Supporting Information

General

^{1}H, ^{13}C, ^{31}P and ^{19}F spectra were recorded on Varian 400, 500 or 600 MHz spectrometers, and ^{11}B spectra were on an Inova 500 MHz spectrometer at ambient temperature. ^{1}H NMR spectra were reported with the solvent resonance as internal standard. ^{13}C NMR spectra were reported with the solvent resonance as internal standard. ^{11}B NMR spectra were reported with $BF_3 \cdot Et_2O$ (δ 0 ppm) as the external reference. ^{31}P NMR spectra were reported with H_3PO_4 (δ 0 ppm) as the external reference. IR spectra were recorded on a Bruker FTIP Alpha (ATR mode) spectrometer. High-resolution mass spectroscopy data were obtained at the Mass Spectroscopy Facilities at Chemistry Department of Boston College with DART ion source in positive ion mode.

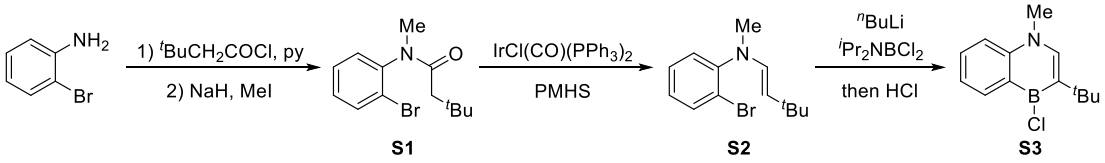
All oxygen- and moisture-sensitive manipulations were carried out under N_2 atmosphere with standard Schlenk techniques or in N_2 glovebox.

Hexanes were purified by distillation before using in column chromatography. Solvents used under N_2 atmosphere (pentane, THF, benzene and CH_2Cl_2) were purified by passing through a neutral alumina column under argon. 1,8-diaminonaphthlene (dan) was purified by distillation under attenuated pressure followed by recrystallization with hexanes/EtOAc. 1, 2-dichlorobenzene (*o*-DCB) was purified by drying with CaH_2 and subsequent distillation under attenuated pressure. Ligand **L5** was prepared according to literature procedures.[1] All other chemicals and solvents were purchased and used as received.

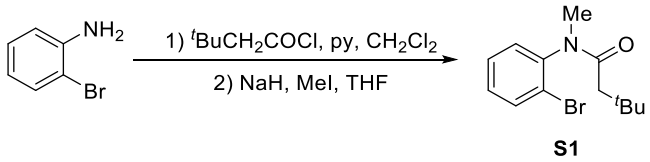
Preparation of Ligand L1 to L4 and CC-L1

Synthesis of ^{t}butyl-substituted 1,4-azaborine precursor S3:

Reaction sequence:



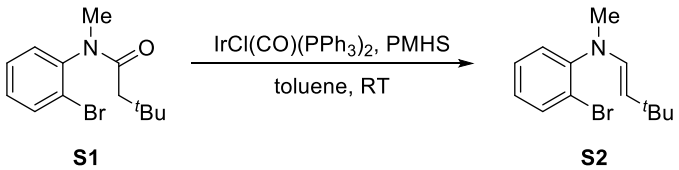
Step 1:



To a solution of 2-bromoaniline (5.10 g, 30.0 mmol, 1.00 equiv.) in CH_2Cl_2 (100 mL) and pyridine (2.50 g, 31.5 mmol, 1.05 equiv.) ^{t}butylacetyl chloride (4.24 g, 31.5 mmol, 1.05 equiv.) was added in a dropwise fashion at 0 °C, and the mixture was allowed to stir for 4 hours. At the conclusion of reaction, H_2O (60 mL) was added, and the organic layer was separated, which was further washed with brine (60 mL) and dried with Na_2SO_4. Removing of all volatiles *in vacuo* resulted in a white solid, which is used for next step without further purification. Then, THF (80 mL) and NaH (1.80 g, 60% in oil, 45.0 mmol, 1.50 equiv.) was added in 5 portions in 20 minutes. The resulting mixture was allowed to stir for another 30 minutes at room temperature, followed by the addition of MeI (6.40 g, 45.0 mmol, 1.50 equiv.). After allowing the mixture to stir for 2 hours, H_2O (60 mL) along with Et_2O (30 mL) were added to the reaction mixture. The organic layer was separated and washed with brine (50 mL) and dried with Na_2SO_4. After removing all volatiles, **S1** was obtained by distillation under attenuated pressure (130 °C, 250 mmTor) as a white solid (88% yield).

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.66 (dt, *J* = 8.0, 1.5 Hz, 1H), 7.37 (tt, *J* = 7.5, 1.3Hz, 1H), 7.25 – 7.19 (m, 2H), 3.16 (d, *J* = 1.6 Hz, 3H), 1.89 (t, *J* = 1.1Hz, 2H), 0.97 (d, *J* = 1.7 Hz, 9H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 171.8, 143.4, 133.9, 130.2, 129.5, 128.9, 123.6, 45.6, 35.8, 31.2, 29.9; IR (ATR) 2952, 2866, 1661, 1475, 1433, 1372, 1361, 1280, 1249, 1117, 1064, 1030, 765, 728, 690, 568, 457 cm^{-1}; HRMS (DART) calcd for $C_{13}H_{19}NOBr$ ($[M+H]^+$) 284.06445, found 284.06500.

Step 2:

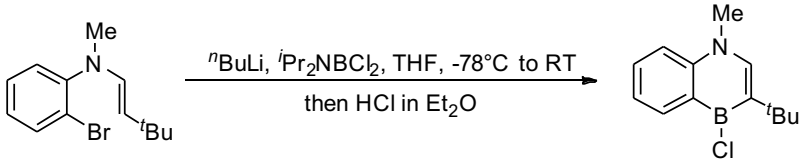


To a 250-mL round bottom flask charged with **S1** (2.80 g, 10.0 mmol, 1.00 equiv.), toluene (30 mL), and PMHS (polymethylhydrosiloxane) (2.60 g, MW 1700-3200, 40.0 mmol, 4.00 equiv.), was added a solution of $IrCl(CO)(PPh_3)_2$ (4 mg, 0.005 mmol, 0.0005 equiv) in toluene (5 mL) in a dropwise fashion under nitrogen at room temperature. Gelation was observed, and the reaction mixture was allowed to stir for another 30 minutes. Et_2O (60 mL) was added, and the mixture was passed through a celite pad. The filter cake was further washed with Et_2O (30 mL) for two times, and the filtrate was combined. All volatiles

were then removed under vacuum and **S2** was obtained by distillation under attenuated pressure (95 °C, 280 mmTor) as a colorless liquid (90% yield).

^{1}H NMR (600 MHz, $CDCl_3$) δ 7.57 (dd, *J* = 8.0, 1.5 Hz, 1H), 7.26 (tdd, *J* = 7.2, 1.6, 0.6 Hz, 1H), 7.09 (dd, *J* = 8.0, 1.6 Hz, 1H), 6.97 (tdd, *J* = 7.2, 1.6, 0.6 Hz, 1H), 6.15 (d, *J* = 14.1 Hz, 1H), 4.64 (d, *J* = 14.1 Hz, 1H), 2.98 (s, 3H), 1.08 (s, 9H); ^{13}C NMR (151 MHz, $CDCl_3$) δ 148.8, 134.0, 132.9, 128.3, 126.3, 125.5, 119.9, 115.2, 38.4, 31.9, 31.3; IR (ATR) 2952, 2900, 2864, 1650, 1584, 1481, 1461, 1420, 1356, 1320, 1251, 1238, 1129, 1117, 1026, 981, 937, 753, 723, 656, 446 cm^{-1}; HRMS (DART) calcd for $C_{13}H_{19}NBr$ ([M+H]$^+$) 268.06954, found 268.06955.

Step 3:

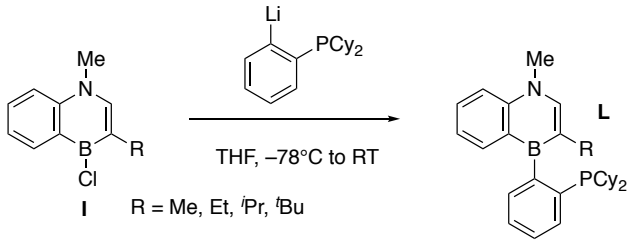


S2 **S3**

To a 100-mL round bottom flask charged with **S2** (2.42 g, 9.02 mmol, 1.00 equiv.) and THF (30 mL), was added ^{n}butyl lithium (3.60 mL, 2.50 M in hexanes, 9.00 mmol, 1.00 equiv.) at –78°C. After allowing the mixture to stir at –78 °C for 20 minutes, a solution of ^{i}Pr$_2$NBCl$_2$ (1.64 g, 9.00 mmol, 1.00 equiv.) in THF (3 mL) was added. The resulting reaction mixture was allowed to warm to room temperature in 2 hours. Then, HCl (4.5 mL, 2.0 M in Et_2O, 9.0 mmol, 1.0 equiv.) was added, and the mixture was allowed to stir for an hour. At the conclusion of the reaction, the formed precipitate was filtered off, and the filtrate was concentrated. The resulting crude material was purified by recrystallization from pentane/CH_2Cl_2 to furnish **S3** as white crystals (36% yield).

^{1}H NMR (500 MHz, $CDCl_3$) δ 8.55 (dd, *J* = 7.9, 1.7 Hz, 1H), 7.78 (s, 1H), 7.69 (ddd, *J* = 8.6, 6.9, 1.7 Hz, 1H), 7.46 (d, *J* = 8.6 Hz, 1H), 7.35 (ddd, *J* = 7.9, 6.9, 1.0 Hz, 1H), 3.89 (s, 3H), 1.50 (s, 9H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 145.8, 143.2, 134.0, 133.7 (br), 131.6, 128.4 (br), 121.4, 114.6, 42.4, 34.9, 31.0; ^{11}B NMR (160 MHz, $CDCl_3$) δ 44.4; HRMS (DART) calcd for $C_{13}H_{18}BNCl$ ([M+H]$^+$) 234.12153, found 234.12340.

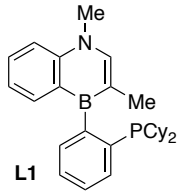
General Procedure for the Synthesis of Ligand L1 to L4:



I R = Me, Et, ^{i}Pr, ^{t}Bu

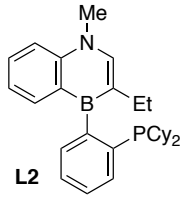
N-Me-*B*-Cl-1,4-Azaborines **I** where R = Me, Et, ^{i}Pr were synthesized according to previous literature.[1]

To a 100-mL round bottom flask charged with 2-bromophenyl dicyclohexylphosphine (706 mg, 2.00 mmol, 1.00 equiv.) and Et_2O (15 mL) was added ^{n}butyllithium (0.80 mL, 2.5 M in hexanes, 2.0 mmol, 1.0 equiv.) at –78 °C. After allowing the mixture to stir at –78 °C for an hour, the corresponding 1,4-azaborine **I** (2.0 mmol, 1.0 equiv.) in THF (3 mL) was added, and the resulting mixture was allowed to warm to room temperature in 2 hours. At the conclusion of reaction, all volatiles were removed under vacuum, and the crude residue was purified by silica gel chromatography under inert atmosphere using pentane/Et_2O (20/1 to 10/1 gradient) as the eluent to afford the desired ligand as white solids.



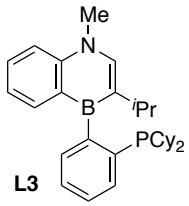
L1

L1, 42% yield. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.74 (dd, *J* = 7.8, 1.6 Hz, 1H), 7.67 (s, 1H), 7.61 – 7.55 (m, 2H), 7.48 (d, *J* = 8.6 Hz, 1H), 7.40 – 7.31 (m, 2H), 7.28 – 7.24 (m, 1H), 7.13 (ddd, *J* = 7.8, 6.8, 0.9 Hz, 1H), 3.90 (s, 3H), 2.06 (d, *J* = 0.9 Hz, 3H), 2.01 (ddd, *J* = 11.1, 5.1, 3.0 Hz, 1H), 1.81 – 1.59 (m, 8H), 1.60 – 1.48 (m, 2H), 1.47 – 0.78 (m, 11H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 146.6, 143.2, 137.6, 137.3 (d, *J* = 11.0 Hz), 131.7 (d, *J* = 15.4 Hz), 131.7 (d, *J* = 2.6 Hz), 130.8 (br), 130.4, 127.5, 125.6, 122.9 (br), 120.2, 114.3, 42.0, 35.1 (d, *J* = 13.7 Hz), 33.6 (d, *J* = 12.4 Hz), 30.7 (d, *J* = 14.2 Hz), 30.3 (d, *J* = 15.9 Hz), 30.0 (d, *J* = 10.6 Hz), 29.2 (d, *J* = 6.0 Hz), 27.7, 27.6 (d, *J* = 6.4 Hz), 27.6, 27.5 (d, *J* = 3.6 Hz), 26.7, 26.6, 19.6 (d, *J* = 4.3 Hz) (one signal of aromatic carbon attached to boron is not observed); ^{11}B NMR (160 MHz, $CDCl_3$) δ 47.3; ^{31}P NMR (202 MHz, $CDCl_3$) δ –3.2; IR (ATR) 3039, 2922, 2849, 1605, 1586, 1491, 1447, 1369, 1269, 1225, 1102, 908, 891, 764, 732, 647 cm^{-1}; HRMS (DART) calcd for $C_{28}H_{38}BNP$ ([M+H]$^+$) 430.28294, found 430.28290.



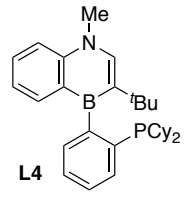
L2

L2, 36% yield. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.71 (dd, *J* = 7.8, 1.7 Hz, 1H), 7.65 (s, 1H), 7.62 – 7.54 (m, 2H), 7.47 (d, *J* = 8.6 Hz, 1H), 7.39 – 7.29 (m, 2H), 7.29 (dd, *J* = 5.5, 3.2 Hz, 1H), 7.11 (t, *J* = 7.3 Hz, 1H), 3.92 (s, 3H), 2.55 (dq, *J* = 14.8, 7.5 Hz, 1H), 2.35 (dq, *J* = 14.7, 7.5 Hz, 1H), 2.08 – 1.94 (m, 1H), 1.79 – 1.59 (m, 8H), 1.57 – 0.79 (m, 16H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 146.0, 143.2, 137.6, 137.2 (d, *J* = 11.0 Hz), 132.2 (d, *J* = 15.4 Hz), 131.7 (d, *J* = 2.5 Hz), 130.5, 127.3, 125.6, 120.1, 114.3, 42.1, 35.3 (d, *J* = 13.8 Hz), 33.5 (d, *J* = 12.3 Hz), 30.7 (d, *J* = 14.0 Hz), 30.3 (d, *J* = 15.9 Hz), 30.0 (d, *J* = 11.3 Hz), 29.1 (d, *J* = 5.7 Hz), 27.7, 27.6 (d, *J* = 1.5 Hz), 27.6 (d, *J* = 3.7 Hz), 27.5 (d, *J* = 8.6 Hz), 26.8, 26.6 (d, *J* = 4.3 Hz), 26.6, 16.5 (three signals of aromatic carbons attached to boron are not observed); ^{11}B NMR (160 MHz, $CDCl_3$) δ 47.1; ^{31}P NMR (202 MHz, $CDCl_3$) δ –3.6; IR (ATR) 3040, 2924, 2850, 1604, 1585, 1491, 1448, 1375, 1266, 1223, 1105, 912, 764, 750, 733, 663 cm^{-1}; HRMS (DART) calcd for $C_{29}H_{40}BNP$ ([M+H]$^+$) 444.29859, found 444.29726.



L3

L3, 48% yield. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.71 – 7.64 (m, 2H), 7.62 – 7.53 (m, 2H), 7.47 (d, *J* = 8.6 Hz, 1H), 7.40 – 7.29 (m, 3H), 7.10 (t, *J* = 7.3 Hz, 1H), 3.93 (s, 3H), 2.89 (hept, *J* = 7.2 Hz, 1H), 1.96 (tt, *J* = 12.1, 3.5 Hz, 1H), 1.80 – 1.59 (m, 8H), 1.56 (d, *J* = 9.0 Hz, 3H), 1.43 (d, *J* = 13.2 Hz, 1H), 1.34 – 0.79 (m, 15H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 144.3, 143.1, 137.7, 137.5 (d, *J* = 11.0 Hz), 134.9 (br), 132.1 (d, *J* = 15.3 Hz), 131.8 (d, *J* = 2.8 Hz), 131.3 (br), 130.5, 127.3, 125.6, 120.1, 114.3, 42.4, 35.2 (d, *J* = 14.0 Hz), 34.1 (d, *J* = 12.9 Hz), 30.6 (d, *J* = 14.2 Hz), 30.4 (d, *J* = 16.0 Hz), 29.9 (d, *J* = 10.3 Hz), 29.7 (d, *J* = 2.4 Hz), 29.3 (d, *J* = 6.7 Hz), 27.7, 27.6, 27.5, 27.5, 27.1, 26.7, 26.6, 22.7 (one signal of the aromatic carbon attached to boron is not observed); ^{11}B NMR (160 MHz, $CDCl_3$) δ 47.5; ^{31}P NMR (202 MHz, $CDCl_3$) δ –4.3; IR (ATR) 3039, 2923, 2849, 1605, 1585, 1491, 1457, 1428, 1383, 1372, 1265, 1223, 908, 765, 750, 733, 667 cm^{-1}; HRMS (DART) calcd for $C_{30}H_{42}BNP$ ([M+H]$^+$) 458.31424, found 458.31565.



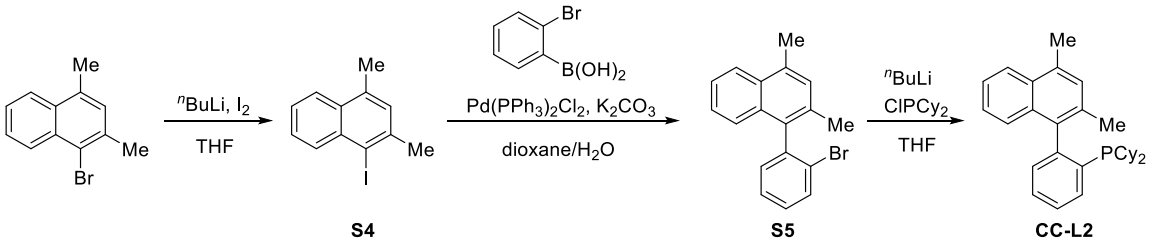
L4

L4, 38% yield. ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.83 (s, 1H), 7.57 – 7.49 (m, 2H), 7.46 – 7.37 (m, 3H), 7.36 – 7.28 (m, 2H), 7.04 (ddd, *J* = 7.9, 6.8, 1.0 Hz, 1H), 3.93 (s, 3H), 2.10 (tdd, *J* = 11.1, 6.7, 3.1 Hz, 1H), 1.83 – 0.70 (m, 30H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 145.1, 142.1, 138.8 (d, *J* = 9.7 Hz), 138.1, 132.2 (d, *J* = 14.9 Hz), 131.2 (d, *J* = 2.3 Hz), 130.5, 126.5, 125.2, 119.9, 113.8, 42.5, 36.0 (d, *J* = 14.7 Hz), 35.9, 33.6 (d, *J* =

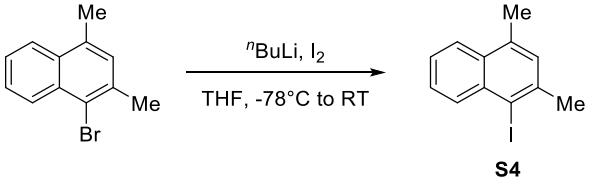
14.1 Hz), 33.0 (d, *J* = 1.6 Hz), 32.0 (d, *J* = 16.6 Hz), 31.1 (d, *J* = 13.3 Hz), 30.5 (d, *J* = 15.7 Hz), 28.3 (d, *J* = 4.9 Hz), 28.0 (d, *J* = 2.0 Hz), 27.9 (d, *J* = 3.4 Hz), 27.8, 27.4 (d, *J* = 10.1 Hz), 26.7, 26.6 (three signals of aromatic carbon attached to boron are not observed); ^{11}B NMR (160 MHz, $CDCl_3$) δ 47.3; ^{31}P NMR (202 MHz, $CDCl_3$) δ –3.4; IR (ATR) 3039, 2920, 2849, 1604, 1581, 1490, 1459, 1447, 1390, 1376, 1264, 1220, 1086, 918, 765, 742, 669 cm^{-1}; HRMS (DART) calcd for $C_{31}H_{44}BNP$ ([M+H]$^+$) 472.32989, found 472.32950.

Synthesis of ligand CC-L1

Reaction sequence:

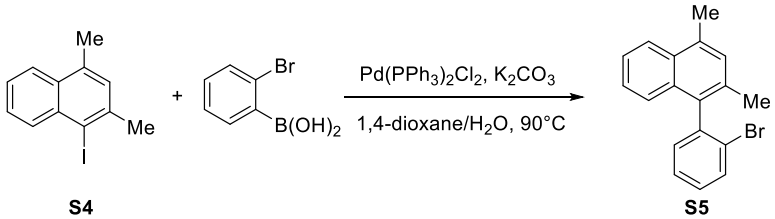


Step 1:



^{n}Butyllithium (1.30 mL, 2.50 M in hexanes, 3.24 mmol, 1.20 equiv.) was added in a dropwise fashion into a 20-mL vial charged with a solution 1-bromo-2,4-dimethylnaphthalene (634 mg, 2.70 mmol, 1.00 equiv., synthesized according to previous literature[2].) in THF (12 mL) at –78 °C. The resulting mixture was allowed to stir for 30 minutes at the same temperature. Then a solution of I_2 (1.35 g, 5.40 mmol, 2.00 equiv.) in THF (3 mL) was added to the reaction mixture, and the resulting mixture was gradually allowed to warm to room temperature in 2 hours. At the conclusion of the reaction, THF was removed, and the residue was taken up in Et_2O (15 mL) and washed with saturated $Na_2S_2O_3$ (10 mL) and H_2O (10 mL). The organic layer was then concentrated under reduced pressure, and the crude material was purified via silica gel chromatography using hexanes as the eluent to afford **S4** as a colorless liquid (88% yield). ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.33 – 8.24 (m, 1H), 7.92 (dd, *J* = 8.3, 1.6 Hz, 1H), 7.58 (ddd, *J* = 8.4, 6.8, 1.3 Hz, 1H), 7.52 (td, *J* = 6.8, 1.4 Hz, 1H), 7.24 (s, 1H), 2.69 (s, 3H), 2.65 (d, *J* = 2.0 Hz, 3H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 140.4, 135.0, 134.6, 132.9, 131.8, 129.2, 127.4, 125.7, 124.4, 103.3, 30.3, 19.2; IR (ATR) 3060, 3007, 2917, 1600, 1510, 1475, 1432, 1387, 1379, 1049, 1026, 875, 752, 731, 709, 669, 655, 453 cm^{-1}; HRMS (DART) calcd for $C_{12}H_{11}I$ ([M]$^+$) 281.98999, found 281.99087.

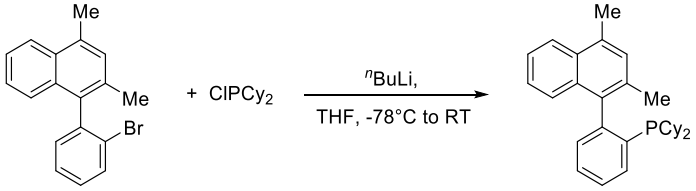
Step 2:



A 20-mL vial was charged with $Pd(PPh_3)_2Cl_2$ (16.5 mg, 0.0235 mmol, 0.0500 equiv.), potassium carbonate (130 mg, 0.940 mmol, 2.00 equiv.) and (2-bromophenyl)boronic acid (104 mg, 0.517 mmol, 1.10 equiv.) under nitrogen. To this mixture 1,4-dioxane (3.5 mL), H_2O (0.5 mL) and **S4** (134 mg, 0.470 mmol, 1.00 equiv.) were added, and the reaction mixture was allowed to stir at 90 °C for 3 hours. At the conclusion of the reaction, Et_2O (5 mL) and H_2O (2 mL) were added to the mixture. The organic layer was separated and the aqueous layer was extracted with Et_2O (10 mL). The combined organic layers were concentrated under reduced pressure. The resulting crude material was purified via silica gel chromatography using hexanes as the eluent to afford **S5** as a colorless liquid (68% yield).

^{1}H NMR (500 MHz, $CDCl_3$) δ 8.07 (dt, *J* = 8.5, 1.0 Hz, 1H), 7.81 (dd, *J* = 8.1, 1.3 Hz, 1H), 7.49 (dtd, *J* = 18.1, 7.1, 1.3 Hz, 2H), 7.41 (ddd, *J* = 8.2, 6.7, 1.3 Hz, 1H), 7.37 – 7.32 (m, 2H), 7.29 (td, *J* = 7.2, 1.4 Hz, 2H), 2.78 (d, *J* = 1.0 Hz, 3H), 2.22 (s, 3H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 140.9, 135.5, 134.2, 133.2, 132.9, 132.4, 132.1, 131.1, 129.5, 129.0, 127.6, 126.1, 125.9, 125.1, 124.9, 124.2, 20.3, 19.6; IR (ATR) 2967, 2943, 2913, 2856, 1599, 1555, 1503, 1438, 1326, 1263, 1026, 961, 884, 867, 747, 639, 567, 417 cm^{-1}; HRMS (DART) calcd for $C_{18}H_{16}Br$ ([M+H]$^+$) 311.04299, found 311.04305.

Step 3:



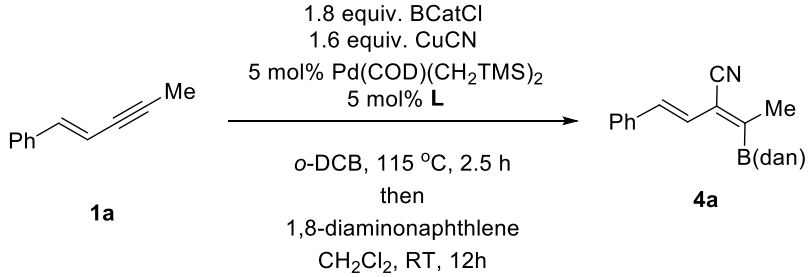
S5 **CC-L1**

To a 20-mL vial charged with **S5** (99 mg, 0.32 mmol, 1.0 equiv.) and THF (2 mL) was added *n*butyllithium (0.15 mL, 2.5 M in hexanes, 0.38 mmol, 1.2 equiv.) at –78 °C. The mixture was allowed to stir at –78 °C for 30 minutes, then a solution of chlorodicyclohexylphosphine (89 mg, 0.38 mmol, 1.2 equiv.) in THF (1 mL) was added. The resulting mixture was gradually allowed to warm to room temperature in 2 hours. THF was removed *in vacuo*, and the residue was purified via silica gel chromatography using hexanes/EtOAc (100/1) as the eluent to afford **CC-L1** as a white solid (72% yield).

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.97 (d, *J* = 8.3 Hz, 1H), 7.67 (dt, *J* = 6.6, 2.3 Hz, 1H), 7.46 – 7.42 (m, 2H), 7.40 (ddd, *J* = 8.2, 6.5, 1.5 Hz, 1H), 7.30 – 7.17 (m, 4H), 2.72 (s, 3H), 2.18 (d, *J* = 2.0 Hz, 3H), 1.91 (ddd, *J* = 15.2, 10.1, 3.2 Hz, 1H), 1.78 – 0.79 (m, 21H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 147.5 (d, *J* = 31.1 Hz), 136.9 (d, *J* = 19.4 Hz), 136.7 (d, *J* = 6.2 Hz), 133.5 (d, *J* = 1.8 Hz), 133.4, 133.0 (d, *J* = 3.2 Hz), 132.7 (d, *J* = 2.0 Hz), 131.6 (d, *J* = 5.9 Hz), 131.0, 129.5, 128.6, 127.7, 126.6, 124.8, 124.4, 124.0, 34.9 (d, *J* = 15.1 Hz), 33.7 (d, *J* = 14.1 Hz), 30.4 (d, *J* = 4.8 Hz), 30.2, 30.1 (d, *J* = 11.9 Hz), 29.8 (d, *J* = 12.9 Hz), 27.6, 27.6 (d, *J* = 18.5 Hz), 27.5 (d, *J* = 4.0 Hz), 27.4 (d, *J* = 6.2 Hz), 26.7, 26.5, 21.4 (d, *J* = 4.3 Hz), 19.7; ^{31}P NMR (202 MHz, $CDCl_3$) δ –9.4; IR (ATR) 3051, 3006, 2921, 2848, 1600, 1511, 1446, 1386, 1034, 1000, 909, 875, 851, 757, 733, 669 cm^{-1}; HRMS (DART) calcd for $C_{30}H_{38}P$ ([M+H]$^+$) 429.27056, found 429.26989.

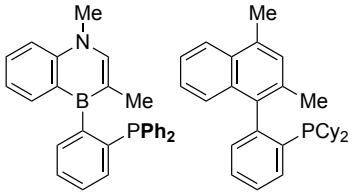
Procedure for *trans*-Selective Cyanoboration, Ligand Screening (Table 1)

To a 4-mL vial charged with $Pd(COD)(CH_2TMS)_2$ (3.9 mg, 0.010 mmol, 5.0 mol %), corresponding ligand in **Table 1** (0.010 mmol, 5.0 mol %), CuCN (29 mg, 0.32 mmol, 1.6 equiv.), BCatCl (55 mg, 0.36 mmol, 1.8 equiv.), and *o*-DCB (0.30 mL) was added enyne **1a** (28.4 mg, 0.200 mmol, 1.00 equiv) and a solution of hexamethylbenzene in *o*-DCB (5.0 µL, 3.3 M) as the internal standard. The resulting mixture was allowed to stir for 2.5 hours at 115 °C. At the conclusion of the reaction, the mixture was passed through an acrodisc under an inert atmosphere using CH_2Cl_2 as the solvent, and 1,8-diaminonaphthlene (64 mg, 0.40 mmol, 2.0 equiv) was added to the filtrate. After allowing the mixture to stir for 12 hours, volatiles were removed under reduced pressure, and the *trans*:*cis* ratios and yields were determined by ^1H NMR of the resulting crude material against hexamethylbenzene as the internal standard.



1a **4a**

entry	**L**	**4a** yield *(trans:cis)*
1	none	3% (89:11)
2	$PhPCy_2$	13% (95:5)
3	XPhos	10% (90:10)
4	dppe	0.3% (ND)
5	**L1**	**92% (96:4)**
6	**L2**	69% (95:5)
7	**L3**	48% (95:5)
8	**L4**	24% (95:5)
9	**L5**	46% (96:4)
10	**CC-L1**	6% (89:11)



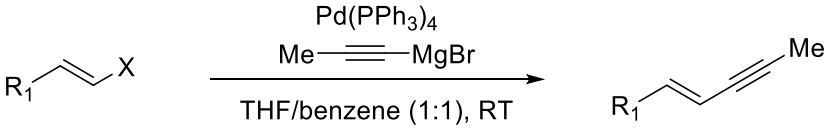
L5 **CC-L1**

o-DCB: *ortho*-dichlorobenzene

Preparation of Enynes 1 and 2 (Table 2 and Table 3)

Enynes in **Table 2**

General Method for Enyne Synthesis by Kumada Coupling:

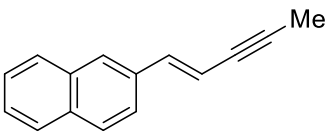


X = Br or I

II

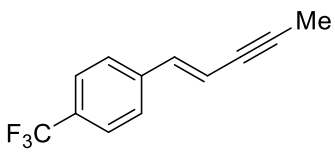
The corresponding *(E)*-styrenyl bromide[3,4] (to synthesize **1a**-**1b**, **1d**-**1h**, **1k**, **1m** and **1s**) or alkenyl iodide[5,6,7] (to synthesize **1n**-**1q** and **1t**) precursors are known compounds. *(E)*-3-(2-bromovinyl) thiophene was obtained using reported methods.[8,9]

To a 20-mL vial charged with $Pd(PPh_3)_4$ (34 mg, 0.030 mmol, 0.015 equiv.), *(E)*-styrenyl bromide or alkenyl iodide **II** (2.0 mmol, 1.0 equiv.) and benzene (5 mL) was added 1-propynyl magnesium bromide (5.2 mL, 0.50 M in THF, 2.6 mmol, 1.3 equiv.) in a dropwise fashion at room temperature under nitrogen. The mixture was allowed to stir for 14 hours at the same temperature. At the conclusion of reaction, aqueous HCl solution (5.0 mL, 1.0 M) was added slowly along with Et_2O (6 mL). The organic layer was separated, and the aqueous layer was further extracted with Et_2O (5 ml). The organic layers were then combined, and dried with Na_2SO_4. All violates were removed *in vacuo*, and the residue was purified by silica gel chromatography using hexanes as the eluent to afford the internal enynes as colorless oils. Enyne **1s** and **1t** were synthesized with the same procedure using 1-butynyl magnesium bromide and 1-ethynyl magnesium bromide, respectively. The characterization data for enynes are consistent with those reported in the literature: **1a**[10], (**1d**, **1e**, **1g**, **1h**, **1n**, **1p**, **1s**)[1], **1t**[11].



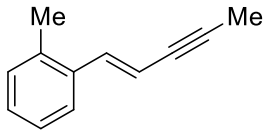
1b

1b, 87% yield. ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.86 – 7.76 (m, 3H), 7.73 (d, *J* = 1.6 Hz, 1H), 7.58 (dd, *J* = 8.6, 1.7 Hz, 1H), 7.52 – 7.42 (m, 2H), 7.06 (d, *J* = 16.1 Hz, 1H), 6.29 (dq, *J* = 16.2, 2.4, Hz, 1H), 2.07 (d, *J* = 2.4 Hz, 3H); ^{13}C NMR (151 MHz, $CDCl_3$) δ 140.3, 134.1, 133.6, 133.4, 128.4, 128.2, 127.8, 126.5, 126.5, 126.3, 122.9, 109.3, 88.8, 79.2, 4.7; IR (ATR) 3055, 3029, 2912, 2850, 2216, 1507, 1362, 1185, 959, 867, 828, 816, 740, 486 cm^{-1}; HRMS (DART) calcd for $C_{15}H_{13}$ ([M+H]$^+$) 193.10118, found 193.10037.



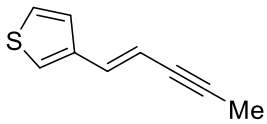
1f

1f, 66% yield. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.56 (d, *J* = 8.2 Hz, 2H), 7.44 (d, *J* = 8.2 Hz, 2H), 6.87 (d, *J* = 16.2 Hz, 1H), 6.22 (dq, *J* = 16.2, 2.4 Hz, 1H), 2.03 (dd, *J* = 2.5, 0.8 Hz, 3H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 140.1 (d, *J* = 1.7 Hz), 138.5, 130.0 (d, *J* = 32.5 Hz), 126.3, 125.7 (q, *J* = 3.8 Hz), 124.2 (q, *J* = 271.9 Hz), 111.8, 90.2, 78.7, 4.6; ^{19}F NMR (470 MHz, $CDCl_3$) δ –62.6; IR (ATR) 3020, 2924, 2854, 2217, 1612, 1411, 1327, 1165, 1120, 1109, 1070, 954, 860, 820, 599, 517 cm^{-1}; HRMS (DART) calcd for $C_{12}H_{10}F_3$ ([M+H]$^+$) 211.07291, found 211.07317.



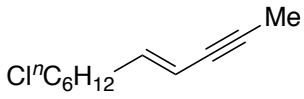
1k

1k, 71% yield. ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.47 (dd, *J* = 7.0, 2.1 Hz, 1H), 7.23 – 7.13 (m, 4H), 6.09 (dq, *J* = 16.1, 2.4 Hz, 1H), 2.39 (s, 3H), 2.06 (d, *J* = 2.4 Hz, 3H); ^{13}C NMR (151 MHz, $CDCl_3$) δ 138.0, 135.6, 135.6, 130.5, 128.2, 126.2, 124.9, 109.9, 88.0, 79.4, 19.8, 4.6; IR (ATR) 3014, 3019, 2949, 2913, 2849, 2217, 1482, 1458, 1436, 1377, 1048, 951, 746, 714, 608, 537, 458 cm^{-1}; HRMS (DART) calcd for $C_{12}H_{13}$ ([M+H]$^+$) 157.10118, found 157.10142.



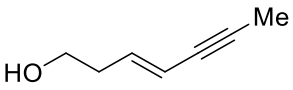
1m

1m, 83% yield. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.28 – 7.25 (m, 1H), 7.20 – 7.14 (m, 2H), 6.86 (d, *J* = 16.1 Hz, 1H), 5.97 (dq, *J* = 16.2, 2.4 Hz, 1H), 2.00 (d, *J* = 2.4 Hz, 3H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 139.5, 134.3, 126.4, 124.5, 122.9, 108.8, 88.3, 78.9, 4.7; IR (ATR) 3097, 3033, 2912, 2847, 2218, 1411, 1244, 1183, 947, 865, 834, 766, 623, 687, 472 cm^{-1}; HRMS (DART) calcd for C_9H_9S ([M+H]$^+$) 149.04195, found 149.04177.



1o

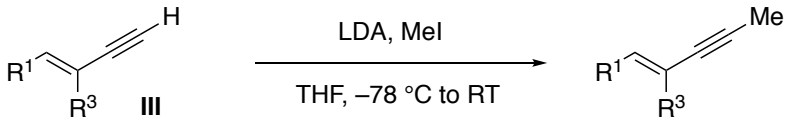
1o, 87% yield. ^{1}H NMR (500 MHz, $CDCl_3$) δ 6.07 – 5.96 (m, 1H), 5.41 (dq, *J* = 15.8, 1.9 Hz, 1H), 3.51 (t, *J* = 6.7 Hz, 2H), 2.07 (qd, *J* = 7.3, 1.5 Hz, 2H), 1.91 (d, *J* = 2.3 Hz, 3H), 1.75 (dt, *J* = 14.7, 6.8 Hz, 2H), 1.48 – 1.19 (m, 6H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 143.1, 110.2, 84.2, 78.5, 45.2, 32.9, 32.7, 28.8, 28.4, 26.8, 4.3; IR (ATR) 3019, 2929, 2855, 2225, 1462, 1444, 1309, 1172, 955, 727, 651 cm^{-1}; HRMS (DART) calcd for $C_{11}H_{18}Cl$ ([M+H]$^+$) 185.10915, found 185.10880.



1q

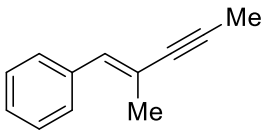
1q, with 2.6 equiv. 1-propynyl magnesium bromide, 81% yield. ^{1}H NMR (500 MHz, $CDCl_3$) δ 5.99 (dtd, *J* = 15.5, 7.3, 0.7 Hz, 1H), 5.60 – 5.42 (m, 1H), 3.63 (t, *J* = 6.4 Hz, 2H), 2.32 (qd, *J* = 6.5, 1.4 Hz, 2H), 1.94 – 1.87 (m, 3H), 1.85 (s, br, 1H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 138.8, 112.9, 85.1, 78.1, 61.7, 36.3, 4.2; IR (ATR) 3330, 2917, 2879, 2224, 1428, 1376, 1171, 1043, 954, 636, 543 cm^{-1}; HRMS (DART) calcd for $C_7H_{11}O$ ([M+H]$^+$) 111.08044, found 111.08026.

General Method for Enyne Synthesis by Terminal Enyne Methylation:



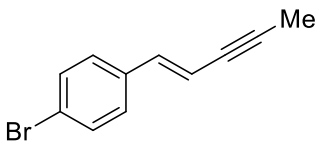
Terminal enynes precursors **III** for synthesizing **1c**, **1i** and **1l** are known compounds.[12,1,13]

To a 20-mL vial charged with diisopropylamine (242 mg, 2.40 mmol, 1.20 equiv.) and THF (6 mL), *n*butyl lithium (0.88 mL, 2.5 M in hexanes, 2.2 mmol, 1.1 equiv.) was added in dropwise fashion at –78 °C. The mixture was allowed to stir at the same temperature for 15 minutes. Then the terminal enyne (2.0 mmol, 1.0 equiv.) in THF (2.0 mL) was added to the LDA solution at –78 °C. After allowing the mixture to stir at –78 °C for another 20 minutes, MeI (355 mg, 2.50 mmol, 1.25 equiv.) was added at once. The resulting mixture was allowed to stir at –78 °C for 30 min and then gradually allowed to warm to room temperature in an hour. At the conclusion of the reaction, THF was removed *in vacuo*, and the residue was dissolved in Et_2O (10 mL). The organic layer was further washed by H_2O (5 mL), brine (5 mL) and concentrated. The residue was purified by silica gel column chromatography using hexanes as the eluent to afford the internal enynes as colorless oils.



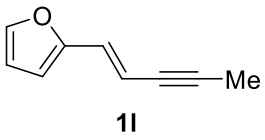
1c

1c, 77% yield. ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.39 – 7.33 (m, 2H), 7.31 – 7.27 (m, 2H), 7.25 (td, *J* = 7.3, 1.3 Hz, 1H), 6.80 (s, 1H), 2.07 (t, *J* = 1.3 Hz, 3H), 2.03 (d, *J* = 0.9 Hz, 3H); ^{13}C NMR (151 MHz, $CDCl_3$) δ 137.2, 134.7, 129.0, 128.3, 126.9, 120.6, 84.8, 83.6, 19.5, 4.4; IR (ATR) 3022, 2915, 2852, 2220, 1492, 1440, 1376, 1246, 1030, 917, 866, 762, 724, 694, 506 cm^{-1}; HRMS (DART) calcd for $C_{12}H_{13}$ ([M+H]$^+$) 157.10118, found 157.10170.



1i

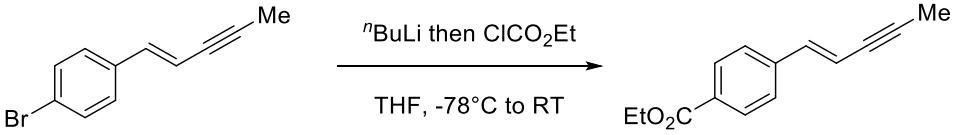
1i, 91% yield. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.46 – 7.39 (m, 2H), 7.24 – 7.16 (m, 2H), 6.78 (d, *J* = 16.2 Hz, 1H), 6.11 (dq, *J* = 16.2, 2.4 Hz, 1H), 2.01 (dd, *J* = 2.4, 0.7 Hz, 3H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 138.9, 135.6, 131.9, 127.6, 122.2, 109.8, 89.2, 78.8, 4.7; IR (ATR) 3031, 2910, 2845, 2213, 1584, 1486, 1399, 1074, 1008, 962, 946, 854, 806, 786, 519 cm^{-1}; HRMS (DART) calcd for $C_{11}H_{10}Br$ ([M+H]$^+$) 220.99604, found 220.99502.



1l

1l, 81% yield. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.34 (d, *J* = 1.6 Hz, 1H), 6.62 (d, *J* = 16.0 Hz, 1H), 6.38 (dt, *J* = 3.4, 1.6 Hz, 1H), 6.31 – 6.23 (m, 1H), 6.04 (dp, *J* = 16.1, 2.4 Hz, 1H), 2.01 (dd, *J* = 2.6, 1.6 Hz, 3H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 152.5, 142.7, 127.5, 111.8, 109.2, 107.2, 89.3, 79.0, 4.7; IR (ATR) 3397, 3055, 2220, 1600, 1505, 1408, 1373, 1335, 1095, 820, 767 cm^{-1}; HRMS (DART) calcd for C_9H_9O ([M+H]$^+$) 133.06479, found 133.06543.

Synthesis of Enyne **1j** by Esterification:

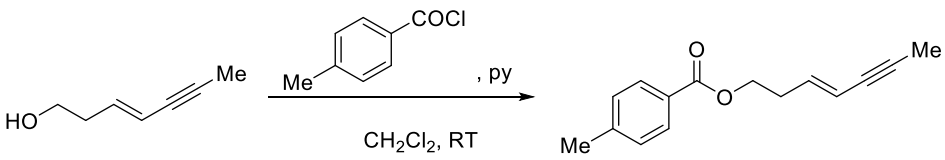


1i **1j**

A solution of enyne **1i** (236 mg, 1.14 mmol, 1.00 equiv.) in THF (4 mL) was placed in a 20-mL vial. ^{n}Butyl lithium (0.500 mL, 2.50 M in hexanes, 1.25 mmol, 1.10 equiv.) was added to this solution in a dropwise fashion at –78 °C. After allowing the mixture to stir at the same temperature for 20 minutes, ethyl chloroformate (186 mg, 1.71 mmol, 1.50 equiv.) was added. The mixture was allowed to stir for an hour at –78 °C and then allowed to warm to room temperature in an hour. The resulting slurry was poured into H_2O (10 mL) and then diluted with Et_2O (5 mL). The organic layer was separated and violates were removed *in vacuo*. The resulting residue was purified by silica gel chromatography using hexanes/EtOAc (20/1) as the eluent to afford **1j** a white solid (47%).

^{1}H NMR (600 MHz, $CDCl_3$) δ 8.03 – 7.86 (m, 2H), 7.48 – 7.30 (m, 2H), 6.85 (d, *J* = 16.2 Hz, 1H), 6.21 (dq, *J* = 16.3, 2.4 Hz, 1H), 4.35 (q, *J* = 7.2 Hz, 2H), 2.08 – 1.89 (m, 3H), 1.37 (t, *J* = 7.1 Hz, 3H); ^{13}C NMR (151 MHz, $CDCl_3$) δ 166.3, 140.8, 139.0, 130.0, 129.9, 125.9, 111.6, 90.1, 78.8, 61.0, 14.4, 4.6; IR (ATR) 3035, 2983, 2912, 2212, 1711, 1607, 1411, 1363, 1279, 1266, 1178, 1127, 1105, 1026, 944, 864, 759, 694, 519 cm^{-1};HRMS (DART) calcd for $C_{14}H_{15}O_2$ ([M+H]$^+$) 215.10666, found 215.10591.

Synthesis of Enyne **1r** by Ester Coupling:



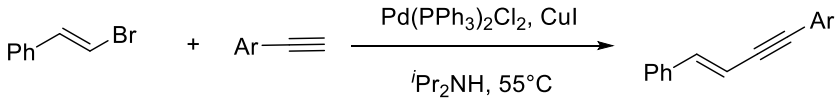
1q **1r**

Under nitrogen, *p*-toluoyl chloride (240 mg, 1.56 mmol, 1.20 equiv.) and pyridine (123 mg, 1.56 mmol, 1.20 equiv.) were added to a 20-mL vial charged with a solution of enyne **1q** (143 mg, 1.30 mmol, 1.00 equiv.) in CH_2Cl_2 (8 mL). The resulting mixture was allowed to stir at room temperature for 14 hours. Then, the solvent was removed under reduced pressure, and the residue was purified by silica gel chromatography with hexans/EtOAc (40/1) as the eluent to afford **1r** as a white solid (68%).

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.98 – 7.80 (m, 2H), 7.23 (d, *J* = 8.2 Hz, 2H), 6.08 (dt, *J* = 15.8, 7.1 Hz, 1H), 5.58 (dp, *J* = 15.8, 1.9 Hz, 1H), 4.32 (t, *J* = 6.6 Hz, 2H), 2.54 (qd, *J* = 6.8, 1.5 Hz, 2H), 2.40 (s, 3H), 1.92 (d, *J* = 2.3 Hz, 3H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 166.6, 143.7, 138.0, 129.7, 129.1, 127.6, 112.8, 85.3, 78.1, 63.6, 32.4, 21.7, 4.3; IR (ATR) 2955, 2916, 2226, 1715, 1612, 1454, 1379, 1271, 1177, 1105, 1020, 955, 841, 753, 691 cm^{-1}; HRMS (DART) calcd for $C_{15}H_{17}O_2$ ([M+H]$^+$) 229.12231, found 229.12131.

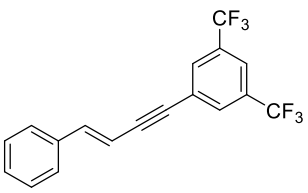
Enynes in **Table 3**

General Method for Enyne Synthesis by Sonogashira Coupling:



IV **2a-d**

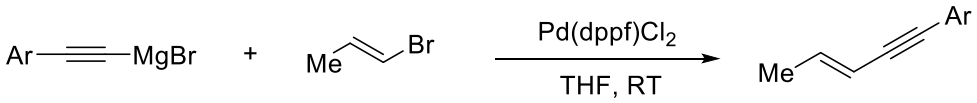
A 50-mL round bottom flask was charged with $PdCl_2(PPh_3)_2$ (84 mg, 0.12 mmol, 0.030 equiv.) and CuI (38 mg, 0.20 mol, 0.050 equiv.) under nitrogen. To this flask ^{i}Pr$_2$NH (20 mL), *(E)*-styrenyl bromide (0.73 g, 4.0 mmol, 1.0 equiv.) and the corresponding terminal alkyne **IV** (4.8 mmol, 1.2 equiv.) were added. The mixture was allowed to stir at 55 °C for 16 h. At the conclusion of the reaction, H_2O (15 mL) and Et_2O (15 mL) were added to the reaction mixture, and the organic layer was separated. The aqueous layer was extracted with another portion of Et_2O (10 mL). The organic layers were combined, dried, and concentrated. The resulting crude residue was purified by silica gel chromatography using hexanes as the eluent to obtain the product as white solids. Characterization data of enyne **2a** to **2c** are consistent with reported in the literature.[14]



2d

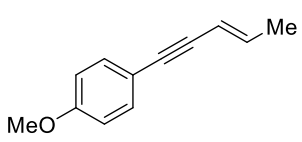
2d, 76% yield. ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.91 (d, *J* = 1.7 Hz, 2H), 7.83 (s, 1H), 7.52 – 7.44 (m, 2H), 7.44 – 7.33 (m, 3H), 7.17 (d, *J* = 16.3 Hz, 1H), 6.41 (d, *J* = 16.2 Hz, 1H); ^{13}C NMR (151 MHz, $CDCl_3$) δ 143.6, 135.9, 132.1 (q, *J* = 33.8 Hz), 131.4 (q, *J* = 4.0 Hz), 129.4, 129.0, 126.7, 126.0, 123.2 (q, *J* = 272.8 Hz), 121.5 (dq, *J* = 7.7, 3.9 Hz), 106.9, 92.6, 88.6; ^{19}F NMR (564 MHz, $CDCl_3$) δ –65.8; IR (ATR) 3033, 2201, 1464, 1385, 1277, 1244, 1174, 1132, 1107, 1048, 953, 896, 848, 748, 684 cm^{-1}; HRMS (DART) calcd for $C_{18}H_{11}F_6$ ([M+H]$^+$) 341.07595, found 341.07569.

General Method for Enyne Synthesis by Kumada Coupling:



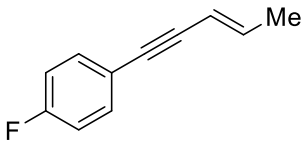
V **2e-g**

The protocol for was adapted from literature procedure.[15] Under nitrogen to a 20-mL vial charged with $Pd(dppf)Cl_2$ (44 mg, 0.060 mmol, 0.020 equiv.) and (*E*)-1-bromopropene (436 mg, 3.60 mmol, 1.20 equiv.) was added alkynyl magnesium bromide **V** (3.0 mmol, 1.0 equiv.) in THF (12 mL) at room temperature. The mixture was allowed to stir for another 14 hours at room temperature. Then the solvent was removed *in vacuo*, and the residue was dissolved in Et_2O (10 mL). This organic solution was further washed by H_2O (10 mL) and brine (10 mL) and dried with Na_2SO_4. Volatiles were removed under reduced pressure, and the resulting crude residue was purified by silica gel column chromatography using hexane as the eluent to afford the product as colorless liquids.



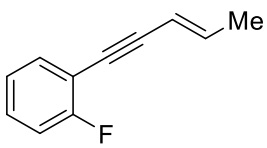
2e

2e, with 1-bromopropene mixture (4.6 equiv., *E*/*Z* = 26:74). Crude ^1H NMR indicates the ratio of *E*/*Z* enyne is 95:5. Purification provides pure **2e,** 56% yield. ^1H NMR (500 MHz, $CDCl_3$) δ 7.40 – 7.31 (m, 2H), 6.87 – 6.76 (m, 2H), 6.21 (dd, *J* = 15.8, 6.8 Hz, 1H), 5.70 (dq, *J* = 15.7, 1.8 Hz, 1H), 3.80 (s, 3H), 1.83 (dd, *J* = 6.8, 1.8 Hz, 3H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 159.4, 139.1, 132.9, 115.9, 114.0, 111.1, 87.7, 87.0, 55.4, 18.8; IR (ATR) 3001, 2959, 2934, 2912, 2837, 1603, 1506, 1441, 1286, 1244, 1171, 1036, 950, 828, 803, 533 cm^{-1}; HRMS (DART) calcd for $C_{12}H_{13}O$ ($[M+H]^+$) 173.09609, found 173.09544.



2f

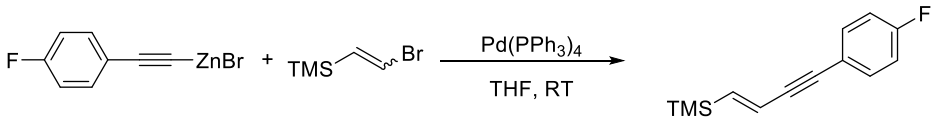
2f, 74% yield. ^1H NMR (500 MHz, $CDCl_3$) δ 7.43 – 7.34 (m, 2H), 7.07 – 6.90 (m, 2H), 6.24 (dqd, *J* = 14.8, 6.8, 1.2 Hz, 1H), 5.69 (dp, *J* = 15.8, 1.8 Hz, 1H), 1.84 (dt, *J* = 6.9, 1.5 Hz, 3H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 162.4 (d, *J* = 248.9 Hz), 140.1, 133.4 (d, *J* = 8.2 Hz), 119.9 (d, *J* = 3.4 Hz), 115.7 (d, *J* = 22.0 Hz), 110.8, 88.0 (d, *J* = 1.4 Hz), 86.7, 18.9; ^{19}F NMR (470 MHz, $CDCl_3$) δ –111.7 (dp, *J* = 13.6, 4.8 Hz); IR (ATR) 2914, 1599, 1504, 1229, 1155, 1092, 950, 909, 831, 678, 527, 503 cm^{-1}; HRMS (DART) calcd for $C_{11}H_{10}F$ ($[M+H]^+$) 161.07610, found 161.07598.



2g

2g, 80% yield. ^1H NMR (500 MHz, $CDCl_3$) δ 7.41 (td, *J* = 7.5, 1.8 Hz, 1H), 7.26 (dddd, *J* = 8.1, 7.2, 5.2, 1.8 Hz, 1H), 7.15 – 6.98 (m, 2H), 6.31 (dq, *J* = 15.7, 6.8 Hz, 1H), 5.75 (dq, *J* = 15.8, 1.8 Hz, 1H), 1.85 (dd, *J* = 6.9, 1.9 Hz, 3H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 162.6 (d, *J* = 250.9 Hz), 140.8, 133.4 (d, *J* = 1.4 Hz), 129.6 (d, *J* = 8.0 Hz), 124.0 (d, *J* = 3.8 Hz), 115.5 (d, *J* = 21.1 Hz), 112.4 (d, *J* = 15.8 Hz), 110.7, 93.5 (d, *J* = 3.3 Hz), 81.1, 18.9 (d, *J* = 2.2 Hz); ^{19}F NMR (470 MHz, $CDCl_3$) δ –110.4 (dt, *J* = 8.7, 6.0 Hz); IR (ATR) 3031, 2914, 2207, 1572, 1491, 1447, 1256, 1218, 1106, 951, 912, 823, 754, 577 cm^{-1}; HRMS (DART) calcd for $C_{11}H_{10}F$ ($[M+H]^+$) 161.07610, found 161.07542.

Synthesis of Enyne **2h** by Negishi Coupling:

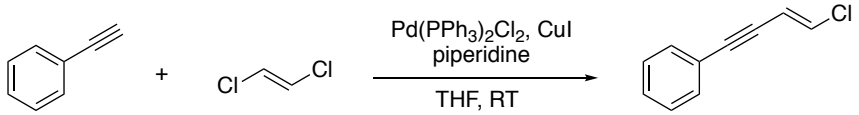


E/*Z* = 90:10 **2h**

The protocol was adapted from literature procedure.[16] Under nitrogen to a 20-mL vial charged with $Pd(PPh_3)_4$ (92 mg, 0.080 mmol, 0.020 equiv.) was added a solution of ((4-fluorophenyl)ethynyl)zinc bromide (3.42 mmol, 0.850 equiv.) in THF (15 mL) followed by (2-bromovinyl)trimethylsilane (716 mg, 4.00 mmol, 1.00 equiv., E/Z = 90/10) at room temperature. The resulting mixture was allowed to stir for 14 hours at room temperature. Then the solvent was removed *in vacuo* and the residue was dissolved in Et_2O (10 mL). This organic solution was further washed by H_2O (10 mL) and concentrated. The crude product was carefully purified by silica gel chromatography using hexanes as the eluent to afford **2h** as a colorless liquid (57% yield).

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.46 – 7.36 (m, 2H), 7.01 (t, *J* = 8.7 Hz, 2H), 6.54 (d, *J* = 19.2 Hz, 1H), 6.15 (d, *J* = 19.2 Hz, 1H), 0.13 (s, 9H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 162.6 (d, *J* = 249.6 Hz), 146.1, 133.6 (d, *J* = 8.2 Hz), 123.3, 119.6 (d, *J* = 3.6 Hz), 115.7 (d, *J* = 22.0 Hz), 89.5 (d, *J* = 1.5 Hz), 88.8, –1.5; ^{19}F NMR (470 MHz, $CDCl_3$) δ –116. 3 (m); IR (ATR) 2956, 1601, 1569, 1505, 1249, 1231, 1155, 975, 863, 833, 740, 727, 694, 658, 529 cm^{-1}; HRMS (DART) calcd for $C_{13}H_{16}FSi$ ([M+H]$^+$) 219.09998, found 219.09980.

Synthesis of Enyne **2i** by Sonogashira Coupling:



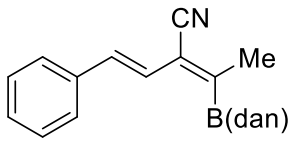
2i

Under nitrogen a 50-mL round bottom flask was charged with $PdCl_2(PPh_3)_2$ (42 mg, 0.060 mmol, 0.020 equiv.) and CuI (23 mg, 0.12 mol, 0.040 equiv.). To this flask Et_2O (6 mL), piperidine (1.02 g, 12.0 mmol, 4.00 equiv.), phenylacetylene (306 mg, 3.00 mmol, 1.00 equiv.) and *trans*-dichloroethylene (437 mg, 4.50 mmol, 1.50 equiv.) were added. The mixture was allowed to stir at room temperature for 16 h. At the conclusion of the reaction H_2O (15 mL) and Et_2O (15 mL) were added, and the organic layer was separated. The aqueous layer was further washed by Et_2O (10 mL). The organic layers were combined, concentrated, and purified by silica gel chromatography using pentane as the eluent to obtain **2i** as a colorless liquid (87%).

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.49 – 7.39 (m, 2H), 7.33 (dd, *J* = 5.0, 1.9 Hz, 3H), 6.63 (d, *J* = 13.6 Hz, 1H), 6.16 (d, *J* = 13.6 Hz, 1H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 131.7, 130.3, 128.8, 128.5, 122.8, 114.0, 92.1, 84.5; IR (ATR) 3067, 3031, 2204, 1581, 1488, 1442, 1272, 1224, 912, 843, 752, 687, 528, 498 cm^{-1}; HRMS (DART) calcd for $C_{10}H_7Cl$ ([M+H]$^+$) 162.02308, found 162.02267.

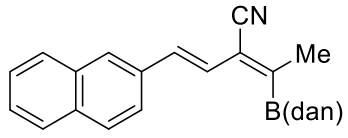
General Procedure for *trans*-Selective Cyanoboration Reaction of 1,3-Enynes (Table 2)

To a 4-mL vial charged with $Pd(COD)(CH_2TMS)_2$ (3.9 mg, 0.010 mmol, 5.0 mol %), **L1** or **L5** (mol % is indicated in the corresponding entries), CuCN (29 mg, 0.32 mmol, 1.6 equiv), BCatCl (55 mg, 0.36 mmol, 1.8 equiv.), and *o*-DCB (0.30 mL) was added the corresponding enyne substrate (0.20 mmol, 1.0 equiv). The resulting mixture was allowed to stir for 2.5 hours at the temperature indicated in the entries. At the conclusion of reaction, the mixture was passed through an acrodisc with CH_2Cl_2 under nitrogen. 1,8-Diaminonaphthlene (64 mg, 0.40 mmol, 2.0 equiv) was then added to the filtrate and the mixture was allowed to stir for another 12 hours. Then the mixture was passed through an acrodisc and concentrated under reduced pressure. The resulting crude residue was purified by silica gel chromatography using hexanes/CH_2Cl_2 (4/1 to 1/1 gradient) as the eluent to afford the pure *trans*-selective cyanoboration products as yellow solids.



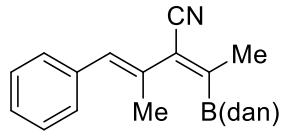
4a

4a, with 5 mol % **L1** at 115 °C, 86% yield (run1: 87%, run2: 85%), 96:4. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.40 (d, *J* = 7.0 Hz, 2H), 7.31 (t, *J* = 7.2 Hz, 2H), 7.27 (d, *J* = 7.0 Hz, 1H), 7.18 – 7.09 (m, 4H), 7.03 (d, *J* = 15.9 Hz, 1H), 6.93 (d, *J* = 15.8 Hz, 1H), 6.39 (dd, *J* = 7.1, 1.3 Hz, 2H), 5.70 (s, 2H), 2.33 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 140.1, 136.4, 135.8, 134.0, 129.0, 128.8, 127.8, 127.1, 123.9, 120.8, 120.1, 118.8, 115.6, 106.7, 22.5 (*B*-alkenyl carbon signal not observed); ^{11}B NMR (160 MHz, $CDCl_3$) δ 28.8; IR (ATR) 3397, 3055, 2220, 1600, 1505, 1408, 1373, 1335, 1095, 820, 767 cm^{-1}; HRMS (DART) calcd for $C_{22}H_{19}BN_3$ ([M+H]$^+$) 336.16665, found 336.16979.



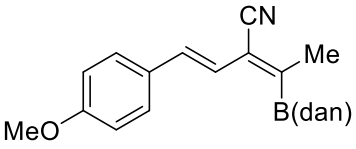
4b

4b, with 5 mol % **L1** at 115 °C, 77% yield (run1: 75%, run2: 79%), 98:2. Crystals for single crystal X-ray diffraction analysis were obtained by recrystallization from hexane/CH_2Cl_2 at room temperature. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.77 (dt, *J* = 7.0, 2.6 Hz, 3H), 7.72 (d, *J* = 8.6 Hz, 1H), 7.53 (dd, *J* = 8.6, 1.7 Hz, 1H), 7.49 – 7.41 (m, 2H), 7.21 – 7.10 (m, 5H), 7.03 (d, *J* = 15.8 Hz, 1H), 6.41 (dd, *J* = 7.2, 1.3 Hz, 2H), 5.77 (s, 2H), 2.34 (s, 3H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 152.5 (br), 140.2, 136.4, 134.0, 133.6, 133.5, 133.3, 128.7, 128.4, 127.9, 127.8, 127.8, 126.6, 126.6, 124.1, 123.3, 120.8, 120.1, 118.8, 115.7, 106.7, 22.6; ^{11}B NMR (160 MHz, $CDCl_3$) δ 28.9; IR (ATR) 3378, 3053, 2924, 2217, 1627, 1600, 1504, 1407, 1373, 1336, 1094, 953, 819, 765 cm^{-1}; HRMS (DART) calcd for $C_{26}H_{21}BN_3$ ([M+H]$^+$) 386.18230, found 386.18179.



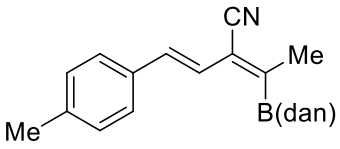
4c

4c, with 5 mol % **L1** at 115 °C, 63% yield (run1: 65%, run2: 61%), >98:2. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.32 (t, *J* = 7.5 Hz, 2H), 7.27 – 7.19 (m, 3H), 7.11 (t, *J* = 7.8 Hz, 2H), 7.05 (d, *J* = 8.2 Hz, 2H), 6.86 (s, 1H), 6.32 (d, *J* = 7.2 Hz, 2H), 5.68 (s, 2H), 2.31 (s, 3H), 2.16 (d, *J* = 1.4 Hz, 3H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 140.1, 136.5, 136.4, 133.0, 132.9, 129.2, 128.5, 127.7, 127.6, 125.4, 119.8, 118.6, 117.0, 106.5, 22.9, 18.1 (*B*-alkenyl carbon signal not observed); ^{11}B NMR (160 MHz, $CDCl_3$) δ 29.0; IR (ATR) 3396, 3054, 2925, 2211, 1599, 1504, 1373, 1332, 1109, 820, 765, 701 cm^{-1}; HRMS (DART) calcd for $C_{23}H_{21}BN_3$ ([M+H]$^+$) 350.18230, found 350.18304.



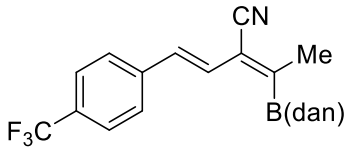
4d

4d, with 1.5 equiv. BcatCl and 5 mol % **L1** at 115 °C, 64% yield (run1: 65%, run2: 62%), 96:4. ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.35 – 7.31 (m, 2H), 7.15 (dd, *J* = 8.3, 7.2 Hz, 2H), 7.11 (dd, *J* = 8.4, 1.1 Hz, 2H), 6.96 (d, *J* = 15.8 Hz, 1H), 6.86 – 6.82 (m, 2H), 6.80 (d, *J* = 15.8 Hz, 1H), 6.39 (dd, *J* = 7.2, 1.1 Hz, 2H), 5.73 (s, 2H), 3.79 (s, 3H), 2.31 (s, 3H); ^{13}C NMR (151 MHz, $CDCl_3$) δ 160.2, 150.9 (br), 140.2, 136.4, 133.4, 128.6, 128.4, 127.8, 121.8, 120.9, 120.1, 118.7, 115.8, 114.4, 106.6, 55.4, 22.4; ^{11}B NMR (160 MHz, $CDCl_3$) δ 28.8; IR (ATR) 3358, 3053, 2932, 2219, 1598, 1508, 1407, 1373, 1333, 1247, 1173, 1032, 1095, 820, 767 cm^{-1}; HRMS (DART) calcd for $C_{23}H_{21}BN_3O$ ([M+H]$^+$) 366.17722, found 366.17843.



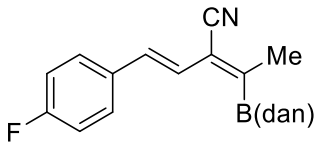
4e

4e, with 5 mol % **L1** at 115 °C, 87% yield (run1: 88%, run2: 85%), 97:3. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.32 – 7.28 (m, 2H), 7.15 (dd, *J* = 8.3, 7.1 Hz, 2H), 7.13 – 7.09 (m, 4H), 7.00 (d, *J* = 15.8 Hz, 1H), 6.88 (d, *J* = 15.8 Hz, 1H), 6.38 (dd, *J* = 7.1, 1.2 Hz, 2H), 5.70 (s, 2H), 2.33 (s, 3H), 2.32 (s, 3H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 140.2, 138.9, 136.4, 133.9, 133.1, 129.7, 127.8, 127.0, 122.9, 120.9, 120.1, 118.8, 115.7, 106.7, 22.4, 21.4 (*B*-alkenyl carbon signal not observed); ^{11}B NMR (160 MHz, $CDCl_3$) δ 28.6; IR (ATR) 3396, 3052, 2917, 2220, 1629, 1600, 1505, 1408, 1373, 1334, 1095, 820, 766 cm^{-1}; HRMS (DART) calcd for $C_{23}H_{21}BN_3$ ([M+H]$^+$) 350.18230, found 350.18279.



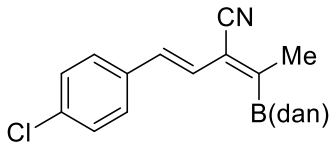
4f

4f, with 5 mol % **L1** at 115 °C, 80% yield (run1: 77%, run2: 82%), >98:2. ^{1}H NMR (600 MHz, THF-d_8) δ 7.65 (d, *J* = 8.2 Hz, 2H), 7.58 (d, *J* = 8.2 Hz, 2H), 7.48 (s, 2H), 7.21 (d, *J* = 15.9 Hz, 1H), 7.06 – 6.99 (m, 3H), 6.96 (dd, *J* = 8.4, 0.9 Hz, 2H), 6.37 (dd, *J* = 7.3, 1.0 Hz, 2H), 2.34 (s, 3H); ^{13}C NMR (126 MHz, THF-d_8) δ 158.0 (br), 142.6, 141.2, 137.7, 131.6, 130.49 (q, *J* = 32.0 Hz), 128.6, 128.4, 128.2, 126.63 (q, *J* = 3.9 Hz), 125.5 (q, *J* = 272.2 Hz), 121.7, 120.2, 118.6, 115.8, 107.0, 22.9; ^{11}B NMR (160 MHz, THF-d_8) δ 29.5; ^{19}F NMR (564 MHz, THF-d_8) δ –63.4; IR (ATR) 3411, 3371, 2922, 2852, 2217, 1602, 1506, 1408, 1329, 1177, 1105, 1068, 820, 764, 690, 455 cm^{-1}; HRMS (DART) calcd for $C_{23}H_{18}BN_3F_3$ ([M+H]$^+$) 404.15404, found 404.15382.



