Supporting Information

Nickel-Catalyzed Asymmetric Reductive Cross-Coupling of α-Chloroesters and (hetero)Aryl Iodides

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Supporting Information

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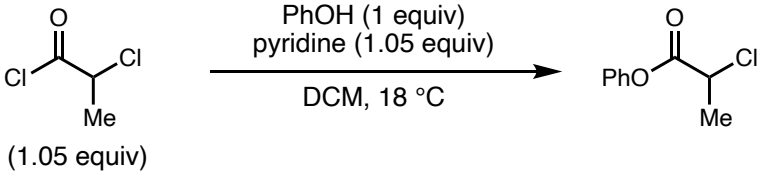
1. Materials and Methods

Unless otherwise stated, reactions were performed under a N_2 atmosphere using freshly dried solvents. Tetrahydrofuran (THF), diethyl ether (Et_2O), methylene chloride (CH_2Cl_2), toluene (PhMe), hexanes, and benzene (C_6H_6) were dried by passing through activated alumina columns under a positive pressure of argon. Triethylamine (Et_3N) and diisopropylamine (*i*-Pr_2NH) were distilled over calcium hydride prior to use. Anhydrous *N*,*N*-dimethylacetamide (DMA) was purchased from Aldrich and stored under N_2. **L1** was synthesized using the procedure reported by Reisman and coworkers.[1] Unless otherwise stated, chemicals and reagents were used as received. All reactions were monitored by thin-layer chromatography using EMD/Merck silica gel 60 F254 pre-coated plates (0.25 mm) and were visualized by UV, CAM, *p*-anisaldehyde, or $KMnO_4$ staining. Flash column chromatography was performed as described by Still et al. using silica gel (230-400 mesh, Silicycle).[2] Purified compounds were dried on a high vacuum line (0.2 torr) to remove trace solvent. Optical rotations were measured on a Jasco P-2000 polarimeter using a 100 mm path-length cell at 589 nm. ^{1}H and ^{13}C NMR spectra were recorded on a Bruker Avance III HD with Prodigy cyroprobe (at 400 MHz and 101 MHz, respectively), a Varian 400 MR (at 400 MHz and 101 MHz, respectively), or a Varian Inova 500 (at 500 MHz and 126 MHz, respectively). ^{1}H NMR spectra were also recorded on a Varian Inova 300 (at 300 MHz). NMR data is reported relative to internal $CHCl_3$ (^{1}H, δ = 7.26) and $CDCl_3$ (^{13}C, δ = 77.0) Data for ^{1}H NMR spectra are reported as follows: chemical shift (δ ppm) (multiplicity, coupling constant (Hz), integration). Multiplicity and qualifier abbreviations are as follows: s = singlet, d = doublet, t = triplet, q = quartet, m = multiplet, br = broad. IR spectra were recorded on a Perkin Elmer Paragon 1000 spectrometer and are reported in frequency of absorption (cm^{-1}). Analytical chiral SFC was performed with a Mettler SFC supercritical CO_2 analytical chromatography system (CO_2 = 1450 psi, column temperature = 40 °C) with Chiralcel AD-H, OD-H, AS-H, OB-H, and OJ-H columns (4.6 mm x 25 cm). HRMS were acquired from the Caltech Mass Spectral Facility using fast-atom bombardment (FAB), electrospray ionization (ESI-TOF), or electron impact (EI).

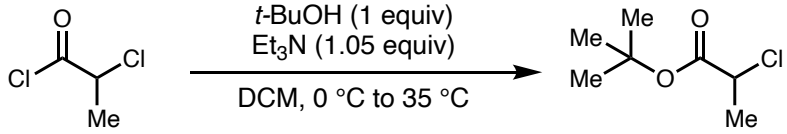
2. Substrate Preparation

phenyl 2-chloropropanoate (1a)



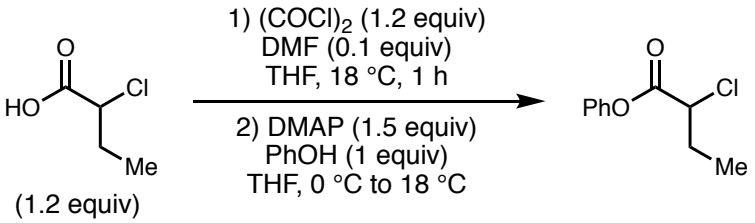
To a 250-mL oven-dried round-bottomed flask equipped with a Teflon-coated stir bar were added phenol (1.88 g, 1 equiv, 20.0 mmol) and DCM (66.7 mL). The reaction was cooled to 0 °C under nitrogen, then 2-chloropropionyl chloride (2.67 g, 1.05 equiv, 21.0 mmol) was added via syringe in a single portion. The reaction was allowed to slowly stir to room temperature while stirring for 20 hours. The reaction solution was then transferred to a separatory funnel and diluted with water and DCM. The layers were separated, then the organic layer was washed thrice with water, dried with Na_2SO_4, filtered, and concentrated under reduced pressure. The crude material was purified by flash column chromatography over silica gel, eluting with 7% Et2O/hexanes to afford **1a** as a colorless oil (3.69 g, 97% yield). Spectral data matched those reported in the literature.[3]

***tert*-butyl 2-chloropropanoate (S1)**



To a 25-mL oven-dried round-bottomed flask equipped with a Teflon-coated stir bar were added DCM (10 mL), 2-chloropropionyl chloride (1.27 g, 1 equiv, 10.0 mmol), and *tert*-butanol (741 mg, 1.0 equiv, 10.0 mmol). The reaction was cooled to 0 °C, then triethylamine (1.01 g, 1 equiv, 10.0 mmol) was added dropwise to the reaction over 2 minutes. The reaction was warmed to 35 °C. After 24 hours of stirring, the reaction was cooled to room temperature, transferred to a separatory funnel, and diluted with water and DCM. The layers were separated, and the aqueous layer was extracted twice with DCM. Combined organics were dried with $MgSO_4$, filtered, and concentrated. The crude material was purified using a silica plug, eluting with 20% Et_2O/pentane to afford **S1** as a colorless oil (905 mg, 55% yield). Spectral data matched those reported in the literature.[4]

phenyl 2-chlorobutanoate (1b)



To a 25-mL oven-dried round-bottomed flask equipped with a Teflon-coated stir bar were added THF (6.4 mL), DMF (60.9 mg, 0.1 equiv, 0.83 mmol), and 2-chlorobutylric acid (1.23 g, 1.2 equiv, 10.0 mmol), under nitrogen. Oxalyl chloride (1.27 g, 1.2 equiv, 10.0 mmol) was added dropwise via syringe to the reaction, over the course of five minutes. The reaction was allowed to stir for 1 hour at 18 °C to form the acyl chloride. To a 50-mL oven-dried round-bottomed flask equipped with a Teflon-coated stir bar were added phenol (784 mg, 1 equiv, 8.33 mmol), 4-(dimethylamino)pyridine (1.53 g, 1.5 equiv, 12.5 mmol), and THF (6.4 mL), under nitrogen. This solution was cooled to 0 °C, then the acyl chloride solution was added dropwise over 2 minutes, resulting in a slurry that was slowly warmed to 18 °C. After 20 hours of stirring, the reaction was transferred to a separatory funnel and diluted with water and Et_2O. The layers were separated, then the organic layer was washed sequentially with 1 M aqueous HCl, saturated aqueous $NaHCO_3$, and brine. The organic layer was dried with Na_2SO_4, filtered, and concentrated. The crude material was purified by flash column chromatography over silica gel, eluting with 6% Et_2O/hexanes to afford **1b** as a colorless oil (1.01 g, 61% yield).

R_f = 0.50 (silica, 8% Et_2O/hexanes, UV)

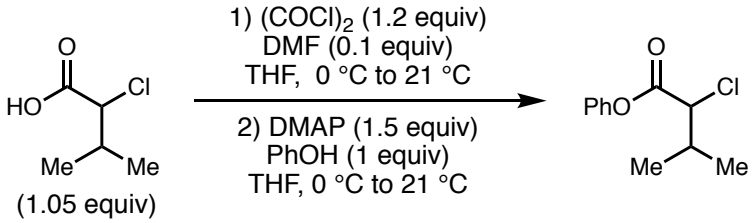
^{1}H NMR (400 MHz, $CDCl_3$): δ 7.45 – 7.36 (m, 2H), 7.30 – 7.23 (m, 1H), 7.16 – 7.10 (m, 2H), 4.46 (dd, *J* = 7.6, 6.0 Hz, 1H), 2.29 – 2.04 (m, 2H), 1.15 (t, *J* = 7.4 Hz, 3H).

^{13}C NMR (101 MHz, $CDCl_3$): δ 168.3, 150.5, 129.7, 126.4, 121.3, 58.8, 28.5, 10.7

FTIR (NaCl, thin film, cm^{-1}): 3522, 3066, 2974, 2880, 1942, 1766, 1592, 1486, 1191

HRMS (FAB, *m/z*): calc'd for $C_{10}H_{12}ClO_2$ $[M+H]^+$: 199.0526; found: 199.0508.

phenyl 2-chloro-3-methylbutanoate (1c)



To a flame-dried 100 mL round bottom flask equipped with a Teflon-coated stir bar were added 2-chloro-3-methylbutyric acid (3.52 g, 1.00 equiv, 23.2 mmol) (synthesized according to known procedure from *rac*-valine[5]) and THF (15.5 mL). The reaction mixture was cooled to 0 ºC in an ice bath. Once cool, oxalyl chloride (4.2 g, 1.4 equiv, 33.1 mmol) dropwise followed by DMF (0.18 mL, 0.1 equiv, 2.32 mmol). The reaction was allowed to stir at room temperature for 1 h. Once complete, the reaction was concentrated and the acid chloride was taken forward without further purification. To a flame-dried 200 mL round bottom flask were added phenol (2.1 g, 1.0 equiv, 22.1 mmol), 4-(dimethylamino)pyridine (4.1 g, 1.5 equiv, 33.1 mmol), and THF (20 mL). The reaction mixture was cooled to 0 ºC in an ice bath. Once cool, the acid chloride was added as a solution in 20 mL THF dropwise. Once the addition was complete, the ice bath was removed and the reaction was allowed to stir at 21 ºC overnight. After 22 h, the reaction was stopped. The reaction was diluted with 40 mL *tert*-butyl methyl ether and washed with 40 mL 1.0 M aq HCl, 40 mL 5% aq $NaHCO_3$, and 40 mL brine. The organic layer was dried over sodium sulfate, filtered, and concentrated. The crude material was purified by flash column chromatography over silica gel, eluting with a gradient of 20 to 50% toluene/hexanes to afford **1c** as a colorless oil (891 mg g, 19% yield).

R_f = 0.25 (silica, 30% toluene/hexanes, UV)

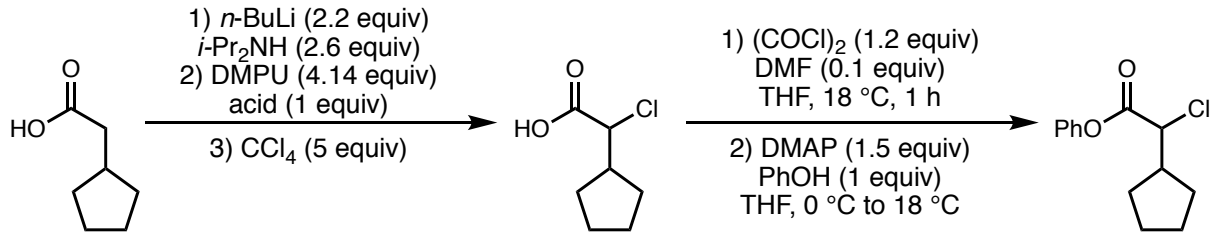
^{1}H NMR (400 MHz, $CDCl_3$): δ 7.39 – 7.27 (m, 2H), 7.23 – 7.14 (m, 1H), 7.08 – 7.00 (m, 2H), 4.26 (d, J = 6.7 Hz, 1H), 2.39 (dp, J = 13.3, 6.7 Hz, 1H), 1.09 (d, J = 6.7 Hz, 7H).

^{13}C NMR (101 MHz, $CDCl_3$): δ 168.1, 150.5, 129.7, 126.4, 121.3, 64.1, 33.0, 19.8, 18.4.

FTIR (NaCl, thin film, cm^{-1}): 3064, 2967, 2936, 2876, 1770, 1593, 1494, 1297, 1232, 1194, 1138, 1079, 927, 726, 688.

HRMS (FAB, *m/z*): calc'd for $C_{11}H_{13}ClO_2$ $[M+H]^+$: 213.0682; found: 213.0692.

phenyl 2-chloro-2-cyclopentylacetate (1d)



To a 200-mL oven-dried round-bottomed flask equipped with a Teflon-coated stir bar were added diisopropylamine (2.63 g, 2.6 equiv, 26.0 mmol) and THF (20 mL). The reaction was cooled to -20 °C in a dry ice/acetone bath, then *n*-butyllithium (2.5 M in hexane, 8.80 mL, 2.2 equiv, 22.0 mmol) was added to the solution dropwise via syringe over 5 minutes. The reaction was stirred at -20 °C for 30 minutes. DMPU (5.31 g, 4.14 equiv, 41.4 mmol) was added to the reaction, followed by 2-cyclopentylacetic acid (1.28 g, 1.0 equiv, 10.0 mmol). The resulting yellow solution was stirred at -20 °C for 2 hours, then cooled to -78 °C. Carbon tetrachloride (7.69 g, 5.0 equiv, 50.0 mmol) was dissolved in THF (20 mL) and the resulting solution was added to the reaction in a single portion via syringe, resulting in an immediate color change to black. The reaction was stirred for 1 hour at -78 °C, then warmed to room temperature. A solution of sodium chloride (4.00 g, 6.84 equiv, 68.4 mmol) in HCl (2 M in water, 26.0 mL, 5.2 equiv, 52.0 mmol) was added to the reaction dropwise over 5 minutes via syringe. The reaction was transferred to a separatory funnel and diluted with water and Et_2O. The layers were separated, and the aqueous layer extracted thrice with Et_2O. The combined organics were dried with Na_2SO_4, filtered, and concentrated. The crude material was purified by flash column chromatography over silica gel, eluting with 50:50:0.1 hexanes/EtOAc/TFA. All fractions staining with bromocresol green were collected together and concentrated, resulting in a brown oil. This oil was added to a separatory funnel and diluted with EtOAc and half-saturated aqueous Na_2CO_3. The layers were separated and the aqueous layer was washed twice with EtOAc. The aqueous layer was acidified to pH=2 with 2 M HCl, then extracted thrice with EtOAc. These final three organic extractions were combined, dried with Na_2SO_4, filtered, and concentrated to afford 1.51 pale yellow oil, which was not fully-pure by TLC or NMR, but was carried forward as-is without further purification (the impurities proved much easier to remove after esterification).

To a 10-mL oven-dried round-bottomed flask equipped with a Teflon-coated stir bar were added THF (2.0 mL), DMF (18.3 mg, 0.1 equiv, 0.25 mmol), and the impure 2-chloro-2-cyclopentylacetic acid (488 mg, 3.00 mmol if pure), under nitrogen. Oxalyl chloride (381 mg, 1.2 equiv, 3.00 mmol) was added dropwise via syringe to the reaction, over the course of five minutes. The reaction was allowed to stir for 1 hour at 18 °C to form the acyl chloride. To a 25-mL oven-dried round-bottomed flask equipped with a Teflon-coated stir bar were added phenol (235 mg, 1 equiv, 2.5 mmol), 4-(dimethylamino)pyridine (458

mg, 1.5 equiv, 3.75 mmol), and THF (2.0 mL), under nitrogen. This solution was cooled to 0 °C, then the acyl chloride solution was added dropwise over 2 minutes, resulting in a slurry that was slowly warmed to 18 °C. After 20 hours of stirring, the reaction was transferred to a separatory funnel and diluted with water and Et_2O. The layers were separated, then the organic layer was washed sequentially with 1 M aqueous HCl, saturated aqueous $NaHCO_3$, and brine. The organic layer was dried with Na_2SO_4, filtered, and concentrated. The crude material was purified by flash column chromatography over silica gel, eluting with 2.2% Et_2O/hexanes to afford **1d** as a colorless oil (106 mg, 18% yield).

R_f = 0.48 (silica, 8% Et_2O/hexanes, UV)

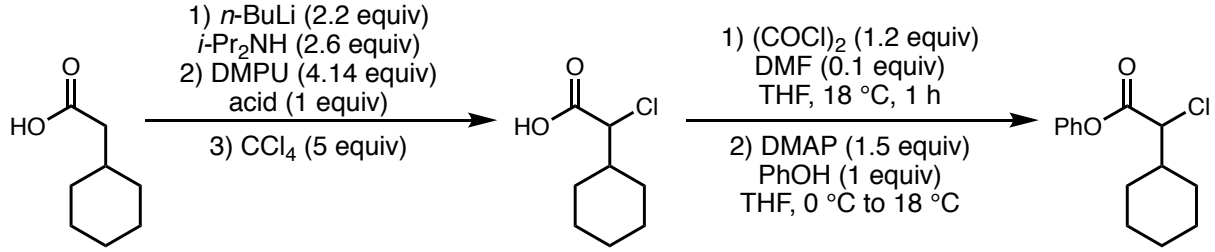
^{1}H NMR (400 MHz, $CDCl_3$): δ 7.44 – 7.36 (m, 2H), 7.30 – 7.23 (m, 1H), 7.15 – 7.09 (m, 2H), 4.35 (d, *J* = 8.6 Hz, 1H), 2.72 – 2.58 (m, 1H), 2.08 – 1.83 (m, 2H), 1.82 – 1.40 (m, 6H).

^{13}C NMR (101 MHz, $CDCl_3$): δ 168.3, 150.5, 129.7, 126.4, 121.3, 61.8, 44.0, 30.1, 30.0, 26.0, 25.4.

FTIR (NaCl, thin film, cm^{-1}): 3044, 2958, 2870, 1769, 1593, 1493, 1162, 1132

HRMS (FAB, *m/z*): calc'd for $C_{13}H_{16}ClO$ $[M+H]^+$: 239.0839 ; found: 239.0832.

phenyl 2-chloro-2-cyclohexylacetate (1e)



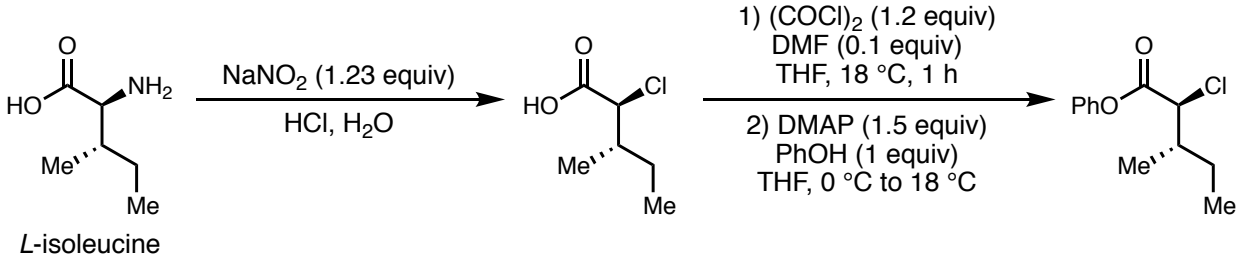
To a 200-mL oven-dried round-bottomed flask equipped with a Teflon-coated stir bar were added diisopropylamine (2.63 g, 2.6 equiv, 26.0 mmol) and THF (20 mL). The reaction was cooled to -20 °C in a dry ice/acetone bath, then *n*-butyllithium (2.5 M in hexane, 8.80 mL, 2.2 equiv, 22.0 mmol) was added to the solution dropwise via syringe over 5 minutes. The reaction was stirred at -20 °C for 30 minutes. DMPU (5.31 g, 4.14 equiv, 41.4 mmol) was added to the reaction, followed by 2-cyclohexyllacetic acid (1.42 g, 1.0 equiv, 10.0 mmol). The resulting yellow solution was stirred at -20 °C for 2 hours, then cooled to -78 °C. Carbon tetrachloride (7.69 g, 5.0 equiv, 50.0 mmol) was dissolved in THF (20 mL) and the resulting solution was added to the reaction in a single portion via syringe, resulting in an immediate color change to black. The reaction was stirred for 1 hour at -78 °C, then warmed to room temperature. A solution of sodium chloride (4.00 g, 6.84 equiv, 68.4 mmol) in HCl (2 M in water, 26.0 mL, 5.2 equiv, 52.0 mmol) was added to the reaction dropwise over 5 minutes via syringe. The reaction was transferred to a separatory funnel and diluted with water and Et_2O. The layers were separated, and the aqueous layer

extracted thrice with Et_2O. The combined organics were dried with Na_2SO_4, filtered, and concentrated. The crude material was purified by flash column chromatography over silica gel, eluting with 50:50:0.1 hexanes/EtOAc/TFA. All fractions staining with bromocresol green were collected together and concentrated, resulting in a brown oil. This oil was added to a separatory funnel and diluted with EtOAc and half-saturated aqueous Na_2CO_3. The layers were separated and the aqueous layer was washed twice with EtOAc. The aqueous layer was acidified to pH=2 with 2 M HCl, then extracted thrice with EtOAc. These final three organic extractions were combined, dried with Na_2SO_4, filtered, and concentrated to afford 1.42 g pale yellow amorphous solid, which was not fully-pure by TLC or NMR, but was carried forward as-is without further purification (the impurities proved much easier to remove after esterification).

To a 10-mL oven-dried round-bottomed flask equipped with a Teflon-coated stir bar were added THF (3.2 mL), DMF (30.5 mg, 0.1 equiv, 0.42 mmol), and the impure 2-chloro-2-cyclohexylacetic acid (883 mg, 5.00 mmol if pure), under nitrogen. Oxalyl chloride (635 mg, 1.2 equiv, 5.00 mmol) was added dropwise via syringe to the reaction, over the course of five minutes. The reaction was allowed to stir for 1 hour at 18 °C to form the acyl chloride. To a 25-mL oven-dried round-bottomed flask equipped with a Teflon-coated stir bar were added phenol (392 mg, 1 equiv, 4.17 mmol), 4-(dimethylamino)pyridine (764 mg, 1.5 equiv, 6.25 mmol), and THF (3.2 mL), under nitrogen. This solution was cooled to 0 °C, then the acyl chloride solution was added dropwise over 2 minutes, resulting in a slurry that was slowly warmed to 18 °C. After 20 hours of stirring, the reaction was transferred to a separatory funnel and diluted with water and Et_2O. The layers were separated, then the organic layer was washed sequentially with 1 M aqueous HCl, saturated aqueous $NaHCO_3$, and brine. The organic layer was dried with Na_2SO_4, filtered, and concentrated. The crude material was purified by flash column chromatography over silica gel, eluting with 6% Et_2O/hexanes to afford **1e** as a colorless oil (488 mg, 46% yield).

R_f = 0.52 (silica, 8% Et_2O/hexanes, UV)
^{1}H NMR (400 MHz, $CDCl_3$): δ 7.44 – 7.37 (m, 2H), 7.30 – 7.23 (m, 1H), 7.15 – 7.09 (m, 2H), 4.29 (d, *J* = 7.4 Hz, 1H), 2.16 – 2.01 (m, 2H), 1.89 – 1.66 (m, 4H), 1.40 – 1.13 (m, 5H).
^{13}C NMR (101 MHz, $CDCl_3$): δ 168.1, 150.5, 129.7, 126.4, 121.4, 63.0, 42.0, 30.1, 28.9, 26.0, 25.9, 25.7.
FTIR (NaCl, thin film, cm^{-1}): 2930, 2854, 1769, 1492, 1450, 1233, 1193, 1163, 1143
HRMS (FAB, *m/z*): calc'd for $C_{14}H_{18}ClO$ $[M+H]^+$: 253.0995 ; found: 253.0988.

phenyl (2*S*,3*S*)-2-chloro-3-methylpentanoate (1f)



L-isoleucine

L-isoleucine was converted to the corresponding α-chloroacid in 12:1 dr using the procedure reported by Bercaw and coworkers. Spectral data matched those reported.[6]

To a 25-mL oven-dried round-bottomed flask equipped with a Teflon-coated stir bar were added THF (4.3 mL), DMF (40.4 mg, 0.1 equiv, 0.55 mmol), and (2*S*,3*S*)-2-chloro-3-methylpentanoic acid (1.00 g, 1.2 equiv, 6.64 mmol), under nitrogen. Oxalyl chloride (843 mg, 1.2 equiv, 6.64 mmol) was added dropwise via syringe to the reaction, over the course of five minutes. The reaction was allowed to stir for 1 hour at 18 °C to form the acyl chloride. To a 50-mL oven-dried round-bottomed flask equipped with a Teflon-coated stir bar were added phenol (521 mg, 1 equiv, 5.53 mmol), 4-(dimethylamino)pyridine (1.01 g, 1.5 equiv, 8.30 mmol), and THF (4.3 mL), under nitrogen. This solution was cooled to 0 °C, then the acyl chloride solution was added dropwise over 2 minutes, resulting in a slurry that was slowly warmed to 18 °C. After 20 hours of stirring, the reaction was transferred to a separatory funnel and diluted with water and Et_2O. The layers were separated, then the organic layer was washed sequentially with 1 M aqueous HCl, saturated aqueous $NaHCO_3$, and brine. The organic layer was dried with Na_2SO_4, filtered, and concentrated. The crude material was purified by flash column chromatography over silica gel, eluting with 4% Et_2O/hexanes to afford **1f** as a colorless oil (679 mg, 54% yield, >20:1 dr).

R_f = 0.54 (silica, 8% EtOAc/hexanes, UV)

$[\alpha]_D^{21}$ = 2° (c = 1.0, $CHCl_3$).

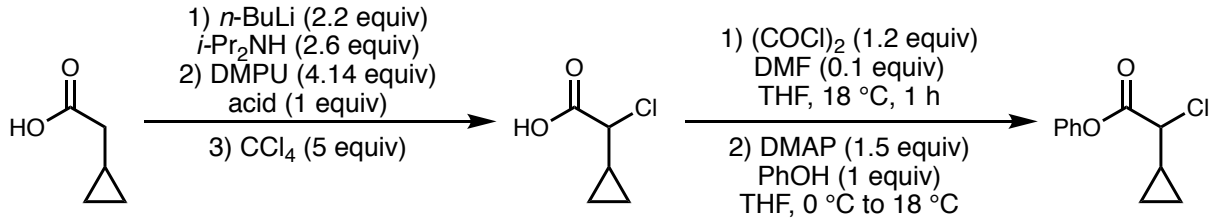
^{1}H NMR (400 MHz, $CDCl_3$): δ 7.49 – 7.35 (m, 2H), 7.31 – 7.21 (m, 1H), 7.17 – 7.08 (m, 2H), 4.38 (d, *J* = 7.1 Hz, 1H), 2.32 – 2.14 (m, 1H), 1.84 – 1.70 (m, 1H), 1.50 – 1.35 (m, 1H), 1.14 (d, *J* = 6.8 Hz, 3H), 0.99 (t, *J* = 7.5 Hz, 3H).

^{13}C NMR (101 MHz, $CDCl_3$): δ 168.1, 150.6, 129.7, 126.4, 121.3, 62.8, 39.2, 25.3, 16.1, 11.0.

FTIR (NaCl, thin film, cm^{-1}): 2926, 2852, 1755, 1492, 1196, 1140, 1107

HRMS (FAB, *m/z*): calc'd for $C_{21}H_{25}O_2$ $[M+H]^+$: 227.0839 ; found: 227.0848.

phenyl 2-chloro-2-cyclopropylacetate (11)

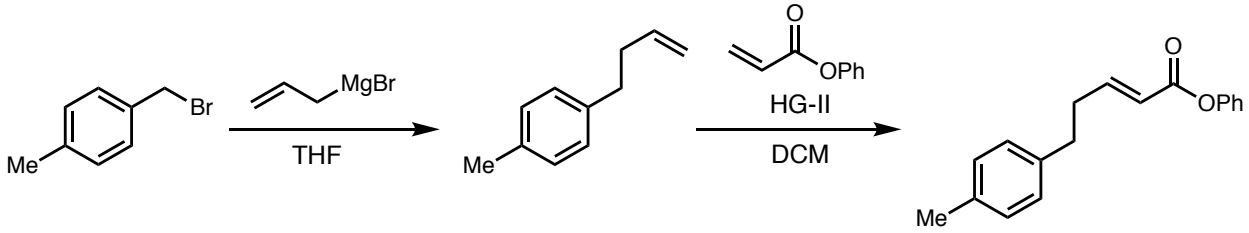


To a 200-mL oven-dried round-bottomed flask equipped with a Teflon-coated stir bar were added diisopropylamine (2.63 g, 2.6 equiv, 26.0 mmol) and THF (20 mL). The reaction was cooled to -20 °C in a dry ice/acetone bath, then *n*-butyllithium (2.5 M in hexane, 8.80 mL, 2.2 equiv, 22.0 mmol) was added to the solution dropwise via syringe over 5 minutes. The reaction was stirred at -20 °C for 30 minutes. DMPU (5.31 g, 4.14 equiv, 41.4 mmol) was added to the reaction, followed by 2-cyclopropyllacetic acid (1.00 g, 1.0 equiv, 10.0 mmol). The resulting yellow solution was stirred at -20 °C for 2 hours, then cooled to -78 °C. Carbon tetrachloride (7.69 g, 5.0 equiv, 50.0 mmol) was dissolved in THF (20 mL) and the resulting solution was added to the reaction in a single portion via syringe, resulting in an immediate color change to black. The reaction was stirred for 1 hour at -78 °C, then warmed to room temperature. A solution of sodium chloride (4.00 g, 6.84 equiv, 68.4 mmol) in HCl (2 M in water, 26.0 mL, 5.2 equiv, 52.0 mmol) was added to the reaction dropwise over 5 minutes via syringe. The reaction was transferred to a separatory funnel and diluted with water and Et_2O. The layers were separated, and the aqueous layer extracted thrice with Et_2O. The combined organics were dried with Na_2SO_4, filtered, and concentrated. The crude material was purified by flash column chromatography over silica gel, eluting with 50:50:0.1 hexanes/EtOAc/TFA. All fractions staining with bromocresol green were collected together and concentrated, resulting in a brown oil. This oil was added to a separatory funnel and diluted with EtOAc and half-saturated aqueous Na_2CO_3. The layers were separated and the aqueous layer was washed twice with EtOAc. The aqueous layer was acidified to pH=2 with 2 M HCl, then extracted thrice with EtOAc. These final three organic extractions were combined, dried with Na_2SO_4, filtered, and concentrated to afford 1.97 g pale yellow oil, which was not fully-pure by TLC or NMR (56 wt. % EtOAc, other small impurities), but was carried forward as-is without further purification (the impurities proved much easier to remove after esterification).

To a 10-mL oven-dried round-bottomed flask equipped with a Teflon-coated stir bar were added THF (2.6 mL), DMF (24.4 mg, 0.1 equiv, 0.33 mmol), and the impure 2-chloro-2-cyclopropylacetic acid (1.22 g, 44% pure), under nitrogen. Oxalyl chloride (508 mg, 1.2 equiv, 4.00 mmol) was added dropwise via syringe to the reaction, over the course of five minutes. The reaction was allowed to stir for 1 hour at 18 °C to form the acyl chloride. To a 25-mL oven-dried round-bottomed flask equipped with a Teflon-coated

stir bar were added phenol (314 mg, 1 equiv, 3.33 mmol), 4-(dimethylamino)pyridine (611 mg, 1.5 equiv, 5.00 mmol), and THF (2.6 mL), under nitrogen. This solution was cooled to 0 °C, then the acyl chloride solution was added dropwise over 2 minutes, resulting in a slurry that was slowly warmed to 18 °C. After 20 hours of stirring, the reaction was transferred to a separatory funnel and diluted with water and Et_2O. The layers were separated, then the organic layer was washed sequentially with 1 M aqueous HCl, saturated aqueous $NaHCO_3$, and brine. The organic layer was dried with Na_2SO_4, filtered, and concentrated. The crude material was purified by flash column chromatography over silica gel, eluting with 2.4% Et_2O/hexanes to afford **11** as a colorless oil (195.1 mg, 28% yield).

phenyl (*E*)-5-(*p*-tolyl)pent-2-enoate (12)



1-(bromomethyl)-4-methylbenzenewas converted to 1-(but-3-en-1-yl)-4-methylbenzene using the procedure reported by Wang and coworkers. Spectral data matched those reported.[7]

Olefin metathesis was carried out following the procedure of Matsubara.[8] In a nitrogen-filled glovebox, to a 2-dram oven-dried vial equipped with a Teflon-coated stir bar was added Hoveyda-Grubbs second generation catalyst (10.7 mg, 0.1 equiv, 0.0171 mmol, followed by anhydrous CH_2Cl_2 (3.42 mL, 0.1 M). Phenyl acrylate (101 mg, 5.0 equiv, 0.684 mmol) was added to the vial, followed by 1-(but-3-en-1-yl)-4-methylbenzene (50.0 mg, 1 equiv, 0.342 mmol). The reaction was sealed with a rubber septum, removed from the glovebox, and stirred under nitrogen at 18 °C for 18 hours. The reaction was filtered through a short plug of silica, eluting with CH_2Cl_2, then concentrated. NMR analysis of the crude material showed a 4:1 ratio of phenyl acrylate to desired product. An aliquot (~5%) of the crude reaction was purified by preparative TLC (10% Et2O/hexanes) to afford **12** as a colorless oil (1.4 mg, 1.5% yield).

$\mathbf{R_f}$ = 0.38 (silica, 10% Et_2O/hexanes, UV)

^{1}H NMR (400 MHz, $CDCl_3$): δ 7.43 – 7.35 (m, 1H), 7.25 – 7.16 (m, 1H), 7.16 – 7.07 (m, 3H), 6.05 (dt, *J* = 15.7, 1.6 Hz, 0H), 2.87 – 2.75 (m, 1H), 2.67 – 2.53 (m, 1H), 2.33 (s, 2H).

^{13}C NMR (101 MHz, $CDCl_3$): δ 165.05, 150.88, 150.75, 137.70, 135.91, 129.53, 129.37, 128.36, 125.84, 121.77, 121.20, 34.39, 33.96, 21.17.

FTIR (NaCl, thin film, cm^{-1}): 2920, 1854, 1732, 1651, 1594, 1494, 1245, 1024, 810.

HRMS (FAB, *m/z*): calc'd for $C_{18}H_{19}O_2$ $[M+H]^+$: 267.1385 ; found: 267.1398.

R_f = 0.41 (silica, 8%% Et_2O/hexanes, UV)

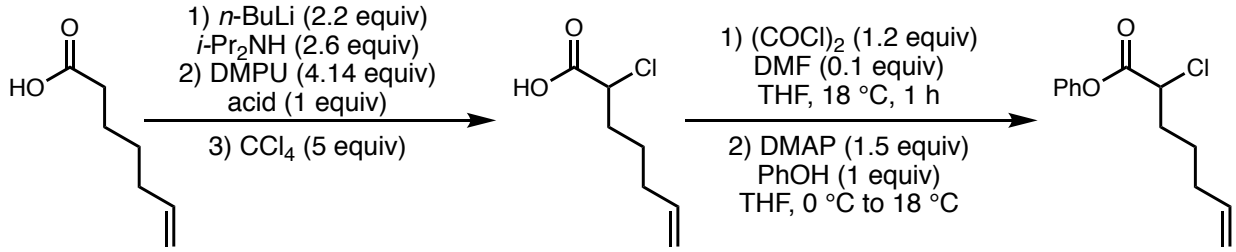
^{1}H NMR (400 MHz, $CDCl_3$): δ 7.45 – 7.37 (m, 2H), 7.30 – 7.24 (m, 1H), 7.18 – 7.12 (m, 2H), 3.86 (d, *J* = 9.7 Hz, 1H), 1.60 (dtt, *J* = 9.6, 8.1, 4.8 Hz, 1H), 0.92 – 0.80 (m, 2H), 0.71 – 0.64 (m, 1H), 0.62 – 0.55 (m, 1H).

^{13}C NMR (101 MHz, $CDCl_3$): δ 167.7, 150.6, 129.7, 126.5, 121.3, 62.4, 15.8, 6.2, 5.4.

FTIR (NaCl, thin film, cm^{-1}): 2987, 1770, 1492, 1302, 1243, 1194, 1162, 1025, 680.

HRMS (FAB, *m/z*): calc'd for $C_{11}H_{12}ClO_2$ $[M+H]^+$: 211.0526; found: 211.0529.

phenyl 2-chlorohept-6-enoate (S3)



To a 500-mL oven-dried round-bottomed flask equipped with a Teflon-coated stir bar were added diisopropylamine (9.61 g, 2.6 equiv, 94.9 mmol) and THF (73 mL). The reaction was cooled to -20 °C in a dry ice/acetone bath, then *n*-butyllithium (2.5 M in hexane, 32.1 mL, 2.2 equiv, 80.3 mmol) was added to the solution dropwise via syringe over 5 minutes. The reaction was stirred at -20 °C for 30 minutes. DMPU (19.4 g, 4.14 equiv, 151 mmol) was added to the reaction, followed by hept-6-enoic acid (4.68 g, 1.0 equiv, 36.5 mmol). The resulting yellow solution was stirred at -20 °C for 2 hours, then cooled to -78 °C. Carbon tetrachloride (28.1 g, 5.0 equiv, 183 mmol) was dissolved in THF (73 mL) and the resulting solution was added to the reaction in a single portion via syringe, resulting in an immediate color change to black. The reaction was stirred for 1 hour at -78 °C, then warmed to room temperature.

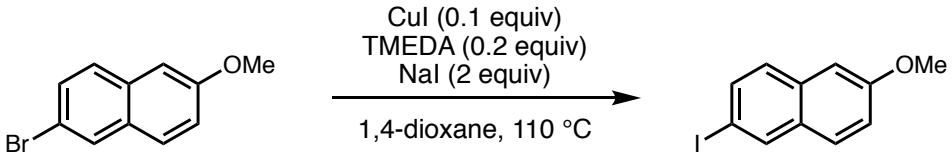
A solution of sodium chloride (14.6 g, 6.84 equiv, 250 mmol) in HCl (2 M in water, 95 mL, 5.2 equiv, 190 mmol) was added to the reaction dropwise over 5 minutes via syringe. The reaction was transferred to a separatory funnel and diluted with water and Et_2O. The layers were separated, and the aqueous layer extracted thrice with Et_2O. The combined organics were dried with Na_2SO_4, filtered, and concentrated. The crude material was purified by flash column chromatography over silica gel, eluting with 50:50:0.1 hexanes/EtOAc/TFA. All fractions staining with bromocresol green were collected together and concentrated, resulting in a brown oil. This oil was added to a separatory funnel and diluted with EtOAc and half-saturated aqueous Na_2CO_3. The layers were separated and the aqueous layer was washed twice with EtOAc. The aqueous layer was acidified to pH=2 with 2 M HCl, then extracted thrice with EtOAc.

These final three organic extractions were combined, dried with Na_2SO_4, filtered, and concentrated to afford 5.54 g pale yellow oil, which was not fully-pure by TLC or NMR (16 wt. % EtOAc, other small impurities), but was carried forward as-is without further purification (the impurities proved much easier to remove after esterification).

To a 25-mL oven-dried round-bottomed flask equipped with a Teflon-coated stir bar were added THF (7.9 mL), DMF (74.9 mg, 0.1 equiv, 1.02 mmol), and the impure 2-chlorohept-6-enoic acid (2.38 g, 84% pure), under nitrogen. Oxalyl chloride (1.56 mg, 1.2 equiv, 12.3 mmol) was added dropwise via syringe to the reaction, over the course of five minutes. The reaction was allowed to stir for 1 hour at 18 °C to form the acyl chloride. To a 50-mL oven-dried round-bottomed flask equipped with a Teflon-coated stir bar were added phenol (965 mg, 1 equiv, 10.2 mmol), 4-(dimethylamino)pyridine (1.88 g, 1.5 equiv, 15.4 mmol), and THF (7.9 mL), under nitrogen. This solution was cooled to 0 °C, then the acyl chloride solution was added dropwise over 2 minutes, resulting in a slurry that was slowly warmed to 18 °C. After 20 hours of stirring, the reaction was transferred to a separatory funnel and diluted with water and Et_2O. The layers were separated, then the organic layer was washed sequentially with 1 M aqueous HCl, saturated aqueous $NaHCO_3$, and brine. The organic layer was dried with Na_2SO_4, filtered, and concentrated. The crude material was purified by flash column chromatography over silica gel, eluting with 3% Et_2O/hexanes to afford **S3** as a colorless oil (1.03 g, 42% yield).

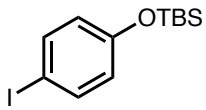
R_f = 0.52 (silica, 8%% Et_2O/hexanes, UV)
^{1}H NMR (400 MHz, $CDCl_3$): δ 7.46 – 7.36 (m, 2H), 7.30 – 7.23 (m, 1H), 7.16 – 7.09 (m, 2H), 5.90 – 5.74 (m, 1H), 5.13 – 4.98 (m, 2H), 4.51 (dd, *J* = 7.9, 6.2 Hz, 1H), 2.26 – 2.02 (m, 4H), 1.79 – 1.55 (m, 2H).
^{13}C NMR (101 MHz, $CDCl_3$): δ 168.3, 150.5, 137.7, 129.7, 126.5, 121.3, 115.6, 57.2, 34.3, 33.0, 25.3.
FTIR (NaCl, thin film, cm^{-1}): 3076, 2931, 1768, 1593, 1494, 1243, 1192, 1164, 917, 688.
HRMS (FAB, *m/z*): calc'd for $C_{13}H_{16}ClO_2$ $[M+H]^+$: 239.0839; found: 239.0842.

2-iodo-6-methoxynaphthalene (7)



In a nitrogen-filled glovebox, to an oven-dried 150-mL pressure flask equipped with a Teflon-coated stir bar were added 2-bromo-6-methoxynaphthalene (3.56 g, 1.0 equiv, 15.0 mmol), copper(I) iodide (286 mg, 0.10 equiv, 1.50 mmol), and sodium iodide (4.50 g, 2.0 equiv, 30.0 mmol). 1,4-dioxane (37.5 mL) was added to flask, followed by *N*,*N*,*N'*,*N'*-tetramethylethylenediamine (264 mg, 0.20 equiv, 3.00 mmol). The pressure flask was sealed and removed from the glovebox, then heated to 110 °C for 17 hours. The reaction was cooled to room temperature, then filtered over a plug of Celite, eluting with DCM. The resulting filtrate was concentrated to afford **7** (4.12 g, 97% yield) as a colorless amorphous solid. Spectral data matched those reported.[9]

***tert*-butyl(4-iodophenoxy)dimethylsilane (2k)**



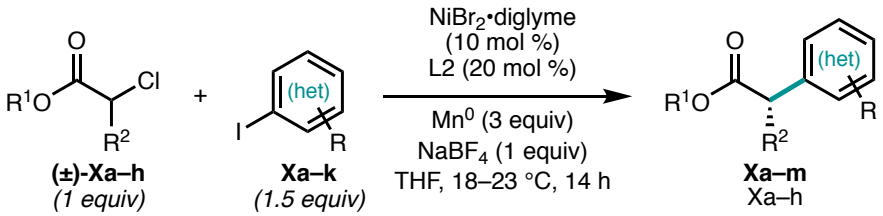
Prepared as previously described from 4-iodophenol (660 mg, 1.0 equiv, 3.0 mmol), *tert*-butyldimethylsilyl chloride (0.74 mL, 1.4 equiv, 4.3 mmol), triethylamine (0.5 mL, 1.2 equiv, 3.6 mmol), and DCM (6.8 mL, 0.44 M). The crude residue was purified by filtration over a silica plug with hexanes to yield **2k** (897 mg, 89% yield) as a colorless oil. Spectral data matched those reported in the literature.[10]

^{1}H NMR (400 MHz, $CDCl_3$): δ 7.53 – 7.46 (m, 2H), 6.65 – 6.58 (m, 2H), 0.97 (s, 9H), 0.18 (s, 6H).

^{13}C NMR (101 MHz, $CDCl_3$): δ 155.8, 138.4, 122.7, 83.9, 25.8, 18.3, -4.3.

3. Reductive Cross-Coupling

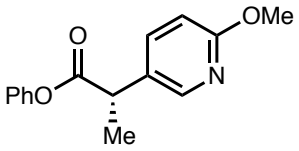
a. General Procedure 1: Reaction on 0.2 mmol scale.



