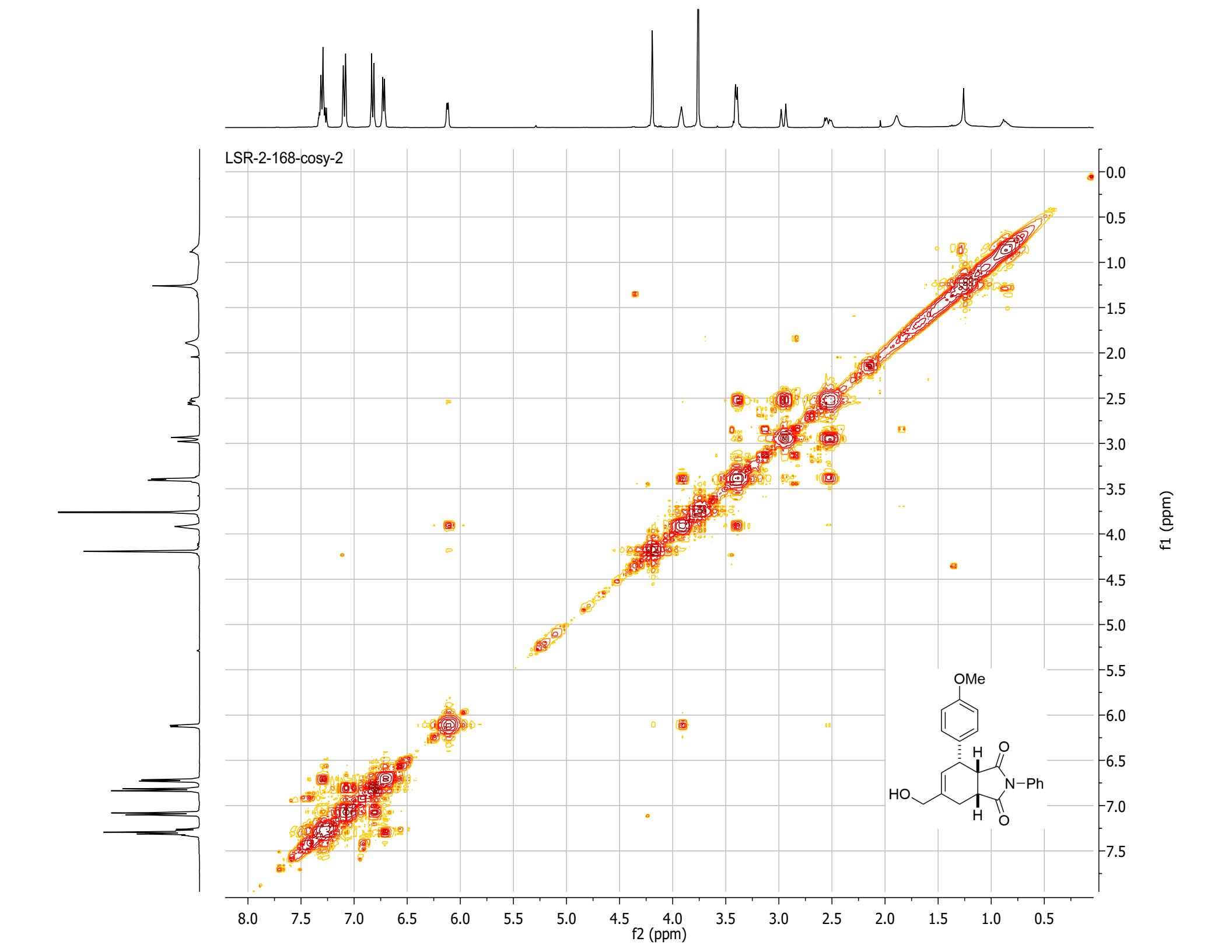


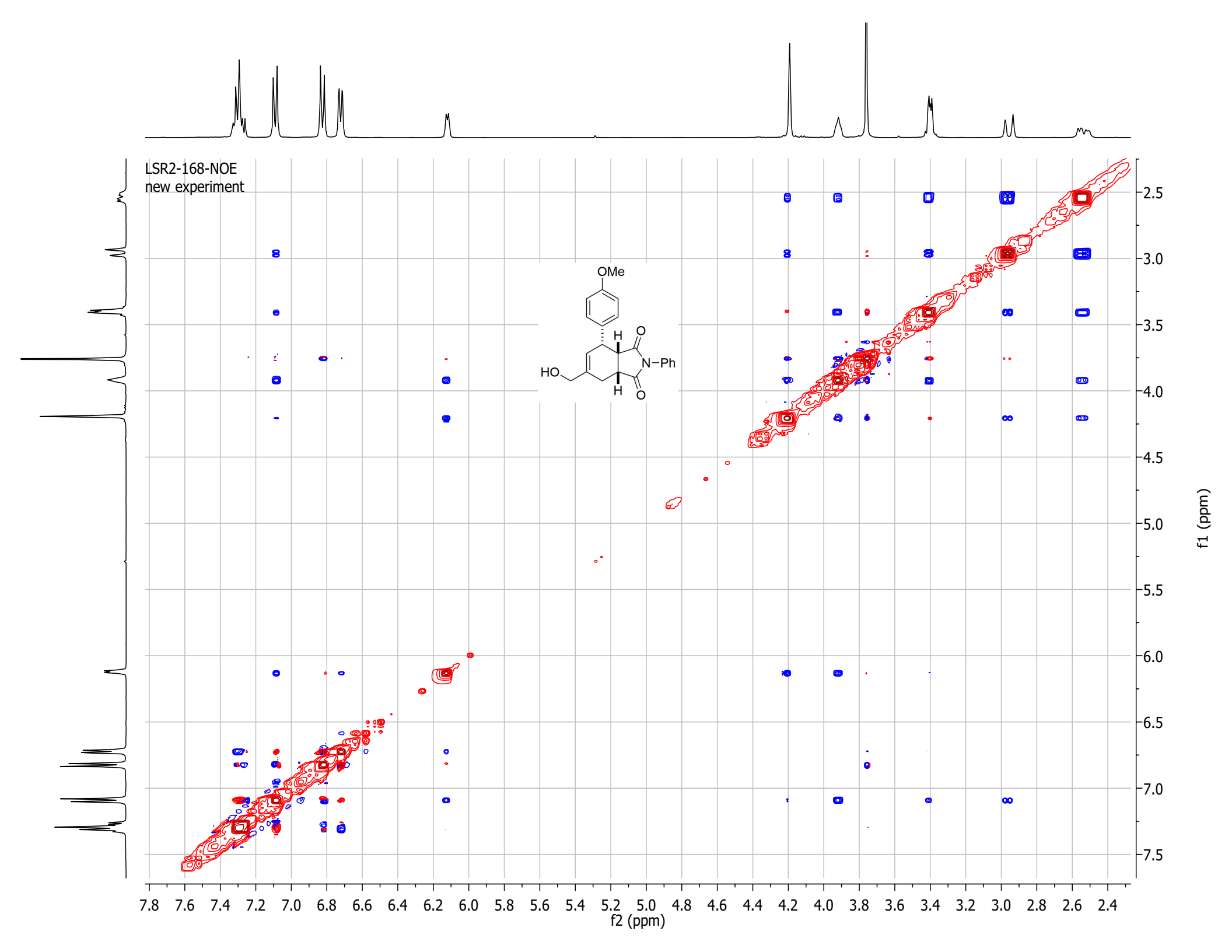


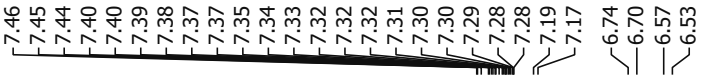
Parameter	Value
1 Title	LSR2-168-TM2
2 Solvent	cdcl3
3 Relaxation Delay	4.8000
4 Spectrometer Frequency	399.78