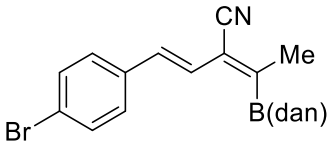
4g

4g, with 5 mol % **L1** at 115 °C, 66% yield (run1: 66%, run2: 65%), 96:4. ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.35 (dd, *J* = 8.6, 5.5 Hz, 2H), 7.16 (t, *J* = 7.7 Hz, 2H), 7.12 (d, *J* = 8.2 Hz, 2H), 7.01 – 6.93 (m, 3H), 6.84 (d, *J* = 15.8 Hz, 1H), 6.40 (d, *J* = 7.2 Hz, 2H), 5.74 (s, 2H), 2.33 (s, 3H); ^{13}C NMR (151 MHz, $CDCl_3$) δ 163.0 (d, *J* = 249.1 Hz), 152.7 (br), 140.1, 136.4, 132.6, 132.03 (d, *J* = 3.4 Hz), 128.7 (d, *J* = 8.1 Hz), 127.8, 123.63 (d, *J* = 2.6 Hz), 120.4, 120.1, 118.8, 116.0 (d, *J* = 21.9 Hz), 115.6, 106.7, 22.5; ^{11}B NMR (160 MHz, $CDCl_3$) δ 28.7; ^{19}F NMR (564 MHz, $CDCl_3$) δ –112.3 (tt, *J* = 8.6, 5.3 Hz); IR (ATR) 3404, 3385, 3052, 2216, 1601, 1505, 1407, 1376, 1334, 1227, 1092, 819, 763, 681 cm^{-1}; HRMS (DART) calcd for $C_{22}H_{18}BN_3F$ ([M+H]$^+$) 354.15723, found 354.15886.



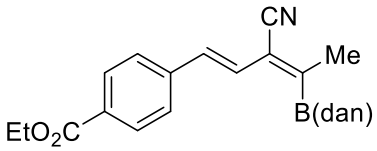
4h

4h, with 5 mol % **L1** at 115 °C, 84% yield (run1: 82%, run2: 86%), >98:2. ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.32 (d, *J* = 8.5 Hz, 2H), 7.27 (d, *J* = 8.4 Hz, 2H), 7.18 – 7.08 (m, 4H), 6.96 (d, *J* = 15.8 Hz, 1H), 6.89 (d, *J* = 15.8 Hz, 1H), 6.39 (d, *J* = 7.1 Hz, 2H), 5.70 (s, 2H), 2.33 (s, 3H); ^{13}C NMR (151 MHz, $CDCl_3$) δ 153.2 (br), 140.0, 136.4, 134.5, 134.3, 132.6, 129.2, 128.2, 127.8, 124.4, 120.5, 120.1, 118.9, 115.4, 106.7, 22.6; ^{11}B NMR (160 MHz, $CDCl_3$) δ 28.8; IR (ATR) 3403, 3379, 2217, 1604, 1508, 1411, 1337, 1095, 820, 765 cm^{-1}; HRMS (DART) calcd for $C_{22}H_{18}BN_3Cl$ ([M+H]$^+$) 370.12768, found 370.12759.



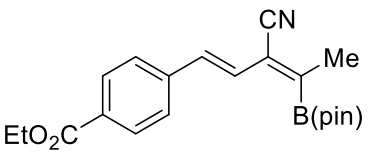
4i

4i, with 5 mol % **L1** at 115 °C, 55% yield (run1: 53%, run2: 57%), 95:5. ^{1}H NMR (500 MHz, THF-d_8) δ 7.49 – 7.34 (m, 6H), 7.10 (dd, *J* = 15.9, 1.0 Hz, 1H), 7.03 (ddd, *J* = 8.3, 7.2, 1.0 Hz, 2H), 6.97 – 6.88 (m, 3H), 6.36 (dd, *J* = 7.3, 1.1 Hz, 2H), 2.31 (s, 3H); ^{13}C NMR (126 MHz, THF-d_8) δ 142.7, 137.7, 136.5, 132.9, 132.0, 129.5, 128.4, 126.8, 122.9, 121.6, 120.3, 118.5, 115.9, 107.0, 22.8 (*B*-alkenyl carbon signal not observed); ^{11}B NMR (160 MHz, THF-d_8) δ 29.0; IR (ATR) 3403, 3374, 2216, 1603, 1506, 1408, 1376, 1335, 1094, 1072, 1007, 819, 763, 754, 686 cm^{-1}; HRMS (DART) calcd for $C_{22}H_{18}BN_3Br$ ([M+H]$^+$) 414.07717, found 414.07770.



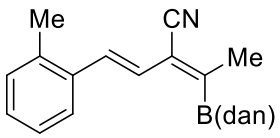
4j

4j, with 5 mol % **L1** at 115 °C, 69% yield, (run1: 71%, run2: 67%), >98:2. ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.99 – 7.94 (m, 2H), 7.47 – 7.41 (m, 2H), 7.18 – 7.09 (m, 4H), 7.02 (d, *J* = 4.1 Hz, 2H), 6.39 (dd, *J* = 7.0, 1.2 Hz, 2H), 5.73 (s, 2H), 4.35 (q, *J* = 7.1 Hz, 2H), 2.35 (s, 3H), 1.37 (t, *J* = 7.1 Hz, 3H); ^{13}C NMR (151 MHz, $CDCl_3$) δ 166.3, 140.1, 140.0, 136.4, 132.8, 130.3, 130.2, 127.8, 126.9, 126.0, 120.5, 120.1, 119.0, 115.3, 106.8, 61.2, 22.7, 14.5 (*B*-alkenyl carbon signal not observed); ^{11}B NMR (160 MHz, $CDCl_3$) δ 28.9; IR (ATR) 3372, 2223, 1691, 1603, 1510, 1409, 1335, 1290, 1272, 1182, 1097, 765, 698 cm^{-1}; HRMS (DART) calcd for $C_{25}H_{23}BN_3O_2$ ([M+H]$^+$) 408.18778, found 408.18712.



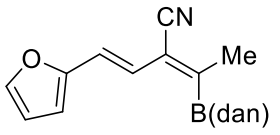
4j-B(pin)

4j-B(pin), with 5 mol % **L1** at 115 °C, pinacol (236 mg, 2.00 mmol, 10.0 equiv.) in CH_2Cl_2 (5 mL) was used rather than 1,8-diaminonaphthlene, purified by silica gel chromatography using hexanes/EtOAc (10/1) as the eluent, 56% yield (run1: 58%, run2: 53%), >98:2. Crystals for single crystal X-ray diffraction analysis were obtained by recrystallization from hexane/CH_2Cl_2 at room temperature. ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.06 – 8.00 (m, 2H), 7.76 (d, *J* = 16.0 Hz, 1H), 7.51 – 7.45 (m, 2H), 7.03 (d, *J* = 16.0 Hz, 1H), 4.38 (q, *J* = 7.1 Hz, 2H), 2.25 (s, 3H), 1.40 (t, *J* = 7.1 Hz, 3H), 1.35 (s, 12H); ^{13}C NMR (151 MHz, $CDCl_3$) δ 166.4, 140.9, 133.1, 130.2 (2 signals), 127.1, 126.9, 125.7, 115.5, 84.7, 61.1, 25.0, 21.9, 14.5 (*B*-alkenyl carbon signal not observed); ^{11}B NMR (160 MHz, $CDCl_3$) δ 29.4; IR (ATR) 2979, 2929, 2221, 1712, 1605, 1361, 1269, 1141, 1102, 1019, 764, 847, 679, 627 cm^{-1}; HRMS (DART) calcd for $C_{21}H_{27}BNO_4$ ([M+H]$^+$) 368.20277, found 368.20267.



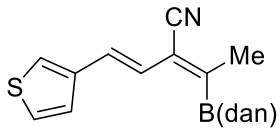
4k

4k, with 5 mol % **L1** at 115 °C, 58% yield (run1: 60%, run2: 56%), 94:6. ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.40 (d, *J* = 7.7 Hz, 1H), 7.32 – 7.23 (m, 1H), 7.20 – 7.08 (m, 7H), 6.86 (d, *J* = 15.7 Hz, 1H), 6.39 (dd, *J* = 7.2, 1.2 Hz, 2H), 5.74 (s, 2H), 2.42 (s, 3H), 2.34 (s, 3H); ^{13}C NMR (151 MHz, $CDCl_3$) δ 152.6 (br), 140.1, 136.5, 136.3, 134.8, 131.6, 130.7, 128.6, 127.8, 126.4, 125.6, 125.0, 120.9, 120.0, 118.7, 115.7, 106.7, 22.5, 19.9; ^{11}B NMR (160 MHz, $CDCl_3$) δ 28.9; IR (ATR) 3395, 3055, 2926, 2219, 1629, 1600, 1505, 1408, 1373, 1335, 1093, 957, 908, 820, 766, 732 cm^{-1}; HRMS (DART) calcd for $C_{23}H_{21}BN_3$ ([M+H]$^+$) 350.18230, found 350.18173.



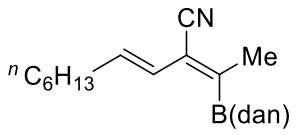
4l

4l, with 5 mol% **L5** at 105 °C, 71% yield (run1: 69%, run2: 73%), 98:2. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.34 (d, *J* = 1.6 Hz, 1H), 7.20 – 7.05 (m, 4H), 6.91 – 6.74 (m, 2H), 6.39 (m, 4H), 5.73 (s, 2H), 2.31 (s, 3H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 151.8, 143.3, 140.2, 136.3, 127.8, 122.2, 121.2, 120.4, 120.1, 118.7, 115.5, 112.1, 111.3, 106.7, 22.5 (*B*-alkenyl carbon signal not observed); ^{11}B NMR (160 MHz, $CDCl_3$) δ 28.8; IR (ATR) 3389, 3053, 2924, 2220, 1629, 1598, 1503, 1407, 1334, 1263, 1094, 1013, 820, 766, 736 cm^{-1}; HRMS (DART) calcd for $C_{20}H_{17}BN_3O$ ([M+H]$^+$) 326.14592, found 326.14575.



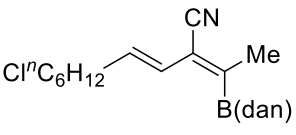
4m

4m, with 5 mol % **L1** at 115 °C, 72% yield (run1: 70%, run2: 74%), 97:3. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.28 (dd, *J* = 3.1, 1.2 Hz, 1H), 7.24 (dd, *J* = 3.0, 0.6 Hz, 1H), 7.19 – 7.09 (m, 5H), 7.03 (d, *J* = 15.8 Hz, 1H), 6.77 (d, *J* = 15.8 Hz, 1H), 6.38 (dd, *J* = 7.1, 1.2 Hz, 2H), 5.71 (s, 2H), 2.31 (s, 3H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 140.1, 138.6, 136.4, 128.0, 127.8, 126.8, 125.0, 124.6, 123.8, 120.7, 120.1, 118.8, 115.6, 106.7, 22.4 (*B*-alkenyl carbon signal not observed); ^{11}B NMR (160 MHz, $CDCl_3$) δ 28.9; IR (ATR) 3394, 3053, 2219, 1628, 1599, 1504, 1407, 1373, 1335, 1095, 820, 766, 650 cm^{-1}; HRMS (DART) calcd for $C_{20}H_{17}BN_3S$ ([M+H]$^+$) 342.12308, found 342.12416.



4n

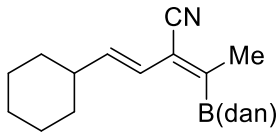
4n, with 7 mol % **L1** at 125 °C, 60% yield (run1: 62%, run2: 57%), 96:4. ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.14 (dd, *J* = 8.3, 7.3 Hz, 2H), 7.09 (dd, *J* = 8.3, 1.0 Hz, 2H), 6.37 (dd, *J* = 7.2, 1.0 Hz, 2H), 6.24 (d, *J* = 15.4 Hz, 1H), 6.18 (dt, *J* = 15.4, 6.7 Hz, 1H), 5.69 (d, *J* = 4.4 Hz, 2H), 2.24 (s, 3H), 2.14 (q, *J* = 7.2 Hz, 2H), 1.41 (h, *J* = 6.8 Hz, 2H), 1.34 – 1.20 (m, 6H), 0.88 (t, *J* = 6.9 Hz, 3H); ^{13}C NMR (151 MHz, $CDCl_3$) δ 149.8 (br), 140.2, 137.1, 136.3, 127.7, 125.5, 120.4, 120.0, 118.6, 115.9, 106.5, 32.7, 31.7, 29.1, 29.0, 22.7, 22.0, 14.2; ^{11}B NMR (160 MHz, $CDCl_3$) δ 28.8; IR (ATR) 3367, 3054, 2954, 2853, 2218, 1598, 1505, 1406, 1372, 1361, 1333, 1095, 957, 820, 764, 664 cm^{-1}; HRMS (DART) calcd for $C_{22}H_{27}BN_3$ ([M+H]$^+$) 344.22925, found 344.22994.



4o

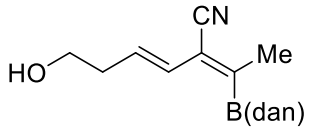
4o, with 7 mol % **L1** at 125 °C, 55% yield (run1: 57%, run2: 53%), 96:4. ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.14 (t, *J* = 7.8 Hz, 2H), 7.09 (d, *J* = 8.3 Hz, 2H), 6.37 (d, *J* = 7.2 Hz, 2H), 6.23 (d, *J* = 15.4 Hz, 1H), 6.16 (dt, *J* = 14.9, 6.8 Hz, 1H), 5.65 (s, 2H), 3.50 (t, *J* = 6.7 Hz, 2H), 2.24 (s, 3H), 2.14 (apparent q, *J* = 7.2 Hz, 2H), 1.74 (apparent p, *J* = 7.0 Hz, 2H), 1.42 (apparent h, *J* = 7.5 Hz, 4H), 1.32 (apparent p, *J* = 7.6 Hz, 2H); ^{13}C NMR (151 MHz, $CDCl_3$) δ 140.2,

136.8, 136.4, 127.7, 125.8, 120.4, 120.0, 118.7, 115.8, 106.5, 45.2, 32.6, 32.6, 29.0, 28.5, 26.8, 22.0 (*B*-alkenyl carbon signal not observed); ^{11}B NMR (160 MHz, $CDCl_3$) δ 29.0; IR (ATR) 3393, 3054, 2927, 2854, 2218, 1628, 1598, 1504, 1406, 1373, 1333, 1095, 820, 765, 730, 665 cm^{-1}; HRMS (DART) calcd for $C_{22}H_{26}BN_3Cl$ ([M+H]$^+$) 378.19028, found 378.18893.



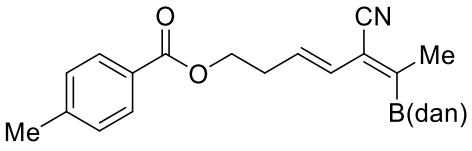
4p

4p, with 7 mol % **L1** at 125 °C, 60% yield (run1: 61%, run2: 59%), 93:7. ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.14 (dd, *J* = 8.3, 7.2 Hz, 2H), 7.09 (dd, *J* = 8.3, 1.0 Hz, 2H), 6.37 (dd, *J* = 7.3, 1.0 Hz, 2H), 6.20 (dd, *J* = 15.5, 1.0 Hz, 1H), 6.12 (dd, *J* = 15.5, 7.1 Hz, 1H), 5.66 (s, 2H), 2.24 (s, 3H), 2.06 (tdt, *J* = 10.9, 7.0, 3.4 Hz, 1H), 1.71 (ddq, *J* = 13.6, 7.2, 3.4 Hz, 4H), 1.64 (dtd, *J* = 12.4, 3.6, 1.7 Hz, 1H), 1.25 (m, 2H), 1.20 – 1.06 (m, 3H); ^{13}C NMR (151 MHz, $CDCl_3$) δ 149.8 (br), 142.6, 140.2, 136.4, 127.7, 123.3, 120.7, 120.0, 118.6, 115.9, 106.5, 41.1, 32.8, 26.0, 25.9, 22.1; ^{11}B NMR (160 MHz, $CDCl_3$) δ 28.7; IR (ATR) 3429, 3393, 2926, 2852, 2218, 1600, 1504, 1408, 1335, 1264, 1093, 963, 820, 732, 703 cm^{-1}; HRMS (DART) calcd for $C_{22}H_{25}BN_3$ ([M+H]$^+$) 342.21360, found 342.21457.



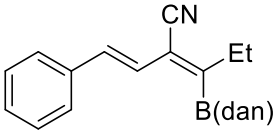
4q

1q was pre-treated with HBCat (29 mg, 0.24 mmol, 1.2 equiv.) in CH_2Cl_2 (1.0 mL) followed by removal of volatiles under high vacuum (150 mmTor) for 30 min at room temperature. This material was then used for the *trans*-selective cyanoboration reaction with 7 mol % **L1** at 125 °C, 35% yield (run1: 32%, run2: 37%), 98:2. **4q** appears to decompose slowly on silica gel column. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.13 (dd, *J* = 8.3, 7.2 Hz, 2H), 7.08 (dd, *J* = 8.4, 1.2 Hz, 2H), 6.39 – 6.31 (m, 3H), 6.17 (dt, *J* = 15.0, 7.1 Hz, 1H), 5.66 (s, 2H), 3.73 (t, *J* = 6.4 Hz, 2H), 2.46 – 2.35 (m, 2H), 2.25 (s, 3H), 1.39 (s, 1H); ^{13}C NMR (151 MHz, $CDCl_3$) δ 151.2 (br), 140.2, 136.3, 132.5, 128.1, 127.7, 120.1, 120.0, 118.6, 115.7, 106.6, 61.7, 35.9, 22.1; ^{11}B NMR (160 MHz, $CDCl_3$) δ 28.9; IR (ATR) 3387, 3053, 2926, 2219, 1599, 1509, 1408, 1373, 1335, 1096, 1036, 821, 768 cm^{-1}; HRMS (DART) calcd for $C_{18}H_{19}BN_3O$ ([M+H]$^+$) 304.16157, found 304.16183.



4r

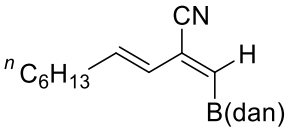
4r, with 7 mol % **L1** at 135 °C, 73% yield (run1: 71%, run2: 75%), 96:4. ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.93 – 7.83 (m, 2H), 7.18 (d, *J* = 8.0 Hz, 2H), 7.15 – 7.04 (m, 4H), 6.44 – 6.36 (m, 1H), 6.32 (dd, *J* = 7.2, 1.1 Hz, 2H), 6.23 (dt, *J* = 14.9, 7.1 Hz, 1H), 5.69 (s, 2H), 4.36 (t, *J* = 6.5 Hz, 2H), 2.60 (q, *J* = 6.7 Hz, 2H), 2.39 (s, 3H), 2.24 (s, 3H); ^{13}C NMR (151 MHz, $CDCl_3$) δ 166.6, 151.6 (br), 143.8, 140.1, 136.3, 131.5, 129.7, 129.2, 128.1, 127.7, 127.4, 120.0, 120.0, 118.7, 115.6, 106.6, 63.6, 32.0, 22.2, 21.8; ^{11}B NMR (160 MHz, $CDCl_3$) δ 28.5; IR (ATR) 3367, 2957, 2219, 1702, 1599, 1508, 1407, 1373, 1335, 1274, 1178, 1096, 908, 820, 768, 754, 731 cm^{-1}; HRMS (DART) calcd for $C_{26}H_{25}BN_3O_2$ ([M+H]$^+$) 422.20343, found 422.20384.



4s

4s, with 5 mol % **L1** at 115 °C, 66% yield (run1: 63%, run2: 68%), 93:7. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.40 (d, *J* = 7.4 Hz, 2H), 7.31 (t, *J* = 7.3 Hz, 2H), 7.27 (d, *J* = 6.9 Hz, 1H), 7.17 (t, *J* = 7.7 Hz, 2H), 7.12 (d, *J* = 8.2 Hz, 2H), 7.04 (d, *J* = 15.9 Hz, 1H), 6.91 (d, *J* = 15.8 Hz, 1H), 6.40 (d, *J* = 7.1 Hz, 2H), 5.74 (s, 2H), 2.71 (q, *J* = 7.6 Hz, 2H), 1.22 (t, *J* = 7.6 Hz, 3H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 159.2 (br), 140.1, 136.4, 135.9, 134.1, 128.9, 128.7, 127.8,

127.1, 124.1, 120.1, 119.5, 118.8, 115.5, 106.7, 30.1, 14.0; ^{11}B NMR (160 MHz, $CDCl_3$) δ 29.0; IR (ATR) 3382, 3052, 2966, 2214, 1599, 1504, 1406, 1373, 1333, 1166, 1103, 951, 818, 761, 750, 686 cm^{-1}; HRMS (DART) calcd for $C_{23}H_{21}BN_3$ ([M+H]$^+$) 350.18230, found 350.18183.



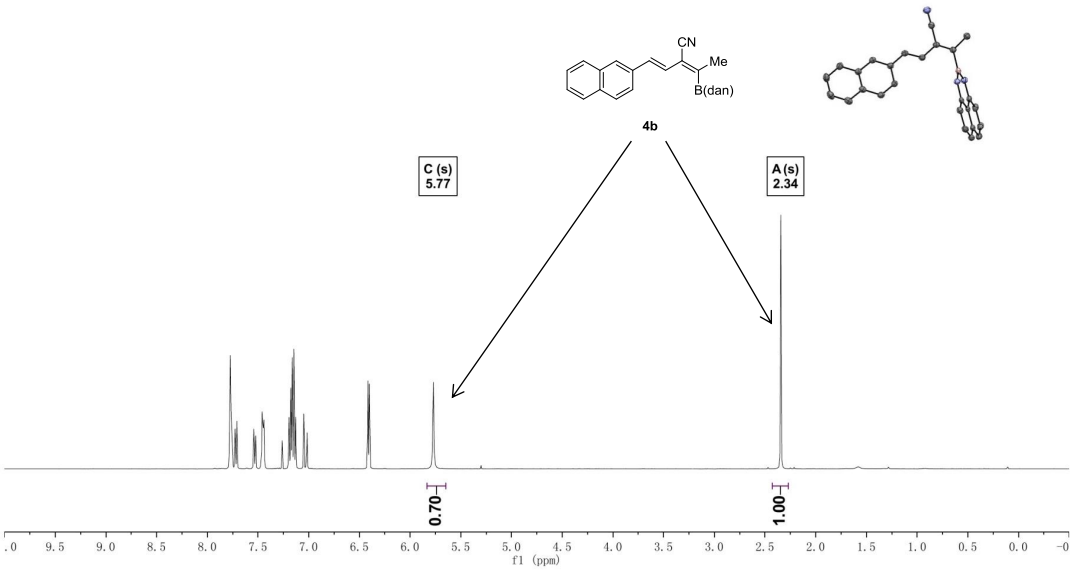
4t

4t, with 10 mol % Pd(COD)($CH_2TMS)_2$ and 10 mol% **L5** at 90 °C for 40 min, 45% yield (run1: 47%, run2: 43%), 96:4. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.13 (dd, *J* = 8.3, 7.2 Hz, 2H), 7.07 (dd, *J* = 8.3, 1.0 Hz, 2H), 6.42 – 6.23 (m, 5H), 5.68 (s, 2H), 2.20 (td, *J* = 7.5, 5.9 Hz, 2H), 1.50 – 1.38 (m, 2H), 1.36 – 1.23 (m, 6H), 0.92 – 0.82 (m, 3H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 141.3, 140.2, 137.7 (br), 136.4, 127.7, 126.6, 125.0, 120.1, 118.7, 117.9, 106.5, 32.9, 31.8, 29.0, 28.9, 22.7, 14.2; ^{11}B NMR (160 MHz, $CDCl_3$) δ 27.5; IR (ATR) 3387, 2923, 2853, 2223, 1629, 1598, 1502, 1406, 1373, 1331, 1165, 1143, 1047, 962, 819, 763 cm^{-1}; HRMS (DART) calcd for $C_{21}H_{25}BN_3$ ([M+H]$^+$) 330.21360, found 330.21405.

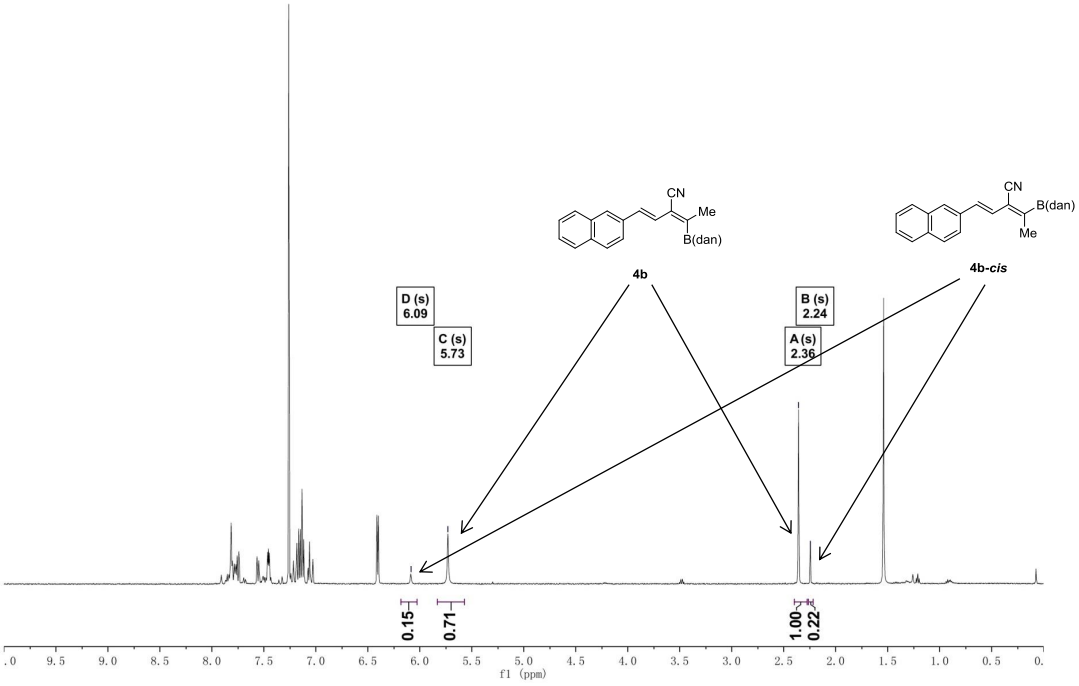
Assignment of the *trans/cis* Configuration of the Products

The trans/cis configuration of **4b** and **4j-B(pin)** was unambiguously determined by single-crystal X-ray diffraction analysis of the corresponding major pure isolated product. The assignment of the trans/cis configuration of the other products shown in Table 2 and Table 3 are made by analogy based on characteristic ^{1}H NMR signature of the Me and NH(Bdan) signals: the Me signal of the *trans* product (signal A) appears more downfield than the Me signal (signal B) of the *cis* product, and the NH(Bdan) signal of the *trans* product (signal C) appears more upfield than the NH(Bdan) signal (signal D) of the *cis* product (see below spectra). A mixture of *trans/cis* products can oftentimes be obtained in small quantities during the silica gel chromatography purification process. The labeled ^{1}H NMR spectra are shown using compound **4b** as the representative example.

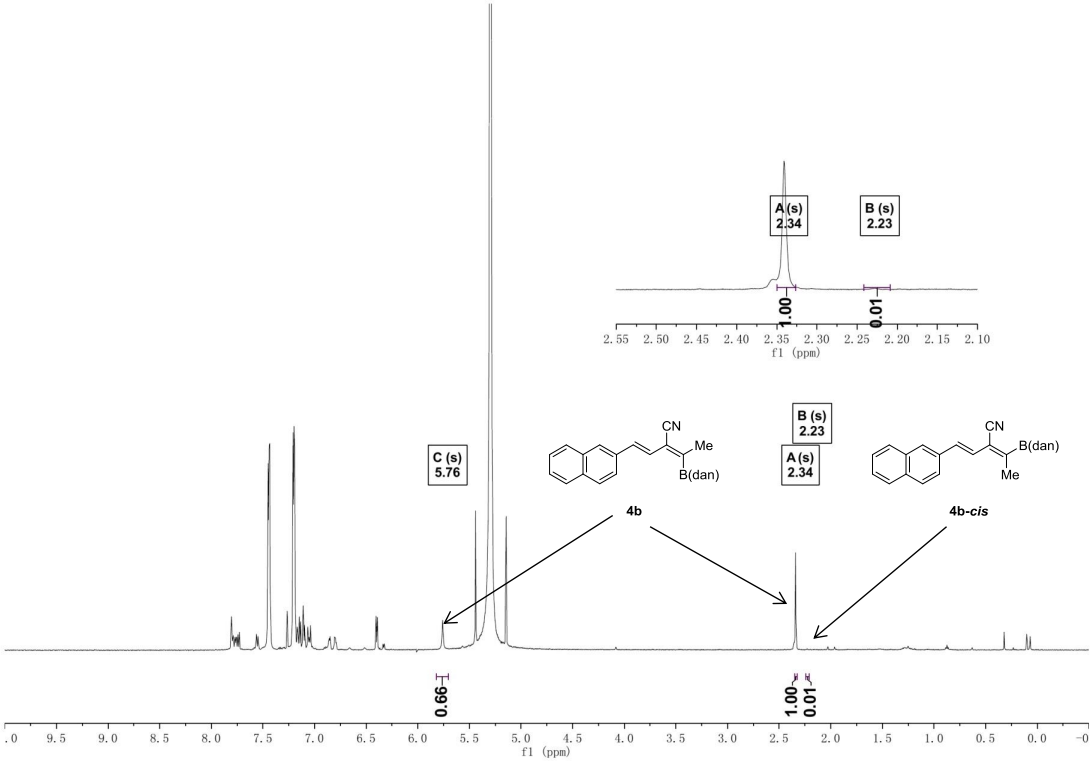
Fraction 2 of the crude mixture after column purification, pure **4b**.



Fraction 1 of the crude mixture after column purification, **4b** and **4b-cis** mixture.

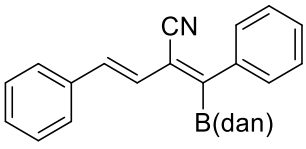


Crude mixture of **4b** and **4b-cis** after quenching with dan.



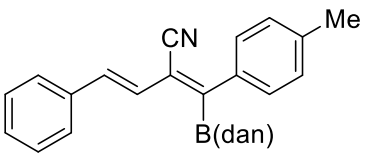
General Procedure for *trans*-Selective Cyanoboration Reaction of 1,3-Enynes (Table 3)

To a 4-mL vial charged with $Pd(COD)(CH_2TMS)_2$ (3.9 mg, 0.010 mmol, 10 mol %), **L5** (4.3 mg, 0.010 mmol, 10 mol %), CuCN (16 mg, 0.18 mmol, 1.8 equiv), BCatCl (28 mg, 0.18 mmol, 1.8 equiv.) and *o*-DCB (0.10 mL) was added the corresponding enyne (0.10 mmol, 1.0 equiv). The resulting mixture was allowed to stir for 1 hour at 105 °C. At the conclusion of the reaction, the mixture was passed through an acrodisc with CH_2Cl_2 under nitrogen. 1,8-diaminonaphthlene (32 mg, 0.20 mmol, 2.0 equiv) was then added to the filtrate, and the mixture was allowed to stir for another 12 hours. The reaction mixture was then again passed through an acrodisc and concentrated under reduced pressure. The resuting crude residue was purified by silica gel chromatography using hexanes/CH_2Cl_2 (4/1 to 1/1 gradient) as the eluent to afford the pure *trans*-selective cyanoboration product as yellow solids.



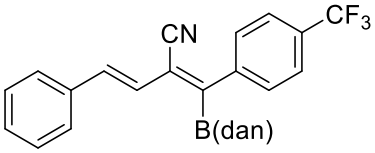
5a

5a, 60% yield (run1: 62%, run2: 57%), 86:14. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.59 (d, *J* = 7.5 Hz, 2H), 7.49 – 7.38 (m, 5H), 7.32 (m, 3H), 7.24 (d, *J* = 15.4 Hz, 1H), 7.14 (m, 5H), 6.37 (d, *J* = 6.8 Hz, 2H), 5.79 (s, 2H); ^{13}C NMR (151 MHz, $CDCl_3$) δ 140.2, 138.9, 136.4, 135.7, 129.5, 129.1, 129.0, 129.0, 128.8, 127.8, 127.6, 127.3, 124.9, 120.1, 119.1, 118.9, 116.6, 106.8 (*B*-alkenyl carbon signal not observed); ^{11}B NMR (160 MHz, $CDCl_3$) δ 29.1; IR (ATR) 3396, 3055, 2219, 1628, 1599, 1504, 1407, 1373, 1336, 1149, 820, 766, 695 cm^{-1}; HRMS (DART) calcd for $C_{27}H_{21}BN_3$ ($[M+H]^+$) 398.18230, found 398.18286.



5b

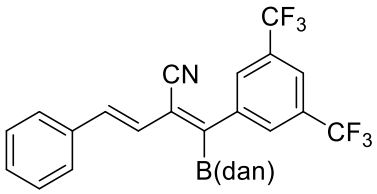
5b, 48% yield (run1: 46%, run2: 50%), 75:25. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.51 (d, *J* = 7.9 Hz, 2H), 7.45 (d, *J* = 7.0 Hz, 2H), 7.37 – 7.18 (m, 6H), 7.19 – 7.09 (m, 5H), 6.36 (dd, *J* = 7.0, 1.4 Hz, 2H), 5.79 (s, 2H), 2.40 (s, 3H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 140.2, 139.8, 136.4, 136.0, 135.9, 135.3, 129.7, 129.0, 129.0, 128.9, 127.8, 127.3, 125.0, 120.1, 118.8, 118.3, 116.9, 106.8, 21.5 (*B*-alkenyl carbon signal not observed); ^{11}B NMR (160 MHz, $CDCl_3$) δ 28.8; IR (ATR) 3419, 3055, 2923, 2219, 1599, 1507, 1406, 1374, 1338, 1260, 1147, 1052, 961, 908, 819, 765, 732 cm^{-1}; HRMS (DART) calcd for $C_{28}H_{23}BN_3$ ($[M+H]^+$) 412.19795, found 412.19878.



5c

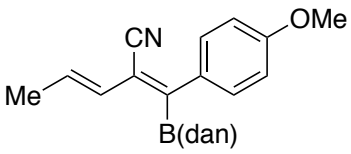
5c, 84% yield (run1: 82%, run2: 86%), 93:7. ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.70 (d, *J* = 8.5 Hz, 2H), 7.67 (d, *J* = 8.3 Hz, 2H), 7.49 – 7.42 (m, 2H), 7.37 – 7.30 (m, 3H), 7.27 (d, *J* = 15.6 Hz, 1H), 7.18 – 7.12 (m, 5H), 6.38 (dd, *J* = 6.7, 1.6 Hz, 2H), 5.78 (s, 2H); ^{13}C NMR (151 MHz, $CDCl_3$) δ 152.3 (br), 142.6, 139.9, 137.0, 136.3, 135.4, 131.1 (q, *J* = 32.9 Hz), 129.5, 129.1, 129.1, 127.8, 127.5, 126.0 (q, *J* = 3.8 Hz), 124.4, 124.0 (q, *J* = 272.4 Hz), 120.9, 120.1, 119.1, 116.1, 106.9; ^{11}B NMR (160 MHz, $CDCl_3$) δ 29.0; ^{19}F NMR (564 MHz, $CDCl_3$) δ –62.8; IR (ATR) 3394, 3055, 2921, 2217, 1628, 1598, 1502, 1408, 1373, 1334, 1148, 907, 820, 767, 730, 692, 648 cm^{-1}; HRMS (DART) calcd for $C_{28}H_{20}BN_3F_3$ ($[M+H]^+$) 466.16969, found 466.16856.

5d, 86% yield (run1: 88%, run2: 83%), >98:2. ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.96 (d, *J* = 1.5 Hz, 2H), 7.93 (s, 1H), 7.52 – 7.45 (m, 2H), 7.39 – 7.34 (m, 3H), 7.32 (d, *J* = 15.8 Hz, 1H), 7.20 – 7.13 (m, 5H), 6.41 (dd,



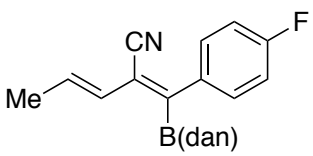
5d

J = 5.9, 2.4 Hz, 2H), 5.79 (s, 2H); ^{13}C NMR (151 MHz, $CDCl_3$) δ 150.1 (br), 141.2, 139.7, 138.2, 136.3, 135.2, 132.5 (q, *J* = 33.7 Hz), 129.8, 129.2, 128.8 (d, *J* = 3.5 Hz), 128.7 (d, *J* = 4.1 Hz), 127.8, 127.6, 123.8, 123.1 (q, *J* = 273.0 Hz), 122.9 (p, *J* = 3.8 Hz), 122.7, 119.4, 115.5, 107.1; ^{11}B NMR (160 MHz, $CDCl_3$) δ 28.7; ^{19}F NMR (564 MHz, $CDCl_3$) δ –62.8; IR (ATR) 3394, 3057, 2224, 1600, 1503, 1407, 1372, 1275, 1176, 1129, 820, 736, 680 cm^{-1}; HRMS (DART) calcd for $C_{29}H_{19}BN_3F_6$ ([M+H]$^+$) 534.15707, found 534.15663.



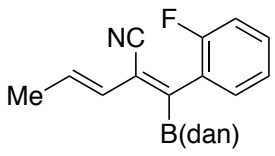
5e

5e, obtained by using hexane/Et_2O (5/1) as eluent, 71% yield (run1: 69%, run2: 73%), 94:6. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.58 – 7.48 (m, 2H), 7.18 – 7.07 (m, 4H), 6.96 – 6.89 (m, 2H), 6.47 – 6.31 (m, 4H), 5.73 (s, 2H), 3.83 (s, 3H), 1.88 (dd, *J* = 6.3, 1.1 Hz, 3H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 160.4, 151.5 (br), 140.3, 136.3, 132.9, 131.0, 130.4, 128.1, 127.7, 120.0, 118.6, 117.3, 116.8, 114.3, 106.6, 55.4, 18.4; ^{11}B NMR (160 MHz, $CDCl_3$) δ 29.0; IR (ATR) 3366, 2930, 2214, 1629, 1598, 1507, 1409, 1373, 1333, 1248, 1180, 1154, 1031, 953, 908, 821, 768, 732 cm^{-1}; HRMS (DART) calcd for $C_{23}H_{21}BN_3O$ ([M+H]$^+$) 366.17722, found 366.17607.



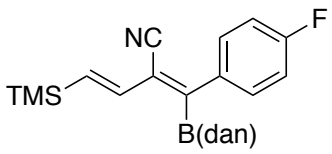
5f

5f, 70% yield (run1: 67%, run2: 72%), 95:5. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.52 (dd, *J* = 8.4, 5.3 Hz, 2H), 7.17 – 7.04 (m, 6H), 6.47 – 6.39 (m, 2H), 6.35 (dd, *J* = 7.0, 1.2 Hz, 2H), 5.70 (s, 2H), 1.90 (d, *J* = 4.9 Hz, 3H); ^{13}C NMR (151 MHz, $CDCl_3$) δ 163.1 (d, *J* = 250.1 Hz), 150.6 (br), 140.1, 136.3, 134.9 (d, *J* = 3.5 Hz), 134.3 (two signals), 130.6 (d, *J* = 8.3 Hz), 127.8, 120.0, 119.0, 118.9, 116.7, 116.0 (d, *J* = 21.8 Hz), 106.7, 18.5; ^{11}B NMR (160 MHz, $CDCl_3$) δ 29.0; ^{19}F NMR (470 MHz, $CDCl_3$) δ –111.5 (tt, *J* = 9.1, 5.2 Hz); IR (ATR) 3369, 2919, 2213,1600, 1504, 1413, 1374, 1335, 1231, 1159, 959, 820, 768 cm^{-1}; HRMS (DART) calcd for $C_{22}H_{18}BN_3F$ ([M+H]$^+$) 354.15723, found 354.15671.



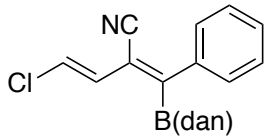
5g

5g, 63% yield (run1: 64%, run2: 61%), 98:2. Crystals for single crystal X-ray diffraction analysis were obtained by recrystallization from hexane/CH_2Cl_2 at –30 °C. ^{1}H NMR (500 MHz, THF-d_8) δ 7.51 – 7.35 (m, 3H), 7.30 (tdd, *J* = 7.3, 5.1, 1.8 Hz, 1H), 7.16 (td, *J* = 7.6, 1.1 Hz, 1H), 7.10 (ddd, *J* = 9.7, 8.4, 1.1 Hz, 1H), 6.97 (t, *J* = 7.8 Hz, 2H), 6.89 (dd, *J* = 8.3, 1.0 Hz, 2H), 6.59 (dq, *J* = 15.3, 1.6 Hz, 1H), 6.37 – 6.23 (m, 3H), 1.84 (dd, *J* = 6.8, 1.6 Hz, 3H); ^{13}C NMR (126 MHz, THF-d_8) δ 160.6 (d, *J* = 247.6 Hz), 142.6, 137.5, 133.8, 131.5 (d, *J* = 2.8 Hz), 131.1 (d, *J* = 8.2 Hz), 129.2, 128.8 (d, *J* = 14.8 Hz), 128.2, 125.1 (d, *J* = 3.5 Hz), 122.6, 121.5, 118.3, 116.6 (d, *J* = 22.0 Hz), 116.3, 106.8, 18.2 (*B*-alkenyl carbon signal not observed); ^{11}B NMR (160 MHz, THF-d_8) δ 25.4; ^{19}F NMR (470 MHz, THF-d_8) δ –110.2 (m); IR (ATR) 3060, 2977, 2923, 2218, 1638, 1555, 1447, 1394, 1360, 1334, 1266, 1229, 1139, 976, 953, 850, 801, 755 cm^{-1}; HRMS (DART) calcd for $C_{22}H_{18}BN_3F$ ([M+H]$^+$) 354.15723, found 354.15738.



5h

5h, 38% yield (run1: 40%, run2: 36%), 94:6. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.56 – 7.48 (m, 2H), 7.19 – 7.06 (m, 6H), 6.89 (d, *J* = 18.5 Hz, 1H), 6.67 (d, *J* = 18.5 Hz, 1H), 6.34 (dd, *J* = 7.0, 1.4 Hz, 2H), 5.70 (s, 2H), 0.13 (s, 9H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 163.3 (d, *J* = 250.7 Hz), 153.5 (br), 140.0, 139.2, 138.6, 136.3, 134.9 (d, *J* = 3.6 Hz), 130.8 (d, *J* = 8.5 Hz), 127.8, 121.5, 120.0, 118.9, 116.5, 116.1 (d, *J* = 21.8 Hz), 106.6, -1.3; ^{11}B NMR (160 MHz, $CDCl_3$) δ 29.8; ^{19}F NMR (470 MHz, $CDCl_3$) δ –110.9 (m); IR (ATR) 3360, 3056, 2955, 2897, 2218, 1599, 1505, 1409, 1373, 1336, 1247, 1235, 1160, 1145, 839, 820, 766 cm^{-1}; HRMS (DART) calcd for $C_{24}H_{24}BN_3FSi$ ([M+H]$^+$) 412.18111, found 412.18054.

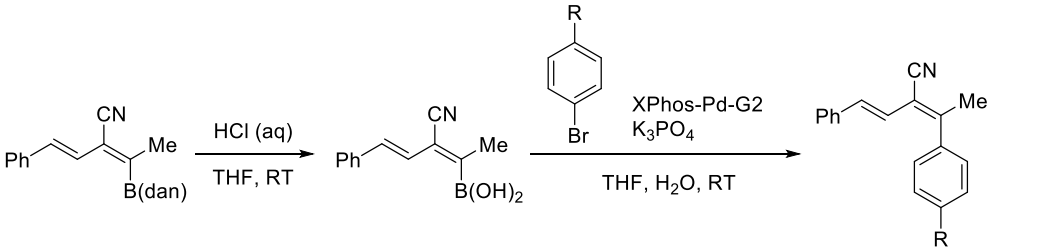


5i

5i, with 15 mol % **L5**, 1.2 equiv. CuCN and 1.6 equiv. BCatCl at 90 °C for 25 min, obtained by using hexane/Et_2O (8/1) as the eluent, 28% yield (run1: 27%, run2: 28%), 96:4. ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.59 – 7.49 (m, 2H), 7.49 – 7.35 (m, 3H), 7.18 – 7.04 (m, 4H), 6.89 (d, *J* = 1.1 Hz, 2H), 6.36 (dt, *J* = 6.9, 1.3 Hz, 2H), 5.71 (s, 2H); ^{13}C NMR (151 MHz, $CDCl_3$) δ 139.8, 138.1, 136.3, 130.1, 129.9, 129.1, 128.7, 127.8, 126.2, 120.1, 119.1, 115.8, 115.2, 106.9 (*B*-alkenyl carbon signal not observed); ^{11}B NMR (160 MHz, $CDCl_3$) δ 29.0; IR (ATR) 3397, 3365, 3062, 2220, 1629, 1599, 1505, 1407, 1374, 1336, 1151, 1051, 820, 766, 732, 696 cm^{-1}; HRMS (DART) calcd for $C_{21}H_{16}BN_3Cl$ ([M+H]$^+$) 356.11203, found 356.11198.

Functionalization of Cyanoboration Product 4a (Scheme 4)

Reaction sequence:



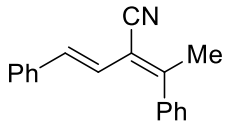
4a **6a** **R = H 6b**
R = 4-B(dan) 6c

Step 1:

Aqueous HCl (1.4 mL, 3.0 M) was added into a 20-mL vial charged with **4a** (33 mg, 0.10 mmol, 1.0 equiv.) and THF (2.8 mL). The resulting mixture was allowed to stir at room temperature for 30 minutes. At the conclusion of reaction, the mixture was diluted with Et_2O (4 mL), and the organic layer was separated. The aqueous layer was extracted with Et_2O (5 mL). The organic layers were combined and concentrated to afford **6a** as a mixture of boronic acid and the trimer boroxine. **6a** was used for the next step without further purification (quant. yield).

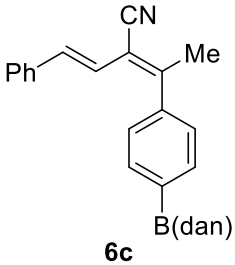
Step 2:

Under nitrogen to a 4-mL vial charged with **6a** (from Step 1)**,** XPhos-Pd-G2 (4 mg, 0.005 mmol, 0.05 equiv.), THF (0.3 mL), and aqueous K_3PO_4 (0.3 mL, 0.5 M) the corresponding aryl bromide (0.15 mmol, 1.5 equiv.) was added. The resulting mixture was allowed to stir for 3 hours at room temperature. Then, H_2O (1 mL) was added, and the organic layer was separated. The aqueous layer was further extracted with Et_2O (3 mL), and the organic layers were combined and concentrated. The resulting crude material was purified by silica gel chromatography using hexanes/EtOAc (10/1) as the eluent to afford **6b-c**.



6b

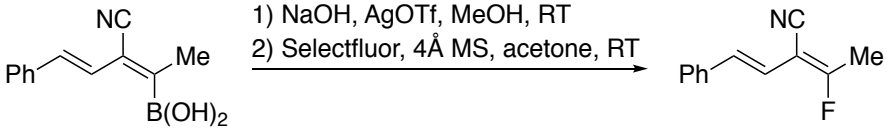
6b, 86% yield. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.48 – 7.36 (m, 3H), 7.31 – 7.16 (m, 7H), 7.01 (d, *J* = 16.0 Hz, 1H), 6.71 (d, *J* = 16.0 Hz, 1H), 2.53 (s, 3H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 153.7, 139.3, 136.3, 133.2, 129.1, 128.8, 128.8, 128.4, 128.1, 126.9, 122.2, 117.0, 112.2, 25.3; IR (ATR) 3058, 2922, 2219, 1492, 1441, 1274, 1025, 960, 765, 754, 699, 693 cm^{-1}; HRMS (DART) calcd for $C_{18}H_{16}N$ ($[M+H]^+$) 246.12773, found 246.12774.



6c

6c, 85% yield. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.72 (d, *J* = 7.8 Hz, 2H), 7.38 – 7.22 (m, 7H), 7.18 (t, *J* = 7.8 Hz, 2H), 7.10 (d, *J* = 8.3 Hz, 2H), 7.05 (d, *J* = 16.0 Hz, 1H), 6.74 (d, *J* = 16.0 Hz, 1H), 6.46 (d, *J* = 7.2 Hz, 2H), 6.09 (s, 2H), 2.56 (s, 3H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 153.1, 141.0, 140.9, 136.5, 136.2, 133.6, 131.9, 128.8, 128.5, 127.9, 127.8, 127.0, 122.0, 120.0, 118.2, 116.9, 112.4, 106.3, 25.2 (*B*-aryl carbon signal not observed); ^{11}B NMR (160 MHz, $CDCl_3$) δ 29.0; IR (ATR) 3416, 3054, 2218, 1599, 1524, 1493,1408, 1374, 1332, 1088, 820, 764, 692 cm^{-1}; HRMS (DART) calcd for $C_{28}H_{23}BN_3$ ($[M+H]^+$) 412.19795, found 412.19759.

Synthesis of Compound **6d**

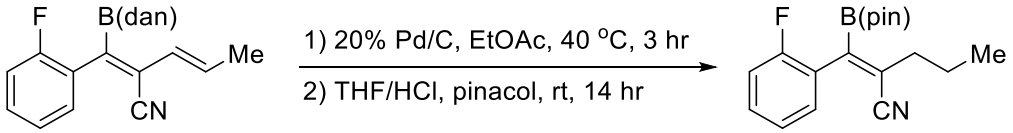


6a **6d**

Under nitrogen to a 4-mL vial charged with a solution of NaOH (9.6 mg, 0.24 mmol, 1.2 equiv.) in MeOH (2.0 mL) was added **6a** (0.20 mmol, 1.0 equiv.) at room temperature. The resulting mixture was allowed to stir for 15 minutes, and then the mixture was cooled to 0 °C. AgOTf (154 mg, 0.600 mmol, 3.00 equiv.) was added in the absence of light, and the resulting mixture was allowed to stir for 30 minutes at 0°C. Then, methanol was removed *in vacuo,* and anhydrous acetone (1 mL) was added and then removed under reduced pressure to help remove methanol. After repeating for four times, 4Å Molecular sieve (100 mg), Selectfluor (85 mg, 0.24 mmol, 1.2 equiv.), and acetone (2 mL) were added to the residue. The resulting slurry was allowed to stir for 2 hours at room temperature. At the conclusion of reaction, the mixture was passed through an acrodisc and washed with acetone. The filtrate was concentrated, dissolved in Et_2O (5 mL) and further washed with H_2O (5 mL). The organic layer was dried with Na_2SO_4, and **6d** was obtained via silica gel chromatography using hexanes/EtOAc (15/1) as the eluent as a white solid (67% yield).

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.45 (d, *J* = 7.2 Hz, 2H), 7.35 (t, *J* = 7.4 Hz, 2H), 7.33 – 7.27 (m, 1H), 6.88 (s, 2H), 2.39 (d, *J* = 17.0 Hz, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 168.7 (d, *J* = 280.5 Hz), 135.9 (d, *J* = 1.3 Hz), 132.7 (d, *J* = 4.2 Hz), 128.9, 128.8, 127.0, 115.6 (d, *J* = 3.6 Hz), 115.3 (d, *J* = 13.7 Hz), 98.8 (d, *J* = 28.6 Hz), 18.3 (d, *J* = 24.7 Hz); ^{19}F NMR (564 MHz, $CDCl_3$) δ –75.6 (q, *J* = 17.0 Hz); IR (ATR) 3027, 2960, 2923, 2229, 1651, 1625, 1496, 1430, 1388, 1312, 1303, 1216, 1184, 1059, 1028, 953, 802, 688 cm^{-1}; HRMS (DART) calcd for $C_{12}H_{11}NF$ ($[M+H]^+$) 188.08700, found 188.08652.

Synthesis of Compound **6e** (eq1)



5g **6e**

Palladium on carbon (12 mg, 0.011 mmol, 10% wt, 0.20 equiv.), **5g** (20 mg, 0.057 mmol, 1.0 equiv.), and EtOAc (0.60 mL) were added into a 4-mL vial. The vial was quickly placed under vacuum and then back filled with H_2 (1 atm) twice, and the mixture was allowed to heat at 40 °C for 3 hours under a H_2 balloon pressue. At the conclusion of reaction, the reaction mixture was passed through an acrodisc, and all volaties were removed *in vacuo*. Pinacol (47 mg, 0.40 mmol, 7.0 equiv.) was added to this residue along with THF (1.5 mL) and aqueous HCl (0.75 mL, 4.3 M). The resulting mixture was allowed to stir for 14 hours at room temperature followed by addition of Et_2O (5 mL) and H_2O (5 mL). The organic layer was separated and the aqueous layer was further washed with Et_2O (5 mL). The combined organic layers were concentrated, and the crude material was purified via silica gel chromatography using hexanes/EtOAc (8/1) as the eluent to afford **6e** as a white solid (54% yield).

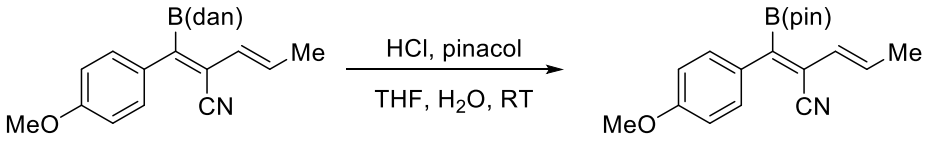
^{1}H NMR (500 MHz, $CDCl_3$) δ 7.39 (td, *J* = 7.7, 1.8 Hz, 1H), 7.35 – 7.29 (m, 1H), 7.17 (td, *J* = 7.6, 1.1 Hz, 1H), 7.06 (ddd, *J* = 9.6, 8.3, 1.1 Hz, 1H), 2.68 – 2.61 (m, 2H), 1.71 (h, *J* = 7.4 Hz, 2H), 1.28 (s, 12H), 1.01 (t, *J* = 7.4 Hz, 3H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 159.6 (d, *J* = 246.5 Hz), 130.4, 130.4 (d, *J* = 10.6 Hz),

128.0, 127.5 (d, *J* = 15.1 Hz), 124.4 (d, *J* = 3.4 Hz), 118.4, 115.5 (d, *J* = 21.9 Hz), 84.7, 36.0, 24.8, 22.3, 13.4 (*B*-alkenyl carbon signal not observed); ^{11}B NMR (160 MHz, $CDCl_3$) δ 29.9; ^{19}F NMR (470 MHz, $CDCl_3$) δ –112.8 (m); IR (ATR) 2963, 2929, 2873, 2213, 1486, 1450, 1357, 1327, 1268, 1140, 1081, 971, 846, 753 cm^{-1}; HRMS (DART) calcd for $C_{18}H_{24}BNO_2F$ ([M+H]$^+$) 316.18786, found 316.18866.

Synthesis of Satigrel (Scheme 5)

Reaction sequence:

Step 1:

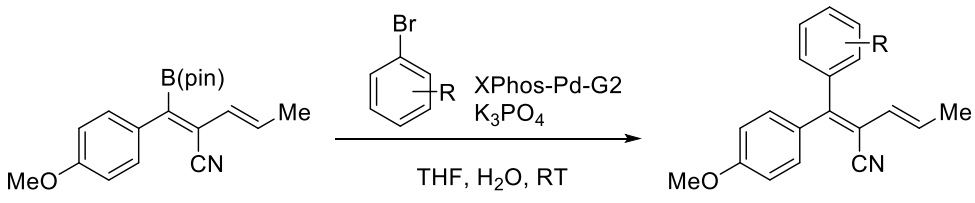


5e **8a-S1**

To a 20-mL vial charged with **5e** (146 mg, 0.400 mmol, 1.00 equiv.), pinacol (236 mg, 2.00 mmol, 5.00 equiv.) and THF (8 mL) was added followed by aqueous HCl (6.0 mL, 4.3 M). The resulting mixture was allowed to stir at room temperature for 20 hours. At the conclusion of reaction, Et_2O (4 mL) was added to the mixture, and the organic layer was separated. The aqueous layer was further extracted with additional Et_2O (5 mL). The combined organic layers were concentrated under reduce pressure, and the resulting crude material was further purified by silica gel chromatography using hexanes/EtOAc (5/1) as the eluent to afford **8a-S1** as a white solid (84% yield).

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.40 – 7.34 (m, 2H), 6.94 – 6.86 (m, 2H), 6.69 (dq, *J* = 15.4, 1.6 Hz, 1H), 6.38 (dq, *J* = 15.3, 6.8 Hz, 1H), 3.82 (s, 3H), 1.90 (dd, *J* = 6.8, 1.7 Hz, 3H), 1.33 (s, 12H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 159.9, 133.7, 131.4, 130.1, 127.9, 121.9, 116.9, 113.9, 84.8, 55.4, 24.9, 18.6 (*B*-alkenyl carbon signal not observed); ^{11}B NMR (160 MHz, $CDCl_3$) δ 30.0; IR (ATR) 2978, 2934, 2838, 2218, 1604, 1509, 1357, 1328, 1291, 1250, 1178, 1137, 1032, 972, 849, 832, 732 cm^{-1}; HRMS (DART) calcd for $C_{19}H_{25}BNO_3$ ([M+H]$^+$) 326.19220, found 326.19142.

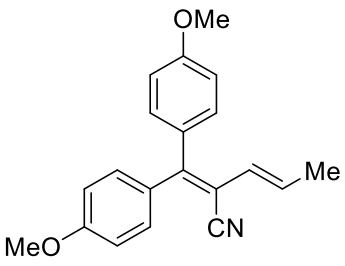
Step 2:



8a-S1

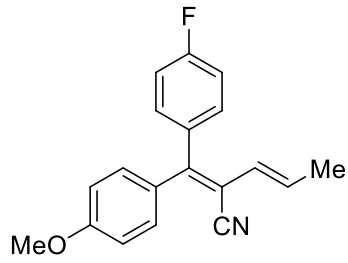
R = 4-OMe 8a
R = 4-F 8b
R = 3-OMe 8c

Under nitrogen to a 20-mL vial charged with **8a-S1** (109 mg, 0.330 mmol, 1.00 equiv.) and XPhos-Pd-G2 (13 mg, 0.016 mmol, 0.050 equiv.) was added THF (2.7 mL), aqueous K_3PO_4 (0.9 mL, 0.6 M) and the corresponding aryl bromide (0.50 mmol, 1.5 equiv.). The resulting mixture was allowed to stir for 15 hours at room temperature. Then, H_2O (1 mL) was added and the organic layer was separated. The aqueous layer was further extracted with Et_2O (3 mL), and the organic layers were combined and concentrated. This crude material was purified by silica gel chromatography using hexanes/EtOAc (15/1) as the eluent to afford **8a**-**8c** as white solids.



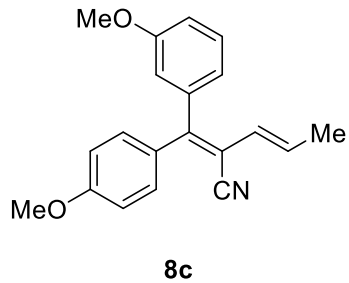
8a

8a with 4-bromo-anisole, 88% yield. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.33 – 7.28 (m, 2H), 7.13 – 7.07 (m, 2H), 6.93 – 6.85 (m, 4H), 6.32 (dq, *J* = 15.4, 6.6 Hz, 1H), 6.21 (dq, *J* = 15.4, 1.5 Hz, 1H), 3.85 (s, 3H), 3.84 (s, 3H), 1.82 (dd, *J* = 6.7, 1.5 Hz, 3H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 160.7, 160.3, 153.3, 132.7, 132.1, 131.7, 131.4, 131.3, 126.6, 118.8, 113.8, 113.7, 108.8, 55.4, 55.4, 18.4; IR (ATR) 3005, 2930, 2838, 2214, 1602, 1573, 1506, 1461, 1442, 1302, 1282, 1247, 1172, 1029, 960, 829, 737, 603, 572 cm^{-1}; HRMS (DART) calcd for $C_{20}H_{20}NO_2$ ([M+H]$^+$) 306.14886, found 306.14963.



8b

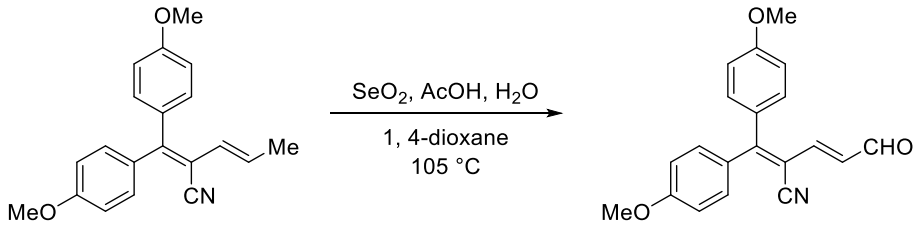
8b with 4-bromo-fluorobenzene, 80% yield. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.35 – 7.27 (m, 2H), 7.15 (ddt, *J* = 8.2, 5.1, 2.5 Hz, 2H), 7.12 – 7.04 (m, 2H), 6.92 – 6.84 (m, 2H), 6.35 (dq, *J* = 15.4, 6.8 Hz, 1H), 6.10 (dq, *J* = 15.4, 1.6 Hz, 1H), 3.83 (s, 3H), 1.82 (dd, *J* = 6.8, 1.6 Hz, 3H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 163.1 (d, *J* = 249.9 Hz), 160.9, 152.2, 135.2 (d, *J* = 3.4 Hz), 132.5, 132.4, 132.2, 131.6, 126.2, 118.4, 115.6 (d, *J* = 21.5 Hz), 113.9, 110.0, 55.5, 18.5; ^{19}F NMR (470 MHz, $CDCl_3$) δ –111.6 (ddd, *J* = 13.5, 8.4, 5.1 Hz); IR (ATR) 2960, 2926, 2850, 2216, 1602, 1575, 1505, 1461, 1444, 1289, 1251, 1228, 1173, 1158, 1095,1028, 960 831, 804, 736, 566 cm^{-1}; HRMS (DART) calcd for $C_{19}H_{16}NOF$ ([M+H]$^+$) 293.12104, found 293.11995.



8c

8c with 3-bromo-anisole, 90% yield. ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.35 – 7.24 (m, 3H), 6.93 (dd, *J* = 8.4, 2.5 Hz, 1H), 6.91 – 6.84 (m, 2H), 6.76 (dt, *J* = 7.6, 1.2 Hz, 1H), 6.68 (dd, *J* = 2.7, 1.5 Hz, 1H), 6.38 – 6.25 (m, 1H), 6.15 (dq, *J* = 15.4, 1.5 Hz, 1H), 3.83 (d, *J* = 0.9 Hz, 3H), 3.78 (d, *J* = 0.9 Hz, 3H), 1.81 (dt, *J* = 6.8, 1.2 Hz, 3H); ^{13}C NMR (151 MHz, $CDCl_3$) δ 160.7, 159.6, 153.2, 140.5, 132.2, 132.0, 131.5, 129.5, 126.4, 122.8, 118.5, 115.9, 114.5, 113.8, 109.9, 55.5, 55.5, 18.5; IR (ATR) 3004, 2935, 2913, 2837, 2216, 1604, 1576, 1509, 1462, 1446, 1287, 1253, 1178, 1034, 961, 837, 802, 787, 700 cm^{-1}; HRMS (DART) calcd for $C_{20}H_{20}NO_2$ ([M+H]$^+$) 306.14886, found 306.14950.

Step 3:



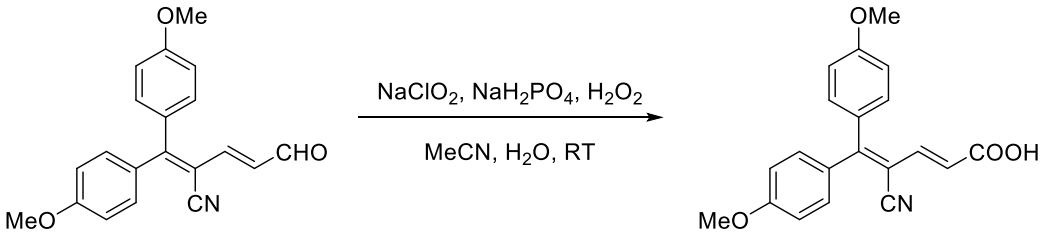
8a **9a-S1**

SeO_2 (162 mg, 1.45 mmol, 5.00 equiv.) and **8a** (89 mg, 0.29 mmol, 1.0 equiv.) were placed in a 20-mL vial. To this vial 1,4-dioxane (1.8 mL), H_2O (0.10 mL) and AcOH (0.050 mL) were added successively.

The resulting mixture was allowed to stir at 105 °C for 12 hours. Then, another portion of SeO_2 (64 mg, 0.58 mmol, 2.0 equiv.) was added, and the mixture was allowed to stir for another 12 hours at 105 °C. At the conclusion of reaction, the reaction mixture was passed through celite, and the filtrate was concentrated. This crude residue was purified by silica gel chromatography using hexanes/EtOAc (4/1) as the eluent to afford **9a-S1** as a yellow solid (77% yield).

^{1}H NMR (500 MHz, $CDCl_3$) δ 9.55 (d, *J* = 7.5 Hz, 1H), 7.46 – 7.36 (m, 2H), 7.25 (d, *J* = 15.5 Hz, 1H), 7.18 – 7.12 (m, 2H), 7.00 – 6.95 (m, 2H), 6.95 – 6.91 (m, 2H), 6.67 (dd, *J* = 15.5, 7.5 Hz, 1H), 3.89 (s, 3H), 3.87 (s, 3H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 192.6, 164.5, 162.4, 162.0, 147.1, 133.1, 132.9, 131.3, 131.0 (two signals), 130.1, 114.2, 114.0, 105.7, 55.6, 55.6; IR (ATR) 3007, 2934, 2839, 2730, 2214, 1672, 1593, 1573, 1501, 1253, 1171, 1116, 1027, 835, 732 cm^{-1}; HRMS (DART) calcd for $C_{20}H_{18}NO_3$ ([M+H]$^+$) 320.12812, found 320.12696.

Step 4:

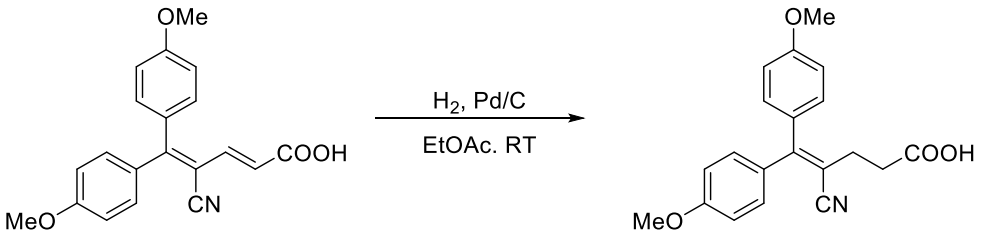


9a-S1 **9a**

H_2O (0.50 mL), MeCN (0.13 mL) and aqueous H_2O_2 (35% v/v, 0.25 mmol, 25 μl, 2.0 equiv.) were added to a 4-mL vial charged with **9a-S1** (40.4 mg, 0.125 mmol, 1.00 equiv.) and NaH_2PO_4 (7.8 mg, 0.065 mmol, 0.52 equiv.). The mixture was cooled to 0 °C and then a pre-cooled solution (0 °C) of $NaClO_2$ (35 mg, 0.31 mmol, 2.5 equiv.) in H_2O (0.31 mL) was added in a dropwise fashion. The mixture was allowed to stir for 30 min and then allowed to warm to room temperature. At the conclusion of reaction, Et_2O (5 mL) and H_2O (3 mL) were added to this mixture. The organic layer was separated, and the concentrated organic layer was purified by silica gel chromatography using hexanes/EtOAc (1/1) as the eluent to afford **9a** as a yellow solid (69% yield).

^{1}H NMR (500 MHz, CDCl3) δ 11.79 (s, br, 1H), 7.53 (d, *J* = 15.4 Hz, 1H), 7.41 – 7.35 (m, 2H), 7.14 – 7.07 (m, 2H), 6.98 – 6.88 (m, 4H), 6.42 (d, *J* = 15.5 Hz, 1H), 3.88 (s, 3H), 3.86 (s, 3H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 171.8, 164.0, 162.2, 161.9, 142.4, 133.2, 132.8, 131.6, 130.3, 120.6, 117.8, 114.2, 114.0, 105.5, 55.6, 55.6; IR (ATR) 2934, 2839, 2213, 1685, 1598, 1508, 1286, 1255, 1210, 1173, 1029, 836, 732 cm^{-1}; HRMS (DART) calcd for $C_{20}H_{18}NO_4$ ([M+H]$^+$) 336.12303, found 336.12345.

Step 5:



9a **7**

A 4-mL vial was charged with **9a** (10.2 mg, 0.0300 mmol, 1.00 equiv), Pd/C (3.1 mg, 0.0030 mmol, 10% wt, 0.10 equiv) and EtOAc (0.4 mL). The vial was quickly placed under vacuum and then and back filled with H_2 (1 atm) twice. The resulting mixture was allowed to stir at room temperature for 2 hours under a H_2 balloon pressure. At the conclusion of reaction, all violates were removed *in vacuo*, and the residue was purified by silica gel chromatography using EtOAc as the eluent to afford **7** as a white solid (91% yield, 97:3 hydrogenation selectivity (**7** *vs.* fully hydrogenated byproduct)).

^{1}H NMR (600 MHz, $CDCl_3$) δ 7.27 (d, *J* = 8.8 Hz, 2H), 7.07 – 7.01 (m, 2H), 6.92 – 6.83 (m, 4H), 3.83 (s, 3H), 3.82 (s, 3H), 2.71 (apparent s, 4H), (COOH signal not observed); ^{13}C NMR (151 MHz, $CDCl_3$) δ 173.6 (br), 160.7, 160.3, 158.2, 132.4, 131.3, 131.1, 131.0, 120.0, 114.0, 113.8, 107.0, 55.5, 55.5, 32.8, 27.4; IR (ATR) 2931, 2839, 2204, 1709, 1605, 1509, 1283, 1249, 1174, 1030, 833 cm^{-1}; HRMS (DART) calcd for $C_{20}H_{20}NO_4$ ($[M+H]^+$) 338.13868, found 338.13898.