On the benchtop, to a 1-dram vial were added a 12 mm Teflon-coated stir bar, Mn^0 (3 equiv, 0.6 mmol, 33.0 mg), aryl iodide (if solid) (1.5 equiv, 0.3 mmol), and (*R*,*R*) 4-heptyl BiOX (20 mol %, 0.04 mmol, 13.5 mg). The vial was sealed under argon and transferred into a N_2-filled glovebox. Once in the glovebox, the vial was charged with $NiBr_2$·diglyme (10 mol %, 0.2 mmol, 7.05 mg), sodium tetrafluoroborate (1 equiv, 0.2 mmol, 22.0 mg), and anhydrous THF (0.1 M, 2.00 mL). The vial was briefly swirled to complex the nickel and ligand. Finally, the aryl iodide (if liquid) (1.5 equiv, 0.3 mmol) and the α-chloroester (1 equiv, 0.2 mmol) were added. The vial was sealed with a Teflon-coated cap and electrical tape then removed from the glovebox. The mixture was stirred at 700 rpm for 14 hours. Due to fluctuation in ambient laboratory temperature, the reactions were run between 18 °C and 23 °C; results were consistent across this temperature range. The reaction was quenched by diluting with 1 mL of 20% EtOAc/hexanes then pushing through a ~8 mm by 6 cm plug of silica (in a monster pipette) into a scintillation vial. The reaction vial was rinsed twice with 1 mL of 20% EtOAc/hexanes, which were also pushed through the silica plug. The plug was eluted further with 20% EtOAc/hexanes (approximately 10 mL collected). The solution was concentrated *in vacuo*. The crude material was purified by column chromatography to afford the desired product.

b. Characterization of Reaction Products

phenyl (*S*)-2-(6-methoxypyridin-3-yl)propanoate (3a)



Prepared from phenyl 2-chloropropanoate (**1a**, 36.9 mg, 0.2 mmol) and 5-iodo-2-methoxypyridine (**2a**, 70.5 mg, 0.3 mmol) according to General Procedure 1. The crude residue was purified by column chromatography (silica, 50:47:3 to 50:42.5:7.5 DCM/hexanes/EtOAc) to yield **3a** (39.8 mg, 77% yield) in 85% ee as a colorless oil.

$\mathbf{R}_f$ = 0.35 (silica, 20% EtOAc/hexanes, UV)

$[\boldsymbol{\alpha}]_{\boldsymbol{D}}^{\mathbf{22}}$ = +73 (c = 0.1.465, CH_2Cl_2).

^{1}H NMR (400 MHz, $CDCl_3$): δ 8.18 (dt, *J* = 2.6, 0.6 Hz, 1H), 7.65 (dd, *J* = 8.6, 2.5 Hz, 1H), 7.39 – 7.30 (m, 2H), 7.21 (ddt, *J* = 8.0, 6.9, 1.1 Hz, 1H), 7.04 – 6.94 (m, 2H), 6.77 (dd, *J* = 8.6, 0.7 Hz, 1H), 3.95 (s, 3H), 3.94 – 3.88 (m, 1H), 1.61 (d, *J* = 7.2 Hz, 3H).

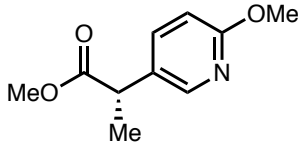
^{13}C NMR (101 MHz, $CDCl_3$): δ 172.9, 163.8, 150.8, 146.1, 137.8, 129.5, 128.5, 126.0, 121.4, 111.2, 53.6, 42.5, 18.6.

FTIR (NaCl, thin film, cm^{-1}): 2980, 2945, 2848, 1755, 1608, 1494, 1395, 1296, 1280, 1194, 1141, 1072, 1026, 919, 834, 755, 689.

HRMS (FAB, *m/z*): calc'd for $C_{17}H_{16}O_3$ $[M+H]^+$: 258.1130 ; found: 258.1133.

Chiral SFC: (OJ-H 2.5 mL/min, 10% IPA in CO_2, λ = 210 nm): t_R (major) = 5.6 min, t_R (minor) = 6.1 min.

methyl (*S*)-2-(6-methoxypyridin-3-yl)propanoate (S4)



Prepared from methyl 2-chloropropanoate (24.5 mg, 0.2 mmol) and 5-iodo-2-methoxypyridine (**2a**, 70.5 mg, 0.3 mmol) according to General Procedure 1. The crude residue was purified by column chromatography (silica, 70:15:15 hexanes/DCM/Et_2O) to yield **S4** (15.8 mg, 40% yield) in 84% ee as a colorless oil.

$\mathbf{R}_f$ = 0.30 (70:15:15 hexanes/DCM/Et_2O, UV)

$[\boldsymbol{\alpha}]_{\boldsymbol{D}}^{\mathbf{21}}$ = +61 (c = 1.0, $CHCl_3$)

^{1}H NMR (400 MHz, $CDCl_3$): δ 8.10 – 8.02 (m, 1H), 7.59 – 7.50 (m, 1H), 6.75 – 6.68 (m, 1H), 3.92 (s, 3H), 3.73 – 3.62 (m, 4H), 1.48 (d, *J* = 7.2 Hz, 3H).

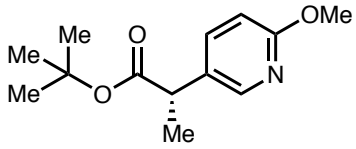
^{13}C NMR (101 MHz, $CDCl_3$): δ 174.8, 163.6, 145.9, 137.8, 128.9, 111.1, 53.6, 52.3, 42.3, 18.6.

FTIR (NaCl, thin film, cm^{-1}): 2951, 1738, 1607, 1494, 1395, 1279, 1166, 1027.

HRMS (FAB, *m/z*): calc'd for $C_{10}H_{14}NO_3$ $[M+H]^+$: 196.0974; found: 196.0988.

Chiral SFC: (IC, 2.5 mL/min, 5% IPA in CO_2, λ = 280 nm): t_R (major) = 3.5 min, t_R (minor) = 3.8 min.

***tert*-butyl (*S*)-2-(6-methoxypyridin-3-yl)propanoate (S5)**



Prepared from *tert*-butyl 2-chloropropanoate (**S1**, 32.9 mg, 0.2 mmol) and 5-iodo-2-methoxypyridine (**2b**, 70.5 mg, 0.3 mmol) according to General Procedure 1. The crude residue was purified by column chromatography (silica, 80:10:10 hexanes/DCM/Et_2O) to yield **S5** (9.7 mg, 20% yield) in 89% ee as a colorless oil.

R_f = 0.27 (80:10:10 hexanes/DCM/Et_2O, UV)

$[\boldsymbol{\alpha}]_{\boldsymbol{D}}^{\mathbf{21}}$ = +31 (c = 0.5, $CHCl_3$)

^{1}H NMR (400 MHz, $CDCl_3$): δ 8.12 – 7.97 (m, 1H), 7.63 – 7.46 (m, 1H), 6.71 (d, *J* = 8.5 Hz, 1H), 3.92 (s, 3H), 3.55 (q, *J* = 7.2 Hz, 1H), 1.47 – 1.37 (m, 10H).

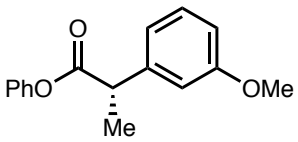
^{13}C NMR (101 MHz, $CDCl_3$): δ 173.6, 163.4, 145.8, 137.8, 129.5, 110.9, 81.0, 53.6, 43.4, 28.1, 18.6.

FTIR (NaCl, thin film, cm^{-1}): 2978, 1728, 1607, 1493, 1394, 1278, 1151, 1029

HRMS (FAB, *m/z*): calc'd for $C_{13}H_{20}NO_3$ $[M+H]^+$: 238.1443; found: 238.1434.

Chiral SFC: (IC, 2.5 mL/min, 5% IPA in CO_2, λ = 280 nm): t_R (major) = 3.3 min, t_R (minor) = 3.7 min.

phenyl (*S*)-2-(3-methoxyphenyl)propanoate (3b)



Prepared from phenyl 2-chloropropanoate (**1a**, 36.9 mg, 0.2 mmol) and 1-iodo-3-methoxybenzene (**2b**, 70.2 mg, 0.3 mmol) according to General Procedure 1. The crude residue was purified by column chromatography (silica, 2.4:3.6:10:84 Et_2O/PhMe/DCM/hexanes) to yield **3b** (45.5 mg, 89% yield) in 84% ee as a colorless oil.

R_f = 0.37 (silica, 40% DCM/hexanes, UV)

$[\boldsymbol{\alpha}]_{\boldsymbol{D}}^{\mathbf{23}}$ = +58 (c = 1.0, $CHCl_3$).

^{1}H NMR (400 MHz, $CDCl_3$): δ 7.37 – 7.26 (m, 3H), 7.24 – 7.16 (m, 1H), 7.04 – 6.93 (m, 4H), 6.84 (ddd, *J* = 8.2, 2.6, 0.9 Hz, 1H), 3.94 (q, *J* = 7.1 Hz, 1H), 3.83 (s, 3H), 1.61 (d, *J* = 7.1 Hz, 3H).

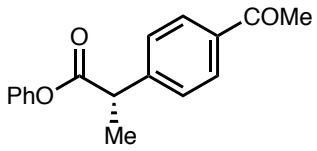
^{13}C NMR (101 MHz, $CDCl_3$): δ 173.0, 160.0, 151.0, 141.7, 129.9, 129.5, 125.9, 121.5, 120.0, 113.5, 112.9, 55.4, 45.8, 18.7.

FTIR (NaCl, thin film, cm^{-1}): 2932, 1748, 1594, 1488, 1456, 1164, 1037.

HRMS (FAB, *m/z*): calc'd for $C_{16}H_{16}O_3$ $[M+\bullet]^+$: 256.1100; found: 256.1104.

Chiral SFC: (AD-H, 2.5 mL/min, 5% IPA in CO_2, λ = 210 nm): t_R (major) = 9.6 min, t_R (minor) = 10.8 min.

phenyl (*S*)-2-(4-acetylphenyl)propanoate (3c)



Prepared from phenyl 2-chloropropanoate (**1a**, 36.9 mg, 0.2 mmol) and 4-iodoacetophenone (**2c**, 73.8 mg, 0.3 mmol) according to General Procedure 1 (run for 48 h). The crude residue was purified by column chromatography (silica, 20–50% EtOAc/hexanes) to yield **3c** (36.3 mg, 68% yield) in 87% ee as a colorless oil.

$\mathbf{R}_f$ = 0.3 (silica, 20% EtOAc/hexanes, UV)

$[\boldsymbol{\alpha}]_{\boldsymbol{D}}^{\mathbf{22}}$ = +79 (c = 1.39, CH_2Cl_2).

^{1}H NMR (400 MHz, $CDCl_3$): ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.01 – 7.94 (m, 2H), 7.55 – 7.47 (m, 2H), 7.39 – 7.29 (m, 2H), 7.25 – 7.16 (m, 1H), 7.02 – 6.95 (m, 2H), 4.04 (q, *J* = 7.2 Hz, 1H), 2.61 (s, 3H), 1.64 (d, *J* = 7.2 Hz, 3H).

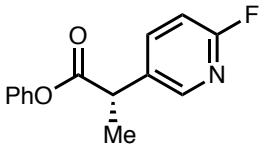
^{13}C NMR (101 MHz, $CDCl_3$): δ 197.8, 172.4, 150.8, 145.4, 136.4, 129.5, 129.0, 128.0, 126.1, 121.4, 45.8, 26.8, 18.5.

FTIR (NaCl, thin film, cm^{-1}): 3058, 2983, 2834, 1752, 1684, 1607, 1492, 1414, 1359, 1268, 1195, 1163, 1144, 1073, 958, 845, 827, 750, 687.

HRMS (FAB, *m/z*): calc'd for $C_{17}H_{16}O_3$ $[M+H]^+$: 269.1178; found:269.1160

Chiral SFC: (AD-H, 2.5 mL/min, 10% IPA in CO_2, λ = 254 nm): t_R (major) = 9.8 min, t_R (minor) = 11.2 min.

phenyl (*S*)-2-(6-fluoropyridin-3-yl)propanoate (3d)



Prepared from phenyl 2-chloropropanoate (**1a**, 36.9 mg, 0.2 mmol) and 2-fluoro-5-iodopyridine (**2d**, 66.9 mg, 0.3 mmol) according to General Procedure 1. The crude residue was purified by column chromatography (silica, 8:10:82 EtOAc/DCM/hexanes) to yield **3d** (36.1 mg, 74% yield) in 87% ee as a pale yellow oil.

$\mathbf{R}_f$ = 0.28 (silica, 8:10:82 EtOAc/DCM/hexanes, UV)

$[\boldsymbol{\alpha}]_{\boldsymbol{D}}^{\mathbf{23}}$ = +45 (c = 0.5, $CHCl_3$).

^{1}H NMR (400 MHz, $CDCl_3$): δ 8.29 – 8.22 (m, 0H), 7.87 (ddd, *J* = 8.5, 7.5, 2.7 Hz, 0H), 7.40 – 7.32 (m, 1H), 7.25 – 7.19 (m, 0H), 7.04 – 6.93 (m, 1H), 4.01 (q, *J* = 7.2 Hz, 0H), 1.66 (d, *J* = 7.2 Hz, 1H).

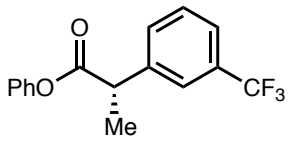
^{13}C NMR (101 MHz, $CDCl_3$): δ 172.3, 163.2 (d, $J_{C–F}$ = 239.4 Hz), 150.6, 147.0 (d, $J_{C–F}$ = 14.8 Hz), 140.3 (d, $J_{C–F}$ = 8.0 Hz), 133.4 (d, $J_{C–F}$ = 4.7 Hz), 129.6, 126.2, 121.3, 109.9 (d, $J_{C–F}$ = 37.6 Hz), 42.5, 18.7.

FTIR (NaCl, thin film, cm^{-1}): 2956, 2930, 1759, 1509, 1264, 1196, 916, 839.

HRMS (FAB, *m/z*): calc'd for $C_{14}H_{13}FNO_2$ $[M+H]^+$: 246.0930; found: 246.0925.

Chiral SFC: (AS-H, 2.5 mL/min, 7% IPA in CO_2, λ = 210 nm): t_R (major) = 4.3 min, t_R (minor) = 4.6 min.

phenyl (*S*)-2-(3-(trifluoromethyl)phenyl)propanoate (3e)



Prepared from phenyl 2-chloropropanoate (**1a**, 36.9 mg, 0.2 mmol) and 1-iodo-3-(trifluoromethyl)benzene (**2e**, 81.6 mg, 0.3 mmol) according to General Procedure 1. The crude residue was purified by column chromatography (silica, 4% EtOAc/hexanes) to yield **3e** (36.2 mg, 61% yield) in 85% ee as a colorless oil.

$\mathbf{R}_f$ = 0.55 (silica, 10% EtOAc/hexanes, UV).

$[\boldsymbol{\alpha}]_{\boldsymbol{D}}^{\mathbf{23}}$ = +55 (c = 0.5, $CHCl_3$).

^{1}H NMR (400 MHz, $CDCl_3$): δ 7.58 (d, *J* = 2.5 Hz, 1H), 7.55 – 7.46 (m, 2H), 7.41 (t, *J* = 7.7 Hz, 1H), 7.31 – 7.21 (m, 2H), 7.12 (td, *J* = 7.3, 1.2 Hz, 1H), 6.94 – 6.87 (m, 2H), 3.95 (q, *J* = 7.2 Hz, 1H), 1.57 (dd, *J* = 7.2, 0.9 Hz, 3H).

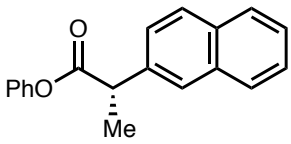
^{13}C NMR (101 MHz, $CDCl_3$): δ 172.5, 150.8, 141.1, 131.3 (q, $^2J_{CF}$ = 32.3 Hz), 131.1, 129.6, 129.4, 126.1, 124.6 ($^3J_{CF}$ = 3.9 Hz), 124.5 ($^3J_{CF}$ = 3.8 Hz), 124.2 ($^1J_{CF}$ = 272.4 Hz), 121.4, 45.6, 18.6.

FTIR (NaCl, thin film, cm^{-1}): 1757, 1593, 1492, 1329, 1194, 1128, 1072, 807, 701.

HRMS (FAB, m/z): calc'd for $C_{15}H_{13}F_3O_2$: 295.0946 [M+H]+; found: 295.0920.

Chiral SFC: (OJ-H, 2.5 mL/min, 7% IPA in CO_2, λ = 210 nm): t_R (major) = 3.6 min, t_R (minor) = 3.0 min.

phenyl (*S*)-2-(naphthalen-2-yl)propanoate (3f)



Prepared from phenyl 2-chloropropanoate (**1a**, 36.9 mg, 0.2 mmol) and 2-iodonapthalene (**2f**, 76.2 mg, 0.3 mmol) according to General Procedure 1. The crude residue was purified by column chromatography (silica, 30% DCM/hexanes) to yield **3f** (51.8 mg, 94% yield) in 86% ee as a colorless oil.

$\mathbf{R}_f$ = 0.37 (silica, 40% DCM/hexanes, UV)

$[\boldsymbol{\alpha}]_{\boldsymbol{D}}^{\mathbf{23}}$ = +80 (c = 1.0, $CHCl_3$).

^{1}H NMR (400 MHz, $CDCl_3$): δ 7.92 – 7.80 (m, 4H), 7.59 – 7.44 (m, 3H), 7.37 – 7.28 (m, 2H), 7.23 – 7.14 (m, 1H), 7.03 – 6.94 (m, 2H), 4.14 (q, *J* = 7.1 Hz, 1H), 1.71 (d, *J* = 7.2 Hz, 3H).

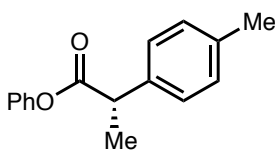
^{13}C NMR (101 MHz, $CDCl_3$): δ 173.2, 150.9, 137.6, 133.7, 132.8, 129.5, 128.7, 128.0, 127.8, 126.5, 126.4, 126.1, 125.9, 125.8, 121.5, 45.9, 18.7.

FTIR (NaCl, thin film, cm^{-1}): 2918, 1750, 1328, 1193, 1160, 823, 746.

HRMS (FAB, *m/z*): calc'd for $C_{19}H_{16}O_2$ $[M+H]^+$: 276.1150; found: 276.1156.

Chiral SFC: (AD-H, 2.5 mL/min, 10% IPA in CO_2, λ = 254 nm): t_R (major) = 13.4 min, t_R (minor) = 13.8 min.

phenyl (*S*)-2-(*p*-tolyl)propanoate (3g)



Prepared from phenyl 2-chloropropanoate (**1a**, 36.9 mg, 0.2 mmol) and 1-iodo-4-methylbenzene (**2g**, 65.4 mg, 0.3 mmol) according to General Procedure 1. The crude residue was purified by column chromatography (silica, 20–50% DCM/hexanes) to yield **3g** (41.2 mg, 86% yield) in 85% ee as a colorless oil.

R_f = 0.3 (silica, 30% DCM/hexanes, UV)

$[\alpha]_D^{22}$ = +73 (c = 1.415, CH_2Cl_2).

^{1}H NMR (400 MHz, $CDCl_3$): δ 7.38 – 7.27 (m, 4H), 7.19 (ddd, *J* = 7.9, 5.9, 1.1 Hz, 3H), 7.03 – 6.95 (m, 2H), 3.93 (q, *J* = 7.1 Hz, 1H), 2.36 (s, 3H), 1.60 (d, *J* = 7.1 Hz, 3H).

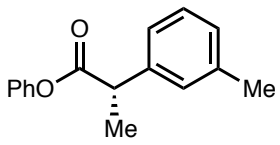
^{13}C NMR (101 MHz, $CDCl_3$): δ 173.3, 151.0, 137.2, 137.2, 129.6, 129.5, 127.5, 125.9, 121.5, 45.4, 21.2, 18.7.

FTIR (NaCl, thin film, cm^{-1}): 2922, 2850, 1752, 1591, 1512, 1492, 1456, 1376, 1331, 1196, 1141, 1070, 917, 808, 755, 724.

HRMS (FAB, *m/z*): calc'd for $C_{16}H_{17}O_2$: 241.1229 $[M+H]^+$; found 241.1234

Chiral SFC: (OB-H, 2.5 mL/min, 30% IPA in CO_2, λ = 210 nm): t_R (major) = 4.2 min, t_R (minor) = 3.6 min.

phenyl (*S*)-2-(*m*-tolyl)propanoate (3h)



Prepared from phenyl 2-chloropropanoate (**1a**, 36.9 mg, 0.2 mmol) and 1-iodo-3-methylbenzene (**2h**, 65.4 mg, 0.3 mmol) according to General Procedure 1. The crude residue was purified by column chromatography (silica, 10% DCM/hexanes) to yield **3h** (41.2 mg, 86% yield) in 84% ee as a colorless oil.

R_f = 0.3 (silica, 20% DCM/hexanes, UV)

$[\alpha]_D^{22}$ = +76 (c = 1.215, CH_2Cl_2)

^{1}H NMR (400 MHz, $CDCl_3$): δ 7.41 – 7.29 (m, 2H), 7.27 (td, *J* = 7.4, 1.0 Hz, 1H), 7.23 – 7.16 (m, 4H), 7.16 – 7.08 (m, 1H), 7.04 – 6.96 (m, 2H), 3.93 (q, *J* = 7.2 Hz, 1H), 2.38 (d, *J* = 0.7 Hz, 3H), 1.61 (d, *J* = 7.2 Hz, 3H).

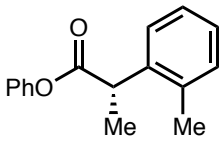
^{13}C NMR (101 MHz, $CDCl_3$): δ 173.3, 151.0, 140.2, 138.6, 129.5, 128.8, 128.4, 128.3, 125.9, 124.7, 121.5, 45.7, 21.6, 18.7.

FTIR (NaCl, thin film, cm^{-1}): 3041, 2978, 2932, 2873, 1765, 1592, 1492, 1333, 1196, 1163, 1143, 1071, 920, 756, 720, 690.

HRMS (FAB, *m/z*): calc'd for $C_{16}H_{17}O_2$: 241.1229 $[M+H]^+$; found 241.1223

Chiral SFC: (IC, 2.5 mL/min, 10% IPA in CO_2, λ = 210 nm): t_R (major) = 3.2 min, t_R (minor) = 3.5 min.

phenyl (*S*)-2-(*o*-tolyl)propanoate (S6)



Prepared from phenyl 2-chloropropanoate (**1a**, 36.9 mg, 0.2 mmol) and 1-iodo-2-methylbenzene (65.4 mg, 0.3 mmol) according to General Procedure 1. The crude residue was purified by column chromatography (silica, 80:17:3 hexanes/DCM/Et_2O) to yield **S6** (41.3 mg, 46% yield) in 47% ee as a colorless oil.

R_f = 0.30 (silica, 80:17:3 hexanes/DCM/Et_2O, UV)

$[\boldsymbol{\alpha}]_{\boldsymbol{D}}^{\mathbf{20}}$ = +50 (c = 1.0, $CHCl_3$)

^{1}H NMR (400 MHz, $CDCl_3$): δ 7.40 – 7.31 (m, 3H), 7.28 – 7.17 (m, 4H), 7.03 – 6.97 (m, 2H), 4.21 (q, *J* = 7.1 Hz, 1H), 2.47 (s, 3H), 1.59 (d, *J* = 7.1 Hz, 3H).

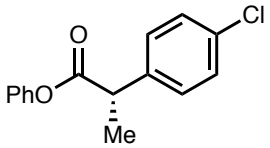
^{13}C NMR (101 MHz, $CDCl_3$): δ 173.5, 151.0, 138.8, 135.9, 130.8, 129.5, 127.3, 126.7, 126.6, 125.9, 121.5, 41.7, 19.8, 18.0.

FTIR (NaCl, thin film, cm^{-1}): 2979, 1759, 1493, 1456, 1196, 1149, 1075, 728.

HRMS (FAB, *m/z*): calc'd for $C_{16}H_{17}O_2$: 241.1229 $[M+H]^+$; found 241.1244.

Chiral SFC: (IC, 2.5 mL/min, 10% IPA in CO_2, λ = 210 nm): t_R (major) = 2.8 min,
t_R (minor) = 3.4 min.

phenyl (*S*)-2-(4-chlorophenyl)propanoate (3i)



Prepared from phenyl 2-chloropropanoate (**1a**, 36.9 mg, 0.2 mmol) and 1-chloro-4-iodobenzene (**2i**, 71.5 mg, 0.3 mmol) according to General Procedure 1. The crude residue was purified by column chromatography (silica, 4% EtOAc/hexanes) to yield **3i** (41.3 mg, 79% yield) in 87% ee as a colorless oil.

R_f = 0.55 (silica, 10% EtOAc/hexanes, UV).

$[\boldsymbol{\alpha}]_{\boldsymbol{D}}^{\mathbf{23}}$ = +37 (c = 1.0, $CHCl_3$).

^{1}H NMR (400 MHz, $CDCl_3$): δ 7.39 – 7.31 (m, 6H), 7.24 – 7.18 (m, 1H), 7.02 – 6.96 (m, 2H), 3.94 (q, *J* = 7.2 Hz, 1H), 1.61 (d, *J* = 7.1 Hz, 3H).

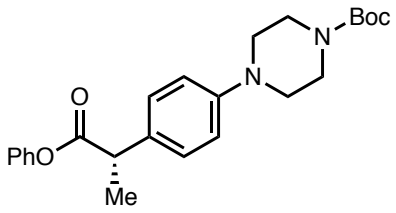
^{13}C NMR (101 MHz, $CDCl_3$): δ 172.8, 150.8, 138.6, 133.4, 129.5, 129.1, 126.0, 121.4, 45.2, 18.6.

FTIR (NaCl, thin film, cm^{-1}): 2981, 1754, 1592, 1492, 1330, 1198, 1138, 1092, 828, 745, 691.

HRMS (FAB, m/z): calc'd for $C_{15}H_{13}ClO_2$: 261.0682 [M+H]+; found: 261.0688.

Chiral SFC: (OJ-H, 2.5 mL/min, 20% IPA in CO_2, λ = 280 nm): t_R (minor) = 4.9 min,
t_R (major) = 5.1 min.

***tert*-butyl (*S*)-4-(4-(1-oxo-1-phenoxypropan-2-yl)phenyl)piperazine-1-carboxylate (3j)**



Prepared from phenyl 2-chloropropanoate (**1a**, 36.9 mg, 0.2 mmol) and *tert*-butyl 4-(4-iodophenyl)piperazine-1-carboxylate (**2j**, 117.0 mg, 0.3 mmol) according to General Procedure 1. The crude residue was purified by column chromatography (silica, 35:10:55 Et_2O/PhMe/hexanes) to yield **3j** (52.9 mg, 64% yield) in 85% ee as a colorless oil.

R_f = 0.28 (silica, 40:10:50 Et_2O/PhMe/hexanes, UV)

$[\alpha]_D^{23}$ = +41 (c = 1.0, $CHCl_3$).

^{1}H NMR (400 MHz, $CDCl_3$): δ 8.21 (d, *J* = 2.6, 0.6 Hz, 1H), 7.57 (dd, *J* = 8.8, 2.6 Hz, 1H), 7.39 – 7.30 (m, 2H), 7.20 (ddt, *J* = 8.0, 6.9, 1.2 Hz, 1H), 7.04 – 6.95 (m, 2H), 6.67 (d, *J* = 8.8 Hz, 1H), 3.87 (q, *J* = 7.2 Hz, 1H), 3.62 – 3.47 (m, 8H), 1.59 (d, *J* = 7.2 Hz, 3H), 1.49 (s, 9H).

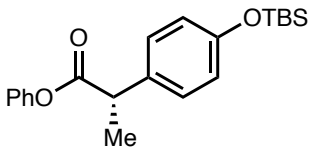
^{13}C NMR (101 MHz, $CDCl_3$): δ 173.1, 158.8, 155.0, 150.9, 147.3, 136.8, 129.5, 126.0, 125.1, 121.5, 107.4, 80.1, 45.3, 42.4, 28.6, 18.5.

FTIR (NaCl, thin film, cm^{-1}): 2976, 2931, 1756, 1696, 1606, 1493, 1408, 1240, 1194, 1164, 1132.

HRMS (FAB, *m/z*): calc'd for $C_{23}H_{30}N_3O_4$ $[M+H]^+$: 412.2236; found: 412.2230.

Chiral SFC: (IC, 2.5 mL/min, 35% IPA in CO_2, λ = 280 nm): t_R (major) = 3.5 min, t_R (minor) = 4.1 min.

phenyl (*S*)-2-(4-((*tert*-butyldimethylsilyl)oxy)phenyl)propanoate (3k)



Prepared from phenyl 2-chloropropanoate (**1a**, 36.9 mg, 0.2 mmol) and *tert*-butyl(4-iodophenoxy)dimethylsilane (**2k**, 100.0 mg, 0.3 mmol) according to General Procedure 1. The crude residue was purified by column chromatography (silica, 30–35% DCM/hexanes) to yield **3k** (56.3 mg, 79% yield) in 84% ee as a colorless oil.

R_f = 0.28 (silica, 35% DCM/hexanes, UV)

$[\alpha]_D^{23}$ = +45 (c = 1.0, $CHCl_3$).

^{1}H NMR (400 MHz, $CDCl_3$): δ 7.36 – 7.30 (m, 2H), 7.28 – 7.23 (m, 2H), 7.23 – 7.15 (m, 1H), 7.02 – 6.94 (m, 2H), 6.88 – 6.79 (m, 2H), 3.90 (q, *J* = 7.2 Hz, 1H), 1.59 (d, *J* = 7.1 Hz, 3H), 0.99 (s, 9H), 0.21 (s, 6H).

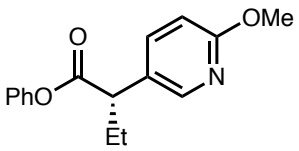
^{13}C NMR (101 MHz, $CDCl_3$): δ 173.5, 155.1, 151.0, 132.8, 129.5, 128.7, 125.9, 121.5, 120.4, 45.0, 25.8, 18.6, 18.3, –4.3.

FTIR (NaCl, thin film, cm^{-1}): 2934, 1756, 1593, 1488, 1398, 1251, 1194, 1164, 1140, 1071, 1024.

HRMS (FAB, *m/z*): calc'd for $C_{21}H_{28}O_3Si$ $[M+\bullet]^+$: 356.1808; found: 356.1802.

Chiral SFC: (AD-H, 2.5 mL/min, 3% IPA in CO_2, λ = 254 nm): t_R (major) = 5.7 min, t_R (minor) = 6.7 min.

phenyl (*S*)-2-(6-methoxypyridin-3-yl)butanoate (6a)



Prepared from phenyl 2-chlorobutanoate (**1b**, 39.7 mg, 0.2 mmol) and 5-iodo-2-methoxypyridine (**2a**, 70.5 mg, 0.3 mmol) according to General Procedure 1. The crude residue was purified by column chromatography (silica, 4% EtOAc/hexanes) to yield **6a** (44.1 mg, 81% yield) in 88% ee as a colorless oil.

$\mathbf{R}_f$ = 0.6 (20% EtOAc/hexanes, UV)

$[\boldsymbol{\alpha}]_{\boldsymbol{D}}^{\mathbf{22}}$ = +67 (c = 1, $CHCl_3$).

^{1}H NMR (400 MHz, $CDCl_3$): δ 8.16 (dt, *J* = 2.5, 0.6 Hz, 1H), 7.67 (dd, *J* = 8.6, 2.5 Hz, 1H), 7.39 – 7.30 (m, 2H), 7.26 – 7.16 (m, 1H), 7.04 – 6.96 (m, 2H), 6.77 (dd, *J* = 8.6, 0.8 Hz, 1H), 3.95 (s, 3H), 3.65 (t, *J* = 7.7 Hz, 1H), 2.22 (dp, *J* = 13.6, 7.4 Hz, 1H), 1.88 (dp, *J* = 13.6, 7.5 Hz, 1H), 1.00 (t, *J* = 7.4 Hz, 3H).

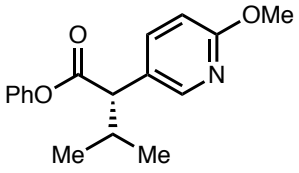
^{13}C NMR (101 MHz, $CDCl_3$): δ 172.5, 163.8, 150.8, 146.5, 138.1, 129.6, 127.0, 126.0, 121.5, 111.3, 53.7, 50.2, 26.8, 12.2.

FTIR (NaCl, thin film, cm^{-1}): 2966, 1755, 1605, 1486, 1394, 1292, 1125, 1025, 829, 689.

HRMS (FAB, *m/z*): calc'd for $C_{16}H_{17}NO_3$: 272.1287 $[M+H]^+$; found: 272.1308.

Chiral SFC: (AD-H, 2.5 mL/min, 10% IPA in CO_2, λ = 230 nm): t_R (major) = 3.8 min, t_R (minor) = 3.6 min.

phenyl (*S*)-2-(6-methoxypyridin-3-yl)-3-methylbutanoate (6b)



Prepared from phenyl 2-chloro-3-methylbutanoate (**1c**, 42.5 mg, 0.2 mmol) and 5-iodo-2-methoxypyridine (**2a**, 70.5 mg, 0.3 mmol) according to General Procedure 1. The crude residue was purified by column chromatography (silica, 2.5–10% EtOAc/hexanes) to yield **6b** (42.7 mg, 75% yield) in 96% ee as a colorless oil.

$\mathbf{R}_f$ = 0.53 (10% EtOAc/hex)

$[\boldsymbol{\alpha}]_{\boldsymbol{D}}^{\mathbf{23}}$ = +56, (c = 1, $CHCl_3$).

^{1}H NMR (400 MHz, $CDCl_3$): δ 8.15 (dd, J = 2.5, 0.7 Hz, 1H), 7.72 (dd, J = 8.6, 2.5 Hz, 1H), 7.41 – 7.30 (m, 2H), 7.25 – 7.16 (m, 1H), 7.05 – 6.94 (m, 2H), 6.80 – 6.71 (m, 1H), 3.95 (s, 3H), 3.36 (d, J = 10.3 Hz, 1H), 2.41 (dhept, J = 10.4, 6.6 Hz, 1H), 1.19 (d, J = 6.5 Hz, 3H), 0.81 (d, J = 6.7 Hz, 3H).

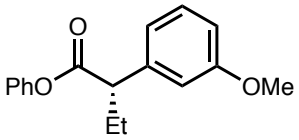
^{13}C NMR (101 MHz, $CDCl_3$): δ 172.3, 163.9, 150.7, 147.0, 138.4, 129.5, 126.3, 126.0, 121.5, 111.2, 56.5, 53.6, 32.1, 21.5, 20.2.

FTIR (NaCl, thin film, cm^{-1}): 2963, 1754, 1605, 1492, 1397, 1286, 1193, 1140, 1105, 1026, 829, 728, 688.

HRMS (FAB, *m/z*): calc'd for $C_{17}H_{20}O_3N$ $[M+H]^+$: 286.1443; found:286.1453.

Chiral SFC: (OJ-H, 2.5 mL/min, 5% IPA in CO_2, λ = 280 nm): t_R (major) = 6.4 min, t_R (minor) = 6.9 min.

phenyl (*S*)-2-(3-methoxyphenyl)butanoate (6c)



Prepared from phenyl 2-chloropropanoate (**1c**, 39.7 mg, 0.2 mmol) and 1-iodo-3-methoxybenzene (**2b**, 70.2 mg, 0.3 mmol) according to General Procedure 1. The crude residue was purified by column chromatography (silica, 2% DCM/PhMe) to yield **6c** (52.2 mg, 97% yield) in 85% ee as a colorless oil.

$\mathbf{R}_f$ = 0.7 (silica, 50% DCM/PhMe, UV)

$[\boldsymbol{\alpha}]_{\boldsymbol{D}}^{\mathbf{23}}$ = +61 (c = 1, $CHCl_3$).

^{1}H NMR (400 MHz, $CDCl_3$): δ 7.40 – 7.25 (m, 3H), 7.24 – 7.15 (m, 1H), 7.04 – 6.93 (m, 4H), 6.84 (ddd, *J* = 8.3, 2.6, 1.0 Hz, 1H), 3.82 (s, 3H), 3.67 (t, *J* = 7.7 Hz, 1H), 2.21 (ddq, *J* = 13.7, 8.1, 7.3 Hz, 1H), 1.90 (dp, *J* = 13.6, 7.4 Hz, 1H), 1.00 (t, *J* = 7.4 Hz, 3H).

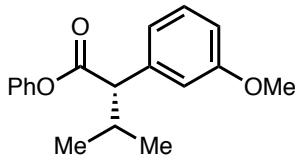
^{13}C NMR (101 MHz, $CDCl_3$): δ 172.6, 160.0, 150.9, 140.3, 129.8, 129.5, 125.9, 121.6, 120.6, 113.9, 112.9, 55.4, 53.7, 26.9, 12.3.

FTIR (NaCl, thin film, cm^{-1}): 3478, 2965, 2935, 2836, 1754, 1609, 1483, 1273, 1069, 955, 774, 693.

HRMS (FAB, *m/z*): calc'd for $C_{17}H_{18}O_3$: 270.1256 $[M+\bullet]^+$; found: 270.1251.

Chiral SFC: (OJ-H, 2.5 mL/min, 20% IPA in CO_2, λ = 210 nm): t_R (major) = 3.2 min, t_R (minor) = 3.9 min.

phenyl 2-(3-methoxyphenyl)-3-methylbutanoate (6d)



Prepared from phenyl 2-chloro-3-methylbutanoate (**1c**, 42.5 mg, 0.2 mmol) and 1-iodo-3-methoxybenzene (**2b**, 70.2 mg, 0.3 mmol) according to General Procedure 1. The crude residue was purified by column chromatography (silica, 1:1.5:5:92.5 PhMe/Et_2O/DCM/hexanes) to yield **6d** (53.5 mg, 94% yield) in 98% ee as a colorless oil.

$\mathbf{R}_f$ = 0.30 (5:5:10:80 PhMe/Et_2O/DCM/hexanes, UV)

$[\boldsymbol{\alpha}]_{\boldsymbol{D}}^{\mathbf{22}}$ = +49 (c = 1, $CHCl_3$).

^{1}H NMR (400 MHz, $CDCl_3$): δ 7.37 – 7.30 (m, 2H), 7.27 (ddd, *J* = 8.1, 7.4, 0.6 Hz, 1H), 7.19 (ddt, *J* = 8.0, 6.9, 1.2 Hz, 1H), 7.04 – 6.95 (m, 4H), 6.84 (ddd, *J* = 8.2, 2.5, 1.0 Hz, 1H), 3.82 (s, 3H), 3.36 (d, *J* = 10.5 Hz, 1H), 2.44 (dp, *J* = 10.6, 6.6 Hz, 1H), 1.18 (d, *J* = 6.5 Hz, 3H), 0.80 (d, *J* = 6.7 Hz, 3H).

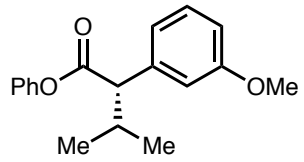
^{13}C NMR (101 MHz, $CDCl_3$): δ 172.5, 159.9, 150.9, 139.5, 129.7, 129.5, 125.9, 121.6, 121.2, 114.3, 113.0, 60.2, 55.4, 32.2, 21.6, 20.4.

FTIR (NaCl, thin film, cm^{-1}): 2962, 2872, 1755, 1748, 1599, 1487, 1267, 1167, 1049, 976, 730, 694.

HRMS (FAB, *m/z*): calc'd for $C_{18}H_{20}O_3$: 285.1491 $[M+H]^+$; found: 285.1498.

Chiral SFC: (AD-H, 2.5 mL/min, 20% IPA in CO_2, λ = 254 nm): t_R (major) = 2.4 min, t_R (minor) = 2.5 min.

phenyl (*S*)-3-methyl-2-(*p*-tolyl)butanoate (6e)



Prepared from phenyl 2-chloro-3-methylbutanoate (**1c**, 42.5 mg, 0.2 mmol) and 1-iodo-4-methylbenzene (**2g**, 65.4 mg, 0.3 mmol) according to General Procedure 1. The crude residue was purified by column chromatography (silica, 10–40% DCM/hexanes) to yield **6e** (42.0 mg, 78% yield) in 97% ee as a colorless oil.

$\mathbf{R}_f$ = 0.5 (30% DCM, hexanes, UV)

$[\boldsymbol{\alpha}]_D^{23}$ = +55 (c = 1.37, $CHCl_3$).

^{1}H NMR (400 MHz, $CDCl_3$): δ 7.38 – 7.28 (m, 4H), 7.22 – 7.11 (m, 3H), 7.11 – 7.04 (m, 0H), 7.03 – 6.91 (m, 2H), 3.36 (d, J = 10.5 Hz, 1H), 2.53 – 2.29 (m, 4H), 1.55 (s, 1H), 1.18 (d, J = 6.5 Hz, 3H), 1.07 (d, J = 6.6 Hz, 0H), 0.79 (d, J = 6.7 Hz, 3H).

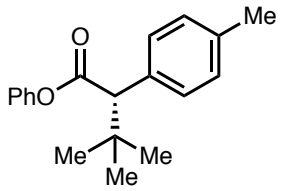
^{13}C NMR (101 MHz, $CDCl_3$): δ 172.7, 150.9, 137.2, 134.9, 129.4, 128.6, 125.9, 121.6, 59.8, 32.1, 21.6, 21.3, 20.4.

FTIR (NaCl, thin film, cm^{-1}): 2961, 2926, 2871, 1756, 1593, 1492, 1197, 1112, 732, 688.

HRMS (FAB, *m/z*): calc'd for $C_{18}H_{21}O_2$: 269.1542 $[M+H]^+$; found: 269.1534.

Chiral SFC: (OJ-H, 2.5 mL/min, 10% IPA in CO_2, λ = 210 nm): t_R (major) = 3.8 min, t_R (minor) = 4.4 min.

phenyl (*S*)-3,3-dimethyl-2-(*p*-tolyl)butanoate (6f)



Prepared from phenyl 2-chloro-3,3-dimethylbutanoate (45.3 mg, 0.2 mmol) and 1-iodo-4-methylbenzene (**2g**, 65.4 mg, 0.3 mmol) according to General Procedure 1. Addition of 1,1,2,2-tetrachloroethane as an internal standard showed 16% yield by NMR. The crude residue was purified by column chromatography (silica, 15–20% DCM/hexanes), followed by preparative TLC (50% DCM/hexanes) to yield **6f** (5.2 mg, 9% yield) in 89% ee as a colorless oil.

$\mathbf{R}_f$ = 0.17 (20% DCM, hexanes, UV)

$[\boldsymbol{\alpha}]_D^{21}$ = –37 (c = 0.3, $CHCl_3$).

^{1}H NMR (400 MHz, $CDCl_3$): δ 7.38 – 7.31 (m, 4H), 7.23 – 7.12 (m, 3H), 7.04 – 6.98 (m, 2H), 3.65 (s, 1H), 2.36 (s, 3H), 1.08 (s, 9H).

^{13}C NMR (101 MHz, $CDCl_3$): δ 172.0, 150.8, 137.1, 132.8, 130.0, 129.7, 129.5, 128.8, 125.9, 121.8, 121.4, 61.2, 35.0, 27.9, 26.7, 21.2.

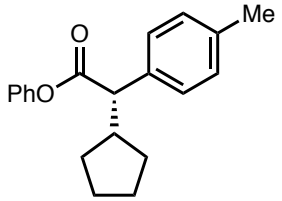
FTIR (NaCl, thin film, cm^{-1}): 2958, 1756, 1593, 1492, 1365, 1197, 1162, 1112, 1024

HRMS (FAB, *m/z*): calc'd for $C_{19}H_{22}O_2$: 283.1698 $[M+H]^+$; found: 283.1693.