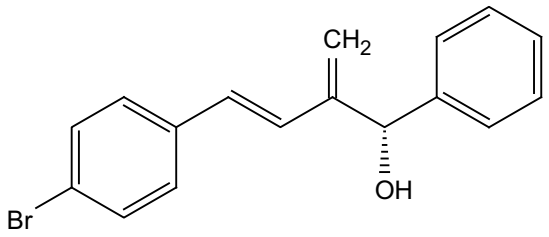

178.61
176.37
158.93
138.42
130.20
130.14
128.82
128.36
126.18
124.16
113.88
66.03
55.27
45.18
40.44
38.63
22.88
Parameter Value
1 Title LSR2-168-TM2-C
2 Solvent cdcl3
3 Relaxation Delay 1.0000
4 Spectrometer Frequency 100.53
OMe
H
O
N−Ph
HO
H
O
230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

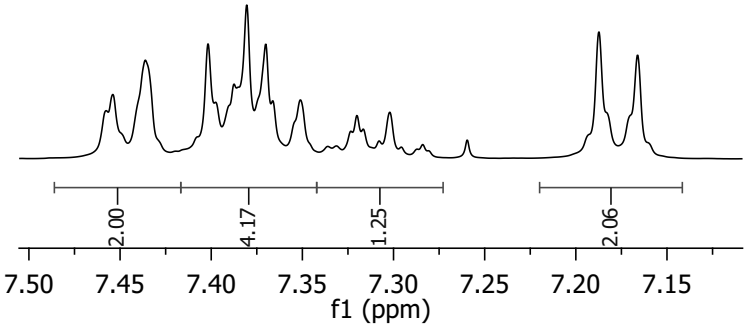

LSR-2-168-cosy-2
f2 (ppm)
f1 (ppm)
OMe
HO
N–Ph
O
H
H

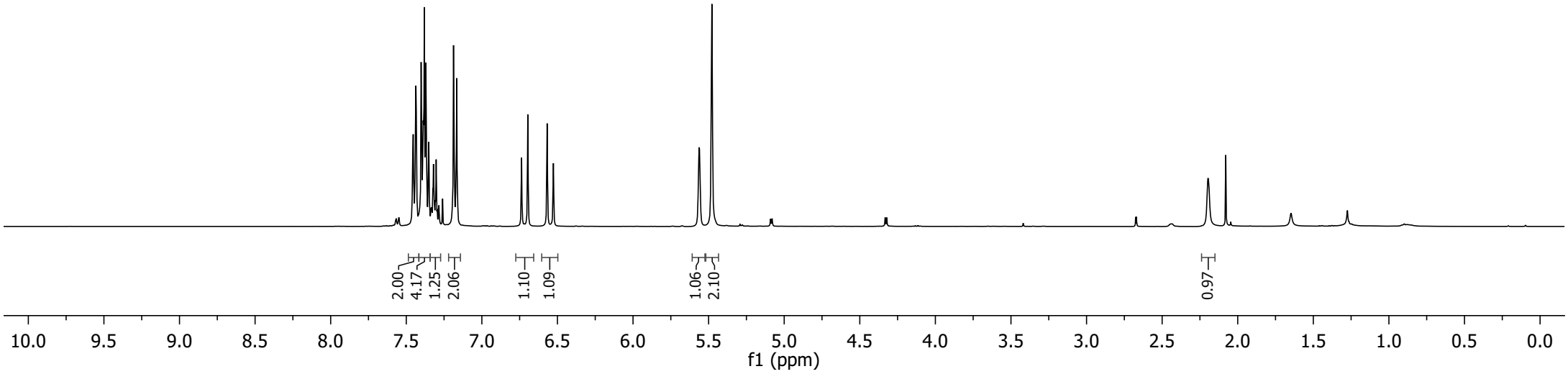

LSR2-168-NOE
new experiment
OMe
H
O
N–Ph
HO
H
O
7.8 7.6 7.4 7.2 7.0 6.8 6.6 6.4 6.2 6.0 5.8 5.6 5.4 5.2 5.0 4.8 4.6 4.4 4.2 4.0 3.8 3.6 3.4 3.2 3.0 2.8 2.6 2.4
f2 (ppm)
2.5 3.0 3.5 4.0 4.5 5.0 5.5 6.0 6.5 7.0 7.5
f1 (ppm)