Crystallographic Data for 4b, 4j-B(pin) and 5g

Crystal Data for 4b:

Identification code	C26H20BN3	
Empirical formula	C26 H20 B N3	
Formula weight	385.26	
Temperature	123(2) K	
Wavelength	1.54178 Å	
Crystal system	Tetragonal	
Space group	$P4_2/n$	
Unit cell dimensions	a = 23.0525(5) Å	α= 90°.
	b = 23.0525(5) Å	β= 90°.
	c = 7.6338(2) Å	γ = 90°.
Volume	4056.7(2) $Å^3$	
Z	8	
Density (calculated)	1.262 Mg/m^3	
Absorption coefficient	0.574 mm^{-1}	
F(000)	1616	
Crystal size	0.560 x 0.220 x 0.160 mm^3	
Theta range for data collection	2.711 to 66.840°.	
Index ranges	-27<=h<=22, -27<=k<=27, -9<=l<=9	
Reflections collected	22309	
Independent reflections	3569 [R(int) = 0.0276]	
Completeness to theta = 66.840°	99.2 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.7528 and 0.6580	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	3569 / 2 / 278	
Goodness-of-fit on F^2	1.060	
Final R indices [I>2sigma(I)]	R1 = 0.0338, wR2 = 0.0869	
R indices (all data)	R1 = 0.0345, wR2 = 0.0874	
Extinction coefficient	n/a	
Largest diff. peak and hole	0.206 and -0.156 $e.Å^{-3}$	

Crystal Data for 4j-B(pin):

Identification code	C21H26BNO4	
Empirical formula	C21 H26 B N O4	
Formula weight	367.24	
Temperature	123(2) K	
Wavelength	1.54178 Å	
Crystal system	Orthorhombic	
Space group	Fdd2	
Unit cell dimensions	a = 31.1427(6) Å	α= 90°.
	b = 37.9695(8) Å	β= 90°.
	c = 13.9845(3) Å	γ = 90°.
Volume	16536.3(6) $Å^3$	
Z	32	
Density (calculated)	1.180 Mg/m^3	
Absorption coefficient	0.645 mm^{-1}	
F(000)	6272	
Crystal size	0.580 x 0.280 x 0.150 mm^3	
Theta range for data collection	3.655 to 66.608°.	
Index ranges	-37<=h<=36, -41<=k<=45, -16<=l<=16	
Reflections collected	30171	
Independent reflections	7254 [R(int) = 0.0267]	
Completeness to theta = 66.608°	99.7 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.7528 and 0.6531	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	7254 / 571 / 575	
Goodness-of-fit on F^2	1.035	
Final R indices [I>2sigma(I)]	R1 = 0.0369, wR2 = 0.1073	
R indices (all data)	R1 = 0.0383, wR2 = 0.1091	
Extinction coefficient	n/a	
Largest diff. peak and hole	0.258 and -0.215 $e.Å^{-3}$	

Crystal Data for 5g:

Identification code	C22H17BFN3	
Empirical formula	C22 H17 B F N3	
Formula weight	353.19	
Temperature	173(2) K	
Wavelength	1.54178 Å	
Crystal system	Monoclinic	
Space group	$P2_1/n$	
Unit cell dimensions	a = 8.7227(4) Å	α= 90°.
	b = 7.3770(3) Å	β= 98.3760(10)°.
	c = 28.3779(11) Å	γ = 90°.
Volume	1806.57(13) $Å^3$	
Z	4	
Density (calculated)	1.299 Mg/m^3	
Absorption coefficient	0.675 mm^{-1}	
F(000)	736	
Crystal size	0.420 x 0.280 x 0.260 mm^3	
Theta range for data collection	3.148 to 66.424°.	
Index ranges	-10<=h<=10, -8<=k<=8, -33<=l<=32	
Reflections collected	19722	
Independent reflections	3171 [R(int) = 0.0228]	
Completeness to theta = 66.424°	99.4 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.7528 and 0.6787	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	3171 / 2 / 251	
Goodness-of-fit on F^2	1.036	
Final R indices [I>2sigma(I)]	R1 = 0.0438, wR2 = 0.1190	
R indices (all data)	R1 = 0.0477, wR2 = 0.1236	
Extinction coefficient	n/a	
Largest diff. peak and hole	0.733 and -0.331 $e.Å^{-3}$	

NMR Spectra Collection

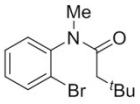
Agilent Technologies

Sample Name:

Data Collected on:
nmr18-vnmrs500
Archive directory:

Sample directory:

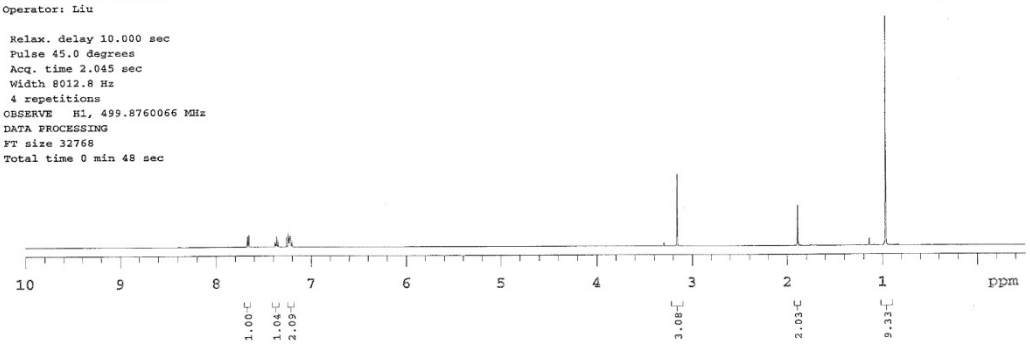
FidFile: yz-4-amide-H



Pulse Sequence: PROTON (s2pul)
Solvent: cdcl3
Data collected on: Dec 17 2019

Temp. 25.0 C / 298.1 K
Operator: Liu

Relax. delay 10.000 sec
Pulse 45.0 degrees
Acq. time 2.045 sec
Width 8012.8 Hz
4 repetitions
OBSERVE H1, 499.8760066 MHz
DATA PROCESSING
FT size 32768
Total time 0 min 48 sec



Agilent Technologies

Sample Name:

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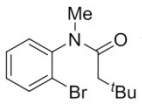
nmr18-vnmrs500
Archive directory:

Sample directory:

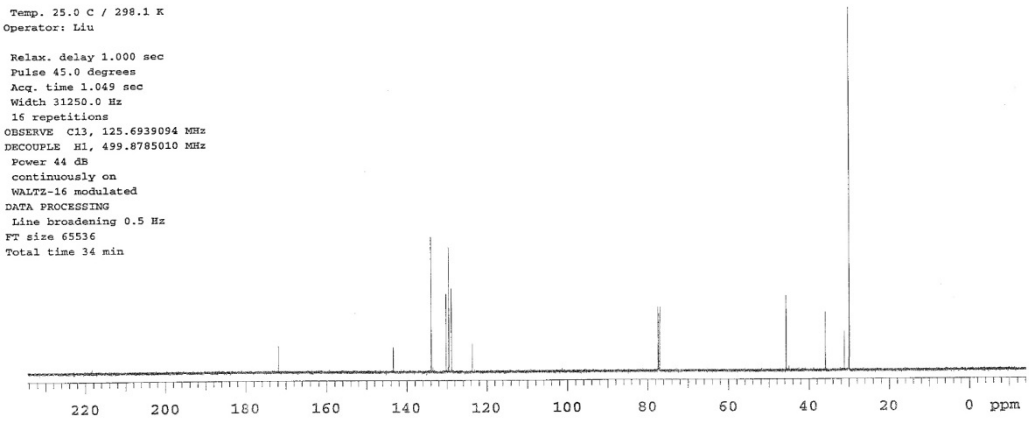
FidFile: yz-4-amide-C



Pulse Sequence: CARBON (s2pul)
Solvent: cdcl3
Data collected on: Feb 20 2020

Temp. 25.0 C / 298.1 K
Operator: Liu

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.049 sec
Width 31250.0 Hz
16 repetitions
OBSERVE C13, 125.6939094 MHz
DECOUPLE H1, 499.8785010 MHz
Power 44 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 0.5 Hz
FT size 65536
Total time 34 min

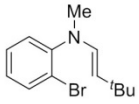


Sample Name:

Data Collected on:
nmr19-vnmrs600
Archive directory:

Sample directory:

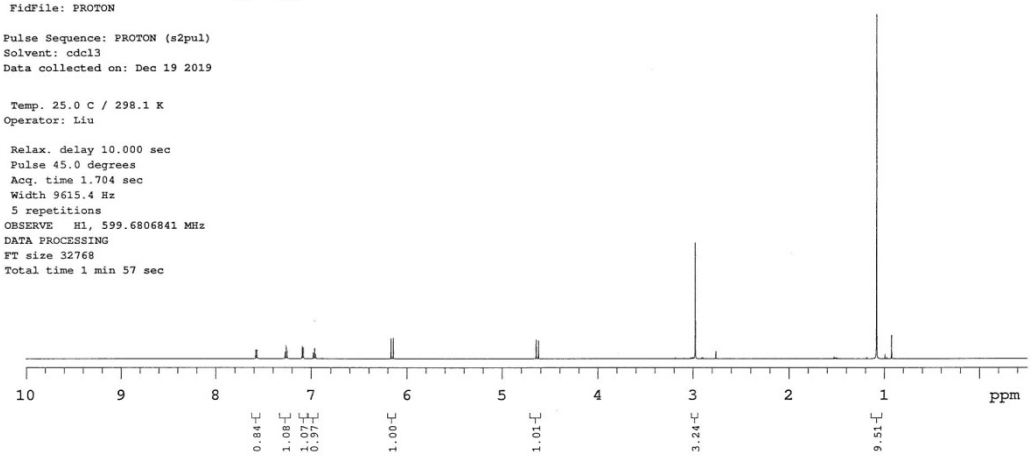
FidFile: PROTON



Pulse Sequence: PROTON (s2pul)
Solvent: cdcl3
Data collected on: Dec 19 2019

Temp. 25.0 C / 298.1 K
Operator: Liu

Relax. delay 10.000 sec
Pulse 45.0 degrees
Acq. time 1.704 sec
Width 9615.4 Hz
5 repetitions
OBSERVE H1, 599.6806841 MHz
DATA PROCESSING
FT size 32768
Total time 1 min 57 sec

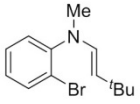


Sample Name:

Data Collected on:
nmr19-vnmrs600
Archive directory:

Sample directory:

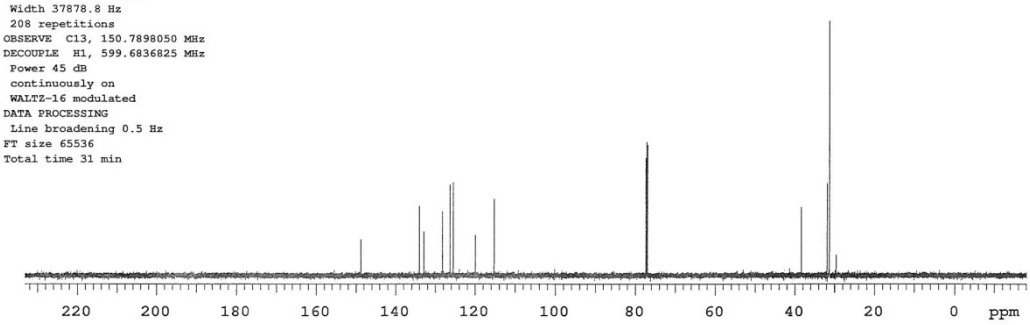
FidFile: CARBON



Pulse Sequence: CARBON (s2pul)
Solvent: cdcl3
Data collected on: Dec 19 2019

Temp. 25.0 C / 298.1 K
Operator: Liu

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 0.865 sec
Width 37878.8 Hz
208 repetitions
OBSERVE C13, 150.7898050 MHz
DECOUPLE H1, 599.6836825 MHz
Power 45 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 0.5 Hz
FT size 65536
Total time 31 min



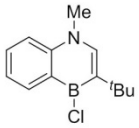
Agilent Technologies

Sample Name:

Data Collected on:
nmr18-vnmrs500
Archive directory:

Sample directory:

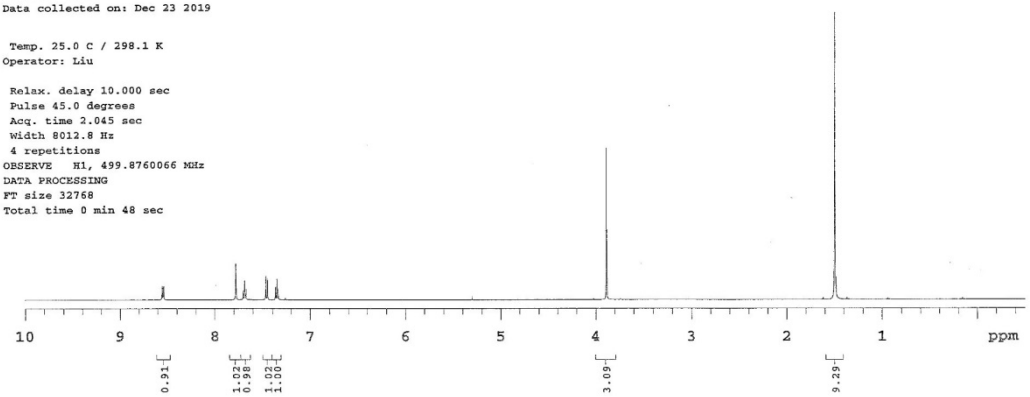
FidFile: PROTON



Pulse Sequence: PROTON (s2pul)
Solvent: cdcl3
Data collected on: Dec 23 2019

Temp. 25.0 C / 298.1 K
Operator: Liu

Relax. delay 10.000 sec
Pulse 45.0 degrees
Acq. time 2.045 sec
Width 8012.8 Hz
4 repetitions
OBSERVE H1, 499.8760066 MHz
DATA PROCESSING
FT size 32768
Total time 0 min 48 sec



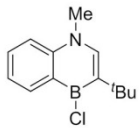
Agilent Technologies

Sample Name:

Data Collected on:
nmr18-vnmrs500
Archive directory:

Sample directory:

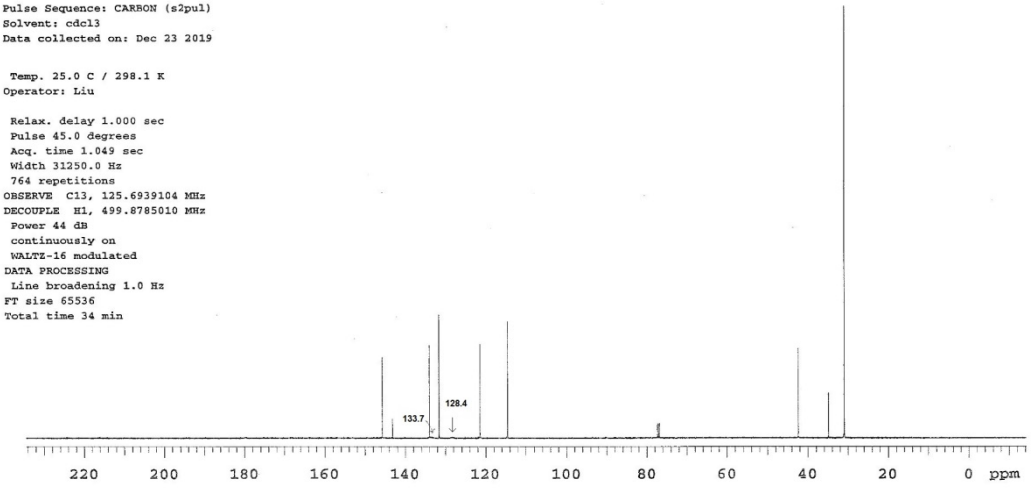
FidFile: CARBON

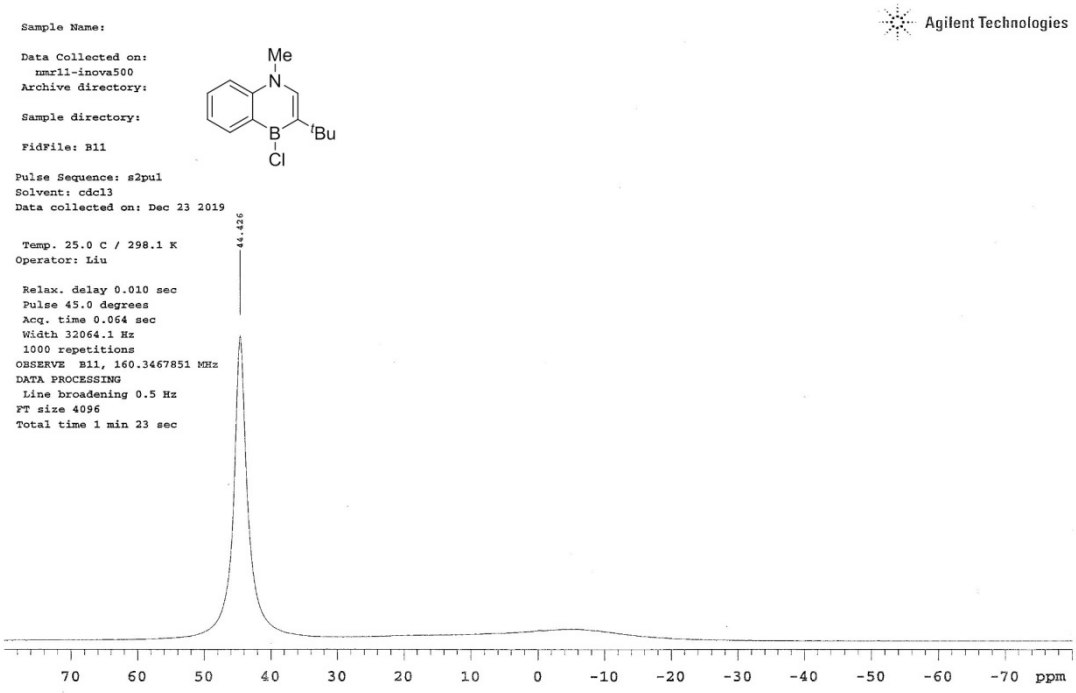


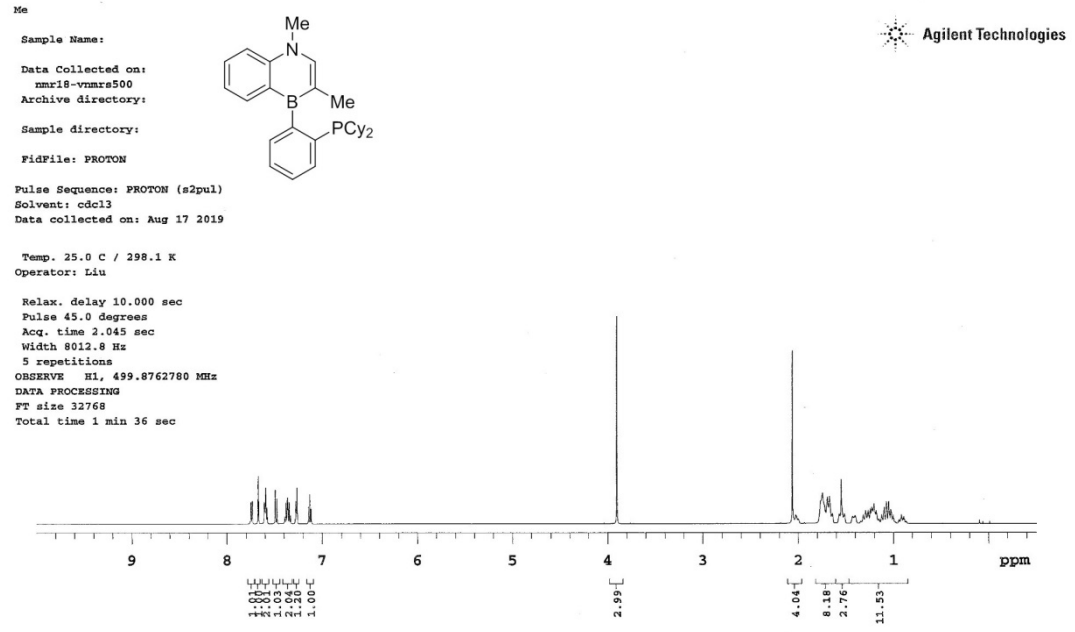
Pulse Sequence: CARBON (s2pul)
Solvent: cdcl3
Data collected on: Dec 23 2019

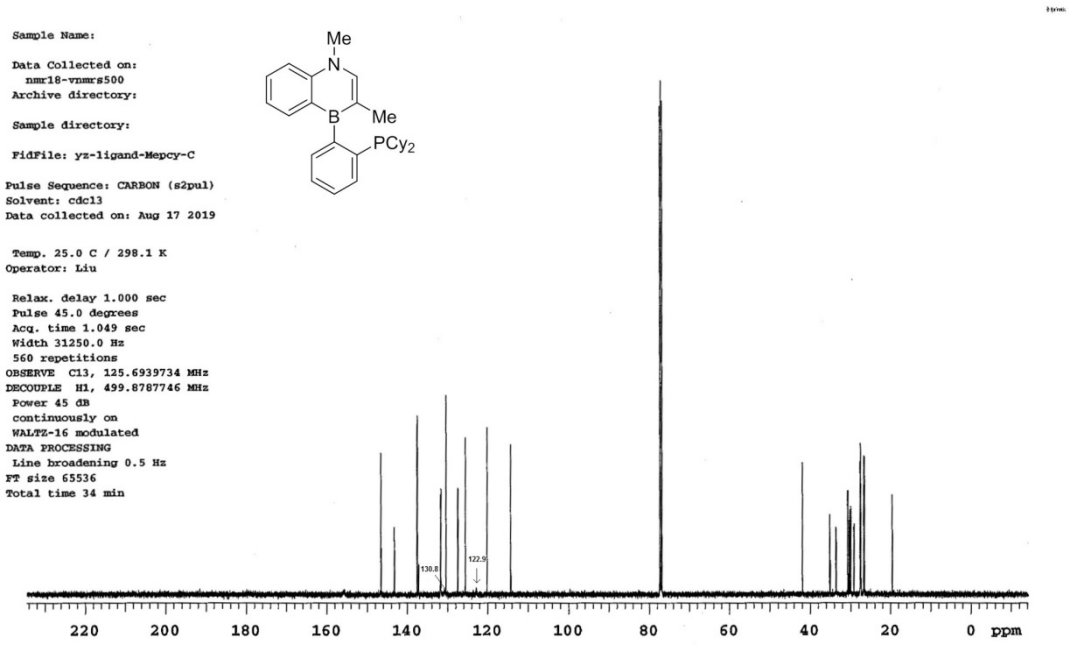
Temp. 25.0 C / 298.1 K
Operator: Liu

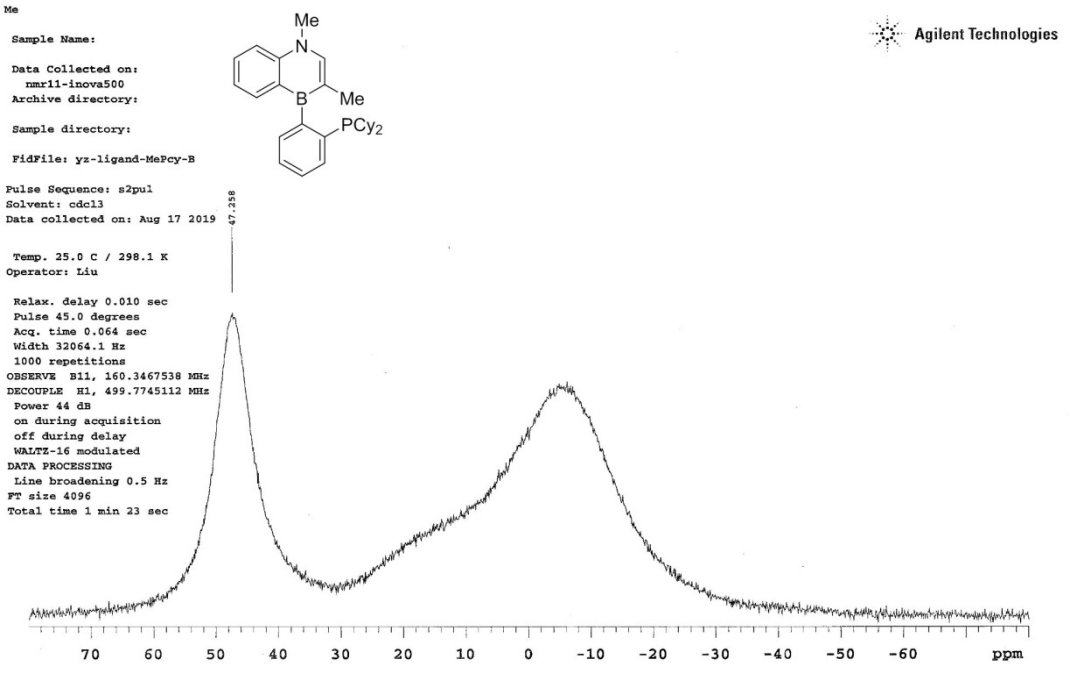
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.049 sec
Width 31250.0 Hz
764 repetitions
OBSERVE C13, 125.6939104 MHz
DECOUPLE H1, 499.8785010 MHz
Power 44 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.0 Hz
FT size 65536
Total time 34 min




Agilent Technologies
Sample Name:
Data Collected on:
nmr11-inova500
Archive directory:
Sample directory:
FidFile: B11
Me
N
B
Cl
tBu
Pulse Sequence: s2pul
Solvent: cdcl3
Data collected on: Dec 23 2019
Temp. 25.0 C / 298.1 K
Operator: Liu
Relax. delay 0.010 sec
Pulse 45.0 degrees
Acq. time 0.064 sec
Width 32064.1 Hz
1000 repetitions
OBSERVE B11, 160.3467851 MHz
DATA PROCESSING
Line broadening 0.5 Hz
FT size 4096
Total time 1 min 23 sec
44.426
70 60 50 40 30 20 10 0 -10 -20 -30 -40 -50 -60 -70 ppm


Me
Agilent Technologies
Sample Name:
Data Collected on:
nmr18-vnmrs500
Archive directory:
Sample directory:
FidFile: PROTON
Me
N
B
Me
PCy2
Pulse Sequence: PROTON (s2pul)
Solvent: cdcl3
Data collected on: Aug 17 2019
Temp. 25.0 C / 298.1 K
Operator: Liu
Relax. delay 10.000 sec
Pulse 45.0 degrees
Acq. time 2.045 sec
Width 8012.8 Hz
5 repetitions
OBSERVE H1, 499.8762780 MHz
DATA PROCESSING
FT size 32768
Total time 1 min 36 sec
9 8 7 6 5 4 3 2 1 ppm
1.01
2.01
3.03
2.04
2.00
1.00
2.99
4.04
8.18
2.76
11.53


Sample Name:
Data Collected on:
nmr18-vnmrs500
Archive directory:
Sample directory:
FidFile: yz-ligand-Mepcy-C
Pulse Sequence: CARBON (s2pul)
Solvent: cdcl3
Data collected on: Aug 17 2019
Temp. 25.0 C / 298.1 K
Operator: Liu
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.049 sec
Width 31250.0 Hz
560 repetitions
OBSERVE C13, 125.6939734 MHz
DECOUPLE H1, 499.8787746 MHz
Power 45 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 0.5 Hz
FT size 65536
Total time 34 min
Me
N
B
Me
PCy2
130.8
122.9
220
200
180
160
140
120
100
80
60
40
20
0
ppm


Me
Sample Name:
Data Collected on:
nmr11-inova500
Archive directory:
Sample directory:
FidFile: yz-ligand-MePcy-B
Pulse Sequence: s2pul
Solvent: cdcl3
Data collected on: Aug 17 2019
Temp. 25.0 C / 298.1 K
Operator: Liu
Relax. delay 0.010 sec
Pulse 45.0 degrees
Acq. time 0.064 sec
Width 32064.1 Hz
1000 repetitions
OBSERVE B11, 160.3467538 MHz
DECOUPLE H1, 499.7745112 MHz
Power 44 dB
on during acquisition
off during delay
WALTZ-16 modulated
DATA PROCESSING
Line broadening 0.5 Hz
FT size 4096
Total time 1 min 23 sec
47.258
N
B
Me
PCy2
Agilent Technologies
70
60
50
40
30
20
10
0
-10
-20
-30
-40
-50
-60
ppm

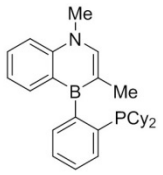
Me

Sample Name:

Data Collected on:
nmr18-vnmrs500
Archive directory:

Sample directory:

FidFile: PHOSPHORUS

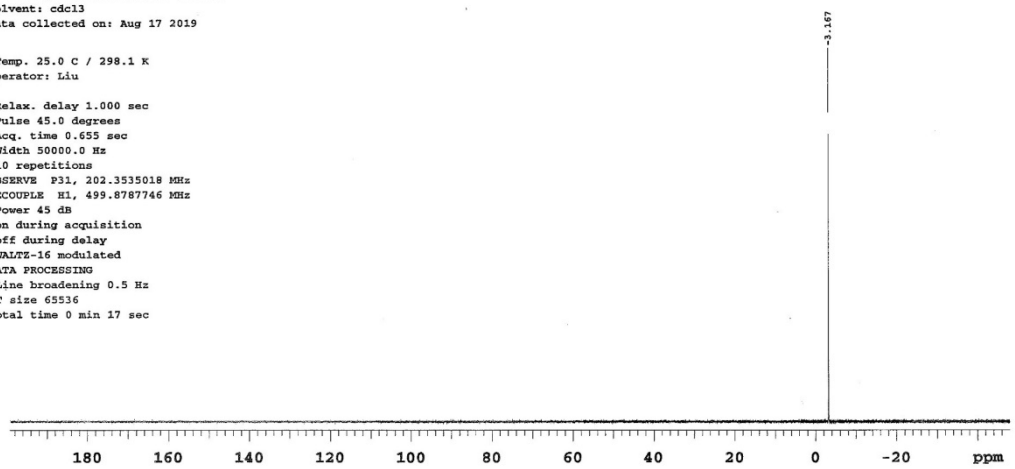


Agilent Technologies

Pulse Sequence: PHOSPHORUS (s2pul)
Solvent: cdcl3
Data collected on: Aug 17 2019

Temp. 25.0 C / 298.1 K
Operator: Liu

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 0.655 sec
Width 50000.0 Hz
10 repetitions
OBSERVE P31, 202.3535018 MHz
DECOUPLE H1, 499.8787746 MHz
Power 45 dB
on during acquisition
off during delay
WALTZ-16 modulated
DATA PROCESSING
Line broadening 0.5 Hz
FT size 65536
Total time 0 min 17 sec



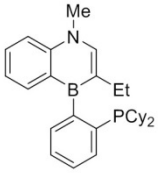
Et

Sample Name:

Data Collected on:
nmr18-vnmrs500
Archive directory:

Sample directory:

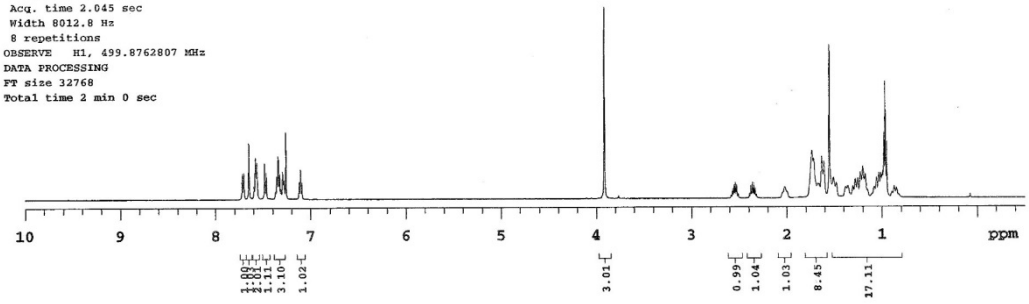
FidFile: yz-ligand-Etpcy-H

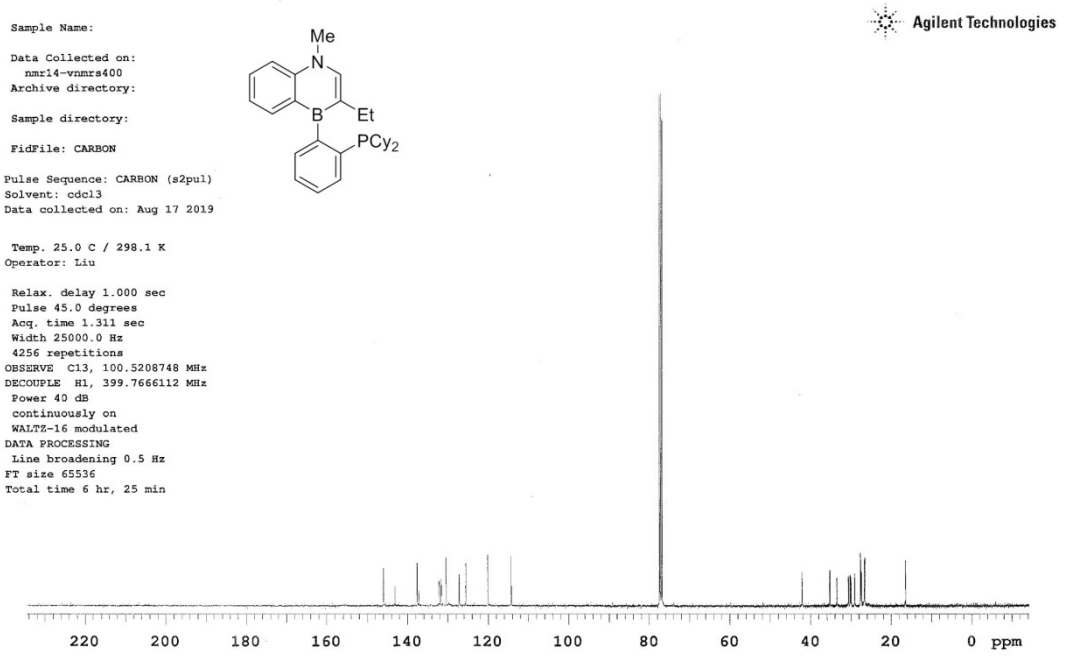


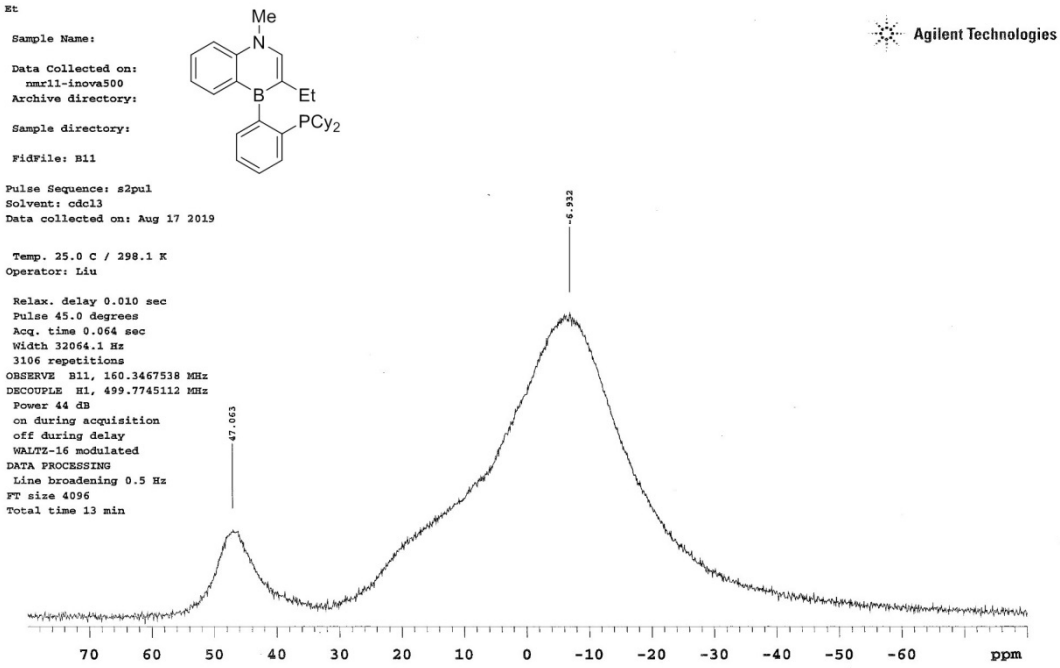
Pulse Sequence: PROTON (s2pul)
Solvent: cdcl3
Data collected on: Aug 17 2019

Temp. 25.0 C / 298.1 K
Operator: Liu

Relax. delay 10.000 sec
Pulse 45.0 degrees
Acq. time 2.045 sec
Width 8012.8 Hz
8 repetitions
OBSERVE H1, 499.8762807 MHz
DATA PROCESSING
FT size 32768
Total time 2 min 0 sec




Agilent Technologies
Sample Name:
Data Collected on:
nmr14-vnmrs400
Archive directory:
Sample directory:
FidFile: CARBON
Pulse Sequence: CARBON (s2pul)
Solvent: cdcl3
Data collected on: Aug 17 2019
Temp. 25.0 C / 298.1 K
Operator: Liu
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.311 sec
Width 25000.0 Hz
4256 repetitions
OBSERVE C13, 100.5208748 MHz
DECOUPLE H1, 399.7666112 MHz
Power 40 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 0.5 Hz
FT size 65536
Total time 6 hr, 25 min
Me
N
B
Et
PCy2
220
200
180
160
140
120
100
80
60
40
20
0 ppm


Et
Agilent Technologies
Sample Name:
Data Collected on:
nmr11-inova500
Archive directory:
Sample directory:
FidFile: B11
Pulse Sequence: s2pul
Solvent: cdcl3
Data collected on: Aug 17 2019
Temp. 25.0 C / 298.1 K
Operator: Liu
Relax. delay 0.010 sec
Pulse 45.0 degrees
Acq. time 0.064 sec
Width 32064.1 Hz
3106 repetitions
OBSERVE B11, 160.3467538 MHz
DECOUPLE H1, 499.7745112 MHz
Power 44 dB
on during acquisition
off during delay
WALTZ-16 modulated
DATA PROCESSING
Line broadening 0.5 Hz
FT size 4096
Total time 13 min
Me
N
B
Et
PCy2
47.063
-6.932
70
60
50
40
30
20
10
0
-10
-20
-30
-40
-50
-60
ppm

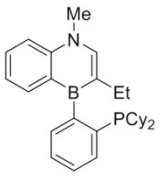
Et

Sample Name:

Data Collected on:
nmr18-vnmrs500
Archive directory:

Sample directory:

FidFile: PHOSPHORUS

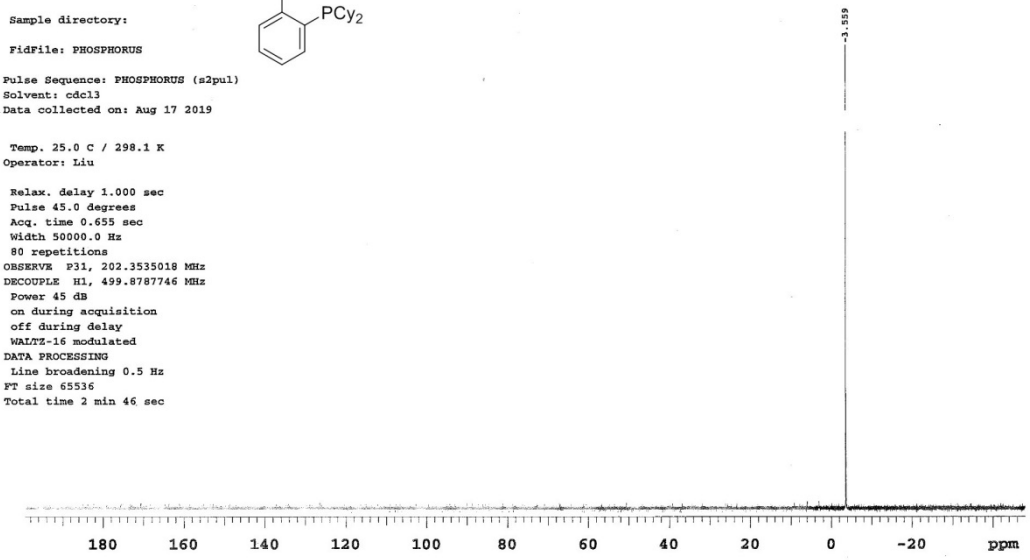


Agilent Technologies

Pulse Sequence: PHOSPHORUS (s2pul)
Solvent: cdcl3
Data collected on: Aug 17 2019

Temp. 25.0 C / 298.1 K
Operator: Liu

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 0.655 sec
Width 50000.0 Hz
80 repetitions
OBSERVE P31, 202.3535018 MHz
DECOUPLE H1, 499.8787746 MHz
Power 45 dB
on during acquisition
off during delay
WALTZ-16 modulated
DATA PROCESSING
Line broadening 0.5 Hz
FT size 65536
Total time 2 min 46 sec



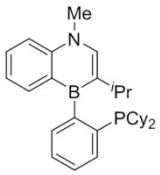
ipr

Sample Name:

Data Collected on:
nmr18-vnmrs500
Archive directory:

Sample directory:

FidFile: PROTON

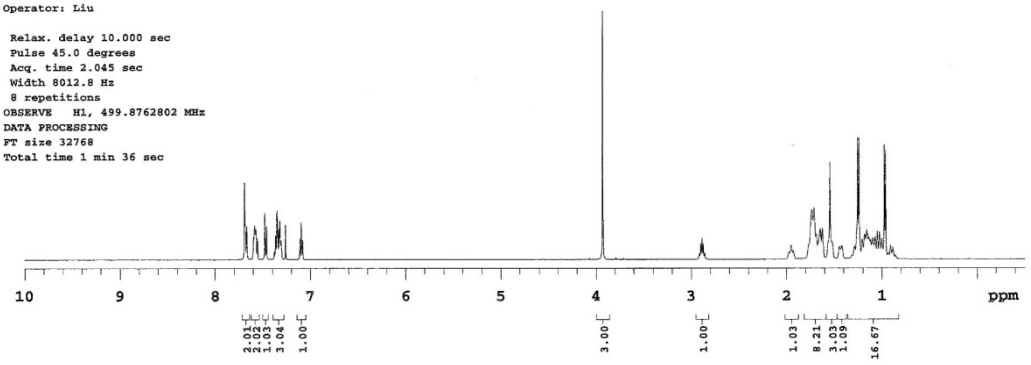


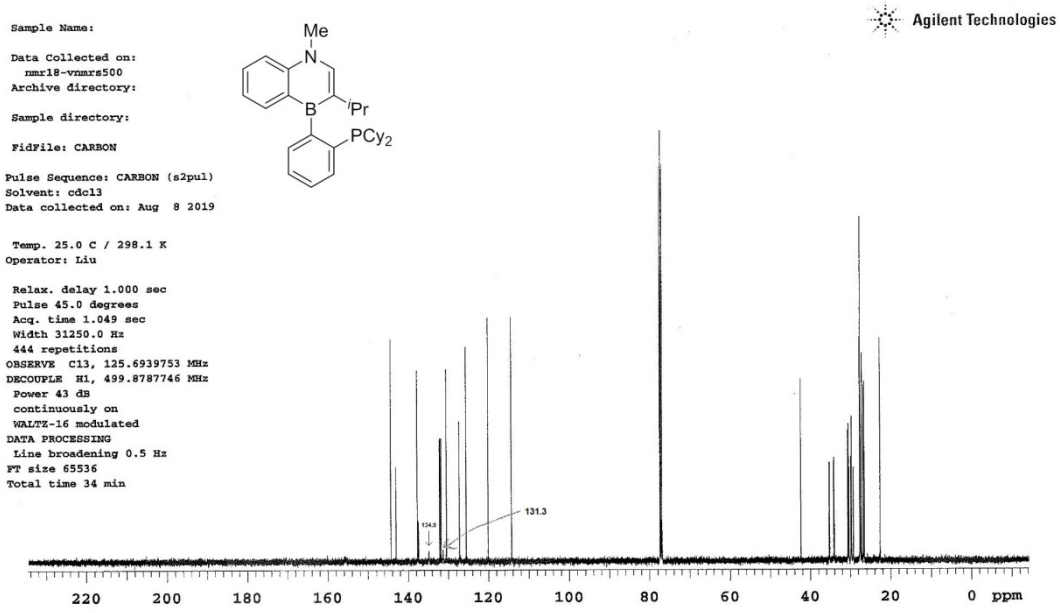
Agilent Technologies

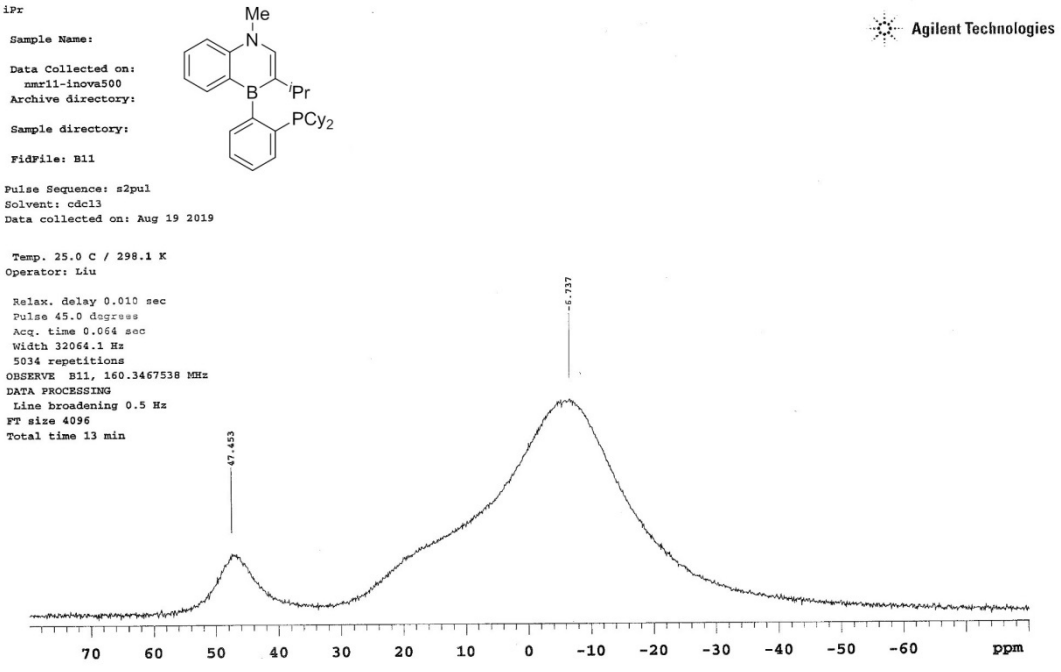
Pulse Sequence: PROTON (s2pul)
Solvent: cdcl3
Data collected on: Aug 7 2019

Temp. 25.0 C / 298.1 K
Operator: Liu

Relax. delay 10.000 sec
Pulse 45.0 degrees
Acq. time 2.045 sec
Width 8012.8 Hz
8 repetitions
OBSERVE H1, 499.8762802 MHz
DATA PROCESSING
FT size 32768
Total time 1 min 36 sec




Agilent Technologies
Sample Name:
Data Collected on:
nmr18-vnmrs500
Archive directory:
Sample directory:
FidFile: CARBON
Pulse Sequence: CARBON (s2pul)
Solvent: cdcl3
Data collected on: Aug 8 2019
Temp. 25.0 C / 298.1 K
Operator: Liu
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.049 sec
Width 31250.0 Hz
444 repetitions
OBSERVE C13, 125.6939753 MHz
DECOUPLE H1, 499.8787746 MHz
Power 43 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 0.5 Hz
FT size 65536
Total time 34 min
Me
N
B
iPr
PCy2
134.9
131.3
220
200
180
160
140
120
100
80
60
40
20
0
ppm


iPr
Agilent Technologies
Sample Name:
Data Collected on:
nmr11-inova500
Archive directory:
Sample directory:
FidFile: B11
Pulse Sequence: s2pul
Solvent: cdcl3
Data collected on: Aug 19 2019
Temp. 25.0 C / 298.1 K
Operator: Liu
Relax. delay 0.010 sec
Pulse 45.0 degrees
Acq. time 0.064 sec
Width 32064.1 Hz
5034 repetitions
OBSERVE B11, 160.3467538 MHz
DATA PROCESSING
Line broadening 0.5 Hz
FT size 4096
Total time 13 min
Me
N
B
iPr
PCy2
47.453
6.737
70
60
50
40
30
20
10
0
-10
-20
-30
-40
-50
-60
ppm

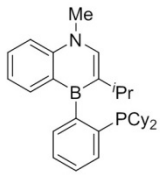
STANDARD PHOSPHORUS PARAMETERS

Sample Name:

Data Collected on:
nmr18-vnmrs500
Archive directory:

Sample directory:

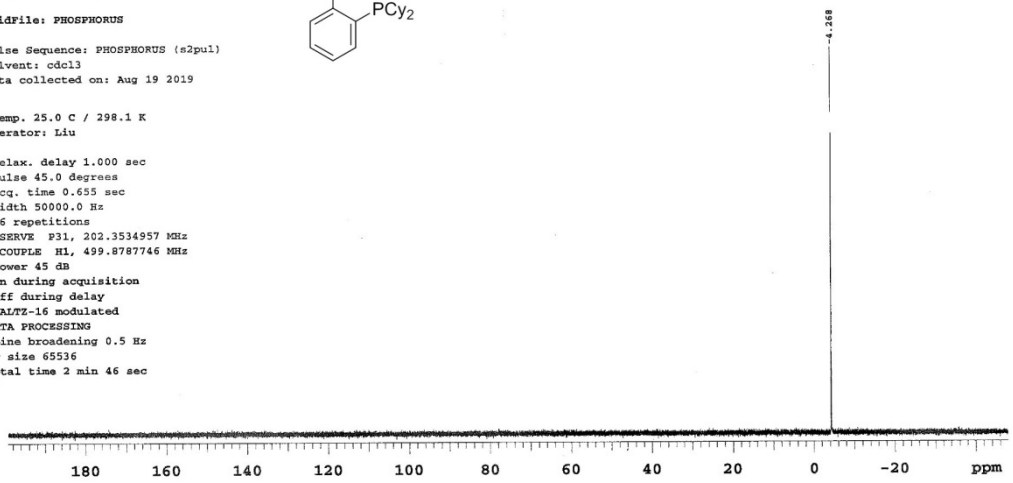
FidFile: PHOSPHORUS



Pulse Sequence: PHOSPHORUS (s2pul)
Solvent: cdcl3
Data collected on: Aug 19 2019

Temp. 25.0 C / 298.1 K
Operator: Liu

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 0.655 sec
Width 50000.0 Hz
86 repetitions
OBSERVE P31, 202.3534957 MHz
DECOUPLE H1, 499.8787746 MHz
Power 45 dB
on during acquisition
off during delay
WALTZ-16 modulated
DATA PROCESSING
Line broadening 0.5 Hz
FT size 65536
Total time 2 min 46 sec

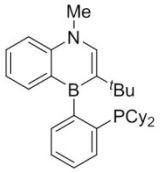


Sample Name:

Data Collected on:
nmr19-vnmrs600
Archive directory:

Sample directory:

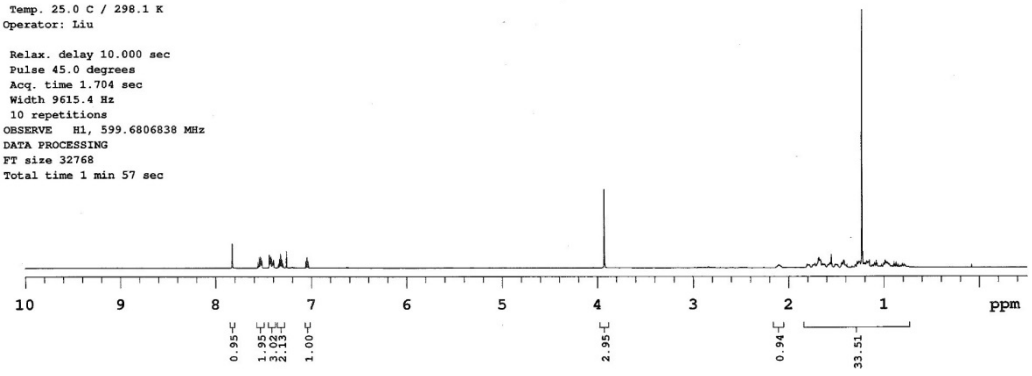
FidFile: PROTON



Pulse Sequence: PROTON (s2pul)
Solvent: cdcl3
Data collected on: Sep 7 2019

Temp. 25.0 C / 298.1 K
Operator: Liu

Relax. delay 10.000 sec
Pulse 45.0 degrees
Acq. time 1.704 sec
Width 9615.4 Hz
10 repetitions
OBSERVE H1, 599.6806838 MHz
DATA PROCESSING
FT size 32768
Total time 1 min 57 sec

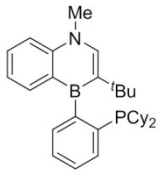


Sample Name:

Data Collected on:
nmr18-vnmrs500
Archive directory:

Sample directory:

FidFile: CARBON

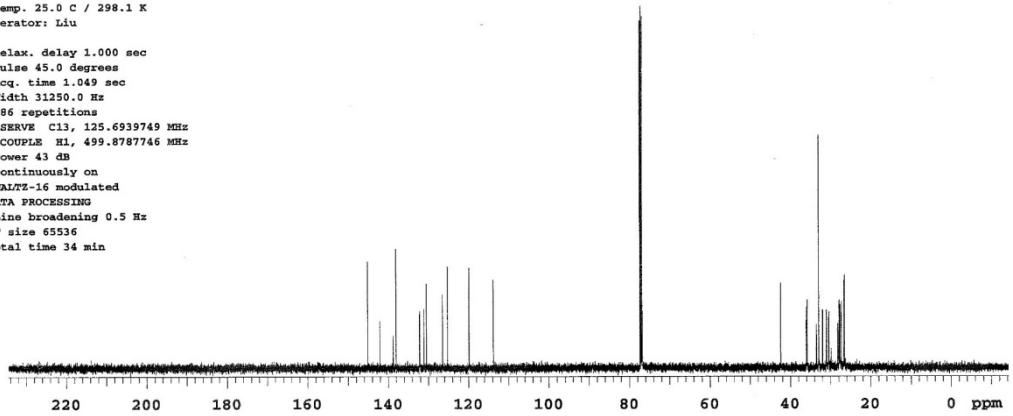


Agilent Technologies

Pulse Sequence: CARBON (s2pul)
Solvent: cdcl3
Data collected on: Aug 7 2019

Temp. 25.0 C / 298.1 K
Operator: Liu

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.049 sec
Width 31250.0 Hz
186 repetitions
OBSERVE C13, 125.6939749 MHz
DECOUPLE H1, 499.8787746 MHz
Power 43 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 0.5 Hz
FT size 65536
Total time 34 min



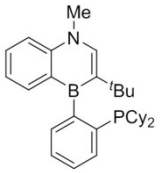
STANDARD PROTON PARAMETERS

Sample Name:

Data Collected on:
nmr11-inova500
Archive directory:

Sample directory:

FidFile: B11

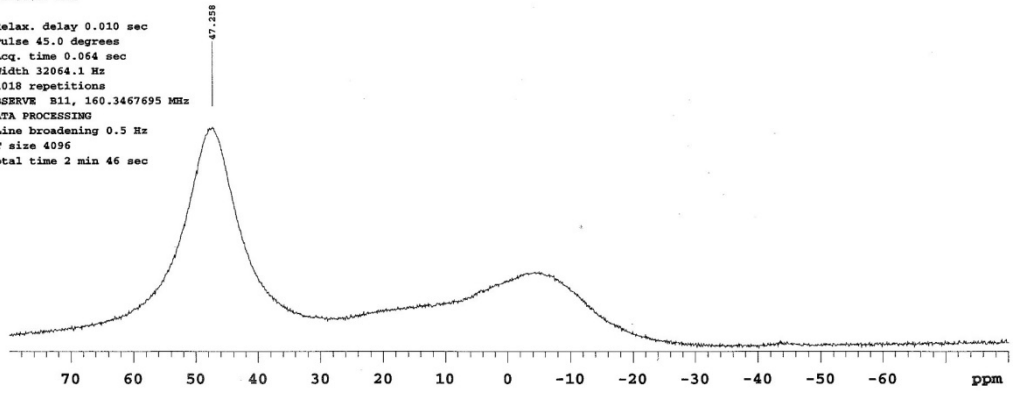


Agilent Technologies

Pulse Sequence: s2pul
Solvent: cdcl3
Data collected on: Sep 7 2019

Temp. 25.0 C / 298.1 K
Operator: Liu

Relax. delay 0.010 sec
Pulse 45.0 degrees
Acq. time 0.064 sec
Width 32064.1 Hz
1018 repetitions
OBSERVE B11, 160.3467695 MHz
DATA PROCESSING
Line broadening 0.5 Hz
FT size 4096
Total time 2 min 46 sec



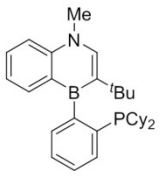
STANDARD PHOSPHORUS PARAMETERS

Sample Name:

Data Collected on:
nmr18-vnmrs500
Archive directory:

Sample directory:

FidFile: PHOSPHORUS

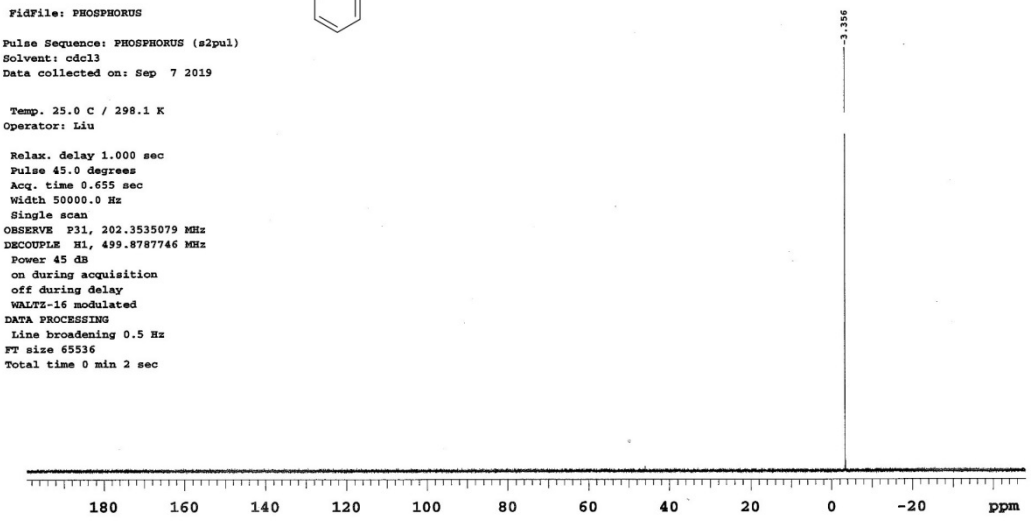


Agilent Technologies

Pulse Sequence: PHOSPHORUS (s2pul)
Solvent: cdcl3
Data collected on: Sep 7 2019

Temp. 25.0 C / 298.1 K
Operator: Liu

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 0.655 sec
Width 50000.0 Hz
Single scan
OBSERVE P31, 202.3535079 MHz
DECOUPLE H1, 499.8787746 MHz
Power 45 dB
on during acquisition
off during delay
WALTZ-16 modulated
DATA PROCESSING
Line broadening 0.5 Hz
FT size 65536
Total time 0 min 2 sec



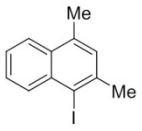
Agilent Technologies

Sample Name:

Data Collected on:
nmr18-vnmrs500
Archive directory:

Sample directory:

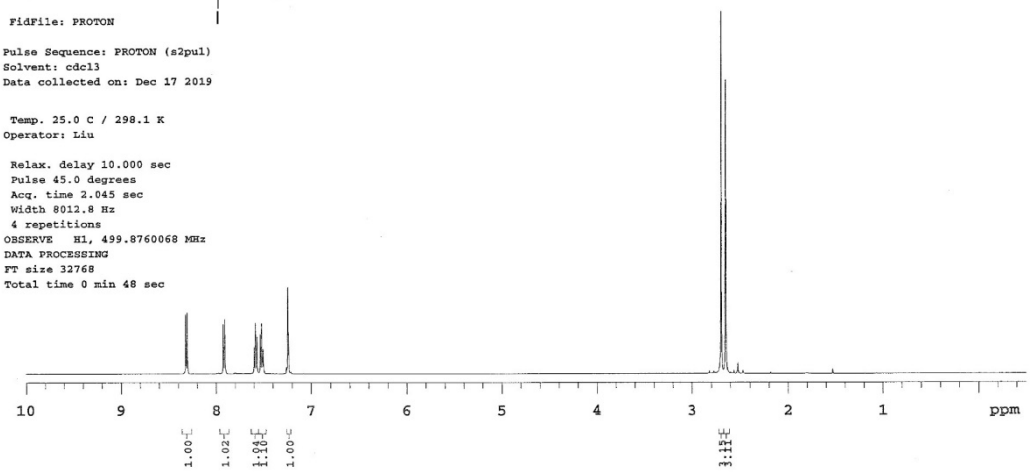
FidFile: PROTON



Pulse Sequence: PROTON (s2pul)
Solvent: cdcl3
Data collected on: Dec 17 2019

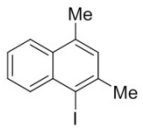
Temp. 25.0 C / 298.1 K
Operator: Liu

Relax. delay 10.000 sec
Pulse 45.0 degrees
Acq. time 2.045 sec
Width 8012.8 Hz
4 repetitions
OBSERVE H1, 499.8760068 MHz
DATA PROCESSING
FT size 32768
Total time 0 min 48 sec



Agilent Technologies

Sample Name:



Data Collected on:
nmr18-vnmrs500
Archive directory:

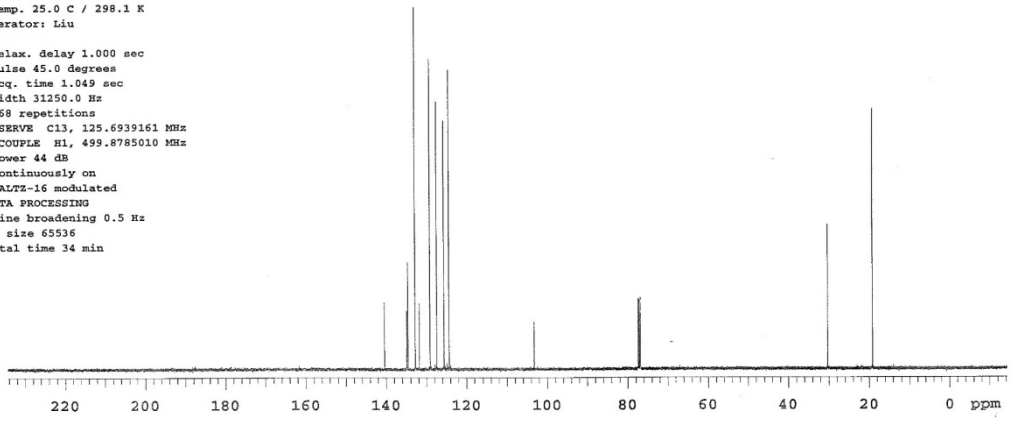
Sample directory:

FidFile: CARBON

Pulse Sequence: CARBON (s2pul)
Solvent: cdcl3
Data collected on: Dec 17 2019

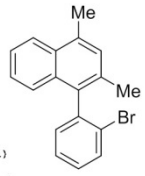
Temp. 25.0 C / 298.1 K
Operator: Liu

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.049 sec
Width 31250.0 Hz
168 repetitions
OBSERVE C13, 125.6939161 MHz
DECOUPLE H1, 499.8785010 MHz
Power 44 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 0.5 Hz
FT size 65536
Total time 34 min



Agilent Technologies

Sample Name:



Data Collected on:
nmr18-vnmrs500
Archive directory:

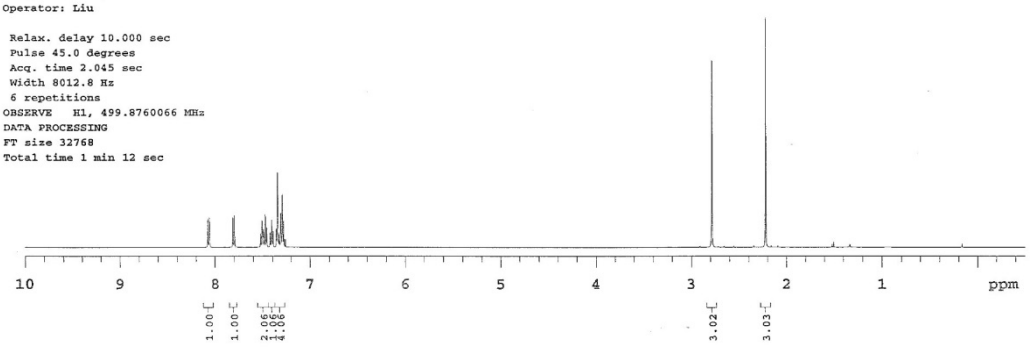
Sample directory:

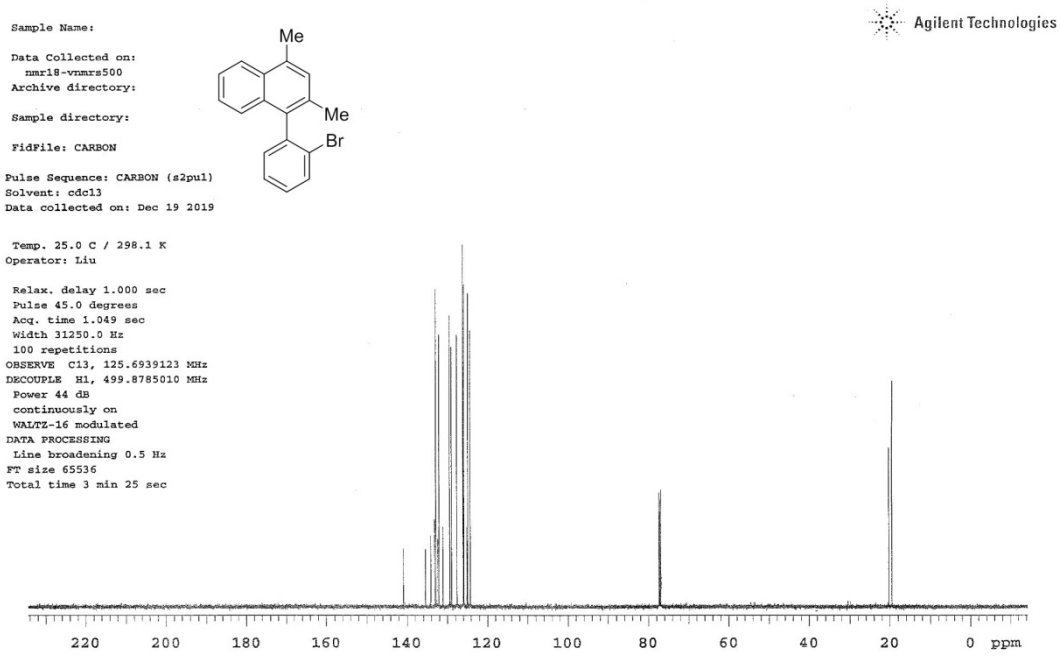
FidFile: PROTON

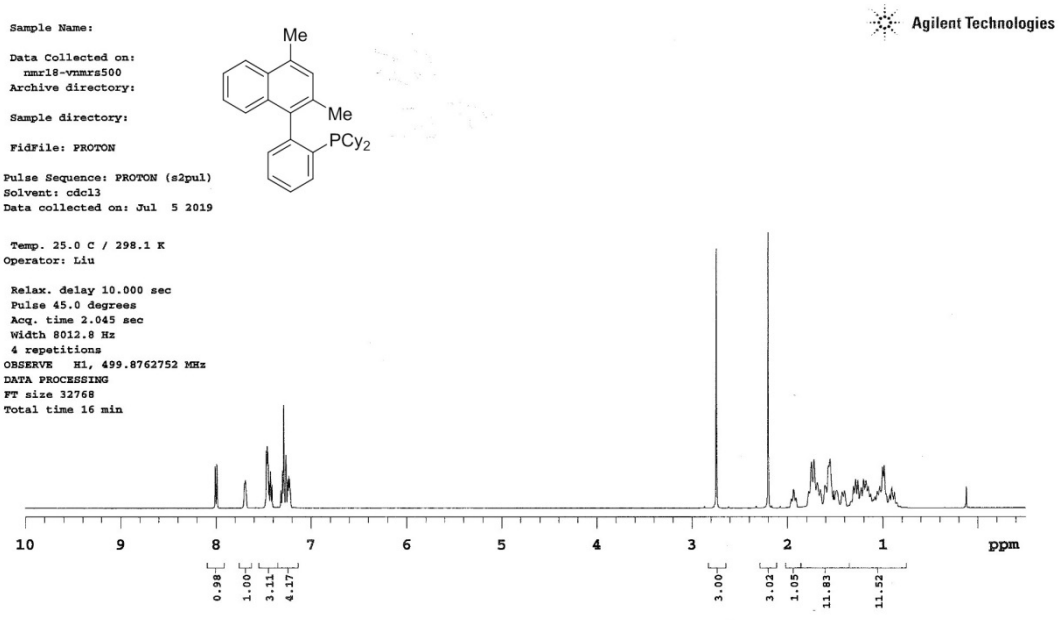
Pulse Sequence: PROTON (s2pul)
Solvent: cdcl3
Data collected on: Dec 19 2019