Chiral SFC: (OJ-H, 2.5 mL/min, 10% IPA in CO_2, λ = 210 nm): t_R (minor) = 4.0 min,

t_R (major) = 5.2 min.

phenyl (*S*)-2-cyclopentyl-2-(*p*-tolyl)acetate (6g)



Prepared from phenyl 2-chloro-2-cyclopentylacetate (**1d**, 47.7 mg, 0.2 mmol) and 1-iodo-4-methylbenzene (**2g**, 65.4 mg, 0.3 mmol) according to General Procedure 1. The crude residue was purified by column chromatography (silica, 5% Et_2O/hexanes) to yield **6g** (55.7 mg, 2.1 wt% ArAr homocoupling, 93% yield) in 97% ee as a colorless oil.

$\mathbf{R}_f$ = 0.46 (silica, 8% Et_2O/hexanes, UV)

$[\boldsymbol{\alpha}]_{\boldsymbol{D}}^{\mathbf{21}}$ = +45 (c = 1.0, $CHCl_3$).

^{1}H NMR (400 MHz, $CDCl_3$): δ 7.37 – 7.30 (m, 4H), 7.22 – 7.14 (m, 3H), 7.02 – 6.96 (m, 2H), 3.49 (d, *J* = 11.1 Hz, 1H), 2.74 – 2.60 (m, 1H), 2.35 (s, 3H), 2.13 – 1.99 (m, 1H), 1.82 – 1.36 (m, 6H), 1.17 – 1.02 (m, 1H).

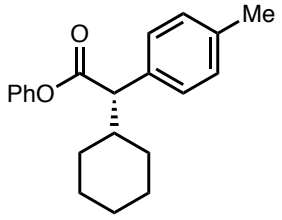
^{13}C NMR (101 MHz, $CDCl_3$): δ 172.8, 151.0, 137.1, 135.6, 129.5, 128.3, 125.8, 121.6, 57.7, 43.6, 31.7, 30.9, 25.4, 25.0, 21.2.

FTIR (NaCl, thin film, cm^{-1}): 3027, 2951, 2869, 1756, 1494, 1196, 1118

HRMS (FAB, *m/z*): calc'd for $C_{20}H_{23}O_2$ [M+H]+: 295.1698; found: 295.1689.

Chiral SFC: (IC, 2.5 mL/min, 5% IPA in CO_2, λ = 210 nm): t_R (major) = 4.4 min, t_R (minor) = 4.8 min.

phenyl (*S*)-2-cyclohexyl-2-(*p*-tolyl)acetate (6h)



Prepared from phenyl 2-chloro-2-cyclohexylacetate (**1e**, 50.5 mg, 0.2 mmol) and 1-iodo-4-methylbenzene (**2g**, 65.4 mg, 0.3 mmol) according to General Procedure 1. The crude residue was purified by column chromatography (silica, 5% Et_2O/hexanes) to yield **6h** (51.4 mg, 81% yield) in 98% ee as a colorless oil.

$\mathbf{R}_f$ = 0.48 (silica, 8% Et_2O/hexanes, UV)

$[\boldsymbol{\alpha}]_{\boldsymbol{D}}^{\mathbf{23}}$ = +37 (c = 1.0, $CHCl_3$).

^{1}H NMR (400 MHz, $CDCl_3$): δ 7.37 – 7.27 (m, 4H), 7.22 – 7.12 (m, 3H), 7.02 – 6.95 (m, 2H), 3.43 (d, *J* = 10.6 Hz, 1H), 2.35 (s, 3H), 2.11 (qt, *J* = 11.0, 3.4 Hz, 1H), 2.04 – 1.95 (m, 1H), 1.85 – 1.74 (m, 1H), 1.72 – 1.59 (m, 2H), 1.48 – 1.09 (m, 5H), 0.94 – 0.75 (m, 1H).

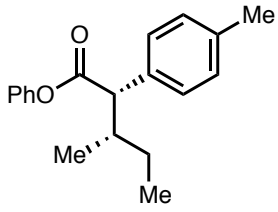
^{13}C NMR (101 MHz, $CDCl_3$): δ 172.7, 150.9, 137.2, 134.4, 129.4, 129.4, 128.7, 125.8, 121.7, 58.6, 41.3, 32.2, 30.6, 26.46, 26.2, 26.1, 21.2.

FTIR (NaCl, thin film, cm^{-1}): 2926, 2852, 1755, 1593, 1492, 1196, 1165, 1140, 1107

HRMS (FAB, m/z): calc'd for $C_{21}H_{25}ClO_2$ [M+H]+: 309.1855; found: 309.1839.

Chiral SFC: (IC, 2.5 mL/min, 5% IPA in CO_2, λ = 210 nm): t_R (major) = 4.1 min, t_R (minor) = 4.4 min.

phenyl (2*S*,3*S*)-3-methyl-2-(*p*-tolyl)pentanoate (6i)



Prepared from phenyl (2*S*,3*S*)-2-chloro-3-methylpentanoate (**1f**, 45.3 mg, 0.2 mmol) and 1-iodo-4-methylbenzene (**2g**, 65.4 mg, 0.3 mmol) according to General Procedure 1, using (*R*,*R*)-**L1**. The crude residue was purified by column chromatography (silica, 4% Et_2O/hexanes) to yield **6i** (47.9 mg, 85% yield) as a colorless oil in >20:1 dr.

$\mathbf{R_f}$ = 0.46 (silica, 8% Et_2O/hexanes, UV)

$[\boldsymbol{\alpha}]_{\boldsymbol{D}}^{\mathbf{21}}$ = +50 (c = 1.0, $CHCl_3$).

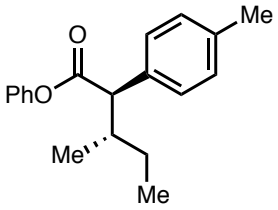
^{1}H NMR (400 MHz, $CDCl_3$): δ 7.37 – 7.27 (m, 4H), 7.22 – 7.13 (m, 3H), 7.01 – 6.94 (m, 2H), 3.47 (d, *J* = 10.5 Hz, 1H), 2.35 (s, 3H), 2.33 – 2.19 (m, 1H), 1.78 – 1.63 (m, 1H), 1.43 – 1.28 (m, 1H), 1.01 (t, *J* = 7.4 Hz, 3H), 0.74 (d, *J* = 6.8 Hz, 3H).

^{13}C NMR (101 MHz, $CDCl_3$): δ 172.8, 150.9, 137.2, 134.8, 129.5, 129.4, 128.7, 125.8, 121.6, 58.2, 38.0, 28.2, 21.3, 16.3, 11.4.

FTIR (NaCl, thin film, cm^{-1}): 2964, 2926, 2876, 1755, 1593, 1514, 1493, 1281, 1197, 1113.

HRMS (FAB, m/z): calc'd for $C_{19}H_{23}O_2$ [M+H]+: 283.1698; found: 283.1718.

phenyl (2*R*,3*S*)-3-methyl-2-(*p*-tolyl)pentanoate (6j)



Prepared from phenyl (2*S*,3*S*)-2-chloro-3-methylpentanoate (**1f**, 45.3 mg, 0.2 mmol) and 1-iodo-4-methylbenzene (**2g**, 65.4 mg, 0.3 mmol) according to General Procedure 1, using (*S*,*S*)-**L1**. The crude residue was purified by column chromatography (silica, 4% to 4.5% Et_2O/hexanes) to yield **6j** (46.6 mg, 83% yield) as a colorless oil in >20:1 dr.

$\mathbf{R}_f$ = 0.46 (silica, 8% Et_2O/hexanes, UV)

$[\boldsymbol{\alpha}]_D^{\mathbf{21}}$ = –44 (c = 1.0, $CHCl_3$).

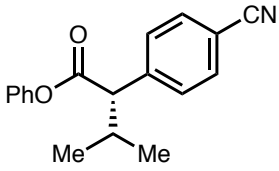
^{1}H NMR (400 MHz, $CDCl_3$): δ 7.37 – 7.28 (m, 4H), 7.22 – 7.13 (m, 3H), 7.01 – 6.95 (m, 2H), 3.47 (d, *J* = 10.7 Hz, 1H), 2.35 (s, 3H), 2.32 – 2.18 (m, 1H), 1.40 – 1.23 (m, 2H), 1.15 (d, *J* = 6.6 Hz, 3H), 1.03 – 0.93 (m, 1H), 0.83 (t, *J* = 7.4 Hz, 3H).

^{13}C NMR (101 MHz, $CDCl_3$): δ 172.8, 150.9, 137.2, 134.8, 129.5, 128.7, 125.9, 121.6, 58.3, 37.9, 26.2, 21.3, 17.5, 10.8.

FTIR (NaCl, thin film, cm^{-1}): 2964, 2931, 2876, 1756, 1593, 1513, 1493, 1196, 1163, 1115.

HRMS (FAB, m/z): calc'd for $C_{19}H_{23}O_2$ [M+H]+: 283.1698; found: 283.1712.

phenyl (*S*)-2-(4-cyanophenyl)-3-methylbutanoate (6k)



Prepared from phenyl 2-chloro-3-methylbutanoate (**1c**, 42.5 mg, 0.2 mmol) and 4-iodobenzonitrile (**2l**, 68.7 mg, 0.3 mmol) according to General Procedure 1 for 48 hours. The crude residue was purified by column chromatography (silica, 4% EtOAc/hexanes) to yield **6k** (37.8 mg, 68% yield) in 96% ee as a colorless oil.

$\mathbf{R}_f$ = 0.3 (20% EtOAc/hexanes, UV)

$[\boldsymbol{\alpha}]_D^{\mathbf{22}}$ = +50 (c = 1, $CHCl_3$).

^{1}H NMR (400 MHz, $CDCl_3$): δ 7.70 – 7.63 (m, 2H), 7.59 – 7.53 (m, 2H), 7.39 – 7.31 (m, 2H), 7.25 – 7.18 (m, 1H), 7.01 – 6.94 (m, 2H), 3.47 (d, *J* = 10.4 Hz, 1H), 2.46 (dp, *J* = 10.4, 6.6 Hz, 1H), 1.20 (d, *J* = 6.5 Hz, 3H), 0.78 (d, *J* = 6.7 Hz, 3H).

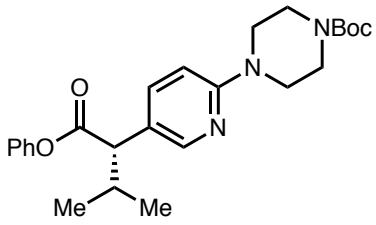
^{13}C NMR (101 MHz, $CDCl_3$): δ 171.6, 150.6, 143.3, 132.6, 129.6, 129.6, 126.2, 121.4, 118.8, 111.7, 60.1, 32.5, 21.5, 20.3.

FTIR (NaCl, thin film, cm^{-1}): 2964, 2229, 1759, 1747, 1493, 1216, 1136, 828, 754, 688.

HRMS (FAB, *m/z*): calc'd for $C_{18}H_{17}NO_2$: 280.1338 $[M+H]^+$; found: 280.1358.

Chiral SFC: (AD-H, 2.5 mL/min, 20% IPA in CO_2, λ = 230 nm): t_R (major) = 2.5 min, t_R (minor) = 2.8 min.

***tert*-butyl (*S*)-4-(5-(3-methyl-1-oxo-1-phenoxybutan-2-yl)pyridin-2-yl)piperazine-1-carboxylatecarboxylate (6l)**



Prepared from phenyl 2-chloro-3-methylbutanoate (**1c**, 42.5 mg, 0.2 mmol) and *tert*-butyl 4-(5-iodopyridin-2-yl)piperazine-1-carboxylate (**2j**, 117 mg, 0.3 mmol) according to General Procedure 1. The crude residue was purified by column chromatography (silica, 4–10% EtOAc/hexanes) to yield **6l** (52.8 mg, 60% yield) in 97% ee as a colorless oil.

R_f = 0.4 (silica, 20% EtOAc/hexanes, UV)

$[\boldsymbol{\alpha}]_{\boldsymbol{D}}^{\mathbf{23}}$ = +35 (c = 0.7, $CHCl_3$).

^{1}H NMR (400 MHz, $CDCl_3$): δ 8.07 (d, *J* = 2.5 Hz, 1H), 7.53 (d, *J* = 8.7 Hz, 1H), 7.29 – 7.19 (m, 2H), 7.13 – 7.03 (m, 1H), 6.93 – 6.85 (m, 2H), 6.57 (d, *J* = 8.8 Hz, 1H), 3.45 (s, 8H), 3.20 (d, *J* = 10.4 Hz, 1H), 2.29 (dp, *J* = 10.3, 6.6 Hz, 1H), 1.39 (s, 9H), 1.07 (d, *J* = 6.5 Hz, 3H), 0.71 (d, *J* = 6.7 Hz, 3H).

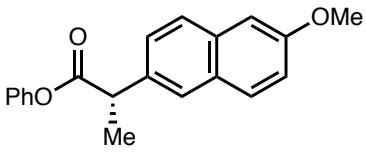
^{13}C NMR (101 MHz, $CDCl_3$): δ 172.5, 158.8, 154.9, 150.8, 148.2, 137.4, 129.5, 125.9, 122.9, 121.5, 107.3, 80.1, 56.5, 45.2, 43.5, 31.9, 28.5, 21.5, 20.2.

FTIR (NaCl, thin film, cm^{-1}): 2965, 1754, 1697, 1494, 1415, 1239, 1167, 930, 754.

HRMS (FAB, *m/z*): calc'd for $C_{25}H_{33}NO_4$: 440.2549 $[M+H]^+$; found: 440.2528.

Chiral SFC: (OD-H, 2.5 mL/min, 15% IPA in CO_2, λ = 230 nm): t_R (major) = 4.4 min, t_R (minor) = 4.9 min.

phenyl 2-(6-methoxynaphthalen-2-yl)propanoate (8)



Prepared from phenyl 2-chloropropanoate (**1a**, 36.9 mg, 0.2 mmol) and 2-iodo-6-methoxynaphthalene (**7**, 85.2 mg, 0.3 mmol) according to General Procedure 1. The crude residue was purified by column chromatography (silica, 5–20% EtOAc/hexanes) to yield **8** (59.3 mg, 97% yield) in 86% ee as a white powder.

R_f = 0.55 (silica, 20% EtOAc/hexanes, UV)

$[\boldsymbol{\alpha}]_{\boldsymbol{D}}^{\mathbf{21}}$ = +83 (c = 0.4, CH_3CN).

^{1}H NMR (400 MHz, $CDCl_3$): δ 7.81 – 7.70 (m, 3H), 7.51 (dd, *J* = 8.5, 1.9 Hz, 1H), 7.37 – 7.29 (m, 2H), 7.23 – 7.12 (m, 3H), 7.03 – 6.95 (m, 2H), 4.11 (q, *J* = 7.1 Hz, 1H), 3.93 (s, 3H), 1.70 (d, *J* = 7.1 Hz, 3H).

^{13}C NMR (101 MHz, $CDCl_3$): δ 173.3, 157.9, 151.0, 135.3, 134.0, 129.5, 129.1, 127.5, 126.3, 125.9, 121.5, 119.2, 105.8, 55.5, 45.7, 18.7.

FTIR (NaCl, thin film, cm^{-1}): 1755, 1744, 1604, 1484, 1264, 1134, 1025, 851.

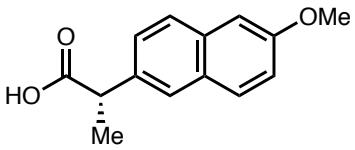
HRMS (FAB, *m/z*): calc'd for $C_{20}H_{18}O_3$: 307.1334 $[M+H]^+$; found: 307.1316.

Chiral SFC: (IC, 2.5 mL/min, 20% IPA in CO_2, λ = 210 nm): t_R (major) = 3.7 min, t_R (minor) = 4.0 min.

c. 1.0 mmol scale preparation of phenyl 2-(6-methoxynaphthalen-2-yl)propanoate (8)

Compound **8** was also prepared on 1.0 mmol scale. On the benchtop, to a 50-mL round-bottomed flask were added a 12.5 cm football-shaped Teflon-coated stir bar, Mn^0 (3 equiv, 3.0 mmol, 165mg and (*R*,*R*) 4-heptyl BiOX (20 mol %, 0.2 mmol, 67.3 mg). The flask was sealed under argon and transferred into a N_2-filled glovebox. Once in the glovebox, the vial was charged with $NiBr_2$·diglyme (10 mol %, 0.1 mmol, 35.3 mg), sodium tetrafluoroborate (1 equiv, 1.0 mmol, 110 mg), and anhydrous THF (5 mL). The reaction was stirred for one minute at 700 rpm. Finally, 2-iodo-6-methoxynaphthalene (**7**, 426 mg, 1.5 mmol) and phenyl 2-chloropropanoate (**1a**, 185 mg, 1.0 mmol) were added as a single portion as a solution in anhydrous THF (5 mL). The flask was sealed with a rubber septum and electrical tape then removed from the glovebox. The mixture was stirred at 700 rpm for 14 hours. The reaction was quenched by diluting with 5 mL of 20% EtOAc/hexanes then eluting through 3.5 cm by 5.0 cm plug of silica. The reaction flask was rinsed twice with 5 mL of 20% EtOAc/hexanes, which were also eluted through the silica plug. The plug was eluted further with 20% EtOAc/hexanes (approximately 50 mL collected). The solution was concentrated *in vacuo*. The crude material was purified by flash column chromatography over silica gel, eluting with 3:1:6 to 3.5:1:5.5 DCM/PhMe/hexanes to afford **8** (284 mg, 93% yield) as a white solid in 84% ee.

(S)-2-(6-methoxynaphthalen-2-yl)propanoic acid (9)



Following a procedure adapted from Shi et al,[11] to a 1-dram vial equipped with a Teflon-coated stir bar were added phenyl 2-(6-methoxynaphthalen-2-yl)propanoate **8** (277 mg, 0.905 mmol, 1 equiv), PhMe (181 μL), KOH (79.8 mg, 1.57 equiv, 1.42 mmol), and water (181 μL). The vial was sealed with a Teflon-lined cap and heated to 90 °C while stirring for 17 hours. The reaction was then cooled to 18 °C and transferred to a separatory funnel with water, then acidified to pH = 1 with 2M HCl. The aqueous phase was extracted thrice with EtOAc. Combined organics were then extracted with saturated aqueous $NaHCO_3$. The resulting aqueous solution was acidified to pH = 1 with s M HCl, then extracted thrice with EtOAc. Combined organics from these three extractions were dried with Na_2SO_4, filtered, and concentrated under reduced pressure. The crude material was purified by flash column chromatography over silica gel, eluting with 3:1 hexanes/EtOAc to give **9** as a white amorphous solid (201 mg, 96% yield). Spectral data matched those reported.[11]

To determine the enantiomeric excess of **9**, an aliquot was converted to its methyl ester for SFC analysis.[12] To a 1-dram vial equipped with a Teflon-coated stir bar were added **9** (15 mg, 0.065 mmol),

MeOH (2 mL), and HCl (12 M, 0.10 mL). The vial was sealed with a Teflon-lined cap and heated to 70 °C while stirring for one hour. The reaction was then cooled to room temperature, concentrated under reduced pressure, diluted with water, and extracted thrice with Et2O. Combined organic extracts were dried with Na_2SO_4, filtered, and concentrated to give **9-OMe** as a white solid (15.2 mg, 96% yield) in 83% ee. The same procedure was followed for a commercial sample of (S)-naproxen and a commercial sample of racemic naproxen, showing no racemization under the acidic esterification conditions. Comparison on these traces was used to assign the product formed with **(*R*,*R*)-L1** as (*S*)-naproxen. All other coupled products were assigned in analogy to this compound.

The enantiopurity of **9** was further enriched by recrystallization.[13] To a 20-mL vial equipped with a 12-mm Teflon-coated stir bar were added **9** (185 mg, 1.0 equiv, 0.80 mmol), MeCN (5.9 mL), and *n*-octylamine (104 mg, 1.0 equiv, 0.80 mmol). The vial was sealed with a Teflon-lined cap and heated to 75 °C while stirring for one hour, resulting in a colorless solution. The reaction was cooled to room temperature (18 °C) while stirring; precipitating and white solid, which was collected by filtration, washing with 1 mL MeCN. This white solid was added to a 100-mL round-bottomed flask equipped with a Teflon-coated stir bar, followed by anhydrous MTBE (32 mL). The flask was equipped with a waterless condenser and heated to 60 °C while stirring until dissolved. After full dissolution, the reaction was allowed to cool to 18 °C while stirring for one hour. A white precipitate formed, which was then collected by filtration, washing with 5 mL MTBE. This material was resubjected to the similar conditions. This white solid was added to a 100-mL round-bottomed flask equipped with a Teflon-coated stir bar, followed by anhydrous MTBE (25 mL). The flask was equipped with a waterless condenser and heated to 60 °C while stirring until dissolved. After full dissolution, the reaction was allowed to cool to 18 °C *without* stirring and left for 16 hours. A white precipitate formed, which was then collected by filtration, washed with 5 mL MTBE. This solid was transferred to a separatory funnel with water, acidified to pH = 1 with 2 M HCl, then extracted twice with EtOAc. Combined organics were dried with Na2SO4, filtered, and concentrated under reduced pressure to give **9** (141 mg, 76% recovery). Methyl esterification of 15 mg of this material as above showed 92% ee.

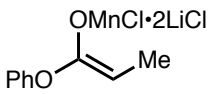
Chiral SFC: (OD-H, 2.5 mL/min, 5% MeOH in CO_2, λ = 254 nm): t_R (minor) = 5.6 min, t_R (major) = 5.9 min.

d. Mechanistic Experiments

Manganese enolate of phenyl propionate (10)

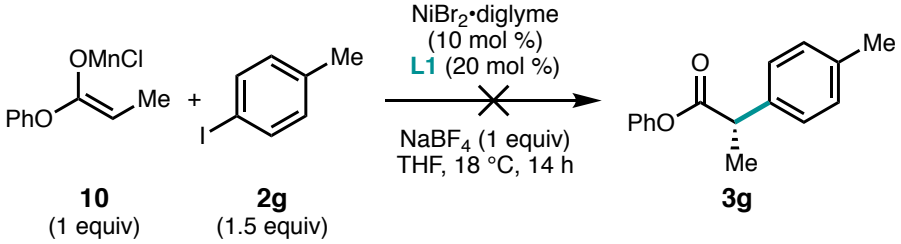
To a flame-dried 25-mL round-bottomed flask equipped with a Teflon-coated stir bar were added $MnCl_2$ (629 mg, 1.0 equiv, 5.00 mmol) and LiCl (424 mg, 2.0 equiv, 10.0 mmol, freshly ground with mortar and pestle). The flask was sealed with a rubber septum and electrical tape, then evacuated under high-vacuum at 100 °C for 22 hours. The flask was then cooled to 18 °C, and THF (8.0 mL) was added via syringe. The reaction turned light pink, then slowly became yellow as it was stirred for 24 hours at 18 °C. This $MnCl_2$•2LiCl solution was used immediately.

A 50-mL flame-dried round-bottom flask equipped with a Teflon-coated stir bar was cooled to 0 °C under an atmosphere of nitrogen. THF (5.26 mL) was added to the flask, followed by diisopropylamine (336 µL, 243 mg, 1.2 equiv, 2.20 mmol**)**. n-butyllithium (880 µL, 2.5 M in hexanes, 1.1 equiv, 2.20 mmol) was added dropwise to the flask via syringe over one minute. The reaction was stirred for 15 minutes at 0 °



C, then phenyl propionate (300 mg, 1.0 equiv, 2.00 mmol) was added dropwise via syringe over two minutes. The reaction was stirred for 30 minutes at 0 °C, then $MnCl_2$•2LiCl (3.52 mL, 0.625 M in THF, 1.10 equiv) was added to the reaction in a single portion via syringe. The cooling bath was removed and the reaction was allowed to stir for 30 minutes. The resulting manganese enolate solution was used immediately.

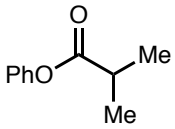
Coupling reaction with 10



The reaction was conducted similarly to General Procedure 1. To a 1-dram vial was added a 12 mm Teflon-coated stir bar and 4-heptyl BiOX (**L2**, 13.5 mg, 0.20 equiv, 0.04 mmol). The vial was sealed under argon and transferred into a nitrogen-filled glovebox. Once in the glovebox, the vial was charged with NiBr2•diglyme (7.05 mg, 0.10 equiv, 0.02 mmol), sodium tetrafluoroborate (22.0 mg, 1.0 equiv, 0.2 mmol), and THF (1 mL). The vial was briefly swirled to complex Ni and ligand. 1-iodo-4-methylbenzene (65.4 mg, 1.5 equiv, 0.30 mmol) was added to the vial, which was then sealed with a Teflon-lined septum cap and electrical tape. The vial was removed from the glovebox, then the manganese enolate solution (0.20 M, 1.0 mL, 1 equiv) was added dropwise over 30 seconds. The vial was sealed with vacuum grease

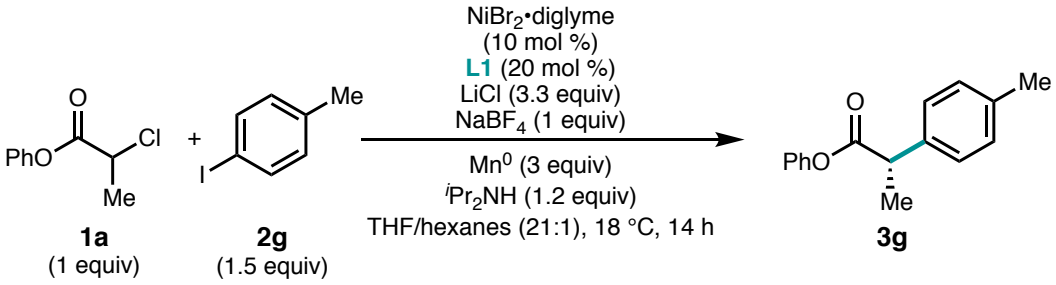
and parafilm, then allowed to stir at 18 °C and 700 rpm. After 14 hours, the reaction was worked following General Procedure 1. No product formation was observed. Note: productive reactivity was also not observed when 2.0 equiv Mn^0 was included.

phenyl isobutyrate



To test the viability of the manganese enolate as a nucleophile, the same batch of enolate solution was treated with iodomethane.[14] To a 10-mL oven dried round-bottomed flask equipped with a Teflon-coated stir bar was added Mn enolate solution (2.00 mL, 0.40 mmol). Iodomethane (68.1 mg, 1.20 equiv, 0.48 mmol) was added dropwise as a solution in DMSO (1.00 mL). The reaction was allowed to stir at 18 °C for 19 hours. The reaction was diluted with water and Et_2O, then the layers were separated. The organic layer was washed thrice with water, then dried with Na_2SO_4, filtered, and concentrated. The crude material was filtered over a short silica plug, eluting with 15% EtOAc/hexanes to afford 31.6 mg phenyl isobutyrate (contaminated with 6% phenyl propionate, 45% yield) as a colorless oil. Spectral data match those reported.[15]

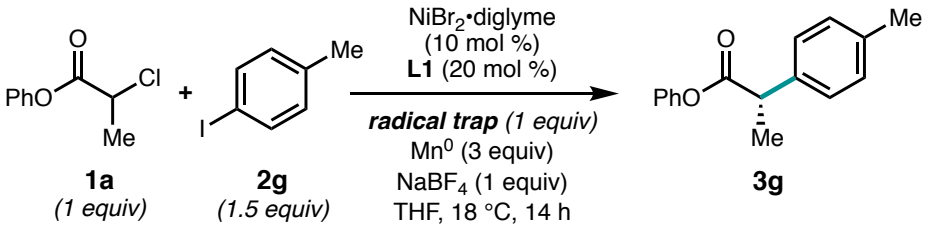
Control with Mn enolate additives



1a (1 equiv) **2g** (1.5 equiv) **3g**

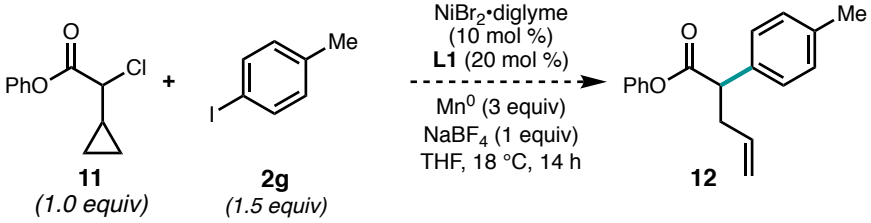
A control reaction was conducted with the byproducts of Mn enolate formation (LiCl, hexanes, and diisopropylamine). The reaction was set up according to a modified General Procedure 1 using phenyl 2-chloropropionate **1a** (36.9 mg, 1.0 equiv, 0.20 mmol) and 1-iodo-4-methylbenzene **2g** (65.4 mg, 1.5 equiv, 0.30 mmol). After the addition of $NaBF_4$, LiCl (28.0 mg, 3.3 equiv, 0.66 mmol) was added to the vial. THF (1.88 mL) and hexanes (89.5 µL) were added. After addition of the electrophiles, diisopropylamine was added (24.3 mg, 1.20 equiv, 0.24 mmol). After the typical workup from General Procedure 1, 0.10 mmol 1,1,2,2-tetrachloroethane was added to the crude residue as a stock solution in $CDCl_3$. NMR analysis showed **3g** in 73% yield. An aliquot of the crude material was purified by preparative TLC (silica, 20:5:75 DCM/Et_2O/hexanes) then analyzed by chiral SFC using the conditions reported above for **3g** to give 81% ee.

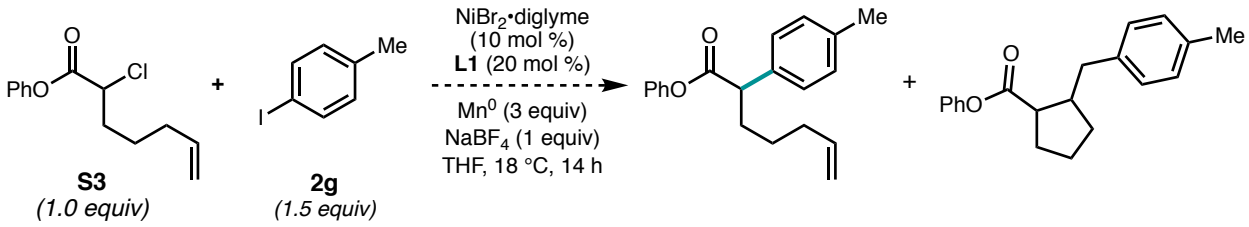
Radical trapping experiments



Radical trapping experiments were conducted according to a modified General Procedure 1 using phenyl 2-chloropropionate **1a** (36.9 mg, 1.0 equiv, 0.20 mmol) and 1-iodo-4-methylbenzene **2g** (65.4 mg, 1.5 equiv, 0.30 mmol). After the addition of solvent, 1.0 equiv radical trap was added (TEMPO, 31.3 mg, 0.2 mmol), (9,10-dihydroanthracene, 36.5 mg, 0.2 mmol), or (1,1-diphenylethylene, 36.0 mg, 0.2 mmol). The remainder of the procedure followed General Procedure 1. The addition of TEMPO resulted in 0% yield of **3g**, with both electrophiles remaining. The addition of 9,10-dihydroanthracene resulted in 0% yield of **3g**, but 20% phenyl propionate was formed, possibly through abstraction of a hydrogen atom by an intermediate α-ester radical. The addition of 1,1-diphenylethylene resulted in a 60% yield of **3g** in 84% ee; none of the product from radical addition to 1,1-diphenylethylene was detected.

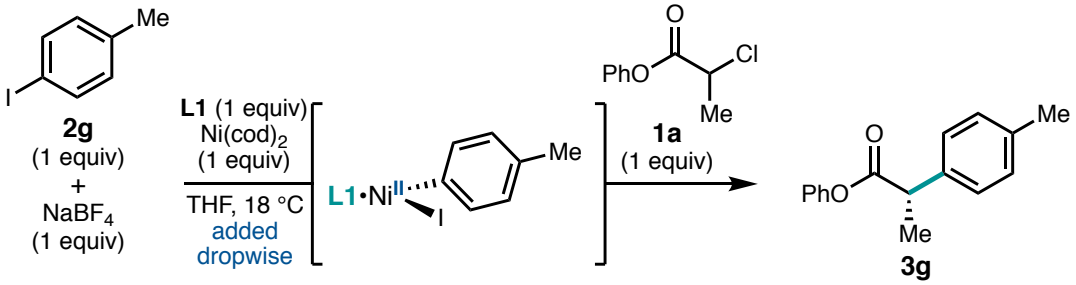
Radical clock experiments





Radical clock substrates **S2** and **S3** were subjected to standard reaction conditions using General Procedure 1. Shown are the expected rearranged and un-rearranged products. In both cases, no species could be cleanly isolated from the crude reaction mixture. ^{1}H-NMR spectra of the crude reaction mixtures are included for reference. For the reaction of **11**, no direct coupling was observed. Comparison of the crude NMR to independently-synthesized **12** shows a 10% yield of the ring-opened then coupled product.

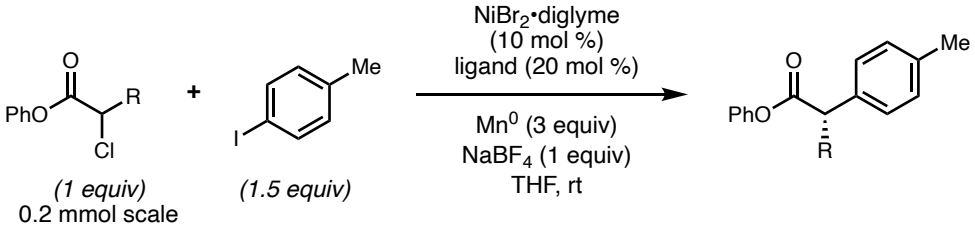
Stoichiometric Reaction



On the benchtop to a 1-dram vial equipped with a 12 mm Teflon-coated stir bar was added 4-heptyl BiOX **L1** (67.3 mg, 1.0 equiv, 0.2 mmol). The vial was sealed under argon and transferred to a nitrogen-filled glovebox. $Ni(cod)_2$ (55.0 mg, 1.0 equiv, 0.2 mmol) was added to the vial, followed by THF (1.0 mL). The vial was stirred at 50 °C for 5 minutes to fully dissolve; a deep blue solution formed. As the solution cooled to room temperature, a second 1-dram vial equipped with a 12-mm Teflon-coated stir bar was charged with 1-iodo-4-methylbenzene (43.6 mg, 1.0 equiv, 0.2 mmol), $NaBF_4$ (22.0 mg, 1.0 equiv, 0.2 mmol), and THF (1.0 mL). This vial was stirred at 700 rpm at room temperature. Once the solution became homogeneous (~2 minutes), the $Ni(cod)_2$•**L1** solution was added dropwise over five minutes. Each drop of the deep blue solution quickly dissipated upon addition, resulting in the solution turning from colorless to deep red/brown. Phenyl 2-chloropropionate (36.9 mg, 1.0 equiv, 0.2 mmol) was added via syringe. The reaction was sealed with a Teflon-lined cap and electrical tape, then removed from the glovebox and stirred at 18 °C for 14 hours. The reaction was worked up following General Procedure 1. To the crude residue was added 0.10 mmol 1,1,2,2-tetrachloroethane as a an internal standard. NMR analysis showed 72% yield of **3g**. An aliquot of the crude material was purified by preparative TLC (silica, 20:5:75 DCM/Et_2O/hexanes) then analyzed by chiral SFC using the conditions reported above for **3g** to give 81% ee.

e. Dataset Generation for Statistical Modelling

A 5 by 5 matrix of α-chloroesters and BiOX ligands were exhaustively explored for to generate a dataset for statistical modelling. Each of the five phenyl chloroesters (α-methyl, α-ethyl, α-isopropyl, α-cyclopentyl, and α-cyclohexyl) were coupled with 1-iodo-4-methylbenzene using General Procedure 1 and each of five BiOX ligands (isopropyl, 4-heptyl, benzhydril, cyclohexyl, and benzyl). All reactions were run in duplicate on 0.2 mmol scale. Yields were determined by 1H-NMR integration relative to 1,1,2,2-tetrachloroethane as an internal standard. Aliquots of the reactions were purified by preparative TLC to obtain clean material for chiral SFC analysis. The results of all runs are shown below (**Figure S1**), with the first yield and ee representing one trial and the second yield and ee representing the duplicate trial. For statistical modelling, the average ee of the two trials was used (yield was not used).



	S1	S2	S3	S4	S5
L2	48% yield 76% ee 42% yield 75% ee	65% yield 78% ee 66% yield 78% ee	39% yield 92% ee 37% yield 92% ee	57% yield 93% ee 57% yield 92% ee	40% yield 93% ee 38% yield 93% ee
L1	86% yield 85% ee 82% yield 84% ee	82% yield 87% ee 86% yield 87% ee	88% yield 97% ee 78% yield 97% ee	91% yield 97% ee 93% yield 97% ee	79% yield 98% ee 81% yield 98% ee
L5	0% yield –% ee 0% yield –% ee	23% yield 85% ee 24% yield 85% ee	25% yield 95% ee 35% yield 96% ee	12% yield 94% ee 12% yield 94% ee	18% yield 94% ee 17% yield 94% ee
L3	86% yield 64% ee 83% yield 65% ee	82% yield 77% ee 84% yield 77% ee	65% yield 92% ee 63% yield 92% ee	76% yield 94% ee 78% yield 94% ee	66% yield 94% ee 57% yield 94% ee
L6	61% yield 39% ee 79% yield 38% ee	72% yield 42% ee 81% yield 43% ee	54% yield 70% ee 51% yield 70% ee	65% yield 68% ee 70% yield 69% ee	61% yield 69% ee 56% yield 69% ee

Figure S1. Yield and ee data for 5 x 5 matrix of α-chloroesters and BiOX ligands.

f. Computational Methods

Conformational searches were performed with Macromodel[16] version 11.7 with OPLS3e[17] (substrates) or OPLS_2005[18] force field (complexes) and a constant dielectric of 7.58 corresponding to the dielectric constant of THF. To limit the number of conformers, an energy window of 10 kJ/mol relative to the minimum was utilized and mirror image conformations were not retained to avoid conformer duplication. Additionally, ligand conformers were found by performing the conformer searches with the full catalyst structure in order to restrict rotation about the central bond linking the two oxazoline rings. Subsequent DFT optimization of the ligand geometry was performed after removing the Ni and Br atoms. All conformers found under these conditions was submitted to DFT level optimization.

All structures were optimized in the gas phase with the B3LYP density functional,[19,20] the 6-31G* basis set, and ultrafine integration grid as implemented in Gaussian16 (revision C.01).[21] Single point energy calculations were then performed on the optimized structures with the MO6-2X density functional[22] and the triple-ζ valence quality def2-TZVP basis set of Weigend and Ahlrichs.[23] Every geometry was confirmed to be optimized to a minimum as evidenced by the lack of imaginary frequencies. Gaussian input files were written using an in-house Python script and parameters were then collected from the optimized ground-states in a similar fashion to previous reports from one of our labs.[24] Optimized structures were visualized using CYLview.[25]

Parameters Collected

The full compilation of calculated parameters for each ligand and substrate are in the accompanying spreadsheets. Sterimol parameters L, B_1, and B_5 represent the length of a specified axis and the minimum and maximum widths, respectively, of a specified group along that axis. All Sterimol parameters were calculated with a modified version of Paton's Python script and CPK radii.[26] Sterimol values were collected along one distinct axis for the BiOx ligands and three distinct axes for the substrates as identified in Figure S3. Molecular surface area values were calculated in Macromodel.[16] All other parameters were collected using an in-house Python script. Boltzmann-weighting of conformer properties utilizing a 2.5 kcal/mol cutoff (T = 298 K) was performed to obtain Boltzmann averaged properties.

Multivariate Correlation Analysis

All model development was performed using an in-house Python script with a forward stepwise linear regression algorithm. In a similar manner to previous work in our group, the model was evaluated according via three different validation techniques (leave one out (LOO), K-fold, and test R^2) in order to determine the robustness of the model as well as to check for model overfit.[12] The in-house script normalized each molecular feature in order to allow the coefficients of the features describe the relative importance of each feature. The modeling script normalized each parameter in order to allow for direct comparison of features included in a model. The 5 x 5 matrix used as the data set is shown in Figure S2 and the structures of the ligands and substrates used to construct the matrix are in Table S1. The ensuing 25 data points were split via a 75:25 ratio between the training set and test set. The split could be partitioned based on the response values using either the "equidistant", "random", or "kennard-stone" functions written into the Python script. As noted in the main text, the same 2-parameter models were generated with only slight variation in the statistics of each model, regardless of the split method used. All three models are shown below in Figure S4; the model using the "equidistant" partition is included in the main text.

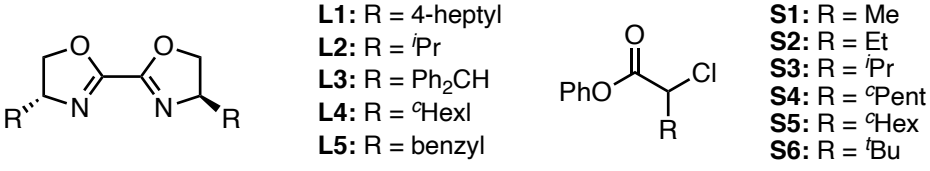


Figure S2. Structures of substrates/ligands used to construct the matrix

Table S1. Matrix with enantiomeric excess for each substrate/ligand combination.

Entry	L1	L2	L3	L4	L5
S1	84.5	75.5	64.5	-	38.5
S2	87	78	77	85	42.5
S3	97	92	92	95.5	70
S4	97	92.5	94	94	68.5
S5	98	93	94	94	69
S6	-	89	-	-	-

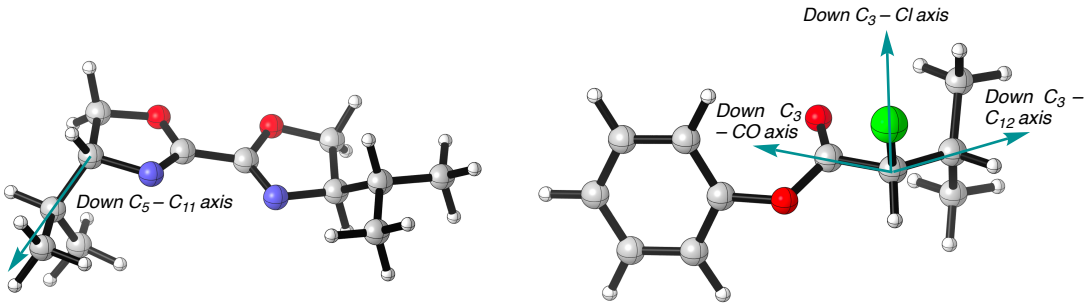


Figure S3. Axes along which Sterimol values were calculated for ligand and substrate.