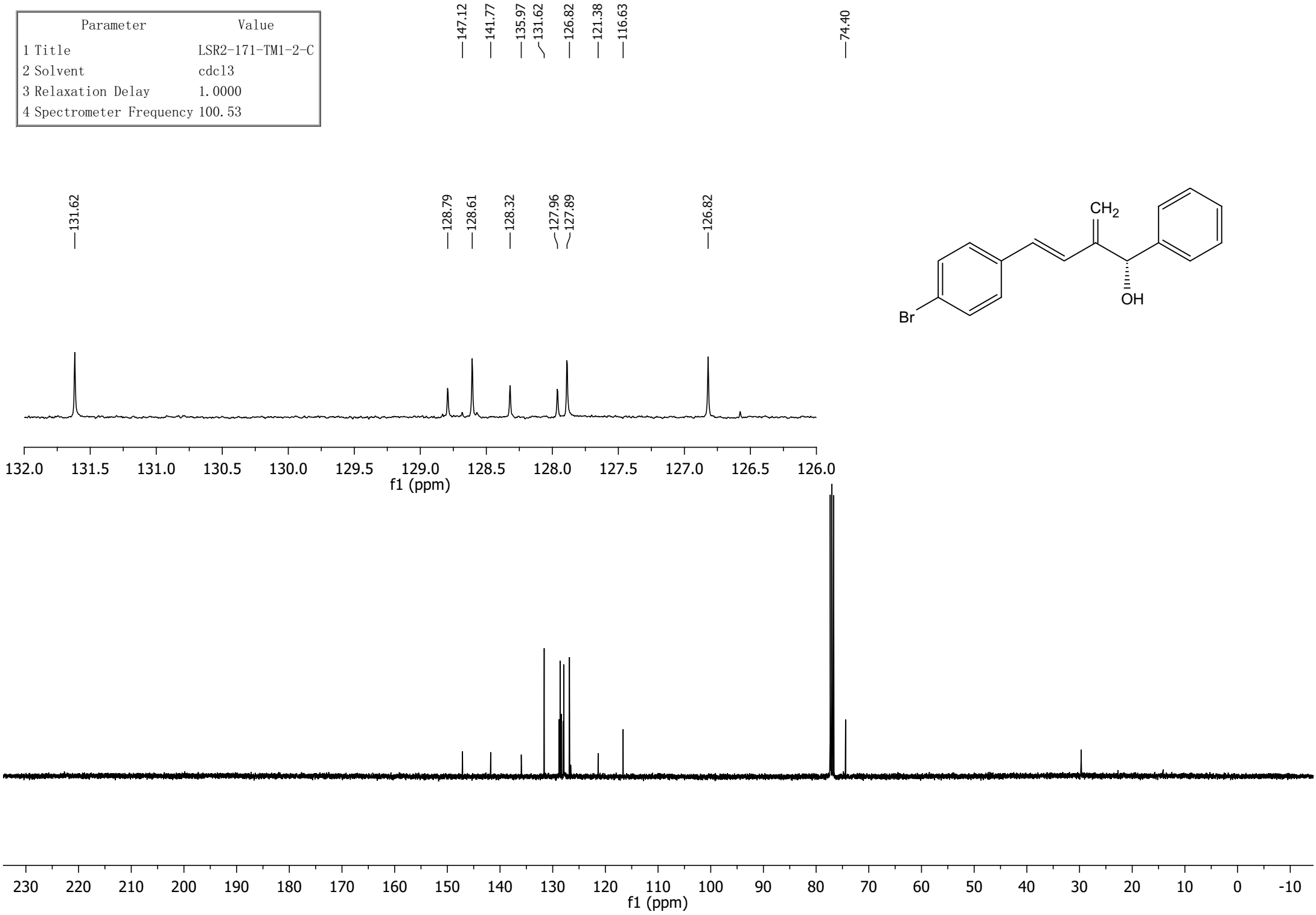
Parameter	Value
1 Title	LSR2-171-TM1
2 Solvent	cdcl3
3 Relaxation Delay	4.8000
4 Spectrometer Frequency	399.78