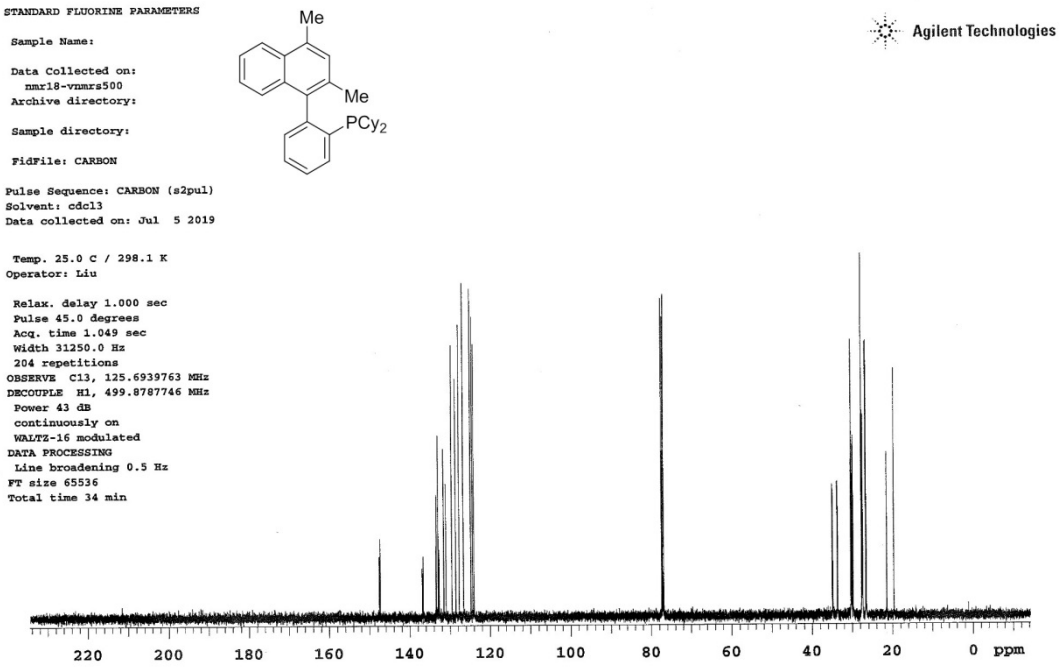
Temp. 25.0 C / 298.1 K
Operator: Liu

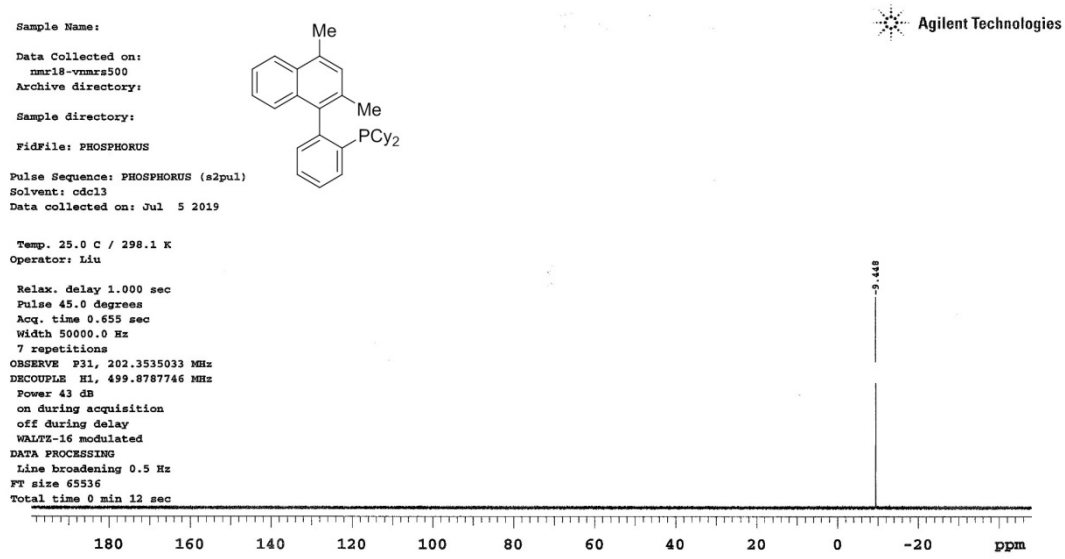
Relax. delay 10.000 sec
Pulse 45.0 degrees
Acq. time 2.045 sec
Width 8012.8 Hz
6 repetitions
OBSERVE H1, 499.8760066 MHz
DATA PROCESSING
FT size 32768
Total time 1 min 12 sec




Agilent Technologies
Sample Name:
Data Collected on:
nmr18-vnmrs500
Archive directory:
Sample directory:
FidFile: CARBON
Me
Me
Br
Pulse Sequence: CARBON (s2pul)
Solvent: cdcl3
Data collected on: Dec 19 2019
Temp. 25.0 C / 298.1 K
Operator: Liu
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.049 sec
Width 31250.0 Hz
100 repetitions
OBSERVE C13, 125.6939123 MHz
DECOUPLE H1, 499.8785010 MHz
Power 44 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 0.5 Hz
FT size 65536
Total time 3 min 25 sec
220
200
180
160
140
120
100
80
60
40
20
0
ppm


Agilent Technologies
Sample Name:
Data Collected on:
nmr18-vnmrs500
Archive directory:
Sample directory:
FidFile: PROTON
Me
Me
PCy2
Pulse Sequence: PROTON (s2pul)
Solvent: cdcl3
Data collected on: Jul 5 2019
Temp. 25.0 C / 298.1 K
Operator: Liu
Relax. delay 10.000 sec
Pulse 45.0 degrees
Acq. time 2.045 sec
Width 8012.8 Hz
4 repetitions
OBSERVE H1, 499.8762752 MHz
DATA PROCESSING
FT size 32768
Total time 16 min
10
9
8
7
6
5
4
3
2
1
ppm
0.98
1.00
3.11
4.17
3.00
3.02
1.05
11.83
11.52


STANDARD FLUORINE PARAMETERS
Sample Name:
Data Collected on:
nmr18-vnmrs500
Archive directory:
Sample directory:
FidFile: CARBON
Pulse Sequence: CARBON (s2pul)
Solvent: cdcl3
Data collected on: Jul 5 2019
Temp. 25.0 C / 298.1 K
Operator: Liu
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.049 sec
Width 31250.0 Hz
204 repetitions
OBSERVE C13, 125.6939763 MHz
DECOUPLE H1, 499.8787746 MHz
Power 43 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 0.5 Hz
FT size 65536
Total time 34 min
Me
Me
PCy2
Agilent Technologies
220
200
180
160
140
120
100
80
60
40
20
0
ppm

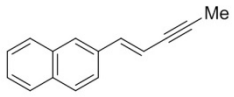

Sample Name:
Data Collected on:
nmr18-vnmrs500
Archive directory:
Sample directory:
FidFile: PHOSPHORUS
Pulse Sequence: PHOSPHORUS (s2pul)
Solvent: cdcl3
Data collected on: Jul 5 2019
Temp. 25.0 C / 298.1 K
Operator: Liu
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 0.655 sec
Width 50000.0 Hz
7 repetitions
OBSERVE P31, 202.3535033 MHz
DECOUPLE H1, 499.8787746 MHz
Power 43 dB
on during acquisition
off during delay
WALTZ-16 modulated
DATA PROCESSING
Line broadening 0.5 Hz
FT size 65536
Total time 0 min 12 sec
-9.448
Me
Me
PCy2
Agilent Technologies
180
160
140
120
100
80
60
40
20
0
-20
ppm

Sample Name:

Data Collected on:
nmr19-vnmrs600
Archive directory:

Sample directory:

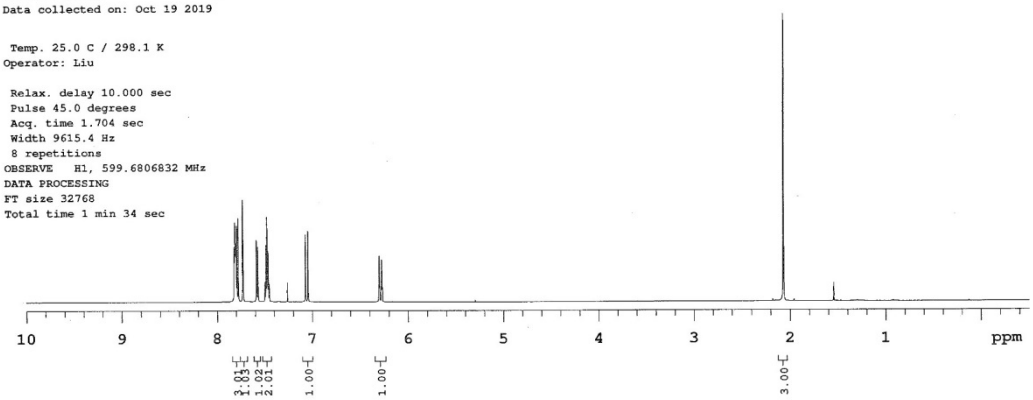
FidFile: PROTON



Pulse Sequence: PROTON (s2pul)
Solvent: cdcl3
Data collected on: Oct 19 2019

Temp. 25.0 C / 298.1 K
Operator: Liu

Relax. delay 10.000 sec
Pulse 45.0 degrees
Acq. time 1.704 sec
Width 9615.4 Hz
8 repetitions
OBSERVE H1, 599.6806832 MHz
DATA PROCESSING
FT size 32768
Total time 1 min 34 sec

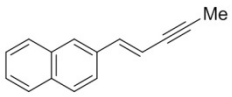


Sample Name:

Data Collected on:
nmr19-vnmrs600
Archive directory:

Sample directory:

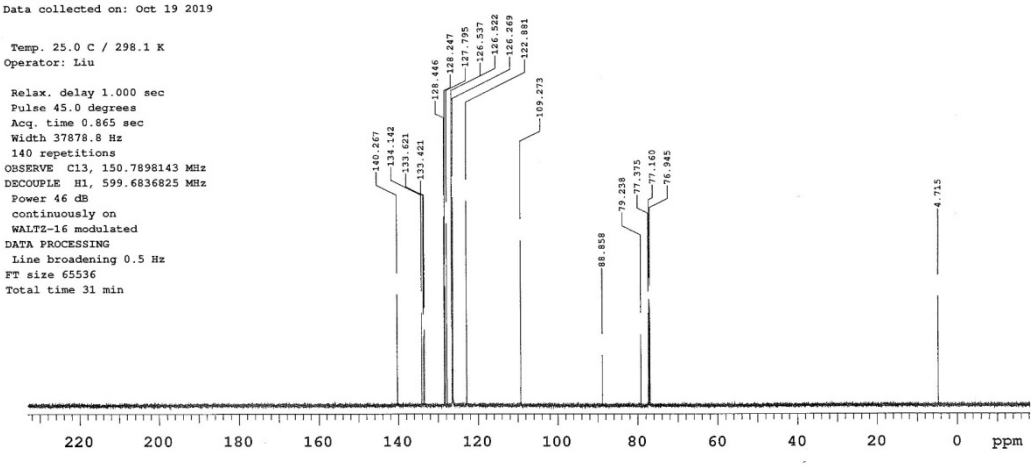
FidFile: CARBON



Pulse Sequence: CARBON (s2pul)
Solvent: cdcl3
Data collected on: Oct 19 2019

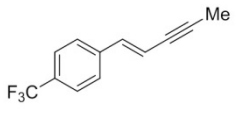
Temp. 25.0 C / 298.1 K
Operator: Liu

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 0.865 sec
Width 37878.8 Hz
140 repetitions
OBSERVE C13, 150.7898143 MHz
DECOUPLE H1, 599.6836825 MHz
Power 46 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 0.5 Hz
FT size 65536
Total time 31 min



Agilent Technologies

Sample Name:



Data Collected on:
nmr18-vnmrs500
Archive directory:

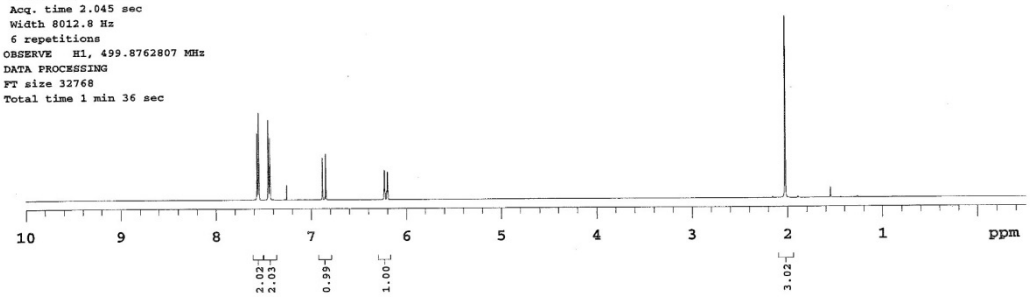
Sample directory:

FidFile: PROTON

Pulse Sequence: PROTON (s2pul)
Solvent: cdcl3
Data collected on: Oct 21 2019

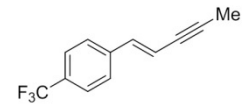
Temp. 25.0 C / 298.1 K
Operator: Liu

Relax. delay 10.000 sec
Pulse 45.0 degrees
Acq. time 2.045 sec
Width 8012.8 Hz
6 repetitions
OBSERVE H1, 499.8762807 MHz
DATA PROCESSING
FT size 32768
Total time 1 min 36 sec



Agilent Technologies

Sample Name:



Data Collected on:
nmr18-vnmrs500
Archive directory:

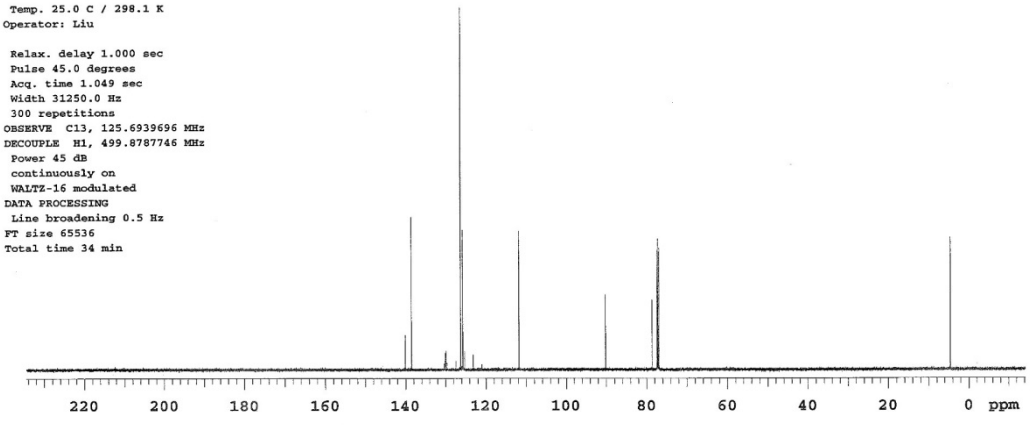
Sample directory:

FidFile: CARBON

Pulse Sequence: CARBON (s2pul)
Solvent: cdcl3
Data collected on: Oct 21 2019

Temp. 25.0 C / 298.1 K
Operator: Liu

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.049 sec
Width 31250.0 Hz
300 repetitions
OBSERVE C13, 125.6939696 MHz
DECOUPLE H1, 499.8787746 MHz
Power 45 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 0.5 Hz
FT size 65536
Total time 34 min



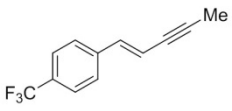
STANDARD FLUORINE PARAMETERS

Sample Name:

Data Collected on:
nmr18-vnmrs500
Archive directory:

Sample directory:

FidFile: FLUORINE

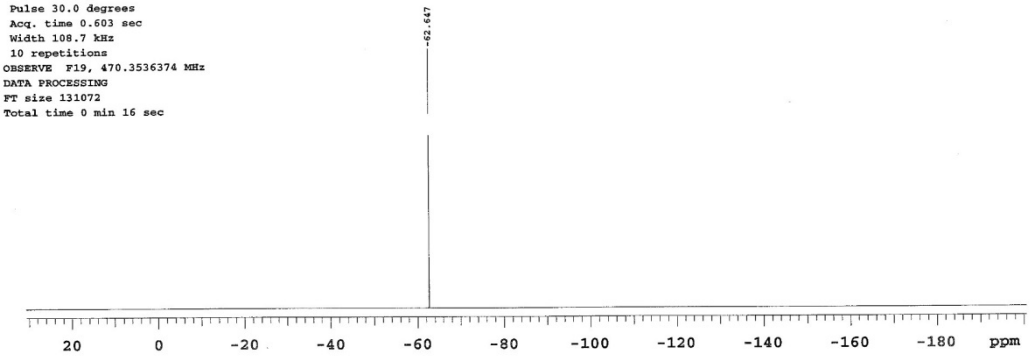


Agilent Technologies

Pulse Sequence: FLUORINE (s2pul)
Solvent: cdcl3
Data collected on: Oct 21 2019

Temp. 25.0 C / 298.1 K
Operator: Liu

Relax. delay 1.000 sec
Pulse 30.0 degrees
Acq. time 0.603 sec
Width 108.7 kHz
10 repetitions
OBSERVE F19, 470.3536374 MHz
DATA PROCESSING
FT size 131072
Total time 0 min 16 sec

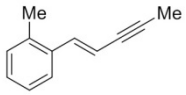


Sample Name:

Data Collected on:
nmr19-vnmrs600
Archive directory:

Sample directory:

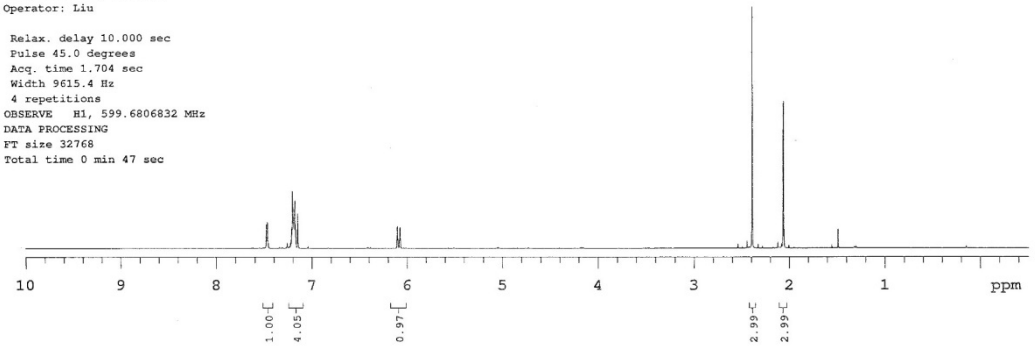
FidFile: PROTON



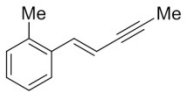
Pulse Sequence: PROTON (s2pul)
Solvent: cdcl3
Data collected on: Jan 2 2020

Temp. 25.0 C / 298.1 K
Operator: Liu

Relax. delay 10.000 sec
Pulse 45.0 degrees
Acq. time 1.704 sec
Width 9615.4 Hz
4 repetitions
OBSERVE H1, 599.6806832 MHz
DATA PROCESSING
FT size 32768
Total time 0 min 47 sec



Sample Name:



Data Collected on:
nmr19-vnmrs600
Archive directory:

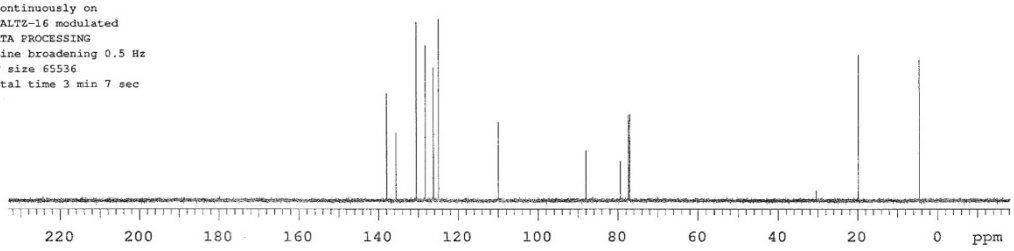
Sample directory:

FidFile: CARBON

Pulse Sequence: CARBON (s2pul)
Solvent: cdcl3
Data collected on: Jan 2 2020

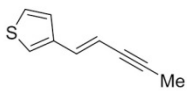
Temp. 25.0 C / 298.1 K
Operator: Liu

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 0.865 sec
Width 37878.8 Hz
16 repetitions
OBSERVE C13, 150.7898189 MHz
DECOUPLE H1, 599.6836825 MHz
Power 45 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 0.5 Hz
FT size 65536
Total time 3 min 7 sec



Agilent Technologies

Sample Name:



Data Collected on:
nmr18-vnmrs500
Archive directory:

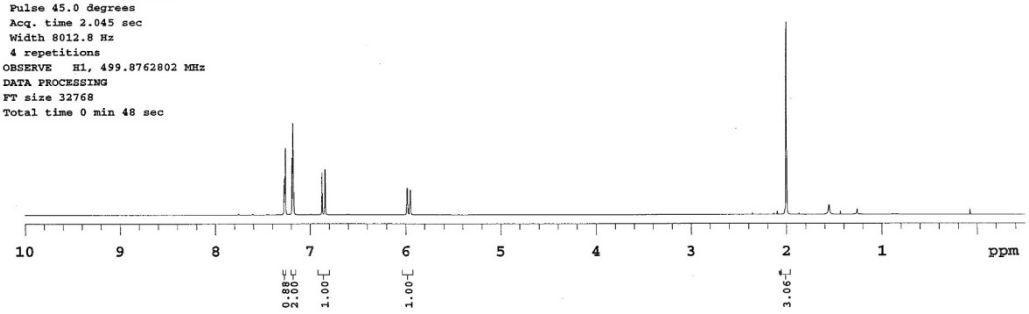
Sample directory:

FidFile: PROTON

Pulse Sequence: PROTON (s2pul)
Solvent: cdcl3
Data collected on: Oct 23 2019

Temp. 25.0 C / 298.1 K
Operator: Liu

Relax. delay 10.000 sec
Pulse 45.0 degrees
Acq. time 2.045 sec
Width 8012.8 Hz
4 repetitions
OBSERVE H1, 499.8762802 MHz
DATA PROCESSING
FT size 32768
Total time 0 min 48 sec



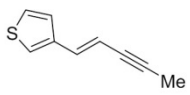
Agilent Technologies

Sample Name:

Data Collected on:
nmr18-vnmrs500
Archive directory:

Sample directory:

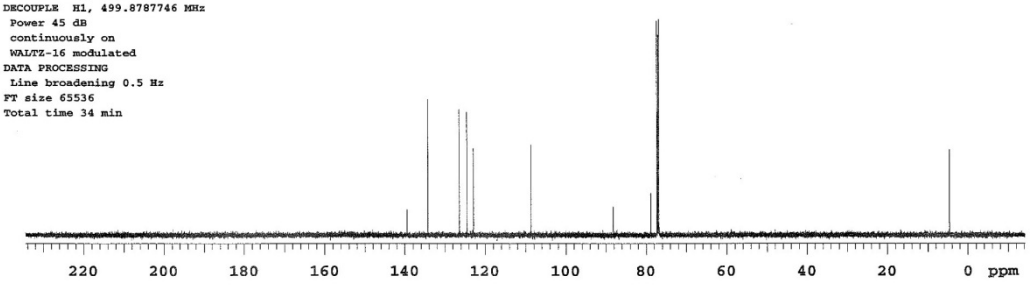
FidFile: CARBON



Pulse Sequence: CARBON (s2pul)
Solvent: cdcl3
Data collected on: Oct 23 2019

Temp. 25.0 C / 298.1 K
Operator: Liu

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.049 sec
Width 31250.0 Hz
202 repetitions
OBSERVE C13, 125.6939715 MHz
DECOUPLE H1, 499.8787746 MHz
Power 45 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 0.5 Hz
FT size 65536
Total time 34 min



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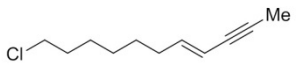
Sample Name:

Data Collected on:
nmr18-vnmrs500
Archive directory:

Sample directory:

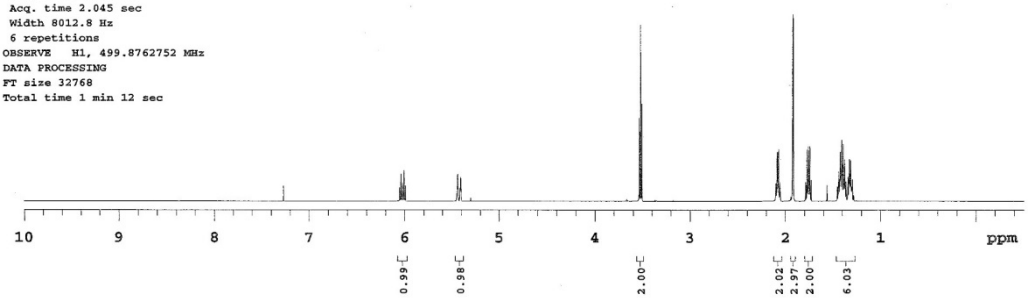
FidFile: PROTON



Pulse Sequence: PROTON (s2pul)
Solvent: cdcl3
Data collected on: Oct 20 2019

Temp. 25.0 C / 298.1 K
Operator: Liu

Relax. delay 10.000 sec
Pulse 45.0 degrees
Acq. time 2.045 sec
Width 8012.8 Hz
6 repetitions
OBSERVE H1, 499.8762752 MHz
DATA PROCESSING
FT size 32768
Total time 1 min 12 sec



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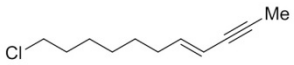
Sample Name:

Data Collected on:
nmr18-vnmrs500
Archive directory:



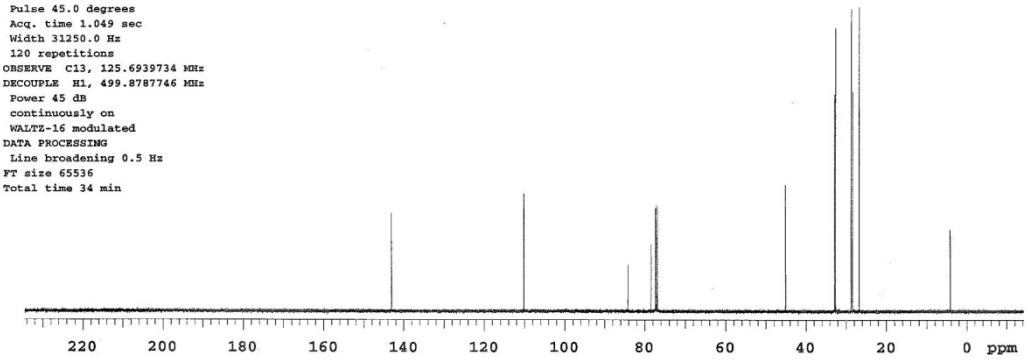
Sample directory:

FidFile: CARBON

Pulse Sequence: CARBON (s2pul)
Solvent: cdcl3
Data collected on: Oct 20 2019

Temp. 25.0 C / 298.1 K
Operator: Liu

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.049 sec
Width 31250.0 Hz
120 repetitions
OBSERVE C13, 125.6939734 MHz
DECOUPLE H1, 499.8787746 MHz
Power 45 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 0.5 Hz
FT size 65536
Total time 34 min



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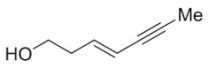
Sample Name:

Data Collected on:
nmr18-vnmrs500
Archive directory:



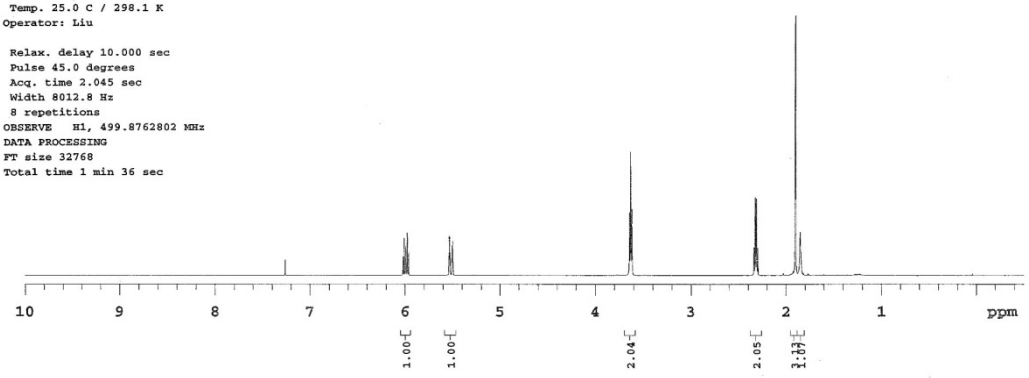
Sample directory:

FidFile: PROTON

Pulse Sequence: PROTON (s2pul)
Solvent: cdcl3
Data collected on: Oct 24 2019

Temp. 25.0 C / 298.1 K
Operator: Liu

Relax. delay 10.000 sec
Pulse 45.0 degrees
Acq. time 2.045 sec
Width 8012.8 Hz
8 repetitions
OBSERVE H1, 499.8762802 MHz
DATA PROCESSING
FT size 32768
Total time 1 min 36 sec



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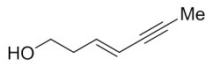
Sample Name:

Data Collected on:
nmr18-vnmrs500
Archive directory:

Sample directory:

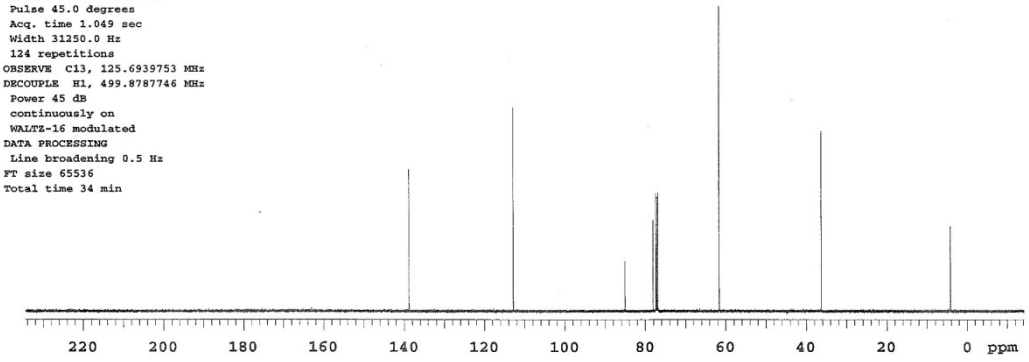
FidFile: CARBON



Pulse Sequence: CARBON (s2pul)
Solvent: cdcl3
Data collected on: Oct 24 2019

Temp. 25.0 C / 298.1 K
Operator: Liu

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.049 sec
Width 31250.0 Hz
124 repetitions
OBSERVE C13, 125.6939753 MHz
DECOUPLE H1, 499.8787746 MHz
Power 45 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 0.5 Hz
FT size 65536
Total time 34 min

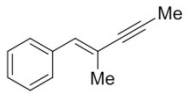


Sample Name:

Data Collected on:
nmr19-vnmrs600
Archive directory:

Sample directory:

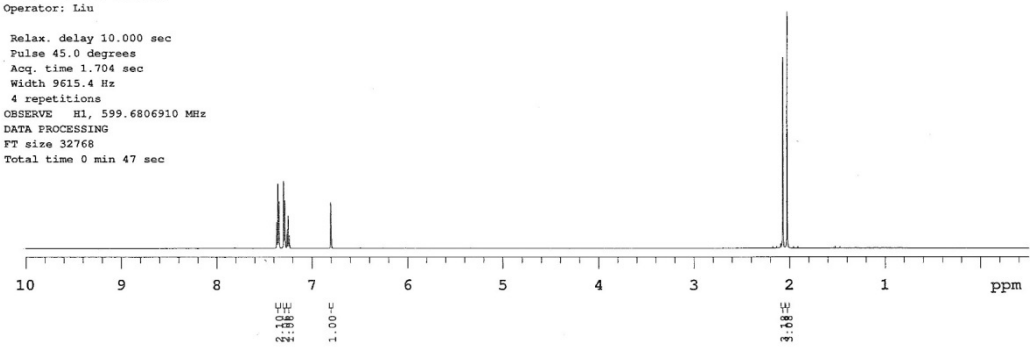
FidFile: PROTON



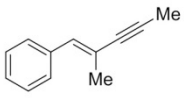
Pulse Sequence: PROTON (s2pul)
Solvent: cdcl3
Data collected on: Nov 7 2019

Temp. 25.0 C / 298.1 K
Operator: Liu

Relax. delay 10.000 sec
Pulse 45.0 degrees
Acq. time 1.704 sec
Width 9615.4 Hz
4 repetitions
OBSERVE H1, 599.6806910 MHz
DATA PROCESSING
FT size 32768
Total time 0 min 47 sec



Sample Name:



Data Collected on:
nmr19-vnmrs600
Archive directory:

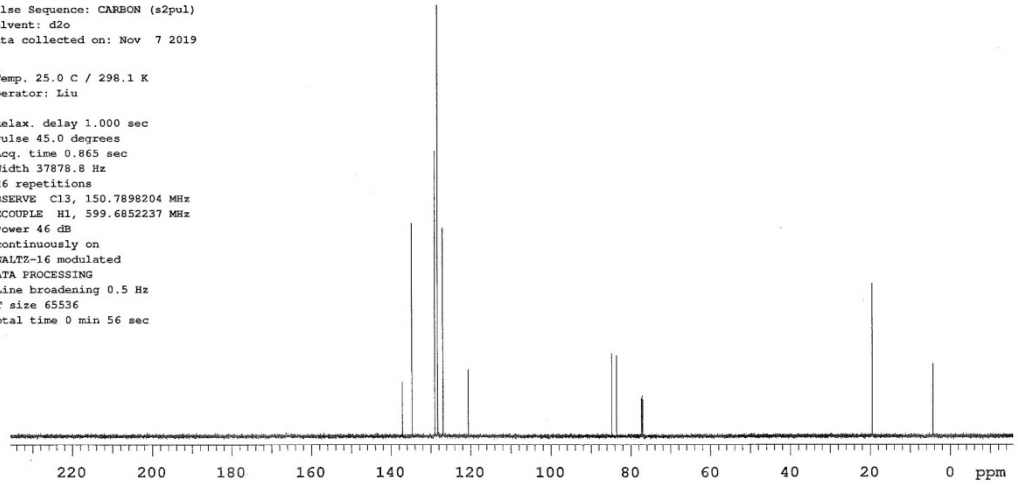
Sample directory:

FidFile: CARBON

Pulse Sequence: CARBON (s2pul)
Solvent: d2o
Data collected on: Nov 7 2019

Temp. 25.0 C / 298.1 K
Operator: Liu

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 0.865 sec
Width 37878.8 Hz
26 repetitions
OBSERVE C13, 150.7898204 MHz
DECOUPLE H1, 599.6852237 MHz
Power 46 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 0.5 Hz
FT size 65536
Total time 0 min 56 sec



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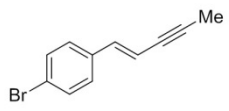
Sample Name:



Data Collected on:
nmr18-vnmrs500
Archive directory:

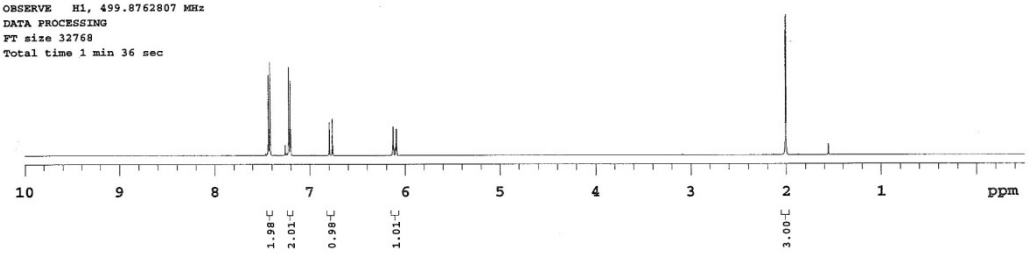
Sample directory:

FidFile: PROTON

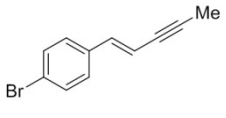
Pulse Sequence: PROTON (s2pul)
Solvent: cdcl3
Data collected on: Oct 23 2019

Temp. 25.0 C / 298.1 K
Operator: Liu

Relax. delay 10.000 sec
Pulse 45.0 degrees
Acq. time 2.045 sec
Width 8012.8 Hz
5 repetitions
OBSERVE H1, 499.8762807 MHz
DATA PROCESSING
FT size 32768
Total time 1 min 36 sec



Sample Name:



Data Collected on:
nmr18-vnmrs500
Archive directory:

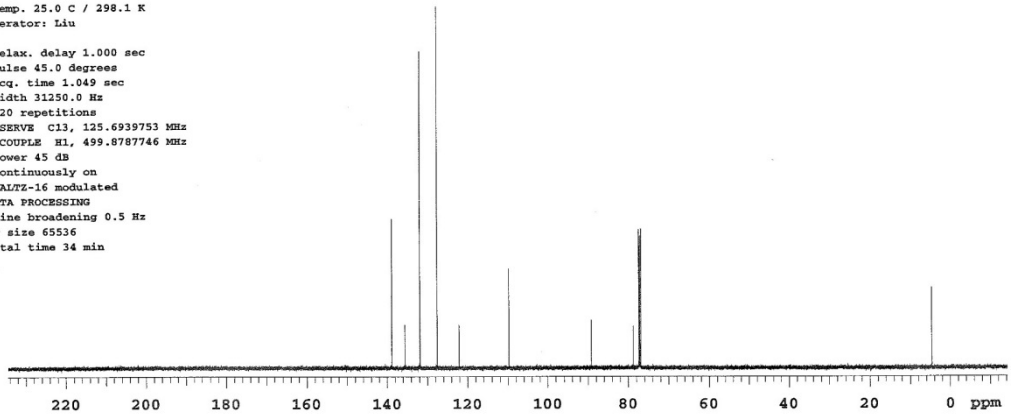
Sample directory:

FidFile: CARBON

Pulse Sequence: CARBON (s2pul)
Solvent: cdcl3
Data collected on: Oct 23 2019

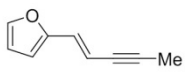
Temp. 25.0 C / 298.1 K
Operator: Liu

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.049 sec
Width 31250.0 Hz
120 repetitions
OBSERVE C13, 125.6939753 MHz
DECOUPLE H1, 499.8787746 MHz
Power 45 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 0.5 Hz
FT size 65536
Total time 34 min



2-furan

Sample Name:



Data Collected on:
nmr18-vnmrs500
Archive directory:

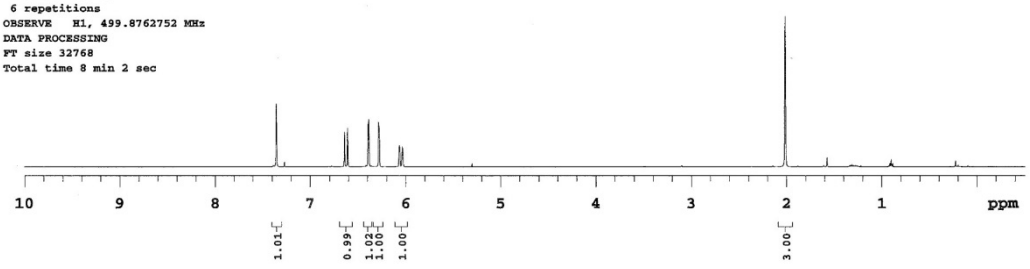
Sample directory:

FidFile: PROTON

Pulse Sequence: PROTON (s2pul)
Solvent: cdcl3
Data collected on: Jun 26 2019

Temp. 25.0 C / 298.1 K
Operator: Liu

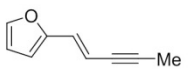
Relax. delay 10.000 sec
Pulse 45.0 degrees
Acq. time 2.045 sec
Width 8012.8 Hz
6 repetitions
OBSERVE H1, 499.8762752 MHz
DATA PROCESSING
FT size 32768
Total time 8 min 2 sec



2-furan

Agilent Technologies

Sample Name:



Data Collected on:
nmr18-vnmrs500
Archive directory:

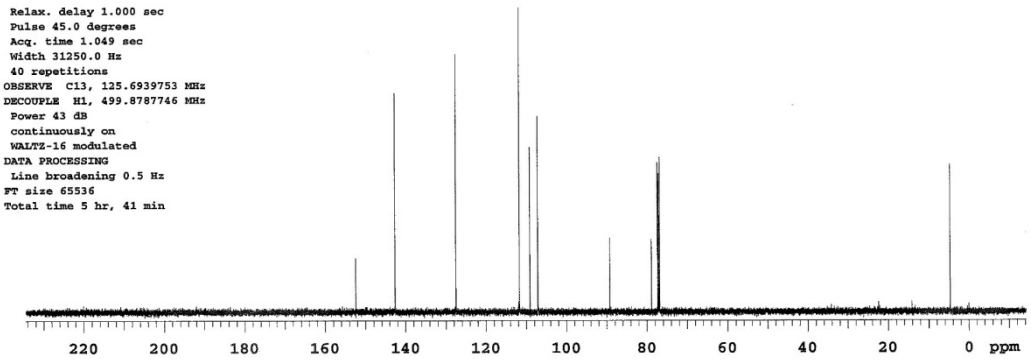
Sample directory:

FidFile: CARBON

Pulse Sequence: CARBON (s2pul)
Solvent: cdcl3
Data collected on: Jun 26 2019

Temp. 25.0 C / 298.1 K
Operator: Liu

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.049 sec
Width 31250.0 Hz
40 repetitions
OBSERVE C13, 125.6939753 MHz
DECOUPLE H1, 499.8787746 MHz
Power 43 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 0.5 Hz
FT size 65536
Total time 5 hr, 41 min

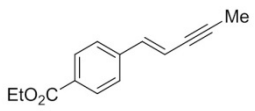


Sample Name:

Data Collected on:
nmr19-vnmrs600
Archive directory:

Sample directory:

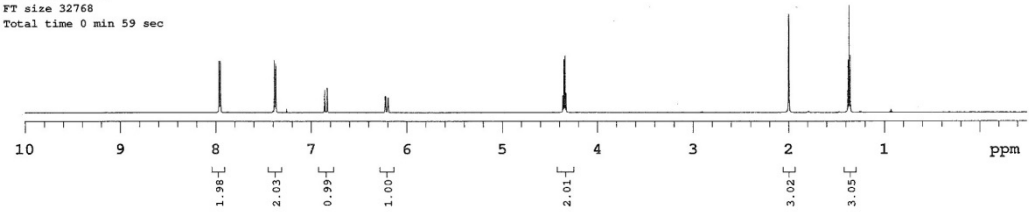
FidFile: PROTON



Pulse Sequence: PROTON (s2pul)
Solvent: cdcl3
Data collected on: Oct 22 2019

Temp. 25.0 C / 298.1 K
Operator: Liu

Relax. delay 10.000 sec
Pulse 45.0 degrees
Acq. time 1.704 sec
Width 9615.4 Hz
2 repetitions
OBSERVE H1, 599.6806841 MHz
DATA PROCESSING
FT size 32768
Total time 0 min 59 sec

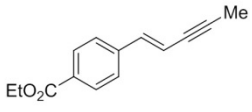


Sample Name:

Data Collected on:
nmr19-vnmrs600
Archive directory:

Sample directory:

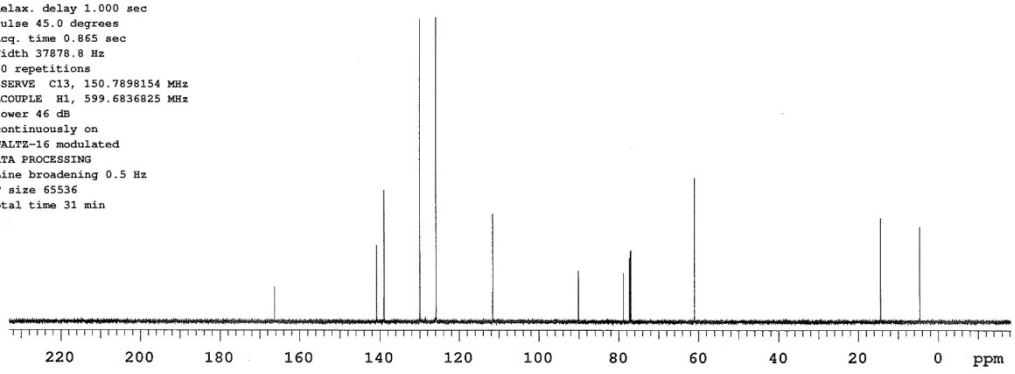
FidFile: CARBON



Pulse Sequence: CARBON (s2pul)
Solvent: cdcl3
Data collected on: Oct 22 2019

Temp. 25.0 C / 298.1 K
Operator: Liu

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 0.865 sec
Width 37878.8 Hz
40 repetitions
OBSERVE C13, 150.7898154 MHz
DECOUPLE H1, 599.6836825 MHz
Power 46 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 0.5 Hz
FT size 65536
Total time 31 min



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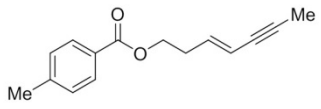
Sample Name:

Data Collected on:
nmr18-vnmrs500
Archive directory:

Sample directory:

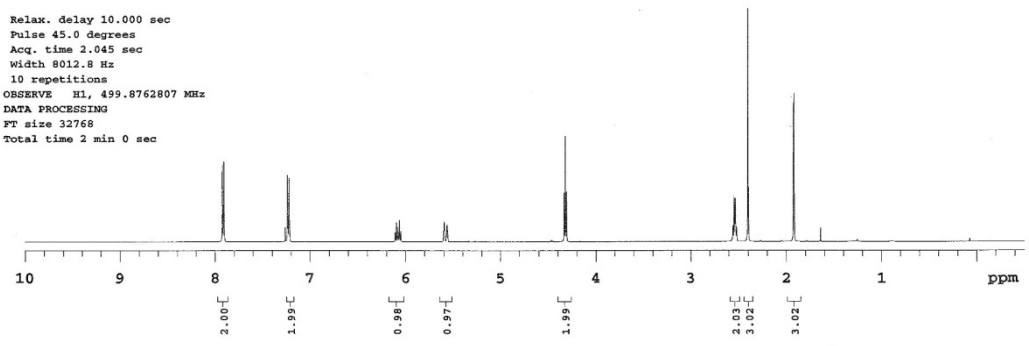
FidFile: PROTON



Pulse Sequence: PROTON (s2pul)
Solvent: cdcl3
Data collected on: Oct 29 2019

Temp. 25.0 C / 298.1 K
Operator: Liu

Relax. delay 10.000 sec
Pulse 45.0 degrees
Acq. time 2.045 sec
Width 8012.8 Hz
10 repetitions
OBSERVE H1, 499.8762807 MHz
DATA PROCESSING
FT size 32768
Total time 2 min 0 sec



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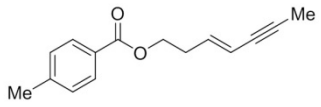
Sample Name:

Data Collected on:
nmr18-vnmrs500
Archive directory:

Sample directory:

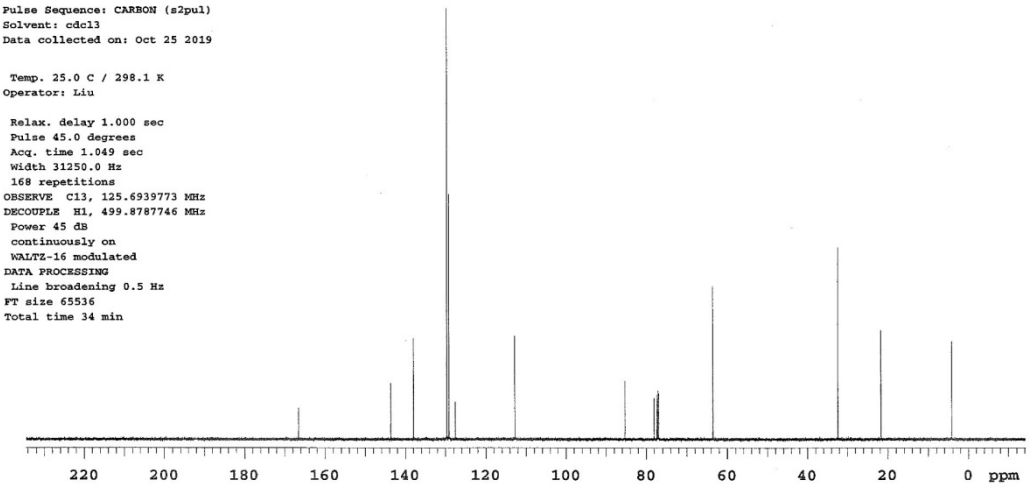
FidFile: CARBON



Pulse Sequence: CARBON (s2pul)
Solvent: cdcl3
Data collected on: Oct 25 2019

Temp. 25.0 C / 298.1 K
Operator: Liu

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.049 sec
Width 31250.0 Hz
168 repetitions
OBSERVE C13, 125.6939773 MHz
DECOUPLE H1, 499.8787746 MHz
Power 45 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 0.5 Hz
FT size 65536
Total time 34 min

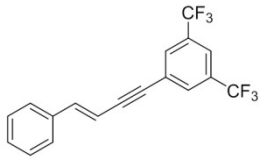


Sample Name:

Data Collected on:
nmr19-vnmrs600
Archive directory:

Sample directory:

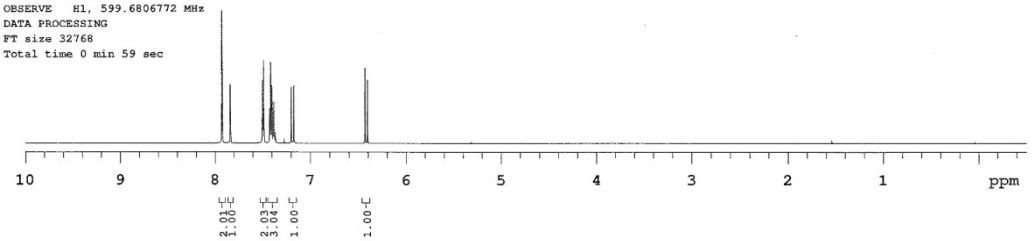
FidFile: PROTON



Pulse Sequence: PROTON (s2pul)
Solvent: cdcl3
Data collected on: Oct 26 2019

Temp. 25.0 C / 298.1 K
Operator: Liu

Relax. delay 10.000 sec
Pulse 45.0 degrees
Acq. time 1.704 sec
Width 9615.4 Hz
5 repetitions
OBSERVE H1, 599.6806772 MHz
DATA PROCESSING
FT size 32768
Total time 0 min 59 sec

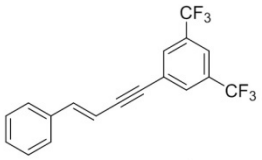


Sample Name:

Data Collected on:
nmr19-vnmrs600
Archive directory:

Sample directory:

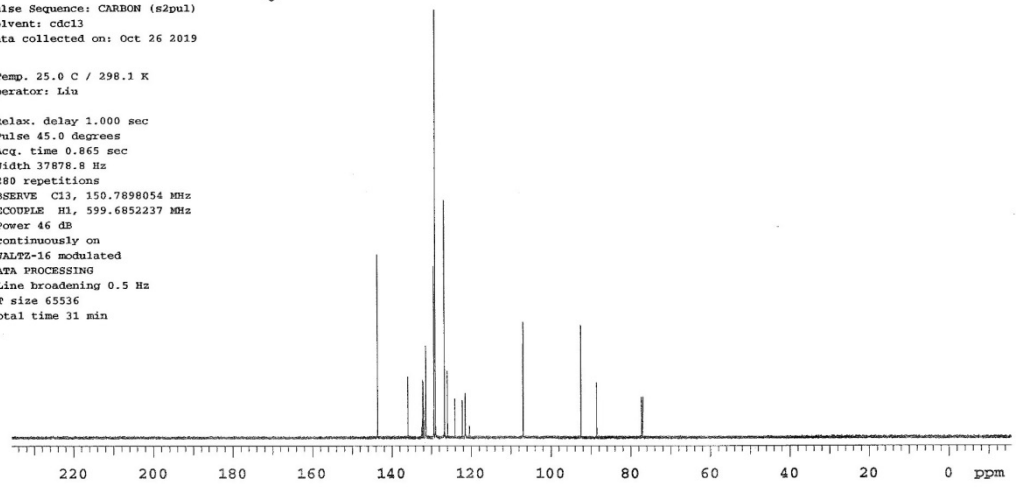
FidFile: yz-3-191026-ph-ph-cf32-C



Pulse Sequence: CARBON (s2pul)
Solvent: cdcl3
Data collected on: Oct 26 2019

Temp. 25.0 C / 298.1 K
Operator: Liu

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 0.865 sec
Width 37878.8 Hz
280 repetitions
OBSERVE C13, 150.7898054 MHz
DECOUPLE H1, 599.6852237 MHz
Power 46 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 0.5 Hz
FT size 65536
Total time 31 min



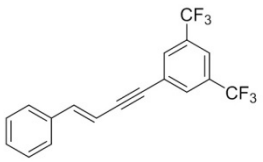
STANDARD FLUORINE PARAMETERS

Sample Name:

Data Collected on:
nmr19-vnmrs600
Archive directory:

Sample directory:

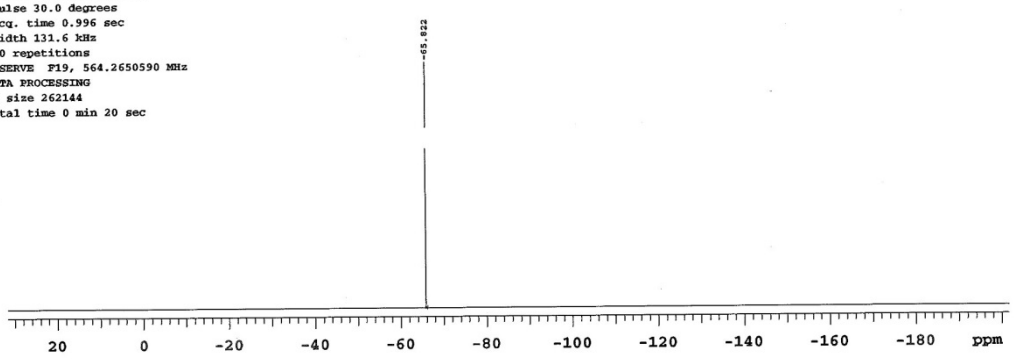
FidFile: yz-3-191026-ph-ph-cf32-F

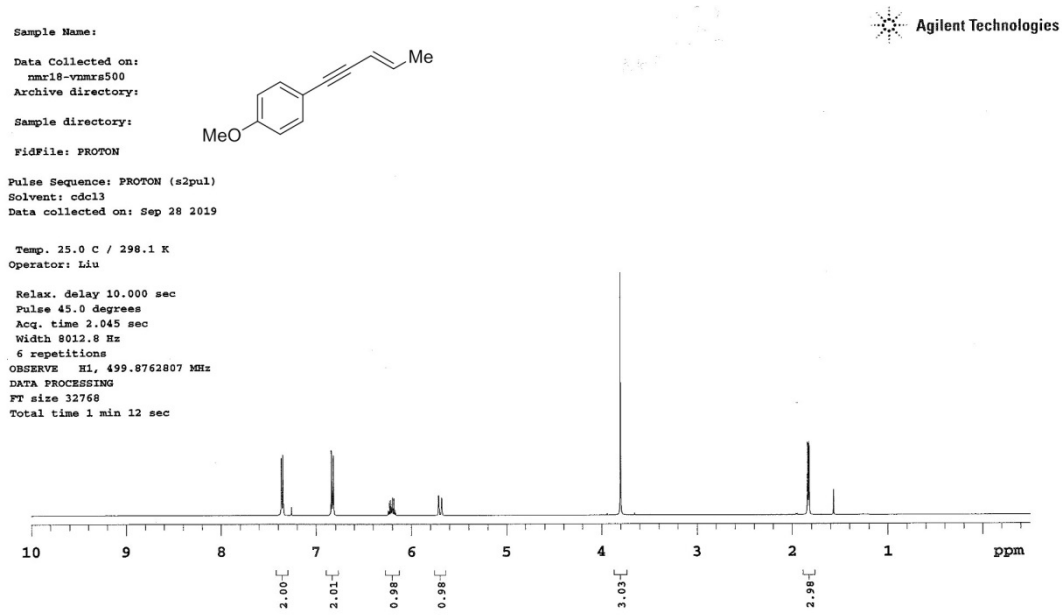


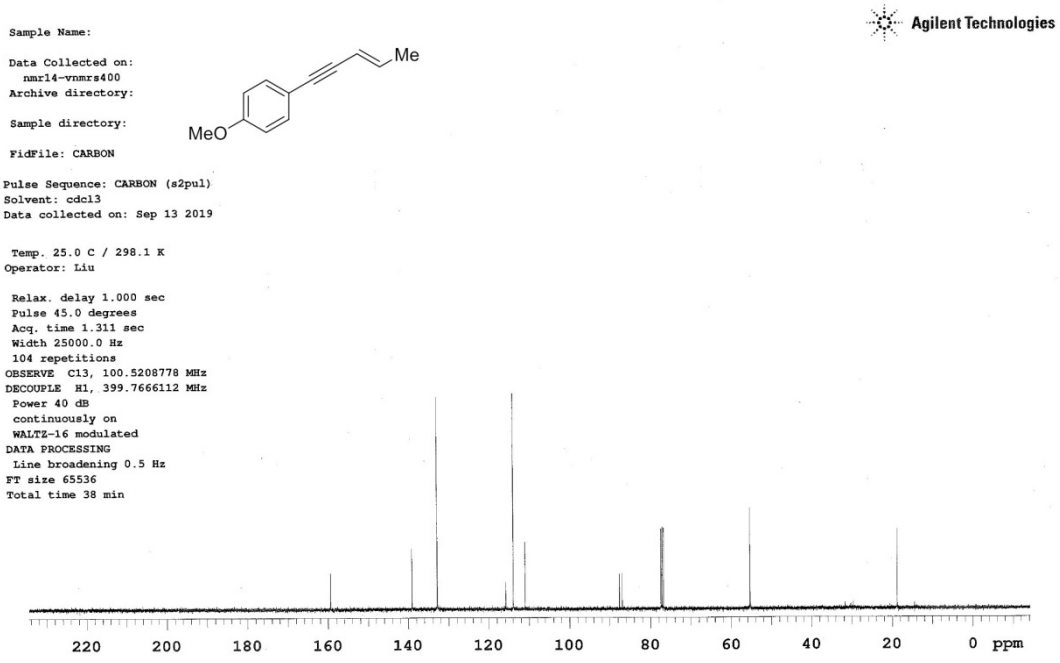
Pulse Sequence: FLUORINE (s2pul)
Solvent: cdcl3
Data collected on: Oct 26 2019

Temp. 25.0 C / 298.1 K
Operator: Liu

Relax. delay 1.000 sec
Pulse 30.0 degrees
Acq. time 0.996 sec
Width 131.6 kHz
10 repetitions
OBSERVE F19, 564.2650590 MHz
DATA PROCESSING
FT size 262144
Total time 0 min 20 sec




Agilent Technologies
Sample Name:
Data Collected on:
nmr18-vnmrs500
Archive directory:
Sample directory:
FidFile: PROTON
Me
MeO
Pulse Sequence: PROTON (s2pul)
Solvent: cdcl3
Data collected on: Sep 28 2019
Temp. 25.0 C / 298.1 K
Operator: Liu
Relax. delay 10.000 sec
Pulse 45.0 degrees
Acq. time 2.045 sec
Width 8012.8 Hz
6 repetitions
OBSERVE H1, 499.8762807 MHz
DATA PROCESSING
FT size 32768
Total time 1 min 12 sec
10
9
8
7
6
5
4
3
2
1
ppm
2.00
2.01
0.98
0.98
3.03
2.98


Agilent Technologies
Sample Name:
Data Collected on:
nmr14-vnmrs400
Archive directory:
Sample directory:
FidFile: CARBON
Me
MeO
Pulse Sequence: CARBON (s2pul)
Solvent: cdcl3
Data collected on: Sep 13 2019
Temp. 25.0 C / 298.1 K
Operator: Liu
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.311 sec
Width 25000.0 Hz
104 repetitions
OBSERVE C13, 100.5208778 MHz
DECOUPLE H1, 399.7666112 MHz
Power 40 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 0.5 Hz
FT size 65536
Total time 38 min
220
200
180
160
140
120
100
80
60
40
20
0 ppm

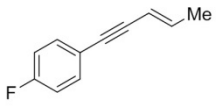
Agilent Technologies

Sample Name:

Data Collected on:
nmr18-vnmrs500
Archive directory:

Sample directory:

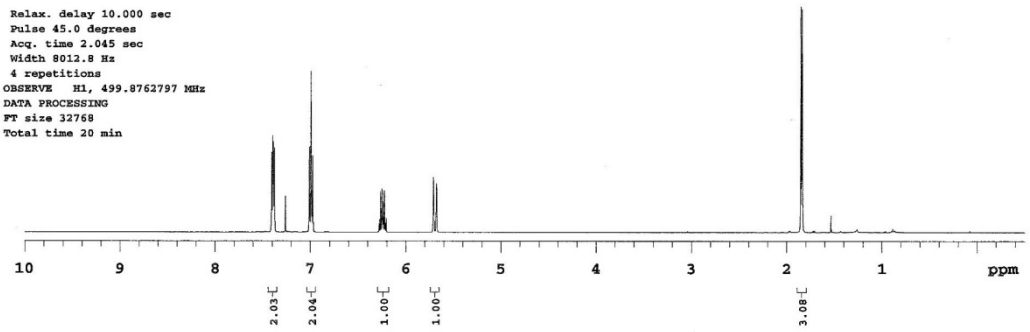
FidFile: PROTON



Pulse Sequence: PROTON (s2pul)
Solvent: cdcl3
Data collected on: Jul 5 2019

Temp. 25.0 C / 298.1 K
Operator: Liu

Relax. delay 10.000 sec
Pulse 45.0 degrees
Acq. time 2.045 sec
Width 8012.8 Hz
4 repetitions
OBSERVE H1, 499.8762797 MHz
DATA PROCESSING
FT size 32768
Total time 20 min



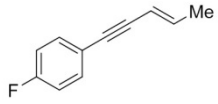
Agilent Technologies

Sample Name:

Data Collected on:
nmr18-vnmrs500
Archive directory:

Sample directory:

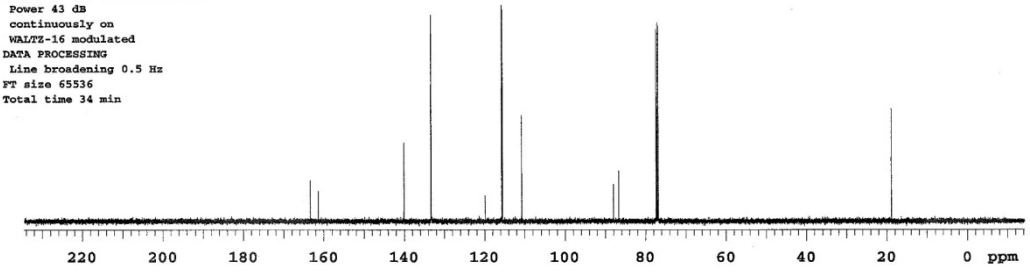
FidFile: CARBON



Pulse Sequence: CARBON (s2pul)
Solvent: cdcl3
Data collected on: Jul 5 2019

Temp. 25.0 C / 298.1 K
Operator: Liu

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.049 sec
Width 31250.0 Hz
300 repetitions
OBSERVE C13, 125.6939696 MHz
DECOUPLE H1, 499.8787746 MHz
Power 43 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 0.5 Hz
FT size 65536
Total time 34 min



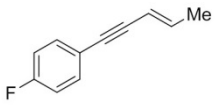
STANDARD FLUORINE PARAMETERS

Sample Name:

Data Collected on:
nmr18-vnmrs500
Archive directory:

Sample directory:

FidFile: FLUORINE

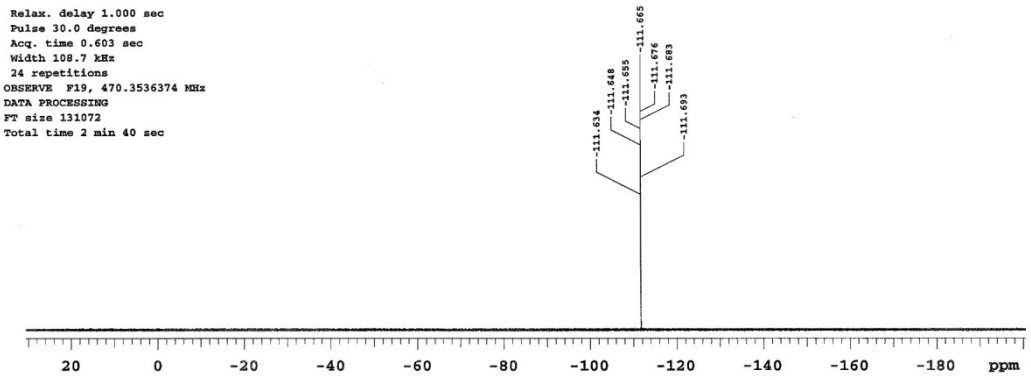


Agilent Technologies

Pulse Sequence: FLUORINE (s2pul)
Solvent: cdcl3
Data collected on: Jul 5 2019

Temp. 25.0 C / 298.1 K
Operator: Liu

Relax. delay 1.000 sec
Pulse 30.0 degrees
Acq. time 0.603 sec
Width 108.7 kHz
24 repetitions
OBSERVE F19, 470.3536374 MHz
DATA PROCESSING
FT size 131072
Total time 2 min 40 sec

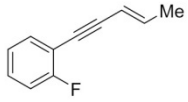


Sample Name:

Data Collected on:
nmr18-vnmrs500
Archive directory:

Sample directory:

FidFile: PROTON

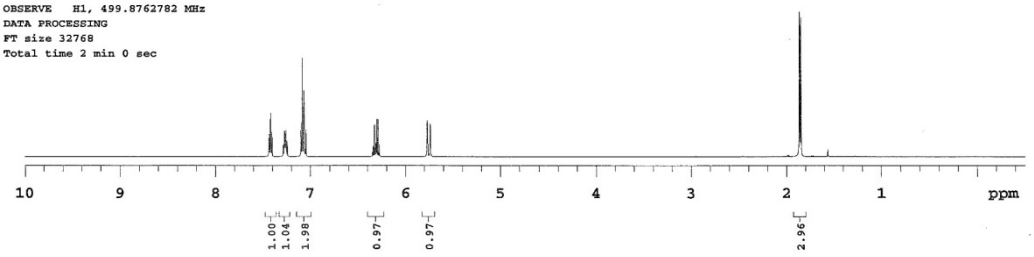


Agilent Technologies

Pulse Sequence: PROTON (s2pul)
Solvent: cdcl3
Data collected on: Oct 21 2019

Temp. 25.0 C / 298.1 K
Operator: Liu

Relax. delay 10.000 sec
Pulse 45.0 degrees
Acq. time 2.045 sec
Width 8012.8 Hz
3 repetitions
OBSERVE H1, 499.8762782 MHz
DATA PROCESSING
FT size 32768
Total time 2 min 0 sec



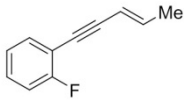
Agilent Technologies

Sample Name:

Data Collected on:
nmr18-vnmrs500
Archive directory:

Sample directory:

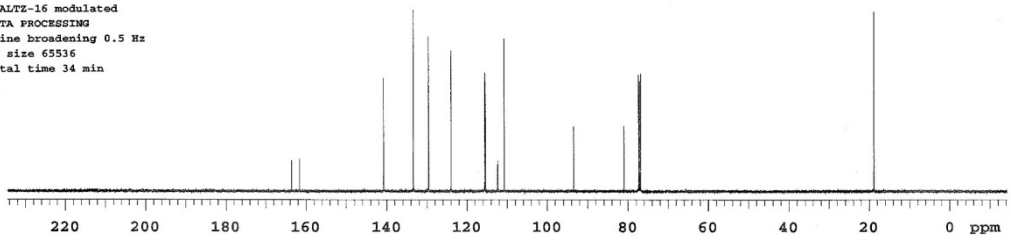
FidFile: CARBON



Pulse Sequence: CARBON (s2pul)
Solvent: cdcl3
Data collected on: Oct 21 2019

Temp. 25.0 C / 298.1 K
Operator: Liu

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.049 sec
Width 31250.0 Hz
162 repetitions
OBSERVE C13, 125.6939753 MHz
DECOUPLE H1, 499.8787746 MHz
Power 45 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 0.5 Hz
FT size 65536
Total time 34 min



STANDARD FLUORINE PARAMETERS

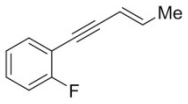
Agilent Technologies

Sample Name:

Data Collected on:
nmr18-vnmrs500
Archive directory:

Sample directory:

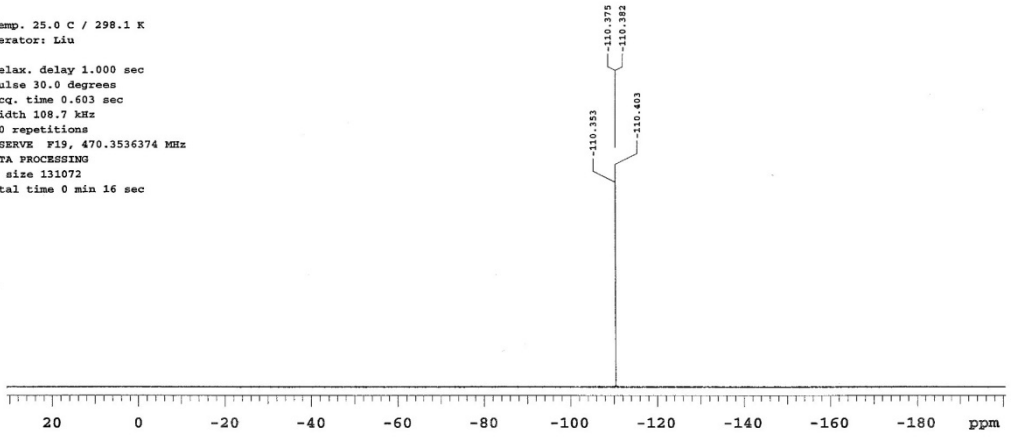
FidFile: yz-3-191021-orthoF-enyne-F



Pulse Sequence: FLUORINE (s2pul)
Solvent: cdcl3
Data collected on: Oct 21 2019

Temp. 25.0 C / 298.1 K
Operator: Liu

Relax. delay 1.000 sec
Pulse 30.0 degrees
Acq. time 0.603 sec
Width 108.7 kHz
10 repetitions
OBSERVE F19, 470.3536374 MHz
DATA PROCESSING
FT size 131072
Total time 0 min 16 sec



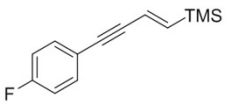
Agilent Technologies

Sample Name:

Data Collected on:
nmr18-vnmrs500
Archive directory:

Sample directory:

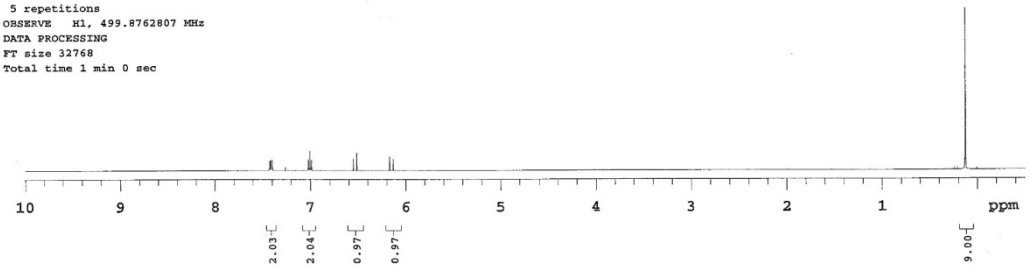
FidFile: PROTON



Pulse Sequence: PROTON (s2pul)
Solvent: cdcl3
Data collected on: Nov 1 2019

Temp. 25.0 C / 298.1 K
Operator: Liu

Relax. delay 10.000 sec
Pulse 45.0 degrees
Acq. time 2.045 sec
Width 8012.8 Hz
5 repetitions
OBSERVE H1, 499.8762807 MHz
DATA PROCESSING
FT size 32768
Total time 1 min 0 sec



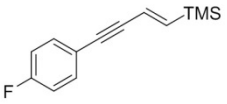
Agilent Technologies

Sample Name:

Data Collected on:
nmr18-vnmrs500
Archive directory:

Sample directory:

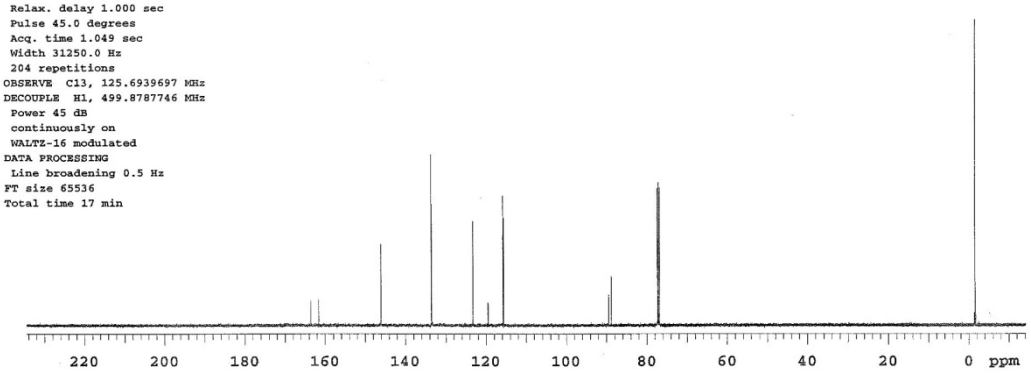
FidFile: CARBON



Pulse Sequence: CARBON (s2pul)
Solvent: cdcl3
Data collected on: Nov 1 2019

Temp. 25.0 C / 298.1 K
Operator: Liu

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.049 sec
Width 31250.0 Hz
204 repetitions
OBSERVE C13, 125.6939697 MHz
DECOUPLE H1, 499.8787746 MHz
Power 45 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 0.5 Hz
FT size 65536
Total time 17 min



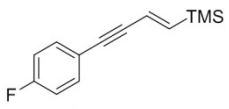
STANDARD FLUORINE PARAMETERS

Sample Name:

Data Collected on:
nmr18-vnmrs500
Archive directory:

Sample directory:

FidFile: FLUORINE

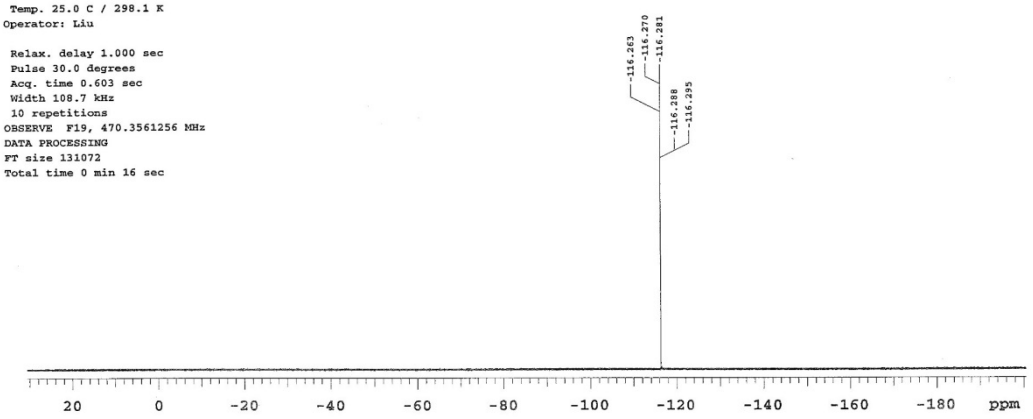


Agilent Technologies

Pulse Sequence: FLUORINE (s2pul)
Solvent: cd3cn
Data collected on: Nov 1 2019

Temp. 25.0 C / 298.1 K
Operator: Liu

Relax. delay 1.000 sec
Pulse 30.0 degrees
Acq. time 0.603 sec
Width 108.7 kHz
10 repetitions
OBSERVE F19, 470.3561256 MHz
DATA PROCESSING
FT size 131072
Total time 0 min 16 sec



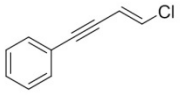
STANDARD PROTON PARAMETERS

Sample Name:

Data Collected on:
nmr18-vnmrs500
Archive directory:

Sample directory:

FidFile: PROTON

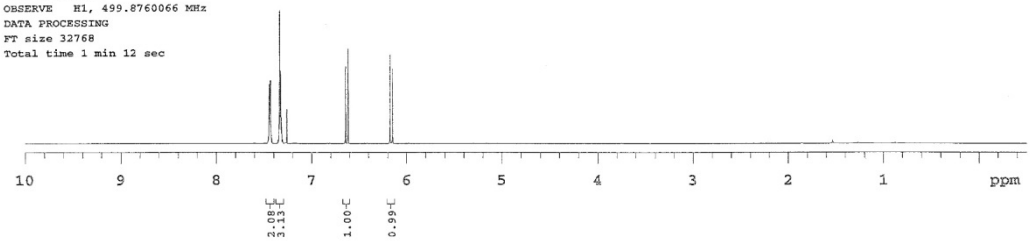


Agilent Technologies

Pulse Sequence: PROTON (s2pul)
Solvent: cdcl3
Data collected on: Mar 17 2020

Temp. 25.0 C / 298.1 K
Operator: Liu

Relax. delay 10.000 sec
Pulse 45.0 degrees
Acq. time 2.045 sec
Width 8012.8 Hz
6 repetitions
OBSERVE H1, 499.8760066 MHz
DATA PROCESSING
FT size 32768
Total time 1 min 12 sec



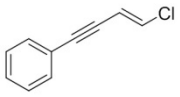
Agilent Technologies

Sample Name:

Data Collected on:
nmr18-vnmrs500
Archive directory:

Sample directory:

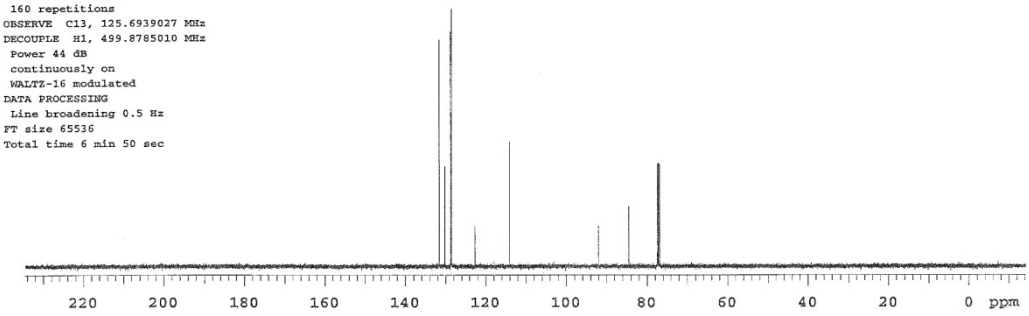
FidFile: CARBON



Pulse Sequence: CARBON (s2pul)
Solvent: cdcl3
Data collected on: Mar 17 2020

Temp. 25.0 C / 298.1 K
Operator: Liu

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.049 sec
Width 31250.0 Hz
160 repetitions
OBSERVE C13, 125.6939027 MHz
DECOUPLE H1, 499.8785010 MHz
Power 44 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 0.5 Hz
FT size 65536
Total time 6 min 50 sec



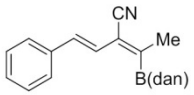
Agilent Technologies

Sample Name:

Data Collected on:
nmr18-vnmrs500
Archive directory:

Sample directory:

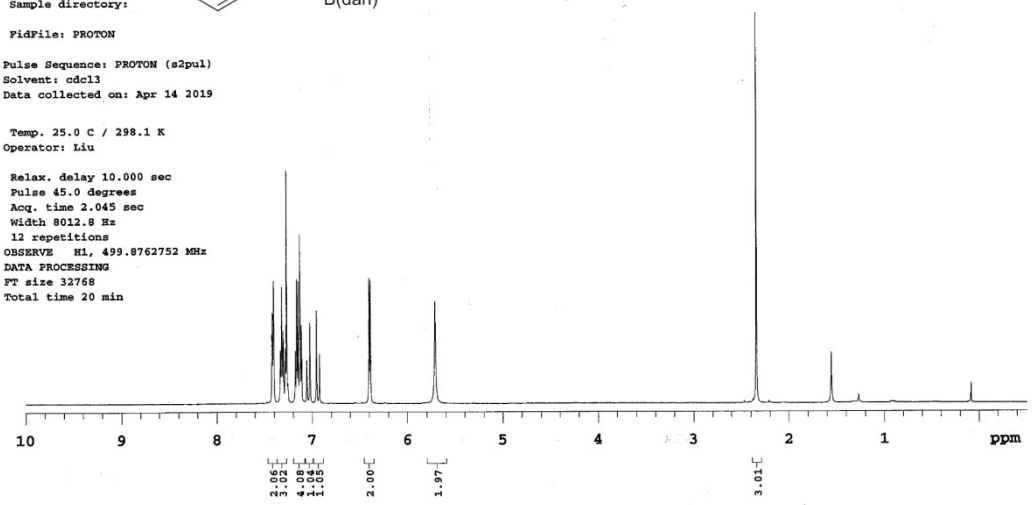
FidFile: PROTON



Pulse Sequence: PROTON (s2pul)
Solvent: cdcl3
Data collected on: Apr 14 2019

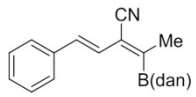
Temp. 25.0 C / 298.1 K
Operator: Liu

Relax. delay 10.000 sec
Pulse 45.0 degrees
Acq. time 2.045 sec
Width 8012.8 Hz
12 repetitions
OBSERVE H1, 499.8762752 MHz
DATA PROCESSING
FT size 32768
Total time 20 min



H

Sample Name:



Data Collected on:
nmr14-vnmrs400
Archive directory:

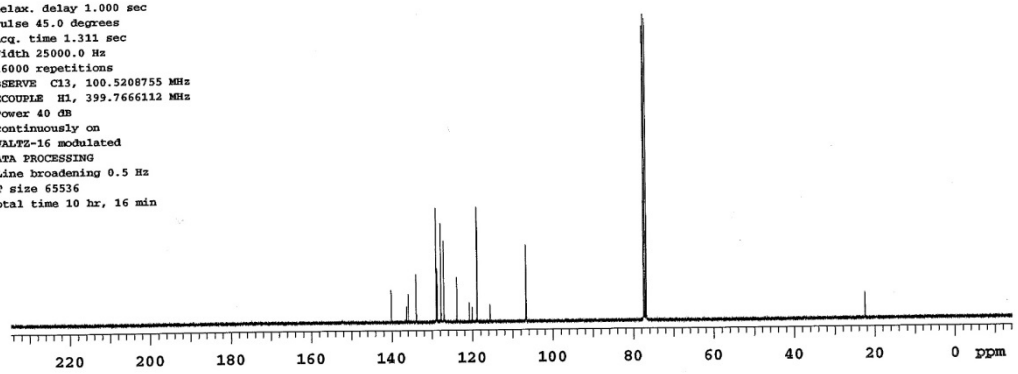
Sample directory:

FidFile: yz-3-190417-H-C

Pulse Sequence: CARBON (s2pul)
Solvent: cdcl3
Data collected on: Apr 17 2019

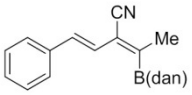
Temp. 25.0 C / 298.1 K
Operator: Liu

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.311 sec
Width 25000.0 Hz
16000 repetitions
OBSERVE C13, 100.5208755 MHz
DECOUPLE H1, 399.7666112 MHz
Power 40 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 0.5 Hz
FT size 65536
Total time 10 hr, 16 min



Agilent Technologies

Sample Name:



Data Collected on:
nmr11-inova500
Archive directory:

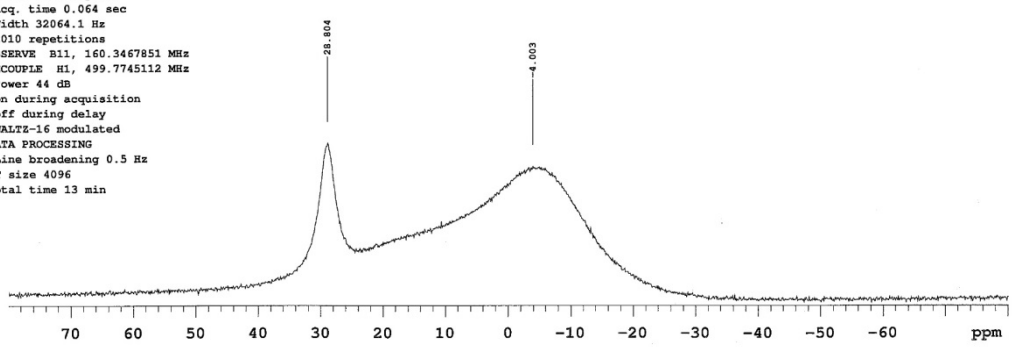
Sample directory:

FidFile: B11

Pulse Sequence: s2pul
Solvent: cdcl3
Data collected on: Apr 18 2019

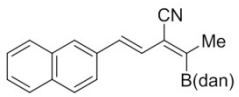
Temp. 25.0 C / 298.1 K
Operator: Liu

Relax. delay 0.010 sec
Pulse 45.0 degrees
Acq. time 0.064 sec
Width 32064.1 Hz
2010 repetitions
OBSERVE B11, 160.3467851 MHz
DECOUPLE H1, 499.7745112 MHz
Power 44 dB
on during acquisition
off during delay
WALTZ-16 modulated
DATA PROCESSING
Line broadening 0.5 Hz
FT size 4096
Total time 13 min



Agilent Technologies

Sample Name:



Data Collected on:
nmr18-vnmrs500
Archive directory:

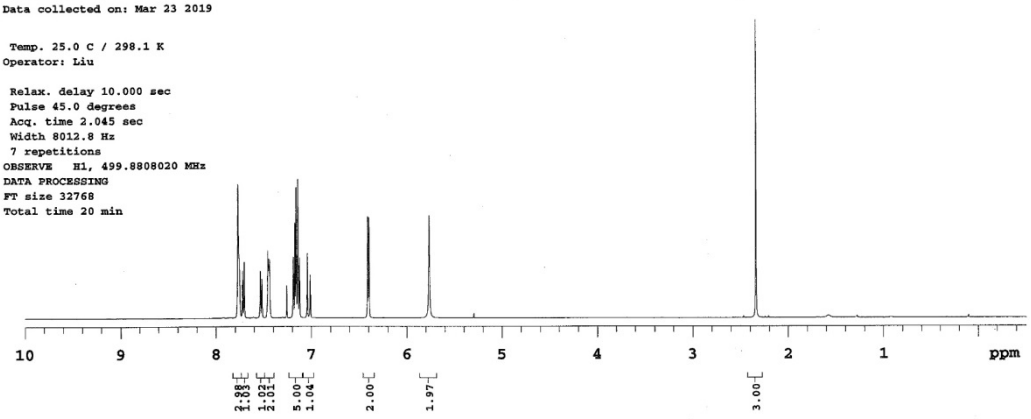
Sample directory:

FidFile: PROTON

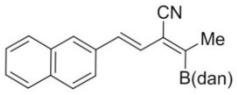
Pulse Sequence: PROTON (s2pul)
Solvent: cdcl3
Data collected on: Mar 23 2019

Temp. 25.0 C / 298.1 K
Operator: Liu

Relax. delay 10.000 sec
Pulse 45.0 degrees
Acq. time 2.045 sec
Width 8012.8 Hz
7 repetitions
OBSERVE H1, 499.8808020 MHz
DATA PROCESSING
FT size 32768
Total time 20 min



Sample Name:



Data Collected on:
nmr18-vnmrs500
Archive directory:

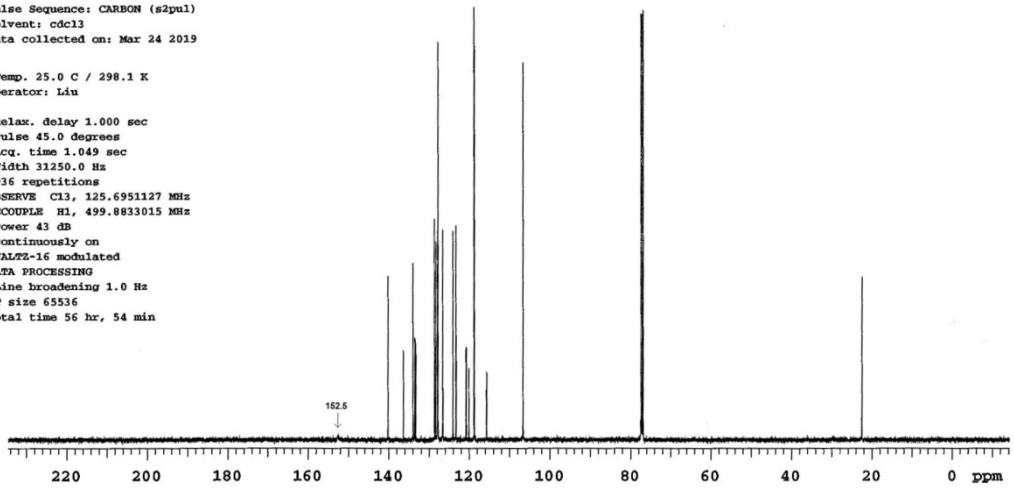
Sample directory:

FidFile: yz-3-190320-2-naph-C

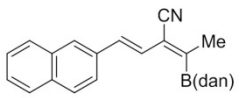
Pulse Sequence: CARBON (s2pul)
Solvent: cdcl3
Data collected on: Mar 24 2019

Temp. 25.0 C / 298.1 K
Operator: Liu

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.049 sec
Width 31250.0 Hz
936 repetitions
OBSERVE C13, 125.6951127 MHz
DECOUPLE H1, 499.8833015 MHz
Power 43 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.0 Hz
FT size 65536
Total time 56 hr, 54 min



2-naph



Agilent Technologies

Sample Name:

Data Collected on:
nmr11-inova500
Archive directory:

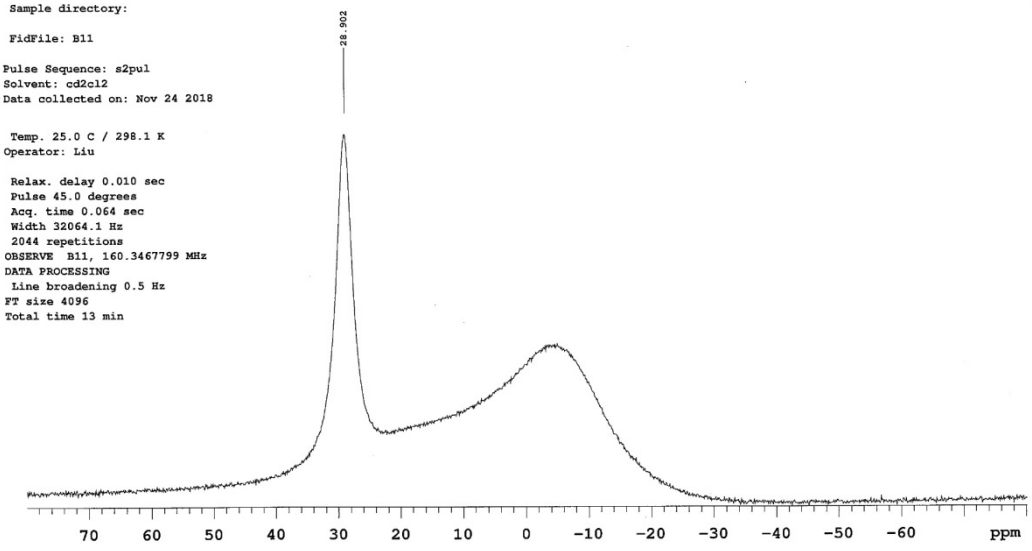
Sample directory:

FidFile: B11

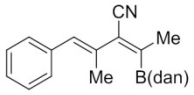
Pulse Sequence: s2pul
Solvent: cd2cl2
Data collected on: Nov 24 2018

Temp. 25.0 C / 298.1 K
Operator: Liu

Relax. delay 0.010 sec
Pulse 45.0 degrees
Acq. time 0.064 sec
Width 32064.1 Hz
2044 repetitions
OBSERVE B11, 160.3467799 MHz
DATA PROCESSING
Line broadening 0.5 Hz
FT size 4096
Total time 13 min



Sample Name:



Data Collected on:
nmr19-vnmrs600
Archive directory:

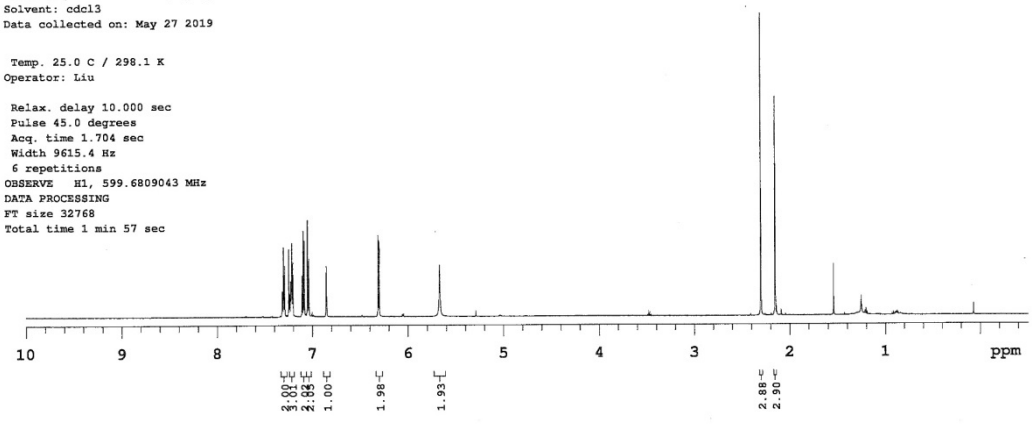
Sample directory:

FidFile: PROTON

Pulse Sequence: PROTON (s2pul)
Solvent: cdcl3
Data collected on: May 27 2019

Temp. 25.0 C / 298.1 K
Operator: Liu

Relax. delay 10.000 sec
Pulse 45.0 degrees
Acq. time 1.704 sec
Width 9615.4 Hz
6 repetitions
OBSERVE H1, 599.6809043 MHz
DATA PROCESSING
FT size 32768
Total time 1 min 57 sec



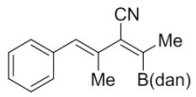
Phco2CH2CH2enyne

Sample Name:

Data Collected on:
nmr18-vnmrs500
Archive directory:

Sample directory:

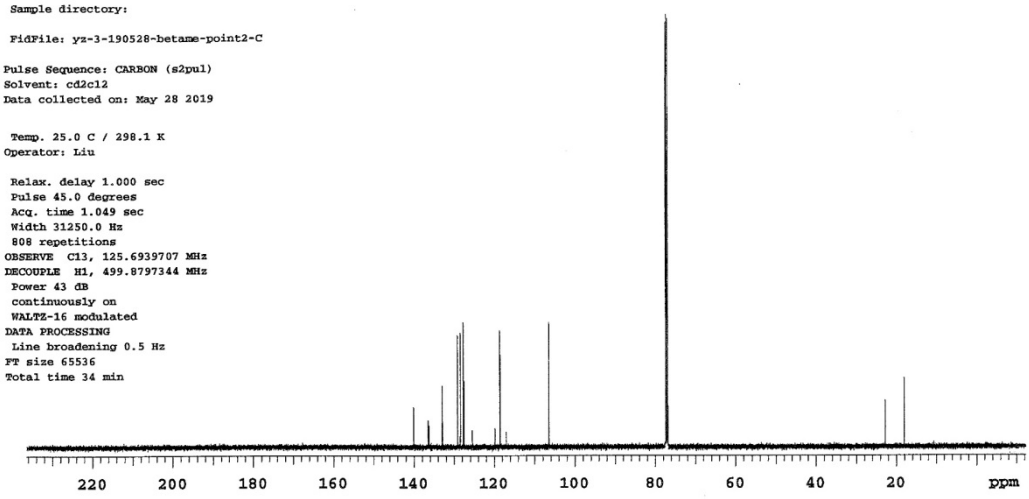
FidFile: yz-3-190528-betame-point2-C



Pulse Sequence: CARBON (s2pul)
Solvent: cd2c12
Data collected on: May 28 2019

Temp. 25.0 C / 298.1 K
Operator: Liu

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.049 sec
Width 31250.0 Hz
808 repetitions
OBSERVE C13, 125.6939707 MHz
DECOUPLE H1, 499.8797344 MHz
Power 43 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 0.5 Hz
FT size 65536
Total time 34 min



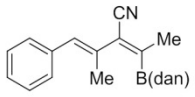
Agilent Technologies

Sample Name:

Data Collected on:
nmr11-inova500
Archive directory:

Sample directory:

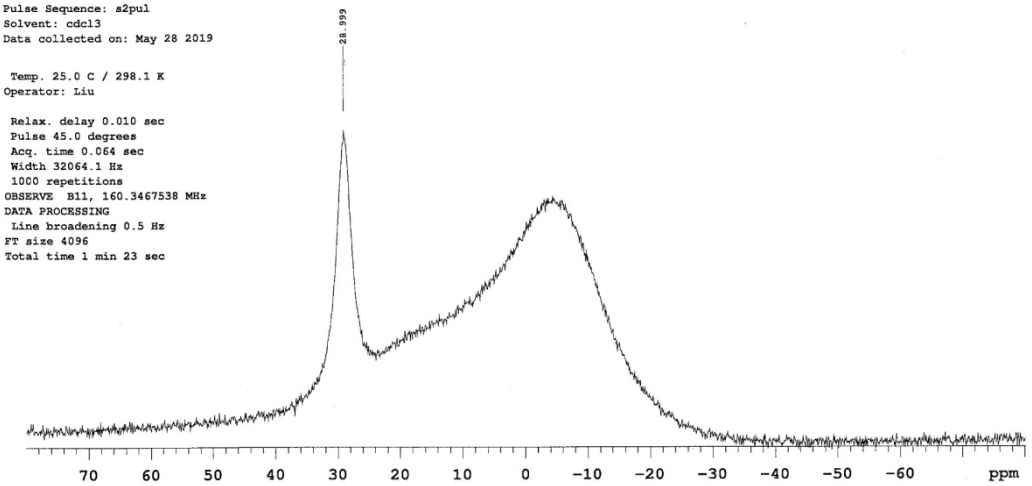
FidFile: B11



Pulse Sequence: s2pul
Solvent: cdcl3
Data collected on: May 28 2019

Temp. 25.0 C / 298.1 K
Operator: Liu

Relax. delay 0.010 sec
Pulse 45.0 degrees
Acq. time 0.064 sec
Width 32064.1 Hz
1000 repetitions
OBSERVE B11, 160.3467538 MHz
DATA PROCESSING
Line broadening 0.5 Hz
FT size 4096
Total time 1 min 23 sec

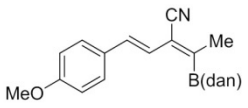


Sample Name:

Data Collected on:
nmr19-vnmrs600
Archive directory:

Sample directory:

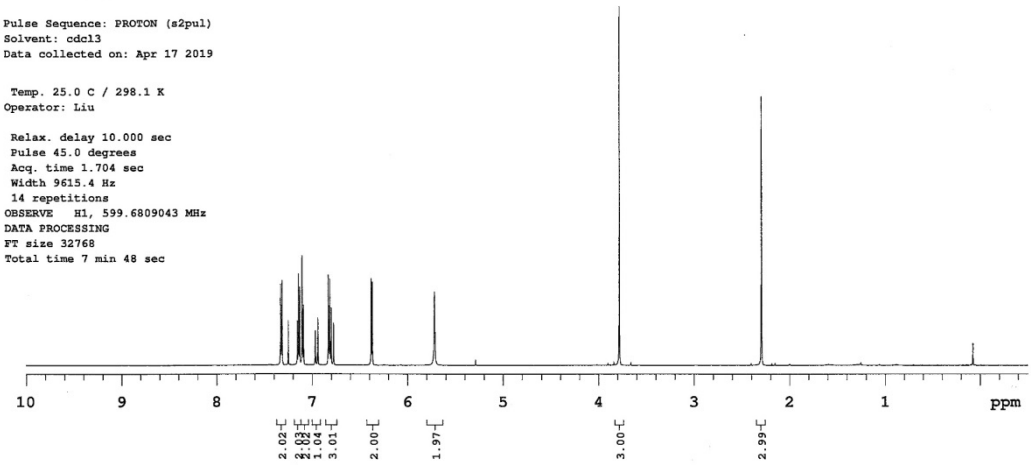
FidFile: PROTON



Pulse Sequence: PROTON (s2pul)
Solvent: cdcl3
Data collected on: Apr 17 2019

Temp. 25.0 C / 298.1 K
Operator: Liu

Relax. delay 10.000 sec
Pulse 45.0 degrees
Acq. time 1.704 sec
Width 9615.4 Hz
14 repetitions
OBSERVE H1, 599.6809043 MHz
DATA PROCESSING
FT size 32768
Total time 7 min 48 sec

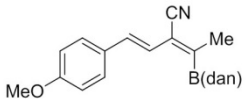


Sample Name:

Data Collected on:
nmr19-vnmrs600
Archive directory:

Sample directory:

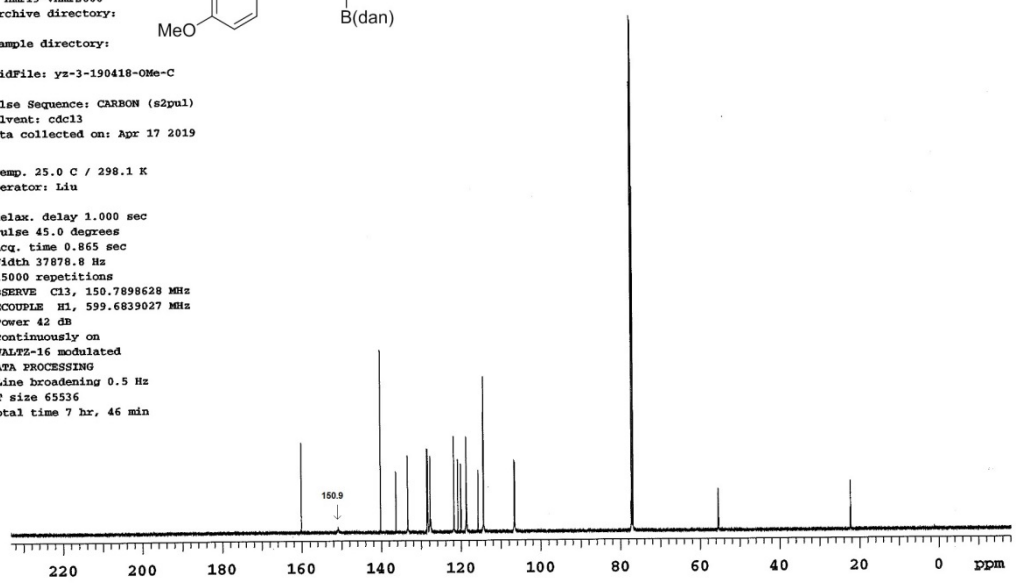
FidFile: yz-3-190418-OMe-C

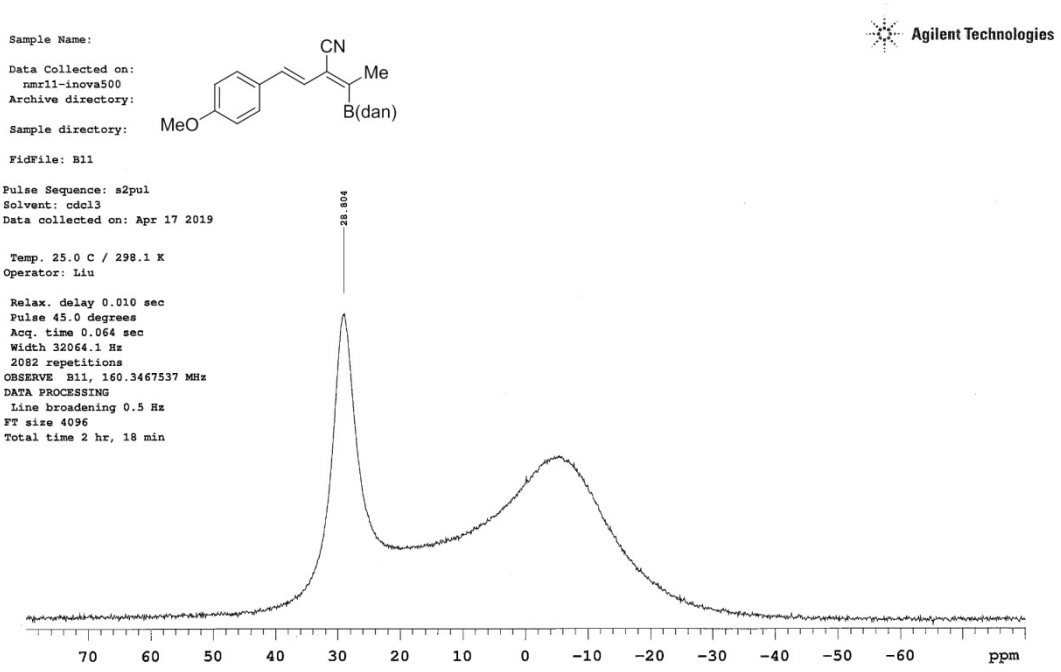


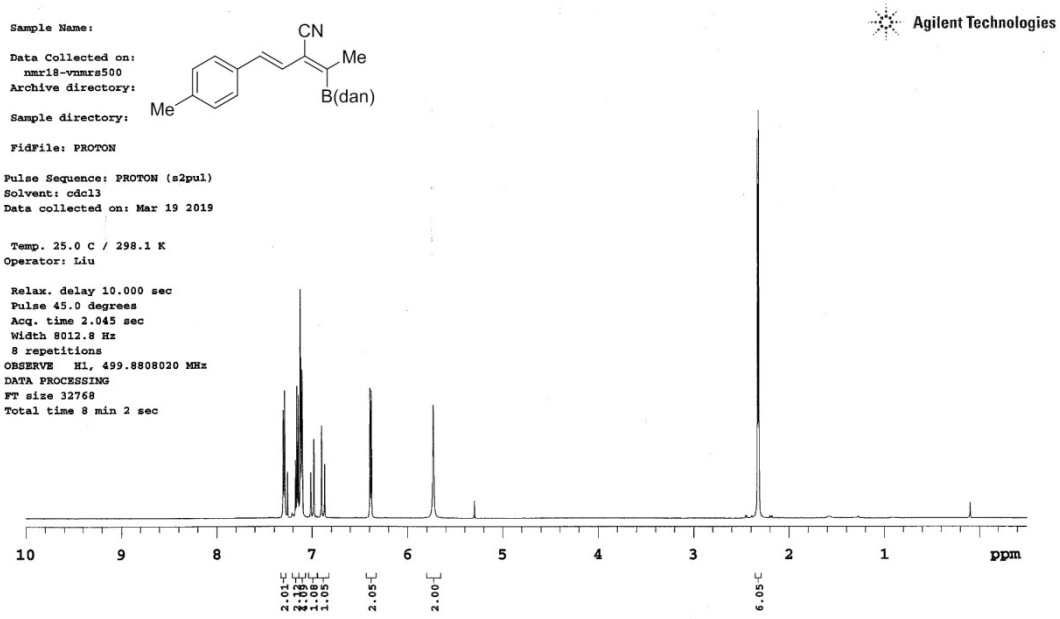
Pulse Sequence: CARBON (s2pul)
Solvent: cdcl3
Data collected on: Apr 17 2019

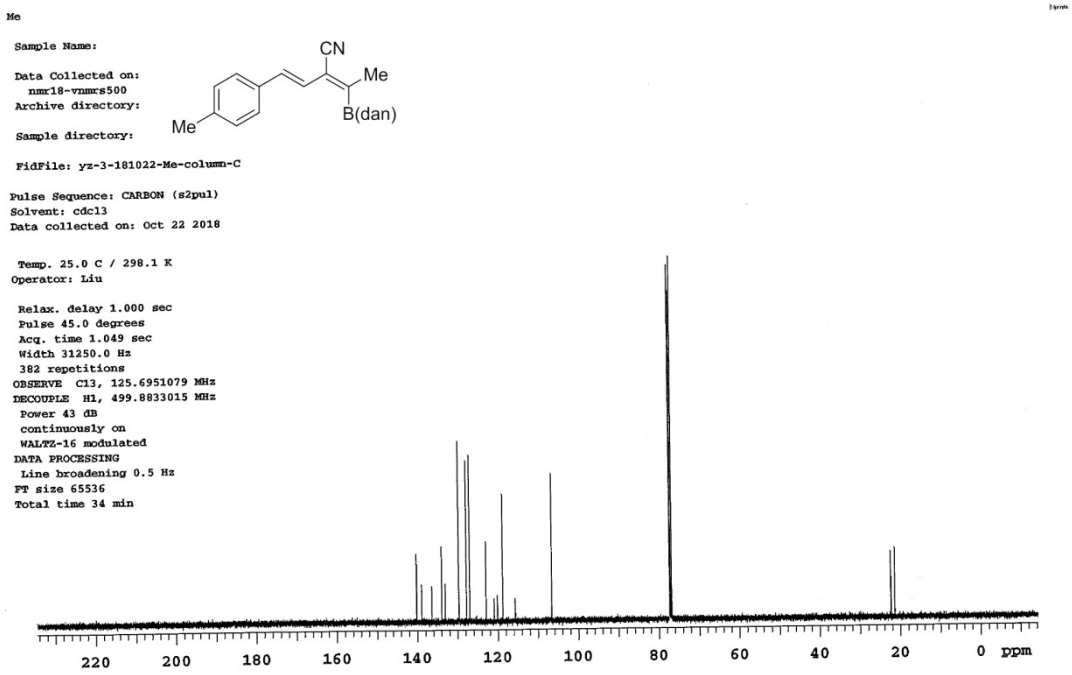
Temp. 25.0 C / 298.1 K
Operator: Liu

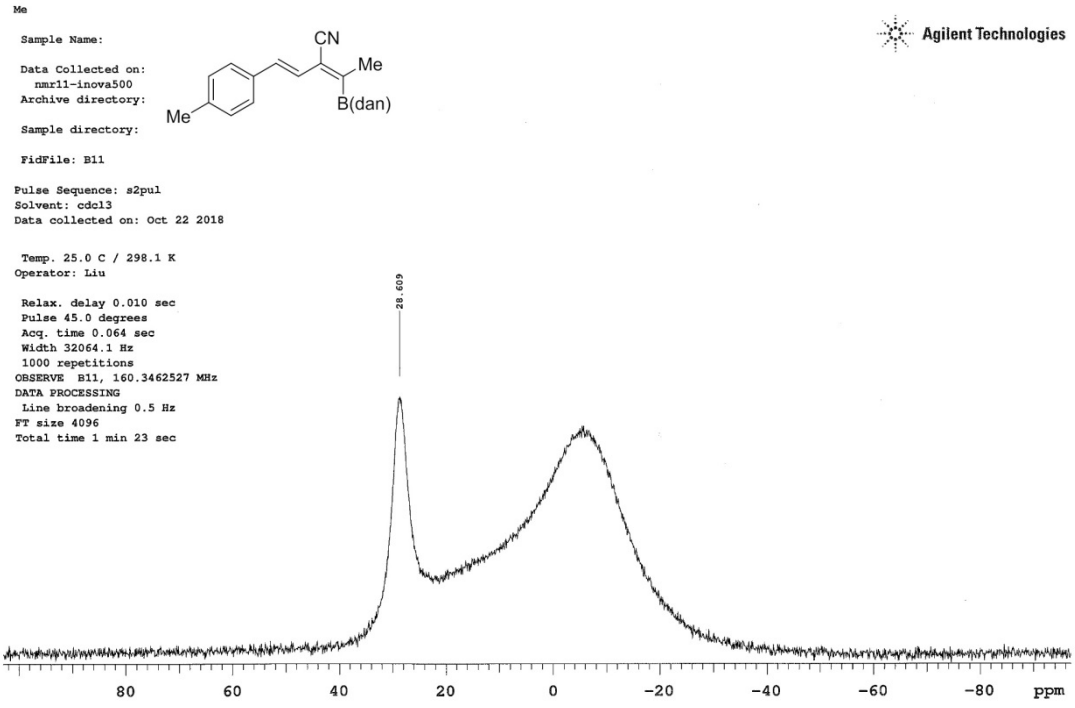
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 0.865 sec
Width 37878.8 Hz
15000 repetitions
OBSERVE C13, 150.7898628 MHz
DECOUPLE H1, 599.6839027 MHz
Power 42 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 0.5 Hz
FT size 65536
Total time 7 hr, 46 min




Agilent Technologies
Sample Name:
Data Collected on:
nmr11-inova500
Archive directory:
Sample directory:
FidFile: B11
CN
Me
B(dan)
MeO
Pulse Sequence: s2pul
Solvent: cdcl3
Data collected on: Apr 17 2019
Temp. 25.0 C / 298.1 K
Operator: Liu
Relax. delay 0.010 sec
Pulse 45.0 degrees
Acq. time 0.064 sec
Width 32064.1 Hz
2082 repetitions
OBSERVE B11, 160.3467537 MHz
DATA PROCESSING
Line broadening 0.5 Hz
FT size 4096
Total time 2 hr, 18 min
28.804
70 60 50 40 30 20 10 0 -10 -20 -30 -40 -50 -60 ppm


Agilent Technologies
Sample Name:
Data Collected on:
nmr18-vnmrs500
Archive directory:
Sample directory:
FidFile: PROTON
CN
Me
B(dan)
Me
Pulse Sequence: PROTON (s2pul)
Solvent: cdcl3
Data collected on: Mar 19 2019
Temp. 25.0 C / 298.1 K
Operator: Liu
Relax. delay 10.000 sec
Pulse 45.0 degrees
Acq. time 2.045 sec
Width 8012.8 Hz
8 repetitions
OBSERVE H1, 499.8808020 MHz
DATA PROCESSING
FT size 32768
Total time 8 min 2 sec
10 9 8 7 6 5 4 3 2 1 ppm
2.01
2.05
1.05
2.05
2.00
6.05

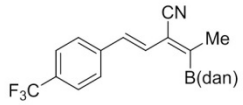

Me
Sample Name:
Data Collected on:
nmr18-vnmrs500
Archive directory:
Sample directory:
FidFile: yz-3-181022-Me-column-C
Pulse Sequence: CARBON (s2pul)
Solvent: cdcl3
Data collected on: Oct 22 2018
Temp. 25.0 C / 298.1 K
Operator: Liu
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.049 sec
Width 31250.0 Hz
382 repetitions
OBSERVE C13, 125.6951079 MHz
DECOUPLE H1, 499.8833015 MHz
Power 43 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 0.5 Hz
FT size 65536
Total time 34 min
CN
Me
B(dan)
Me
220
200
180
160
140
120
100
80
60
40
20
0
ppm


Me
Sample Name:
Data Collected on:
nmr11-inova500
Archive directory:
Sample directory:
FidFile: B11
Pulse Sequence: s2pul
Solvent: cdcl3
Data collected on: Oct 22 2018
Temp. 25.0 C / 298.1 K
Operator: Liu
Relax. delay 0.010 sec
Pulse 45.0 degrees
Acq. time 0.064 sec
Width 32064.1 Hz
1000 repetitions
OBSERVE B11, 160.3462527 MHz
DATA PROCESSING
Line broadening 0.5 Hz
FT size 4096
Total time 1 min 23 sec
28.609
CN
Me
B(dan)
Me
Agilent Technologies
80
60
40
20
0
-20
-40
-60
-80
ppm

Sample Name:

Data Collected on:
nmr19-vnmrs600
Archive directory:

Sample directory:

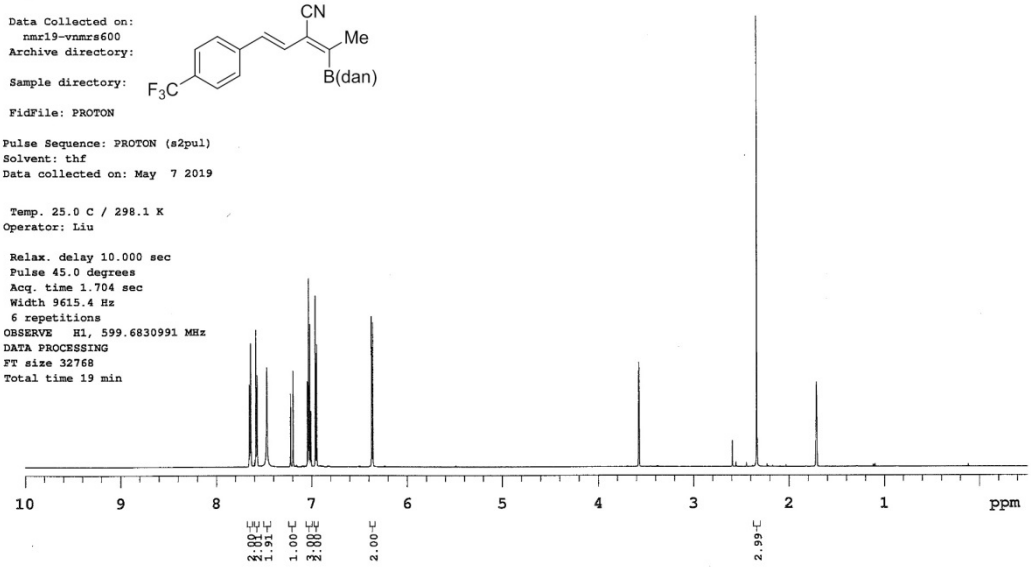


FidFile: PROTON

Pulse Sequence: PROTON (s2pul)
Solvent: thf
Data collected on: May 7 2019

Temp. 25.0 C / 298.1 K
Operator: Liu

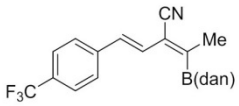
Relax. delay 10.000 sec
Pulse 45.0 degrees
Acq. time 1.704 sec
Width 9615.4 Hz
6 repetitions
OBSERVE H1, 599.6830991 MHz
DATA PROCESSING
FT size 32768
Total time 19 min



Sample Name:

Data Collected on:
nmr19-vnmrs600
Archive directory:

Sample directory:

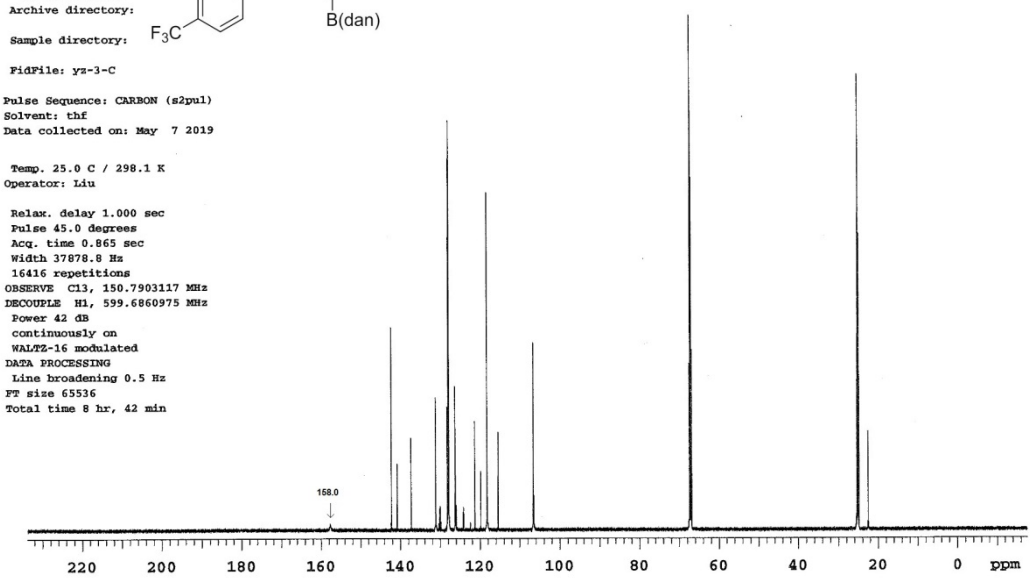


FidFile: yz-3-C

Pulse Sequence: CARBON (s2pul)
Solvent: thf
Data collected on: May 7 2019

Temp. 25.0 C / 298.1 K
Operator: Liu

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 0.865 sec
Width 37878.8 Hz
16416 repetitions
OBSERVE C13, 150.7903117 MHz
DECOUPLE H1, 599.6860975 MHz
Power 42 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 0.5 Hz
FT size 65536
Total time 8 hr, 42 min

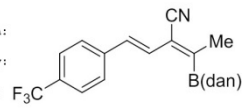


Agilent Technologies

Sample Name:

Data Collected on:
nmr11-inova500
Archive directory:

Sample directory:

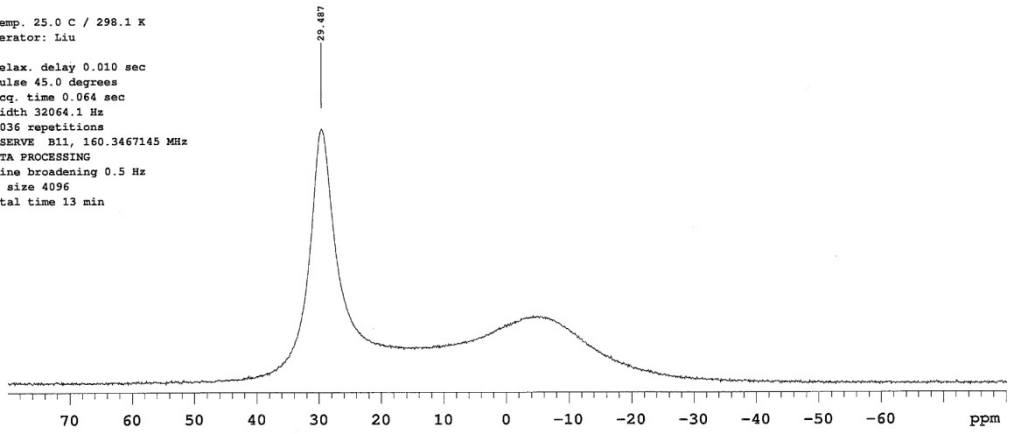


FidFile: B11

Pulse Sequence: s2pul
Solvent: thf
Data collected on: May 7 2019

Temp. 25.0 C / 298.1 K
Operator: Liu

Relax. delay 0.010 sec
Pulse 45.0 degrees
Acq. time 0.064 sec
Width 32064.1 Hz
1036 repetitions
OBSERVE B11, 160.3467145 MHz
DATA PROCESSING
Line broadening 0.5 Hz
FT size 4096
Total time 13 min

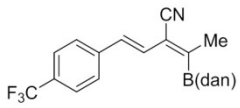


STANDARD FLUORINE PARAMETERS

Sample Name:

Data Collected on:
nmr19-vnmrs600
Archive directory:

Sample directory:

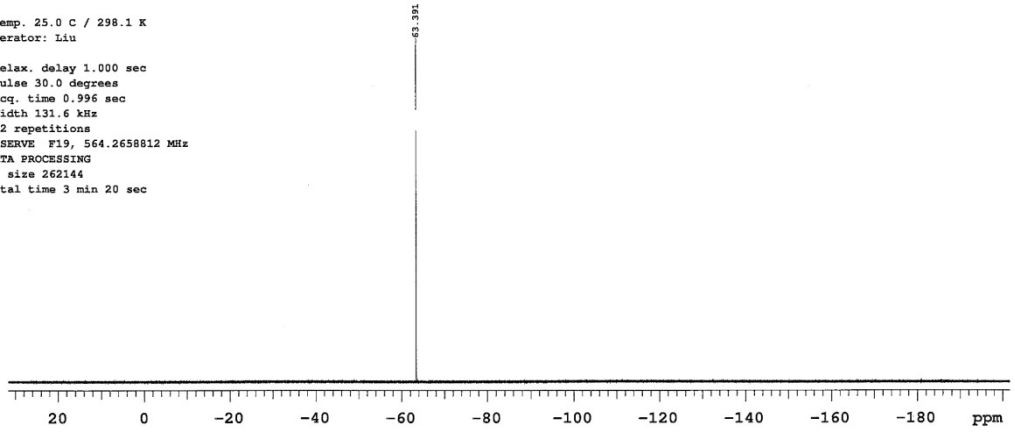


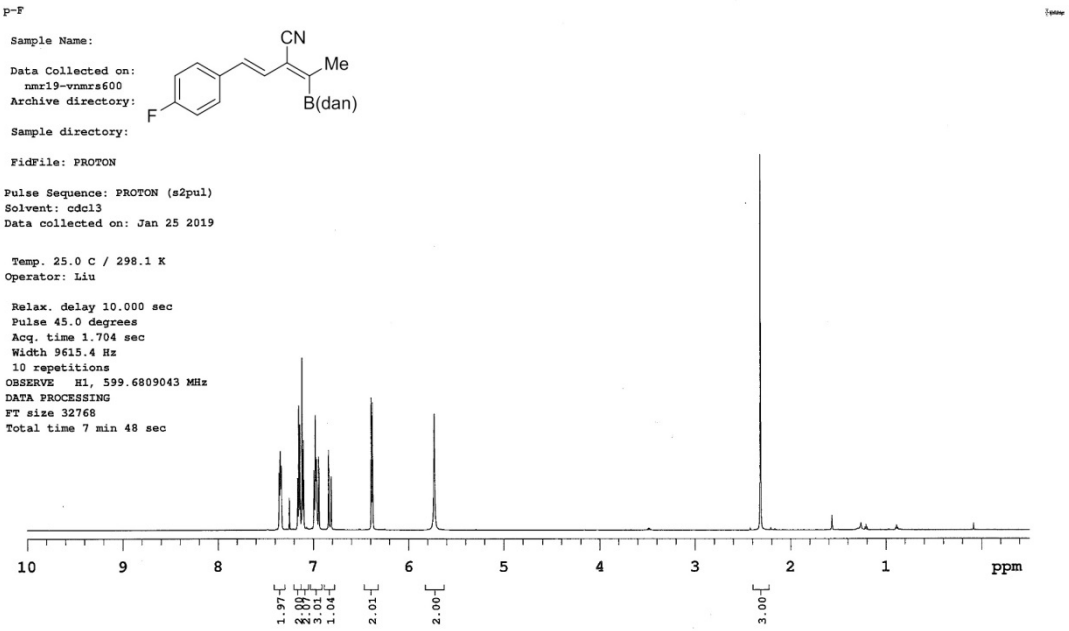
FidFile: FLUORINE

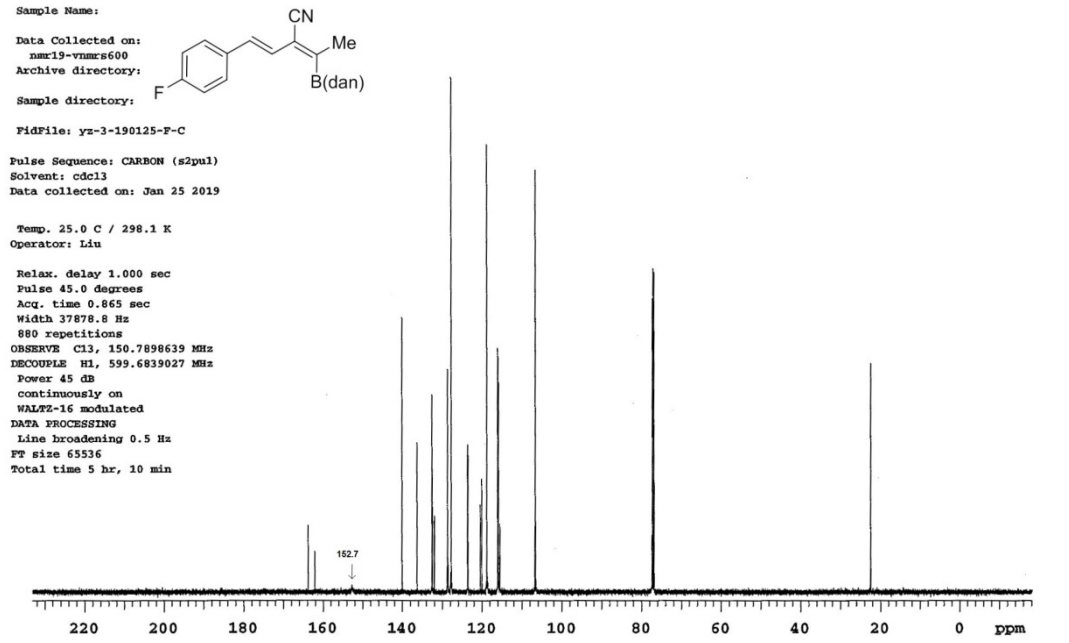
Pulse Sequence: FLUORINE (s2pul)
Solvent: thf
Data collected on: May 7 2019

Temp. 25.0 C / 298.1 K
Operator: Liu

Relax. delay 1.000 sec
Pulse 30.0 degrees
Acq. time 0.996 sec
Width 131.6 kHz
12 repetitions
OBSERVE F19, 564.2658812 MHz
DATA PROCESSING
FT size 262144
Total time 3 min 20 sec

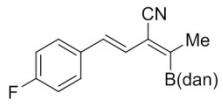



p-F
Sample Name:
Data Collected on:
nmr19-vnmrs600
Archive directory:
Sample directory:
FidFile: PROTON
Pulse Sequence: PROTON (s2pul)
Solvent: cdcl3
Data collected on: Jan 25 2019
Temp. 25.0 C / 298.1 K
Operator: Liu
Relax. delay 10.000 sec
Pulse 45.0 degrees
Acq. time 1.704 sec
Width 9615.4 Hz
10 repetitions
OBSERVE H1, 599.6809043 MHz
DATA PROCESSING
FT size 32768
Total time 7 min 48 sec
CN
Me
B(dan)
F
10
9
8
7
6
5
4
3
2
1
ppm
1.97
2.09
3.01
1.04
2.01
2.00
3.00


Sample Name:
Data Collected on:
nmr19-vnmrs600
Archive directory:
Sample directory:
FidFile: yz-3-190125-F-C
Pulse Sequence: CARBON (s2pul)
Solvent: cdcl3
Data collected on: Jan 25 2019
Temp. 25.0 C / 298.1 K
Operator: Liu
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 0.865 sec
Width 37878.8 Hz
880 repetitions
OBSERVE C13, 150.7898639 MHz
DECOUPLE H1, 599.6839027 MHz
Power 45 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 0.5 Hz
FT size 65536
Total time 5 hr, 10 min
CN
Me
B(dan)
F
152.7
220
200
180
160
140
120
100
80
60
40
20
0
ppm

p-F

Sample Name:



Data Collected on:
nmr11-inova500
Archive directory:

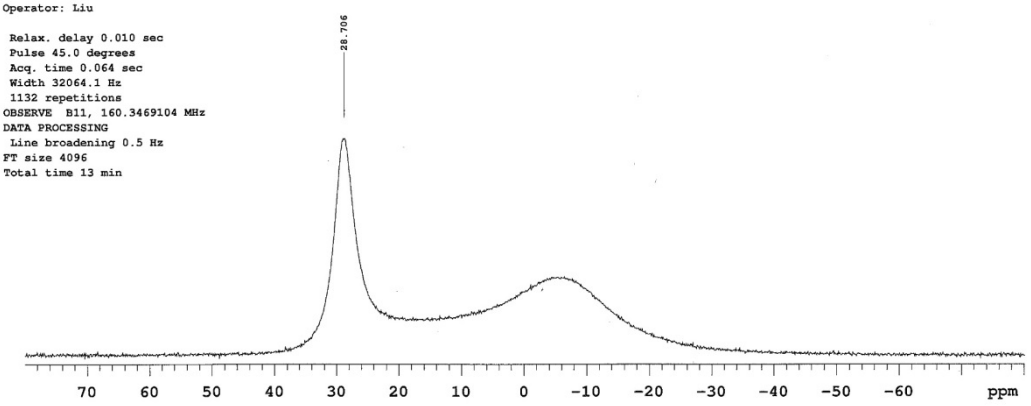
Sample directory:

FidFile: B11

Pulse Sequence: s2pul
Solvent: cdcl3
Data collected on: Jan 25 2019

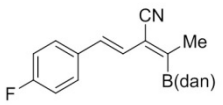
Temp. 25.0 C / 298.1 K
Operator: Liu

Relax. delay 0.010 sec
Pulse 45.0 degrees
Acq. time 0.064 sec
Width 32064.1 Hz
1132 repetitions
OBSERVE B11, 160.3469104 MHz
DATA PROCESSING
Line broadening 0.5 Hz
FT size 4096
Total time 13 min



p-F

Sample Name:



Data Collected on:
nmr19-vnmrs600
Archive directory:

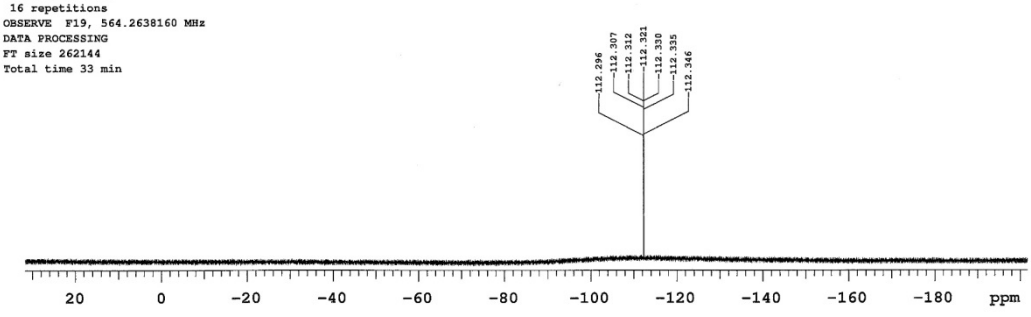
Sample directory:

FidFile: yz-3-190123-F-F

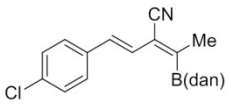
Pulse Sequence: FLUORINE (s2pul)
Solvent: cdcl3
Data collected on: Jan 23 2019

Temp. 25.0 C / 298.1 K
Operator: Liu

Relax. delay 1.000 sec
Pulse 30.0 degrees
Acq. time 0.996 sec
Width 131.6 kHz
16 repetitions
OBSERVE F19, 564.2638160 MHz
DATA PROCESSING
FT size 262144
Total time 33 min



p-Cl



Sample Name:

Data Collected on:
nmr19-vnmrs600
Archive directory:

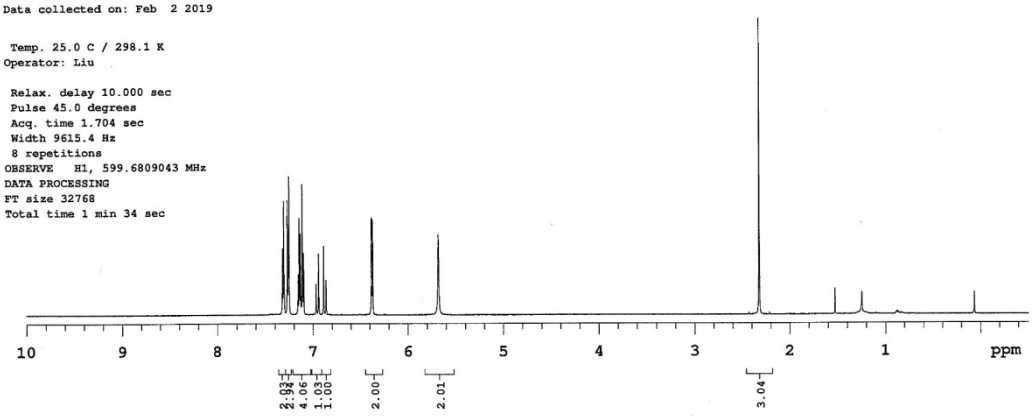
Sample directory:

FidFile: yz-3-190202-Cl-H

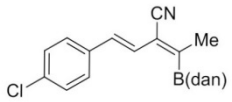
Pulse Sequence: PROTON (s2pul)
Solvent: cdcl3
Data collected on: Feb 2 2019

Temp. 25.0 C / 298.1 K
Operator: Liu

Relax. delay 10.000 sec
Pulse 45.0 degrees
Acq. time 1.704 sec
Width 9615.4 Hz
8 repetitions
OBSERVE H1, 599.6809043 MHz
DATA PROCESSING
FT size 32768
Total time 1 min 34 sec



Sample Name:



Data Collected on:
nmr19-vnmrs600
Archive directory:

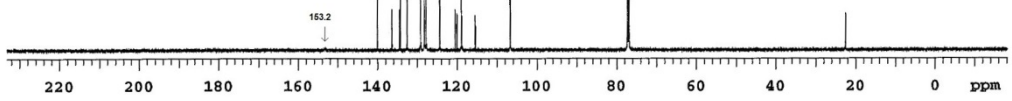
Sample directory:

FidFile: yz-3-190506-Cl-C

Pulse Sequence: CARBON (s2pul)
Solvent: cdcl3
Data collected on: May 6 2019

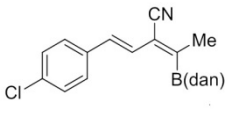
Temp. 25.0 C / 298.1 K
Operator: Liu

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 0.865 sec
Width 37878.8 Hz
15000 repetitions
OBSERVE C13, 150.7898581 MHz
DECOUPLE H1, 599.6839027 MHz
Power 42 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 0.5 Hz
FT size 65536
Total time 7 hr, 46 min



p-Cl

Sample Name:



Data Collected on:
nmr11-inova500
Archive directory:

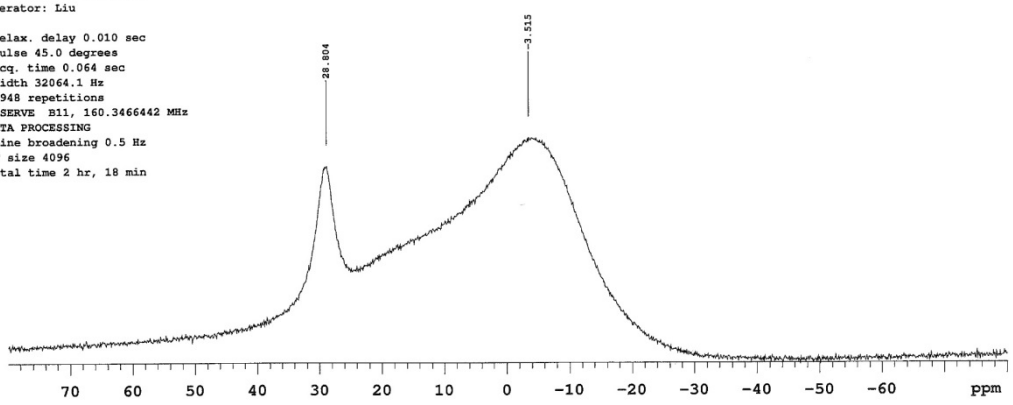
Sample directory:

FidFile: B11

Pulse Sequence: s2pul
Solvent: cdcl3
Data collected on: Feb 4 2019

Temp. 25.0 C / 298.1 K
Operator: Liu

Relax. delay 0.010 sec
Pulse 45.0 degrees
Acq. time 0.064 sec
Width 32064.1 Hz
2948 repetitions
OBSERVE B11, 160.3466442 MHz
DATA PROCESSING
Line broadening 0.5 Hz
FT size 4096
Total time 2 hr, 18 min



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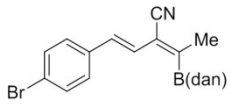
Sample Name:



Data Collected on:
nmr18-vnmrs500
Archive directory:

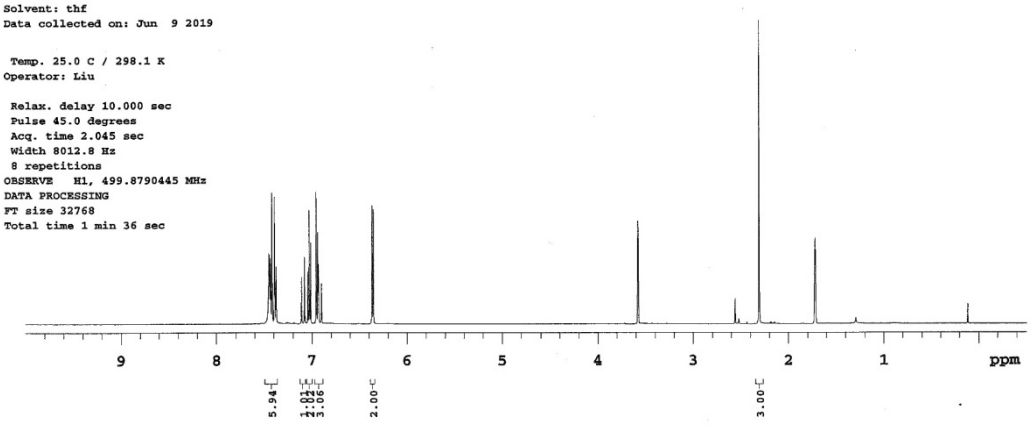
Sample directory:

FidFile: PROTON

Pulse Sequence: PROTON (s2pul)
Solvent: thf
Data collected on: Jun 9 2019

Temp. 25.0 C / 298.1 K
Operator: Liu

Relax. delay 10.000 sec
Pulse 45.0 degrees
Acq. time 2.045 sec
Width 8012.8 Hz
8 repetitions
OBSERVE H1, 499.8790445 MHz
DATA PROCESSING
FT size 32768
Total time 1 min 36 sec



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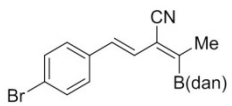
Sample Name:

Data Collected on:
nmr18-vnmrs500
Archive directory:

Sample directory:

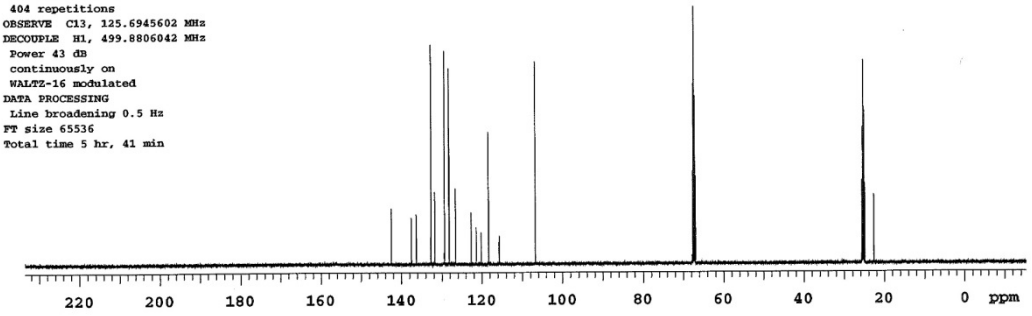


FidFile: yz-3-190609-pbr-thf-C

Pulse Sequence: CARBON (s2pul)
Solvent: thf
Data collected on: Jun 9 2019

Temp. 25.0 C / 298.1 K
Operator: Liu

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.049 sec
Width 31250.0 Hz
404 repetitions
OBSERVE C13, 125.6945602 MHz
DECOUPLE H1, 499.8806042 MHz
Power 43 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 0.5 Hz
FT size 65536
Total time 5 hr, 41 min