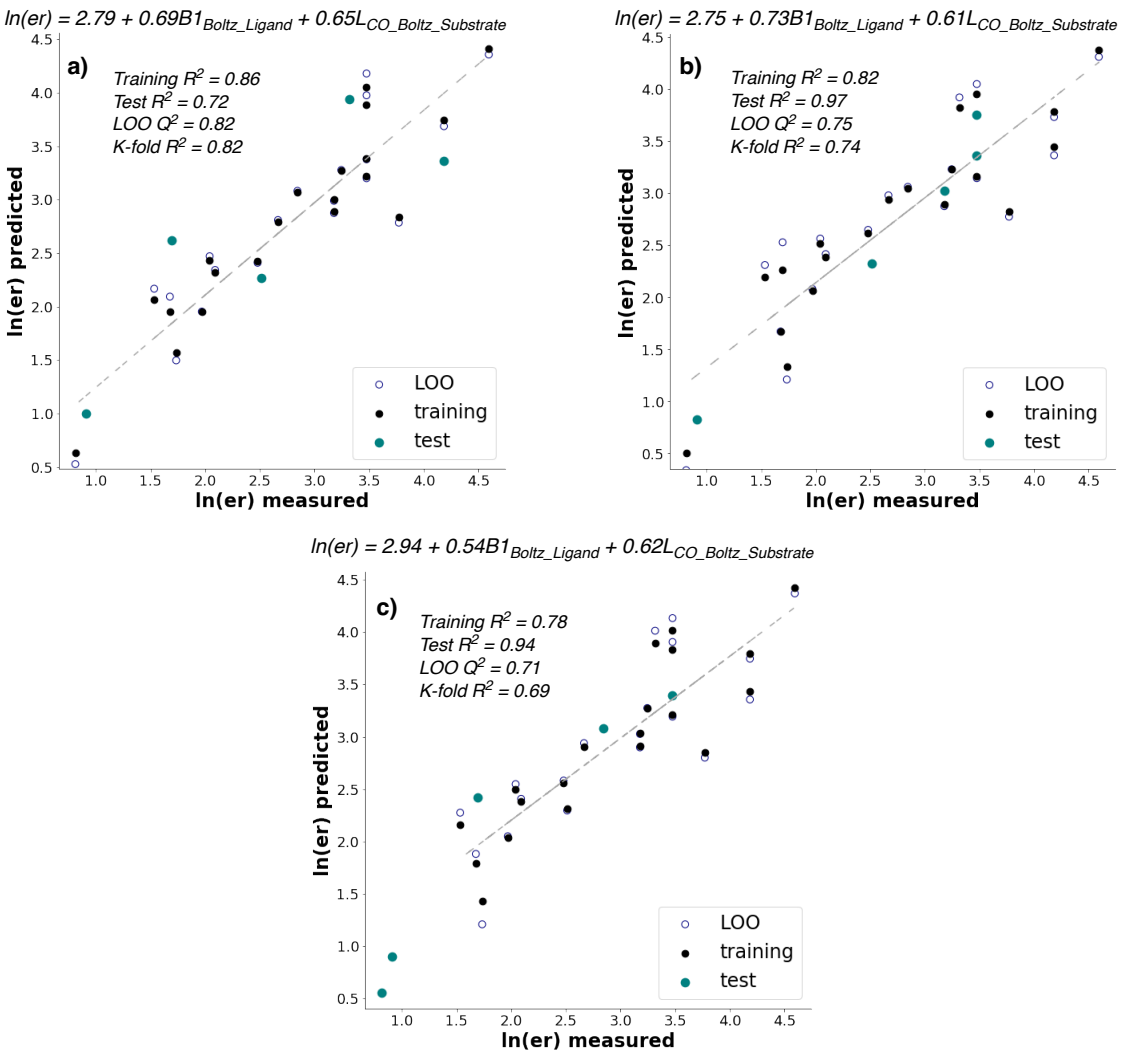
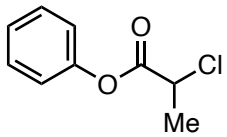


Figure S4a). Model generated with equidistant splitting method to develop training and test sets. **b)** Model generated with random splitting method to develop training and test sets. **c)** Model generated with the kennard-stone splitting method to develop training and test sets. Training/test split ratio of 0.25 used for all splits.

Cartesian Coordinates of Substrate Conformers (B3LYP/6-31G* Geometry)



S1_1 Ground State

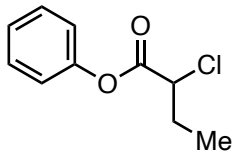
O	-0.07004	-0.36813	-0.59645
C	-0.99939	-0.39202	0.39348
C	-2.39074	-0.53421	-0.21291
O	-0.77011	-0.31675	1.57397
C	1.27561	-0.14518	-0.28117
C	2.19730	-1.02673	-0.83535
C	3.55782	-0.80996	-0.61691
C	3.98058	0.27633	0.15014
C	3.03841	1.15070	0.69558
C	1.67543	0.94870	0.48183
Cl	-2.89064	1.13596	-0.77212
C	-3.39549	-1.08679	0.77826
H	-2.33095	-1.12956	-1.12483
H	1.84260	-1.86232	-1.42960
H	4.28486	-1.49223	-1.04728
H	5.03986	0.44261	0.32121
H	3.36292	1.99864	1.29136
H	0.93692	1.62091	0.90126
H	-3.42293	-0.46880	1.67782
H	-4.39101	-1.12580	0.33016
H	-3.09737	-2.10078	1.06814

S1_2 Ground State

O	0.07003	0.36806	-0.59639
C	0.99948	0.39220	0.39338
C	2.39077	0.53404	-0.21324
O	0.77040	0.31734	1.57397
C	-1.27564	0.14521	-0.28101
C	-2.19727	1.02679	-0.83520
C	-3.55782	0.80998	-0.61691
C	-3.98062	-0.27633	0.15007
C	-3.03847	-1.15074	0.69551
C	-1.67547	-0.94874	0.48188
Cl	2.89043	-1.13635	-0.77168
C	3.39566	1.08707	0.77759
H	2.33091	1.12904	-1.12538
H	-1.84255	1.86240	-1.42939
H	-4.28482	1.49227	-1.04731
H	-5.03990	-0.44266	0.32108
H	-3.36304	-1.99873	1.29119
H	-0.93701	-1.62096	0.90138
H	3.42313	0.46949	1.67742
H	4.39115	1.12582	0.32940
H	3.09762	2.10122	1.06703

S1_3 Ground State

O	-0.21152	0.37875	-0.18310
C	-1.01539	-0.15561	0.77084
C	-2.47508	0.17101	0.48311
O	-0.64391	-0.78101	1.73187
C	1.17083	0.16820	-0.13198
C	1.97331	1.29485	-0.27556
C	3.35914	1.14015	-0.30749
C	3.92555	-0.13007	-0.19372
C	3.10142	-1.24828	-0.05275
C	1.71420	-1.10910	-0.02362
Cl	-2.99490	-0.77447	-0.98994
C	-2.73682	1.65600	0.27998
H	-3.05425	-0.23565	1.31135
H	1.50750	2.27075	-0.36414
H	3.99336	2.01432	-0.42111
H	5.00456	-0.24916	-0.21651
H	3.53771	-2.23895	0.03397
H	1.06726	-1.97052	0.08672
H	-2.17198	2.03281	-0.57493
H	-3.80240	1.83228	0.11319
H	-2.42807	2.20535	1.17747



S2_1 Ground State

O	0.23996	-0.37140	0.67727
C	-0.75687	-0.34364	-0.25847
C	-2.07782	-0.49598	0.49137
O	-0.59885	-0.18566	-1.43789
C	1.57012	-0.16809	0.29173
C	2.50065	-1.07372	0.79079
C	3.85272	-0.88405	0.50614
C	4.26013	0.19974	-0.27278
C	3.31058	1.09768	-0.76366
C	1.95567	0.92318	-0.48288
Cl	-3.40116	-0.92547	-0.65942
C	-2.41061	0.78101	1.28105
C	-2.48738	2.04760	0.42837
H	-1.98832	-1.33798	1.18015

H	2.15803	-1.90790	1.39399
H	4.58520	-1.58606	0.89337
H	5.31271	0.34475	-0.49639
H	3.62243	1.94258	-1.37047
H	1.21370	1.61241	-0.86610
H	-3.35920	0.61168	1.80112
H	-1.63432	0.88529	2.04853
H	-3.24718	1.95113	-0.35234
H	-2.74488	2.90848	1.05327
H	-1.53052	2.26268	-0.05998

S2_2 Ground State

O	-0.17726	-0.00130	-0.70598
C	0.79138	0.14116	0.23548
C	2.16270	-0.01875	-0.41073
O	0.60381	0.35969	1.40594
C	-1.52414	0.01333	-0.32402
C	-2.36574	0.85034	-1.04847
C	-3.73086	0.85106	-0.76172
C	-4.23715	0.02326	0.24104
C	-3.37474	-0.81119	0.95499
C	-2.00862	-0.82538	0.67619
Cl	2.49581	-1.81768	-0.45980
C	3.25764	0.71138	0.35203
C	3.06882	2.23164	0.29242
H	2.11262	0.29104	-1.45576
H	-1.94703	1.48265	-1.82437
H	-4.39599	1.50010	-1.32356
H	-5.29968	0.02638	0.46472
H	-3.76476	-1.45860	1.73474
H	-1.33130	-1.46824	1.22497
H	4.22224	0.43005	-0.08218
H	3.24567	0.36757	1.39038
H	3.05820	2.59416	-0.74249
H	2.13353	2.53259	0.77398
H	3.88955	2.73468	0.81330

S2_3 Ground State

O	-0.17723	-0.00136	-0.70579
C	0.79143	0.14107	0.23570
C	2.16270	-0.01875	-0.41061
O	0.60386	0.35961	1.40615
C	-1.52408	0.01322	-0.32401
C	-2.36553	0.85070	-1.04808
C	-3.73068	0.85156	-0.76143
C	-4.23721	0.02335	0.24085
C	-3.37496	-0.81159	0.95447
C	-2.00884	-0.82589	0.67579
Cl	2.49589	-1.81763	-0.45992
C	3.25759	0.71142	0.35217
C	3.06869	2.23169	0.29227
H	2.11252	0.29118	-1.45559
H	-1.94667	1.48335	-1.82364
H	-4.39559	1.50101	-1.32305
H	-5.29975	0.02650	0.46448
H	-3.76518	-1.45930	1.73388
H	-1.33170	-1.46915	1.22429
H	4.22222	0.43006	-0.08196
H	3.24555	0.36777	1.39056
H	2.13325	2.53267	0.77352
H	3.88922	2.73486	0.81335
H	3.05838	2.59403	-0.74270

S2_4 Ground State

O	0.29579	-0.27033	-0.61269
C	-0.64054	-0.24725	0.37173
C	-2.03316	-0.28197	-0.24496
O	-0.41330	-0.20970	1.55455
C	1.65104	-0.14673	-0.28510
C	2.51372	-1.08101	-0.84794
C	3.88436	-0.96249	-0.61771
C	4.37560	0.07942	0.16985
C	3.49218	1.00808	0.72378
C	2.12009	0.90446	0.49829
Cl	-2.41354	1.44054	-0.74280
C	-3.07593	-0.82610	0.71976
C	-4.47566	-0.93483	0.11698
H	-2.00593	-0.84331	-1.18064
H	2.10641	-1.88032	-1.45815
H	4.56561	-1.68646	-1.05484
H	5.44256	0.16919	0.35024
H	3.87023	1.82185	1.33545
H	1.42670	1.61935	0.92413
H	-3.07717	-0.20405	1.61971
H	-2.72232	-1.81823	1.03184
H	-4.47636	-1.57089	-0.77626
H	-5.16842	-1.37372	0.84187
H	-4.86123	0.04812	-0.16869

S2_5 Ground State

O	0.29578	0.27114	0.61284
C	-0.64052	0.24744	-0.37158
C	-2.03316	0.28205	0.24499
O	-0.41320	0.20947	-1.55435

C	1.65105	0.14708	0.28522
C	2.51401	1.08124	0.84775
C	3.88460	0.96231	0.61729
C	4.37546	-0.07991	-0.17005
C	3.49169	-1.00846	-0.72370
C	2.11969	-0.90439	-0.49804
Cl	-2.41334	-1.44044	0.74294
C	-3.07591	0.82596	-0.71987
C	-4.47575	0.93443	-0.11724
H	-2.00613	0.84347	1.18065
H	2.10701	1.88086	1.45775
H	4.56613	1.68618	1.05417
H	5.44238	-0.17001	-0.35053
H	3.86945	-1.82242	-1.33531
H	1.42603	-1.61913	-0.92371
H	-3.07693	0.20394	-1.61984
H	-2.72247	1.81817	-1.03187
H	-4.47664	1.57043	0.77605
H	-5.16850	1.37326	-0.84218
H	-4.86117	-0.04861	0.16831

S2_6 Ground State

O	-0.03892	0.04530	-0.36089
C	-0.83938	-0.23177	0.70086
C	-2.30520	-0.13592	0.29988
O	-0.45981	-0.48711	1.81572
C	1.35172	0.01051	-0.21419
C	2.05045	1.11847	-0.68152
C	3.44421	1.11283	-0.62803
C	4.12117	0.00846	-0.10899
C	3.40035	-1.09458	0.35280
C	2.00681	-1.10447	0.30145
Cl	-2.69543	-1.54252	-0.79449
C	-2.66630	1.18550	-0.37420
C	-2.34889	2.38379	0.52774
H	-2.88695	-0.29663	1.20769
H	1.49963	1.96281	-1.08288
H	3.99807	1.97290	-0.99250
H	5.20612	0.00586	-0.06584
H	3.92319	-1.95687	0.75580
H	1.43888	-1.95449	0.65883
H	-3.73379	1.16173	-0.61675
H	-2.11689	1.25964	-1.31707
H	-1.27544	2.45666	0.73462
H	-2.65815	3.31506	0.04302
H	-2.87225	2.31388	1.48796

S2_7 Ground State

O	0.25493	0.69218	-0.30309
C	-0.72924	-0.23321	-0.43369
C	-2.08061	0.46501	-0.56400
O	-0.55716	-1.42573	-0.48512
C	1.57786	0.27818	-0.11265
C	2.53456	0.85288	-0.94219
C	3.87872	0.53451	-0.74817
C	4.25081	-0.35128	0.26376
C	3.27438	-0.91550	1.08711
C	1.92759	-0.60247	0.90747
Cl	-2.41784	1.36698	0.99094
C	-3.22713	-0.47402	-0.93017
C	-3.60959	-1.51235	0.12645
H	-1.97486	1.25196	-1.31459
H	2.21925	1.54052	-1.71990
H	4.63279	0.98034	-1.38999
H	5.29732	-0.59982	0.41225
H	3.55940	-1.60344	1.87756
H	1.16280	-1.03498	1.54103
H	-2.92533	-0.97962	-1.85657
H	-4.09432	0.14931	-1.17499
H	-3.94059	-1.02839	1.04987
H	-4.43350	-2.13068	-0.24460
H	-2.76590	-2.16603	0.35624

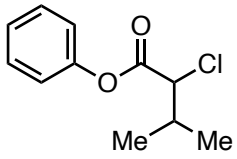
S2_8 Ground State

O	0.10239	0.20547	-0.21598
C	-0.64837	-0.36811	0.75878
C	-2.13072	-0.21331	0.45149
O	-0.21971	-0.89865	1.75270
C	1.49865	0.15752	-0.14321
C	2.16927	1.36026	-0.33745
C	3.56400	1.36425	-0.35045
C	4.27019	0.17467	-0.16770
C	3.57726	-1.02234	0.02334
C	2.18296	-1.04197	0.03423
Cl	-2.52363	-1.23408	-1.01201
C	-2.54899	1.24141	0.24288
C	-4.05995	1.42867	0.10998
H	-2.67258	-0.67019	1.27994
H	1.59617	2.27057	-0.47924
H	4.09572	2.29872	-0.50334
H	5.35597	0.17921	-0.17581
H	4.12259	-1.95088	0.16383
H	1.63713	-1.96537	0.18303
H	-2.02517	1.63439	-0.63360

H	-2.17939	1.80174	1.11353
H	-4.58508	1.05106	0.99504
H	-4.30417	2.49013	0.00101
H	-4.44663	0.89907	-0.76543

S2_9 Ground State

O	-0.02946	-0.09479	-0.39085
C	-0.79305	-0.74796	0.51088
C	-2.28592	-0.61134	0.23912
O	-0.38972	-1.32711	1.49098
C	1.35790	-0.01919	-0.22112
C	1.92031	1.24107	-0.39785
C	3.30469	1.38380	-0.31103
C	4.10884	0.27339	-0.05003
C	3.52428	-0.98290	0.11915
C	2.14115	-1.14218	0.03230
Cl	-2.68377	-0.36232	-1.51477
C	-2.87971	0.50718	1.11125
C	-2.27543	1.89176	0.87473
H	-2.73899	-1.56502	0.51118
H	1.27167	2.08544	-0.60601
H	3.75199	2.36371	-0.44887
H	5.18665	0.38556	0.01893
H	4.14625	-1.85022	0.31982
H	1.68093	-2.11245	0.16684
H	-2.72429	0.19807	2.15245
H	-3.96042	0.52492	0.93597
H	-2.38018	2.19322	-0.17163
H	-2.78387	2.63474	1.49720
H	-1.21070	1.91491	1.12999



S3_1 Ground State

O	-0.40235	0.00308	-0.79087
C	0.59106	-0.44410	0.03294
C	1.93046	-0.11335	-0.61249
O	0.42306	-0.95764	1.10771
C	-1.73596	-0.04639	-0.36739
C	-2.31743	-1.21823	0.10996
C	-3.67037	-1.20030	0.44892
C	-4.42452	-0.03403	0.30725
C	-3.82284	1.12755	-0.17891
C	-2.47018	1.12586	-0.51832
Cl	3.02133	-1.55917	-0.50322
C	2.58172	1.13885	0.01604
C	2.90403	0.98364	1.50519
C	1.68953	2.36527	-0.23636
H	1.77236	0.05500	-1.67750
H	-1.72423	-2.11677	0.22145
H	-4.13498	-2.10662	0.82575
H	-5.47722	-0.03146	0.57341
H	-4.40364	2.03778	-0.29511
H	-1.97825	2.01398	-0.90115
H	3.52163	1.27855	-0.53280
H	3.55608	0.12508	1.68437
H	3.41363	1.88366	1.86565
H	1.99401	0.84453	2.09610
H	0.75461	2.30251	0.33181
H	2.21052	3.27351	0.08328
H	1.43409	2.47401	-1.29613

S3_2 Ground State

O	0.48836	-0.16599	0.68807
C	-0.43287	-0.51087	-0.26268
C	-1.80702	-0.44316	0.39602
O	-0.18271	-0.76847	-1.40856
C	1.83816	-0.04406	0.33824
C	2.75096	-0.70564	1.15290
C	4.11501	-0.56044	0.90054
C	4.55148	0.23596	-0.15894
C	3.61902	0.89192	-0.96481
C	2.25240	0.75953	-0.72086
Cl	-2.98914	-1.43029	-0.54936
C	-2.26049	1.02580	0.56356
C	-3.54999	1.11829	1.38477
C	-2.38473	1.76283	-0.77399
H	-1.74127	-0.91100	1.38010
H	2.38572	-1.31895	1.96992
H	4.83421	-1.07249	1.53288
H	5.61355	0.34575	-0.35618
H	3.95371	1.51259	-1.79069
H	1.52298	1.26123	-1.34471
H	-1.45076	1.48886	1.14425
H	-3.79747	2.16727	1.57895
H	-4.38913	0.66481	0.84842
H	-3.44741	0.60956	2.35011
H	-1.45826	1.71784	-1.35530
H	-3.18189	1.32787	-1.38452
H	-2.62551	2.81639	-0.59844

S3_3 Ground State

O	0.48163	0.03168	-0.79256
C	-0.53956	-0.11791	0.09485
C	-1.86297	0.07782	-0.63725
O	-0.40270	-0.36772	1.26622
C	1.80331	-0.00580	-0.33327
C	2.66893	-0.87481	-0.98804
C	4.01419	-0.89585	-0.61925
C	4.47641	-0.05681	0.39535
C	3.59034	0.80947	1.03916
C	2.24431	0.84404	0.67747
Cl	-2.16214	1.88419	-0.68104
C	-3.05863	-0.68858	-0.05787
C	-3.47392	-0.26946	1.35666
C	-2.76471	-2.19635	-0.13584
H	-1.71580	-0.19650	-1.68272
H	2.28453	-1.51573	-1.77457
H	4.69834	-1.56965	-1.12644
H	5.52334	-0.07592	0.68275
H	3.94626	1.46549	1.82798
H	1.54785	1.51191	1.17008
H	-3.89216	-0.46926	-0.73797
H	-3.69458	0.80056	1.40319
H	-4.37886	-0.81483	1.64613
H	-2.68638	-0.49104	2.07935
H	-3.65507	-2.76480	0.15165
H	-2.48356	-2.50495	-1.14997
H	-1.95521	-2.47286	0.54721

S3_4 Ground State

O	0.55839	0.70966	-0.11360
C	-0.41556	-0.20965	-0.33946
C	-1.78244	0.46410	-0.25364
O	-0.22261	-1.36971	-0.60622
C	1.89746	0.30595	-0.07479
C	2.78927	1.02912	-0.85917
C	4.14801	0.71861	-0.80146
C	4.59856	-0.30650	0.03111
C	3.68640	-1.01907	0.81217
C	2.32620	-0.71607	0.76789
Cl	-2.04087	0.98308	1.48332
C	-2.93638	-0.39416	-0.78490
C	-4.19048	0.46227	-0.99495
C	-3.24167	-1.63081	0.06840
H	-1.72291	1.40453	-0.80702
H	2.41363	1.82283	-1.49637
H	4.85193	1.27964	-1.40897
H	5.65622	-0.54849	0.07334
H	4.03272	-1.81610	1.46342
H	1.61047	-1.26266	1.36998
H	-2.58296	-0.73920	-1.76732
H	-3.99162	1.31798	-1.65102
H	-4.98526	-0.13622	-1.45198
H	-4.56460	0.84653	-0.04013
H	-3.62298	-1.33920	1.05199
H	-4.01000	-2.23556	-0.42503
H	-2.35227	-2.24860	0.20409

S3_4 Ground State

O	-0.49262	0.03461	-0.69218
C	0.46032	0.02988	0.27740
C	1.83861	-0.08675	-0.36224
O	0.25234	0.10041	1.46234
C	-1.84570	0.04412	-0.33238
C	-2.37472	-0.90104	0.54245
C	-3.74491	-0.87843	0.79995
C	-4.56745	0.06963	0.18805
C	-4.01686	1.00386	-0.69016
C	-2.64711	0.99560	-0.95380
Cl	2.16769	-1.88790	-0.45130
C	2.91727	0.66312	0.42069
C	2.55676	2.15856	0.45511
C	4.31054	0.45739	-0.18093
H	1.79377	0.24479	-1.40105
H	-1.72773	-1.63126	1.01296
H	-4.16951	-1.60844	1.48267
H	-5.63351	0.07857	0.39411
H	-4.65092	1.74197	-1.17231
H	-2.19420	1.70951	-1.63379
H	2.89830	0.27665	1.44584
H	1.59634	2.33484	0.94713
H	3.32236	2.71194	1.00848
H	2.51331	2.57652	-0.55863
H	4.34643	0.81628	-1.21737
H	5.05227	1.02229	0.39334
H	4.60409	-0.59512	-0.17541

S3_6 Ground State

O	0.20923	-0.44638	-0.09139
C	-0.62326	0.12268	0.80902
C	-2.07764	-0.26461	0.58306
O	-0.29751	0.90744	1.66788
C	1.58052	-0.16849	-0.06789
C	2.42440	-1.27023	-0.16350

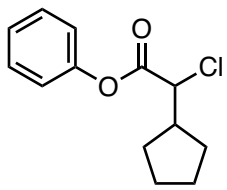
C	3.80221	-1.06483	-0.22426
C	4.32056	0.23065	-0.18878
C	3.45586	1.32254	-0.09619
C	2.07510	1.13298	-0.03717
Cl	-2.25796	-2.01328	0.11489
C	-2.78250	0.66025	-0.43750
C	-2.12727	0.65156	-1.82231
C	-2.88411	2.08460	0.12838
H	-2.56811	-0.17113	1.55200
H	1.99266	-2.26500	-0.19234
H	4.46842	-1.91910	-0.29941
H	5.39379	0.38925	-0.23425
H	3.85462	2.33233	-0.06929
H	1.39905	1.97456	0.04239
H	-3.79772	0.25544	-0.53129
H	-2.01757	-0.36556	-2.20767
H	-2.74346	1.22158	-2.52551
H	-1.13420	1.11290	-1.79812
H	-1.89558	2.53587	0.25970
H	-3.45630	2.71563	-0.55969
H	-3.38719	2.09788	1.10124

S3_7 Ground State

O	0.25432	-0.04221	-0.33569
C	-0.49676	-0.38695	0.74265
C	-1.97583	-0.37698	0.38515
O	-0.06973	-0.63393	1.84218
C	1.64668	0.02301	-0.22302
C	2.25041	1.18656	-0.68782
C	3.64172	1.28329	-0.66706
C	4.41067	0.22435	-0.18268
C	3.78455	-0.93588	0.27713
C	2.39469	-1.04808	0.25816
Cl	-2.27836	-1.75995	-0.76937
C	-2.45497	0.96333	-0.19076
C	-2.04789	2.09883	0.76329
C	-3.96839	0.96414	-0.42502
H	-2.52026	-0.62942	1.29608
H	1.62918	1.99356	-1.06232
H	4.12167	2.18735	-1.02992
H	5.49361	0.30140	-0.16498
H	4.37920	-1.76308	0.65321
H	1.89965	-1.94298	0.61431
H	-1.94006	1.10690	-1.14733
H	-0.96185	2.16834	0.88256
H	-2.40271	3.05792	0.37233
H	-2.49002	1.95807	1.75682
H	-4.50865	0.81622	0.51842
H	-4.28386	1.92567	-0.84360
H	-4.26979	0.17474	-1.11830

S3_8 Ground State

O	0.33753	-0.41446	-0.04860
C	-0.47104	0.19250	0.84580
C	-1.94152	-0.16011	0.66434
O	-0.12384	0.99410	1.68047
C	1.71280	-0.15384	-0.05734
C	2.22602	1.14088	-0.05064
C	3.60772	1.30969	-0.14172
C	4.45489	0.20478	-0.24210
C	3.91772	-1.08336	-0.25351
C	2.53877	-1.26836	-0.16085
Cl	-2.20109	-1.80058	-0.07271
C	-2.66332	0.95981	-0.11978
C	-4.18172	0.76167	-0.10219
C	-2.12887	1.13002	-1.54585
H	-2.36480	-0.22115	1.66786
H	1.56407	1.99280	0.03586
H	4.02119	2.31387	-0.13382
H	5.52897	0.34774	-0.31246
H	4.56982	-1.94786	-0.33508
H	2.09272	-2.25714	-0.17160
H	-2.42800	1.86785	0.45310
H	-4.55974	0.65526	0.92095
H	-4.67797	1.62430	-0.55916
H	-4.46736	-0.13223	-0.66509
H	-2.30307	0.22557	-2.13694
H	-2.64111	1.96283	-2.03862
H	-1.05457	1.33883	-1.56078



S4_1 Ground State

O	1.07413	0.17878	-0.70748
C	0.08948	0.16268	0.22935
C	-1.23361	0.56558	-0.40903
O	0.23345	-0.12820	1.39014
C	2.39745	-0.06982	-0.32512
C	3.00798	0.64929	0.69897
C	4.35120	0.40185	0.97939
C	5.06822	-0.54383	0.24356

C	4.43811	-1.24878	-0.78266
C	3.09360	-1.01451	-1.07120
Cl	-1.27015	2.39921	-0.37888
C	-2.42522	-0.03073	0.31443
C	-3.79507	0.35863	-0.26715
C	-4.71206	-0.76453	0.23299
C	-3.86583	-2.03552	0.02975
C	-2.39597	-1.58956	0.25895
H	-1.22901	0.30026	-1.46787
H	2.44252	1.37995	1.26437
H	4.83810	0.95418	1.77763
H	6.11426	-0.72876	0.46859
H	4.99023	-1.98332	-1.36142
H	2.58072	-1.54764	-1.86487
H	-2.37247	0.28770	1.36050
H	-4.11290	1.35885	0.03852
H	-3.75331	0.34666	-1.36566
H	-5.67335	-0.80170	-0.28959
H	-4.92399	-0.61682	1.29996
H	-3.99111	-2.39954	-0.99669
H	-4.16198	-2.85178	0.69584
H	-1.97340	-1.99010	1.18334
H	-1.75221	-1.94359	-0.55632

S4_2 Ground State

O	1.07418	0.17868	-0.70760
C	0.08956	0.16253	0.22927
C	-1.23354	0.56552	-0.40906
O	0.23357	-0.12845	1.39003
C	2.39749	-0.06987	-0.32518
C	3.09358	-1.01492	-1.07086
C	4.43809	-1.24912	-0.78225
C	5.06823	-0.54376	0.24366
C	4.35127	0.40226	0.97911
C	3.00806	0.64963	0.69859
Cl	-1.26999	2.39915	-0.37875
C	-2.42519	-0.03078	0.31434
C	-3.79498	0.35883	-0.26718
C	-4.71228	-0.76415	0.23283
C	-3.86622	-2.03543	0.03042
C	-2.39617	-1.58957	0.25847
H	-1.22894	0.30030	-1.46792
H	2.58067	-1.54835	-1.86430
H	4.99017	-1.98394	-1.36069
H	6.11427	-0.72863	0.46875
H	4.83819	0.95491	1.77710
H	2.44263	1.38058	1.26368
H	-2.37241	0.28739	1.36050
H	-4.11265	1.35907	0.03855
H	-3.75319	0.34694	-1.36570
H	-5.67333	-0.80132	-0.29020
H	-4.92472	-0.61608	1.29964
H	-3.99203	-2.40057	-0.99556
H	-4.16213	-2.85090	0.69757
H	-1.97286	-1.99044	1.18239
H	-1.75318	-1.94334	-0.55752

S4_3 Ground State

O	-0.74913	0.25854	-0.33666
C	-0.07919	0.71738	0.75223
C	1.37199	1.00998	0.40064
O	-0.54245	0.83862	1.85852
C	-2.09982	-0.08711	-0.22991
C	-2.46025	-1.33339	-0.73110
C	-3.80409	-1.70667	-0.71823
C	-4.76796	-0.83754	-0.20550
C	-4.38505	0.41012	0.29076
C	-3.04563	0.79809	0.28015
Cl	1.41761	2.44953	-0.72371
C	2.08898	-0.19034	-0.20287
C	3.59618	0.00667	-0.43063
C	4.11261	-1.43381	-0.53841
C	3.35032	-2.18255	0.57456
C	1.99373	-1.43769	0.72453
H	1.85788	1.33853	1.32014
H	-1.69117	-1.98882	-1.12655
H	-4.09461	-2.67725	-1.10929
H	-5.81364	-1.12982	-0.19399
H	-5.13202	1.09038	0.68899
H	-2.73860	1.76292	0.66435
H	1.61118	-0.41839	-1.16151
H	3.81361	0.62154	-1.30790
H	4.04268	0.50303	0.44265
H	5.19980	-1.51029	-0.43626
H	3.84737	-1.84363	-1.52154
H	3.91208	-2.12564	1.51348
H	3.21813	-3.24484	0.34766
H	1.13887	-2.06074	0.44494
H	1.83089	-1.13511	1.76558

S4_4 Ground State

O	0.72187	-0.62782	0.76162
C	-0.25589	-0.76427	-0.18393
C	-1.58204	-1.03583	0.51790

O	-0.08472	-0.63999	-1.36801
C	2.00565	-0.24717	0.34612
C	3.05178	-1.11775	0.62631
C	4.35306	-0.73779	0.29538
C	4.59153	0.49633	-0.31048
C	3.52536	1.35602	-0.58361
C	2.22135	0.98972	-0.25409
Cl	-2.39947	-2.43337	-0.30696
C	-2.50075	0.19840	0.54135
C	-1.88784	1.34559	1.40484
C	-2.14205	2.63455	0.60300
C	-2.04226	2.17037	-0.85656
C	-2.78518	0.82399	-0.85532
H	-1.37950	-1.36912	1.53567
H	2.83932	-2.07195	1.09672
H	5.17847	-1.40964	0.51104
H	5.60481	0.78854	-0.56900
H	3.70690	2.31711	-1.05541
H	1.38445	1.64760	-0.45999
H	-3.43574	-0.14522	0.99339
H	-2.32049	1.37116	2.40969
H	-0.80964	1.19785	1.53132
H	-1.43983	3.43502	0.85908
H	-3.15434	3.00938	0.80275
H	-0.99152	2.01398	-1.13232
H	-2.46263	2.88679	-1.56971
H	-2.48013	0.17043	-1.67438
H	-3.86258	0.99489	-0.95493

S4_5 Ground State

O	-1.04296	0.38327	0.70463
C	-0.15172	0.75355	-0.26364
C	1.20878	0.91169	0.40519
O	-0.40466	0.86589	-1.43283
C	-2.34897	0.02801	0.34738
C	-3.37463	0.62427	1.07305
C	-4.69360	0.25148	0.81419
C	-4.97359	-0.70415	-0.16335
C	-3.92921	-1.29096	-0.88054
C	-2.60568	-0.93136	-0.62879
Cl	2.24019	2.03166	-0.57212
C	1.86017	-0.47047	0.59273
C	2.17878	-1.21417	-0.74053
C	3.70043	-1.45696	-0.72121
C	4.04072	-1.54758	0.77388
C	3.18917	-0.42613	1.38815
H	1.07275	1.39169	1.37580
H	-3.13018	1.36463	1.82749
H	-5.50042	0.71111	1.37728
H	-6.00101	-0.99109	-0.36593
H	-4.14217	-2.03479	-1.64258
H	-1.78984	-1.37726	-1.18444
H	1.12214	-1.04564	1.16473
H	1.64225	-2.16937	-0.76104
H	1.85710	-0.64513	-1.61647
H	4.21713	-0.59600	-1.16190
H	3.99467	-2.34607	-1.28816
H	5.10902	-1.43219	0.98443
H	3.72873	-2.52254	1.17199
H	3.02697	-0.53852	2.46513
H	3.68641	0.53644	1.22633

S4_6 Ground State

O	1.20394	0.79928	-0.08751
C	0.15715	-0.04095	-0.29861
C	-1.15314	0.72381	-0.15190
O	0.24875	-1.20958	-0.58033
C	2.50895	0.29459	-0.08499
C	3.43806	0.96763	-0.87082
C	4.77028	0.55467	-0.84838
C	5.15769	-0.52136	-0.04893
C	4.20912	-1.18222	0.73420
C	2.87501	-0.77717	0.72497
Cl	-1.38918	1.03836	1.64016
C	-2.34001	-0.00444	-0.76993
C	-2.75331	-1.33808	-0.07405
C	-4.24156	-1.16835	0.29387
C	-4.76946	-0.15252	-0.73022
C	-3.62156	0.86261	-0.82150
H	-1.02930	1.71837	-0.58596
H	3.11146	1.80250	-1.48193
H	5.50298	1.07582	-1.45739
H	6.19464	-0.84314	-0.03414
H	4.50641	-2.01871	1.35969
H	2.13159	-1.28352	1.32853
H	-2.02128	-0.22763	-1.79639
H	-2.61494	-2.16852	-0.77192
H	-2.13371	-1.55524	0.79820
H	-4.32934	-0.74510	1.30216
H	-4.78969	-2.11612	0.28598
H	-5.72077	0.30507	-0.43946
H	-4.92036	-0.64080	-1.70246
H	-3.66053	1.49140	-1.71748
H	-3.65582	1.52660	0.05045

S4_7 Ground State

O	0.63033	-0.51448	0.87717
C	-0.34896	-0.84210	-0.01876
C	-1.68736	-0.82814	0.70837
O	-0.16742	-1.04589	-1.19052
C	1.93320	-0.29604	0.41075
C	2.51030	0.93046	0.72307
C	3.82857	1.17549	0.33805
C	4.54965	0.20084	-0.35285
C	3.95100	-1.02363	-0.65619
C	2.63522	-1.28364	-0.27412
Cl	-2.70357	-2.21052	0.11798
C	-2.43617	0.50918	0.53440
C	-1.60326	1.70908	1.07614
C	-1.05989	2.41279	-0.17732
C	-2.22869	2.29483	-1.16574
C	-2.75812	0.86161	-0.94903
H	-1.51096	-1.01772	1.76704
H	1.92826	1.67123	1.26108
H	4.28886	2.12913	0.57886
H	5.57494	0.39378	-0.65380
H	4.50886	-1.78423	-1.19423
H	2.15843	-2.22747	-0.50842
H	-3.35646	0.40016	1.11567
H	-2.27608	2.38876	1.61171
H	-0.82365	1.40501	1.78052
H	-0.18258	1.88223	-0.56811
H	-0.75599	3.44693	0.01656
H	-1.93663	2.47926	-2.20431
H	-3.00114	3.03060	-0.90638
H	-2.24417	0.16714	-1.61821
H	-3.82742	0.77284	-1.15759

S4_8 Ground State

O	-1.02201	0.44431	0.68666
C	-0.12691	0.76704	-0.29586
C	1.23024	0.95700	0.37176
O	-0.37541	0.82423	-1.46948
C	-2.32718	0.07368	0.34294
C	-3.35403	0.69979	1.04131
C	-4.67260	0.31588	0.79701
C	-4.95117	-0.68049	-0.13936
C	-3.90570	-1.29689	-0.82967
C	-2.58260	-0.92648	-0.59187
Cl	2.30136	1.95530	-0.69050
C	1.84517	-0.41563	0.70174
C	2.00314	-1.34164	-0.53390
C	3.32397	-2.09038	-0.29674
C	4.20947	-1.02856	0.37159
C	3.25570	-0.33047	1.35843
H	1.09740	1.53175	1.28978
H	-3.11074	1.47164	1.76391
H	-5.48021	0.79877	1.33913
H	-5.97828	-0.97613	-0.33076
H	-4.11752	-2.07250	-1.55967
H	-1.76614	-1.39510	-1.12756
H	1.14081	-0.86569	1.41078
H	1.14433	-2.00904	-0.66008
H	2.07988	-0.73664	-1.44342
H	3.75233	-2.49462	-1.21961
H	3.16621	-2.93250	0.39051
H	4.55306	-0.31030	-0.38208
H	5.09439	-1.44647	0.86262
H	3.24143	-0.86864	2.31285
H	3.55432	0.70007	1.57034

S4_9 Ground State

O	0.72183	-0.62751	0.76153
C	-0.25590	-0.76415	-0.18393
C	-1.58201	-1.03581	0.51792
O	-0.08482	-0.63999	-1.36806
C	2.00566	-0.24696	0.34607
C	3.05167	-1.11764	0.62646
C	4.35302	-0.73789	0.29557
C	4.59168	0.49613	-0.31043
C	3.52564	1.35591	-0.58374
C	2.22154	0.98982	-0.25427
Cl	-2.39939	-2.43339	-0.30697
C	-2.50081	0.19833	0.54141
C	-1.88795	1.34557	1.40489
C	-2.14207	2.63451	0.60297
C	-2.04244	2.17027	-0.85657
C	-2.78531	0.82388	-0.85526
H	-1.37946	-1.36913	1.53568
H	2.83904	-2.07175	1.09697
H	5.17833	-1.40983	0.51136
H	5.60501	0.78818	-0.56891
H	3.70733	2.31692	-1.05563
H	1.38477	1.64779	-0.46034
H	-3.43576	-0.14533	0.99349
H	-2.32074	1.37120	2.40967
H	-0.80976	1.19780	1.53148
H	-1.43972	3.43493	0.85890
H	-3.15428	3.00949	0.80282

H	-0.99172	2.01391	-1.13239
H	-2.46285	2.88667	-1.56973
H	-3.86273	0.99470	-0.95483
H	-2.48024	0.17030	-1.67430

S4_10 Ground State

O	0.51740	-0.46899	0.89530
C	-0.41908	-0.93353	0.01188
C	-1.79726	-0.77576	0.64296
O	-0.17575	-1.33629	-1.09404
C	1.83692	-0.31098	0.45080
C	2.59005	-1.40006	0.02358
C	3.91646	-1.18846	-0.35149
C	4.47386	0.09063	-0.29511
C	3.70086	1.16857	0.13825
C	2.37148	0.97164	0.51294
Cl	-2.87129	-2.11194	0.05386
C	-2.42920	0.60176	0.33413
C	-1.72202	1.75454	1.11765
C	-1.32974	2.80830	0.05877
C	-1.18672	2.00480	-1.24186
C	-2.34834	1.00144	-1.16286
H	-1.71245	-0.91007	1.72195
H	2.14281	-2.38577	-0.02071
H	4.51485	-2.02900	-0.69001
H	5.50772	0.24600	-0.58832
H	4.12909	2.16541	0.18507
H	1.74945	1.79313	0.85299
H	-3.47159	0.51415	0.65146
H	-2.37926	2.16642	1.88943
H	-0.83063	1.37990	1.62770
H	-0.42253	3.35893	0.33083
H	-2.13436	3.54590	-0.05314
H	-0.22578	1.47620	-1.26091
H	-1.22751	2.62905	-2.14033
H	-3.28216	1.49892	-1.44846
H	-2.22250	0.13869	-1.82123

S4_11 Ground State

O	-0.63040	-0.51457	-0.87722
C	0.34888	-0.84208	0.01874
C	1.68729	-0.82818	-0.70837
O	0.16734	-1.04571	1.19053
C	-1.93326	-0.29605	-0.41078
C	-2.51031	0.93047	-0.72312
C	-3.82856	1.17556	-0.33807
C	-4.54965	0.20096	0.35290
C	-3.95103	-1.02352	0.65626
C	-2.63528	-1.28360	0.27416
Cl	2.70344	-2.21063	-0.11795
C	2.43616	0.50909	-0.53443
C	1.60328	1.70904	-1.07613
C	1.06012	2.41286	0.17736
C	2.22903	2.29483	1.16565
C	2.75819	0.86150	0.94899
H	1.51090	-1.01780	-1.76703
H	-1.92826	1.67118	-1.26120
H	-4.28883	2.12920	-0.57889
H	-5.57491	0.39397	0.65388
H	-4.50891	-1.78407	1.19436
H	-2.15851	-2.22743	0.50848
H	3.35642	0.40005	-1.11572
H	2.27610	2.38863	-1.61181
H	0.82356	1.40501	-1.78039
H	0.18283	1.88238	0.56829
H	0.75629	3.44702	-0.01651
H	1.93711	2.47937	2.20424
H	3.00156	3.03046	0.90615
H	3.82747	0.77251	1.15755
H	2.24410	0.16717	1.61821

S4_12 Ground State

O	1.01132	0.53973	-0.76082
C	-0.11309	0.16678	-0.09342
C	-1.31593	0.87926	-0.70302
O	-0.14168	-0.60870	0.82955
C	2.25857	0.09049	-0.31156
C	3.08195	-0.51666	-1.25305
C	4.36426	-0.91474	-0.87428
C	4.80580	-0.70665	0.43291
C	3.96305	-0.09359	1.36245
C	2.68086	0.31329	0.99616
Cl	-1.31830	2.57339	0.00178
C	-2.65662	0.19135	-0.48230
C	-2.68926	-1.21853	-1.13623
C	-3.65815	-2.01749	-0.25158
C	-3.31105	-1.53290	1.16389
C	-3.09423	-0.01521	1.00114
H	-1.12494	1.02676	-1.76725
H	2.71514	-0.66536	-2.26324
H	5.01557	-1.38785	-1.60318
H	5.80339	-1.01899	0.72665
H	4.30346	0.07214	2.38026
H	2.01834	0.79017	1.70856

H	-3.39570	0.82363	-0.98542
H	-2.98685	-1.17802	-2.18923
H	-1.69805	-1.68485	-1.09089
H	-3.55377	-3.09996	-0.38013
H	-4.69514	-1.75333	-0.49948
H	-2.37585	-1.99981	1.49031
H	-4.08324	-1.77299	1.90211
H	-4.02781	0.52915	1.17733
H	-2.35766	0.37099	1.70696

S4_13 Ground State

O	0.81241	-0.33214	-0.37211
C	0.13906	-0.98353	0.60415
C	-1.33332	-1.17783	0.26950
O	0.59657	-1.31479	1.67098
C	2.15111	0.02646	-0.17816
C	2.47749	1.35020	-0.45344
C	3.80787	1.75538	-0.34887
C	4.79186	0.84075	0.02910
C	4.44268	-0.48388	0.29838
C	3.11695	-0.90442	0.19411
Cl	-1.59841	-1.56246	-1.48857
C	-2.14704	0.04179	0.73057
C	-1.86291	1.36664	-0.04045
C	-3.25119	1.94133	-0.40829
C	-4.22716	1.26395	0.56778
C	-3.67559	-0.16425	0.66512
H	-1.65776	-2.06396	0.81586
H	1.69300	2.03963	-0.74733
H	4.07237	2.78654	-0.56358
H	5.82706	1.15782	0.11183
H	5.20534	-1.19939	0.59118
H	2.83636	-1.92896	0.40367
H	-1.86407	0.17203	1.78363
H	-1.30564	2.05714	0.60123
H	-1.25227	1.19139	-0.92879
H	-3.50834	1.65284	-1.43451
H	-3.28284	3.03438	-0.35916
H	-5.26815	1.29844	0.23027
H	-4.18175	1.75243	1.55040
H	-4.05381	-0.72743	1.52484
H	-3.93720	-0.72130	-0.24188