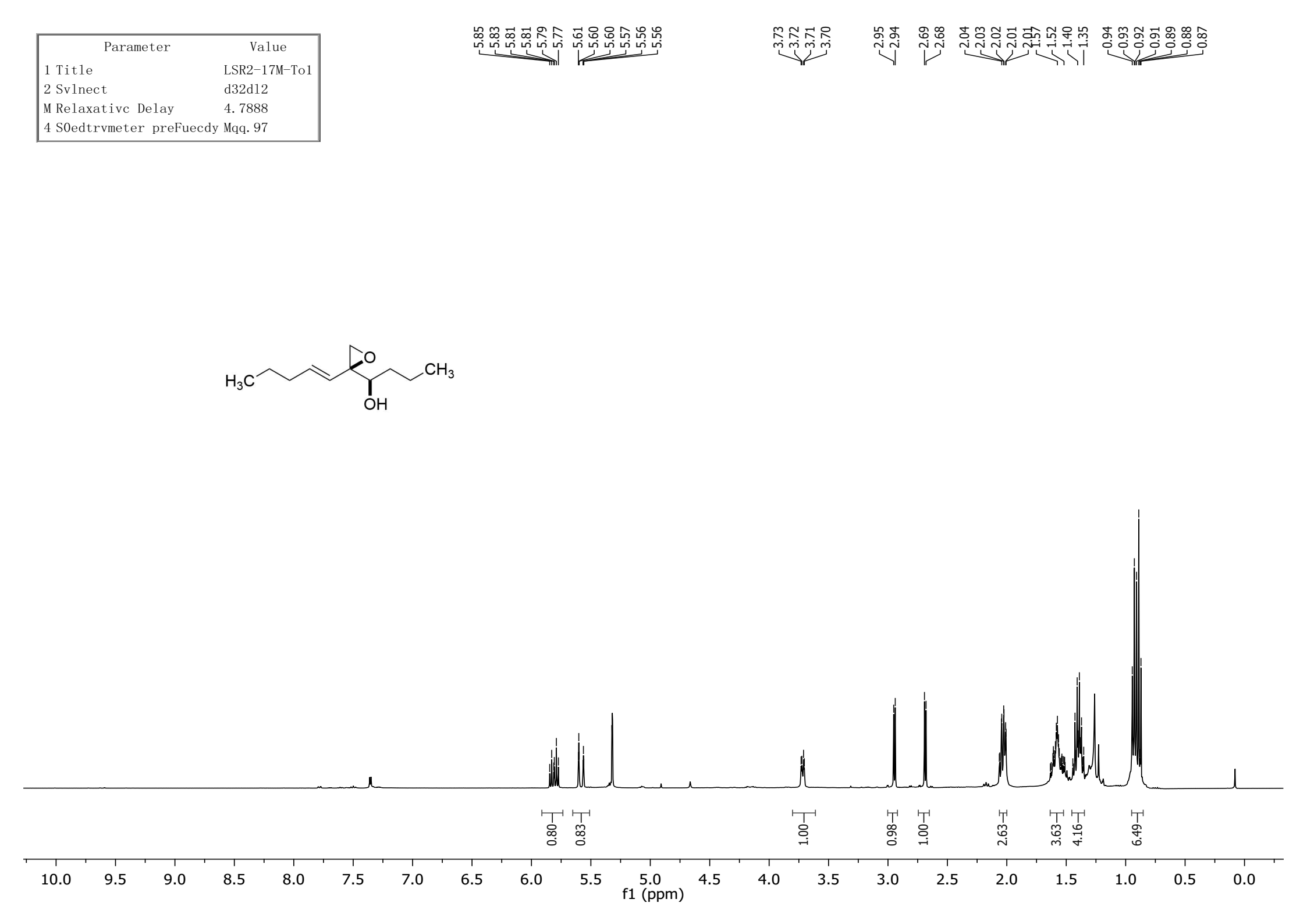




Parameter	Value
1 Title	LSR2-171-TM1-2-C
2 Solvent	cdcl3
3 Relaxation Delay	1.0000
4 Spectrometer Frequency	100.53



Parameter	Value
1 Title	LSR2-17M-To1
2 Svlnect	d32d12
M Relaxativc Delay	4.7888
4 SOedtrvmeter preFuecdy	Mqq.97



Parameter	Value
1 Title	LSR2-17M-To1-C
2 Svlnect	d32dl2
M Relaxativc Delay	1.8888
4 SOedtrvmeter preFuecdy	188.54