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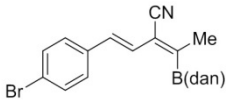
Sample Name:

Data Collected on:
nmr11-inova500
Archive directory:

Sample directory:

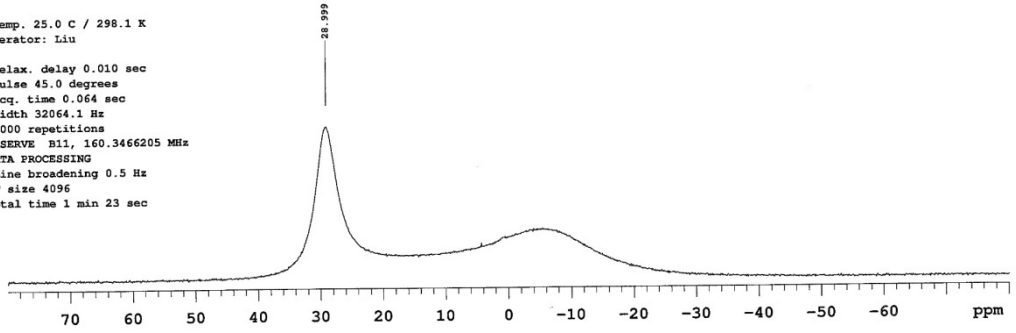


FidFile: B11

Pulse Sequence: s2pul
Solvent: thf
Data collected on: Jun 9 2019

Temp. 25.0 C / 298.1 K
Operator: Liu

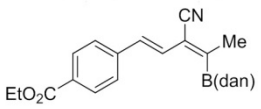
Relax. delay 0.010 sec
Pulse 45.0 degrees
Acq. time 0.064 sec
Width 32064.1 Hz
1000 repetitions
OBSERVE B11, 160.3466205 MHz
DATA PROCESSING
Line broadening 0.5 Hz
FT size 4096
Total time 1 min 23 sec



Sample Name:

Data Collected on:
nmr19-vnmrs600
Archive directory:

Sample directory:

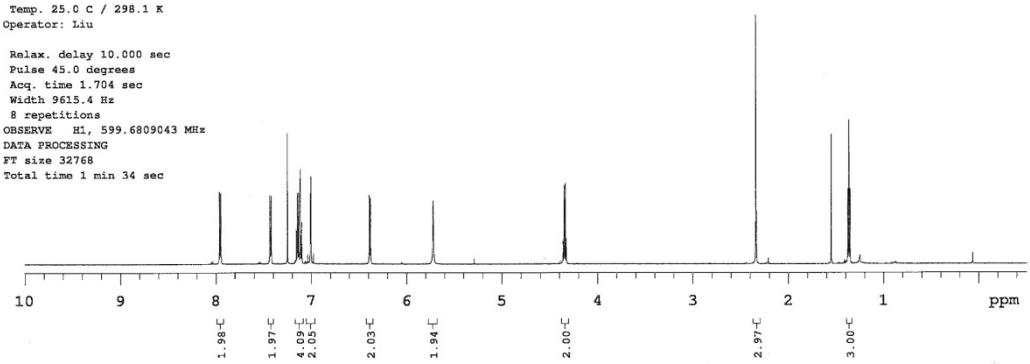


FidFile: PROTON

Pulse Sequence: PROTON (s2pul)
Solvent: cdcl3
Data collected on: May 30 2019

Temp. 25.0 C / 298.1 K
Operator: Liu

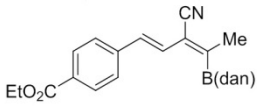
Relax. delay 10.000 sec
Pulse 45.0 degrees
Acq. time 1.704 sec
Width 9615.4 Hz
8 repetitions
OBSERVE H1, 599.6809043 MHz
DATA PROCESSING
FT size 32768
Total time 1 min 34 sec



Sample Name:

Data Collected on:
nmr19-vnmrs600
Archive directory:

Sample directory:

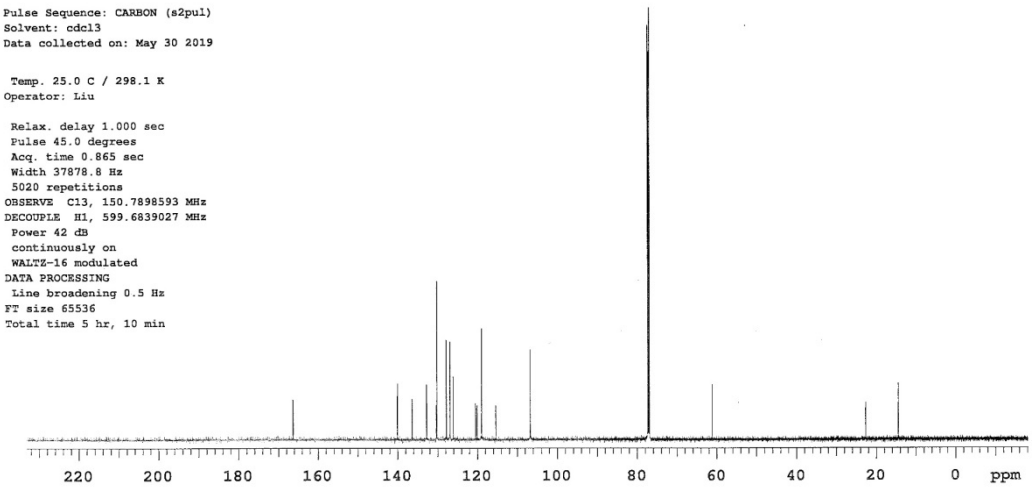


FidFile: CARBON

Pulse Sequence: CARBON (s2pul)
Solvent: cdcl3
Data collected on: May 30 2019

Temp. 25.0 C / 298.1 K
Operator: Liu

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 0.865 sec
Width 37878.8 Hz
5020 repetitions
OBSERVE C13, 150.7898593 MHz
DECOUPLE H1, 599.6839027 MHz
Power 42 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 0.5 Hz
FT size 65536
Total time 5 hr, 10 min



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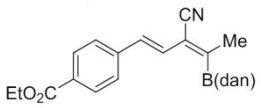
Sample Name:

Data Collected on:
nmr11-inova500
Archive directory:

Sample directory:

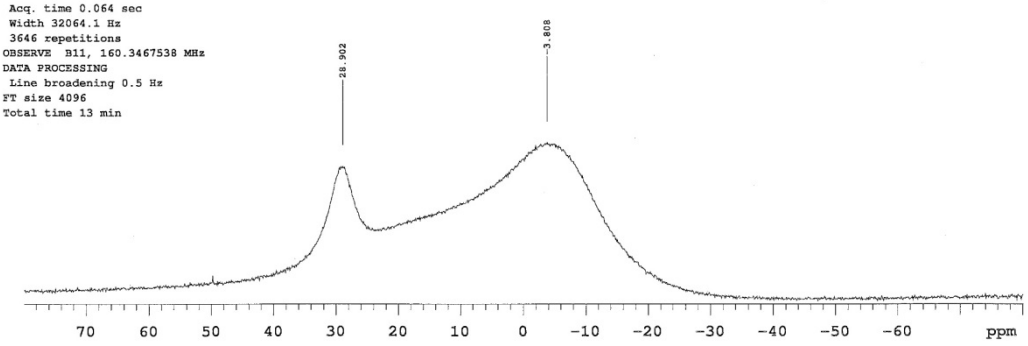


FidFile: B11

Pulse Sequence: s2pul
Solvent: cdcl3
Data collected on: May 31 2019

Temp. 25.0 C / 298.1 K
Operator: Liu

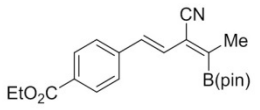
Relax. delay 0.010 sec
Pulse 45.0 degrees
Acq. time 0.064 sec
Width 32064.1 Hz
3646 repetitions
OBSERVE B11, 160.3467538 MHz
DATA PROCESSING
Line broadening 0.5 Hz
FT size 4096
Total time 13 min



Sample Name:

Data Collected on:
nmr19-vnmrs600
Archive directory:

Sample directory:

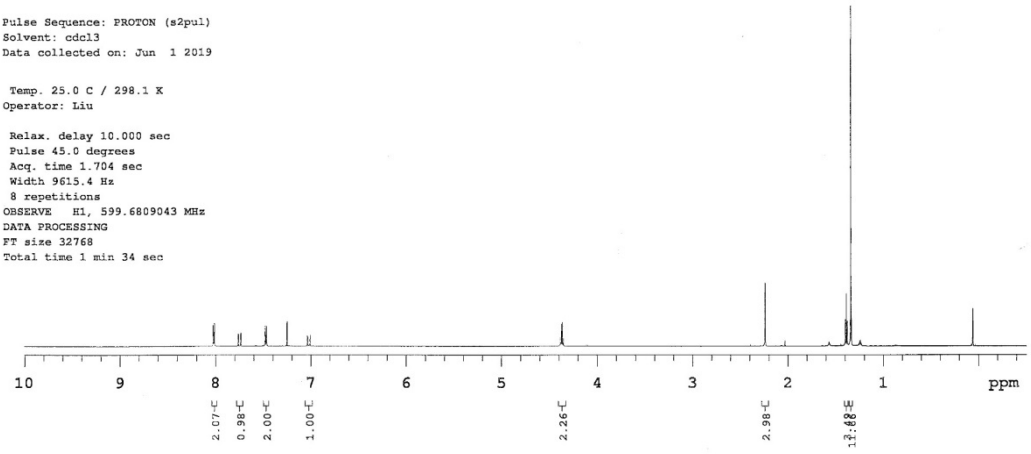


FidFile: PROTON

Pulse Sequence: PROTON (s2pul)
Solvent: cdcl3
Data collected on: Jun 1 2019

Temp. 25.0 C / 298.1 K
Operator: Liu

Relax. delay 10.000 sec
Pulse 45.0 degrees
Acq. time 1.704 sec
Width 9615.4 Hz
8 repetitions
OBSERVE H1, 599.6809043 MHz
DATA PROCESSING
FT size 32768
Total time 1 min 34 sec

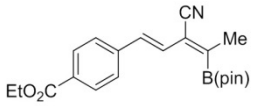


Sample Name:

Data Collected on:
nmr19-vnmrs600
Archive directory:

Sample directory:

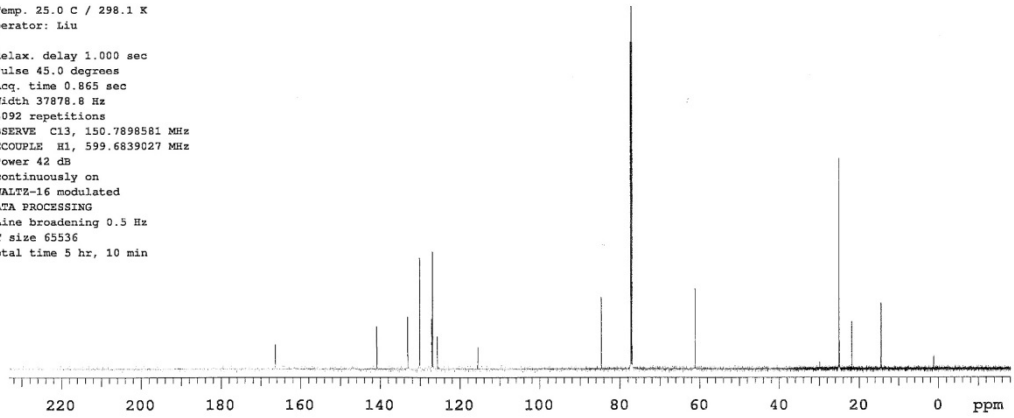
FidFile: CARBON



Pulse Sequence: CARBON (s2pul)
Solvent: cdcl3
Data collected on: Jun 1 2019

Temp. 25.0 C / 298.1 K
Operator: Liu

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 0.865 sec
Width 37878.8 Hz
4092 repetitions
OBSERVE C13, 150.7898581 MHz
DECOUPLE H1, 599.6839027 MHz
Power 42 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 0.5 Hz
FT size 65536
Total time 5 hr, 10 min



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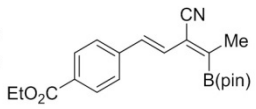
Sample Name:

Data Collected on:
nmr11-inova500
Archive directory:

Sample directory:

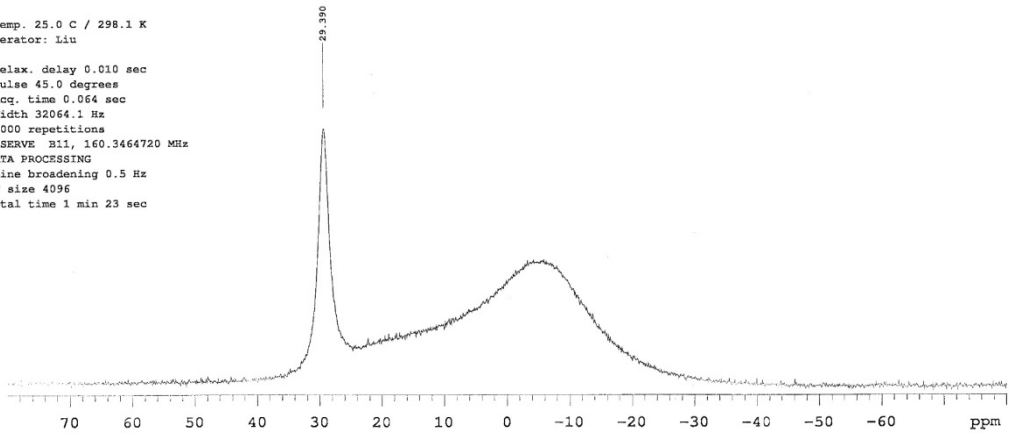
FidFile: B11



Pulse Sequence: s2pul
Solvent: cdcl3
Data collected on: Jun 2 2019

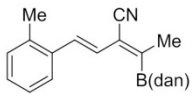
Temp. 25.0 C / 298.1 K
Operator: Liu

Relax. delay 0.010 sec
Pulse 45.0 degrees
Acq. time 0.064 sec
Width 32064.1 Hz
1000 repetitions
OBSERVE B11, 160.3464720 MHz
DATA PROCESSING
Line broadening 0.5 Hz
FT size 4096
Total time 1 min 23 sec



Agilent Technologies

Sample Name:



Data Collected on:
nmr18-vnmrs500
Archive directory:

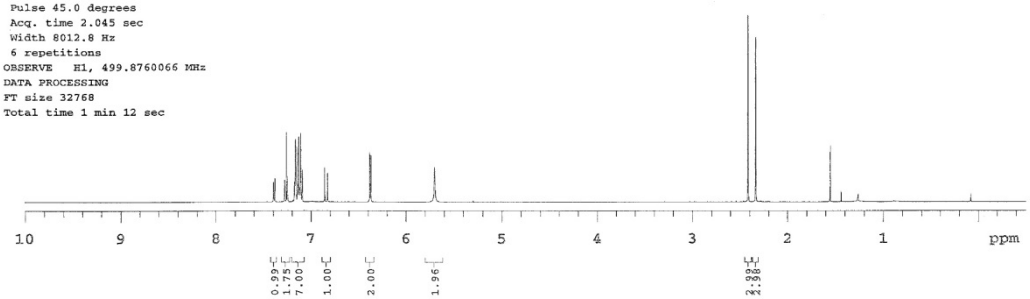
Sample directory:

FidFile: PROTON

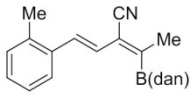
Pulse Sequence: PROTON (s2pul)
Solvent: cdcl3
Data collected on: Feb 6 2020

Temp. 25.0 C / 298.1 K
Operator: Liu

Relax. delay 10.000 sec
Pulse 45.0 degrees
Acq. time 2.045 sec
Width 8012.8 Hz
6 repetitions
OBSERVE H1, 499.8760066 MHz
DATA PROCESSING
FT size 32768
Total time 1 min 12 sec



Sample Name:



Data Collected on:
nmr19-vnmrs600
Archive directory:

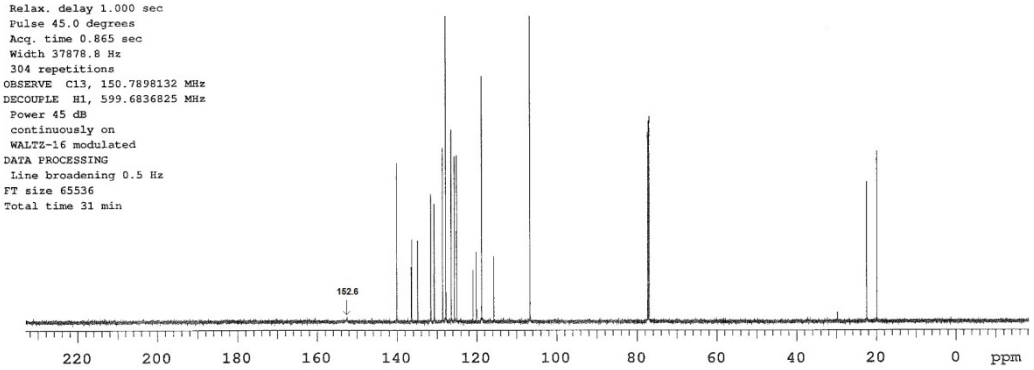
Sample directory:

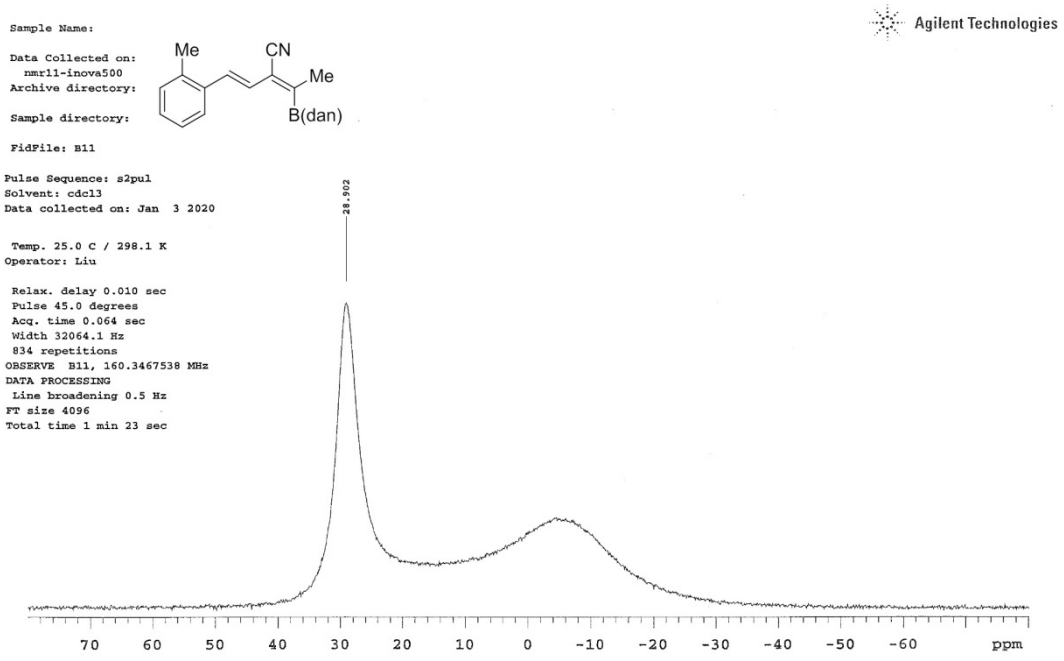
FidFile: CARBON

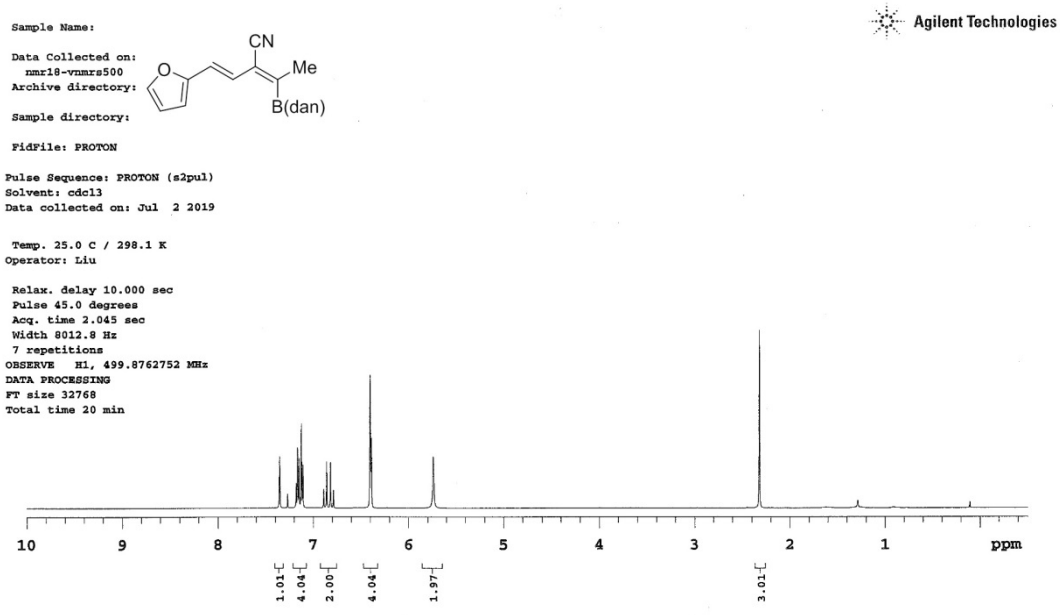
Pulse Sequence: CARBON (s2pul)
Solvent: cdcl3
Data collected on: Jan 3 2020

Temp. 25.0 C / 298.1 K
Operator: Liu

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 0.865 sec
Width 37878.8 Hz
304 repetitions
OBSERVE C13, 150.7898132 MHz
DECOUPLE H1, 599.6836825 MHz
Power 45 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 0.5 Hz
FT size 65536
Total time 31 min




Agilent Technologies
Sample Name:
Data Collected on:
nmr11-inova500
Archive directory:
Sample directory:
FidFile: B11
Me
CN
Me
B(dan)
Pulse Sequence: s2pul
Solvent: cdcl3
Data collected on: Jan 3 2020
Temp. 25.0 C / 298.1 K
Operator: Liu
Relax. delay 0.010 sec
Pulse 45.0 degrees
Acq. time 0.064 sec
Width 32064.1 Hz
834 repetitions
OBSERVE B11, 160.3467538 MHz
DATA PROCESSING
Line broadening 0.5 Hz
FT size 4096
Total time 1 min 23 sec
28.902
70 60 50 40 30 20 10 0 -10 -20 -30 -40 -50 -60 ppm


Agilent Technologies
Sample Name:
Data Collected on:
nmr18-vnmrs500
Archive directory:
Sample directory:
FidFile: PROTON
CN
Me
O
B(dan)
Pulse Sequence: PROTON (s2pul)
Solvent: cdcl3
Data collected on: Jul 2 2019
Temp. 25.0 C / 298.1 K
Operator: Liu
Relax. delay 10.000 sec
Pulse 45.0 degrees
Acq. time 2.045 sec
Width 8012.8 Hz
7 repetitions
OBSERVE H1, 499.8762752 MHz
DATA PROCESSING
FT size 32768
Total time 20 min
10 9 8 7 6 5 4 3 2 1 ppm
1.01
4.04
2.00
4.04
1.97
3.01

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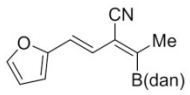
Sample Name:



Data Collected on:
nmr18-vnmrs500
Archive directory:

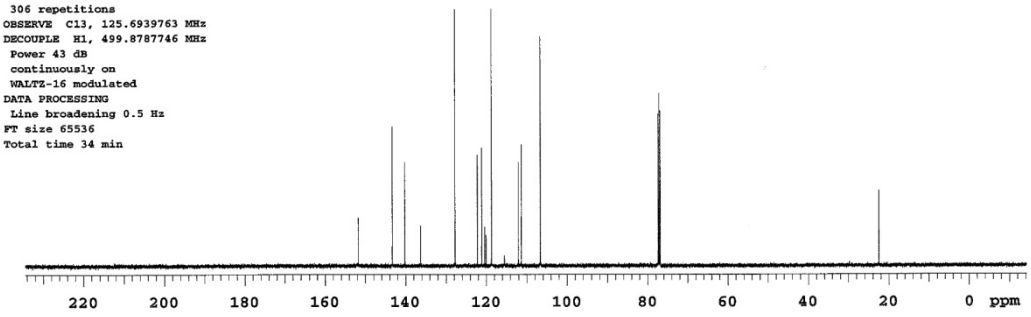
Sample directory:

FidFile: CARBON

Pulse Sequence: CARBON (s2pul)
Solvent: cdcl3
Data collected on: Jul 2 2019

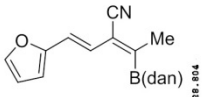
Temp. 25.0 C / 298.1 K
Operator: Liu

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.049 sec
Width 31250.0 Hz
306 repetitions
OBSERVE C13, 125.6939763 MHz
DECOUPLE H1, 499.8787746 MHz
Power 43 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 0.5 Hz
FT size 65536
Total time 34 min



Agilent Technologies

Sample Name:



Data Collected on:
nmr11-inova500
Archive directory:

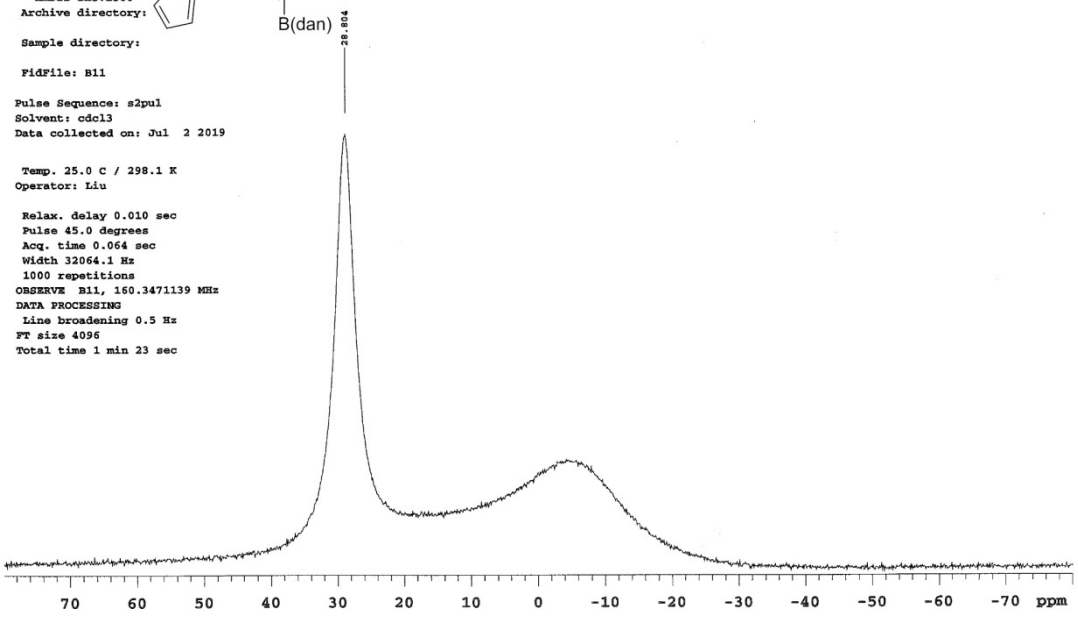
Sample directory:

FidFile: B11

Pulse Sequence: s2pul
Solvent: cdcl3
Data collected on: Jul 2 2019

Temp. 25.0 C / 298.1 K
Operator: Liu

Relax. delay 0.010 sec
Pulse 45.0 degrees
Acq. time 0.064 sec
Width 32064.1 Hz
1000 repetitions
OBSERVE B11, 160.3471139 MHz
DATA PROCESSING
Line broadening 0.5 Hz
FT size 4096
Total time 1 min 23 sec



thio

Sample Name:

Data Collected on:
nmr18-vnmrs500
Archive directory:

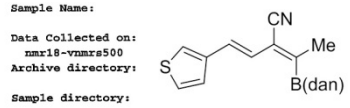
Sample directory:

FidFile: PROTON

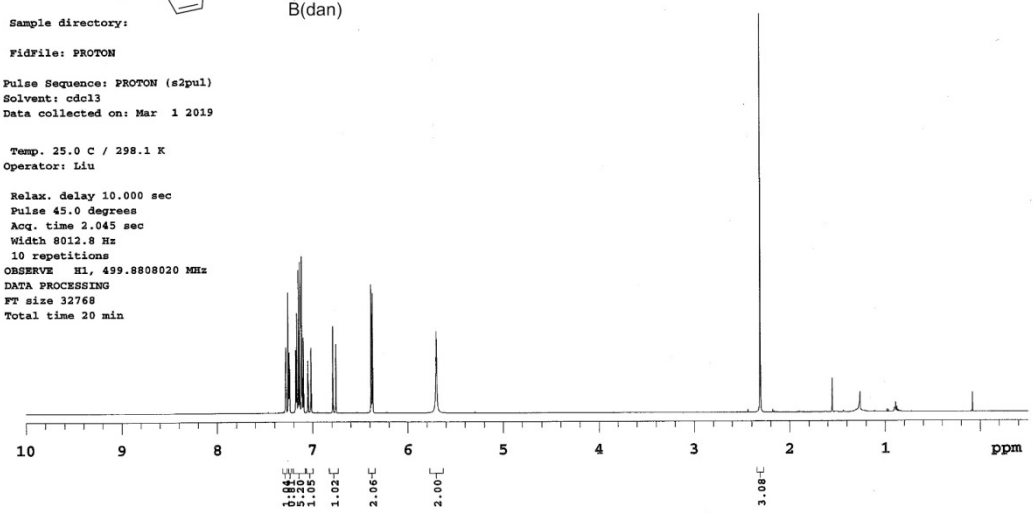
Pulse Sequence: PROTON (s2pul)
Solvent: cdcl3
Data collected on: Mar 1 2019

Temp. 25.0 C / 298.1 K
Operator: Liu

Relax. delay 10.000 sec
Pulse 45.0 degrees
Acq. time 2.045 sec
Width 8012.8 Hz
10 repetitions
OBSERVE H1, 499.8808020 MHz
DATA PROCESSING
FT size 32768
Total time 20 min



Agilent Technologies



thio

Sample Name:

Data Collected on:
nmr18-vnmrs500
Archive directory:

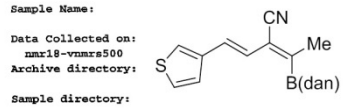
Sample directory:

FidFile: CARBON

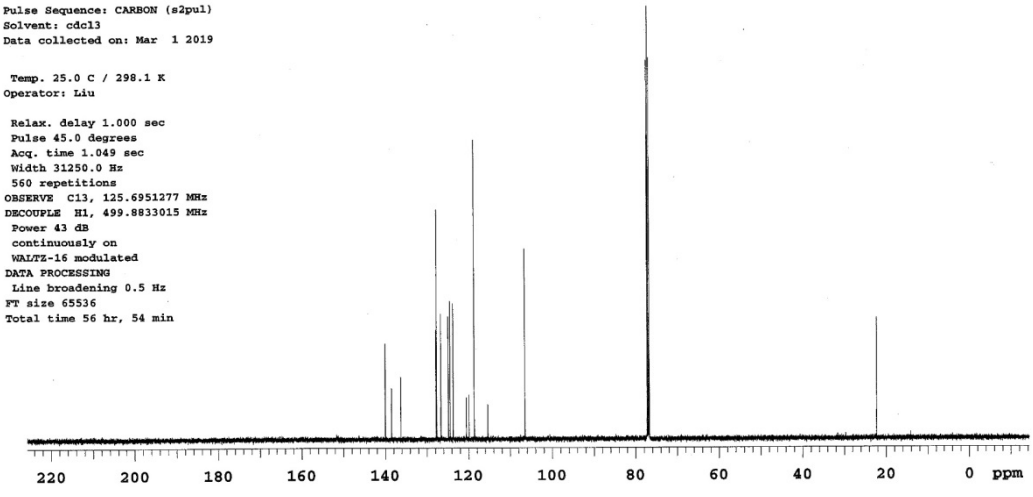
Pulse Sequence: CARBON (s2pul)
Solvent: cdcl3
Data collected on: Mar 1 2019

Temp. 25.0 C / 298.1 K
Operator: Liu

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.049 sec
Width 31250.0 Hz
560 repetitions
OBSERVE C13, 125.6951277 MHz
DECOUPLE H1, 499.8833015 MHz
Power 43 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 0.5 Hz
FT size 65536
Total time 56 hr, 54 min



Agilent Technologies



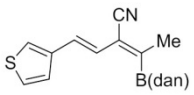
thio

Agilent Technologies

Sample Name:

Data Collected on:
nmr11-inova500
Archive directory:

Sample directory:

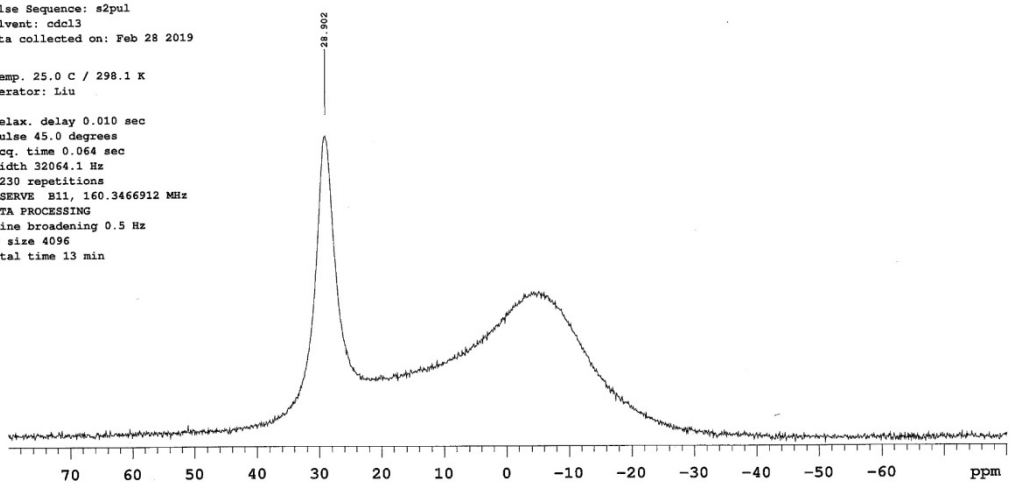


FidFile: yz-3-190228-thio-B

Pulse Sequence: s2pul
Solvent: cdcl3
Data collected on: Feb 28 2019

Temp. 25.0 C / 298.1 K
Operator: Liu

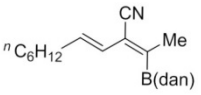
Relax. delay 0.010 sec
Pulse 45.0 degrees
Acq. time 0.064 sec
Width 32064.1 Hz
1230 repetitions
OBSERVE B11, 160.3466912 MHz
DATA PROCESSING
Line broadening 0.5 Hz
FT size 4096
Total time 13 min



Sample Name:

Data Collected on:
nmr19-vnmrs600
Archive directory:

Sample directory:

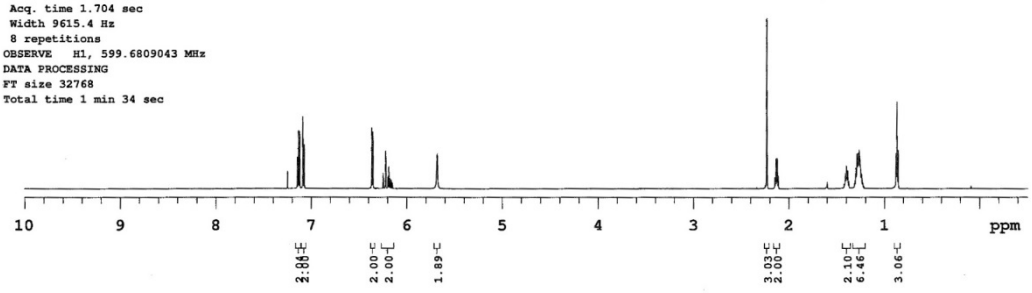


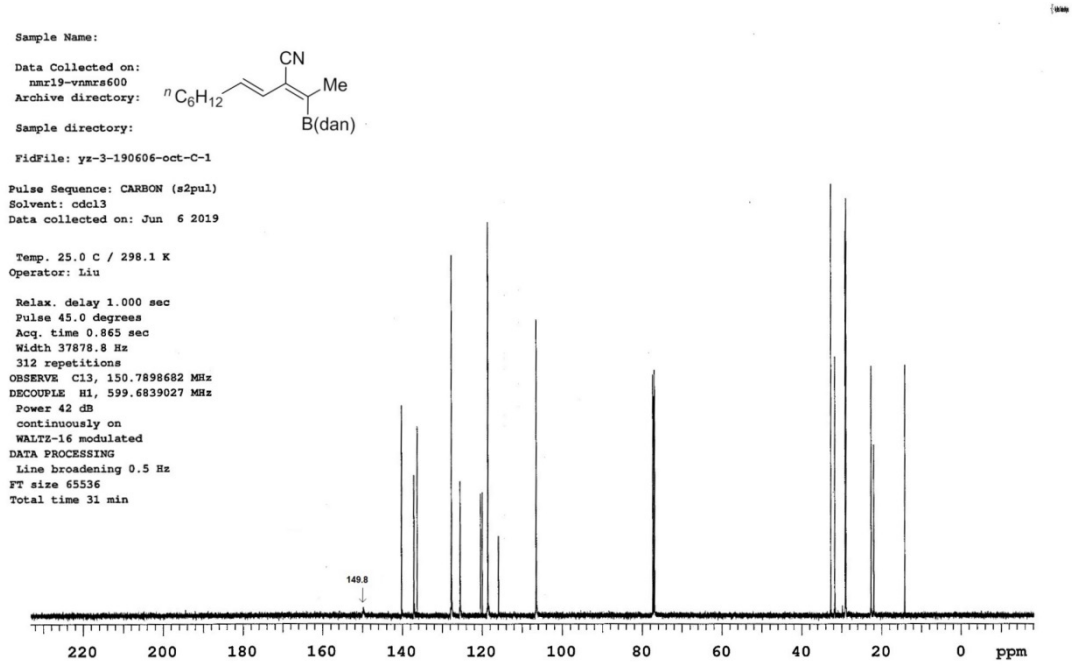
FidFile: PROTON

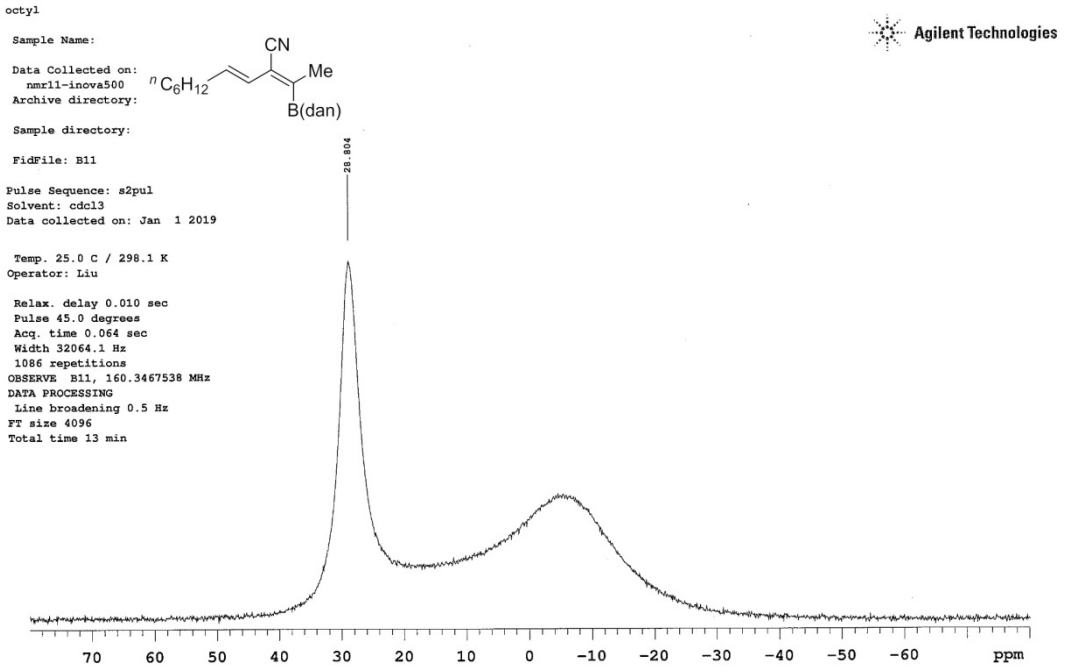
Pulse Sequence: PROTON (s2pul)
Solvent: cdcl3
Data collected on: Jun 6 2019

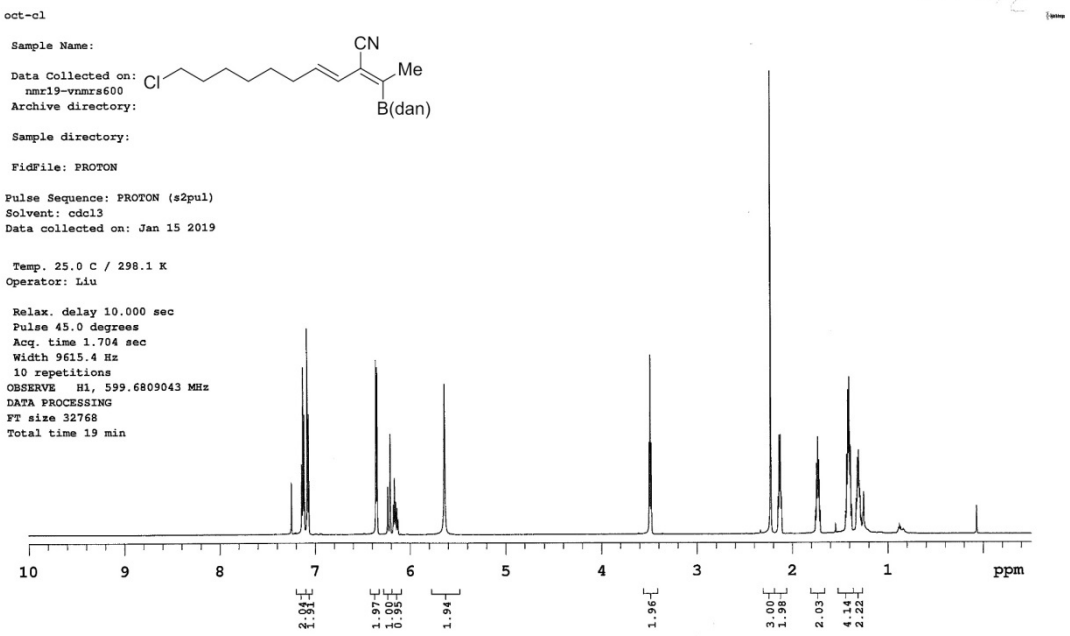
Temp. 25.0 C / 298.1 K
Operator: Liu

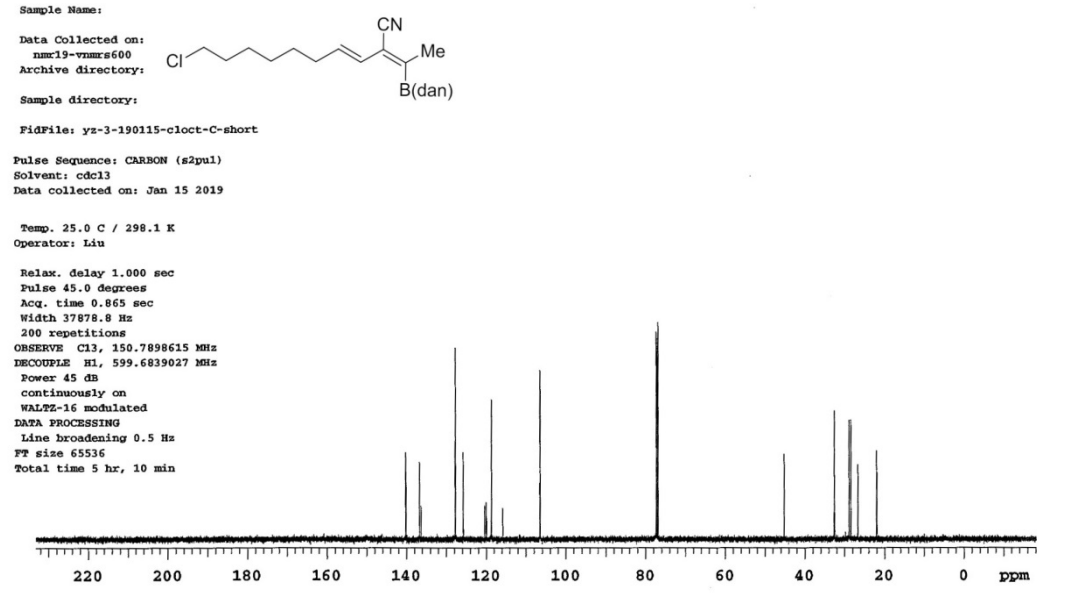
Relax. delay 10.000 sec
Pulse 45.0 degrees
Acq. time 1.704 sec
Width 9615.4 Hz
8 repetitions
OBSERVE H1, 599.6809043 MHz
DATA PROCESSING
FT size 32768
Total time 1 min 34 sec




Sample Name:
Data Collected on:
nmr19-vnmrs600
Archive directory:
Sample directory:
FidFile: yz-3-190606-oct-C-1
Pulse Sequence: CARBON (s2pul)
Solvent: cdcl3
Data collected on: Jun 6 2019
Temp. 25.0 C / 298.1 K
Operator: Liu
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 0.865 sec
Width 37878.8 Hz
312 repetitions
OBSERVE C13, 150.7898682 MHz
DECOUPLE H1, 599.6839027 MHz
Power 42 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 0.5 Hz
FT size 65536
Total time 31 min
CN
Me
B(dan)
149.8
220
200
180
160
140
120
100
80
60
40
20
0
ppm


octyl
Agilent Technologies
Sample Name:
Data Collected on:
nmr11-inova500
Archive directory:
Sample directory:
FidFile: B11
Pulse Sequence: s2pul
Solvent: cdcl3
Data collected on: Jan 1 2019
Temp. 25.0 C / 298.1 K
Operator: Liu
Relax. delay 0.010 sec
Pulse 45.0 degrees
Acq. time 0.064 sec
Width 32064.1 Hz
1086 repetitions
OBSERVE B11, 160.3467538 MHz
DATA PROCESSING
Line broadening 0.5 Hz
FT size 4096
Total time 13 min
CN
Me
B(dan)
28.804
70
60
50
40
30
20
10
0
-10
-20
-30
-40
-50
-60
ppm


oct-cl
Sample Name:
Data Collected on:
nmr19-vnmrs600
Archive directory:
Sample directory:
FidFile: PROTON
Pulse Sequence: PROTON (s2pul)
Solvent: cdcl3
Data collected on: Jan 15 2019
Temp. 25.0 C / 298.1 K
Operator: Liu
Relax. delay 10.000 sec
Pulse 45.0 degrees
Acq. time 1.704 sec
Width 9615.4 Hz
10 repetitions
OBSERVE H1, 599.6809043 MHz
DATA PROCESSING
FT size 32768
Total time 19 min
CN
Me
Cl
B(dan)
10
9
8
7
6
5
4
3
2
1
ppm
2.04
2.01
1.97
1.00
0.95
1.94
1.96
3.00
1.98
2.03
4.14
2.22


Sample Name:
Data Collected on:
nmr19-vnmrs600
Archive directory:
Sample directory:
FidFile: yz-3-190115-cloct-C-short
Pulse Sequence: CARBON (s2pul)
Solvent: cdcl3
Data collected on: Jan 15 2019
Temp. 25.0 C / 298.1 K
Operator: Liu
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 0.865 sec
Width 37878.8 Hz
200 repetitions
OBSERVE C13, 150.7898615 MHz
DECOUPLE H1, 599.6839027 MHz
Power 45 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 0.5 Hz
FT size 65536
Total time 5 hr, 10 min
CN
Me
Cl
B(dan)
220
200
180
160
140
120
100
80
60
40
20
0
ppm

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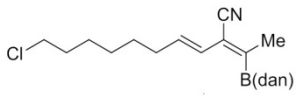
Sample Name:



Data Collected on:
nmr11-inova500
Archive directory:

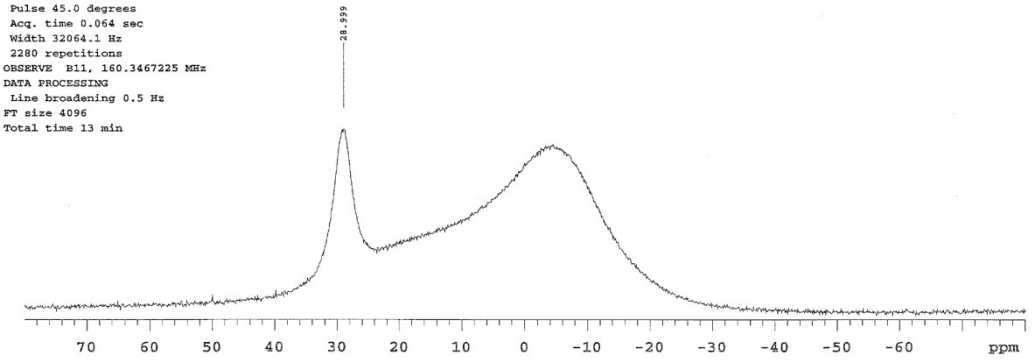
Sample directory:

FidFile: B11

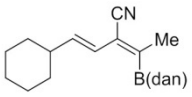
Pulse Sequence: s2pul
Solvent: cdcl3
Data collected on: Jan 25 2020

Temp. 25.0 C / 298.1 K
Operator: Liu

Relax. delay 0.010 sec
Pulse 45.0 degrees
Acq. time 0.064 sec
Width 32064.1 Hz
2280 repetitions
OBSERVE B11, 160.3467225 MHz
DATA PROCESSING
Line broadening 0.5 Hz
FT size 4096
Total time 13 min



Sample Name:



Data Collected on:
nmr19-vnmrs600
Archive directory:

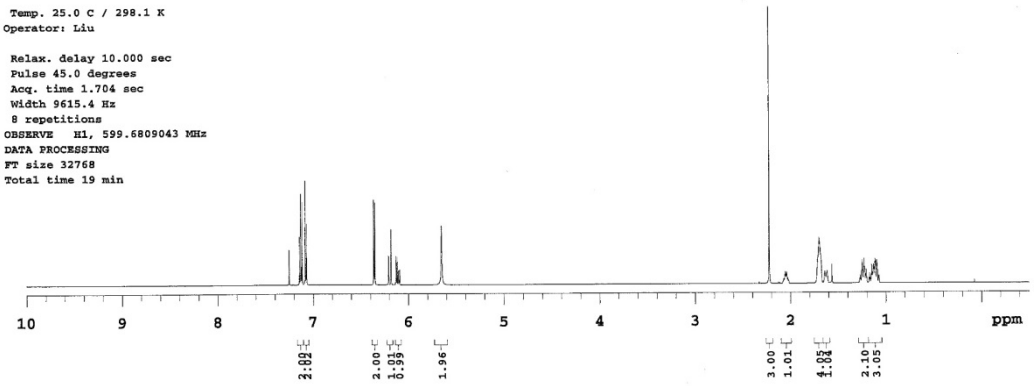
Sample directory:

FidFile: yz-3-190331-chex-H

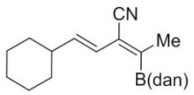
Pulse Sequence: PROTON (s2pul)
Solvent: cdcl3
Data collected on: Mar 31 2019

Temp. 25.0 C / 298.1 K
Operator: Liu

Relax. delay 10.000 sec
Pulse 45.0 degrees
Acq. time 1.704 sec
Width 9615.4 Hz
8 repetitions
OBSERVE H1, 599.6809043 MHz
DATA PROCESSING
FT size 32768
Total time 19 min



Sample Name:



Data Collected on:
nmr19-vnmrs600
Archive directory:

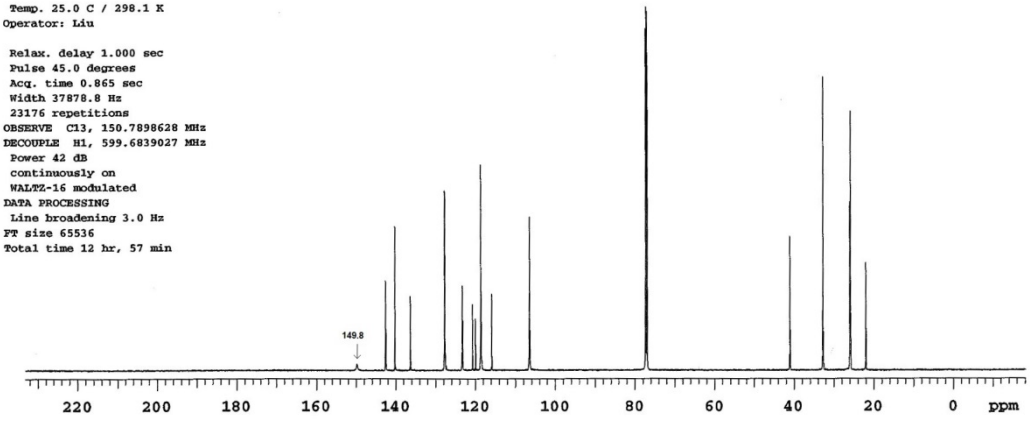
Sample directory:

FidFile: yz-3-190331-chex-c

Pulse Sequence: CARBON (s2pul)
Solvent: cdcl3
Data collected on: Mar 31 2019

Temp. 25.0 C / 298.1 K
Operator: Liu

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 0.865 sec
Width 37878.8 Hz
23176 repetitions
OBSERVE C13, 150.7898628 MHz
DECOUPLE H1, 599.6839027 MHz
Power 42 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 3.0 Hz
FT size 65536
Total time 12 hr, 57 min



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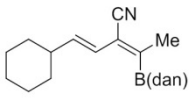
Sample Name:



Data Collected on:
nmr11-inova500
Archive directory:

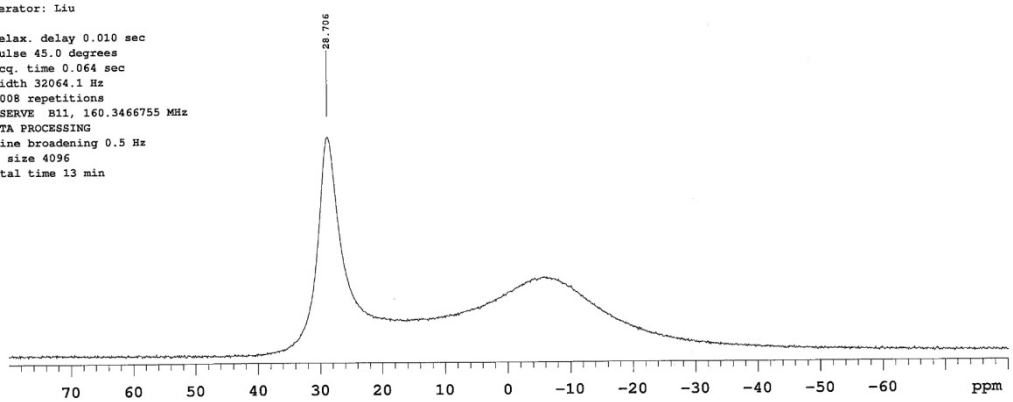
Sample directory:

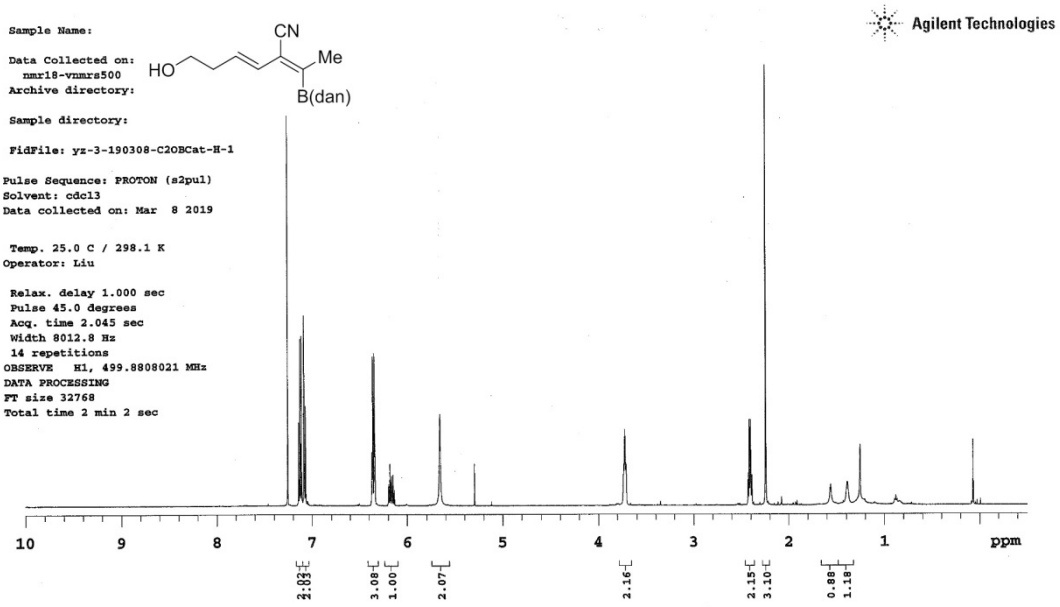
FidFile: B11

Pulse Sequence: s2pul
Solvent: cdcl3
Data collected on: Apr 1 2019

Temp. 25.0 C / 298.1 K
Operator: Liu

Relax. delay 0.010 sec
Pulse 45.0 degrees
Acq. time 0.064 sec
Width 32064.1 Hz
2008 repetitions
OBSERVE B11, 160.3466755 MHz
DATA PROCESSING
Line broadening 0.5 Hz
FT size 4096
Total time 13 min

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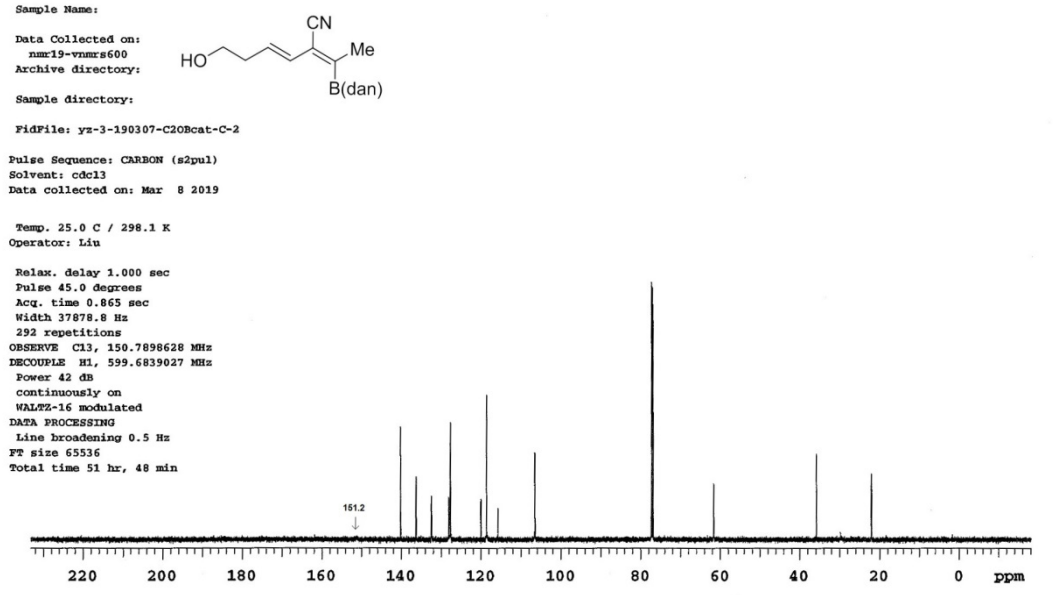
Sample Name:
Data Collected on:
nmr18-vnmrs500
Archive directory:
Sample directory:
FidFile: yz-3-190308-C2OBCat-H-1
Pulse Sequence: PROTON (s2pul)
Solvent: cdcl3
Data collected on: Mar 8 2019
Temp. 25.0 C / 298.1 K
Operator: Liu
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 2.045 sec
Width 8012.8 Hz
14 repetitions
OBSERVE H1, 499.8808021 MHz
DATA PROCESSING
FT size 32768
Total time 2 min 2 sec
CN
Me
HO
B(dan)
10
9
8
7
6
5
4
3
2
1
ppm
2.03
3.08
1.00
2.07
2.16
2.15
3.10
0.88
1.18


Sample Name:
Data Collected on:
nmr19-vnmrs600
Archive directory:
Sample directory:
FidFile: yz-3-190307-C2OBcat-C-2
Pulse Sequence: CARBON (s2pul)
Solvent: cdcl3
Data collected on: Mar 8 2019
Temp. 25.0 C / 298.1 K
Operator: Liu
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 0.865 sec
Width 37878.8 Hz
292 repetitions
OBSERVE C13, 150.7898628 MHz
DECOUPLE H1, 599.6839027 MHz
Power 42 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 0.5 Hz
FT size 65536
Total time 51 hr, 48 min
CN
Me
HO
B(dan)
151.2
220
200
180
160
140
120
100
80
60
40
20
0
ppm

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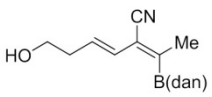
Sample Name:

Data Collected on:
nmr11-inova500
Archive directory:

Sample directory:

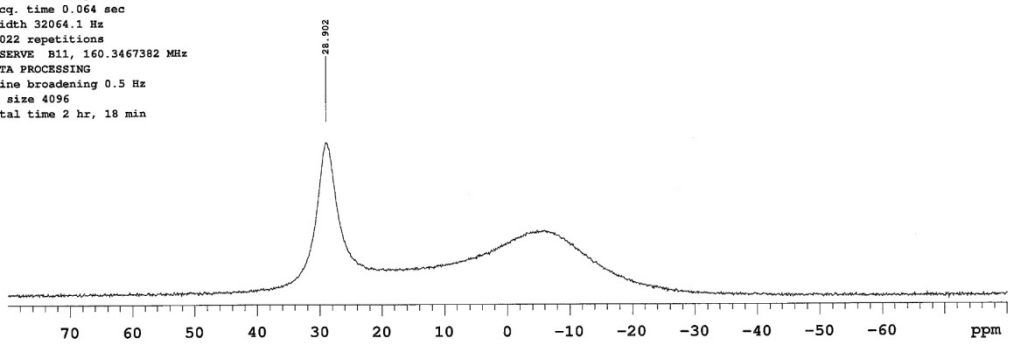
FidFile: B11



Pulse Sequence: s2pul
Solvent: cdcl3
Data collected on: Mar 8 2019

Temp. 25.0 C / 298.1 K
Operator: Liu

Relax. delay 0.010 sec
Pulse 45.0 degrees
Acq. time 0.064 sec
Width 32064.1 Hz
1022 repetitions
OBSERVE B11, 160.3467382 MHz
DATA PROCESSING
Line broadening 0.5 Hz
FT size 4096
Total time 2 hr, 18 min

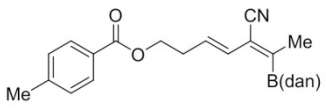


Sample Name:

Data Collected on:
nmr19-vnmrs600
Archive directory:

Sample directory:

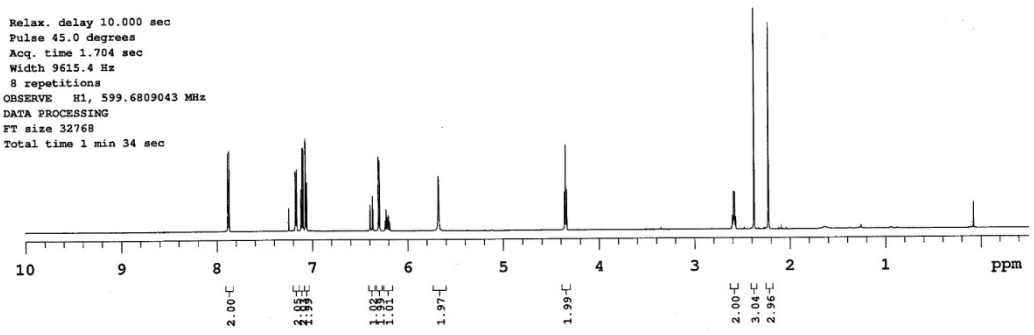
FidFile: PROTON



Pulse Sequence: PROTON (s2pul)
Solvent: cdcl3
Data collected on: Jun 14 2019

Temp. 25.0 C / 298.1 K
Operator: Liu

Relax. delay 10.000 sec
Pulse 45.0 degrees
Acq. time 1.704 sec
Width 9615.4 Hz
8 repetitions
OBSERVE H1, 599.6809043 MHz
DATA PROCESSING
FT size 32768
Total time 1 min 34 sec

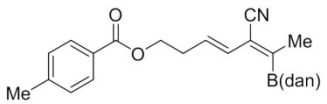


Sample Name:

Data Collected on:
nmr19-vnmrs600
Archive directory:

Sample directory:

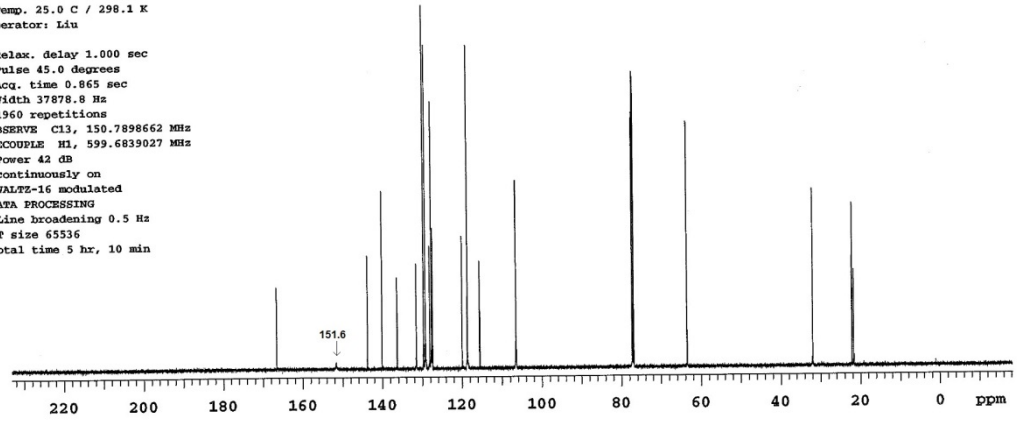
FidFile: yz-3-190614-phco2-C



Pulse Sequence: CARBON (s2pul)
Solvent: cdcl3
Data collected on: Jun 14 2019

Temp. 25.0 C / 298.1 K
Operator: Liu

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 0.865 sec
Width 37878.8 Hz
1960 repetitions
OBSERVE C13, 150.7898662 MHz
DECOUPLE H1, 599.6839027 MHz
Power 42 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 0.5 Hz
FT size 65536
Total time 5 hr, 10 min



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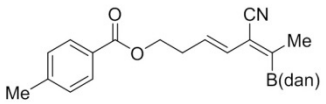
Sample Name:

Data Collected on:
nmr11-inova500
Archive directory:

Sample directory:

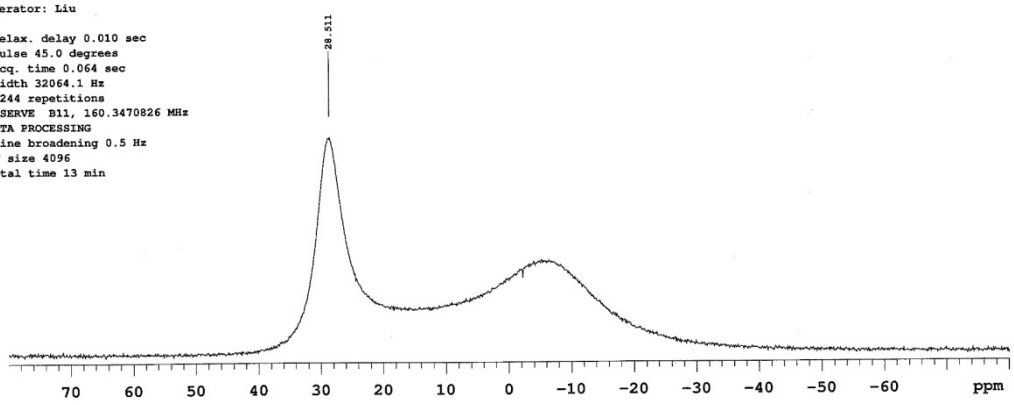
FidFile: B11



Pulse Sequence: s2pul
Solvent: cdcl3
Data collected on: Jun 12 2019

Temp. 25.0 C / 298.1 K
Operator: Liu

Relax. delay 0.010 sec
Pulse 45.0 degrees
Acq. time 0.064 sec
Width 32064.1 Hz
1244 repetitions
OBSERVE B11, 160.3470826 MHz
DATA PROCESSING
Line broadening 0.5 Hz
FT size 4096
Total time 13 min

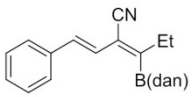


Sample Name:

Data Collected on:
nmr18-vnmrs500
Archive directory:

Sample directory:

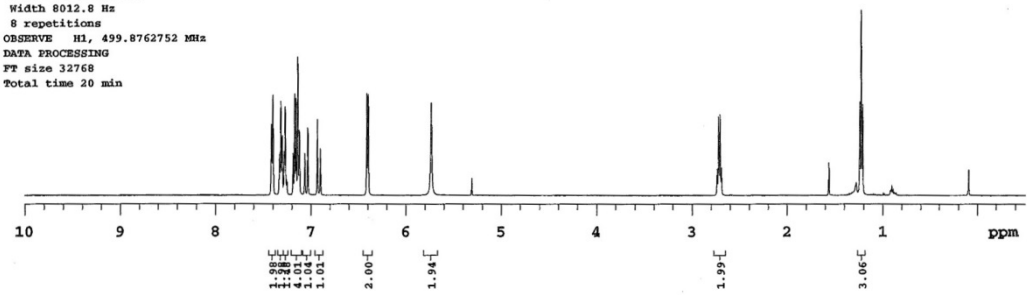
FidFile: yz-3-190509-Et-H



Pulse Sequence: PROTON (s2pul)
Solvent: cdcl3
Data collected on: May 9 2019

Temp. 25.0 C / 298.1 K
Operator: Liu

Relax. delay 10.000 sec
Pulse 45.0 degrees
Acq. time 2.045 sec
Width 8012.8 Hz
8 repetitions
OBSERVE H1, 499.8762752 MHz
DATA PROCESSING
FT size 32768
Total time 20 min



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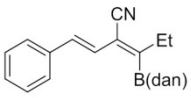
Sample Name:

Data Collected on:
nmr18-vnmrs500
Archive directory:

Sample directory:

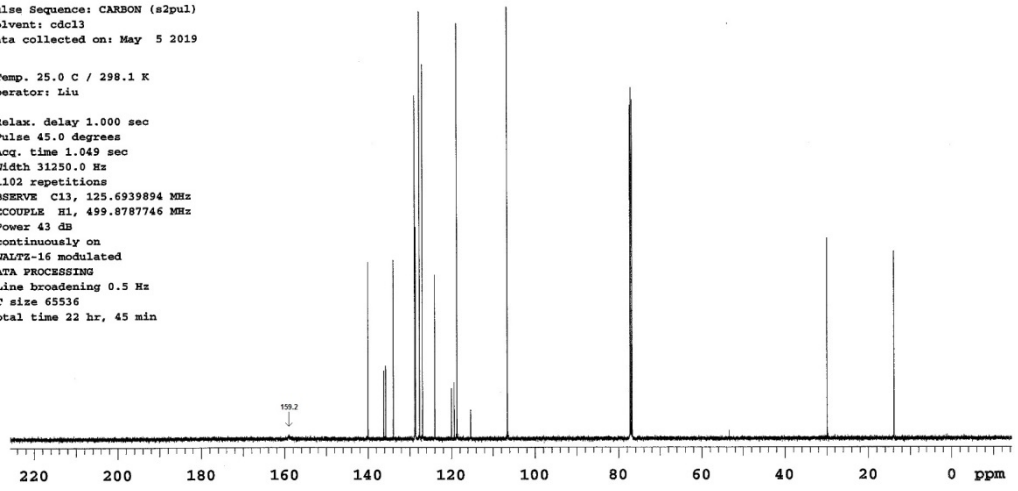
FidFile: CARBON



Pulse Sequence: CARBON (s2pul)
Solvent: cdcl3
Data collected on: May 5 2019

Temp. 25.0 C / 298.1 K
Operator: Liu

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.049 sec
Width 31250.0 Hz
1102 repetitions
OBSERVE C13, 125.6939894 MHz
DECOUPLE H1, 499.8787746 MHz
Power 43 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 0.5 Hz
FT size 65536
Total time 22 hr, 45 min



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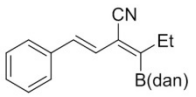
Sample Name:



Data Collected on:
nmr11-inova500
Archive directory:

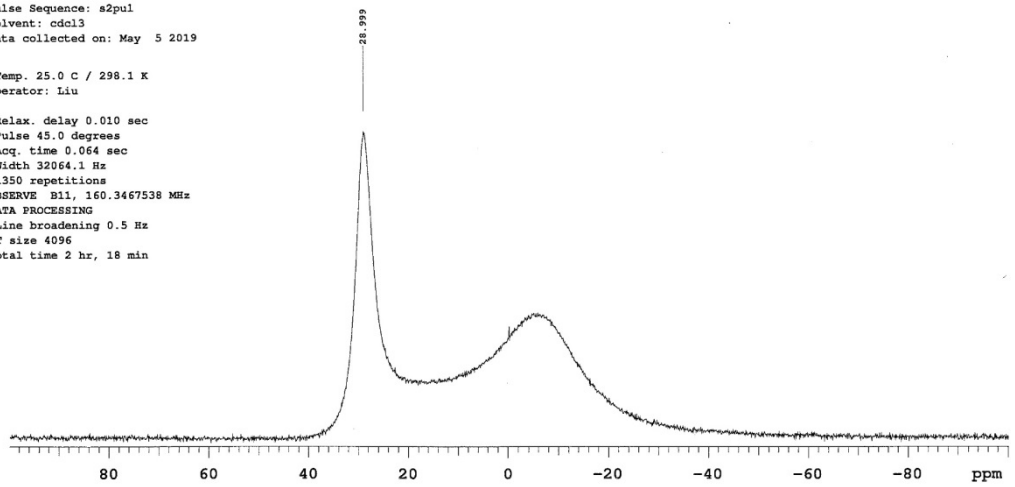
Sample directory:

FidFile: B11

Pulse Sequence: s2pul
Solvent: cdcl3
Data collected on: May 5 2019

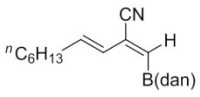
Temp. 25.0 C / 298.1 K
Operator: Liu

Relax. delay 0.010 sec
Pulse 45.0 degrees
Acq. time 0.064 sec
Width 32064.1 Hz
1350 repetitions
OBSERVE B11, 160.3467538 MHz
DATA PROCESSING
Line broadening 0.5 Hz
FT size 4096
Total time 2 hr, 18 min



Agilent Technologies

Sample Name:



Data Collected on:
nmr18-vnmrs500
Archive directory:

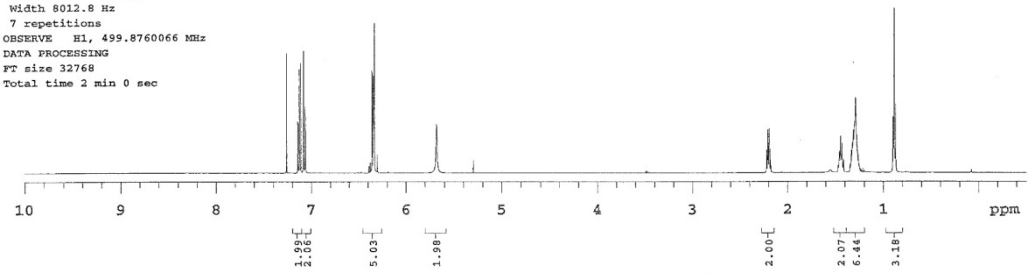
Sample directory:

FidFile: PROTON

Pulse Sequence: PROTON (s2pul)
Solvent: cdcl3
Data collected on: Mar 17 2020

Temp. 25.0 C / 298.1 K
Operator: Liu

Relax. delay 10.000 sec
Pulse 45.0 degrees
Acq. time 2.045 sec
Width 8012.8 Hz
7 repetitions
OBSERVE H1, 499.8760066 MHz
DATA PROCESSING
FT size 32768
Total time 2 min 0 sec



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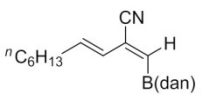
Sample Name:

Data Collected on:
nmr18-vnmrs500
Archive directory:

Sample directory:

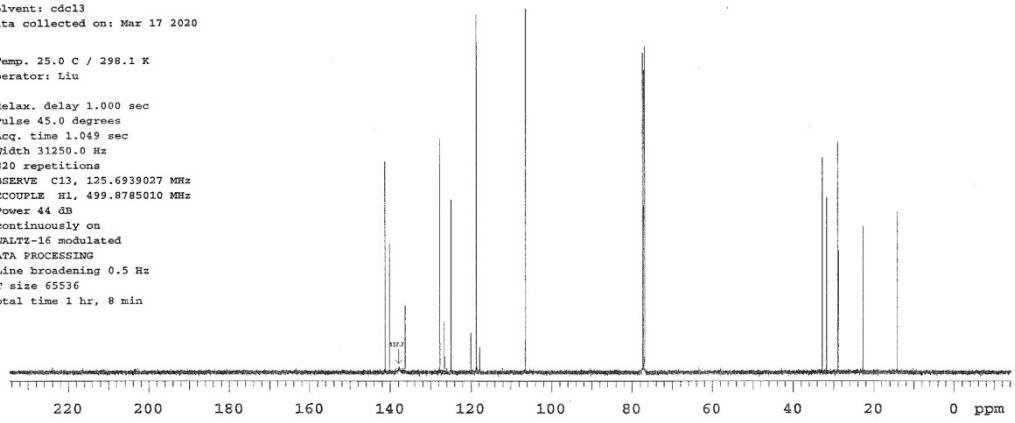
FidFile: CARBON



Pulse Sequence: CARBON (s2pul)
Solvent: cdcl3
Data collected on: Mar 17 2020

Temp. 25.0 C / 298.1 K
Operator: Liu

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.049 sec
Width 31250.0 Hz
820 repetitions
OBSERVE C13, 125.6939027 MHz
DECOUPLE H1, 499.8785010 MHz
Power 44 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 0.5 Hz
FT size 65536
Total time 1 hr, 8 min



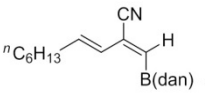
Agilent Technologies

Sample Name:

Data Collected on:
nmr11-inova500
Archive directory:

Sample directory:

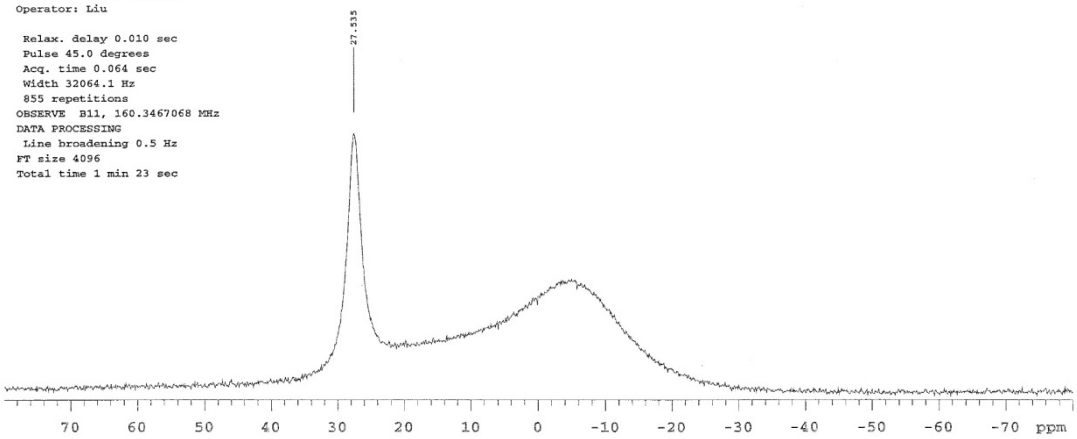
FidFile: B11



Pulse Sequence: s2pul
Solvent: cdcl3
Data collected on: Mar 17 2020

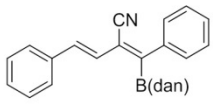
Temp. 25.0 C / 298.1 K
Operator: Liu

Relax. delay 0.010 sec
Pulse 45.0 degrees
Acq. time 0.064 sec
Width 32064.1 Hz
855 repetitions
OBSERVE B11, 160.3467068 MHz
DATA PROCESSING
Line broadening 0.5 Hz
FT size 4096
Total time 1 min 23 sec



Agilent Technologies

Sample Name:



Data Collected on:
nmr18-vnmrs500
Archive directory:

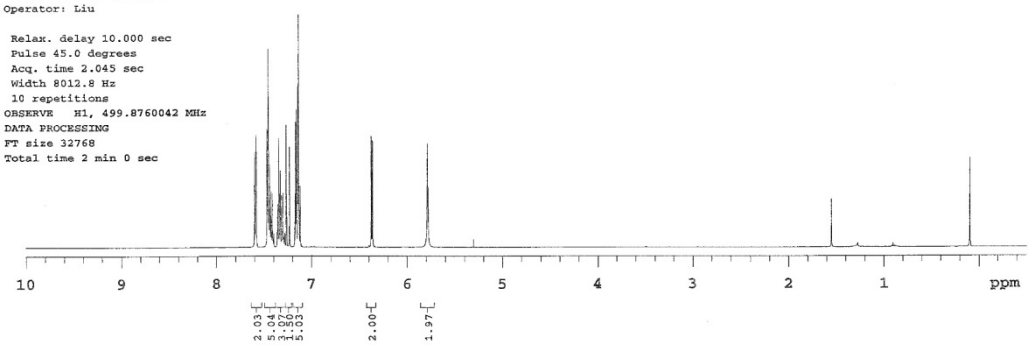
Sample directory:

FidFile: PROTON

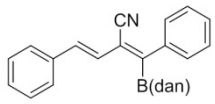
Pulse Sequence: PROTON (s2pul)
Solvent: cdcl3
Data collected on: Feb 3 2020

Temp. 25.0 C / 298.1 K
Operator: Liu

Relax. delay 10.000 sec
Pulse 45.0 degrees
Acq. time 2.045 sec
Width 8012.8 Hz
10 repetitions
OBSERVE H1, 499.8760042 MHz
DATA PROCESSING
FT size 32768
Total time 2 min 0 sec



Sample Name:



Data Collected on:
nmr19-vnmrs600
Archive directory:

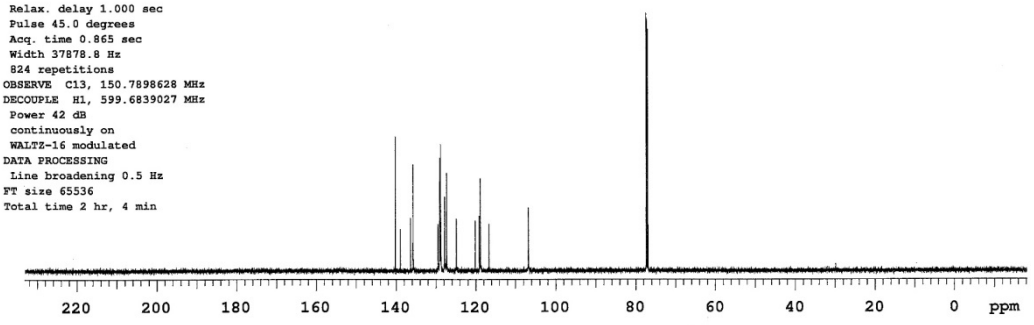
Sample directory:

FidFile: CARBON

Pulse Sequence: CARBON (s2pul)
Solvent: cdcl3
Data collected on: May 22 2019

Temp. 25.0 C / 298.1 K
Operator: Liu

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 0.865 sec
Width 37878.8 Hz
824 repetitions
OBSERVE C13, 150.7898628 MHz
DECOUPLE H1, 599.6839027 MHz
Power 42 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 0.5 Hz
FT size 65536
Total time 2 hr, 4 min



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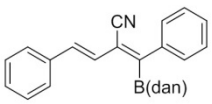
Sample Name:

Data Collected on:
nmr11-inova500
Archive directory:

Sample directory:

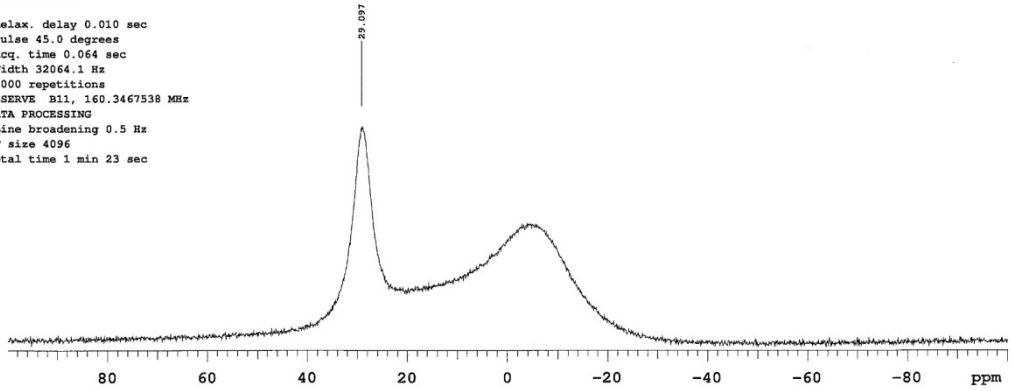
FidFile: B11



Pulse Sequence: s2pul
Solvent: cdcl3
Data collected on: May 22 2019

Temp. 25.0 C / 298.1 K
Operator: Liu

Relax. delay 0.010 sec
Pulse 45.0 degrees
Acq. time 0.064 sec
Width 32064.1 Hz
1000 repetitions
OBSERVE B11, 160.3467538 MHz
DATA PROCESSING
Line broadening 0.5 Hz
FT size 4096
Total time 1 min 23 sec



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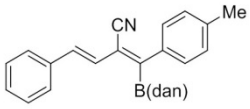
Sample Name:

Data Collected on:
nmr18-vnmrs500
Archive directory:

Sample directory:

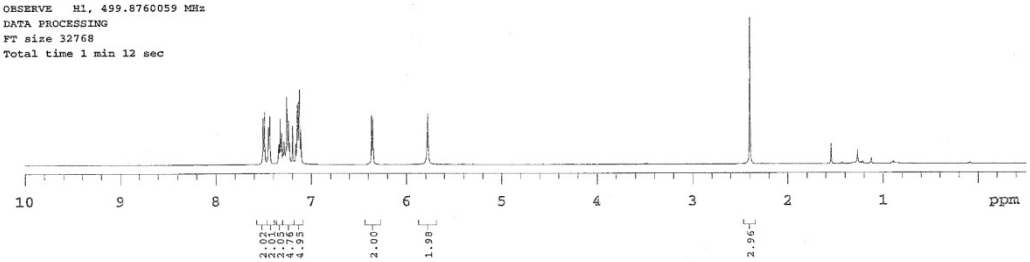
FidFile: PROTON



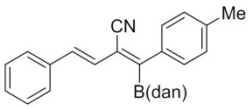
Pulse Sequence: PROTON (s2pul)
Solvent: cdcl3
Data collected on: Feb 23 2020

Temp. 25.0 C / 298.1 K
Operator: Liu

Relax. delay 10.000 sec
Pulse 45.0 degrees
Acq. time 2.045 sec
Width 8012.8 Hz
6 repetitions
OBSERVE H1, 499.8760059 MHz
DATA PROCESSING
FT size 32768
Total time 1 min 12 sec



Sample Name:



Data Collected on:
nmr18-vnmrs500
Archive directory:

Sample directory:

FidFile: CARBON

Pulse Sequence: CARBON (s2pul)
Solvent: cdcl3
Data collected on: May 26 2019

Temp. 25.0 C / 298.1 K
Operator: Liu

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.049 sec
Width 31250.0 Hz
800 repetitions
OBSERVE C13, 125.6939658 MHz
DECOUPLE H1, 499.8787746 MHz
Power 43 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 0.5 Hz
FT size 65536
Total time 1 hr, 42 min

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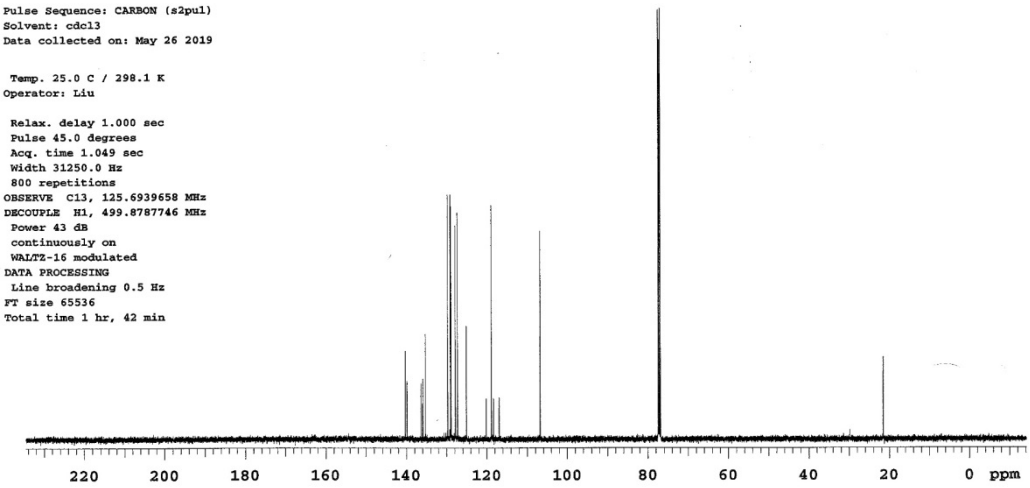
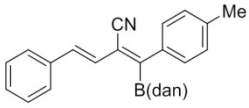


STANDARD PROTON PARAMETERS

Sample Name:



Data Collected on:
nmr11-inova500
Archive directory:

Sample directory:

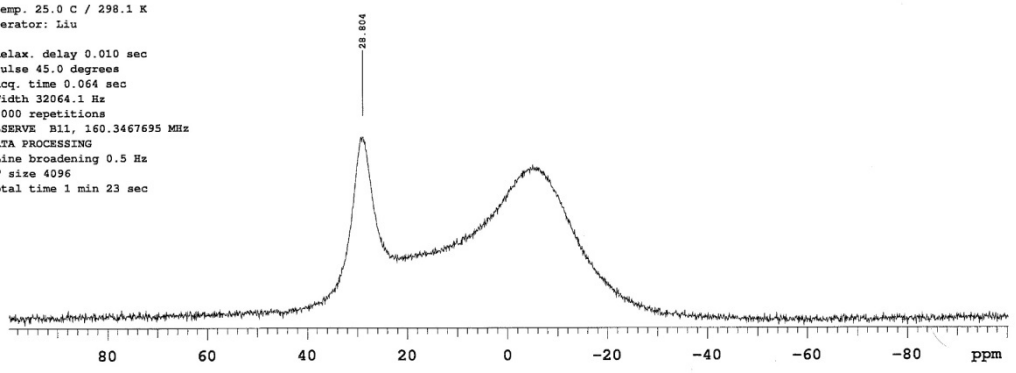
FidFile: B11

Pulse Sequence: s2pul
Solvent: cdcl3
Data collected on: May 26 2019

Temp. 25.0 C / 298.1 K
Operator: Liu

Relax. delay 0.010 sec
Pulse 45.0 degrees
Acq. time 0.064 sec
Width 32064.1 Hz
1000 repetitions
OBSERVE B11, 160.3467695 MHz
DATA PROCESSING
Line broadening 0.5 Hz
FT size 4096
Total time 1 min 23 sec

Agilent Technologies

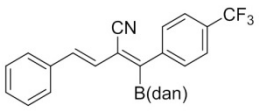


Sample Name:

Data Collected on:
nmr19-vnmrs600
Archive directory:

Sample directory:

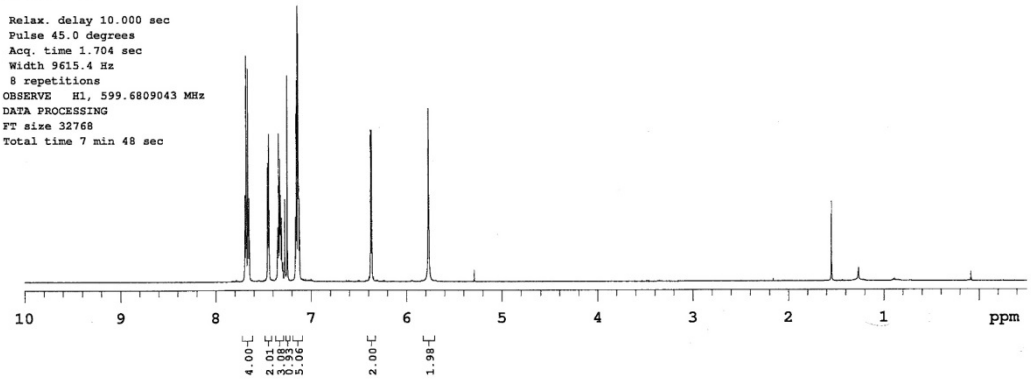
FidFile: PROTON



Pulse Sequence: PROTON (s2pul)
Solvent: cdcl3
Data collected on: May 24 2019

Temp. 25.0 C / 298.1 K
Operator: Liu

Relax. delay 10.000 sec
Pulse 45.0 degrees
Acq. time 1.704 sec
Width 9615.4 Hz
8 repetitions
OBSERVE H1, 599.6809043 MHz
DATA PROCESSING
FT size 32768
Total time 7 min 48 sec

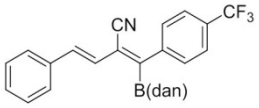


Sample Name:

Data Collected on:
nmr19-vnmrs600
Archive directory:

Sample directory:

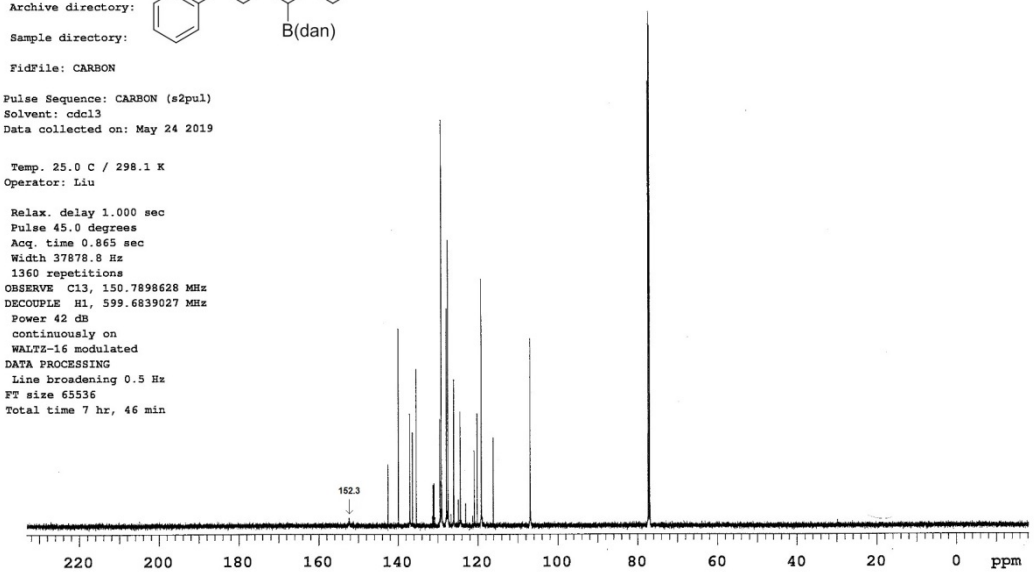
FidFile: CARBON



Pulse Sequence: CARBON (s2pul)
Solvent: cdcl3
Data collected on: May 24 2019

Temp. 25.0 C / 298.1 K
Operator: Liu

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 0.865 sec
Width 37878.8 Hz
1360 repetitions
OBSERVE C13, 150.7898628 MHz
DECOUPLE H1, 599.6839027 MHz
Power 42 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 0.5 Hz
FT size 65536
Total time 7 hr, 46 min



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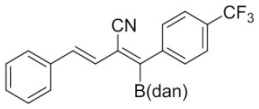
Sample Name:



Data Collected on:
nmr11-inova500
Archive directory:

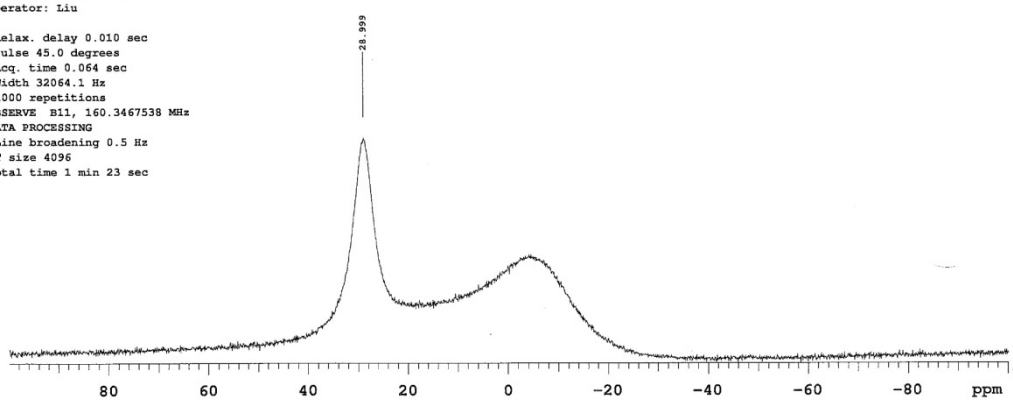
Sample directory:

FidFile: B11

Pulse Sequence: s2pul
Solvent: cdcl3
Data collected on: May 24 2019

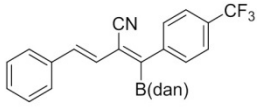
Temp. 25.0 C / 298.1 K
Operator: Liu

Relax. delay 0.010 sec
Pulse 45.0 degrees
Acq. time 0.064 sec
Width 32064.1 Hz
1000 repetitions
OBSERVE B11, 160.3467538 MHz
DATA PROCESSING
Line broadening 0.5 Hz
FT size 4096
Total time 1 min 23 sec



STANDARD FLUORINE PARAMETERS

Sample Name:



Data Collected on:
nmr19-vnmrs600
Archive directory:

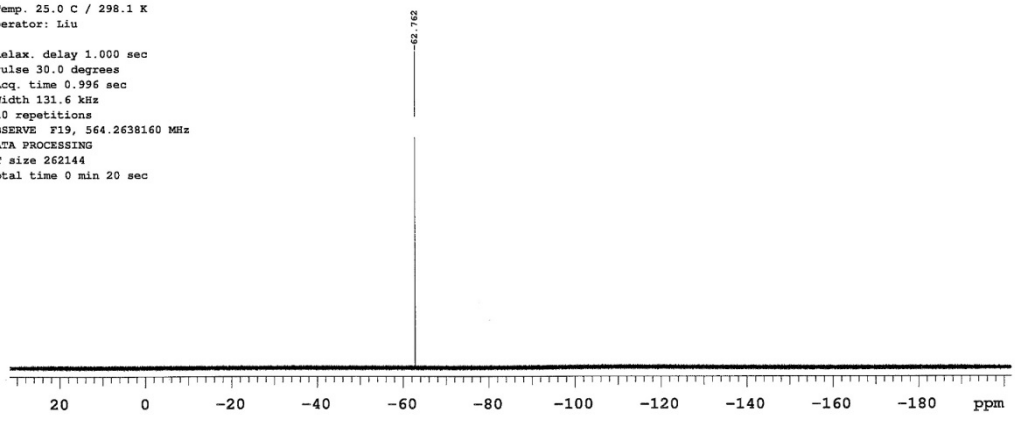
Sample directory:

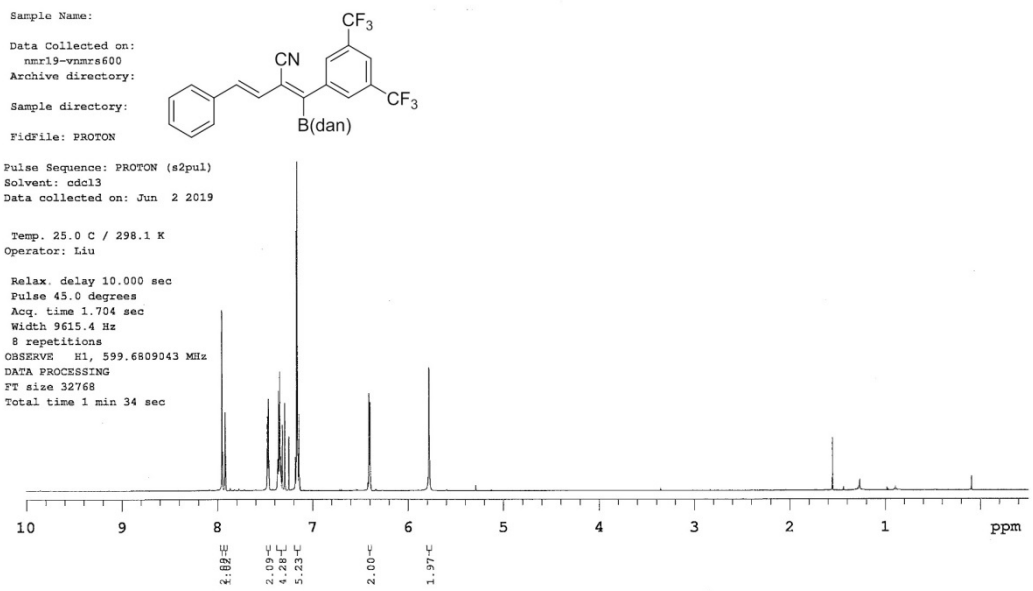
FidFile: FLUORINE

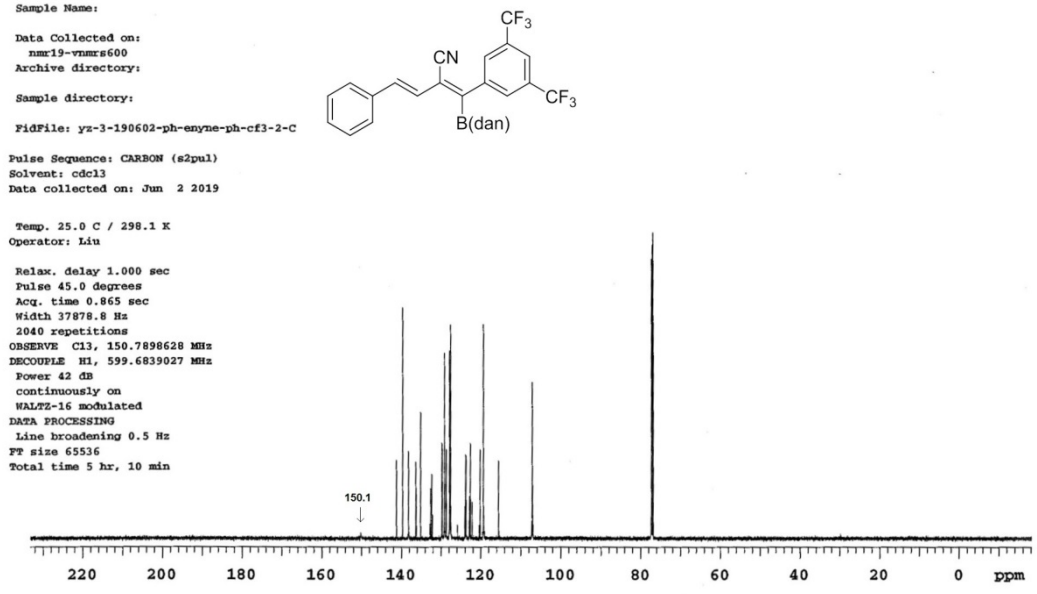
Pulse Sequence: FLUORINE (s2pul)
Solvent: cdcl3
Data collected on: May 24 2019

Temp. 25.0 C / 298.1 K
Operator: Liu

Relax. delay 1.000 sec
Pulse 30.0 degrees
Acq. time 0.996 sec
Width 131.6 kHz
10 repetitions
OBSERVE F19, 564.2638160 MHz
DATA PROCESSING
FT size 262144
Total time 0 min 20 sec




Sample Name:
Data Collected on:
nmr19-vnmrs600
Archive directory:
Sample directory:
FidFile: PROTON
CF3
CN
CF3
B(dan)
Pulse Sequence: PROTON (s2pul)
Solvent: cdcl3
Data collected on: Jun 2 2019
Temp. 25.0 C / 298.1 K
Operator: Liu
Relax. delay 10.000 sec
Pulse 45.0 degrees
Acq. time 1.704 sec
Width 9615.4 Hz
8 repetitions
OBSERVE H1, 599.6809043 MHz
DATA PROCESSING
FT size 32768
Total time 1 min 34 sec
10
9
8
7
6
5
4
3
2
1
ppm
2.88
2.09
4.28
5.23
2.00
1.97


Sample Name:
Data Collected on:
nmr19-vnmrs600
Archive directory:
Sample directory:
FidFile: yz-3-190602-ph-enyne-ph-cf3-2-C
CF3
CN
CF3
B(dan)
Pulse Sequence: CARBON (s2pul)
Solvent: cdcl3
Data collected on: Jun 2 2019
Temp. 25.0 C / 298.1 K
Operator: Liu
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 0.865 sec
Width 37878.8 Hz
2040 repetitions
OBSERVE C13, 150.7898628 MHz
DECOUPLE H1, 599.6839027 MHz
Power 42 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 0.5 Hz
FT size 65536
Total time 5 hr, 10 min
150.1
220
200
180
160
140
120
100
80
60
40
20
0
ppm

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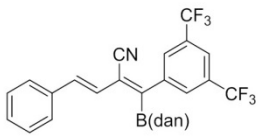
Sample Name:

Data Collected on:
nmr11-inova500
Archive directory:

Sample directory:

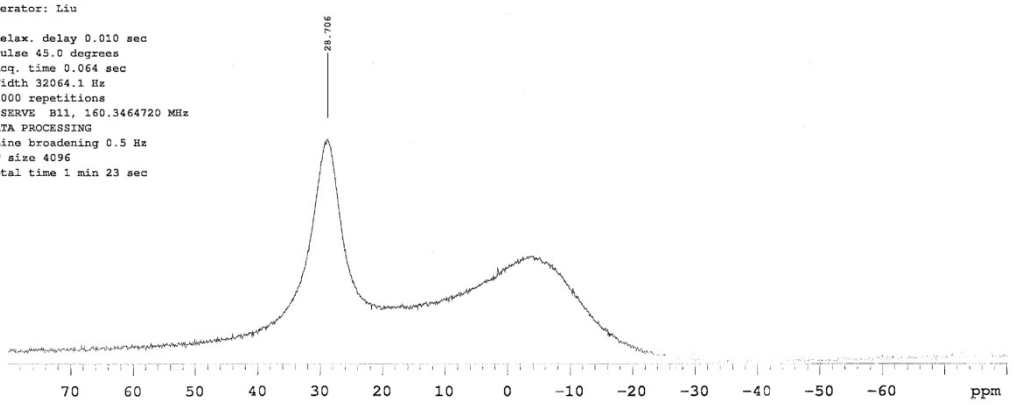
FidFile: B11



Pulse Sequence: s2pul
Solvent: cdcl3
Data collected on: Jun 2 2019

Temp. 25.0 C / 298.1 K
Operator: Liu

Relax. delay 0.010 sec
Pulse 45.0 degrees
Acq. time 0.064 sec
Width 32064.1 Hz
1000 repetitions
OBSERVE B11, 160.3464720 MHz
DATA PROCESSING
Line broadening 0.5 Hz
FT size 4096
Total time 1 min 23 sec



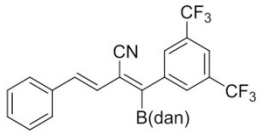
STANDARD FLUORINE PARAMETERS

Sample Name:

Data Collected on:
nmr19-vnmrs600
Archive directory:

Sample directory:

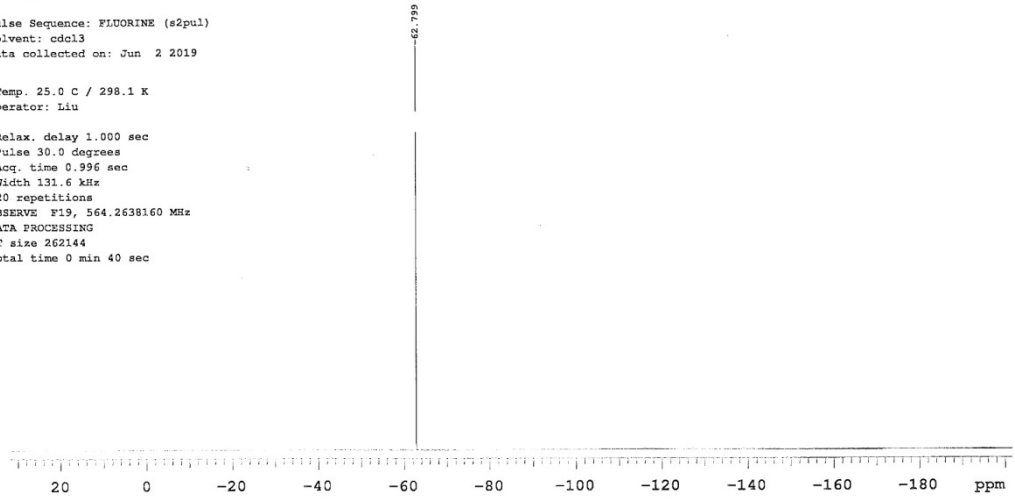
FidFile: FLUORINE



Pulse Sequence: FLUORINE (s2pul)
Solvent: cdcl3
Data collected on: Jun 2 2019

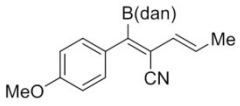
Temp. 25.0 C / 298.1 K
Operator: Liu

Relax. delay 1.000 sec
Pulse 30.0 degrees
Acq. time 0.996 sec
Width 131.6 kHz
20 repetitions
OBSERVE F19, 564.2638160 MHz
DATA PROCESSING
FT size 262144
Total time 0 min 40 sec



Agilent Technologies

Sample Name:



Data Collected on:
nmr18-vnmrs500
Archive directory:

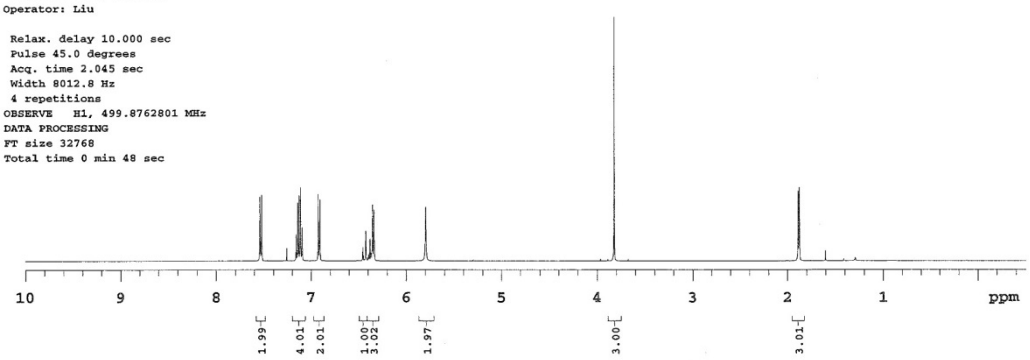
Sample directory:

FidFile: PROTON

Pulse Sequence: PROTON (s2pul)
Solvent: cdcl3
Data collected on: Nov 5 2019

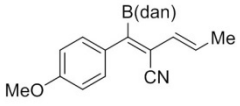
Temp. 25.0 C / 298.1 K
Operator: Liu

Relax. delay 10.000 sec
Pulse 45.0 degrees
Acq. time 2.045 sec
Width 8012.8 Hz
4 repetitions
OBSERVE H1, 499.8762801 MHz
DATA PROCESSING
FT size 32768
Total time 0 min 48 sec



Agilent Technologies

Sample Name:



Data Collected on:
nmr18-vnmrs500
Archive directory:

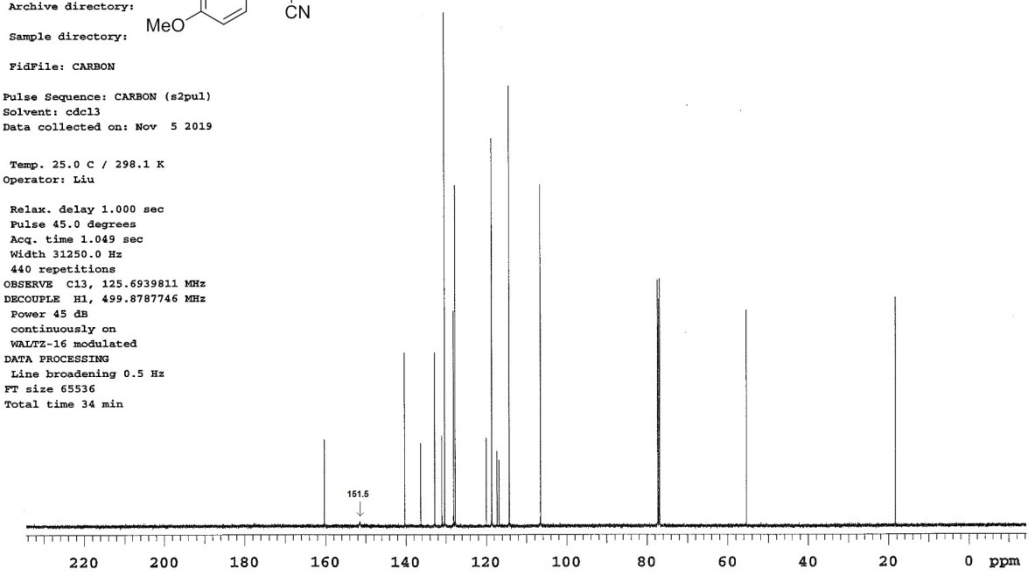
Sample directory:

FidFile: CARBON

Pulse Sequence: CARBON (s2pul)
Solvent: cdcl3
Data collected on: Nov 5 2019

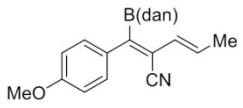
Temp. 25.0 C / 298.1 K
Operator: Liu

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.049 sec
Width 31250.0 Hz
440 repetitions
OBSERVE C13, 125.6939811 MHz
DECOUPLE H1, 499.8787746 MHz
Power 45 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 0.5 Hz
FT size 65536
Total time 34 min



Agilent Technologies

Sample Name:



Data Collected on:
nmr11-inova500
Archive directory:

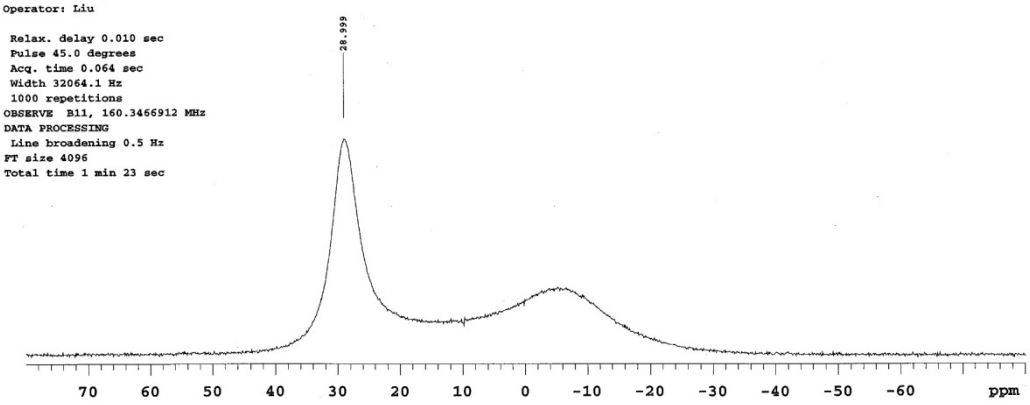
Sample directory:

FidFile: B11

Pulse Sequence: s2pul
Solvent: cdcl3
Data collected on: Sep 19 2019

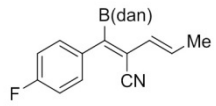
Temp. 25.0 C / 298.1 K
Operator: Liu

Relax. delay 0.010 sec
Pulse 45.0 degrees
Acq. time 0.064 sec
Width 32064.1 Hz
1000 repetitions
OBSERVE B11, 160.3466912 MHz
DATA PROCESSING
Line broadening 0.5 Hz
FT size 4096
Total time 1 min 23 sec



Agilent Technologies

Sample Name:



Data Collected on:
nmr18-vnmrs500
Archive directory:

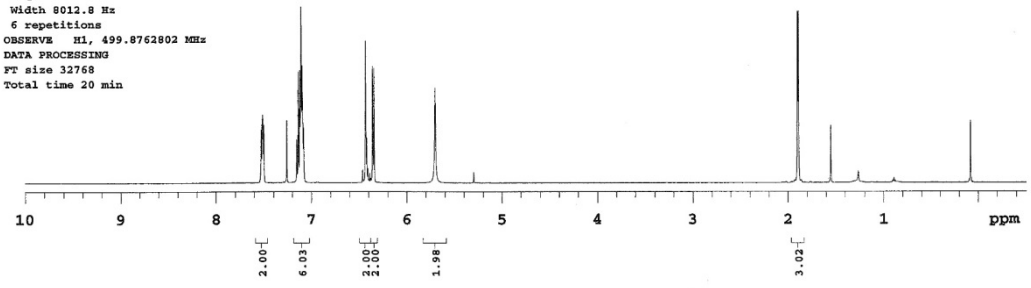
Sample directory:

FidFile: PROTON

Pulse Sequence: PROTON (s2pul)
Solvent: cdcl3
Data collected on: Jul 16 2019

Temp. 25.0 C / 298.1 K
Operator: Liu

Relax. delay 10.000 sec
Pulse 45.0 degrees
Acq. time 2.045 sec
Width 8012.8 Hz
6 repetitions
OBSERVE H1, 499.8762802 MHz
DATA PROCESSING
FT size 32768
Total time 20 min

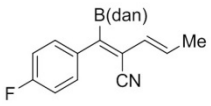


Sample Name:

Data Collected on:
nmr19-vnmrs600
Archive directory:

Sample directory:

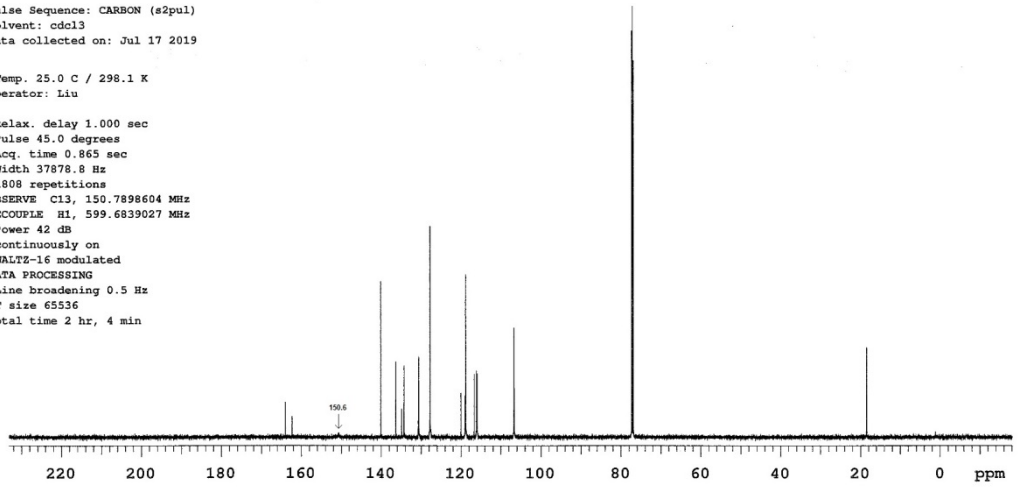
FidFile: CARBON



Pulse Sequence: CARBON (s2pul)
Solvent: cdcl3
Data collected on: Jul 17 2019

Temp. 25.0 C / 298.1 K
Operator: Liu

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 0.865 sec
Width 37878.8 Hz
1808 repetitions
OBSERVE C13, 150.7898604 MHz
DECOUPLE H1, 599.6839027 MHz
Power 42 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 0.5 Hz
FT size 65536
Total time 2 hr, 4 min



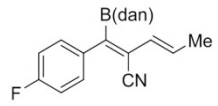
Agilent Technologies

Sample Name:

Data Collected on:
nmr11-inova500
Archive directory:

Sample directory:

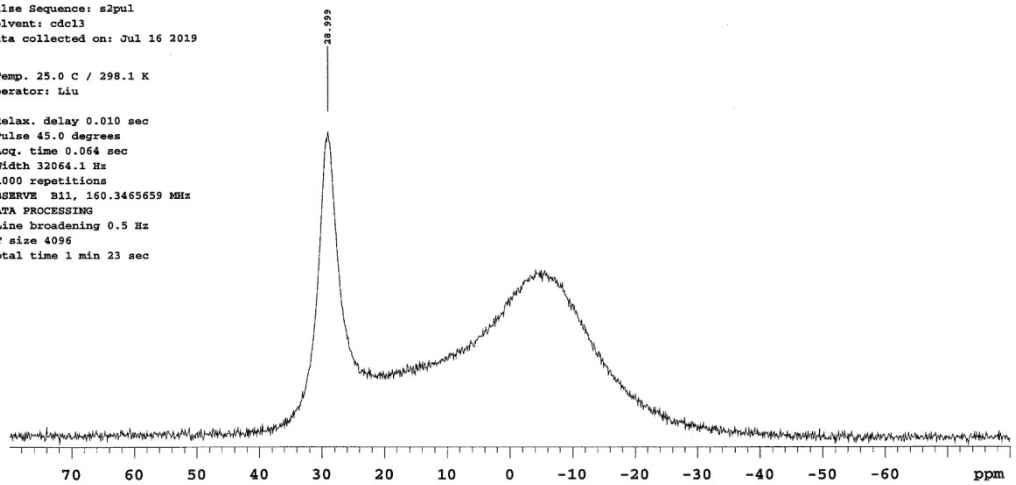
FidFile: B11



Pulse Sequence: s2pul
Solvent: cdcl3
Data collected on: Jul 16 2019

Temp. 25.0 C / 298.1 K
Operator: Liu

Relax. delay 0.010 sec
Pulse 45.0 degrees
Acq. time 0.064 sec
Width 32064.1 Hz
1000 repetitions
OBSERVE B11, 160.3465659 MHz
DATA PROCESSING
Line broadening 0.5 Hz
FT size 4096
Total time 1 min 23 sec



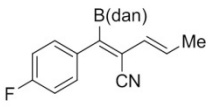
STANDARD FLUORINE PARAMETERS

Sample Name:

Data Collected on:
nmr18-vnmrs500
Archive directory:

Sample directory:

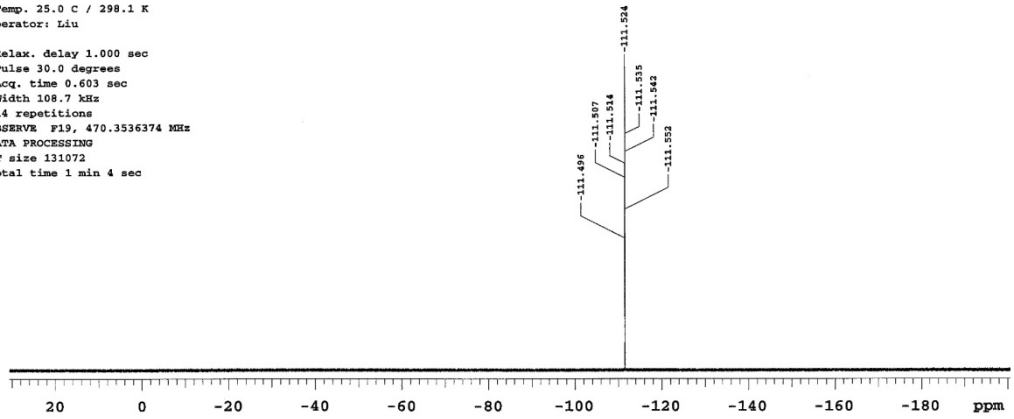
FidFile: FLUORINE



Pulse Sequence: FLUORINE (s2pul)
Solvent: cdcl3
Data collected on: Jul 16 2019

Temp. 25.0 C / 298.1 K
Operator: Liu

Relax. delay 1.000 sec
Pulse 30.0 degrees
Acq. time 0.603 sec
Width 108.7 kHz
14 repetitions
OBSERVE F19, 470.3536374 MHz
DATA PROCESSING
FT size 131072
Total time 1 min 4 sec



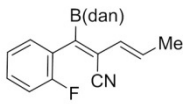
Agilent Technologies

Sample Name:

Data Collected on:
nmr18-vnmrs500
Archive directory:

Sample directory:

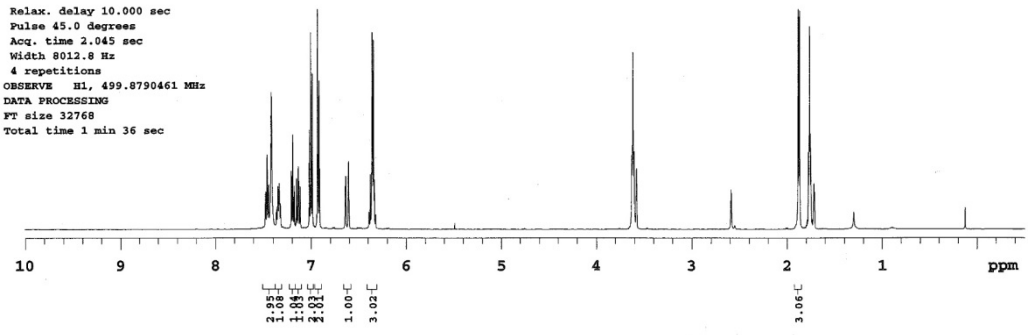
FidFile: yz-3-190909-



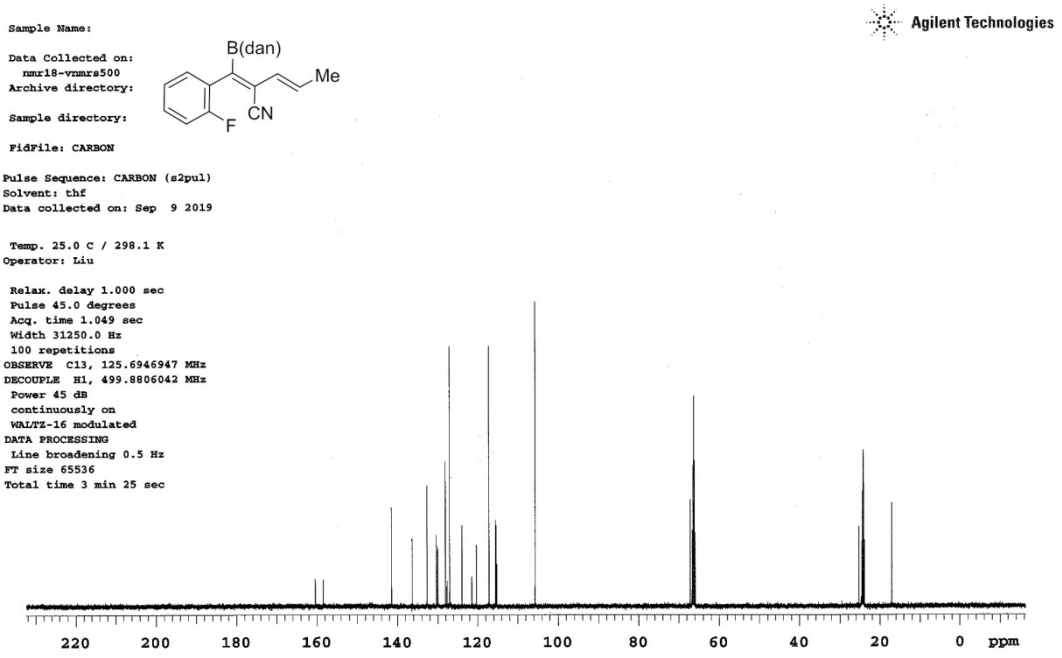
Pulse Sequence: PROTON (s2pul)
Solvent: thf
Data collected on: Sep 9 2019

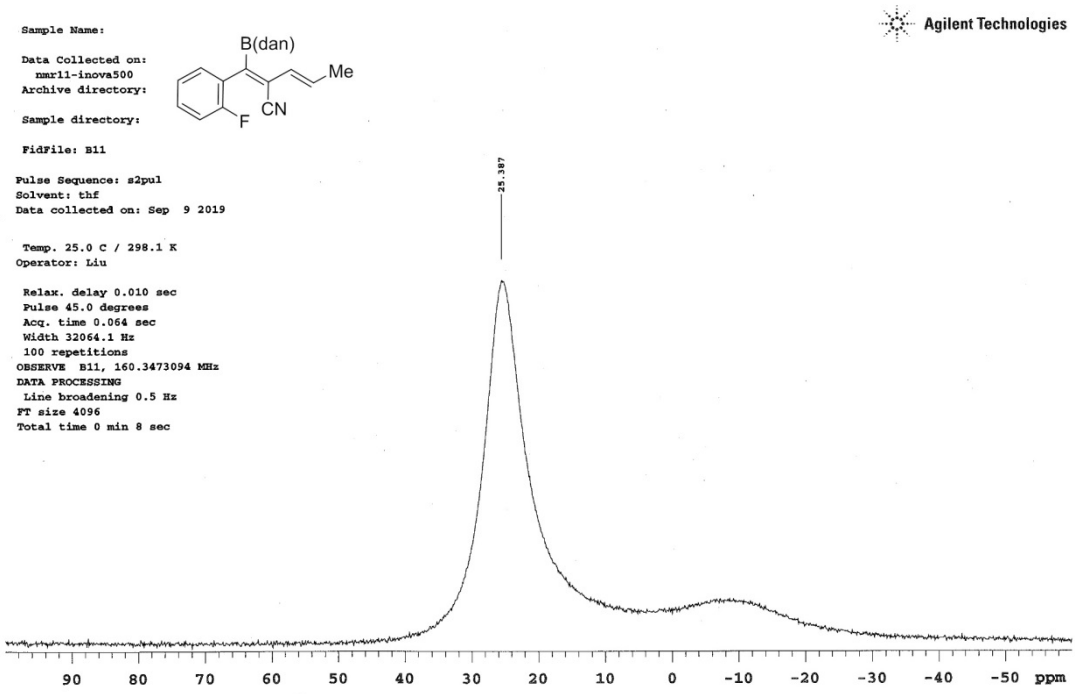
Temp. 25.0 C / 298.1 K
Operator: Liu

Relax. delay 10.000 sec
Pulse 45.0 degrees
Acq. time 2.045 sec
Width 8012.8 Hz
4 repetitions
OBSERVE H1, 499.8790461 MHz
DATA PROCESSING
FT size 32768
Total time 1 min 36 sec



Agilent Technologies


Agilent Technologies
Sample Name:
Data Collected on:
nmr18-vnmrs500
Archive directory:
Sample directory:
FidFile: CARBON
B(dan)
Me
CN
F
Pulse Sequence: CARBON (s2pul)
Solvent: thf
Data collected on: Sep 9 2019
Temp. 25.0 C / 298.1 K
Operator: Liu
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.049 sec
Width 31250.0 Hz
100 repetitions
OBSERVE C13, 125.6946947 MHz
DECOUPLE H1, 499.8806042 MHz
Power 45 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 0.5 Hz
FT size 65536
Total time 3 min 25 sec
220 200 180 160 140 120 100 80 60 40 20 0 ppm


Agilent Technologies
Sample Name:
Data Collected on:
nmr11-inova500
Archive directory:
Sample directory:
FidFile: B11
B(dan)
Me
CN
F
25.387
Pulse Sequence: s2pul
Solvent: thf
Data collected on: Sep 9 2019
Temp. 25.0 C / 298.1 K
Operator: Liu
Relax. delay 0.010 sec
Pulse 45.0 degrees
Acq. time 0.064 sec
Width 32064.1 Hz
100 repetitions
OBSERVE B11, 160.3473094 MHz
DATA PROCESSING
Line broadening 0.5 Hz
FT size 4096
Total time 0 min 8 sec
90 80 70 60 50 40 30 20 10 0 -10 -20 -30 -40 -50 ppm

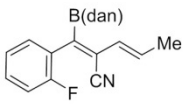
STANDARD FLUORINE PARAMETERS

Sample Name:

Data Collected on:
nmr18-vnmrs500
Archive directory:

Sample directory:

FidFile: FLUORINE

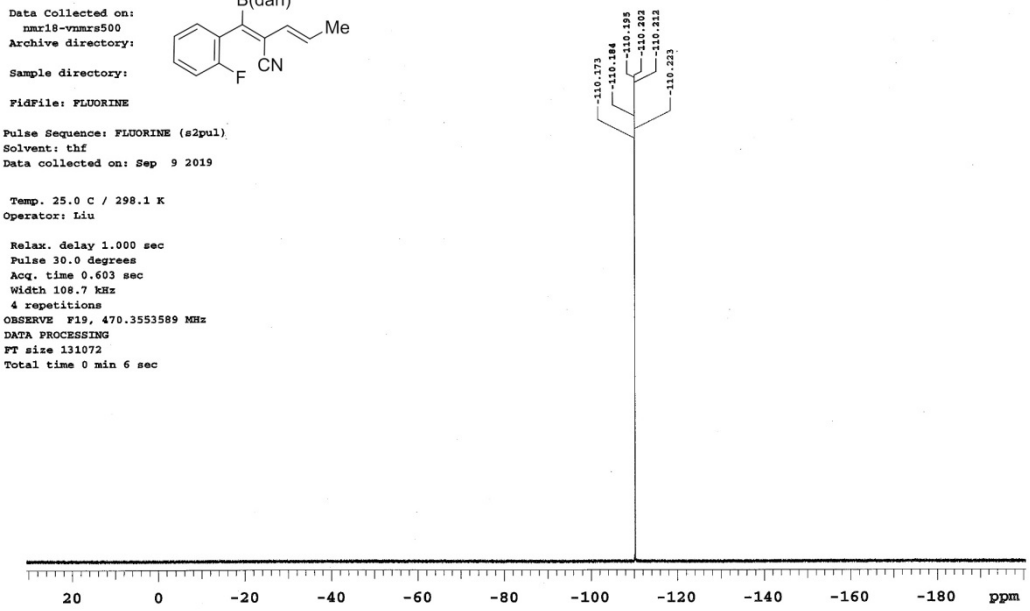


Agilent Technologies

Pulse Sequence: FLUORINE (s2pul)
Solvent: thf
Data collected on: Sep 9 2019

Temp. 25.0 C / 298.1 K
Operator: Liu

Relax. delay 1.000 sec
Pulse 30.0 degrees
Acq. time 0.603 sec
Width 108.7 kHz
4 repetitions
OBSERVE F19, 470.3553589 MHz
DATA PROCESSING
FT size 131072
Total time 0 min 6 sec

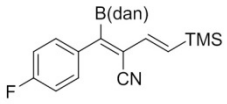


Sample Name:

Data Collected on
nmr18-vnmrs500
Archive directory

Sample directory:

FidFile: PROTON

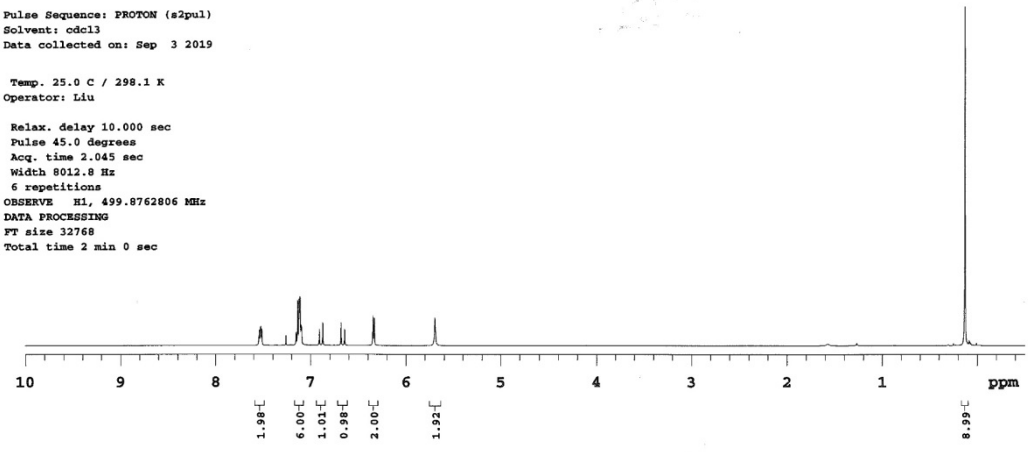


Agilent Technologies

Pulse Sequence: PROTON (s2pul)
Solvent: cdcl3
Data collected on: Sep 3 2019

Temp. 25.0 C / 298.1 K
Operator: Liu

Relax. delay 10.000 sec
Pulse 45.0 degrees
Acq. time 2.045 sec
Width 8012.8 Hz
6 repetitions
OBSERVE H1, 499.8762806 MHz
DATA PROCESSING
FT size 32768
Total time 2 min 0 sec

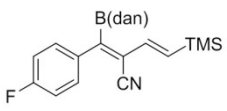


Agilent Technologies

Sample Name:

Data Collected on:
nmr18-vnmrs500
Archive directory:

Sample directory:

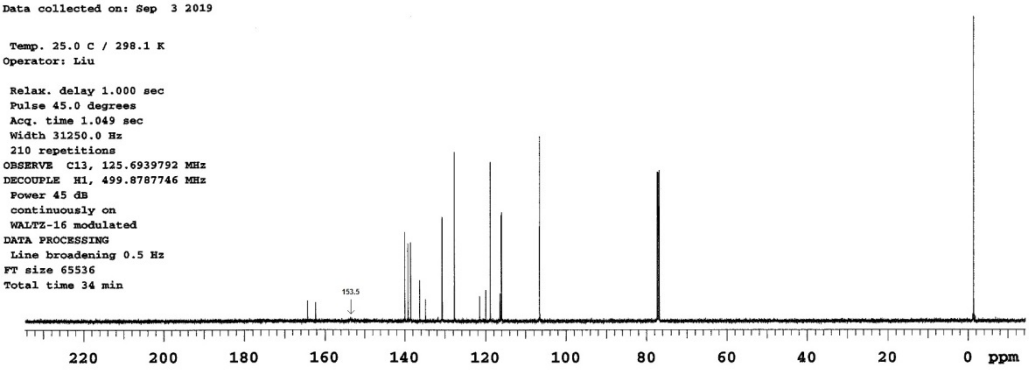


FidFile: CARBON

Pulse Sequence: CARBON (s2pul)
Solvent: cdcl3
Data collected on: Sep 3 2019

Temp. 25.0 C / 298.1 K
Operator: Liu

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.049 sec
Width 31250.0 Hz
210 repetitions
OBSERVE C13, 125.6939792 MHz
DECOUPLE H1, 499.8787746 MHz
Power 45 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 0.5 Hz
FT size 65536
Total time 34 min

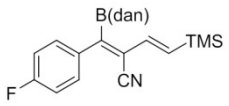


Agilent Technologies

Sample Name:

Data Collected on:
nmr11-inova500
Archive directory:

Sample directory:

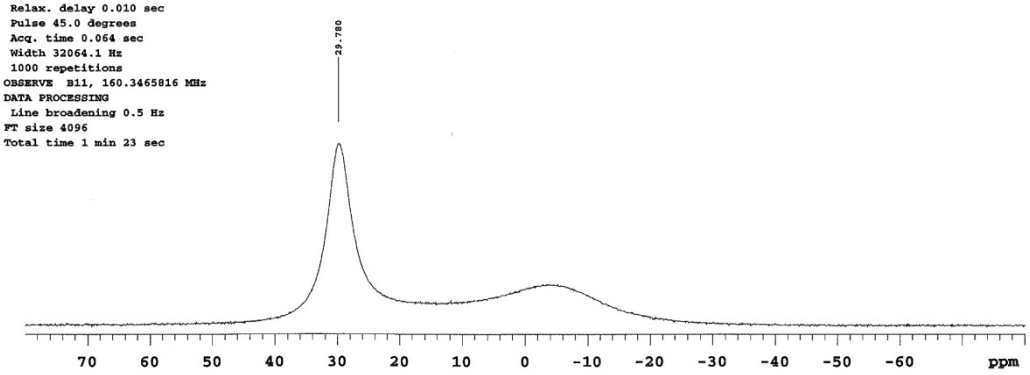


FidFile: B11

Pulse Sequence: s2pul
Solvent: cdcl3
Data collected on: Sep 3 2019

Temp. 25.0 C / 298.1 K
Operator: Liu

Relax. delay 0.010 sec
Pulse 45.0 degrees
Acq. time 0.064 sec
Width 32064.1 Hz
1000 repetitions
OBSERVE B11, 160.3465816 MHz
DATA PROCESSING
Line broadening 0.5 Hz
FT size 4096
Total time 1 min 23 sec