S4_14 Ground State

O	1.01136	0.53961	-0.76070
C	-0.11308	0.16675	-0.09331
C	-1.31586	0.87933	-0.70291
O	-0.14176	-0.60877	0.82962
C	2.25862	0.09041	-0.31149
C	3.08225	-0.51606	-1.25320
C	4.36459	-0.91409	-0.87452
C	4.80594	-0.70664	0.43284
C	3.96297	-0.09425	1.36261
C	2.68073	0.31257	0.99641
Cl	-1.31824	2.57339	0.00207
C	-2.65659	0.19143	-0.48236
C	-2.68921	-1.21841	-1.13638
C	-3.65830	-2.01738	-0.25197
C	-3.31153	-1.53288	1.16361
C	-3.09436	-0.01522	1.00101
H	-1.12479	1.02693	-1.76711
H	2.71558	-0.66427	-2.26352
H	5.01608	-1.38666	-1.60360
H	5.80356	-1.01894	0.72652
H	4.30322	0.07099	2.38055
H	2.01805	0.78891	1.70902
H	-3.39561	0.82375	-0.98550
H	-2.98660	-1.17782	-2.18943
H	-1.69802	-1.68478	-1.09089
H	-3.55388	-3.09985	-0.38055
H	-4.69524	-1.75324	-0.50011
H	-2.37654	-2.00000	1.49034
H	-4.08401	-1.77281	1.90158
H	-4.02782	0.52934	1.17722
H	-2.35774	0.37073	1.70693

S4_15 Ground State

O	1.19933	0.76352	-0.25956
C	0.15594	-0.10764	-0.29359
C	-1.15397	0.67097	-0.32312
O	0.25577	-1.30860	-0.31766
C	2.50498	0.27611	-0.13650
C	3.43962	0.76151	-1.04451
C	4.77216	0.36772	-0.92104
C	5.15431	-0.50387	0.09938
C	4.20015	-0.97819	1.00190
C	2.86574	-0.58911	0.89307
Cl	-1.41848	1.33603	1.36690
C	-2.34477	-0.14509	-0.81448
C	-2.72483	-1.37434	0.05339
C	-4.25862	-1.43726	-0.01327
C	-4.67071	0.04108	-0.00493
C	-3.64581	0.70778	-0.94170
H	-1.01319	1.56169	-0.93849

H	3.11709	1.43966	-1.82760
H	5.50918	0.74363	-1.62450
H	6.19149	-0.81132	0.19295
H	4.49338	-1.65489	1.79904
H	2.11782	-0.95144	1.58790
H	-2.04236	-0.49331	-1.81095
H	-2.22920	-2.28360	-0.29012
H	-2.41096	-1.20676	1.08898
H	-4.69459	-2.01368	0.80942
H	-4.57965	-1.90979	-0.95168
H	-4.56365	0.44569	1.00872
H	-5.70509	0.20894	-0.32245
H	-4.00326	0.67519	-1.97695
H	-3.47881	1.76004	-0.69122

S4_16 Ground State

O	1.00410	0.54228	-0.76889
C	-0.12183	0.16857	-0.10356
C	-1.32456	0.86418	-0.73400
O	-0.14725	-0.59416	0.83025
C	2.25180	0.11258	-0.30179
C	2.66419	0.37239	1.00219
C	3.94669	-0.01583	1.38704
C	4.79936	-0.64720	0.47899
C	4.36752	-0.89262	-0.82495
C	3.08493	-0.51350	-1.22194
Cl	-1.38439	2.54843	-0.00952
C	-2.65457	0.13930	-0.56540
C	-2.57709	-1.32480	-1.11524
C	-2.93485	-2.23308	0.07696
C	-3.86182	-1.35931	0.93379
C	-3.18628	0.02029	0.88722
H	-1.10474	1.02955	-1.78955
H	1.99367	0.86335	1.69747
H	4.27957	0.17878	2.40222
H	5.79717	-0.94482	0.78691
H	5.02662	-1.38024	-1.53708
H	2.72548	-0.69130	-2.23008
H	-3.37662	0.70611	-1.16244
H	-3.30474	-1.44593	-1.92493
H	-1.59536	-1.56750	-1.53807
H	-2.02811	-2.46721	0.64411
H	-3.39192	-3.17725	-0.23749
H	-3.98600	-1.73437	1.95494
H	-4.86001	-1.31046	0.47713
H	-3.86202	0.84244	1.13811
H	-2.35411	0.04475	1.59390

S4_17 Ground State

O	-0.42776	0.60500	-0.09248
C	0.35454	0.53312	1.00859
C	1.79731	0.92778	0.72232
O	-0.00171	0.14747	2.09679
C	-1.77751	0.23816	-0.05937
C	-2.62964	1.05152	-0.80073
C	-3.97974	0.71718	-0.89062
C	-4.46482	-0.42101	-0.24411
C	-3.59297	-1.22532	0.49087
C	-2.23825	-0.90533	0.59018
Cl	1.88820	2.48280	-0.22256
C	2.61894	-0.18183	0.03796
C	2.49483	-1.53325	0.80809
C	1.62439	-2.42514	-0.09211
C	2.07117	-2.02876	-1.50547
C	2.20253	-0.49499	-1.42987
H	2.23235	1.15398	1.69539
H	-2.22335	1.92737	-1.29538
H	-4.65046	1.34756	-1.46683
H	-5.51701	-0.68017	-0.31306
H	-3.96514	-2.11209	0.99543
H	-1.56276	-1.51906	1.17034
H	3.65442	0.17025	0.06846
H	3.49188	-1.97657	0.90817
H	2.09029	-1.41391	1.81733
H	0.56183	-2.18538	0.04270
H	1.74735	-3.49144	0.12379
H	1.37657	-2.35217	-2.28746
H	3.04560	-2.48559	-1.72284
H	1.24240	-0.02649	-1.65737
H	2.92772	-0.09636	-2.14414

S4_18 Ground State

O	0.46475	-0.63757	-0.10908
C	-0.34782	-0.53750	0.96765
C	-1.77111	-0.98089	0.65792
O	-0.02775	-0.09557	2.04578
C	1.79792	-0.21785	-0.04877
C	2.72262	-1.06729	-0.64791
C	4.06135	-0.68179	-0.70256
C	4.46176	0.54124	-0.16198
C	3.51739	1.38020	0.43163
C	2.17382	1.00940	0.49275
Cl	-1.78555	-2.56407	-0.24447
C	-2.60055	0.08220	-0.08800

C	-2.73461	1.38742	0.76025
C	-2.46944	2.54396	-0.22251
C	-1.47300	1.94554	-1.22513
C	-2.02127	0.52911	-1.45990
H	-2.23218	-1.19165	1.62283
H	2.38148	-2.00971	-1.06296
H	4.78942	-1.33903	-1.16858
H	5.50487	0.83988	-0.20368
H	3.82389	2.33295	0.85317
H	1.43948	1.65086	0.96185
H	-3.58421	-0.37438	-0.23099
H	-3.71403	1.45433	1.24338
H	-1.98592	1.40204	1.55917
H	-2.09923	3.44419	0.27890
H	-3.39591	2.81625	-0.74456
H	-0.47163	1.89630	-0.77868
H	-1.38653	2.52557	-2.14968
H	-1.27550	-0.16622	-1.84920
H	-2.83810	0.57045	-2.18919

S4_19 Ground State

O	0.90390	-0.00612	-0.61056
C	0.02496	0.31780	0.37593
C	-1.36853	0.48177	-0.21708
O	0.30094	0.45438	1.54066
C	2.26603	-0.12969	-0.31278
C	2.96662	0.88103	0.34024
C	4.33746	0.72130	0.53921
C	4.99245	-0.42621	0.08759
C	4.27186	-1.42396	-0.57002
C	2.89933	-1.27943	-0.77226
Cl	-1.50219	2.25059	-0.67680
C	-2.45944	0.06289	0.76493
C	-3.87772	0.20882	0.18762
C	-4.05372	-1.01137	-0.74209
C	-3.12853	-2.11902	-0.15891
C	-2.37365	-1.46052	1.02251
H	-1.42808	-0.05857	-1.16193
H	2.44917	1.76648	0.68843
H	4.89466	1.50109	1.04986
H	6.06046	-0.54085	0.24647
H	4.77500	-2.31765	-0.92712
H	2.31621	-2.03918	-1.28215
H	-2.31529	0.63653	1.68404
H	-4.58976	0.15499	1.01963
H	-4.04049	1.16390	-0.31833
H	-3.74994	-0.75689	-1.76381
H	-5.09917	-1.32877	-0.79951
H	-2.42651	-2.47751	-0.91966
H	-3.69508	-2.99340	0.17530
H	-2.88696	-1.67072	1.96724
H	-1.34831	-1.82600	1.13702

S4_20 Ground State

O	0.36435	-0.63722	-0.37383
C	-0.37686	-0.86895	0.73767
C	-1.85516	-1.04647	0.42437
O	0.04910	-0.86639	1.86728
C	1.71534	-0.29761	-0.23772
C	2.11767	0.89395	-0.83187
C	3.46486	1.25268	-0.78268
C	4.38786	0.42418	-0.14325
C	3.96213	-0.76844	0.44524
C	2.61910	-1.14131	0.40074
Cl	-2.10770	-2.19833	-0.96249
C	-2.59144	0.28697	0.17999
C	-2.33369	1.28674	1.34538
C	-1.29506	2.27666	0.79539
C	-1.72314	2.45033	-0.66900
C	-2.16392	1.03839	-1.11690
H	-2.28329	-1.54153	1.29549
H	1.37994	1.51828	-1.32508
H	3.78980	2.17994	-1.24514
H	5.43591	0.70540	-0.10442
H	4.67787	-1.41606	0.94278
H	2.27603	-2.06234	0.85591
H	-3.65190	0.02169	0.13697
H	-3.26674	1.81830	1.56518
H	-2.01256	0.79447	2.26804
H	-1.27491	3.21810	1.35396
H	-0.28795	1.84680	0.85396
H	-0.93102	2.86217	-1.30397
H	-2.57054	3.14566	-0.72064
H	-2.98405	1.07285	-1.83905
H	-1.33939	0.51406	-1.60329

S4_21 Ground State

O	0.78905	-0.36521	-0.37868
C	0.12482	-1.00886	0.60797
C	-1.35510	-1.18514	0.29976
O	0.59403	-1.34545	1.66833
C	2.12930	-0.00401	-0.20230
C	2.45184	1.31301	-0.51305
C	3.78189	1.72325	-0.42636

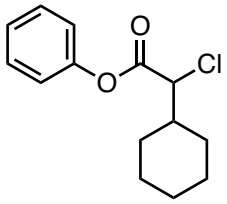
C	4.76983	0.82012	-0.03135
C	4.42469	-0.49796	0.27276
C	3.09920	-0.92374	0.18716
Cl	-1.67270	-1.49617	-1.46439
C	-2.14724	0.02156	0.83069
C	-1.77367	1.37749	0.17927
C	-3.08943	2.16918	0.16503
C	-4.13228	1.09322	-0.17197
C	-3.69128	-0.12271	0.66617
H	-1.67455	-2.09043	0.81641
H	1.66415	1.99259	-0.82081
H	4.04309	2.74914	-0.66857
H	5.80491	1.14094	0.03744
H	5.19047	-1.20461	0.57866
H	2.82237	-1.94306	0.42446
H	-1.89991	0.05327	1.89914
H	-0.96395	1.88394	0.71420
H	-1.43488	1.21264	-0.84884
H	-3.07728	2.99989	-0.54821
H	-3.29132	2.59020	1.15918
H	-4.07194	0.84848	-1.23920
H	-5.16085	1.40237	0.04027
H	-3.96954	-1.07065	0.19710
H	-4.16496	-0.09720	1.65358

S4_22 Ground State

O	0.36432	-0.63746	-0.37375
C	-0.37700	-0.86895	0.73774
C	-1.85532	-1.04633	0.42433
O	0.04885	-0.86621	1.86739
C	1.71527	-0.29779	-0.23766
C	2.11758	0.89364	-0.83208
C	3.46476	1.25243	-0.78294
C	4.38778	0.42412	-0.14330
C	3.96208	-0.76840	0.44544
C	2.61907	-1.14132	0.40099
Cl	-2.10784	-2.19829	-0.96252
C	-2.59138	0.28715	0.17981
C	-2.33369	1.28688	1.34531
C	-1.29480	2.27661	0.79550
C	-1.72261	2.45039	-0.66893
C	-2.16357	1.03856	-1.11697
H	-2.28358	-1.54136	1.29539
H	1.37986	1.51782	-1.32546
H	3.78968	2.17959	-1.24561
H	5.43581	0.70538	-0.10450
H	4.67785	-1.41587	0.94313
H	2.27602	-2.06227	0.85634
H	-3.65187	0.02203	0.13666
H	-3.26672	1.81855	1.56494
H	-2.01281	0.79452	2.26801
H	-0.28779	1.84654	0.85425
H	-1.27449	3.21804	1.35408
H	-0.93036	2.86221	-1.30375
H	-2.56992	3.14584	-0.72067
H	-2.98360	1.07323	-1.83923
H	-1.33912	0.51408	-1.60335

S4_23 Ground State

O	-0.78529	0.32143	-0.40497
C	0.03034	0.41547	0.67586
C	1.45862	0.70811	0.24673
O	-0.30375	0.23960	1.82125
C	-2.13991	0.02216	-0.22673
C	-2.64547	-1.03507	-0.97530
C	-4.00534	-1.33453	-0.89236
C	-4.83969	-0.58159	-0.06523
C	-4.31177	0.47691	0.67683
C	-2.95515	0.79021	0.59996
Cl	1.51513	2.36174	-0.52338
C	2.01966	-0.36510	-0.69560
C	3.53372	-0.20518	-0.92067
C	4.19182	-0.81506	0.33942
C	3.15627	-1.82680	0.91248
C	1.93879	-1.76201	-0.03807
H	2.04491	0.79231	1.16111
H	-1.97476	-1.60304	-1.61156
H	-4.40959	-2.15704	-1.47495
H	-5.89771	-0.81690	0.00014
H	-4.95797	1.06635	1.32048
H	-2.53492	1.60821	1.17211
H	1.44964	-0.31975	-1.62743
H	3.80996	-0.78386	-1.80983
H	3.82992	0.83121	-1.10390
H	4.41217	-0.03344	1.07468
H	5.14683	-1.29157	0.09896
H	2.86096	-1.54425	1.92843
H	3.55901	-2.84208	0.97501
H	2.03503	-2.51139	-0.83216
H	0.99032	-1.95783	0.47231



S5_1 Ground State

O	-1.11863	0.56696	0.70775
C	-0.19514	0.98361	-0.20860
C	1.08822	1.33386	0.53438
O	-0.36500	1.01244	-1.39885
C	-2.34622	0.05062	0.27725
C	-3.48057	0.54739	0.91038
C	-4.72785	0.01622	0.58249
C	-4.82992	-0.99805	-0.37046
C	-3.67890	-1.48381	-0.99371
C	-2.42506	-0.96463	-0.67300
Cl	1.76060	2.88124	-0.13373
C	2.12521	0.19489	0.47112
C	1.59972	-1.05346	1.20807
C	2.66609	-2.15630	1.24408
C	3.14414	-2.51560	-0.16839
C	3.64455	-1.27270	-0.91540
C	2.57957	-0.16840	-0.95068
H	0.84322	1.54412	1.57545
H	-3.37366	1.33560	1.64815
H	-5.61829	0.39817	1.07289
H	-5.80178	-1.40884	-0.62677
H	-3.75325	-2.27281	-1.73621
H	-1.52890	-1.33074	-1.15838
H	2.99927	0.56660	1.02420
H	1.28438	-0.79008	2.22524
H	0.70699	-1.43580	0.69493
H	2.26628	-3.04228	1.75185
H	3.52237	-1.81067	1.84085
H	3.93207	-3.27702	-0.12048
H	2.30882	-2.96086	-0.72838
H	3.93978	-1.53520	-1.93823
H	4.54727	-0.89018	-0.41717
H	1.71506	-0.50924	-1.53352
H	2.96622	0.72099	-1.45742

S5_2 Ground State

O	-1.18992	0.35044	0.69010
C	-0.42196	1.00558	-0.23340
C	0.95570	1.20809	0.38940
O	-0.77750	1.31120	-1.33890
C	-2.48487	-0.06200	0.35694
C	-3.48544	0.24739	1.27241
C	-4.78460	-0.20122	1.03545
C	-5.07141	-0.94676	-0.10875
C	-4.05279	-1.24737	-1.01494
C	-2.74828	-0.80966	-0.78811
Cl	1.82915	2.53255	-0.47713
C	1.74541	-0.11719	0.40513
C	1.98818	-0.69990	-0.99607
C	2.72179	-2.04527	-0.91399
C	4.03473	-1.92174	-0.13057
C	3.79080	-1.33752	1.26669
C	3.06124	0.01015	1.18761
H	0.82324	1.55631	1.41576
H	-3.23626	0.82859	2.15401
H	-5.57086	0.03509	1.74627
H	-6.08386	-1.29260	-0.29393
H	-4.27096	-1.82706	-1.90697
H	-1.95445	-1.03446	-1.48949
H	1.09482	-0.81275	0.95628
H	1.03886	-0.81705	-1.53191
H	2.58706	0.01160	-1.57773
H	2.91352	-2.42511	-1.92459
H	2.07354	-2.78306	-0.41879
H	4.72261	-1.26417	-0.68125
H	4.52599	-2.89933	-0.05387
H	4.73990	-1.21543	1.80227
H	3.18663	-2.04417	1.85411
H	3.70413	0.74604	0.68924
H	2.85893	0.39553	2.19549

S5_3 Ground State

O	-1.51878	0.77523	0.19546
C	-0.43102	-0.03751	0.20786
C	0.84072	0.80653	0.17940
O	-0.46826	-1.24104	0.27616
C	-2.80186	0.21921	0.15680
C	-3.71463	0.69693	1.09085
C	-5.02980	0.23374	1.05145
C	-5.41665	-0.69835	0.08780
C	-4.48493	-1.16352	-0.84238
C	-3.16827	-0.70544	-0.81760
Cl	0.89421	1.69230	-1.42280
C	2.11796	0.01093	0.45410
C	2.50142	-0.98924	-0.64979
C	3.75390	-1.78440	-0.25778

C	4.93067	-0.85639	0.06802
C	4.55116	0.15203	1.15974
C	3.29539	0.94595	0.77700
H	0.72490	1.60332	0.91892
H	-3.38902	1.42318	1.82817
H	-5.74970	0.60317	1.77574
H	-6.44019	-1.05972	0.05970
H	-4.78195	-1.88707	-1.59577
H	-2.43820	-1.06041	-1.53475
H	1.88666	-0.56890	1.36119
H	1.66499	-1.66481	-0.84441
H	2.69949	-0.43557	-1.57596
H	4.02354	-2.47224	-1.06826
H	3.52869	-2.40768	0.61980
H	5.22179	-0.31063	-0.84115
H	5.80537	-1.44084	0.37882
H	5.38280	0.84053	1.35261
H	4.36467	-0.38698	2.10007
H	3.50823	1.56797	-0.10232
H	3.01850	1.63133	1.58939

S5_4 Ground State

O	1.36984	0.24265	-0.72607
C	0.37866	0.28090	0.20409
C	-0.91412	0.75723	-0.44693
O	0.50047	-0.01056	1.36707
C	2.67339	-0.08500	-0.33460
C	3.31763	0.59314	0.69677
C	4.64165	0.26521	0.98591
C	5.30663	-0.71906	0.25179
C	4.64351	-1.38197	-0.78163
C	3.31756	-1.06703	-1.07917
Cl	-0.90495	2.57978	-0.23534
C	-2.15224	0.10693	0.16286
C	-3.45814	0.66522	-0.42373
C	-4.68545	-0.04169	0.16555
C	-4.61378	-1.55981	-0.03601
C	-3.30977	-2.12627	0.53673
C	-2.08058	-1.42055	-0.05176
H	-0.86551	0.59874	-1.52532
H	2.79215	1.35380	1.26106
H	5.15456	0.78477	1.78984
H	6.33808	-0.96664	0.48383
H	5.15530	-2.14619	-1.35903
H	2.77976	-1.56603	-1.87852
H	-2.12664	0.30295	1.24212
H	-3.52027	1.74251	-0.24373
H	-3.44636	0.52599	-1.51545
H	-5.59867	0.36293	-0.28707
H	-4.74407	0.17849	1.24114
H	-5.47828	-2.04881	0.42925
H	-4.66479	-1.78489	-1.11140
H	-3.24203	-3.20426	0.34690
H	-3.30550	-1.99809	1.62827
H	-2.02570	-1.62772	-1.13121
H	-1.17003	-1.82401	0.40287

S5_5 Ground State

O	-0.98585	0.66780	-0.14379
C	-0.19363	0.69370	0.95206
C	1.13651	1.38683	0.69576
O	-0.45067	0.17752	2.01358
C	-2.22020	0.00990	-0.10580
C	-2.34051	-1.30984	0.32188
C	-3.59215	-1.92144	0.25373
C	-4.69775	-1.22473	-0.23742
C	-4.55270	0.09555	-0.66610
C	-3.30789	0.72095	-0.60139
Cl	0.95484	2.84860	-0.37415
C	2.20660	0.42312	0.14160
C	2.57335	-0.64540	1.18948
C	3.71001	-1.54194	0.67910
C	3.35712	-2.18570	-0.66786
C	2.97051	-1.12346	-1.70487
C	1.82879	-0.23469	-1.19454
H	1.46521	1.77286	1.66090
H	-1.47944	-1.84070	0.70794
H	-3.70027	-2.94921	0.58754
H	-5.66801	-1.70974	-0.28668
H	-5.40765	0.64264	-1.05213
H	-3.16441	1.74465	-0.93039
H	3.09624	1.04602	-0.02538
H	2.86051	-0.16486	2.13292
H	1.69239	-1.26071	1.41146
H	3.93652	-2.31313	1.42508
H	4.62178	-0.93829	0.56389
H	2.51198	-2.87529	-0.52717
H	4.19764	-2.78858	-1.03249
H	2.67801	-1.59881	-2.64872
H	3.84617	-0.49660	-1.92730
H	0.92912	-0.84920	-1.05843
H	1.57565	0.53304	-1.93251

S5_6 Ground State

O	1.38508	0.35779	-0.80556
C	0.26056	0.21439	-0.05239
C	-0.91297	0.84699	-0.79310
O	0.21767	-0.32930	1.02287
C	2.61912	-0.05170	-0.28815
C	3.08424	0.41510	0.93838
C	4.35439	0.02694	1.36248
C	5.14378	-0.80800	0.56889
C	4.66045	-1.25904	-0.65992
C	3.38947	-0.88233	-1.09440
Cl	-0.84139	2.64126	-0.42059
C	-2.28959	0.25510	-0.48728
C	-2.31635	-1.23042	-0.90368
C	-3.72089	-1.82453	-0.72895
C	-4.22977	-1.64168	0.70636
C	-4.18776	-0.16597	1.12341
C	-2.78125	0.42511	0.95948
H	-0.70935	0.78663	-1.86324
H	2.46346	1.06246	1.54597
H	4.72744	0.38197	2.31858
H	6.13236	-1.10387	0.90682
H	5.27024	-1.90558	-1.28400
H	2.99093	-1.21761	-2.04619
H	-2.98834	0.79499	-1.14301
H	-1.98771	-1.33789	-1.94623
H	-1.60638	-1.78971	-0.28152
H	-3.71005	-2.88702	-1.00072
H	-4.41177	-1.32785	-1.42543
H	-5.24845	-2.03768	0.79978
H	-3.59810	-2.22724	1.38953
H	-4.51712	-0.05500	2.16347
H	-4.89829	0.40445	0.50693
H	-2.08484	-0.07709	1.63749
H	-2.78292	1.48687	1.22659

S5_7 Ground State

O	-0.97960	0.32279	-0.32324
C	-0.38336	0.86924	0.76890
C	1.05401	1.25445	0.45230
O	-0.89602	1.00209	1.85140
C	-2.30163	-0.12474	-0.24147
C	-2.54469	-1.42151	-0.68146
C	-3.85478	-1.90033	-0.68912
C	-4.90146	-1.08482	-0.25703
C	-4.63575	0.21480	0.17904
C	-3.33141	0.70793	0.18784
Cl	1.00917	2.65873	-0.71774
C	1.88825	0.08886	-0.08727
C	3.36041	0.48030	-0.28814
C	4.19325	-0.70677	-0.78849
C	4.08054	-1.91030	0.15484
C	2.61426	-2.30286	0.36971
C	1.77907	-1.11650	0.87010
H	1.48195	1.65379	1.37254
H	-1.71275	-2.03330	-1.01475
H	-4.05421	-2.91097	-1.03293
H	-5.92071	-1.45916	-0.26138
H	-5.44760	0.85325	0.51459
H	-3.11410	1.71365	0.52582
H	1.46070	-0.20082	-1.05542
H	3.43260	1.31755	-0.98905
H	3.76730	0.83206	0.67188
H	5.24115	-0.40383	-0.90038
H	3.84175	-0.99609	-1.78934
H	4.53159	-1.65361	1.12437
H	4.64786	-2.76139	-0.24089
H	2.53844	-3.13376	1.08123
H	2.19222	-2.66183	-0.58000
H	2.12992	-0.81638	1.86805
H	0.73272	-1.42318	0.98346

S5_8 Ground State

O	0.92560	0.18634	-0.63334
C	0.18507	0.97649	0.19897
C	-1.27327	0.89497	-0.22437
O	0.61062	1.57973	1.14835
C	2.27705	-0.04414	-0.35054
C	2.68238	-1.37502	-0.33293
C	4.02875	-1.67046	-0.12072
C	4.94989	-0.64012	0.07346
C	4.52205	0.68867	0.05098
C	3.17941	0.99957	-0.16397
Cl	-1.89571	2.58647	-0.47058
C	-2.09383	0.14626	0.84346
C	-3.56058	-0.05040	0.41867
C	-3.71238	-1.05308	-0.73455
C	-3.06078	-2.40235	-0.40057
C	-1.59338	-2.23285	0.01716
C	-1.45917	-1.22653	1.16855
H	-1.33720	0.41665	-1.19912
H	1.94540	-2.15629	-0.48823
H	4.35483	-2.70625	-0.10716
H	5.99761	-0.87114	0.24068

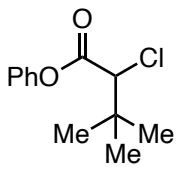
H	5.23589	1.49310	0.20136
H	2.83672	2.02644	-0.17807
H	-2.05361	0.76770	1.74513
H	-4.11020	-0.42605	1.29236
H	-4.00978	0.91189	0.15453
H	-3.25950	-0.64364	-1.64848
H	-4.77617	-1.19181	-0.96135
H	-3.13777	-3.08521	-1.25538
H	-3.61388	-2.87039	0.42680
H	-1.17281	-3.19857	0.32342
H	-0.99828	-1.89666	-0.84243
H	-1.98115	-1.62232	2.04987
H	-0.41015	-1.11184	1.46433

S5_9 Ground State

O	1.16073	-0.59093	-0.14706
C	0.38315	-0.59696	0.95685
C	-1.01420	-1.14762	0.70544
O	0.69231	-0.15686	2.03869
C	2.44987	-0.04740	-0.10498
C	2.70757	1.21497	0.42386
C	4.00805	1.71430	0.35202
C	5.02597	0.96584	-0.24153
C	4.74322	-0.29436	-0.77064
C	3.44854	-0.80801	-0.70414
Cl	-1.07404	-2.35689	-0.65051
C	-2.01035	0.01393	0.50901
C	-1.71540	0.87413	-0.73026
C	-2.70340	2.04340	-0.84010
C	-4.15715	1.55501	-0.83592
C	-4.44717	0.70095	0.40465
C	-3.46683	-0.47463	0.51231
H	-1.28876	-1.70369	1.60305
H	1.91498	1.78620	0.88983
H	4.22316	2.69583	0.76401
H	6.03490	1.36403	-0.29237
H	5.52898	-0.88101	-1.23724
H	3.19839	-1.78207	-1.11085
H	-1.86292	0.63921	1.40293
H	-0.68755	1.25340	-0.69858
H	-1.78789	0.24396	-1.62535
H	-2.49536	2.61944	-1.74968
H	-2.55022	2.72790	0.00702
H	-4.33875	0.95373	-1.73835
H	-4.84551	2.40769	-0.88071
H	-5.47678	0.32438	0.37915
H	-4.36357	1.32821	1.30399
H	-3.61800	-1.15498	-0.33480
H	-3.66215	-1.05399	1.42403

S5_10 Ground State

O	-1.03944	0.44824	-0.38408
C	-0.19622	0.43626	0.67951
C	1.20649	0.84278	0.26102
O	-0.48842	0.09818	1.79986
C	-2.37093	0.05386	-0.21820
C	-3.19831	0.64944	0.72975
C	-4.53356	0.25237	0.79352
C	-5.02900	-0.71789	-0.07989
C	-4.18338	-1.29734	-1.02669
C	-2.84448	-0.91283	-1.09876
Cl	1.16925	2.57022	-0.32810
C	1.80189	-0.09672	-0.80210
C	3.28797	0.20569	-1.07166
C	4.19206	-0.16820	0.11222
C	4.00103	-1.63311	0.52942
C	2.52692	-1.95371	0.81344
C	1.63968	-1.57567	-0.38077
H	1.80201	0.86382	1.17099
H	-2.80335	1.39966	1.40366
H	-5.18864	0.70692	1.53078
H	-6.07061	-1.01937	-0.02337
H	-4.56258	-2.04999	-1.71159
H	-2.16602	-1.34496	-1.82698
H	1.22616	0.06822	-1.71915
H	3.59099	-0.37989	-1.95014
H	3.41630	1.25989	-1.33705
H	3.97883	0.48696	0.96839
H	5.23933	0.01690	-0.15485
H	4.61699	-1.86257	1.40729
H	4.35629	-2.28416	-0.28283
H	2.40697	-3.02072	1.03564
H	2.19119	-1.41572	1.70997
H	1.92118	-2.19162	-1.24546
H	0.58960	-1.80797	-0.16868



S6_1 Ground State

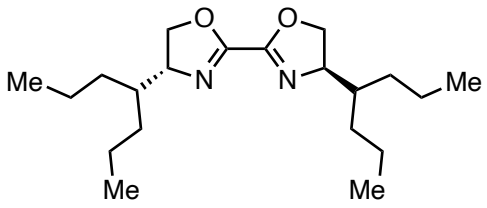
O	-0.65651	-0.01946	-0.76855
C	0.28659	-0.49984	0.09440

C	1.66218	-0.26945	-0.51832
O	0.05482	-0.97930	1.17360
C	-2.00149	0.00006	-0.37978
C	-2.65798	-1.14986	0.05046
C	-4.01600	-1.06683	0.35718
C	-4.70096	0.14317	0.23030
C	-4.02429	1.28247	-0.20751
C	-2.66530	1.21514	-0.51412
Cl	2.56635	-1.84742	-0.49097
C	2.43443	0.88623	0.17627
C	1.52231	2.13100	0.13887
C	3.71344	1.17630	-0.62576
C	2.79043	0.55195	1.63252
H	1.53383	-0.02965	-1.57382
H	-2.11667	-2.08232	0.15006
H	-4.53917	-1.95569	0.69704
H	-5.75847	0.19703	0.47073
H	-4.55133	2.22630	-0.31121
H	-2.11533	2.08492	-0.85804
H	0.63210	2.00257	0.76381
H	2.07284	2.99688	0.52111
H	1.19456	2.36188	-0.88109
H	4.38017	0.30969	-0.63861
H	3.48006	1.44557	-1.66287
H	4.25368	2.01471	-0.17291
H	3.46817	-0.30439	1.68505
H	3.29107	1.41217	2.09056
H	1.89990	0.31449	2.21929

S6_2 Ground State

O	-0.46482	0.34624	-0.12379
C	0.32113	-0.11803	0.87641
C	1.78683	0.23809	0.66587
O	-0.05774	-0.77692	1.81425
C	-1.84626	0.12367	-0.10648
C	-2.64156	1.23193	-0.37966
C	-4.02451	1.07126	-0.45552
C	-4.59631	-0.18670	-0.25839
C	-3.77987	-1.28623	0.01162
C	-2.39443	-1.14170	0.08764
Cl	1.95359	2.02553	0.34150
C	2.50935	-0.63965	-0.39526
C	4.01873	-0.35298	-0.31739
C	2.00460	-0.38015	-1.82271
C	2.25991	-2.11446	-0.01712
H	2.26333	0.08004	1.63346
H	-2.16855	2.19654	-0.53008
H	-4.65291	1.93092	-0.66854
H	-5.67358	-0.31029	-0.31561
H	-4.22035	-2.26697	0.16514
H	-1.75617	-1.98854	0.30449
H	4.40762	-0.54644	0.68930
H	4.55591	-1.00241	-1.01695
H	4.24197	0.68539	-0.57687
H	0.94200	-0.61309	-1.92622
H	2.15201	0.66423	-2.11088
H	2.56308	-1.00986	-2.52400
H	1.20712	-2.39317	-0.12761
H	2.84718	-2.76267	-0.67591
H	2.55520	-2.32259	1.01704

Cartesian Coordinates of Free Ligand Conformers



L1_1 Ground State

N	-1.26704	-0.75551	0.19939
C	-0.66791	-0.31659	1.23311
O	-1.27571	-0.40316	2.45033
C	-2.52203	-1.10077	2.20164
C	-2.59522	-1.20906	0.65495
C	0.66809	0.31390	1.23377
O	1.27596	0.39778	2.45113
C	2.52226	1.09596	2.20391
C	2.59537	1.20764	0.65746
N	1.26716	0.75510	0.20098
C	-3.71073	-0.35737	0.00727
C	-3.81706	-0.64311	-1.50168
C	-3.50127	1.14424	0.28252
C	3.71083	0.35736	0.00785
C	3.81699	0.64630	-1.50050
C	3.50144	-1.14484	0.27994
C	-4.38695	-2.02002	-1.86021
C	-4.51073	-2.22412	-3.37233
C	-4.76505	1.99322	0.10944
C	-4.51047	3.48054	0.36597
C	4.76522	-1.99345	0.10504
C	4.51068	-3.48127	0.35869
C	4.38617	2.02422	-1.85622

C	4.51013	2.23132	-3.36792
H	-3.33181	-0.51536	2.64452
H	-2.46680	-2.07400	2.69874
H	-2.72622	-2.25253	0.35225
H	3.33207	0.50960	2.64547
H	2.46704	2.06810	2.70314
H	2.72637	2.25177	0.35705
H	-4.65285	-0.66861	0.48779
H	-2.81973	-0.52714	-1.94420
H	-4.45378	0.12137	-1.96511
H	-2.70847	1.51571	-0.37909
H	-3.12859	1.29321	1.30524
H	4.65299	0.66762	0.48893
H	2.81971	0.53075	-1.94324
H	4.45409	-0.11691	-1.96551
H	2.70861	-1.51493	-0.38239
H	3.12882	-1.29595	1.30238
H	-3.75314	-2.81400	-1.44435
H	-5.37413	-2.13743	-1.39054
H	-4.92206	-3.21084	-3.61294
H	-5.16853	-1.46865	-3.81920
H	-3.53233	-2.14028	-3.86015
H	-5.54136	1.62811	0.79697
H	-5.17016	1.86446	-0.90238
H	-5.42566	4.07145	0.24792
H	-4.13309	3.64642	1.38246
H	-3.76288	3.87666	-0.33165
H	5.54160	-1.62969	0.79320
H	5.17021	-1.86271	-0.90657
H	5.42585	-4.07195	0.23935
H	4.13343	-3.64915	1.37489
H	3.76300	-3.87602	-0.33963
H	5.37320	2.14129	-1.38613
H	3.75183	2.81703	-1.43895
H	4.92090	3.21877	-3.60653
H	5.16849	1.47713	-3.81612
H	3.53188	2.14784	-3.85609

L1_2 Ground State

N	1.35585	0.58746	-0.27296
C	0.70688	0.21448	0.75647
O	1.32911	0.17911	1.96728
C	2.67682	0.65172	1.71985
C	2.73146	0.86270	0.17992
C	-0.70689	-0.21455	0.75641
O	-1.32913	-0.17941	1.96723
C	-2.67685	-0.65194	1.71968
C	-2.73144	-0.86270	0.17972
N	-1.35583	-0.58735	-0.27309
C	3.74771	-0.02724	-0.57245
C	3.40229	-1.52021	-0.43439
C	5.19532	0.28192	-0.14929
C	-3.74771	0.02729	-0.57256
C	-3.40224	1.52024	-0.43442
C	-5.19532	-0.28186	-0.14935
C	4.22403	-2.45320	-1.33120
C	3.73350	-3.90177	-1.26286
C	5.63144	1.74417	-0.30409
C	7.12642	1.93681	-0.03664
C	-5.63142	-1.74412	-0.30406
C	-7.12640	-1.93675	-0.03661
C	-4.22412	2.45333	-1.33100
C	-3.73346	3.90187	-1.26269
H	3.36928	-0.10739	2.09116
H	2.82065	1.57494	2.28823
H	2.95300	1.90819	-0.05548
H	-3.36930	0.10716	2.09106
H	-2.82075	-1.57522	2.28793
H	-2.95293	-1.90818	-0.05583
H	3.64028	0.23812	-1.63399
H	2.34177	-1.64813	-0.68031
H	3.51992	-1.83817	0.61246
H	5.87057	-0.34078	-0.74849
H	5.35119	-0.03438	0.89339
H	-3.64033	-0.23801	-1.63411
H	-2.34175	1.64815	-0.68052
H	-3.51967	1.83811	0.61247
H	-5.87057	0.34080	-0.74859
H	-5.35117	0.03451	0.89331
H	5.28413	-2.41908	-1.05022
H	4.16835	-2.09496	-2.36874
H	4.32859	-4.55812	-1.90770
H	3.79745	-4.29125	-0.23934
H	2.68661	-3.97724	-1.57994
H	5.06128	2.38673	0.37942
H	5.39074	2.08894	-1.31942
H	7.42112	2.98676	-0.14159
H	7.38945	1.61540	0.97859
H	7.73079	1.34700	-0.73626
H	-5.06126	-2.38663	0.37951
H	-5.39071	-2.08897	-1.31936
H	-7.42110	-2.98671	-0.14148
H	-7.38945	-1.61526	0.97860

H	-7.73077	-1.34700	-0.73628
H	-5.28416	2.41928	-1.04976
H	-4.16871	2.09514	-2.36857
H	-4.32868	4.55830	-1.90734
H	-3.79713	4.29129	-0.23914
H	-2.68665	3.97728	-1.58004

L1_3 Ground State

N	1.12613	-0.14427	-0.09051
C	0.43438	-0.99151	-0.74123
O	1.01392	-2.15183	-1.15802
C	2.41230	-2.02515	-0.80056
C	2.47733	-0.72170	0.04112
C	-0.99273	-0.83185	-1.09009
O	-1.58407	-1.92649	-1.64774
C	-2.93939	-1.51155	-1.95052
C	-3.05794	-0.10213	-1.31102
N	-1.68018	0.22166	-0.89504
C	3.56881	0.26714	-0.40853
C	4.97275	-0.36984	-0.33315
C	3.45001	1.58887	0.36865
C	-4.02103	-0.02885	-0.10421
C	-4.20606	1.42485	0.36714
C	-3.54802	-0.93774	1.04672
C	5.49277	-0.68244	1.07547
C	6.88151	-1.32607	1.04747
C	4.44836	2.66935	-0.05823
C	4.19496	4.00458	0.64638
C	-4.64947	-1.30262	2.04749
C	-4.13448	-2.18119	3.19011
C	-5.01411	2.31476	-0.58377
C	-5.20127	3.73260	-0.03768
H	2.98791	-1.95779	-1.73043
H	2.70791	-2.92643	-0.25948
H	2.62783	-0.95122	1.10432
H	-3.62307	-2.25074	-1.52518
H	-3.05186	-1.50089	-3.03889
H	-3.37383	0.63062	-2.06011
H	3.36860	0.48598	-1.46892
H	5.68645	0.29896	-0.83010
H	4.98452	-1.29573	-0.92602
H	3.56292	1.39474	1.44487
H	2.42916	1.96303	0.23875
H	-4.99301	-0.40460	-0.46392
H	-3.21290	1.86174	0.53067
H	-4.70910	1.42188	1.34266
H	-2.71958	-0.44179	1.56824
H	-3.12991	-1.87102	0.64515
H	4.79490	-1.35096	1.59715
H	5.53160	0.23901	1.66928
H	7.24566	-1.53986	2.05838
H	6.86862	-2.27033	0.48940
H	7.61046	-0.66618	0.56156
H	4.38666	2.81061	-1.14676
H	5.47555	2.34191	0.14941
H	4.91640	4.76797	0.33395
H	3.18912	4.38069	0.42527
H	4.27378	3.89535	1.73499
H	-5.45928	-1.82422	1.51762
H	-5.09676	-0.39132	2.46463
H	-4.93628	-2.44147	3.89015
H	-3.70732	-3.11602	2.80698
H	-3.34834	-1.66749	3.75635
H	-5.99722	1.85596	-0.76242
H	-4.52018	2.37229	-1.56242
H	-5.78275	4.35565	-0.72644
H	-5.72621	3.71766	0.92532
H	-4.23301	4.22187	0.12147

L1_4 Ground State

N	1.32763	-0.05546	0.00102
C	0.54197	-1.03845	-0.18902
O	1.02514	-2.30942	-0.10280
C	2.45326	-2.15795	0.08901
C	2.65369	-0.63189	0.29424
C	-0.89939	-0.92550	-0.49537
O	-1.59886	-2.09325	-0.45082
C	-2.96431	-1.73644	-0.77932
C	-2.92449	-0.19174	-0.95759
N	-1.50512	0.15910	-0.77306
C	3.75443	-0.01464	-0.58814
C	5.12501	-0.67336	-0.32342
C	3.76805	1.51592	-0.43830
C	-3.82377	0.60782	0.01294
C	-3.38260	0.42190	1.47509
C	-5.31398	0.28247	-0.19588
C	5.73916	-0.41184	1.05739
C	7.08552	-1.11911	1.23281
C	4.78252	2.23346	-1.33404
C	4.65870	3.75678	-1.24620
C	-5.84197	0.48770	-1.62114
C	-7.36049	0.31498	-1.70966
C	-4.07399	1.35476	2.47595
C	-3.48814	1.22905	3.88472

H	2.95110	-2.53244	-0.81239
H	2.74843	-2.77064	0.94337
H	2.87845	-0.40603	1.34505
H	-3.60331	-2.07330	0.04068
H	-3.24328	-2.27114	-1.69141
H	-3.19989	0.08202	-1.98105
H	3.47996	-0.24422	-1.62946
H	5.83025	-0.33215	-1.09141
H	5.04110	-1.75967	-0.47110
H	3.95853	1.78164	0.61138
H	2.76066	1.88299	-0.66068
H	-3.66738	1.66494	-0.24561
H	-2.30146	0.59501	1.52829
H	-3.54678	-0.62021	1.78798
H	-5.90321	0.91316	0.48074
H	-5.51340	-0.75320	0.11897
H	5.05122	-0.74318	1.84671
H	5.87378	0.66669	1.20520
H	7.51780	-0.92103	2.21982
H	6.97847	-2.20555	1.12595
H	7.80682	-0.78336	0.47787
H	4.63779	1.91234	-2.37547
H	5.80500	1.93909	-1.06309
H	5.39014	4.25800	-1.89014
H	3.65877	4.08775	-1.55060
H	4.82261	4.10551	-0.21919
H	-5.36188	-0.21868	-2.31090
H	-5.56387	1.49199	-1.97005
H	-7.72150	0.45523	-2.73448
H	-7.66255	-0.68758	-1.38282
H	-7.87721	1.04016	-1.06957
H	-5.15035	1.14511	2.51436
H	-3.97433	2.39241	2.12770
H	-3.99067	1.90041	4.59003
H	-3.59308	0.20544	4.26491
H	-2.41958	1.47489	3.88918

L1_5 Ground State

N	1.14056	-0.23114	0.09965
C	0.48812	-1.23355	-0.33515
O	1.09748	-2.44849	-0.41435
C	2.46332	-2.22026	0.01380
C	2.49867	-0.71522	0.40442
C	-0.92343	-1.19970	-0.77120
O	-1.51232	-2.41724	-0.94250
C	-2.85076	-2.12660	-1.41725
C	-2.96892	-0.58315	-1.30161
N	-1.60027	-0.14085	-0.97340
C	3.58052	0.09274	-0.33952
C	4.97548	-0.37695	0.11298
C	3.35899	1.61109	-0.20324
C	-3.96809	-0.09820	-0.22655
C	-4.14431	1.42995	-0.28636
C	-3.54588	-0.56129	1.18120
C	6.14511	0.29658	-0.61171
C	7.49870	-0.30122	-0.22012
C	3.47246	2.17322	1.21816
C	3.23867	3.68565	1.25548
C	-4.68281	-0.55396	2.20841
C	-4.21809	-0.99386	3.59883
C	-4.90627	1.94551	-1.51225
C	-5.08958	3.46515	-1.48811
H	3.12063	-2.45836	-0.82907
H	2.67662	-2.90262	0.83988
H	2.65806	-0.59889	1.48395
H	-3.55888	-2.67413	-0.78999
H	-2.92734	-2.48789	-2.44724
H	-3.24995	-0.14961	-2.26637
H	3.47375	-0.15095	-1.40827
H	5.05555	-1.46348	-0.03870
H	5.08214	-0.21954	1.19550
H	2.36133	1.84051	-0.59153
H	4.07571	2.13102	-0.85200
H	-4.93428	-0.56986	-0.47018
H	-3.14994	1.89204	-0.24579
H	-4.67877	1.76245	0.61278
H	-2.72410	0.07718	1.52948
H	-3.13338	-1.57863	1.13736
H	6.14720	1.37136	-0.39323
H	6.00013	0.20480	-1.69726
H	8.32323	0.19771	-0.74123
H	7.67592	-0.20155	0.85775
H	7.54547	-1.36940	-0.46492
H	4.46227	1.94929	1.63846
H	2.73831	1.68051	1.86777
H	3.31759	4.08021	2.27479
H	3.97271	4.21372	0.63421
H	2.24150	3.93570	0.87461
H	-5.48661	-1.21865	1.86094
H	-5.12465	0.44847	2.27466
H	-5.04466	-0.99290	4.31817
H	-3.79810	-2.00681	3.57208
H	-3.43889	-0.32420	3.98216

H	-5.88987	1.45646	-1.56013
H	-4.37913	1.66498	-2.43337
H	-5.63794	3.81840	-2.36858
H	-5.64661	3.78060	-0.59741
H	-4.11972	3.97629	-1.46938

L1_6 Ground State

N	-1.44168	-0.35343	-0.72929
C	-0.84381	-1.07381	0.13320
O	-1.54085	-2.02597	0.81294
C	-2.89253	-1.95567	0.29516
C	-2.85318	-0.77738	-0.71944
C	0.58478	-0.95605	0.49287
O	1.08274	-1.96965	1.25341
C	2.48689	-1.65898	1.43345
C	2.67404	-0.29080	0.71796
N	1.34589	0.00530	0.15212
C	-3.78492	0.41089	-0.38715
C	-3.38955	1.08513	0.93801
C	-5.26699	-0.00496	-0.41489
C	3.77339	-0.30242	-0.36266
C	5.14808	-0.49528	0.30405
C	3.69218	0.93356	-1.27843
C	-4.11711	2.40287	1.22821
C	-3.57429	3.10076	2.47798
C	-5.74882	-0.64701	-1.72176
C	-7.26367	-0.86736	-1.73800
C	3.94225	2.28292	-0.59577
C	3.84120	3.44996	-1.58130
C	6.32470	-0.59977	-0.67142
C	7.64345	-0.92405	0.03476
H	-3.56501	-1.79316	1.14096
H	-3.12764	-2.91813	-0.16766
H	-3.09731	-1.13114	-1.72602
H	3.06793	-2.46487	0.97285
H	2.69258	-1.63544	2.50615
H	2.90865	0.49750	1.44452
H	-3.62290	1.14419	-1.19015
H	-3.55804	0.39336	1.77699
H	-2.31160	1.28232	0.91035
H	-5.87895	0.88527	-0.22587
H	-5.47477	-0.68812	0.42275
H	3.58036	-1.18247	-0.99612
H	5.12561	-1.40884	0.91630
H	5.33366	0.32888	1.00713
H	2.69561	0.95013	-1.73153
H	4.40903	0.81013	-2.10051
H	-5.19285	2.22684	1.35354
H	-4.01284	3.06938	0.36055
H	-4.10255	4.04044	2.67460
H	-3.68457	2.46352	3.36403
H	-2.50793	3.33084	2.36752
H	-5.24661	-1.61011	-1.88114
H	-5.45979	-0.00818	-2.56795
H	-7.59146	-1.33433	-2.67328
H	-7.57596	-1.51792	-0.91190
H	-7.80088	0.08265	-1.63086
H	4.93379	2.29278	-0.12326
H	3.21106	2.42859	0.20912
H	4.01737	4.41152	-1.08605
H	4.57722	3.34929	-2.38865
H	2.84709	3.48637	-2.04208
H	6.43220	0.34100	-1.22486
H	6.10642	-1.37317	-1.42114
H	8.47444	-0.98648	-0.67651
H	7.89385	-0.15337	0.77402
H	7.58352	-1.88258	0.56463

L1_7 Ground State

N	1.19662	-0.51909	0.27217
C	0.64379	-0.58258	-0.87260
O	1.34740	-1.06688	-1.93318
C	2.64238	-1.43711	-1.39748
C	2.57987	-0.99614	0.09234
C	-0.73594	-0.14722	-1.17144
O	-1.27113	-0.64588	-2.32183
C	-2.58185	-0.03486	-2.42464
C	-2.76040	0.71156	-1.07549
N	-1.43145	0.62765	-0.43944
C	3.59503	0.09481	0.50211
C	3.35560	1.40792	-0.26315
C	5.04699	-0.40182	0.36307
C	-3.84292	0.10926	-0.15095
C	-4.06574	0.99537	1.08796
C	-3.49757	-1.33870	0.24745
C	4.17943	2.59916	0.23912
C	3.78799	3.90698	-0.45364
C	5.38469	-1.72095	1.07566
C	5.12774	-1.69400	2.58532
C	-4.69736	-2.15456	0.74009
C	-4.30903	-3.57764	1.14852
C	-4.76108	2.33274	0.81015
C	-4.99669	3.14360	2.08705
H	3.40549	-0.92045	-1.98422

H	2.76451	-2.51654	-1.52408
H	2.71924	-1.85873	0.75162
H	-3.31344	-0.82926	-2.59270
H	-2.57249	0.63580	-3.28921
H	-2.99280	1.76627	-1.25199
H	3.39503	0.29853	1.56239
H	2.29233	1.66140	-0.18025
H	3.55870	1.26157	-1.33473
H	5.71482	0.37640	0.75185
H	5.29322	-0.49853	-0.70449
H	-4.77502	0.09287	-0.73943
H	-3.09234	1.17428	1.56167
H	-4.66984	0.44158	1.81803
H	-2.71949	-1.31447	1.02089
H	-3.05220	-1.86969	-0.60504
H	5.25013	2.41637	0.08406
H	4.03822	2.70138	1.32431
H	4.38400	4.75001	-0.08647
H	3.93847	3.83839	-1.53807
H	2.73088	4.14162	-0.28132
H	6.44423	-1.94377	0.89497
H	4.82695	-2.55207	0.62339
H	5.46640	-2.62136	3.06005
H	5.66227	-0.86086	3.05802
H	4.06341	-1.57450	2.81586
H	-5.45726	-2.19317	-0.05347
H	-5.17231	-1.65054	1.59147
H	-5.17928	-4.15014	1.48854
H	-3.85838	-4.11994	0.30828
H	-3.57584	-3.56546	1.96384
H	-5.72229	2.14507	0.31034
H	-4.16447	2.93376	0.11170
H	-5.49659	4.09497	1.87321
H	-5.62227	2.58821	2.79650
H	-4.04801	3.36827	2.58884

L1_8 Ground State

N	-1.26867	-0.59009	-0.28645
C	-0.65227	-0.31123	0.79162
O	-1.31136	-0.38340	1.98110
C	-2.65024	-0.82993	1.65117
C	-2.65719	-0.90291	0.09763
C	0.76015	0.11429	0.87354
O	1.34934	-0.04494	2.09084
C	2.70177	0.45125	1.93014
C	2.79889	0.81381	0.42118
N	1.43606	0.58964	-0.09456
C	-3.65120	0.05169	-0.60346
C	-3.30969	1.52597	-0.32578
C	-5.11059	-0.28934	-0.25074
C	3.83354	0.00027	-0.38889
C	3.48977	-1.49930	-0.40449
C	5.26999	0.26149	0.10358
C	-4.10823	2.53612	-1.15757
C	-3.61831	3.97173	-0.95097
C	-5.54024	-1.73302	-0.53941
C	-7.04235	-1.94546	-0.33402
C	5.70838	1.73313	0.16865
C	5.61840	2.46683	-1.17273
C	4.33656	-2.33824	-1.36846
C	3.85117	-3.78757	-1.45429
H	-3.35469	-0.10578	2.06712
H	-2.81047	-1.79985	2.13038
H	-2.86978	-1.92304	-0.23655
H	3.38636	-0.34012	2.24406
H	2.82598	1.31389	2.59087
H	3.02696	1.87726	0.29824
H	-3.51309	-0.12051	-1.68054
H	-2.24315	1.67264	-0.53199
H	-3.45430	1.75062	0.74167
H	-5.76818	0.38204	-0.81605
H	-5.29770	-0.06045	0.80949
H	3.74683	0.36158	-1.42212
H	2.43586	-1.60451	-0.68713
H	3.58454	-1.91798	0.60875
H	5.96255	-0.27149	-0.55908
H	5.39833	-0.19448	1.09621
H	-5.17494	2.48083	-0.90663
H	-4.02736	2.26965	-2.22078
H	-4.19690	4.68365	-1.55027
H	-3.70704	4.27047	0.10081
H	-2.56390	4.07153	-1.23463
H	-4.99009	-2.43087	0.10520
H	-5.26872	-1.99263	-1.57217
H	-7.33235	-2.98262	-0.53518
H	-7.33633	-1.70979	0.69615
H	-7.62617	-1.29855	-0.99979
H	6.74558	1.76375	0.52672
H	5.11977	2.27328	0.92242
H	6.02395	3.48156	-1.09573
H	6.18639	1.93670	-1.94712
H	4.58381	2.55027	-1.52339
H	5.38952	-2.32915	-1.06006

H	4.30384	-1.87990	-2.36688
H	4.46421	-4.37614	-2.14605
H	3.89284	-4.27552	-0.47269
H	2.81236	-3.83387	-1.80208

L1_9 Ground State

N	-1.42745	-0.24287	-0.34548
C	-0.72071	-1.28576	-0.16469
O	-1.29595	-2.51452	-0.27894
C	-2.69773	-2.25748	-0.54248
C	-2.79276	-0.70873	-0.64560
C	0.72039	-1.28570	0.16423
O	1.29552	-2.51442	0.27942
C	2.69744	-2.25727	0.54215
C	2.79242	-0.70852	0.64502
N	1.42721	-0.24274	0.34428
C	-3.83777	-0.08800	0.30217
C	-5.24980	-0.51931	-0.13545
C	-3.66284	1.43705	0.43055
C	3.83785	-0.08796	-0.30237
C	5.24965	-0.51959	0.13568
C	3.66327	1.43714	-0.43071
C	-6.38087	-0.02740	0.77315
C	-7.74427	-0.59426	0.36971
C	-3.89269	2.24223	-0.85327
C	-3.69600	3.74380	-0.62950
C	3.89291	2.24221	0.85321
C	3.69654	3.74383	0.62946
C	6.38113	-0.02767	-0.77242
C	7.74430	-0.59479	-0.36859
H	-3.27465	-2.66510	0.29457
H	-2.97130	-2.78586	-1.45856
H	-3.02919	-0.40265	-1.67282
H	3.27391	-2.66487	-0.29523
H	2.97158	-2.78558	1.45808
H	3.02836	-0.40226	1.67230
H	-3.64933	-0.51609	1.29930
H	-5.43631	-0.17605	-1.16276
H	-5.29335	-1.61767	-0.17648
H	-2.64517	1.62873	0.78602
H	-4.34238	1.80493	1.21016
H	3.64965	-0.51595	-1.29958
H	5.29301	-1.61796	0.17650
H	5.43585	-0.17656	1.16312
H	2.64574	1.62903	-0.78648
H	4.34311	1.80492	-1.21011
H	-6.42368	1.06831	0.75175
H	-6.15755	-0.30516	1.81279
H	-8.54155	-0.22537	1.02438
H	-7.99922	-0.31148	-0.65897
H	-7.74854	-1.68990	0.42153
H	-4.90541	2.06314	-1.23902
H	-3.19746	1.90120	-1.63048
H	-3.85859	4.31294	-1.55174
H	-4.39383	4.12471	0.12656
H	-2.67926	3.95600	-0.27860
H	4.90550	2.06293	1.23922
H	3.19742	1.90127	1.63022
H	3.85898	4.31290	1.55177
H	4.39465	4.12465	-0.12639
H	2.67993	3.95622	0.27829
H	6.42408	1.06804	-0.75082
H	6.15814	-0.30521	-1.81220
H	8.54186	-0.22590	-1.02291
H	7.99892	-0.31222	0.66023
H	7.74844	-1.69042	-0.42061

L1_10 Ground State

N	1.22213	-0.05971	0.64658
C	0.63551	-1.14357	0.32815
O	1.26972	-2.33433	0.52444
C	2.52345	-1.99336	1.16766
C	2.56724	-0.44265	1.11659
C	-0.71276	-1.23305	-0.26897
O	-1.28926	-2.46795	-0.23220
C	-2.55548	-2.31450	-0.92122
C	-2.67347	-0.78600	-1.16404
N	-1.34882	-0.25833	-0.78442
C	3.65672	0.13225	0.18309
C	3.74308	1.66370	0.30717
C	3.42097	-0.29658	-1.27950
C	-3.78774	-0.09381	-0.34635
C	-3.94108	1.38093	-0.76027
C	-3.53913	-0.23025	1.16831
C	4.31958	2.17364	1.63256
C	4.42905	3.70005	1.67216
C	4.65138	-0.18582	-2.19226
C	5.76571	-1.18118	-1.85376
C	-4.78849	-0.01383	2.02863
C	-4.49554	-0.13343	3.52618
C	-4.54404	1.60304	-2.15175
C	-4.71525	3.08791	-2.48251
H	3.33136	-2.47809	0.61360
H	2.49613	-2.38973	2.18721

H	2.71114	-0.03272	2.12102
H	-3.34098	-2.72445	-0.28130
H	-2.50573	-2.89443	-1.84783
H	-2.83536	-0.58079	-2.22671
H	4.60775	-0.29729	0.53285
H	2.73890	2.07890	0.15457
H	4.36698	2.05192	-0.50839
H	2.60345	0.31122	-1.68478
H	3.06666	-1.33594	-1.31544
H	-4.72286	-0.62348	-0.59203
H	-2.95465	1.85797	-0.70257
H	-4.57739	1.89237	-0.02669
H	-2.75632	0.48070	1.46159
H	-3.13651	-1.22643	1.39753
H	3.69606	1.83939	2.47190
H	5.31259	1.72894	1.79148
H	4.84460	4.04921	2.62407
H	5.07695	4.06948	0.86787
H	3.44506	4.16658	1.54424
H	5.05183	0.83584	-2.16444
H	4.32798	-0.35294	-3.22775
H	6.59365	-1.10669	-2.56752
H	6.17960	-1.00790	-0.85397
H	5.39152	-2.21239	-1.88334
H	-5.55448	-0.74890	1.74302
H	-5.22223	0.97298	1.82229
H	-5.40060	0.01392	4.12605
H	-4.08860	-1.12227	3.77065
H	-3.75790	0.61375	3.84258
H	-5.51896	1.09793	-2.20965
H	-3.91159	1.13794	-2.91902
H	-5.14957	3.23094	-3.47831
H	-5.37333	3.57995	-1.75591
H	-3.75026	3.60804	-2.45935

L1_11 Ground State

N	-1.34876	-0.25894	-0.78433
C	-0.71282	-1.23352	-0.26849
O	-1.28950	-2.46832	-0.23113
C	-2.55579	-2.31496	-0.92005
C	-2.67352	-0.78657	-1.16362
C	0.63553	-1.14399	0.32845
O	1.26984	-2.33472	0.52460
C	2.52364	-1.99370	1.16762
C	2.56732	-0.44299	1.11662
N	1.22212	-0.06011	0.64684
C	-3.78763	-0.09377	-0.34623
C	-3.94069	1.38080	-0.76089
C	-3.53899	-0.22948	1.16849
C	3.65663	0.13205	0.18298
C	3.74297	1.66348	0.30722
C	3.42063	-0.29665	-1.27960
C	-4.54401	1.60230	-2.15231
C	-4.71471	3.08704	-2.48395
C	-4.78836	-0.01256	2.02867
C	-4.49545	-0.13118	3.52630
C	4.65065	-0.18519	-2.19281
C	5.76582	-1.17967	-1.85455
C	4.31946	2.17331	1.63266
C	4.42900	3.69971	1.67237
H	-3.34129	-2.72442	-0.27979
H	-2.50630	-2.89539	-1.84636
H	-2.83542	-0.58184	-2.22639
H	3.33151	-2.47836	0.61341
H	2.49652	-2.39011	2.18716
H	2.71136	-0.03310	2.12105
H	-4.72285	-0.62338	-0.59162
H	-2.95412	1.85760	-0.70374
H	-4.57663	1.89281	-0.02739
H	-2.75615	0.48158	1.46141
H	-3.13642	-1.22557	1.39821
H	4.60774	-0.29749	0.53253
H	2.73879	2.07869	0.15466
H	4.36688	2.05180	-0.50830
H	2.60269	0.31082	-1.68453
H	3.06681	-1.33617	-1.31557
H	-3.91200	1.13646	-2.91950
H	-5.51916	1.09756	-2.20958
H	-5.14933	3.22963	-3.47968
H	-5.37234	3.57980	-1.75742
H	-3.74950	3.60678	-2.46144
H	-5.55432	-0.74785	1.74351
H	-5.22215	0.97409	1.82166
H	-5.40053	0.01646	4.12605
H	-4.08841	-1.11982	3.77140
H	-3.75788	0.61627	3.84224
H	5.05038	0.83677	-2.16534
H	4.32698	-0.35273	-3.22814
H	6.59334	-1.10487	-2.56877
H	6.18012	-1.00578	-0.85504
H	5.39232	-2.21115	-1.88358
H	5.31245	1.72855	1.79158
H	3.69590	1.83903	2.47196

H	4.84453	4.04879	2.62431
H	5.07695	4.06916	0.86812
H	3.44504	4.16630	1.54443

L1_12 Ground State

N	1.23743	-0.73173	0.17794
C	0.58494	-0.82773	-0.91068
O	1.17507	-1.39312	-2.00148
C	2.48015	-1.82726	-1.54226
C	2.59102	-1.24607	-0.10721
C	-0.80080	-0.35718	-1.11001
O	-1.45467	-0.89812	-2.17817
C	-2.76248	-0.26964	-2.17995
C	-2.78374	0.57158	-0.87386
N	-1.40587	0.47148	-0.35764
C	3.64151	-0.12283	0.04774
C	3.79839	0.28635	1.52346
C	3.30076	1.09014	-0.83949
C	-3.81098	0.14681	0.20668
C	-4.01425	1.29478	1.21686
C	-3.42791	-1.14291	0.95840
C	4.48135	-0.75653	2.41518
C	4.65282	-0.26870	3.85608
C	4.49043	2.01492	-1.11748
C	4.10643	3.21821	-1.98202
C	-3.37101	-2.44279	0.14573
C	-3.11051	-3.65921	1.03882
C	-4.80325	2.49620	0.68432
C	-4.98683	3.58910	1.74062
H	3.22948	-1.44011	-2.23731
H	2.49707	-2.92109	-1.56575
H	2.81580	-2.04197	0.60935
H	-3.51763	-1.05629	-2.21961
H	-2.83295	0.34545	-3.08200
H	-2.97302	1.62045	-1.12215
H	4.59795	-0.54710	-0.29949
H	2.80359	0.52148	1.92224
H	4.38166	1.21461	1.57538
H	2.49029	1.65706	-0.36410
H	2.89992	0.75203	-1.80489
H	-4.76651	-0.02392	-0.31525
H	-3.02936	1.62399	1.57386
H	-4.54354	0.90029	2.09468
H	-4.16424	-1.28144	1.76221
H	-2.46081	-0.98298	1.45083
H	3.90253	-1.68924	2.42167
H	5.46447	-1.00801	1.99191
H	5.14421	-1.02317	4.48058
H	5.25967	0.64424	3.89327
H	3.68151	-0.03838	4.30971
H	5.28425	1.44085	-1.61643
H	4.92056	2.37066	-0.17257
H	4.96982	3.86336	-2.17956
H	3.70071	2.89574	-2.94876
H	3.33873	3.82653	-1.48901
H	-2.58580	-2.39244	-0.61517
H	-4.32045	-2.58093	-0.39210
H	-3.07113	-4.58505	0.45408
H	-2.15559	-3.55605	1.56805
H	-3.89732	-3.77196	1.79470
H	-5.78725	2.15412	0.33304
H	-4.30072	2.92852	-0.19105
H	-5.55959	4.43639	1.34728
H	-5.51927	3.20310	2.61835
H	-4.01731	3.96953	2.08362

L1_13 Ground State

N	1.19139	-0.26780	0.22944
C	0.54151	-1.25660	-0.23918
O	1.13186	-2.48210	-0.29600
C	2.48121	-2.27995	0.19343
C	2.52461	-0.77818	0.59533
C	-0.84813	-1.19546	-0.73814
O	-1.44555	-2.40138	-0.95557
C	-2.75677	-2.08373	-1.48581
C	-2.85910	-0.54091	-1.34894
N	-1.50049	-0.12379	-0.95312
C	3.65399	0.01328	-0.09269
C	5.01639	-0.48366	0.42932
C	3.45598	1.53448	0.04096
C	-3.89809	-0.05977	-0.31048
C	-4.04980	1.47163	-0.35045
C	-3.54540	-0.55336	1.10603
C	6.24697	0.19709	-0.18672
C	6.34418	0.04537	-1.70744
C	3.49274	2.08652	1.47037
C	3.29845	3.60462	1.50239
C	-4.72644	-0.54613	2.08224
C	-4.33019	-1.01723	3.48359
C	-4.74904	2.01997	-1.59925
C	-4.91118	3.54160	-1.55572
H	3.17102	-2.52367	-0.62142
H	2.64645	-2.97104	1.02323
H	2.63423	-0.67066	1.68200

H	-3.50028	-2.63151	-0.90117
H	-2.79084	-2.42655	-2.52438
H	-3.09140	-0.08739	-2.31747
H	3.58628	-0.22501	-1.16424
H	5.09489	-1.56577	0.24820
H	5.04872	-0.35892	1.52003
H	2.48936	1.78794	-0.40650
H	4.22238	2.04357	-0.55836
H	-4.85907	-0.51276	-0.60486
H	-3.05171	1.91790	-0.25759
H	-4.61891	1.79638	0.53006
H	-2.73062	0.06639	1.50144
H	-3.14628	-1.57603	1.06232
H	7.14454	-0.23271	0.27666
H	6.25236	1.26209	0.07695
H	7.27809	0.47368	-2.08758
H	6.31808	-1.01187	-2.00004
H	5.51758	0.55042	-2.21897
H	4.44645	1.83316	1.95249
H	2.70427	1.61112	2.06692
H	3.32020	3.99176	2.52735
H	4.08636	4.11525	0.93478
H	2.33597	3.88421	1.05805
H	-5.52378	-1.19216	1.68789
H	-5.15597	0.46174	2.14700
H	-5.18768	-1.01595	4.16579
H	-3.92440	-2.03596	3.45707
H	-3.55896	-0.36650	3.91284
H	-5.73654	1.54693	-1.69927
H	-4.18567	1.74749	-2.50113
H	-5.41486	3.91850	-2.45292
H	-5.50245	3.84993	-0.68482
H	-3.93579	4.03745	-1.48509

L1_14 Ground State

N	-1.29483	0.12959	-0.67941
C	-0.71978	-1.00501	-0.63055
O	-1.30407	-2.08115	-1.23017
C	-2.49198	-1.55617	-1.87402
C	-2.57625	-0.08798	-1.37765
C	0.56114	-1.27769	0.05336
O	1.12757	-2.48642	-0.22510
C	2.32311	-2.54182	0.59322
C	2.41839	-1.12760	1.22666
N	1.14919	-0.47723	0.84943
C	-3.76505	0.19864	-0.43206
C	-3.86819	1.70141	-0.11462
C	-3.67356	-0.64380	0.85491
C	3.62693	-0.29465	0.74547
C	3.68769	1.02167	1.53948
C	3.60280	-0.08099	-0.78642
C	-4.32555	2.57954	-1.28463
C	-4.45524	4.05337	-0.89154
C	-5.00375	-0.79190	1.60094
C	-4.86614	-1.61458	2.88431
C	4.97415	-0.21067	-1.46035
C	4.91664	0.06231	-2.96468
C	4.88676	1.92322	1.23208
C	4.91944	3.16717	2.12411
H	-3.34124	-2.17559	-1.57459
H	-2.35055	-1.63666	-2.95611
H	-2.62718	0.59905	-2.22794
H	3.16568	-2.79184	-0.05682
H	2.18821	-3.33765	1.33177
H	2.46021	-1.19360	2.32027
H	-4.67260	-0.10458	-0.97954
H	-2.89044	2.04399	0.24675
H	-4.57329	1.84269	0.71455
H	-2.92263	-0.19415	1.51687
H	-3.29993	-1.65046	0.62244
H	4.52055	-0.88832	0.99752
H	3.69730	0.78107	2.61294
H	2.75679	1.57394	1.36015
H	3.17027	0.90346	-1.00637
H	2.92789	-0.80365	-1.26273
H	-3.62060	2.49508	-2.12185
H	-5.29188	2.21150	-1.65838
H	-4.78521	4.66776	-1.73674
H	-5.18158	4.18211	-0.07977
H	-3.49519	4.45131	-0.54195
H	-5.73904	-1.26677	0.93572
H	-5.41050	0.19731	1.84686
H	-5.82736	-1.71955	3.39979
H	-4.48970	-2.62197	2.66838
H	-4.16226	-1.14192	3.57976
H	5.36190	-1.22449	-1.28441
H	5.69194	0.47155	-0.98990
H	5.89998	-0.05590	-3.43343
H	4.22216	-0.62460	-3.46378
H	4.57047	1.08352	-3.16516
H	4.85827	2.23592	0.18078
H	5.81885	1.35442	1.35936
H	5.77644	3.80814	1.88868

H	4.00859	3.76451	1.99713
H	4.98780	2.89150	3.18350

L1_15 Ground State

N	1.11255	-0.11288	0.03156
C	0.45732	-0.81096	-0.80690
O	1.07217	-1.84712	-1.44281
C	2.45707	-1.77973	-1.02222
C	2.47164	-0.68525	0.07931
C	-0.96175	-0.59913	-1.16070
O	-1.52445	-1.57465	-1.92921
C	-2.87611	-1.12010	-2.18824
C	-3.02835	0.14600	-1.30309
N	-1.66667	0.39513	-0.79337
C	3.55181	0.39447	-0.11619
C	4.96761	-0.21766	-0.14456
C	3.38638	1.50762	0.93421
C	-4.02647	-0.01006	-0.13324
C	-4.23928	1.33030	0.59332
C	-3.57836	-1.11454	0.84341
C	5.45409	-0.84842	1.16615
C	6.86417	-1.43024	1.03672
C	4.39434	2.66104	0.83195
C	4.36151	3.39670	-0.51137
C	-4.70509	-1.66233	1.72555
C	-4.21617	-2.73646	2.70022
C	-5.02809	2.37767	-0.20034
C	-5.24539	3.66860	0.59324
H	3.05683	-1.50740	-1.89775
H	2.75613	-2.77138	-0.67620
H	2.59821	-1.13388	1.07350
H	-3.56199	-1.92978	-1.92605
H	-2.95993	-0.90925	-3.25867
H	-3.33067	1.00290	-1.91317
H	3.36688	0.83057	-1.10848
H	5.67907	0.56286	-0.44282
H	5.02099	-0.97495	-0.93987
H	3.44838	1.06576	1.93808
H	2.36930	1.90299	0.84336
H	-4.98394	-0.31673	-0.58554
H	-3.25560	1.73344	0.86498
H	-4.77040	1.14446	1.53570
H	-2.76987	-0.72080	1.47238
H	-3.14040	-1.95588	0.28899
H	4.76365	-1.64152	1.48307
H	5.44278	-0.09819	1.96612
H	7.20323	-1.87540	1.97860
H	6.90124	-2.20940	0.26549
H	7.58514	-0.65324	0.75492
H	5.41202	2.29555	1.02420
H	4.17650	3.37535	1.63648
H	5.03046	4.26448	-0.50378
H	4.67370	2.74851	-1.33815
H	3.34944	3.75401	-0.73699
H	-5.49476	-2.07877	1.08397
H	-5.17200	-0.84577	2.29100
H	-5.03575	-3.12428	3.31551
H	-3.77055	-3.58282	2.16332
H	-3.45093	-2.33480	3.37520
H	-6.00091	1.95562	-0.49091
H	-4.50641	2.61809	-1.13580
H	-5.81299	4.40601	0.01464
H	-5.79782	3.47271	1.52038
H	-4.28718	4.12430	0.86967

L1_16 Ground State

N	1.04511	-0.28374	0.43146
C	0.45012	-1.11033	-0.33173
O	1.08191	-2.25807	-0.70182
C	2.37787	-2.20767	-0.05548
C	2.38686	-0.83820	0.68497
C	-0.91423	-0.93367	-0.87149
O	-1.46697	-2.04357	-1.43835
C	-2.75799	-1.61100	-1.93577
C	-2.91016	-0.16512	-1.39210
N	-1.58423	0.14764	-0.82560
C	3.49575	0.11625	0.19971
C	4.89167	-0.48990	0.48813
C	3.31102	1.51218	0.81629
C	-4.01098	0.00070	-0.31959
C	-4.20464	1.48297	0.04797
C	-3.71235	-0.85409	0.92722
C	5.89058	-0.34494	-0.66604
C	7.27635	-0.89473	-0.32282
C	4.29680	2.57481	0.32098
C	4.00246	3.95682	0.91037
C	-4.93838	-1.13027	1.80387
C	-4.59605	-1.95984	3.04377
C	-4.85790	2.33955	-1.04229
C	-5.06575	3.78971	-0.59806
H	3.14208	-2.28390	-0.83462
H	2.45533	-3.07160	0.60987
H	2.50007	-0.97629	1.76831
H	-3.51450	-2.30691	-1.56421

H	-2.72983	-1.65878	-3.02860
H	-3.10831	0.53134	-2.21266
H	3.37179	0.20627	-0.89084
H	4.80378	-1.55991	0.72519
H	5.30694	-0.02623	1.39383
H	3.39493	1.42604	1.91072
H	2.28720	1.84447	0.61473
H	-4.94334	-0.36934	-0.77690
H	-3.22558	1.90180	0.31249
H	-4.82505	1.54796	0.95102
H	-2.93568	-0.35331	1.51906
H	-3.28217	-1.82021	0.62960
H	5.97270	0.70972	-0.95429
H	5.49269	-0.86808	-1.54709
H	7.96764	-0.79708	-1.16715
H	7.71178	-0.35926	0.52963
H	7.22505	-1.95700	-0.05359
H	4.25380	2.62717	-0.77607
H	5.32530	2.28662	0.57471
H	4.71239	4.70848	0.54726
H	2.99265	4.29033	0.64358
H	4.06495	3.93861	2.00530
H	-5.69732	-1.65575	1.20677
H	-5.39902	-0.18457	2.11682
H	-5.48473	-2.15705	3.65371
H	-4.16055	-2.92672	2.76330
H	-3.86497	-1.43972	3.67424
H	-5.82533	1.89711	-1.32025
H	-4.24377	2.33037	-1.95213
H	-5.53578	4.38861	-1.38617
H	-5.70739	3.84150	0.29006
H	-4.10965	4.26190	-0.34279

L1_17 Ground State

N	1.20482	-0.16078	-0.00457
C	0.48902	-1.04049	-0.58205
O	1.04286	-2.23776	-0.92234
C	2.44853	-2.11034	-0.59521
C	2.54881	-0.74995	0.14721
C	-0.93999	-0.88062	-0.92312
O	-1.55502	-1.99900	-1.40269
C	-2.90677	-1.58220	-1.71841
C	-2.99434	-0.13083	-1.17468
N	-1.60814	0.19469	-0.78986
C	3.64697	0.18506	-0.39266
C	5.04226	-0.46770	-0.29592
C	3.56295	1.56190	0.28724
C	-3.95137	0.03972	0.02661
C	-4.11268	1.52325	0.40256
C	-3.48368	-0.79419	1.23674
C	5.58397	-0.68670	1.12217
C	6.96156	-1.35444	1.11603
C	4.56924	2.59148	-0.23591
C	4.34958	3.97891	0.37262
C	-4.57418	-1.08406	2.27899
C	-5.66504	-2.03890	1.78361
C	-4.91193	2.36056	-0.60194
C	-5.07706	3.81376	-0.14991
H	3.01062	-2.12183	-1.53561
H	2.73734	-2.97463	0.00653
H	2.71491	-0.90318	1.22172
H	-3.59777	-2.27826	-1.23579
H	-3.03207	-1.64376	-2.80365
H	-3.30122	0.55585	-1.96987
H	3.43017	0.32917	-1.46256
H	5.75650	0.15187	-0.85239
H	5.02898	-1.43393	-0.82041
H	3.69332	1.44537	1.37264
H	2.54562	1.94233	0.14833
H	-4.92761	-0.33897	-0.31228
H	-3.11293	1.95575	0.53513
H	-4.61211	1.59092	1.37791
H	-2.64816	-0.26620	1.71126
H	-3.07523	-1.75631	0.89828
H	4.88566	-1.30378	1.70325
H	5.64885	0.27431	1.64702
H	7.34166	-1.50064	2.13309
H	6.92306	-2.33629	0.62847
H	7.69138	-0.74410	0.57034
H	4.48895	2.65338	-1.33062
H	5.59514	2.26328	-0.02312
H	4.44766	3.94881	1.46473
H	5.07629	4.70529	-0.00834
H	3.34545	4.35421	0.14253
H	-5.03367	-0.14548	2.61528
H	-4.09697	-1.51948	3.16635
H	-6.38779	-2.26056	2.57670
H	-6.22426	-1.61899	0.93988
H	-5.23071	-2.99068	1.45242
H	-5.90216	1.90508	-0.74697
H	-4.42128	2.34628	-1.58386
H	-4.10143	4.29871	-0.02667
H	-5.59792	3.86967	0.81380

H	-5.65284	4.39827	-0.87622

L1_18 Ground State

N	1.04914	-0.11317	-0.04164
C	0.34081	-0.93595	-0.70566
O	0.92378	-2.04603	-1.23793
C	2.33855	-1.89910	-0.96077
C	2.42194	-0.65395	-0.03644
C	-1.10987	-0.79946	-0.95030
O	-1.71821	-1.89883	-1.48203
C	-3.10665	-1.51705	-1.65697
C	-3.20089	-0.10963	-1.00557
N	-1.80396	0.23248	-0.68093
C	3.45263	0.39875	-0.48464
C	4.87596	-0.19508	-0.54623
C	3.34891	1.65898	0.39084
C	-4.10692	0.01404	0.24610
C	-4.43990	1.49727	0.50821
C	-3.50347	-0.61367	1.51762
C	5.49623	-0.59200	0.79912
C	6.89806	-1.18486	0.63471
C	4.28396	2.79932	-0.02344
C	4.04093	4.07355	0.78944
C	-3.27937	-2.13131	1.51780
C	-2.80703	-2.63498	2.88470
C	-5.42323	2.12733	-0.48462
C	-5.72607	3.59183	-0.15690
H	2.85053	-1.75086	-1.91799
H	2.69314	-2.82494	-0.50304
H	2.64828	-0.94957	0.99650
H	-3.73063	-2.27502	-1.18073
H	-3.31295	-1.50183	-2.73131
H	-3.55776	0.60984	-1.74909
H	3.17551	0.68374	-1.51147
H	5.53599	0.53148	-1.03620
H	4.87502	-1.07450	-1.20616
H	3.54103	1.39503	1.44068
H	2.31118	2.00665	0.35570
H	-5.04615	-0.51169	0.00939
H	-3.50233	2.06883	0.51801
H	-4.86648	1.58855	1.51622
H	-4.17911	-0.37387	2.35039
H	-2.55438	-0.10884	1.73629
H	4.85377	-1.32001	1.31231
H	5.54753	0.28431	1.45690
H	7.33379	-1.45999	1.60151
H	6.87566	-2.08547	0.00890
H	7.57427	-0.46699	0.15480
H	4.14377	3.01309	-1.09269
H	5.33199	2.49307	0.09187
H	4.71683	4.88049	0.48472
H	3.01182	4.42992	0.66287
H	4.19741	3.89239	1.85992
H	-2.53837	-2.41605	0.76412
H	-4.21549	-2.64019	1.24488
H	-2.64752	-3.71900	2.87952
H	-1.86135	-2.15848	3.16989
H	-3.54140	-2.40661	3.66680
H	-6.35781	1.54834	-0.48294
H	-5.02869	2.06605	-1.50750
H	-6.43648	4.02487	-0.86998
H	-6.15688	3.68986	0.84694
H	-4.81194	4.19675	-0.18432

L1_19 Ground State

N	1.13861	-0.12363	-0.06797
C	0.41874	-0.90383	-0.76992
O	0.97167	-2.02959	-1.30179
C	2.38094	-1.94867	-0.97487
C	2.48589	-0.72359	-0.02633
C	-1.01499	-0.69905	-1.06327
O	-1.65635	-1.76708	-1.61769
C	-3.00712	-1.30672	-1.87040
C	-3.06772	0.08439	-1.18512
N	-1.66591	0.36824	-0.82305
C	3.57593	0.29018	-0.42073
C	4.97362	-0.36418	-0.44353
C	3.49580	1.53982	0.47218
C	-3.97305	0.14542	0.06539
C	-4.06301	1.57913	0.62192
C	-3.50091	-0.83993	1.15209
C	5.52937	-0.80748	0.91548
C	6.90896	-1.45894	0.78905
C	4.49310	2.64473	0.11035
C	4.27731	3.91485	0.93725
C	-4.54721	-1.14067	2.23091
C	-4.04448	-2.15219	3.26399
C	-4.59789	2.64983	-0.34137
C	-5.99209	2.35182	-0.90151
H	2.93142	-1.80705	-1.91156
H	2.67994	-2.89635	-0.52210
H	2.66375	-1.04557	1.00824
H	-3.70001	-2.04100	-1.45202
H	-3.14692	-1.25633	-2.95465

H	-3.40238	0.84234	-1.89961
H	3.34752	0.60306	-1.45142
H	5.68104	0.33981	-0.89912
H	4.95752	-1.23303	-1.11714
H	3.63909	1.25120	1.52333
H	2.47587	1.93291	0.40713
H	-4.97358	-0.17065	-0.26734
H	-3.06245	1.87297	0.96035
H	-4.70689	1.56579	1.51048
H	-2.59140	-0.44115	1.61903
H	-3.20624	-1.79279	0.69146
H	4.83862	-1.51388	1.39499
H	5.59603	0.05609	1.58853
H	7.29900	-1.76656	1.76552
H	6.86895	-2.34878	0.14888
H	7.63172	-0.76474	0.34335
H	4.39938	2.88198	-0.95903
H	5.52234	2.29109	0.25556
H	4.99753	4.69638	0.67010
H	3.26953	4.31790	0.78232
H	4.38872	3.70942	2.00899
H	-5.45958	-1.52498	1.75268
H	-4.83799	-0.21560	2.74379
H	-4.80426	-2.36040	4.02560
H	-3.77774	-3.10344	2.78737
H	-3.14990	-1.77817	3.77625
H	-3.89169	2.80043	-1.16760
H	-4.62586	3.60505	0.19869
H	-6.36639	3.19049	-1.49901
H	-5.99276	1.46499	-1.54586
H	-6.71070	2.17000	-0.09255

L1_20 Ground State

N	-1.42521	0.12569	-0.65453
C	-0.82562	-0.89893	-0.19509
O	-1.48712	-2.08690	-0.11954
C	-2.80507	-1.82792	-0.66342
C	-2.79931	-0.30326	-0.97093
C	0.56725	-0.91636	0.29853
O	1.09708	-2.15236	0.51056
C	2.44420	-1.91510	0.98847
C	2.59731	-0.36612	0.95800
N	1.27303	0.11742	0.52867
C	-3.83437	0.53283	-0.18349
C	-3.56909	0.48030	1.33118
C	-5.27733	0.13177	-0.54040
C	3.71284	0.12297	0.01307
C	5.09132	-0.39239	0.49565
C	3.66303	1.65264	-0.13058
C	-4.40536	1.46027	2.16205
C	-3.99114	1.47004	3.63581
C	-5.63435	0.20629	-2.03012
C	-7.12524	-0.03090	-2.28413
C	4.66094	2.24237	-1.13191
C	4.49667	3.75643	-1.28904
C	5.99309	-0.92107	-0.62614
C	7.36932	-1.36017	-0.12244
H	-3.54021	-2.12912	0.08670
H	-2.93043	-2.44847	-1.55517
H	-2.96098	-0.12801	-2.03909
H	3.13311	-2.43200	0.31385
H	2.52728	-2.34875	1.98858
H	2.79711	0.03032	1.96222
H	-3.68034	1.57180	-0.50842
H	-2.50843	0.70083	1.49850
H	-3.73834	-0.53981	1.70739
H	-5.96368	0.78784	0.00843
H	-5.48099	-0.88408	-0.16878
H	3.49946	-0.31905	-0.97277
H	4.96303	-1.19843	1.23238
H	5.60953	0.41273	1.03508
H	3.83722	2.10349	0.85869
H	2.64624	1.93786	-0.42040
H	-5.47140	1.21060	2.09010
H	-4.29636	2.47042	1.74296
H	-4.59666	2.17334	4.21842
H	-4.10899	0.47600	4.08454
H	-2.93938	1.75955	3.74638
H	-5.05389	-0.53188	-2.59877
H	-5.34502	1.19084	-2.42338
H	-7.36303	0.01665	-3.35252
H	-7.43566	-1.01643	-1.91593
H	-7.73664	0.72069	-1.77042
H	4.52670	1.75571	-2.10827
H	5.68961	2.02228	-0.81779
H	5.21429	4.16637	-2.00866
H	3.48819	4.00753	-1.63831
H	4.65144	4.27005	-0.33228
H	6.11086	-0.15315	-1.39978
H	5.49078	-1.76747	-1.11557
H	7.98944	-1.75049	-0.93695
H	7.90703	-0.52047	0.33448
H	7.28027	-2.14701	0.63684

L1_21 Ground State

N	1.10823	-0.35430	0.34176
C	0.54961	-0.71225	-0.74443
O	1.25899	-1.42670	-1.66174
C	2.56381	-1.62854	-1.06383
C	2.50320	-0.82563	0.26631
C	-0.84361	-0.39877	-1.12264
O	-1.37121	-1.17584	-2.11077
C	-2.70003	-0.64383	-2.34101
C	-2.89170	0.40289	-1.21101
N	-1.55694	0.51165	-0.59126
C	3.48906	0.36118	0.37059
C	3.18998	1.43181	-0.69479
C	4.95409	-0.10810	0.33386
C	-3.95036	0.01440	-0.15380
C	-4.19121	1.16847	0.83607
C	-3.56057	-1.28386	0.57915
C	4.04852	2.70358	-0.61530
C	3.95464	3.43308	0.72811
C	5.33690	-1.15884	1.38333
C	6.84195	-1.43767	1.40615
C	-4.73285	-1.98710	1.27128
C	-4.30097	-3.25870	2.00566
C	-4.92413	2.38057	0.25052
C	-5.17678	3.47000	1.29592
H	3.31402	-1.26705	-1.77094
H	2.70360	-2.70280	-0.91306
H	2.67492	-1.48772	1.12049
H	-3.40897	-1.47473	-2.30119
H	-2.71628	-0.20336	-3.34255
H	-3.15605	1.37650	-1.63502
H	3.30031	0.80404	1.35732
H	2.13527	1.71488	-0.60044
H	3.30669	0.99488	-1.69700
H	5.59983	0.76720	0.47646
H	5.19674	-0.49110	-0.66900
H	-4.88524	-0.16935	-0.70847
H	-3.22075	1.48148	1.24121
H	-4.77640	0.79305	1.68532
H	-2.77820	-1.05216	1.31292
H	-3.10594	-1.99395	-0.12521
H	3.72172	3.38121	-1.41469
H	5.09837	2.46945	-0.83392
H	4.49845	4.38384	0.69930
H	2.91058	3.64952	0.98446
H	4.37728	2.83743	1.54512
H	4.80260	-2.09898	1.19398
H	5.01000	-0.81642	2.37516
H	7.09861	-2.19621	2.15381
H	7.19051	-1.79813	0.43058
H	7.40724	-0.52826	1.64287
H	-5.49735	-2.23610	0.52147
H	-5.21548	-1.30464	1.98246
H	-5.15190	-3.75428	2.48631
H	-3.84153	-3.97623	1.31482
H	-3.56216	-3.03087	2.78330
H	-5.88183	2.05292	-0.17892
H	-4.34703	2.80982	-0.57874
H	-5.70341	4.32822	0.86367
H	-5.78407	3.08695	2.12514
H	-4.23262	3.83366	1.71853