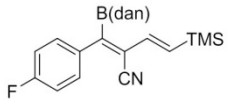
STANDARD FLUORINE PARAMETERS

Sample Name:

Data Collected on:
nmr18-vnmrs500
Archive directory:

Sample directory:

FidFile: yz-3-190223-p-F-tms-F

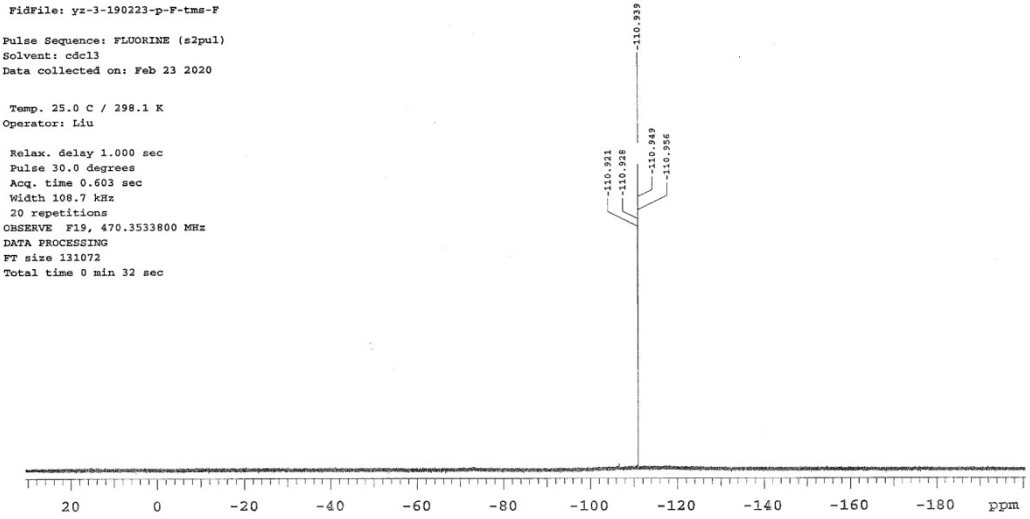


Agilent Technologies

Pulse Sequence: FLUORINE (s2pul)
Solvent: cdcl3
Data collected on: Feb 23 2020

Temp. 25.0 C / 298.1 K
Operator: Liu

Relax. delay 1.000 sec
Pulse 30.0 degrees
Acq. time 0.603 sec
Width 108.7 kHz
20 repetitions
OBSERVE F19, 470.3533800 MHz
DATA PROCESSING
FT size 131072
Total time 0 min 32 sec

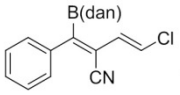


Sample Name:

Data Collected on:
nmr19-vnmrs600
Archive directory:

Sample directory:

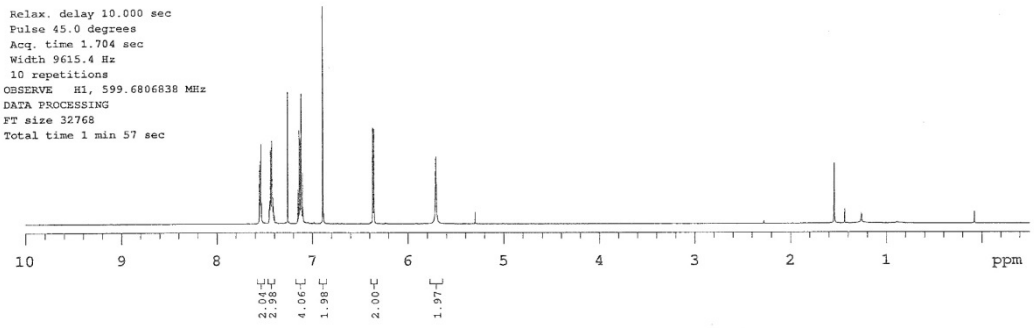
FidFile: PROTON



Pulse Sequence: PROTON (s2pul)
Solvent: cdcl3
Data collected on: Mar 19 2020

Temp. 25.0 C / 298.1 K
Operator: Liu

Relax. delay 10.000 sec
Pulse 45.0 degrees
Acq. time 1.704 sec
Width 9615.4 Hz
10 repetitions
OBSERVE H1, 599.6806838 MHz
DATA PROCESSING
FT size 32768
Total time 1 min 57 sec

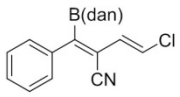


Sample Name:

Data Collected on:
nmr19-vnmrs600
Archive directory:

Sample directory:

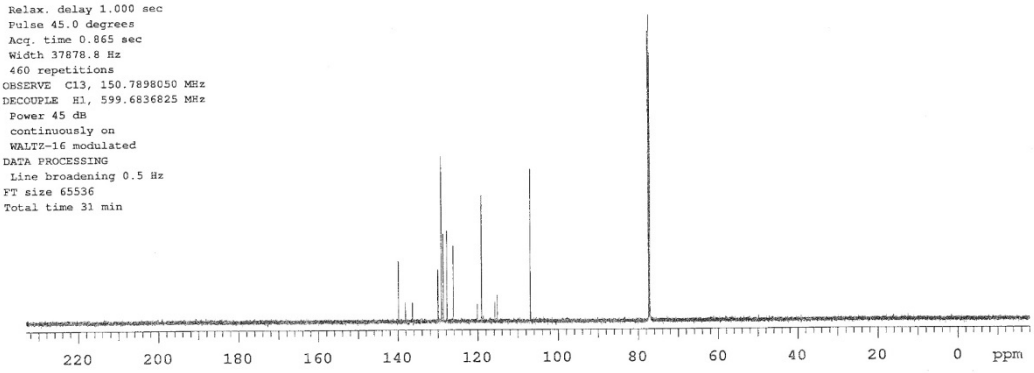
FidFile: CARBON



Pulse Sequence: CARBON (s2pul)
Solvent: cdcl3
Data collected on: Mar 18 2020

Temp. 25.0 C / 298.1 K
Operator: Liu

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 0.865 sec
Width 37878.8 Hz
460 repetitions
OBSERVE C13, 150.7898050 MHz
DECOUPLE H1, 599.6836825 MHz
Power 45 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 0.5 Hz
FT size 65536
Total time 31 min



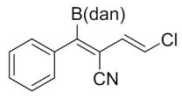
Agilent Technologies

Sample Name:

Data Collected on:
nmr11-inova500
Archive directory:

Sample directory:

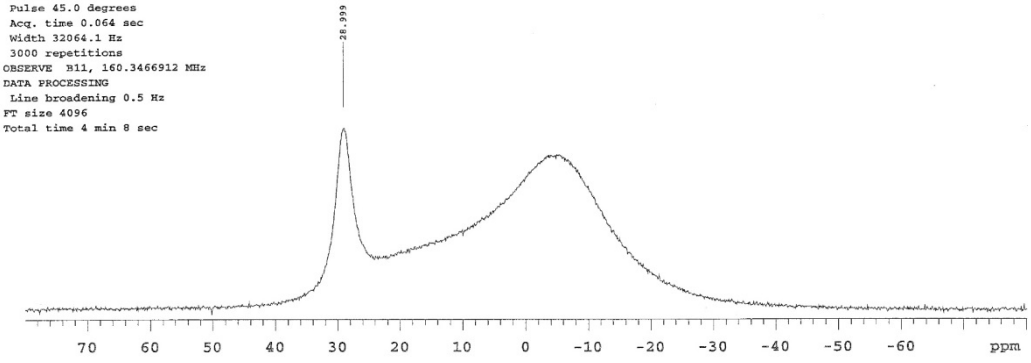
FidFile: B11



Pulse Sequence: s2pul
Solvent: cdcl3
Data collected on: Mar 19 2020

Temp. 25.0 C / 298.1 K
Operator: Liu

Relax. delay 0.010 sec
Pulse 45.0 degrees
Acq. time 0.064 sec
Width 32064.1 Hz
3000 repetitions
OBSERVE B11, 160.3466912 MHz
DATA PROCESSING
Line broadening 0.5 Hz
FT size 4096
Total time 4 min 8 sec



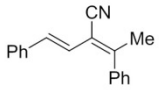
Agilent Technologies

Sample Name:

Data Collected on:
nmr18-vnmrs500
Archive directory:

Sample directory:

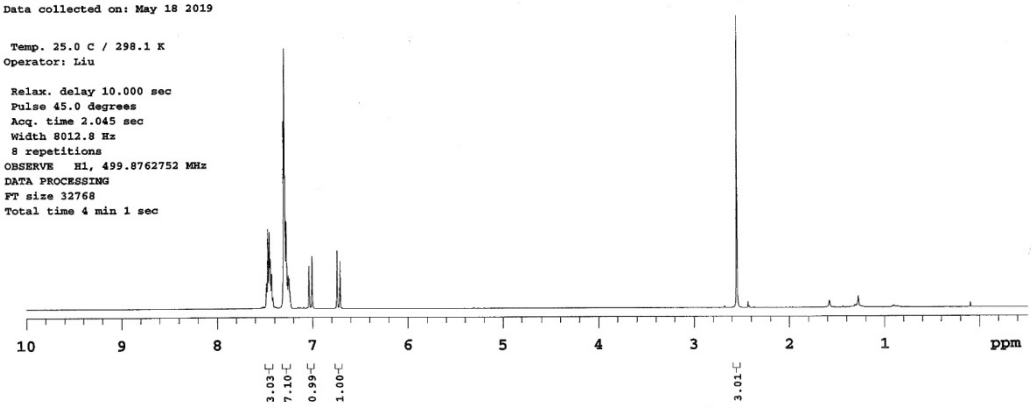
FidFile: PROTON



Pulse Sequence: PROTON (s2pul)
Solvent: cdcl3
Data collected on: May 18 2019

Temp. 25.0 C / 298.1 K
Operator: Liu

Relax. delay 10.000 sec
Pulse 45.0 degrees
Acq. time 2.045 sec
Width 8012.8 Hz
8 repetitions
OBSERVE H1, 499.8762752 MHz
DATA PROCESSING
FT size 32768
Total time 4 min 1 sec



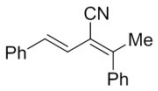
Agilent Technologies

Sample Name:

Data Collected on:
nmr18-vnmrs500
Archive directory:

Sample directory:

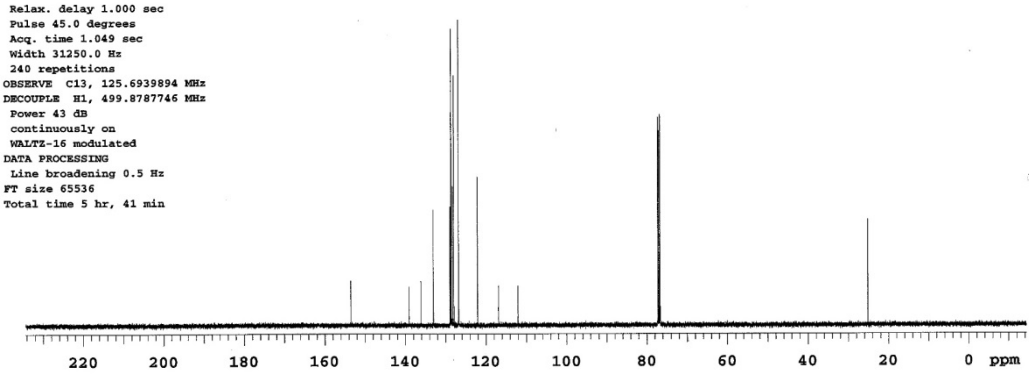
FidFile: CARBON

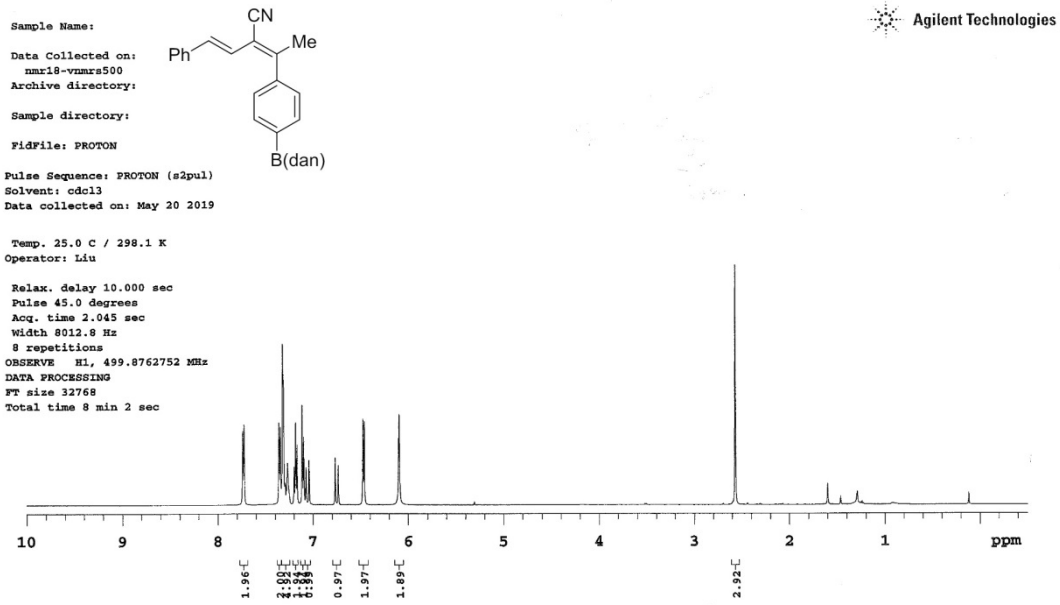


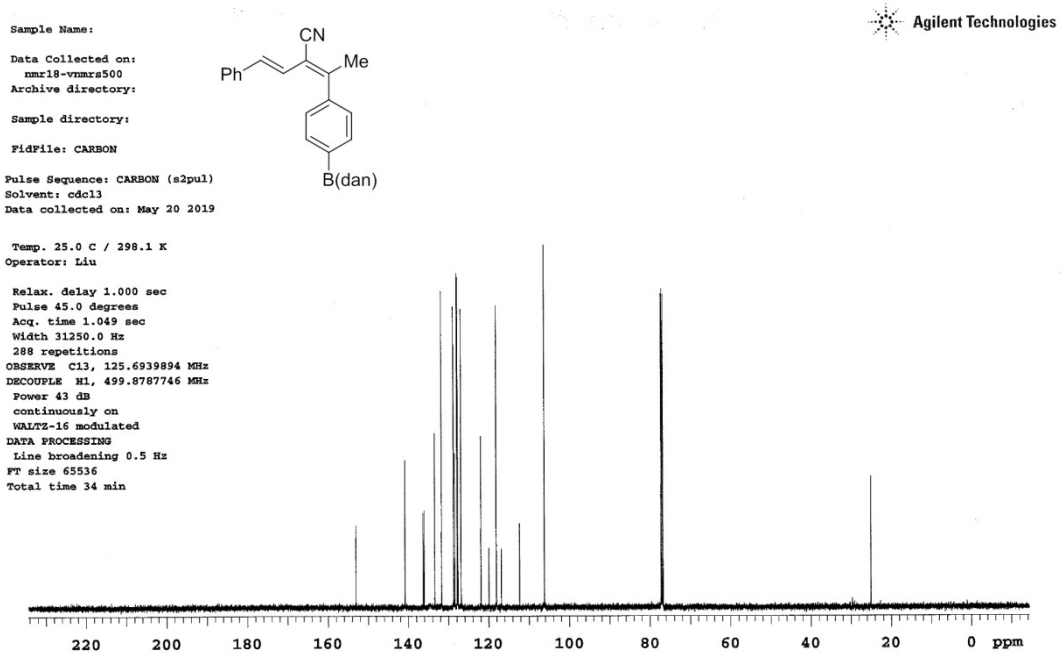
Pulse Sequence: CARBON (s2pul)
Solvent: cdcl3
Data collected on: May 18 2019

Temp. 25.0 C / 298.1 K
Operator: Liu

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.049 sec
Width 31250.0 Hz
240 repetitions
OBSERVE C13, 125.6939894 MHz
DECOUPLE H1, 499.8787746 MHz
Power 43 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 0.5 Hz
FT size 65536
Total time 5 hr, 41 min




Agilent Technologies
Sample Name:
Data Collected on:
nmr18-vnmrs500
Archive directory:
Sample directory:
FidFile: PROTON
CN
Me
Ph
B(dan)
Pulse Sequence: PROTON (s2pul)
Solvent: cdcl3
Data collected on: May 20 2019
Temp. 25.0 C / 298.1 K
Operator: Liu
Relax. delay 10.000 sec
Pulse 45.0 degrees
Acq. time 2.045 sec
Width 8012.8 Hz
8 repetitions
OBSERVE H1, 499.8762752 MHz
DATA PROCESSING
FT size 32768
Total time 8 min 2 sec
10
9
8
7
6
5
4
3
2
1
ppm
1.96
2.00
0.97
1.97
1.89
2.92


Agilent Technologies
Sample Name:
Data Collected on:
nmr18-vnmrs500
Archive directory:
Sample directory:
FidFile: CARBON
CN
Me
Ph
B(dan)
Pulse Sequence: CARBON (s2pul)
Solvent: cdcl3
Data collected on: May 20 2019
Temp. 25.0 C / 298.1 K
Operator: Liu
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.049 sec
Width 31250.0 Hz
288 repetitions
OBSERVE C13, 125.6939894 MHz
DECOUPLE H1, 499.8787746 MHz
Power 43 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 0.5 Hz
FT size 65536
Total time 34 min
220
200
180
160
140
120
100
80
60
40
20
0
ppm

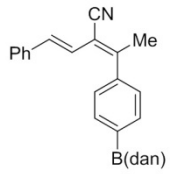
Agilent Technologies

Sample Name:

Data Collected on:
nmr11-inova500
Archive directory:

Sample directory:

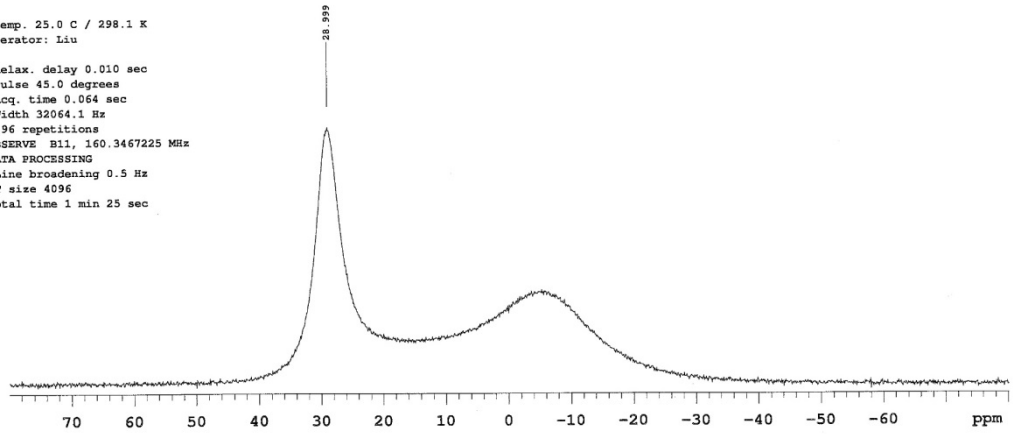
FidFile: B11



Pulse Sequence: s2pul
Solvent: cdcl3
Data collected on: May 20 2019

Temp. 25.0 C / 298.1 K
Operator: Liu

Relax. delay 0.010 sec
Pulse 45.0 degrees
Acq. time 0.064 sec
Width 32064.1 Hz
896 repetitions
OBSERVE B11, 160.3467225 MHz
DATA PROCESSING
Line broadening 0.5 Hz
FT size 4096
Total time 1 min 25 sec

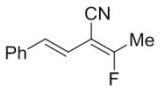


Sample Name:

Data Collected on:
nmr19-vnmrs600
Archive directory:

Sample directory:

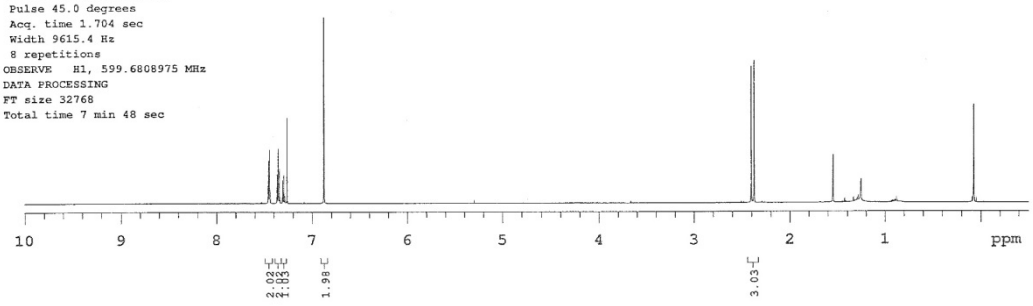
FidFile: yz-3-190622-flouronation-H



Pulse Sequence: PROTON (s2pul)
Solvent: cdcl3
Data collected on: Jun 22 2019

Temp. 25.0 C / 298.1 K
Operator: Liu

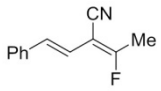
Relax. delay 10.000 sec
Pulse 45.0 degrees
Acq. time 1.704 sec
Width 9615.4 Hz
8 repetitions
OBSERVE H1, 599.6808975 MHz
DATA PROCESSING
FT size 32768
Total time 7 min 48 sec



Sample Name:

Data Collected on:
nmr14-vnmrs400
Archive directory:

Sample directory:

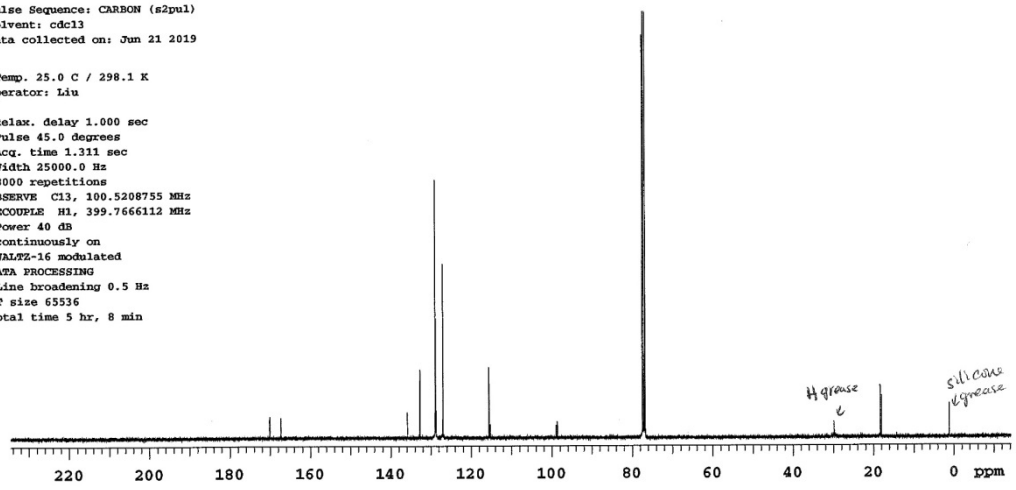


FidFile: yz-3-190622-fluorination-C

Pulse Sequence: CARBON (s2pul)
Solvent: cdcl3
Data collected on: Jun 21 2019

Temp. 25.0 C / 298.1 K
Operator: Liu

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.311 sec
Width 25000.0 Hz
8000 repetitions
OBSERVE C13, 100.5208755 MHz
DECOUPLE H1, 399.7666112 MHz
Power 40 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 0.5 Hz
FT size 65536
Total time 5 hr, 8 min

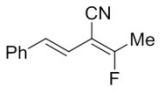


STANDARD FLUORINE PARAMETERS

Sample Name:

Data Collected on:
nmr19-vnmrs600
Archive directory:

Sample directory:

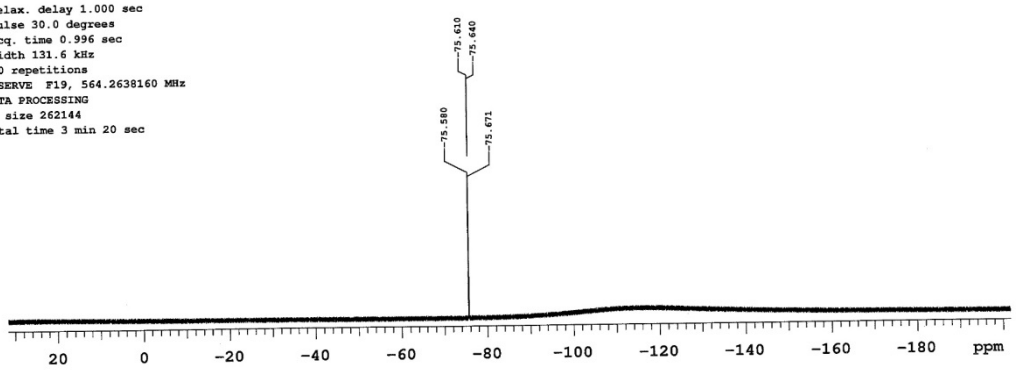


FidFile: FLUORINE

Pulse Sequence: FLUORINE (s2pul)
Solvent: cdcl3
Data collected on: Jun 22 2019

Temp. 25.0 C / 298.1 K
Operator: Liu

Relax. delay 1.000 sec
Pulse 30.0 degrees
Acq. time 0.996 sec
Width 131.6 kHz
20 repetitions
OBSERVE F19, 564.2638160 MHz
DATA PROCESSING
FT size 262144
Total time 3 min 20 sec

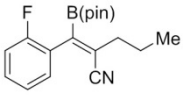


Agilent Technologies

Sample Name:

Data Collected on:
nmr18-vnmrs500
Archive directory:

Sample directory:

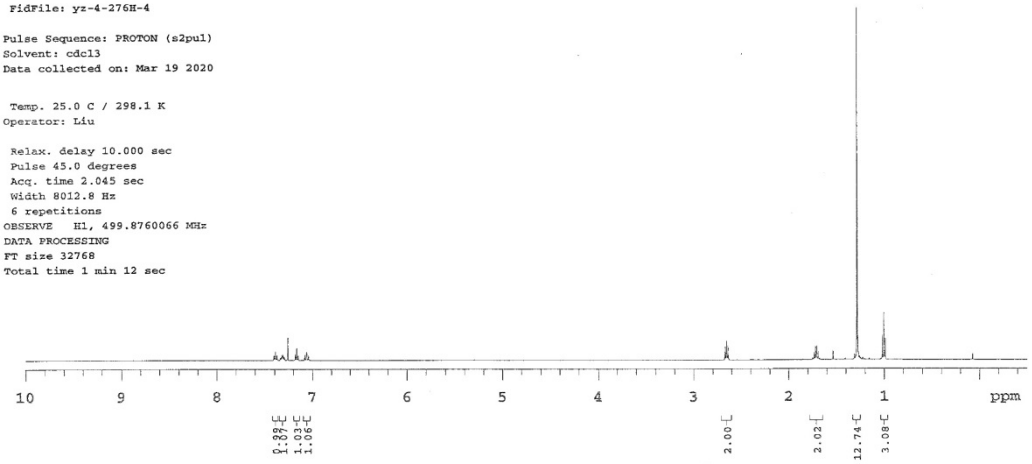


FidFile: yz-4-276H-4

Pulse Sequence: PROTON (s2pul)
Solvent: cdcl3
Data collected on: Mar 19 2020

Temp. 25.0 C / 298.1 K
Operator: Liu

Relax. delay 10.000 sec
Pulse 45.0 degrees
Acq. time 2.045 sec
Width 8012.8 Hz
6 repetitions
OBSERVE H1, 499.8760066 MHz
DATA PROCESSING
FT size 32768
Total time 1 min 12 sec



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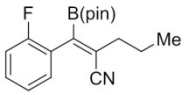
Sample Name:

Data Collected on:
nmr18-vnmrs500
Archive directory:

Sample directory:

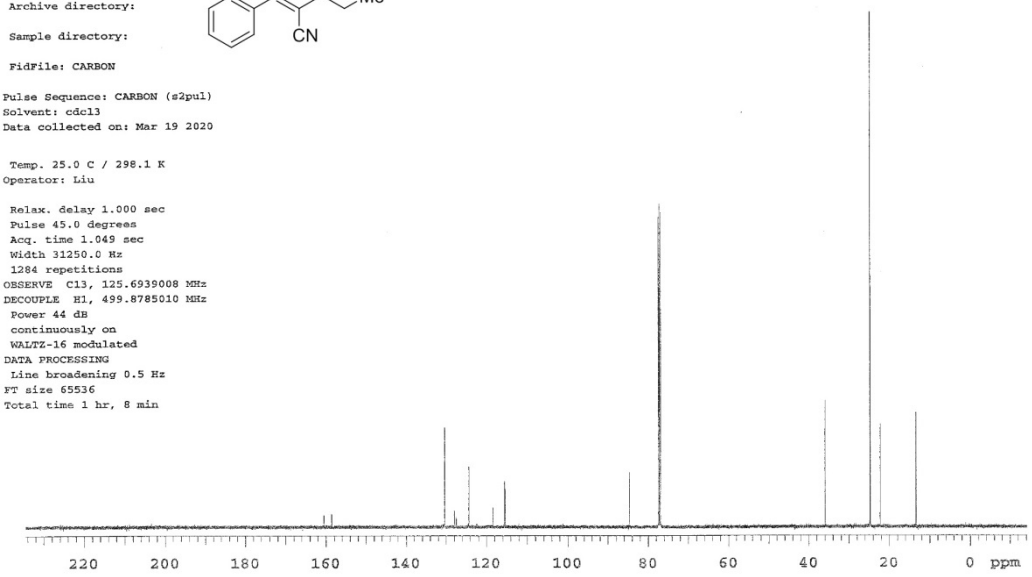


FidFile: CARBON

Pulse Sequence: CARBON (s2pul)
Solvent: cdcl3
Data collected on: Mar 19 2020

Temp. 25.0 C / 298.1 K
Operator: Liu

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.049 sec
Width 31250.0 Hz
1284 repetitions
OBSERVE C13, 125.6939008 MHz
DECOUPLE H1, 499.8785010 MHz
Power 44 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 0.5 Hz
FT size 65536
Total time 1 hr, 8 min



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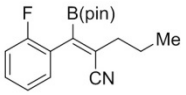
Sample Name:

Data Collected on:
nmr11-inova500
Archive directory:

Sample directory:

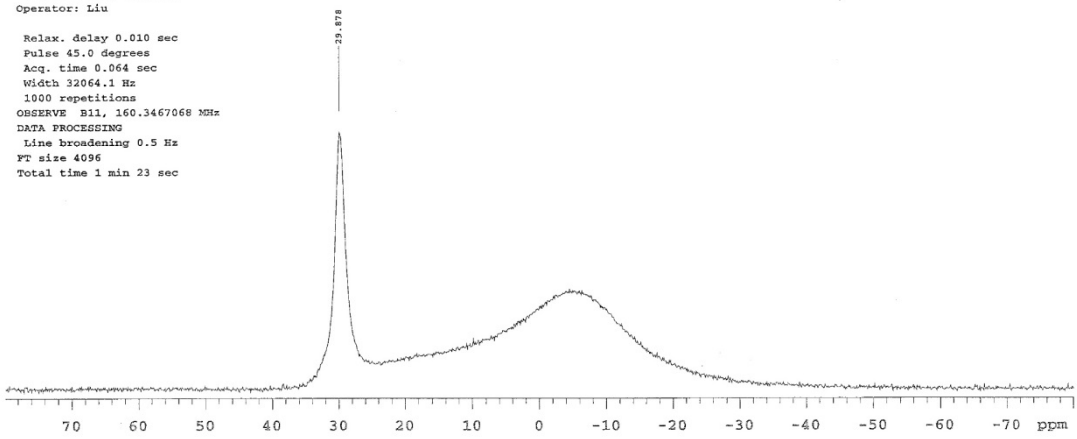
FidFile: B11



Pulse Sequence: s2pul
Solvent: cdcl3
Data collected on: Mar 19 2020

Temp. 25.0 C / 298.1 K
Operator: Liu

Relax. delay 0.010 sec
Pulse 45.0 degrees
Acq. time 0.064 sec
Width 32064.1 Hz
1000 repetitions
OBSERVE B11, 160.3467068 MHz
DATA PROCESSING
Line broadening 0.5 Hz
FT size 4096
Total time 1 min 23 sec



STANDARD FLUORINE PARAMETERS

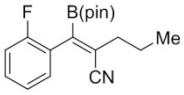
Agilent Technologies

Sample Name:

Data Collected on:
nmr18-vnmrs500
Archive directory:

Sample directory:

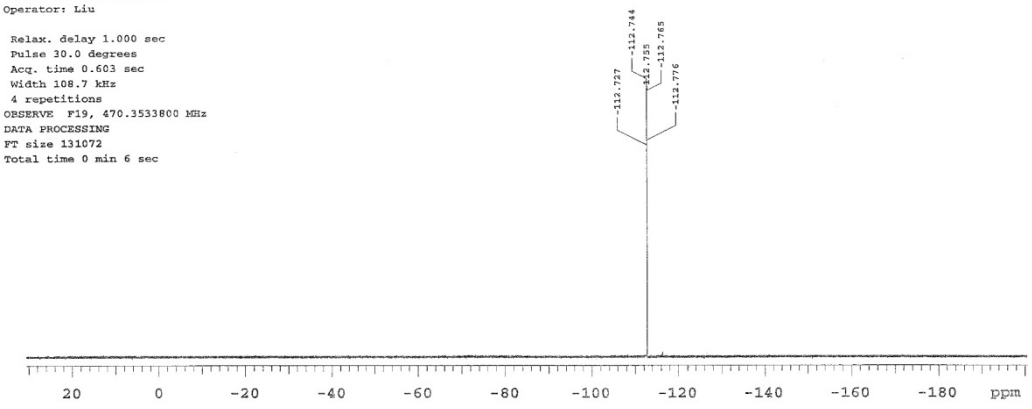
FidFile: yz-4-276F-4



Pulse Sequence: FLUORINE (s2pul)
Solvent: cdcl3
Data collected on: Mar 19 2020

Temp. 25.0 C / 298.1 K
Operator: Liu

Relax. delay 1.000 sec
Pulse 30.0 degrees
Acq. time 0.603 sec
Width 108.7 kHz
4 repetitions
OBSERVE F19, 470.3533800 MHz
DATA PROCESSING
FT size 131072
Total time 0 min 6 sec

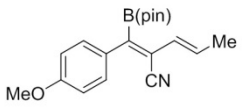


Sample Name:

Data Collected on:
nmr19-vnmrs600
Archive directory:

Sample directory:

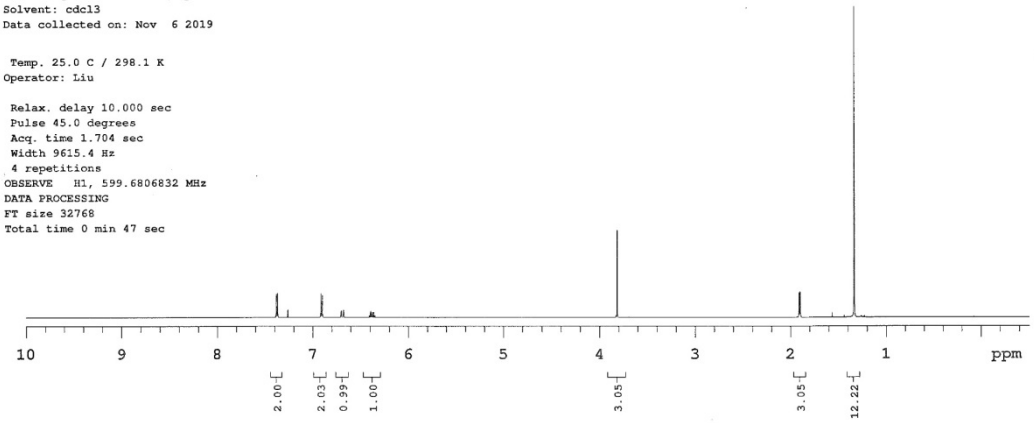
FidFile: PROTON



Pulse Sequence: PROTON (s2pul)
Solvent: cdcl3
Data collected on: Nov 6 2019

Temp. 25.0 C / 298.1 K
Operator: Liu

Relax. delay 10.000 sec
Pulse 45.0 degrees
Acq. time 1.704 sec
Width 9615.4 Hz
4 repetitions
OBSERVE H1, 599.6806832 MHz
DATA PROCESSING
FT size 32768
Total time 0 min 47 sec

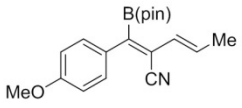


Sample Name:

Data Collected on:
nmr19-vnmrs600
Archive directory:

Sample directory:

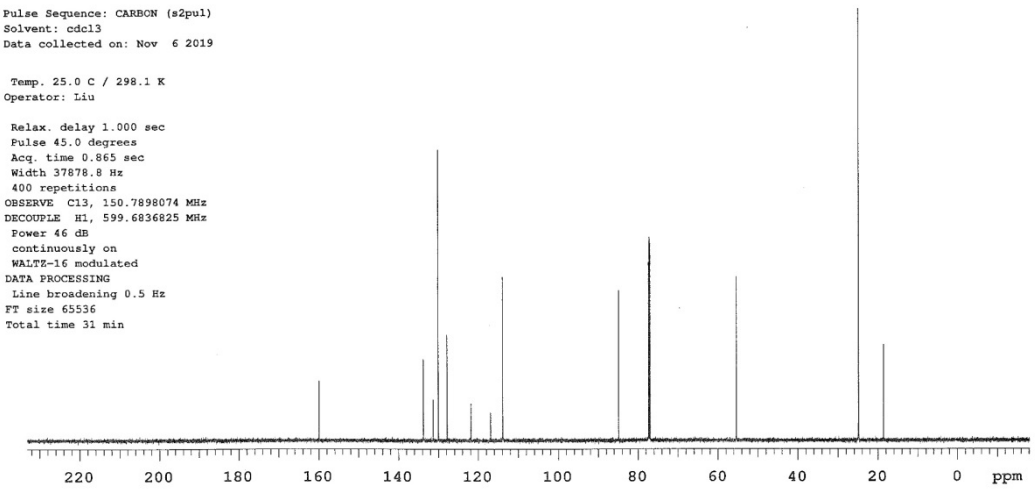
FidFile: CARBON



Pulse Sequence: CARBON (s2pul)
Solvent: cdcl3
Data collected on: Nov 6 2019

Temp. 25.0 C / 298.1 K
Operator: Liu

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 0.865 sec
Width 37878.8 Hz
400 repetitions
OBSERVE C13, 150.7898074 MHz
DECOUPLE H1, 599.6836825 MHz
Power 46 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 0.5 Hz
FT size 65536
Total time 31 min



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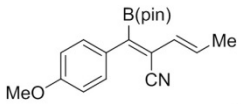
Sample Name:

Data Collected on:
nmr11-inova500
Archive directory:

Sample directory:

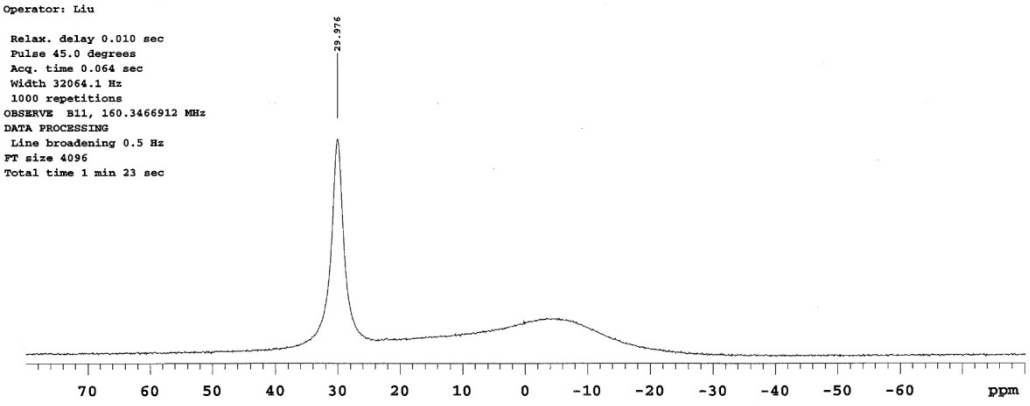
FidFile: B11



Pulse Sequence: s2pul
Solvent: cdcl3
Data collected on: Sep 21 2019

Temp. 25.0 C / 298.1 K
Operator: Liu

Relax. delay 0.010 sec
Pulse 45.0 degrees
Acq. time 0.064 sec
Width 32064.1 Hz
1000 repetitions
OBSERVE B11, 160.3466912 MHz
DATA PROCESSING
Line broadening 0.5 Hz
FT size 4096
Total time 1 min 23 sec



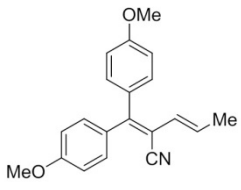
Agilent Technologies

Sample Name:

Data Collected on:
nmr18-vnmrs500
Archive directory:

Sample directory:

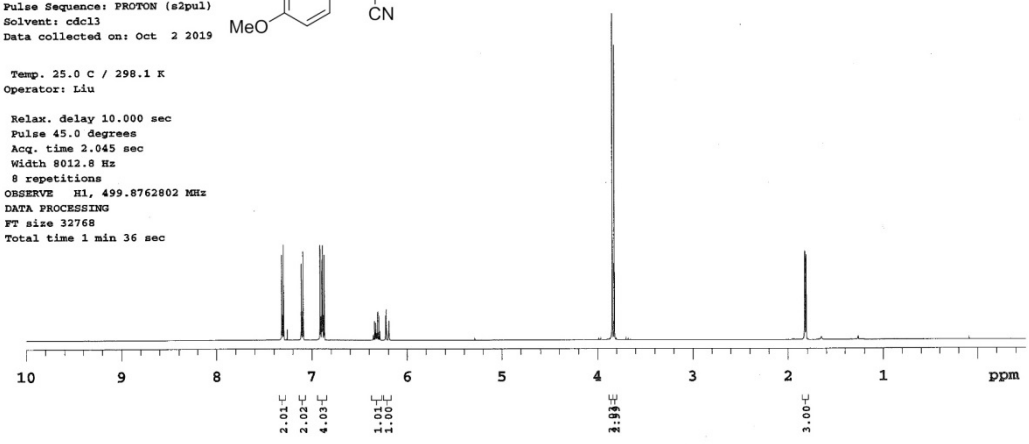
FidFile: PROTON



Pulse Sequence: PROTON (s2pul)
Solvent: cdcl3
Data collected on: Oct 2 2019

Temp. 25.0 C / 298.1 K
Operator: Liu

Relax. delay 10.000 sec
Pulse 45.0 degrees
Acq. time 2.045 sec
Width 8012.8 Hz
8 repetitions
OBSERVE H1, 499.8762802 MHz
DATA PROCESSING
FT size 32768
Total time 1 min 36 sec



Sample Name:

Data Collected on:
nmr18-vnmrs500
Archive directory:

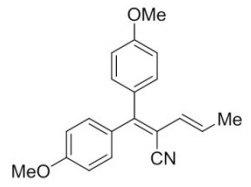
Sample directory:

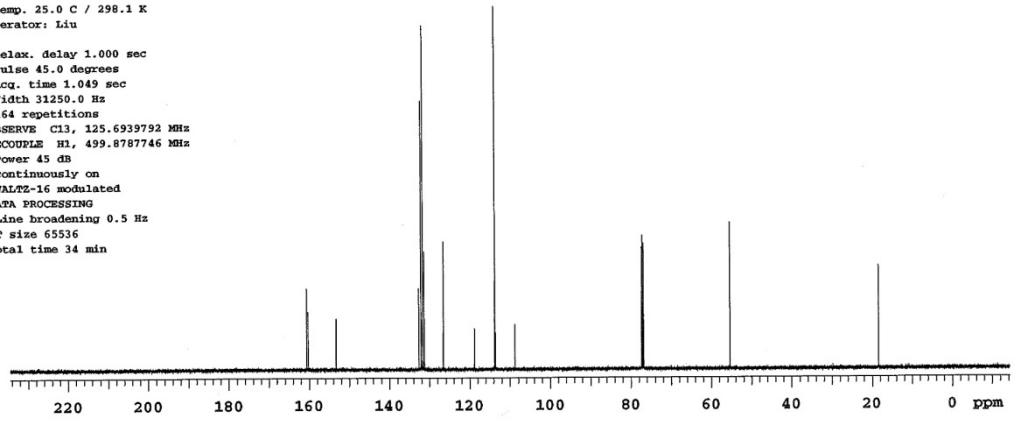
FidFile: yz-4-182C-2-pure

Pulse Sequence: CARBON (s2pul)
Solvent: cdcl3
Data collected on: Oct 2 2019

Temp. 25.0 C / 298.1 K
Operator: Liu

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.049 sec
Width 31250.0 Hz
164 repetitions
OBSERVE C13, 125.6939792 MHz
DECOUPLE H1, 499.8787746 MHz
Power 45 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 0.5 Hz
FT size 65536
Total time 34 min





Sample Name:

Data Collected on:
nmr18-vnmrs500
Archive directory:

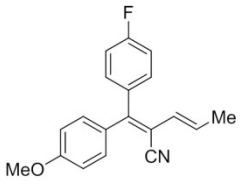
Sample directory:

FidFile: PROTON

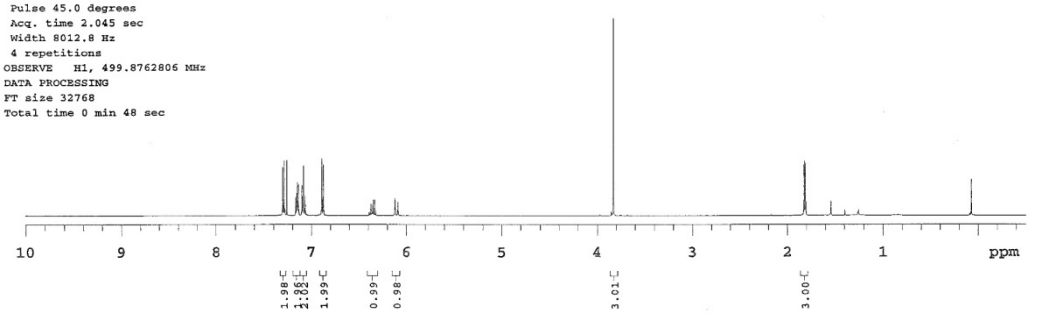
Pulse Sequence: PROTON (s2pul)
Solvent: cdcl3
Data collected on: Nov 15 2019

Temp. 25.0 C / 298.1 K
Operator: Liu

Relax. delay 10.000 sec
Pulse 45.0 degrees
Acq. time 2.045 sec
Width 8012.8 Hz
4 repetitions
OBSERVE H1, 499.8762806 MHz
DATA PROCESSING
FT size 32768
Total time 0 min 48 sec



Agilent Technologies



Sample Name:

Data Collected on:
nmr18-vnmrs500
Archive directory:

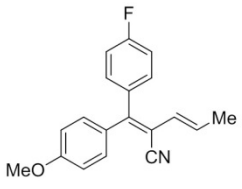
Sample directory:

FidFile: CARBON

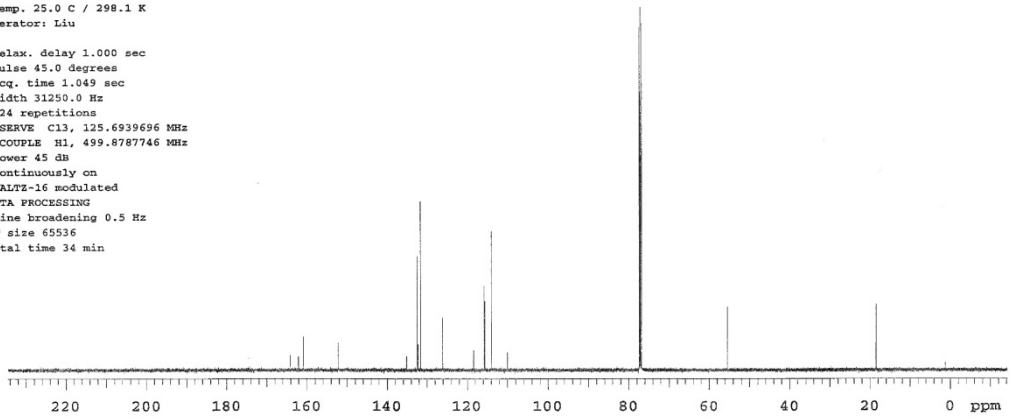
Pulse Sequence: CARBON (s2pul)
Solvent: cdcl3
Data collected on: Nov 15 2019

Temp. 25.0 C / 298.1 K
Operator: Liu

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.049 sec
Width 31250.0 Hz
824 repetitions
OBSERVE C13, 125.6939696 MHz
DECOUPLE H1, 499.8787746 MHz
Power 45 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 0.5 Hz
FT size 65536
Total time 34 min



Agilent Technologies



STANDARD FLUORINE PARAMETERS

Sample Name:

Data Collected on:
nmr18-vnmrs500
Archive directory:

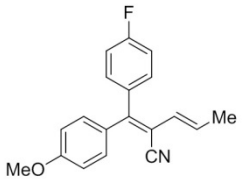
Sample directory:

FidFile: FLUORINE

Pulse Sequence: FLUORINE (s2pul)
Solvent: cdcl3
Data collected on: Nov 15 2019

Temp. 25.0 C / 298.1 K
Operator: Liu

Relax. delay 1.000 sec
Pulse 30.0 degrees
Acq. time 0.603 sec
Width 108.7 kHz
20 repetitions
OBSERVE F19, 470.3536374 MHz
DATA PROCESSING
FT size 131072
Total time 0 min 32 sec



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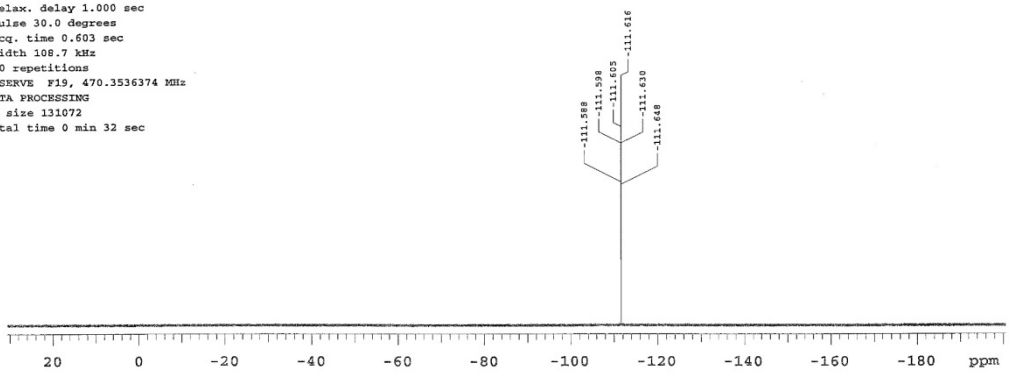


Sample Name:

Data Collected on:
nmr19-vnmrs600
Archive directory:

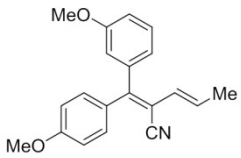
Sample directory:

FidFile: yz-4-242H-1

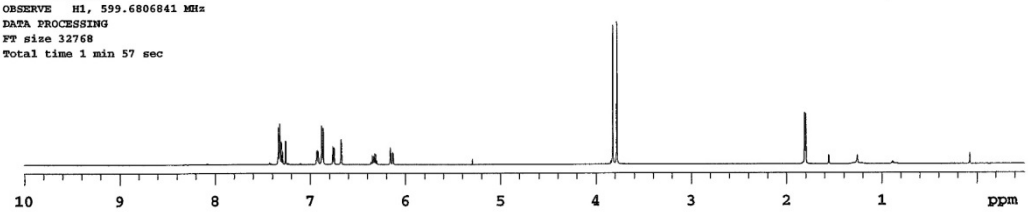
Pulse Sequence: PROTON (s2pul)
Solvent: cdcl3
Data collected on: Jan 3 2020

Temp. 25.0 C / 298.1 K
Operator: Liu

Relax. delay 10.000 sec
Pulse 45.0 degrees
Acq. time 1.704 sec
Width 9615.4 Hz
6 repetitions
OBSERVE H1, 599.6806841 MHz
DATA PROCESSING
FT size 32768
Total time 1 min 57 sec



8c



Sample Name:

Data Collected on:
nmr19-vnmrs600
Archive directory:

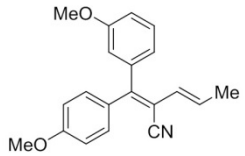
Sample directory:

FidFile: CARBON

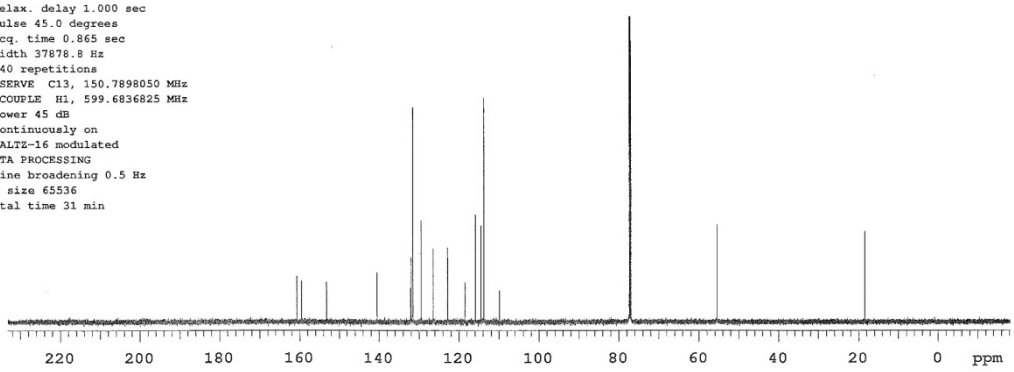
Pulse Sequence: CARBON (s2pul)
Solvent: cdcl3
Data collected on: Jan 3 2020

Temp. 25.0 C / 298.1 K
Operator: Liu

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 0.865 sec
Width 37878.8 Hz
240 repetitions
OBSERVE C13, 150.7898050 MHz
DECOUPLE H1, 599.6836825 MHz
Power 45 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 0.5 Hz
FT size 65536
Total time 31 min



8c



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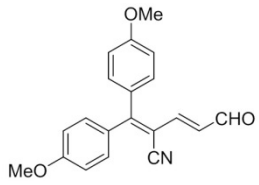
Sample Name:

Data Collected on:
nmr18-vnmrs500
Archive directory:

Sample directory:

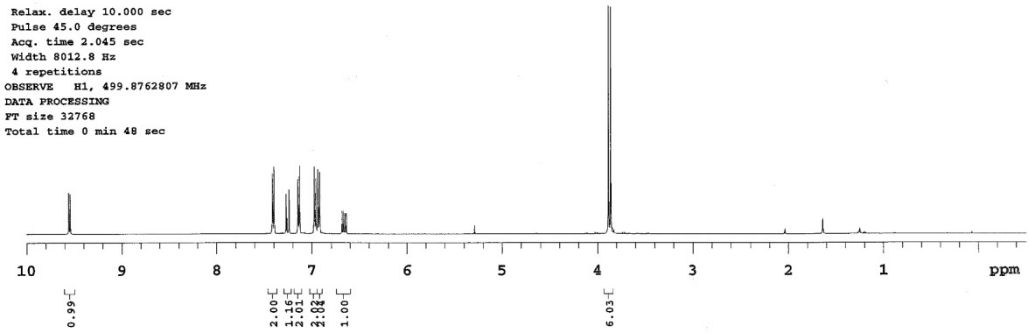
FidFile: PROTON



Pulse Sequence: PROTON (s2pul)
Solvent: cdcl3
Data collected on: Oct 4 2019

Temp. 25.0 C / 298.1 K
Operator: Liu

Relax. delay 10.000 sec
Pulse 45.0 degrees
Acq. time 2.045 sec
Width 8012.8 Hz
4 repetitions
OBSERVE H1, 499.8762807 MHz
DATA PROCESSING
FT size 32768
Total time 0 min 48 sec

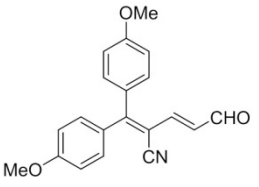


Sample Name:

Data Collected on:
nmr18-vnmrs500
Archive directory:

Sample directory:

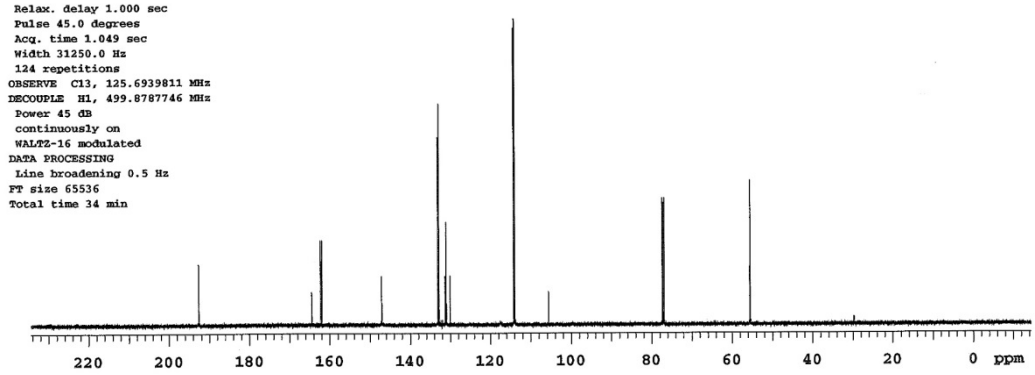
FidFile: yz-4-182C-3

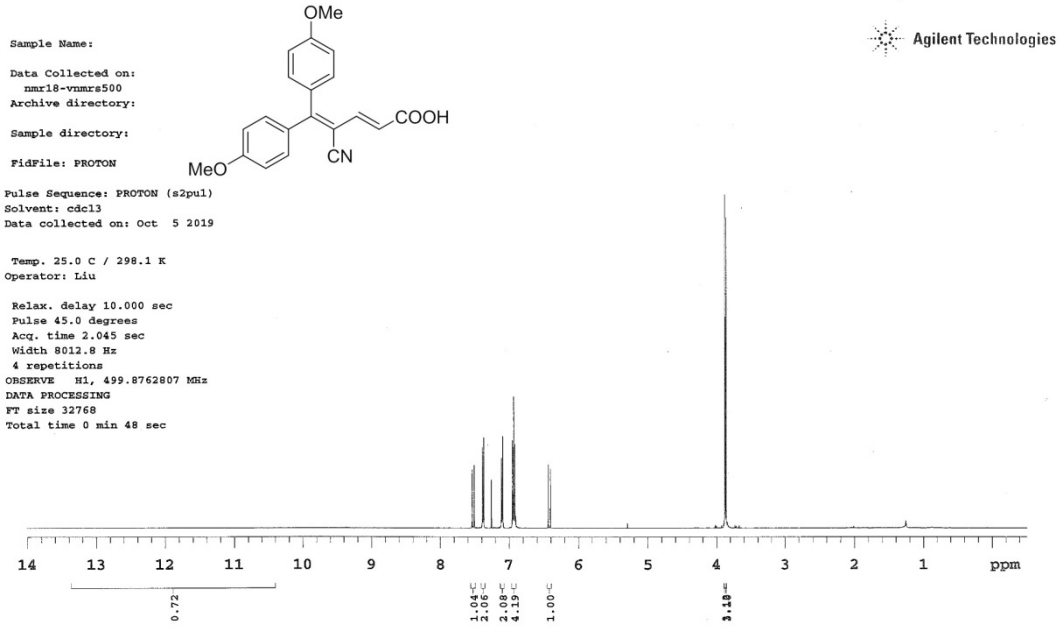


Pulse Sequence: CARBON (s2pul)
Solvent: cdcl3
Data collected on: Oct 4 2019

Temp. 25.0 C / 298.1 K
Operator: Liu

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.049 sec
Width 31250.0 Hz
124 repetitions
OBSERVE C13, 125.6939811 MHz
DECOUPLE H1, 499.8787746 MHz
Power 45 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 0.5 Hz
FT size 65536
Total time 34 min

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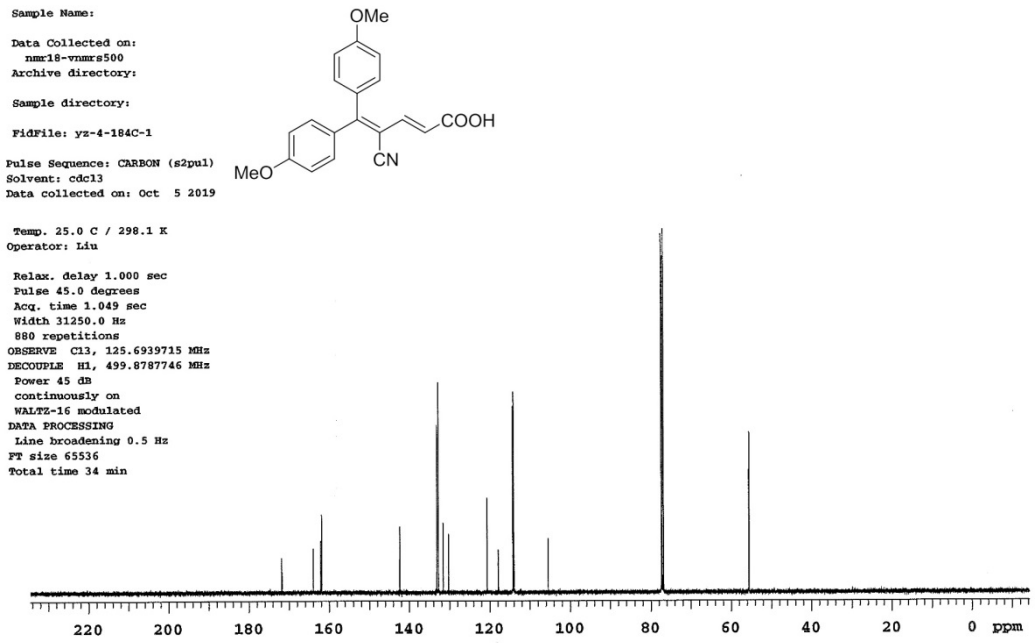
Sample Name:
Data Collected on:
nmr18-vnmrs500
Archive directory:
Sample directory:
FidFile: PROTON
OMe
COOH
CN
MeO
Pulse Sequence: PROTON (s2pul)
Solvent: cdcl3
Data collected on: Oct 5 2019
Temp. 25.0 C / 298.1 K
Operator: Liu
Relax. delay 10.000 sec
Pulse 45.0 degrees
Acq. time 2.045 sec
Width 8012.8 Hz
4 repetitions
OBSERVE H1, 499.8762807 MHz
DATA PROCESSING
FT size 32768
Total time 0 min 48 sec
14 13 12 11 10 9 8 7 6 5 4 3 2 1 ppm
0.72
1.04
2.06
2.08
4.19
1.00
3.18


Sample Name:
Data Collected on:
nmr18-vnmrs500
Archive directory:
Sample directory:
FidFile: yz-4-184C-1
OMe
COOH
CN
MeO
Pulse Sequence: CARBON (s2pul)
Solvent: cdcl3
Data collected on: Oct 5 2019
Temp. 25.0 C / 298.1 K
Operator: Liu
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.049 sec
Width 31250.0 Hz
880 repetitions
OBSERVE C13, 125.6939715 MHz
DECOUPLE H1, 499.8787746 MHz
Power 45 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 0.5 Hz
FT size 65536
Total time 34 min
220 200 180 160 140 120 100 80 60 40 20 0 ppm

Sample Name:

Data Collected on:
nmr19-vnmrs600
Archive directory:

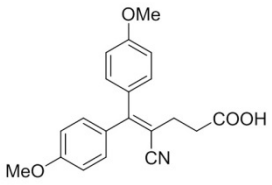
Sample directory:

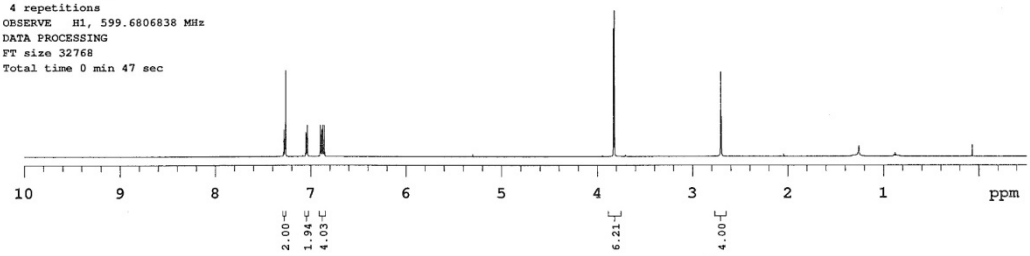
FidFile: yz-4-198-2-H

Pulse Sequence: PROTON (s2pul)
Solvent: cdcl3
Data collected on: Oct 30 2019

Temp. 25.0 C / 298.1 K
Operator: Liu

Relax. delay 10.000 sec
Pulse 45.0 degrees
Acq. time 1.704 sec
Width 9615.4 Hz
4 repetitions
OBSERVE H1, 599.6806838 MHz
DATA PROCESSING
FT size 32768
Total time 0 min 47 sec





Sample Name:

Data Collected on:
nmr19-vnmrs600
Archive directory:

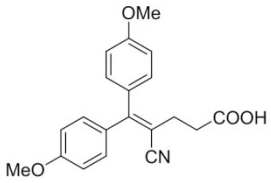
Sample directory:

FidFile: yz-198-2-C

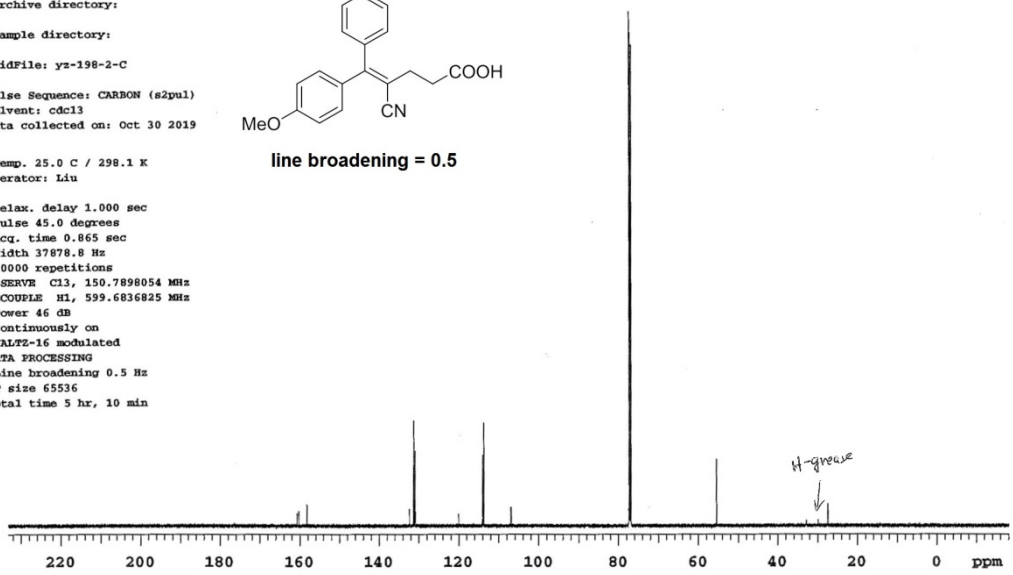
Pulse Sequence: CARBON (s2pul)
Solvent: cdcl3
Data collected on: Oct 30 2019

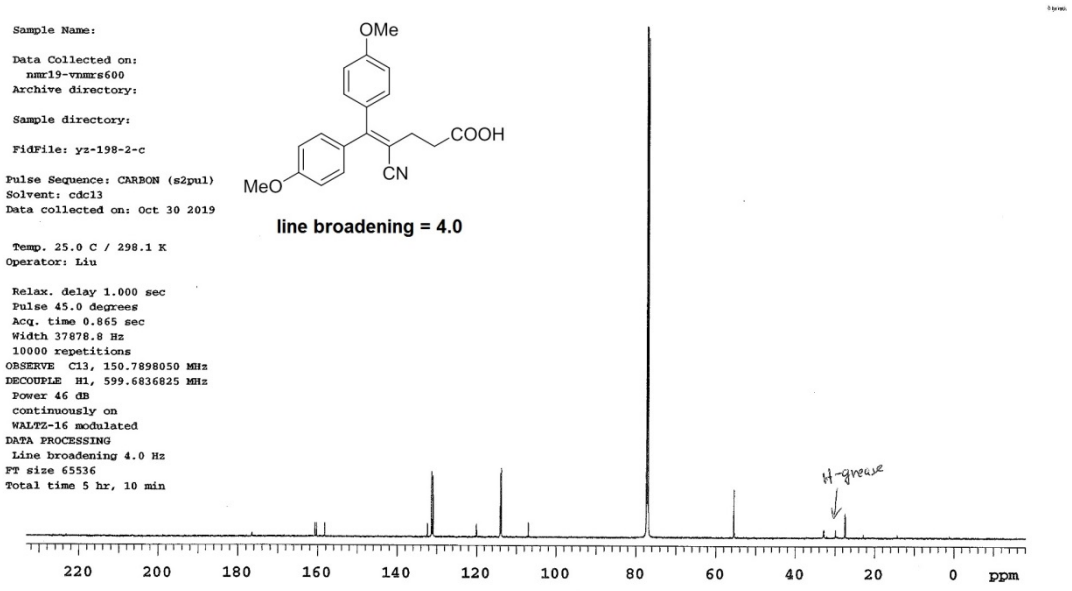
Temp. 25.0 C / 298.1 K
Operator: Liu

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 0.865 sec
Width 37878.8 Hz
10000 repetitions
OBSERVE C13, 150.7898054 MHz
DECOUPLE H1, 599.6836825 MHz
Power 46 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 0.5 Hz
FT size 65536
Total time 5 hr, 10 min



line broadening = 0.5




Sample Name:
Data Collected on:
nmr19-vnmrs600
Archive directory:
Sample directory:
FidFile: yz-198-2-c
Pulse Sequence: CARBON (s2pul)
Solvent: cdcl3
Data collected on: Oct 30 2019
Temp. 25.0 C / 298.1 K
Operator: Liu
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 0.865 sec
Width 37878.8 Hz
10000 repetitions
OBSERVE C13, 150.7898050 MHz
DECOUPLE H1, 599.6836825 MHz
Power 46 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 4.0 Hz
FT size 65536
Total time 5 hr, 10 min
OMe
COOH
CN
MeO
line broadening = 4.0
H-grease
220
200
180
160
140
120
100
80
60
40
20
0
ppm

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