L1_22 Ground State

N	1.17420	-0.11739	-0.13903
C	0.48433	-1.07484	-0.61548
O	1.03659	-2.31668	-0.71040
C	2.41748	-2.14757	-0.30554
C	2.48994	-0.68515	0.21154
C	-0.91271	-0.96206	-1.08424
O	-1.50256	-2.13568	-1.45052
C	-2.82575	-1.76670	-1.91372
C	-2.93129	-0.24954	-1.60086
N	-1.57604	0.12214	-1.15344
C	3.64599	0.13955	-0.38398
C	5.01532	-0.50005	-0.07101
C	3.53838	1.60985	0.05420
C	-3.98201	0.10687	-0.52637
C	-4.08848	1.63672	-0.40449
C	-3.68409	-0.59161	0.82136
C	5.43959	-0.48974	1.40281
C	6.79901	-1.16073	1.61592
C	4.60395	2.53185	-0.54649
C	4.36756	4.00166	-0.18972
C	-4.92653	-1.14550	1.52920
C	-4.59765	-1.77833	2.88276
C	-5.15561	2.14874	0.56723
C	-5.25391	3.67665	0.56642
H	3.04525	-2.31603	-1.18765
H	2.64594	-2.90417	0.44796
H	2.56983	-0.66214	1.30648
H	-3.55461	-2.37953	-1.37675
H	-2.88244	-1.99226	-2.98273
H	-3.16264	0.31939	-2.50920

H	3.51584	0.10829	-1.47691
H	5.78386	0.01477	-0.66087
H	5.02257	-1.53865	-0.43186
H	3.58110	1.67149	1.15104
H	2.54328	1.97064	-0.22602
H	-4.94325	-0.27405	-0.90774
H	-4.29551	2.05235	-1.40181
H	-3.10596	2.02676	-0.11079
H	-3.15944	0.10968	1.48286
H	-2.98478	-1.42464	0.67404
H	4.68505	-0.99829	2.01773
H	5.48340	0.54334	1.76885
H	7.09519	-1.14227	2.67053
H	6.77802	-2.20859	1.29222
H	7.58203	-0.65350	1.03929
H	4.61004	2.41531	-1.63967
H	5.60305	2.23402	-0.20215
H	4.38037	4.14895	0.89719
H	5.13687	4.65010	-0.62395
H	3.39244	4.34306	-0.55667
H	-5.40210	-1.89352	0.87848
H	-5.66883	-0.35020	1.66547
H	-5.49276	-2.18768	3.36426
H	-3.87366	-2.59475	2.77077
H	-4.15839	-1.04007	3.56462
H	-4.93017	1.80402	1.58419
H	-6.13191	1.71692	0.30474
H	-5.51730	4.05471	-0.42891
H	-4.29666	4.13106	0.84881
H	-6.01431	4.03085	1.27144

L1_23 Ground State

N	1.35657	-0.09127	0.06840
C	0.58933	-1.09940	-0.05279
O	1.09856	-2.35277	0.10812
C	2.52471	-2.16193	0.27805
C	2.69676	-0.62213	0.38266
C	-0.85610	-1.03407	-0.35341
O	-1.53451	-2.20732	-0.21694
C	-2.90465	-1.90237	-0.57660
C	-2.89865	-0.37024	-0.84287
N	-1.48313	0.01663	-0.70427
C	3.77514	-0.04152	-0.55085
C	5.16158	-0.65558	-0.26280
C	3.76000	1.49544	-0.49870
C	-3.79326	0.46951	0.09810
C	-3.31312	0.37369	1.55782
C	-5.28098	0.10723	-0.05466
C	5.78722	-0.29463	1.09020
C	7.14964	-0.96311	1.29181
C	4.74992	2.17355	-1.45088
C	4.59566	3.69658	-1.46024
C	-5.83983	0.20357	-1.47956
C	-7.35769	0.00993	-1.52438
C	-4.07595	1.24720	2.56565
C	-4.05726	2.74179	2.23151
H	3.02345	-2.58480	-0.60113
H	2.83776	-2.71204	1.16792
H	2.92823	-0.32483	1.41403
H	-3.54404	-2.20885	0.25470
H	-3.16139	-2.49322	-1.46039
H	-3.19832	-0.16076	-1.87448
H	3.49326	-0.34206	-1.57194
H	5.85054	-0.35080	-1.06034
H	5.09768	-1.75051	-0.33984
H	3.95716	1.83095	0.52953
H	2.74310	1.82831	-0.73127
H	-3.66233	1.50802	-0.23322
H	-2.25377	0.65421	1.58174
H	-3.36564	-0.67191	1.89377
H	-5.86646	0.77702	0.58724
H	-5.45944	-0.90533	0.33801
H	5.11589	-0.58824	1.90826
H	5.90189	0.79355	1.16733
H	7.58995	-0.69434	2.25833
H	7.06317	-2.05601	1.25541
H	7.85465	-0.66217	0.50738
H	4.60094	1.78276	-2.46761
H	5.78103	1.91775	-1.17353
H	5.31002	4.16944	-2.14359
H	3.58608	3.98714	-1.77389
H	4.76278	4.11444	-0.45988
H	-5.36513	-0.54562	-2.12655
H	-5.58011	1.18295	-1.90522
H	-7.74055	0.07301	-2.54893
H	-7.64189	-0.96962	-1.12079
H	-7.86977	0.77387	-0.92706
H	-3.62310	1.09519	3.55400
H	-5.11453	0.90422	2.65801
H	-4.52306	3.33012	3.02990
H	-3.02946	3.10206	2.10313
H	-4.59985	2.95831	1.30435

L1_24 Ground State

N	1.21528	-0.21755	0.16620
C	0.53560	-1.20931	-0.25109
O	1.11707	-2.43811	-0.32586
C	2.49280	-2.23614	0.08324
C	2.56607	-0.72872	0.45914
C	-0.87974	-1.14852	-0.67180
O	-1.49292	-2.35474	-0.83784
C	-2.83026	-2.03922	-1.29977
C	-2.91748	-0.49361	-1.18521
N	-1.53862	-0.07704	-0.86689
C	3.65602	0.04820	-0.30573
C	5.04595	-0.45082	0.13057
C	3.47220	1.57229	-0.17762
C	-3.90357	0.00849	-0.10642
C	-4.05811	1.53856	-0.16396
C	-3.47591	-0.45603	1.30069
C	6.22054	0.19138	-0.61428
C	7.56547	-0.43456	-0.23706
C	3.62391	2.14232	1.23707
C	3.42527	3.65994	1.26658
C	-4.59418	-0.43599	2.35353
C	-5.68673	-1.48323	2.11557
C	-4.81987	2.06521	-1.38517
C	-4.98222	3.58719	-1.36008
H	3.13404	-2.49655	-0.76538
H	2.70147	-2.91538	0.91307
H	2.74143	-0.60599	1.53550
H	-3.54270	-2.57131	-0.66407
H	-2.92410	-2.40083	-2.32820
H	-3.19600	-0.05560	-2.14876
H	3.52831	-0.20054	-1.37101
H	5.09912	-1.53976	-0.01537
H	5.17116	-0.28947	1.21052
H	2.47351	1.82200	-0.55043
H	4.18941	2.07038	-0.84278
H	-4.87484	-0.44650	-0.35328
H	-3.05748	1.98749	-0.12779
H	-4.58327	1.87730	0.73867
H	-2.64472	0.17837	1.63034
H	-3.07254	-1.47700	1.25561
H	6.24995	1.26720	-0.40299
H	6.05871	0.09605	-1.69715
H	8.39389	0.04214	-0.77260
H	7.75961	-0.33209	0.83762
H	7.58466	-1.50508	-0.47533
H	4.61583	1.89897	1.64126
H	2.89076	1.67141	1.90378
H	3.53139	4.06025	2.28116
H	4.15991	4.16636	0.62821
H	2.42741	3.92989	0.90146
H	-5.04798	0.56237	2.40318
H	-4.14360	-0.61015	3.33911
H	-6.43013	-1.47032	2.92037
H	-6.22101	-1.31083	1.17442
H	-5.25830	-2.49263	2.07326
H	-5.81039	1.58970	-1.42751
H	-4.30194	1.77729	-2.30926
H	-5.53081	3.94797	-2.23734
H	-5.52964	3.91021	-0.46613
H	-4.00535	4.08497	-1.34702

L1_25 Ground State

N	-1.38735	-0.65181	-0.21013
C	-0.75324	-0.23871	0.81325
O	-1.39753	-0.14063	2.00905
C	-2.74559	-0.61018	1.75799
C	-2.77453	-0.88984	0.22839
C	0.66500	0.17490	0.82057
O	1.26403	0.18997	2.04374
C	2.61735	0.64880	1.80132
C	2.70862	0.76921	0.25384
N	1.33745	0.49241	-0.21233
C	-3.76509	-0.02252	-0.58249
C	-3.40291	1.47088	-0.50533
C	-5.22419	-0.29431	-0.17343
C	3.72070	-0.18170	-0.42656
C	3.33230	-1.65631	-0.21288
C	5.16574	0.11276	0.01258
C	-4.19547	2.37207	-1.45913
C	-3.68786	3.81631	-1.44644
C	-5.67618	-1.75684	-0.26892
C	-7.17834	-1.91887	-0.02227
C	5.63596	1.55828	-0.19096
C	7.13019	1.72993	0.09403
C	4.21971	-2.68614	-0.92889
C	4.28288	-2.50213	-2.44808
H	-3.43631	0.17181	2.08202
H	-2.90988	-1.50540	2.36438
H	-3.00530	-1.94213	0.03602
H	3.30088	-0.08517	2.23434
H	2.74703	1.60495	2.31644
H	2.95589	1.79503	-0.03589
H	-3.64162	-0.33705	-1.62873

H	-2.33639	1.57470	-0.73616
H	-3.53613	1.83744	0.52361
H	-5.88001	0.30800	-0.81364
H	-5.39534	0.07194	0.85032
H	3.64210	0.03657	-1.49967
H	2.29934	-1.78520	-0.55604
H	3.33367	-1.88391	0.86284
H	5.83783	-0.54675	-0.55024
H	5.29769	-0.16677	1.06887
H	-5.26108	2.36333	-1.19770
H	-4.12465	1.96661	-2.47821
H	-4.26201	4.44981	-2.13185
H	-3.76650	4.25248	-0.44298
H	-2.63419	3.86487	-1.74583
H	-5.12745	-2.37366	0.45468
H	-5.42064	-2.15136	-1.26228
H	-7.48452	-2.96894	-0.08438
H	-7.45650	-1.54753	0.97167
H	-7.76158	-1.35495	-0.76012
H	5.06850	2.23865	0.45734
H	5.41909	1.86818	-1.22284
H	7.44920	2.76859	-0.04629
H	7.36984	1.44272	1.12517
H	7.73282	1.10079	-0.57203
H	3.82410	-3.68534	-0.70508
H	5.23574	-2.66820	-0.51391
H	4.84115	-3.31767	-2.92112
H	3.27637	-2.48587	-2.88318
H	4.77578	-1.56308	-2.72410

L1_26 Ground State

N	1.16319	-0.16426	0.12151
C	0.46941	-1.16375	-0.25186
O	1.03163	-2.40357	-0.26680
C	2.40718	-2.20540	0.14487
C	2.50540	-0.68166	0.44145
C	-0.94373	-1.10027	-0.67918
O	-1.57746	-2.30280	-0.78630
C	-2.90437	-1.98750	-1.27678
C	-2.97249	-0.43837	-1.21558
N	-1.58471	-0.02876	-0.92728
C	3.60771	0.03580	-0.36315
C	4.98952	-0.45627	0.10559
C	3.44438	1.56695	-0.32315
C	-3.93568	0.12018	-0.14446
C	-4.02558	1.65633	-0.21895
C	-3.53545	-0.34148	1.27033
C	6.17471	0.12523	-0.67161
C	7.50974	-0.49704	-0.25517
C	3.59536	2.21468	1.05777
C	3.41550	3.73380	0.99958
C	-4.63916	-0.18477	2.32213
C	-4.20596	-0.68940	3.70083
C	-4.49650	2.24530	-1.55755
C	-5.86911	1.74395	-2.01678
H	3.05107	-2.52266	-0.68201
H	2.59523	-2.84312	1.01184
H	2.68348	-0.50543	1.50985
H	-3.63189	-2.49205	-0.63617
H	-2.98749	-2.37978	-2.29507
H	-3.25842	-0.03455	-2.19135
H	3.47940	-0.27165	-1.41294
H	5.02759	-1.55252	0.02338
H	5.11450	-0.23412	1.17471
H	2.45134	1.80847	-0.71593
H	4.17211	2.01666	-1.01096
H	-4.92468	-0.30575	-0.37274
H	-3.03667	2.06423	0.02125
H	-4.70995	2.00155	0.56638
H	-2.64306	0.21487	1.58404
H	-3.23574	-1.39820	1.24915
H	6.21909	1.21088	-0.52235
H	6.01379	-0.02988	-1.74768
H	8.34603	-0.06368	-0.81476
H	7.70309	-0.33581	0.81243
H	7.51404	-1.57963	-0.43158
H	4.58183	1.98278	1.48161
H	2.85245	1.79143	1.74527
H	3.52104	4.18995	1.99039
H	4.15988	4.19411	0.33800
H	2.42308	3.99454	0.61354
H	-5.53296	-0.73390	1.99289
H	-4.93938	0.86737	2.40103
H	-5.00630	-0.57522	4.44048
H	-3.93194	-1.75090	3.66428
H	-3.33190	-0.13588	4.06444
H	-3.75100	2.05014	-2.33873
H	-4.53149	3.33726	-1.45137
H	-6.20073	2.26887	-2.91953
H	-5.85682	0.67234	-2.24729
H	-6.62672	1.90354	-1.23931

L1_27 Ground State

N	1.33259	-0.08001	0.34237

C	0.56871	-1.04357	0.01434
O	1.04521	-2.31918	0.05175
C	2.44996	-2.18739	0.38183
C	2.62996	-0.67924	0.70611
C	-0.83978	-0.90297	-0.41082
O	-1.52777	-2.07050	-0.54662
C	-2.85950	-1.68546	-0.96743
C	-2.82094	-0.13030	-0.98605
N	-1.42898	0.20278	-0.63565
C	3.79788	-0.00591	-0.03647
C	5.12490	-0.67662	0.36206
C	3.80356	1.52128	0.20876
C	-3.81574	0.56576	-0.02891
C	-3.50854	0.23658	1.44220
C	-5.27635	0.25851	-0.40665
C	6.35848	-0.16875	-0.39127
C	7.63410	-0.91630	0.00516
C	4.04739	2.35032	-1.05780
C	4.09382	3.85332	-0.77609
C	-5.67196	0.59867	-1.84886
C	-7.17417	0.43525	-2.09420
C	-4.30501	1.05808	2.46237
C	-3.84678	0.79787	3.89972
H	3.02836	-2.50119	-0.49456
H	2.66694	-2.85853	1.21518
H	2.77460	-0.52387	1.78525
H	-3.57000	-2.10442	-0.25066
H	-3.04393	-2.12598	-1.95113
H	-3.00320	0.24450	-1.99819
H	3.62769	-0.18611	-1.10918
H	5.05363	-1.76305	0.20692
H	5.27970	-0.53443	1.44251
H	4.56353	1.76944	0.96387
H	2.83687	1.82073	0.62612
H	-3.64930	1.64392	-0.16583
H	-2.43994	0.41163	1.61287
H	-3.68281	-0.83305	1.63283
H	-5.93294	0.82008	0.26882
H	-5.49282	-0.80302	-0.21211
H	6.49266	0.90320	-0.20266
H	6.19042	-0.27197	-1.47212
H	8.50565	-0.53883	-0.54093
H	7.83815	-0.80630	1.07723
H	7.54599	-1.98912	-0.20578
H	3.24310	2.13399	-1.77367
H	4.98146	2.03751	-1.54190
H	4.24615	4.43036	-1.69516
H	3.15857	4.19487	-0.31664
H	4.91079	4.10075	-0.08675
H	-5.12399	-0.03877	-2.55498
H	-5.37162	1.63163	-2.07353
H	-7.43997	0.67291	-3.13010
H	-7.49631	-0.59397	-1.89388
H	-7.75436	1.09589	-1.43881
H	-5.37622	0.83509	2.38082
H	-4.19390	2.12631	2.22888
H	-4.42413	1.38985	4.61869
H	-3.96572	-0.25974	4.16554
H	-2.78801	1.05306	4.02683

L1_28 Ground State

N	1.42379	-0.17561	0.07112
C	0.68257	-1.18916	-0.13616
O	1.20688	-2.44029	-0.00905
C	2.61957	-2.23381	0.23697
C	2.75519	-0.69933	0.43134
C	-0.74676	-1.13366	-0.50914
O	-1.36863	-2.33990	-0.62036
C	-2.74025	-2.03336	-0.97159
C	-2.78505	-0.47832	-1.03406
N	-1.40466	-0.06586	-0.72510
C	3.87083	-0.05121	-0.40907
C	5.25072	-0.66073	-0.08295
C	3.82607	1.47989	-0.27119
C	-3.79845	0.14767	-0.05647
C	-5.23724	-0.30484	-0.40935
C	-3.64237	1.67661	-0.02786
C	5.79695	-0.37221	1.32090
C	7.15852	-1.03131	1.55612
C	4.84989	2.22610	-1.13219
C	4.66927	3.74471	-1.06321
C	-4.52829	2.39990	0.99107
C	-4.25933	3.90672	1.02514
C	-6.09004	-0.69232	0.80464
C	-7.52312	-1.07030	0.42544
H	3.16647	-2.59906	-0.63951
H	2.90292	-2.82582	1.10967
H	2.92383	-0.45363	1.48826
H	-3.38605	-2.45203	-0.19351
H	-2.96082	-2.52320	-1.92337
H	-3.02488	-0.13125	-2.04808
H	3.64784	-0.29705	-1.45894
H	5.97554	-0.29875	-0.82271

H	5.21071	-1.74993	-0.22768
H	3.96595	1.75890	0.78300
H	2.81626	1.81044	-0.53581
H	-3.54508	-0.23988	0.94268
H	-5.21200	-1.16650	-1.09176
H	-5.74000	0.49462	-0.97136
H	-3.85667	2.06977	-1.03370
H	-2.59170	1.91113	0.17304
H	5.88766	0.71097	1.46839
H	5.08842	-0.72433	2.08255
H	7.54186	-0.81460	2.55929
H	7.09379	-2.12121	1.45044
H	7.89871	-0.67337	0.83023
H	4.75862	1.89212	-2.17563
H	5.87028	1.97022	-0.81785
H	5.40816	4.26657	-1.68175
H	3.67150	4.03774	-1.41058
H	4.77909	4.10693	-0.03367
H	-4.35629	1.97385	1.98959
H	-5.58823	2.22838	0.76233
H	-4.89718	4.41278	1.75857
H	-3.21494	4.11318	1.28736
H	-4.44923	4.36210	0.04550
H	-6.10445	0.13340	1.52581
H	-5.60929	-1.53520	1.32100
H	-8.10810	-1.36065	1.30511
H	-8.03742	-0.22940	-0.05559
H	-7.53736	-1.91171	-0.27839

L1_29 Ground State

N	1.30317	-0.71700	0.77797
C	0.74942	-1.41587	-0.13052
O	1.36133	-2.55038	-0.57030
C	2.54508	-2.68422	0.25543
C	2.60157	-1.35698	1.06172
C	-0.53339	-1.08616	-0.78391
O	-1.13877	-2.11420	-1.44282
C	-2.32475	-1.53260	-2.04113
C	-2.38193	-0.09694	-1.45375
N	-1.09005	0.05823	-0.75758
C	3.79306	-0.44427	0.68143
C	4.00338	0.69531	1.70035
C	3.68988	0.04179	-0.77421
C	-3.55564	0.14832	-0.47828
C	-3.62928	1.62939	-0.06496
C	-3.46498	-0.77516	0.75204
C	2.99638	1.85179	1.65091
C	3.25201	2.87759	2.75789
C	4.92440	0.79958	-1.27212
C	4.81396	1.18640	-2.74890
C	-4.78906	-0.94606	1.50396
C	-4.65225	-1.84984	2.73167
C	-4.07939	2.58882	-1.17224
C	-4.18028	4.03613	-0.68370
H	3.40214	-2.83756	-0.40496
H	2.41436	-3.56702	0.88872
H	2.65969	-1.56081	2.13710
H	-3.18038	-2.15708	-1.77207
H	-2.19411	-1.54780	-3.12741
H	-2.43109	0.64215	-2.25924
H	4.68051	-1.09394	0.75404
H	5.01504	1.10163	1.56613
H	3.99340	0.25790	2.70958
H	2.80192	0.67489	-0.88163
H	3.52272	-0.82099	-1.43460
H	-4.47401	-0.10454	-1.03324
H	-2.64278	1.93092	0.30900
H	-4.32533	1.72964	0.77767
H	-2.69804	-0.38179	1.43126
H	-3.11311	-1.77180	0.45225
H	3.05928	2.35206	0.67576
H	1.97865	1.45708	1.72351
H	2.53930	3.70820	2.70485
H	3.15642	2.41996	3.75050
H	4.26276	3.29946	2.68618
H	5.82022	0.18103	-1.11787
H	5.07167	1.70555	-0.67110
H	5.70085	1.73259	-3.08914
H	4.70337	0.29811	-3.38281
H	3.93981	1.82565	-2.92192
H	-5.54059	-1.36505	0.81964
H	-5.17451	0.03286	1.81628
H	-5.60929	-1.96921	3.25176
H	-4.29765	-2.84853	2.44871
H	-3.93150	-1.43457	3.44619
H	-5.05466	2.26235	-1.56107
H	-3.38191	2.54662	-2.01885
H	-4.50514	4.70954	-1.48474
H	-4.89861	4.12447	0.14050
H	-3.21095	4.39401	-0.31682

L1_30 Ground State

N	1.10554	0.24413	0.71464
C	0.52230	-0.78207	1.19144

O	1.20131	-1.61538	2.02687
C	2.50329	-0.99802	2.19990
C	2.49967	0.18655	1.19641
C	-0.88118	-1.14430	0.91375
O	-1.52910	-1.80420	1.91461
C	-2.86714	-2.03534	1.40371
C	-2.91703	-1.21621	0.08555
N	-1.51260	-0.83084	-0.14563
C	3.47545	0.02431	0.00899
C	3.51663	1.30280	-0.84762
C	3.12324	-1.21168	-0.84125
C	-3.83264	0.03053	0.15561
C	-4.03858	0.67710	-1.22487
C	-3.36504	1.05637	1.21703
C	4.19102	2.50744	-0.18188
C	4.24559	3.72780	-1.10453
C	4.27232	-1.71250	-1.72251
C	3.87644	-2.92764	-2.56483
C	-2.28308	2.05990	0.78181
C	-1.74941	2.86475	1.96893
C	-4.84201	-0.16814	-2.21977
C	-5.08725	0.56510	-3.54114
H	3.26560	-1.75304	1.99239
H	2.58559	-0.67812	3.24288
H	2.72372	1.12398	1.71418
H	-3.57937	-1.70050	2.16166
H	-2.98474	-3.11184	1.24564
H	-3.24793	-1.84936	-0.74285
H	4.47366	-0.13192	0.45003
H	2.48776	1.56167	-1.12756
H	4.04864	1.08733	-1.78301
H	2.25129	-0.97392	-1.46359
H	2.80714	-2.03981	-0.19208
H	-4.80994	-0.35569	0.48709
H	-3.06112	0.92089	-1.65752
H	-4.56190	1.63313	-1.08316
H	-3.00739	0.52028	2.10747
H	-4.24457	1.62402	1.55150
H	3.65900	2.78093	0.73852
H	5.21034	2.23021	0.12316
H	4.73203	4.57978	-0.61650
H	4.80346	3.50351	-2.02190
H	3.23703	4.04101	-1.39948
H	5.13015	-1.96958	-1.08476
H	4.61671	-0.90902	-2.38596
H	4.71130	-3.27830	-3.18185
H	3.55666	-3.76162	-1.92815
H	3.04240	-2.68596	-3.23444
H	-2.70276	2.74641	0.03575
H	-1.45258	1.54109	0.29647
H	-1.01223	3.60775	1.64510
H	-2.55482	3.39553	2.49288
H	-1.25795	2.20601	2.69566
H	-5.80541	-0.44498	-1.76774
H	-4.31872	-1.11022	-2.42810
H	-5.66190	-0.05050	-4.24221
H	-5.64398	1.49589	-3.37779
H	-4.13906	0.82803	-4.02508

L1_31 Ground State

N	1.19143	-0.16148	0.02719
C	0.54088	-1.22298	-0.23666
O	1.11802	-2.43636	-0.01647
C	2.45761	-2.14350	0.45299
C	2.50928	-0.59086	0.52750
C	-0.83553	-1.26131	-0.77355
O	-1.40873	-2.49742	-0.82556
C	-2.71213	-2.28585	-1.42408
C	-2.83277	-0.74242	-1.54201
N	-1.49634	-0.24592	-1.16410
C	3.66526	0.02995	-0.28163
C	5.00969	-0.35767	0.36143
C	3.48101	1.54694	-0.47587
C	-3.92444	-0.11886	-0.64470
C	-4.03737	1.38484	-0.94945
C	-3.67727	-0.41944	0.85248
C	6.24764	0.13593	-0.39401
C	7.55136	-0.38888	0.21246
C	3.51391	2.38898	0.80445
C	3.32115	3.87954	0.51371
C	-4.94515	-0.77279	1.63934
C	-4.66721	-1.00784	3.12537
C	-5.14110	2.13056	-0.19391
C	-5.24062	3.59902	-0.61571
H	3.16353	-2.55990	-0.27335
H	2.59499	-2.64310	1.41475
H	2.59404	-0.25568	1.56910
H	-3.46168	-2.73820	-0.76937
H	-2.72392	-2.79527	-2.39221
H	-3.03015	-0.44614	-2.57905
H	3.62714	-0.42712	-1.28295
H	5.06783	-1.45328	0.44014
H	5.04356	0.01653	1.39430

H	2.51966	1.70659	-0.97491
H	4.25584	1.91046	-1.16319
H	-4.86980	-0.60071	-0.94237
H	-4.20692	1.50996	-2.02921
H	-3.06715	1.85153	-0.73820
H	-3.17848	0.44156	1.31566
H	-2.97238	-1.25332	0.96388
H	6.26626	1.23252	-0.39878
H	6.17781	-0.17403	-1.44612
H	8.42552	-0.01940	-0.33496
H	7.65412	-0.07325	1.25791
H	7.58348	-1.48514	0.19396
H	4.46630	2.24306	1.33188
H	2.72387	2.05139	1.48681
H	3.34224	4.47511	1.43336
H	4.11018	4.25759	-0.14824
H	2.35949	4.05922	0.01891
H	-5.39495	-1.67551	1.20129
H	-5.69286	0.02099	1.52594
H	-5.57952	-1.28023	3.66770
H	-3.93862	-1.81547	3.26729
H	-4.25496	-0.10638	3.59477
H	-4.95406	2.07907	0.88600
H	-6.10636	1.63261	-0.36370
H	-6.02759	4.12366	-0.06239
H	-4.29519	4.12397	-0.43363
H	-5.46633	3.68801	-1.68535

L1_32 Ground State

N	-1.34484	-0.20084	-0.93291
C	-0.79043	-1.01302	-0.12447
O	-1.51513	-2.03739	0.40097
C	-2.84172	-1.90176	-0.16867
C	-2.75165	-0.62849	-1.06115
C	0.61713	-0.93747	0.32074
O	1.06021	-2.00344	1.04290
C	2.45704	-1.72822	1.31370
C	2.69746	-0.31802	0.70369
N	1.40750	0.03118	0.08270
C	-3.69511	0.54526	-0.71231
C	-3.58755	0.95729	0.76523
C	-5.13638	0.30631	-1.20581
C	3.85860	-0.27116	-0.30898
C	5.18940	-0.52955	0.42148
C	3.84475	1.02602	-1.13967
C	-4.34501	2.24227	1.11661
C	-4.08999	2.69375	2.55673
C	-5.93783	-0.80273	-0.51291
C	-7.38275	-0.86749	-1.01541
C	4.07318	2.32102	-0.35211
C	4.04207	3.55449	-1.25823
C	6.42051	-0.58192	-0.48874
C	7.69185	-0.97406	0.26810
H	-3.54701	-1.82142	0.65939
H	-3.05883	-2.81036	-0.73681
H	-2.92550	-0.88889	-2.11291
H	3.05085	-2.50996	0.82821
H	2.60826	-1.78106	2.39432
H	2.89502	0.41729	1.49419
H	-3.30364	1.38610	-1.30113
H	-3.94081	0.15176	1.42304
H	-2.52468	1.09907	0.99834
H	-5.10143	0.09273	-2.28390
H	-5.69402	1.24661	-1.11009
H	3.69404	-1.10255	-1.01234
H	5.12174	-1.48335	0.96517
H	5.34118	0.24069	1.19070
H	2.87557	1.08995	-1.64496
H	4.60520	0.94761	-1.92741
H	-5.42294	2.09543	0.96981
H	-4.04607	3.03933	0.42173
H	-4.64115	3.61059	2.79386
H	-4.40071	1.92247	3.27226
H	-3.02419	2.88939	2.72437
H	-5.93937	-0.64225	0.57302
H	-5.45916	-1.77639	-0.68046
H	-7.94457	-1.66854	-0.52246
H	-7.90695	0.07665	-0.82440
H	-7.41623	-1.05052	-2.09627
H	5.03682	2.28207	0.17361
H	3.30020	2.42313	0.41979
H	4.20268	4.47673	-0.68851
H	4.82058	3.49721	-2.02915
H	3.07572	3.63895	-1.76904
H	6.57006	0.39386	-0.96664
H	6.23907	-1.29736	-1.30305
H	8.56267	-0.99843	-0.39631
H	7.90621	-0.26095	1.07350
H	7.59082	-1.96649	0.72420

L1_33 Ground State

N	1.35587	0.50946	-0.28882
C	0.76038	0.15986	0.78030
O	1.41703	0.23371	1.97100

C	2.72564	0.77068	1.65441
C	2.72481	0.89104	0.10383
C	-0.62342	-0.35276	0.84935
O	-1.22935	-0.23856	2.06394
C	-2.53030	-0.85631	1.89839
C	-2.62033	-1.14529	0.37307
N	-1.26384	-0.85968	-0.12720
C	3.77080	0.01712	-0.62640
C	3.51430	-1.48222	-0.39500
C	5.20886	0.42942	-0.26263
C	-3.68005	-0.31488	-0.38606
C	-3.36761	1.18962	-0.31922
C	-5.09740	-0.67627	0.12001
C	4.37162	-2.41871	-1.25403
C	3.96532	-3.88586	-1.09265
C	5.55402	1.90453	-0.50168
C	7.04201	2.19584	-0.29054
C	-6.14624	-0.81924	-0.99013
C	-7.54124	-1.13566	-0.44718
C	-4.31665	2.08934	-1.11709
C	-3.87981	3.55639	-1.09077
H	3.47359	0.07840	2.04798
H	2.82761	1.73362	2.16278
H	2.87708	1.93141	-0.19937
H	-3.28359	-0.15732	2.26787
H	-2.55097	-1.76350	2.50940
H	-2.83879	-2.20448	0.19486
H	3.62175	0.21475	-1.69764
H	2.45842	-1.68375	-0.60944
H	3.66956	-1.73063	0.66571
H	5.90251	-0.18334	-0.85091
H	5.41134	0.17545	0.78902
H	-3.59679	-0.62325	-1.43750
H	-2.34639	1.34297	-0.68740
H	-3.37151	1.52084	0.73019
H	-5.43520	0.07701	0.84604
H	-5.06457	-1.62684	0.67261
H	5.43289	-2.30940	-0.99765
H	4.27748	-2.12518	-2.30899
H	4.58538	-4.54461	-1.71097
H	4.06919	-4.21068	-0.05002
H	2.91902	-4.03788	-1.38304
H	4.96649	2.54681	0.16726
H	5.26499	2.18359	-1.52458
H	7.27136	3.25426	-0.45614
H	7.35208	1.94222	0.73060
H	7.66003	1.60681	-0.97878
H	-5.82659	-1.61570	-1.67609
H	-6.18369	0.09829	-1.58847
H	-8.26993	-1.25239	-1.25697
H	-7.53758	-2.06484	0.13597
H	-7.89883	-0.33442	0.21116
H	-5.33664	2.00952	-0.71973
H	-4.36187	1.73799	-2.15715
H	-4.56612	4.19025	-1.66338
H	-3.84894	3.93943	-0.06332
H	-2.87674	3.67500	-1.51737

L1_34 Ground State

N	-1.57938	0.71193	-0.69021
C	-0.88504	-0.17736	-1.27948
O	-1.39211	-0.80692	-2.37559
C	-2.67027	-0.16825	-2.61930
C	-2.88044	0.75155	-1.38453
C	0.46182	-0.61312	-0.85805
O	1.20211	-1.23846	-1.81436
C	2.45423	-1.57885	-1.16787
C	2.32927	-0.96430	0.25547
N	0.95561	-0.43090	0.30082
C	-4.04284	0.30648	-0.46363
C	-4.42722	1.39647	0.55873
C	-3.76473	-1.06559	0.17337
C	3.35945	0.13902	0.59081
C	3.19819	1.36097	-0.33007
C	4.79817	-0.40907	0.59246
C	-3.46490	1.60022	1.73612
C	-3.90330	2.75795	2.63640
C	-4.94797	-1.64712	0.95308
C	-4.65721	-3.04977	1.49228
C	5.04813	-1.60691	1.51712
C	6.53101	-1.97783	1.60107
C	4.03266	2.58183	0.07377
C	3.71398	3.80971	-0.78322
H	-3.42542	-0.95157	-2.72107
H	-2.59480	0.38525	-3.56027
H	-3.07330	1.78329	-1.70028
H	3.26386	-1.15592	-1.76718
H	2.54577	-2.66862	-1.16186
H	2.40498	-1.74564	1.01785
H	-4.90832	0.19256	-1.13662
H	-5.42608	1.16757	0.95429
H	-4.53558	2.34877	0.01894
H	-2.89264	-0.98789	0.83233

H	-3.48206	-1.78052	-0.61242
H	3.11886	0.46384	1.61327
H	2.14046	1.64866	-0.33139
H	3.44742	1.08634	-1.36608
H	5.47518	0.40025	0.89140
H	5.09333	-0.67546	-0.43388
H	-2.45251	1.77195	1.35879
H	-3.41445	0.68010	2.33271
H	-3.22016	2.88569	3.48355
H	-3.92537	3.70400	2.08109
H	-4.90979	2.59055	3.04099
H	-5.83477	-1.67702	0.30378
H	-5.20376	-0.98421	1.78905
H	-5.50959	-3.45017	2.05247
H	-4.43402	-3.74821	0.67648
H	-3.79006	-3.03922	2.16357
H	4.48106	-2.48081	1.17079
H	4.66833	-1.37508	2.52197
H	6.69264	-2.84003	2.25736
H	6.93028	-2.23130	0.61137
H	7.12430	-1.14252	1.99204
H	5.10365	2.35673	-0.00491
H	3.84300	2.81263	1.13147
H	4.31685	4.67482	-0.48518
H	3.91382	3.61233	-1.84361
H	2.65738	4.08833	-0.69274

L1_35 Ground State

N	-1.48024	-0.25914	-0.48312
C	-0.77174	-1.29941	-0.29421
O	-1.33465	-2.53052	-0.44015
C	-2.73066	-2.27961	-0.73819
C	-2.83267	-0.73069	-0.82968
C	0.65899	-1.29386	0.07719
O	1.24043	-2.51999	0.18880
C	2.63218	-2.25660	0.49551
C	2.71086	-0.70943	0.63019
N	1.35170	-0.24880	0.29581
C	-3.90865	-0.12685	0.09330
C	-5.30382	-0.56459	-0.39391
C	-3.75261	1.39809	0.23954
C	3.78008	-0.06269	-0.27192
C	5.18102	-0.49289	0.20106
C	3.59760	1.46338	-0.37553
C	-6.48486	-0.05603	0.44504
C	-6.43854	-0.49399	1.91171
C	-3.93516	2.21190	-1.04651
C	-3.77265	3.71405	-0.80054
C	3.78083	2.24428	0.93058
C	3.58066	3.74872	0.73034
C	6.33617	0.02554	-0.66133
C	7.69052	-0.54024	-0.22707
H	-3.32674	-2.69788	0.08000
H	-2.97696	-2.80143	-1.66566
H	-3.03955	-0.41591	-1.86068
H	3.23529	-2.64326	-0.33304
H	2.88531	-2.80018	1.40852
H	2.91197	-0.42096	1.66997
H	-3.73754	-0.56258	1.08854
H	-5.43856	-0.23828	-1.43390
H	-5.34548	-1.66352	-0.41607
H	-2.75274	1.59636	0.63930
H	-4.46799	1.75495	0.99227
H	3.62603	-0.47208	-1.28270
H	5.23169	-1.59153	0.22105
H	5.33269	-0.16957	1.24051
H	2.59017	1.65498	-0.75913
H	4.29849	1.85155	-1.12586
H	-7.41318	-0.42299	-0.01173
H	-6.53438	1.03864	0.39028
H	-7.34097	-0.17789	2.44634
H	-6.36640	-1.58578	1.99451
H	-5.57751	-0.06512	2.43584
H	-4.92560	2.02095	-1.48096
H	-3.19857	1.88865	-1.79252
H	-3.89919	4.28933	-1.72461
H	-4.51201	4.07740	-0.07594
H	-2.77743	3.93822	-0.39899
H	4.78202	2.06410	1.34484
H	3.06369	1.88331	1.67831
H	3.70971	4.30038	1.66836
H	4.29949	4.14919	0.00467
H	2.57413	3.96127	0.35132
H	6.37009	1.12085	-0.61608
H	6.14747	-0.23207	-1.71295
H	8.50505	-0.15247	-0.84876
H	7.91117	-0.27707	0.81466
H	7.70455	-1.63452	-0.30115

L1_36 Ground State

N	1.08583	-0.23966	-0.08656
C	0.38271	-1.28173	-0.28508
O	0.94601	-2.51131	-0.13551
C	2.34971	-2.25373	0.12412

C	2.43533	-0.71086	0.28191
C	-1.05032	-1.26425	-0.63986
O	-1.77408	-2.33762	-0.21473
C	-3.12539	-2.08396	-0.67971
C	-3.07672	-0.62297	-1.20625
N	-1.63672	-0.30987	-1.24321
C	3.52580	-0.04516	-0.57763
C	4.92761	-0.59219	-0.23448
C	3.42217	1.48643	-0.48293
C	-3.82701	0.40962	-0.33203
C	-3.23598	0.50998	1.09332
C	-5.33685	0.10551	-0.32909
C	5.46320	-0.23860	1.15852
C	6.84848	-0.83862	1.41250
C	4.42007	2.24670	-1.36177
C	4.17993	3.75841	-1.33751
C	-6.20360	1.29483	0.09907
C	-7.69606	0.95778	0.13326
C	-2.13452	1.56855	1.24450
C	-1.46428	1.52341	2.61840
H	2.91873	-2.62396	-0.73555
H	2.63817	-2.81463	1.01549
H	2.59708	-0.43464	1.33191
H	-3.80067	-2.23560	0.16449
H	-3.35433	-2.81363	-1.46227
H	-3.47950	-0.56389	-2.22357
H	3.31283	-0.32879	-1.61996
H	5.63801	-0.22712	-0.98659
H	4.92813	-1.68621	-0.34442
H	3.54698	1.80005	0.56342
H	2.40169	1.77072	-0.75996
H	-3.68427	1.37898	-0.82947
H	-4.03797	0.73446	1.80850
H	-2.83939	-0.46818	1.40030
H	-5.54350	-0.74692	0.33476
H	-5.65045	-0.20871	-1.33569
H	5.51338	0.85141	1.27060
H	4.76867	-0.59201	1.93237
H	7.22392	-0.57554	2.40752
H	6.82436	-1.93300	1.34208
H	7.57445	-0.47693	0.67423
H	4.34643	1.87939	-2.39531
H	5.44819	2.04011	-1.03660
H	4.90082	4.29068	-1.96824
H	3.17319	4.00190	-1.69702
H	4.27063	4.15426	-0.31853
H	-6.02815	2.12956	-0.59329
H	-5.88711	1.64887	1.08863
H	-8.29609	1.82548	0.42897
H	-8.04931	0.62675	-0.85099
H	-7.90172	0.15043	0.84668
H	-2.57640	2.56115	1.07659
H	-1.37878	1.42624	0.46636
H	-0.70905	2.31076	2.71885
H	-2.19357	1.65087	3.42884
H	-0.96047	0.56105	2.77154

L1_37 Ground State

N	1.06452	-0.19688	-0.02616
C	0.29285	-1.18925	-0.22502
O	0.79755	-2.45224	-0.18193
C	2.22853	-2.28051	-0.01761
C	2.40859	-0.75601	0.21802
C	-1.15911	-1.07879	-0.46810
O	-1.90810	-2.13640	-0.04705
C	-3.27490	-1.78490	-0.38456
C	-3.18337	-0.30484	-0.84856
N	-1.73452	-0.06228	-0.97171
C	3.47306	-0.09735	-0.67843
C	4.86320	-0.73248	-0.46306
C	3.45829	1.42960	-0.49462
C	-3.81625	0.72125	0.12368
C	-3.10459	0.74433	1.49628
C	-5.33097	0.49260	0.28503
C	5.50824	-0.48611	0.90639
C	6.87328	-1.16782	1.03145
C	4.43510	2.18827	-1.39817
C	4.28011	3.70620	-1.27417
C	-6.14429	0.47998	-1.01421
C	-7.65284	0.43154	-0.75805
C	-1.92841	1.72748	1.58549
C	-1.16209	1.60256	2.90324
H	2.71147	-2.62638	-0.93803
H	2.55171	-2.90708	0.81620
H	2.65612	-0.55029	1.26751
H	-3.88581	-1.93998	0.50687
H	-3.61210	-2.46189	-1.17540
H	-3.63900	-0.17889	-1.83481
H	3.17630	-0.30988	-1.71719
H	5.54073	-0.36116	-1.24195
H	4.79757	-1.81713	-0.63109
H	3.66860	1.67624	0.55593
H	2.43840	1.77983	-0.68471

H	-3.67847	1.70430	-0.34765
H	-2.75156	-0.26507	1.75186
H	-3.83645	1.00198	2.27436
H	-5.71772	1.29043	0.93369
H	-5.51146	-0.44310	0.83499
H	4.84879	-0.84811	1.70650
H	5.62420	0.59183	1.07308
H	7.32746	-0.98073	2.01072
H	6.78613	-2.25389	0.90464
H	7.56698	-0.80128	0.26508
H	4.27234	1.88625	-2.44260
H	5.46989	1.91105	-1.15768
H	4.98493	4.23724	-1.92381
H	3.26626	4.02109	-1.54809
H	4.46066	4.03656	-0.24387
H	-5.85916	-0.38159	-1.63225
H	-5.89835	1.37370	-1.60472
H	-8.21902	0.41412	-1.69581
H	-7.92653	-0.46301	-0.18530
H	-7.98270	1.30503	-0.18299
H	-2.31682	2.75012	1.47527
H	-1.24333	1.56081	0.74952
H	-0.35311	2.33894	2.96410
H	-1.81923	1.75148	3.76978
H	-0.70996	0.60724	2.99469

L1_38 Ground State

N	1.35027	-0.07248	-0.06892
C	0.60967	-1.06149	-0.37374
O	1.12708	-2.32136	-0.34403
C	2.53508	-2.14457	-0.05105
C	2.67565	-0.62995	0.26207
C	-0.81311	-0.96720	-0.76181
O	-1.49673	-2.14551	-0.76330
C	-2.82931	-1.81127	-1.22467
C	-2.82698	-0.25763	-1.29572
N	-1.41953	0.11085	-1.06382
C	3.80242	0.07467	-0.51616
C	5.17724	-0.56024	-0.21787
C	3.75859	1.59198	-0.26896
C	-3.76124	0.44245	-0.28285
C	-3.33968	0.14688	1.16638
C	-5.23539	0.08083	-0.58538
C	5.70869	-0.37095	1.20833
C	7.06602	-1.04903	1.41223
C	4.79669	2.39496	-1.05886
C	4.61801	3.90524	-0.88384
C	-6.20837	1.26243	-0.48488
C	-7.65944	0.85645	-0.75042
C	-4.15550	0.86779	2.24409
C	-3.60862	0.61062	3.65071
H	3.09950	-2.44743	-0.93990
H	2.79454	-2.80273	0.78085
H	2.83546	-0.46680	1.33603
H	-3.54566	-2.22665	-0.51263
H	-2.97559	-2.28568	-2.19945
H	-3.11229	0.08146	-2.29834
H	3.59201	-0.09425	-1.58367
H	5.91103	-0.15027	-0.92293
H	5.13638	-1.63673	-0.43783
H	3.88307	1.79390	0.80454
H	2.75358	1.94382	-0.52414
H	-3.62508	1.51943	-0.45352
H	-2.28553	0.42658	1.27849
H	-3.39402	-0.93628	1.35286
H	-5.56613	-0.72230	0.08861
H	-5.31639	-0.33264	-1.60150
H	4.99109	-0.77240	1.93633
H	5.80057	0.69918	1.43109
H	7.43902	-0.90278	2.43191
H	6.99986	-2.12892	1.23142
H	7.81491	-0.64453	0.72050
H	4.72037	2.13691	-2.12480
H	5.81180	2.11419	-0.74865
H	4.71303	4.19241	0.17056
H	5.36718	4.46783	-1.45228
H	3.62618	4.22544	-1.22414
H	-5.90182	2.03323	-1.20529
H	-6.13136	1.72608	0.50523
H	-8.33405	1.71779	-0.69233
H	-7.76991	0.41170	-1.74713
H	-8.00116	0.11444	-0.01835
H	-5.20458	0.54816	2.20106
H	-4.15289	1.94749	2.04049
H	-2.57136	0.95524	3.73777
H	-3.62173	-0.46020	3.88839
H	-4.20054	1.12954	4.41297

L1_39 Ground State

N	-1.47501	-0.07207	-0.84356
C	-0.92281	-1.17345	-0.52533
O	-1.59464	-2.34312	-0.72262
C	-2.84127	-1.95934	-1.35747
C	-2.83247	-0.40492	-1.31440

C	0.41507	-1.30253	0.08629
O	0.99465	-2.53115	-0.02206
C	2.24707	-2.42245	0.70115
C	2.35663	-0.91320	1.04686
N	1.03707	-0.36364	0.67922
C	-3.93058	0.24702	-0.43054
C	-4.23529	1.68727	-0.89346
C	-3.63328	0.19416	1.07983
C	3.48229	-0.16576	0.29610
C	3.62220	1.27918	0.80831
C	3.26050	-0.20349	-1.22839
C	-3.11656	2.71597	-0.68375
C	-3.49640	4.09390	-1.23153
C	-3.67276	-1.19304	1.73369
C	-3.46884	-1.11604	3.24918
C	4.52327	0.07289	-2.05107
C	4.25626	0.04918	-3.55802
C	4.19503	1.41157	2.22376
C	4.35606	2.87217	2.65301
H	-3.66024	-2.41626	-0.79922
H	-2.83011	-2.35732	-2.37664
H	-2.94784	-0.00642	-2.32905
H	3.04580	-2.78835	0.05112
H	2.17966	-3.06255	1.58602
H	2.49900	-0.77860	2.12343
H	-4.84549	-0.33764	-0.61651
H	-5.13795	2.03252	-0.36916
H	-4.49851	1.66193	-1.96155
H	-4.37260	0.83157	1.58553
H	-2.65397	0.64761	1.26745
H	4.41505	-0.70767	0.52329
H	2.63575	1.75732	0.76090
H	4.27210	1.83837	0.12312
H	2.47945	0.52228	-1.48818
H	2.86661	-1.18397	-1.52927
H	-2.89104	2.79978	0.38642
H	-2.19372	2.36280	-1.15539
H	-2.69610	4.82392	-1.06642
H	-3.69106	4.05124	-2.31061
H	-4.40397	4.47823	-0.74895
H	-2.89998	-1.84169	1.30779
H	-4.63825	-1.67322	1.51690
H	-3.49964	-2.10991	3.70954
H	-2.49819	-0.66541	3.48874
H	-4.24475	-0.50196	3.72248
H	5.28792	-0.67615	-1.80029
H	4.94849	1.04596	-1.77409
H	5.17058	0.23857	-4.13143
H	3.85852	-0.92339	-3.87280
H	3.52031	0.81233	-3.83814
H	5.16952	0.90445	2.26984
H	3.54738	0.89764	2.94586
H	4.76853	2.95098	3.66511
H	5.02865	3.41041	1.97404
H	3.39076	3.39213	2.64258

L1_40 Ground State

N	-1.14825	-0.51655	-0.18022
C	-0.49449	-0.14889	0.84835
O	-1.11612	-0.09415	2.05712
C	-2.47408	-0.54053	1.81001
C	-2.53108	-0.75936	0.27108
C	0.93213	0.22971	0.83817
O	1.61652	-0.01547	1.99053
C	2.96823	0.44213	1.72806
C	2.97076	0.76952	0.20902
N	1.54679	0.70716	-0.16815
C	-3.52517	0.14874	-0.48878
C	-3.14600	1.63436	-0.35952
C	-4.98018	-0.12491	-0.06675
C	3.80101	-0.20351	-0.66363
C	3.24875	-1.64705	-0.62006
C	5.29511	-0.16745	-0.29055
C	-3.94360	2.57944	-1.26543
C	-3.42086	4.01704	-1.20489
C	-5.44805	-1.57845	-0.21095
C	-6.94743	-1.73611	0.05463
C	5.95825	1.21398	-0.32940
C	7.47381	1.13961	-0.12622
C	2.19149	-1.95526	-1.68989
C	1.57065	-3.34192	-1.51337
H	-3.15071	0.23524	2.17563
H	-2.63708	-1.45710	2.38375
H	-2.77403	-1.80115	0.04127
H	3.65069	-0.35980	2.01633
H	3.15572	1.31856	2.35587
H	3.32815	1.78807	0.03288
H	-3.42168	-0.12601	-1.54832
H	-2.08207	1.73708	-0.60252
H	-3.26006	1.96199	0.68476
H	-5.63987	0.50783	-0.67266
H	-5.13138	0.20323	0.97295
H	3.70843	0.16567	-1.69449

H	2.82844	-1.85738	0.37392
H	4.08269	-2.35275	-0.73830
H	5.82509	-0.83101	-0.98746
H	5.44263	-0.61263	0.70474
H	-5.00520	2.57084	-0.98812
H	-3.89225	2.21305	-2.30036
H	-3.99858	4.68205	-1.85661
H	-3.48012	4.41488	-0.18433
H	-2.37131	4.06673	-1.51810
H	-4.89358	-2.22792	0.47896
H	-5.21281	-1.93654	-1.22294
H	-7.26481	-2.78014	-0.04276
H	-7.20544	-1.40104	1.06672
H	-7.53723	-1.13873	-0.65095
H	5.52606	1.86454	0.44233
H	5.73787	1.69524	-1.29260
H	7.93117	2.13490	-0.14781
H	7.71968	0.67922	0.83854
H	7.94682	0.53577	-0.90988
H	2.66273	-1.88097	-2.68045
H	1.40378	-1.19713	-1.66039
H	0.84969	-3.55921	-2.30919
H	2.33331	-4.13131	-1.52491
H	1.03683	-3.40783	-0.55729

L1_41 Ground State

N	-1.74851	0.40266	-0.61828
C	-0.98648	-0.39416	-1.25357
O	-1.49472	-1.14665	-2.26966
C	-2.87961	-0.73055	-2.38549
C	-3.10613	0.18313	-1.15069
C	0.43505	-0.62990	-0.93400
O	1.22118	-1.02767	-1.97018
C	2.53999	-1.22245	-1.39800
C	2.37927	-0.79575	0.08926
N	0.94256	-0.49248	0.22540
C	-4.03572	-0.43158	-0.07598
C	-4.41258	0.58558	1.01470
C	-3.47501	-1.74589	0.52023
C	3.24091	0.41064	0.52747
C	2.86039	1.68686	-0.24318
C	4.74522	0.09613	0.43670
C	-5.30016	1.74171	0.54005
C	-5.71484	2.66597	1.68794
C	-2.47182	-1.61021	1.67858
C	-1.83756	-2.95649	2.03527
C	5.21035	-1.13860	1.21860
C	6.73450	-1.28149	1.22797
C	3.50346	2.97195	0.29074
C	2.97316	4.22163	-0.41685
H	-3.50164	-1.62880	-2.39362
H	-2.99277	-0.20241	-3.33731
H	-3.51970	1.14663	-1.46260
H	3.24238	-0.60685	-1.96472
H	2.80782	-2.27555	-1.51994
H	2.60181	-1.63560	0.75440
H	-4.95965	-0.69065	-0.61770
H	-3.49662	0.98797	1.46304
H	-4.94148	0.05119	1.81638
H	-3.00762	-2.33746	-0.27961
H	-4.32421	-2.34868	0.87135
H	2.99251	0.57897	1.58521
H	1.77095	1.79993	-0.19899
H	3.11909	1.57492	-1.30686
H	5.30228	0.96505	0.80727
H	5.03703	-0.01206	-0.61907
H	-6.19769	1.33540	0.05168
H	-4.77755	2.33416	-0.22187
H	-6.34765	3.48768	1.33432
H	-6.27573	2.11614	2.45352
H	-4.83570	3.10517	2.17437
H	-2.98574	-1.20551	2.55952
H	-1.68448	-0.89682	1.42212
H	-1.15657	-2.86082	2.88815
H	-2.59732	-3.70556	2.29336
H	-1.25771	-3.34947	1.19085
H	4.76957	-2.04883	0.79148
H	4.83932	-1.07513	2.25108
H	7.05079	-2.17218	1.78190
H	7.12862	-1.36461	0.20771
H	7.20877	-0.40987	1.69478
H	4.59408	2.93018	0.17769
H	3.30807	3.04969	1.36950
H	3.43978	5.13275	-0.02592
H	3.17401	4.17907	-1.49442
H	1.88858	4.31612	-0.28674

L1_42 Ground State

N	1.08585	-0.23969	-0.08650
C	0.38272	-1.28175	-0.28506
O	0.94602	-2.51134	-0.13555
C	2.34972	-2.25377	0.12407
C	2.43534	-0.71089	0.28191
C	-1.05031	-1.26425	-0.63982

O	-1.77408	-2.33764	-0.21472
C	-3.12539	-2.08395	-0.67971
C	-3.07671	-0.62295	-1.20621
N	-1.63671	-0.30985	-1.24315
C	3.52580	-0.04517	-0.57763
C	4.92763	-0.59217	-0.23449
C	3.42213	1.48642	-0.48296
C	-3.82701	0.40964	-0.33198
C	-3.23597	0.50998	1.09336
C	-5.33685	0.10557	-0.32910
C	5.46323	-0.23853	1.15849
C	6.84851	-0.83855	1.41247
C	4.42005	2.24671	-1.36176
C	4.17985	3.75840	-1.33755
C	-6.20363	1.29481	0.09920
C	-7.69611	0.95777	0.13306
C	-2.13450	1.56854	1.24455
C	-1.46423	1.52336	2.61842
H	2.91872	-2.62398	-0.73563
H	2.63820	-2.81470	1.01541
H	2.59713	-0.43471	1.33191
H	-3.80067	-2.23559	0.16450
H	-3.35433	-2.81360	-1.46227
H	-3.47947	-0.56384	-2.22354
H	3.31282	-0.32881	-1.61996
H	5.63801	-0.22712	-0.98663
H	4.92817	-1.68619	-0.34440
H	3.54688	1.80005	0.56340
H	2.40165	1.77069	-0.76002
H	-3.68424	1.37900	-0.82942
H	-4.03796	0.73444	1.80856
H	-2.83937	-0.46818	1.40033
H	-5.54354	-0.74696	0.33463
H	-5.65042	-0.20852	-1.33576
H	5.51342	0.85148	1.27052
H	4.76870	-0.59190	1.93236
H	7.22396	-0.57546	2.40749
H	6.82438	-1.93294	1.34208
H	7.57448	-0.47689	0.67419
H	4.34650	1.87936	-2.39529
H	5.44816	2.04017	-1.03651
H	4.90077	4.29068	-1.96825
H	3.17313	4.00184	-1.69714
H	4.27046	4.15429	-0.31858
H	-6.02807	2.12970	-0.59293
H	-5.88731	1.64861	1.08889
H	-8.29617	1.82539	0.42893
H	-8.04921	0.62703	-0.85134
H	-7.90189	0.15021	0.84622
H	-2.57637	2.56114	1.07666
H	-1.37879	1.42623	0.46638
H	-0.70898	2.31069	2.71886
H	-2.19349	1.65082	3.42889
H	-0.96043	0.56099	2.77152

L1_43 Ground State

N	1.11136	-0.24916	0.54681
C	0.53656	-1.11021	-0.19347
O	1.17472	-2.27538	-0.48871
C	2.45081	-2.19718	0.19443
C	2.44367	-0.79288	0.86656
C	-0.80997	-0.95559	-0.78259
O	-1.34500	-2.08678	-1.32388
C	-2.61878	-1.67431	-1.87932
C	-2.78730	-0.20859	-1.39721
N	-1.48041	0.12632	-0.80012
C	3.56829	0.14012	0.37241
C	4.95469	-0.44128	0.74745
C	3.35425	1.56311	0.91497
C	-3.92279	-0.00194	-0.36899
C	-4.12623	1.49316	-0.06400
C	-3.66768	-0.80911	0.91868
C	6.03226	-0.31012	-0.34177
C	5.79971	-1.22511	-1.54787
C	4.34716	2.61264	0.40608
C	4.00718	4.01919	0.90635
C	-4.92367	-1.05311	1.76178
C	-4.62519	-1.83274	3.04466
C	-4.74175	2.30835	-1.20667
C	-4.96182	3.77424	-0.82425
H	3.23700	-2.31648	-0.55550
H	2.50226	-3.02644	0.90500
H	2.52358	-0.87844	1.95829
H	-3.38760	-2.35556	-1.50587
H	-2.55524	-1.76438	-2.96800
H	-2.95776	0.45564	-2.25014
H	3.47915	0.17924	-0.72345
H	4.86497	-1.50736	1.00118
H	5.30163	0.04852	1.66686
H	3.39907	1.52944	2.01462
H	2.33583	1.87604	0.66201
H	-4.84004	-0.38855	-0.84285
H	-3.15580	1.92134	0.21684

H	-4.77606	1.59220	0.81497
H	-2.91199	-0.28553	1.51791
H	-3.22768	-1.78537	0.67299
H	7.00927	-0.54646	0.09980
H	6.09280	0.73046	-0.68047
H	6.59569	-1.10962	-2.29172
H	5.77922	-2.27926	-1.24369
H	4.84979	-1.00547	-2.04879
H	4.35232	2.60592	-0.69315
H	5.36710	2.35599	0.71985
H	4.72276	4.76185	0.53584
H	3.00617	4.32170	0.57684
H	4.01959	4.06005	2.00239
H	-5.66077	-1.60298	1.15931
H	-5.39552	-0.09667	2.02076
H	-5.53489	-2.00746	3.62999
H	-4.17963	-2.80913	2.81810
H	-3.91718	-1.28695	3.67975
H	-5.70019	1.85614	-1.49965
H	-4.09788	2.26467	-2.09467
H	-5.40471	4.34333	-1.64931
H	-5.63226	3.85949	0.03968
H	-4.01391	4.25534	-0.55545

L1_44 Ground State

N	1.18701	-0.41599	0.25002
C	0.59705	-0.75078	-0.82701
O	1.26678	-1.48107	-1.76141
C	2.57547	-1.72734	-1.18897
C	2.56562	-0.92787	0.14427
C	-0.79315	-0.39339	-1.17629
O	-1.35969	-1.14182	-2.16496
C	-2.67665	-0.56951	-2.36460
C	-2.81909	0.46630	-1.21742
N	-1.47117	0.52925	-0.62027
C	3.58665	0.22898	0.23313
C	3.30988	1.30715	-0.83037
C	5.03645	-0.28646	0.17265
C	-3.86954	0.09272	-0.14672
C	-4.05988	1.23890	0.86314
C	-3.50401	-1.22633	0.56117
C	4.20202	2.55583	-0.75073
C	4.13769	3.27964	0.59756
C	5.41207	-1.37202	1.19352
C	5.20840	-0.94720	2.65089
C	-4.68376	-1.90647	1.26362
C	-4.27538	-3.19962	1.97340
C	-4.76930	2.47886	0.30776
C	-4.97168	3.56045	1.37206
H	3.32365	-1.38754	-1.90881
H	2.68327	-2.80611	-1.04416
H	2.73459	-1.59894	0.99233
H	-3.40807	-1.38063	-2.32353
H	-2.69761	-0.11479	-3.35967
H	-3.06343	1.45270	-1.62349
H	3.41865	0.68385	1.21643
H	2.26349	1.61814	-0.73054
H	3.41135	0.86968	-1.83403
H	5.71062	0.56632	0.32005
H	5.24635	-0.65797	-0.84097
H	-4.81893	-0.05658	-0.68690
H	-3.07378	1.51919	1.25425
H	-4.63969	0.86789	1.71800
H	-2.70319	-1.02708	1.28449
H	-3.08147	-1.93863	-0.16073
H	3.88728	3.24633	-1.54391
H	5.24368	2.29534	-0.97845
H	4.70346	4.21751	0.56875
H	3.10146	3.51916	0.86501
H	4.55382	2.66956	1.40722
H	6.46662	-1.63476	1.03925
H	4.84637	-2.29280	0.99739
H	5.57614	-1.71420	3.34118
H	5.74841	-0.01667	2.86575
H	4.15145	-0.77470	2.88166
H	-5.46724	-2.12378	0.52361
H	-5.13530	-1.22086	1.99198
H	-5.13171	-3.67814	2.46168
H	-3.84762	-3.91989	1.26530
H	-3.51775	-3.00316	2.74144
H	-5.74366	2.18385	-0.10761
H	-4.19599	2.90320	-0.52665
H	-5.48207	4.43881	0.96131
H	-5.57382	3.18309	2.20762
H	-4.00995	3.89192	1.78127

L1_45 Ground State

N	0.88892	-0.21601	-0.08597
C	0.19212	-1.10765	-0.66806
O	0.77377	-2.28468	-1.02976
C	2.17920	-2.12384	-0.71373
C	2.25097	-0.76892	0.04222
C	-1.24510	-0.98251	-0.98584
O	-1.87361	-2.14355	-1.32581

C	-3.24037	-1.75986	-1.62298
C	-3.31341	-0.25791	-1.22661
N	-1.91275	0.09971	-0.93597
C	3.31526	0.20272	-0.50083
C	4.72967	-0.41055	-0.42598
C	3.19922	1.56987	0.19385
C	-4.25765	0.07594	-0.03963
C	-4.72692	1.54496	-0.09731
C	-3.67480	-0.27294	1.34270
C	5.29358	-0.62724	0.98379
C	6.68982	-1.25448	0.95571
C	4.17006	2.63304	-0.32910
C	3.91694	4.00741	0.29584
C	-3.50660	-1.76563	1.65425
C	-3.02676	-1.99924	3.08933
C	-3.64981	2.60921	0.14959
C	-4.20481	4.02858	0.00675
H	2.73217	-2.11119	-1.65936
H	2.49555	-2.98652	-0.12370
H	2.43484	-0.92872	1.11276
H	-3.90635	-2.40575	-1.04817
H	-3.40638	-1.92690	-2.69153
H	-3.64485	0.33558	-2.08668
H	3.08213	0.35085	-1.56672
H	5.41934	0.23456	-0.98435
H	4.73813	-1.37177	-0.95972
H	3.34428	1.44643	1.27661
H	2.17009	1.92252	0.06922
H	-5.15641	-0.54202	-0.19416
H	-5.53226	1.67719	0.63949
H	-5.18587	1.72598	-1.08083
H	-4.34015	0.16205	2.10212
H	-2.70628	0.22563	1.45798
H	4.62022	-1.26999	1.56652
H	5.33650	0.33017	1.51738
H	7.08549	-1.39928	1.96700
H	6.67428	-2.23232	0.45892
H	7.39534	-0.61792	0.40806
H	4.07648	2.70343	-1.42222
H	5.20711	2.33240	-0.13012
H	4.02727	3.96930	1.38652
H	4.61846	4.75817	-0.08503
H	2.90011	4.35588	0.07976
H	-2.79004	-2.22466	0.96486
H	-4.46481	-2.28278	1.49906
H	-2.90890	-3.06715	3.30452
H	-2.05819	-1.51404	3.25997
H	-3.73643	-1.58588	3.81640
H	-2.81358	2.45875	-0.54093
H	-3.23208	2.48189	1.15584
H	-5.02609	4.20826	0.71210
H	-4.59613	4.20089	-1.00385
H	-3.43122	4.78099	0.19673
H	-6.76647	0.19276	-2.13389
H	-5.13269	-0.11142	-2.67942
H	-5.90385	2.21706	-3.25721
H	-6.11157	2.57505	-1.53486
H	-4.49692	2.27613	-2.18899
H	4.38497	2.35568	-1.42609
H	5.53569	2.25156	-0.10180
H	4.99163	4.64094	-0.58708
H	3.27107	4.32305	-0.30356
H	4.42248	4.20981	1.03405
H	6.02978	0.37425	-1.31413
H	5.46433	-1.26835	-1.54516
H	7.96057	-1.22795	-1.34017
H	7.83476	-0.44942	0.24548
H	7.26272	-2.10939	0.02840

L1_46 Ground State

N	-1.50240	0.17431	-0.63537
C	-0.88326	-0.92450	-0.46362
O	-1.52275	-2.10167	-0.70827
C	-2.84686	-1.73130	-1.16659
C	-2.87021	-0.18047	-1.05478
C	0.51044	-1.04722	0.01257
O	1.07981	-2.27251	-0.15442
C	2.42024	-2.14853	0.38194
C	2.52226	-0.65978	0.82569
N	1.18276	-0.11007	0.55044
C	-3.91423	0.39596	-0.07187
C	-3.64388	-0.05747	1.37327
C	-5.35264	0.07515	-0.52143
C	3.62162	0.12845	0.08663
C	5.01593	-0.46629	0.40470
C	3.52114	1.62678	0.41521
C	-4.49668	0.64837	2.43374
C	-4.07940	0.27131	3.85755
C	-5.71995	0.47433	-1.95941
C	-5.54620	1.96759	-2.25226
C	4.50090	2.52485	-0.34626
C	4.28666	4.00863	-0.03563
C	5.93691	-0.59709	-0.81419

C	7.32635	-1.12550	-0.45270
H	-3.57428	-2.23567	-0.52615
H	-2.96310	-2.09288	-2.19215
H	-3.04024	0.27022	-2.03778
H	3.12334	-2.41239	-0.41364
H	2.52119	-2.86355	1.20269
H	2.70825	-0.58178	1.90497
H	-3.77346	1.48456	-0.09947
H	-2.58710	0.12955	1.59678
H	-3.79393	-1.14401	1.46161
H	-6.04660	0.58112	0.16063
H	-5.53866	-1.00089	-0.39025
H	3.42400	0.00140	-0.98927
H	4.91359	-1.46287	0.85772
H	5.50572	0.15076	1.17092
H	3.67776	1.75978	1.49689
H	2.49600	1.95486	0.21354
H	-5.55784	0.40695	2.29403
H	-4.40782	1.73571	2.30038
H	-4.69642	0.78193	4.60540
H	-4.17786	-0.80851	4.02380
H	-3.03288	0.53997	4.04429
H	-6.76647	0.19276	-2.13389
H	-5.13269	-0.11142	-2.67942
H	-5.90385	2.21706	-3.25721
H	-6.11157	2.57505	-1.53486
H	-4.49692	2.27613	-2.18899
H	4.38497	2.35568	-1.42609
H	5.53569	2.25156	-0.10180
H	4.99163	4.64094	-0.58708
H	3.27107	4.32305	-0.30356
H	4.42248	4.20981	1.03405
H	6.02978	0.37425	-1.31413
H	5.46433	-1.26835	-1.54516
H	7.96057	-1.22795	-1.34017
H	7.83476	-0.44942	0.24548
H	7.26272	-2.10939	0.02840

L1_47 Ground State

N	-1.63565	0.64666	-0.83611
C	-0.89035	-0.19748	-1.42891
O	-1.38171	-0.90751	-2.48305
C	-2.72504	-0.39778	-2.68178
C	-2.96799	0.52389	-1.45594
C	0.48850	-0.53106	-1.02155
O	1.31078	-0.97567	-2.00951
C	2.57345	-1.26438	-1.35614
C	2.34906	-0.82917	0.12029
N	0.92920	-0.43341	0.16879
C	-4.01032	-0.02347	-0.45087
C	-4.39066	1.04911	0.58122
C	-3.58286	-1.36971	0.18364
C	3.25754	0.31937	0.61585
C	3.00899	1.61710	-0.17258
C	4.74128	-0.09132	0.61791
C	-5.58490	0.67144	1.46372
C	-5.95867	1.78127	2.44925
C	-2.64474	-1.29669	1.40035
C	-2.11142	-2.67874	1.78453
C	5.07675	-1.35263	1.42338
C	6.58506	-1.59344	1.52621
C	3.70038	2.85815	0.40346
C	3.29610	4.13889	-0.33130
H	-3.40473	-1.25164	-2.73575
H	-2.74248	0.14067	-3.63434
H	-3.29807	1.51760	-1.77954
H	3.35225	-0.69987	-1.87397
H	2.77304	-2.33381	-1.46661
H	2.47585	-1.68183	0.79416
H	-4.90761	-0.22211	-1.05936
H	-4.63231	1.97938	0.04675
H	-3.51968	1.27856	1.20599
H	-3.10538	-1.99113	-0.58704
H	-4.48720	-1.91928	0.47666
H	2.95490	0.50382	1.65664
H	1.92863	1.80112	-0.19476
H	3.32448	1.48757	-1.21878
H	5.32874	0.74037	1.02516
H	5.09082	-0.21880	-0.41801
H	-5.36383	-0.24762	2.02039
H	-6.44829	0.43978	0.82352
H	-6.81655	1.49708	3.06894
H	-5.12111	2.00779	3.11997
H	-6.21829	2.70726	1.92173
H	-3.18355	-0.86617	2.25402
H	-1.80385	-0.62941	1.19581
H	-1.47854	-2.62574	2.67722
H	-2.92708	-3.38365	1.99120
H	-1.50519	-3.10083	0.97344
H	4.60539	-2.23307	0.96742
H	4.64767	-1.26417	2.43124
H	6.80860	-2.50195	2.09617
H	7.03513	-1.70308	0.53193

H	7.08480	-0.75360	2.02370
H	4.79085	2.74573	0.35668
H	3.44522	2.94933	1.46860
H	3.79629	5.01821	0.08980
H	3.55875	4.08223	-1.39484
H	2.21405	4.30371	-0.26687

L1_48 Ground State

N	1.20080	-0.57079	0.23469
C	0.63102	-0.70606	-0.89568
O	1.29650	-1.32020	-1.91468
C	2.54976	-1.76072	-1.33488
C	2.56661	-1.10461	0.07135
C	-0.72779	-0.22696	-1.22161
O	-1.29336	-0.77876	-2.33252
C	-2.57461	-0.11509	-2.47344
C	-2.70975	0.72963	-1.17834
N	-1.38160	0.62897	-0.54323
C	3.61785	0.01431	0.24953
C	3.63553	0.54729	1.69417
C	3.39419	1.15734	-0.75956
C	-3.81185	0.24219	-0.21023
C	-3.98567	1.22047	0.96558
C	-3.52990	-1.18948	0.28515
C	3.87295	-0.49412	2.79824
C	5.17577	-1.28463	2.64237
C	4.49518	2.22847	-0.79906
C	5.88846	1.68215	-1.12458
C	-4.76164	-1.91332	0.83903
C	-4.43579	-3.32228	1.34047
C	-4.61842	2.56725	0.59819
C	-4.81008	3.47323	1.81722
H	3.36073	-1.43540	-1.99084
H	2.53466	-2.85435	-1.29557
H	2.73419	-1.86628	0.83832
H	-3.34356	-0.88383	-2.58448
H	-2.53910	0.49358	-3.38209
H	-2.89557	1.77921	-1.42610
H	4.58809	-0.45518	0.03472
H	2.68263	1.05611	1.88214
H	4.42163	1.30924	1.77107
H	2.43427	1.63582	-0.53153
H	3.29397	0.73888	-1.77049
H	-4.74779	0.22809	-0.79265
H	-3.00233	1.38494	1.42376
H	-4.61131	0.74722	1.73317
H	-2.74514	-1.14846	1.05112
H	-3.11653	-1.79762	-0.53114
H	3.88709	0.03230	3.76130
H	3.02307	-1.18577	2.85348
H	5.34807	-1.93944	3.50373
H	5.16579	-1.91729	1.74716
H	6.03712	-0.61003	2.55744
H	4.52851	2.77052	0.15396
H	4.21523	2.97274	-1.55579
H	6.61314	2.49489	-1.24574
H	6.26285	1.02444	-0.33202
H	5.87696	1.10356	-2.05710
H	-5.52970	-1.96972	0.05445
H	-5.20493	-1.33147	1.65716
H	-5.32838	-3.82916	1.72393
H	-4.01873	-3.94049	0.53606
H	-3.69517	-3.28961	2.14849
H	-5.58956	2.39172	0.11341
H	-3.99718	3.09056	-0.14021
H	-5.26525	4.43054	1.53958
H	-5.45833	2.99768	2.56338
H	-3.84977	3.68617	2.30172

L1_49 Ground State

N	-1.30462	-0.63788	-0.26484
C	-0.70450	-0.37528	0.82647
O	-1.38700	-0.44567	2.00287
C	-2.72578	-0.86996	1.64485
C	-2.70435	-0.93330	0.09102
C	0.71215	0.02878	0.93794
O	1.27062	-0.13000	2.16997
C	2.63060	0.35386	2.03901
C	2.77258	0.68931	0.52769
N	1.41778	0.48604	-0.01757
C	-3.67178	0.03918	-0.62251
C	-3.31582	1.50693	-0.32887
C	-5.14207	-0.28407	-0.29955
C	3.80637	-0.15951	-0.24671
C	3.42270	-1.65046	-0.24696
C	5.23673	0.07133	0.27487
C	-4.08389	2.53286	-1.17001
C	-3.57948	3.96051	-0.94403
C	-5.58602	-1.71961	-0.60662
C	-7.09441	-1.91273	-0.43036
C	5.71313	1.53175	0.31963
C	5.67309	2.23679	-1.03948
C	4.33037	-2.56498	-1.08430
C	4.42543	-2.16332	-2.55931

H	-3.42717	-0.13787	2.05203
H	-2.90964	-1.84026	2.11472
H	-2.92479	-1.94830	-0.25360
H	3.30048	-0.43576	2.38700
H	2.74205	1.22798	2.68701
H	3.02769	1.74529	0.39399
H	-3.51566	-0.12816	-1.69789
H	-2.24349	1.64024	-0.51304
H	-3.47856	1.72714	0.73689
H	-5.77964	0.40033	-0.87212
H	-5.34585	-0.06001	0.75864
H	3.75106	0.19639	-1.28222
H	2.39722	-1.73441	-0.62501
H	3.40658	-2.02692	0.78600
H	5.92967	-0.49255	-0.36178
H	5.33181	-0.36884	1.27822
H	-5.15616	2.49013	-0.94121
H	-3.98483	2.27207	-2.23308
H	-4.13616	4.68380	-1.55042
H	-3.68591	4.25383	0.10763
H	-2.51823	4.04805	-1.20535
H	-5.05738	-2.42948	0.04284
H	-5.29908	-1.97561	-1.63610
H	-7.39487	-2.94428	-0.64459
H	-7.40405	-1.68049	0.59599
H	-7.65695	-1.25298	-1.10183
H	6.74243	1.54317	0.70084
H	5.12203	2.10397	1.04729
H	6.10727	3.24059	-0.97696
H	6.24123	1.67234	-1.78933
H	4.64908	2.34267	-1.41421
H	3.93514	-3.58677	-1.01559
H	5.33716	-2.60498	-0.64893
H	4.99450	-2.90307	-3.13331
H	3.42839	-2.08232	-3.00875
H	4.92311	-1.19524	-2.68616

L1_50 Ground State

N	-1.60517	-0.99964	-1.14354
C	-1.01468	-1.62883	-0.21006
O	-1.73964	-2.39093	0.65575
C	-3.10933	-2.28895	0.18280
C	-3.04975	-1.19494	-0.91915
C	0.42529	-1.51513	0.10002
O	1.06606	-2.65515	0.47116
C	2.45086	-2.26117	0.67087
C	2.43314	-0.71441	0.52706
N	1.05850	-0.41227	0.08808
C	-3.70842	0.15311	-0.53803
C	-2.99800	0.83465	0.65569
C	-5.21859	-0.03755	-0.30537
C	3.48720	-0.15337	-0.44405
C	4.89292	-0.36225	0.14813
C	3.17598	1.30538	-0.83133
C	-1.88569	1.81053	0.24392
C	-1.06309	2.30762	1.43315
C	-6.02195	1.26501	-0.38930
C	-7.51322	1.06013	-0.11321
C	3.16289	2.31120	0.32538
C	2.80266	3.72165	-0.14782
C	6.04469	0.08144	-0.75912
C	7.41636	-0.27331	-0.17978
H	-3.73566	-2.03113	1.03883
H	-3.40596	-3.26912	-0.20219
H	-3.51283	-1.55241	-1.84545
H	3.05216	-2.75114	-0.10301
H	2.76295	-2.62011	1.65343
H	2.57324	-0.23691	1.50540
H	-3.58816	0.79965	-1.41838
H	-3.73510	1.37531	1.26350
H	-2.57712	0.06947	1.32314
H	-5.38863	-0.50116	0.67748
H	-5.61963	-0.74245	-1.04890
H	3.41840	-0.75045	-1.36672
H	5.02727	-1.42932	0.38090
H	4.96743	0.16385	1.11037
H	2.19347	1.31926	-1.31412
H	3.90117	1.63423	-1.58663
H	-2.34360	2.66221	-0.27962
H	-1.21904	1.31983	-0.47049
H	-0.30606	3.03364	1.11496
H	-1.69365	2.78862	2.19226
H	-0.53621	1.47198	1.90823
H	-5.88671	1.70194	-1.38816
H	-5.61679	1.99769	0.32047
H	-8.06823	2.00152	-0.19145
H	-7.95370	0.35208	-0.82582
H	-7.67616	0.65891	0.89453
H	4.14160	2.33191	0.82392
H	2.43250	1.99419	1.07965
H	2.79753	4.43573	0.68341
H	3.51776	4.08402	-0.89678
H	1.80701	3.73394	-0.60723

H	5.99042	1.16441	-0.92376
H	5.92834	-0.38516	-1.74734
H	8.22729	0.05907	-0.83718
H	7.56461	0.19959	0.79874
H	7.51975	-1.35657	-0.04198

L1_51 Ground State

N	-1.34775	-0.47362	-0.98399
C	-0.75013	-1.25307	-0.17389
O	-1.43078	-2.29269	0.38415
C	-2.74745	-2.25276	-0.22066
C	-2.74670	-0.93223	-1.04209
C	0.65797	-1.11553	0.25283
O	1.19659	-2.20938	0.85851
C	2.57350	-1.85291	1.13808
C	2.69596	-0.37927	0.65592
N	1.36685	-0.06992	0.09915
C	-3.71207	0.15812	-0.52419
C	-3.33314	0.61457	0.89482
C	-5.17596	-0.32872	-0.64830
C	3.82001	-0.15600	-0.37530
C	5.18729	-0.37746	0.29762
C	3.68689	1.20501	-1.08442
C	-4.18240	1.75601	1.46284
C	-3.67764	2.22590	2.82966
C	-6.15312	0.73567	-1.16328
C	-7.59515	0.22904	-1.23258
C	3.84061	2.43849	-0.18760
C	3.69292	3.74164	-0.97719
C	6.39102	-0.25919	-0.64256
C	7.70946	-0.62007	0.04620
H	-3.48707	-2.28124	0.58233
H	-2.85796	-3.14566	-0.84293
H	-3.00243	-1.13094	-2.08929
H	3.21565	-2.54055	0.57782
H	2.74712	-1.99005	2.20795
H	2.86461	0.29375	1.50613
H	-3.57280	1.01667	-1.19577
H	-3.39044	-0.24066	1.58493
H	-2.28354	0.93110	0.88241
H	-5.52551	-0.70485	0.32382
H	-5.22609	-1.18744	-1.33393
H	3.69522	-0.93173	-1.14709
H	5.20458	-1.37725	0.75595
H	5.30652	0.33215	1.12839
H	2.70193	1.23958	-1.56124
H	4.42867	1.25520	-1.89198
H	-5.22914	1.43896	1.55448
H	-4.17549	2.59947	0.75876
H	-4.29304	3.04094	3.22671
H	-3.69616	1.40669	3.55895
H	-2.64402	2.58585	2.76399
H	-5.82647	1.06037	-2.16076
H	-6.10598	1.62543	-0.52507
H	-8.27232	0.99802	-1.62050
H	-7.67545	-0.64809	-1.88652
H	-7.95743	-0.06527	-0.23991
H	4.81870	2.42668	0.31211
H	3.08383	2.41228	0.60637
H	3.80032	4.61915	-0.32961
H	4.45184	3.81287	-1.76626
H	2.70921	3.79705	-1.45796
H	6.45564	0.76280	-1.03528
H	6.23697	-0.91269	-1.51266
H	8.55943	-0.52148	-0.63803
H	7.89586	0.03410	0.90670
H	7.69403	-1.65324	0.41426

L1_52 Ground State

N	1.30181	-0.10983	0.69265
C	0.68088	-1.14404	0.28628
O	1.28787	-2.36296	0.35445
C	2.56323	-2.11488	0.99756
C	2.64557	-0.56791	1.09419
C	-0.68093	-1.14400	-0.28636
O	-1.28794	-2.36290	-0.35465
C	-2.56330	-2.11472	-0.99774
C	-2.64560	-0.56774	-1.09422
N	-1.30184	-0.10973	-0.69262
C	3.73100	0.06787	0.19630
C	3.86047	1.57751	0.46568
C	3.45529	-0.21091	-1.29530
C	-3.73102	0.06797	-0.19627
C	-3.86045	1.57763	-0.46551
C	-3.45532	-0.21097	1.29531
C	4.48384	1.94124	1.81777
C	4.63154	3.45345	2.00438
C	4.67326	-0.05118	-2.21749
C	5.75576	-1.11381	-2.00297
C	-4.67331	-0.05142	2.21750
C	-5.75578	-1.11405	2.00280
C	-4.48375	1.94148	-1.81760
C	-4.63133	3.45371	-2.00414
H	3.34656	-2.56259	0.38057

H	2.54771	-2.60703	1.97474
H	2.81957	-0.25986	2.12983
H	-3.34664	-2.56248	-0.38080
H	-2.54779	-2.60678	-1.97497
H	-2.81959	-0.25957	-2.12982
H	4.67711	-0.41663	0.48173
H	2.86391	2.02913	0.38215
H	4.47327	2.02883	-0.32552
H	2.65142	0.45839	-1.62368
H	3.06614	-1.23032	-1.42348
H	-4.67713	-0.41649	-0.48175
H	-2.86388	2.02922	-0.38191
H	-4.47326	2.02891	0.32570
H	-2.65149	0.45832	1.62378
H	-3.06614	-1.23039	1.42336
H	5.46950	1.46148	1.90356
H	3.87470	1.53885	2.63760
H	5.08062	3.69747	2.97366
H	3.65619	3.95157	1.95142
H	5.26667	3.88666	1.22203
H	5.11117	0.94795	-2.09505
H	4.32700	-0.10151	-3.25783
H	6.57494	-0.99551	-2.72092
H	6.19084	-1.05805	-0.99872
H	5.34391	-2.12302	-2.13009
H	-5.11126	0.94771	2.09520
H	-4.32707	-0.10189	3.25783
H	-6.57499	-0.99588	2.72074
H	-6.19084	-1.05816	0.99854
H	-5.34390	-2.12326	2.12978
H	-3.87462	1.53909	-2.63743
H	-5.46944	1.46180	-1.90344
H	-5.08037	3.69782	-2.97341
H	-3.65594	3.95175	-1.95113
H	-5.26644	3.88693	-1.22177

L1_53 Ground State

N	-1.25206	0.48384	-0.42410
C	-0.61819	-0.43959	-1.02896
O	-1.20457	-1.08098	-2.07945
C	-2.47711	-0.41247	-2.26788
C	-2.58478	0.54853	-1.05379
C	0.73764	-0.90767	-0.67570
O	1.36504	-1.65791	-1.62584
C	2.62340	-2.05239	-1.02425
C	2.68693	-1.23274	0.29184
N	1.33701	-0.65032	0.41753
C	-3.68754	0.16952	-0.03933
C	-3.84001	1.25054	1.04526
C	-3.41836	-1.21419	0.58647
C	3.76028	-0.12168	0.30654
C	3.82477	0.57606	1.67865
C	3.53010	0.90140	-0.82275
C	-4.45712	2.56787	0.56273
C	-4.62820	3.58175	1.69684
C	-4.64423	-1.88350	1.22568
C	-5.71205	-2.31429	0.21516
C	4.74151	1.78921	-1.12813
C	4.47763	2.75739	-2.28407
C	4.12172	-0.32578	2.88647
C	5.43240	-1.11107	2.77772
H	-3.25918	-1.17534	-2.29993
H	-2.44259	0.11013	-3.22864
H	-2.75596	1.57445	-1.39419
H	3.42425	-1.82427	-1.73188
H	2.58948	-3.13296	-0.85405
H	2.85825	-1.89872	1.14268
H	-4.62325	0.12480	-0.61707
H	-2.85198	1.44124	1.48288
H	-4.46741	0.85595	1.85509
H	-2.62571	-1.10055	1.33532
H	-3.01649	-1.89987	-0.17209
H	4.72111	-0.62452	0.11766
H	2.86872	1.08699	1.84278
H	4.59677	1.35470	1.63504
H	2.66798	1.52805	-0.56127
H	3.25046	0.38062	-1.74878
H	-3.83397	3.01409	-0.22315
H	-5.43387	2.36336	0.10100
H	-5.07264	4.51663	1.33741
H	-5.27734	3.18370	2.48635
H	-3.66175	3.82380	2.15470
H	-5.09383	-1.21488	1.97121
H	-4.30396	-2.76672	1.78145
H	-6.53697	-2.83895	0.70985
H	-6.14165	-1.45778	-0.31655
H	-5.28844	-2.99239	-0.53651
H	5.60456	1.15261	-1.37046
H	5.02520	2.36135	-0.23627
H	5.35320	3.38224	-2.49292
H	4.22571	2.21489	-3.20355
H	3.63749	3.42357	-2.05397
H	3.28766	-1.01891	3.05366

H	4.15878	0.31006	3.78046
H	5.64501	-1.65692	3.70363
H	5.40290	-1.84546	1.96439
H	6.27827	-0.43991	2.58297

L1_54 Ground State

N	-1.91703	-0.86073	-0.77437
C	-1.19289	-1.68233	-0.12840
O	-1.77878	-2.67928	0.59246
C	-3.20211	-2.52315	0.35385
C	-3.31301	-1.18420	-0.42494
C	0.27461	-1.58381	0.00580
O	0.96750	-2.75301	0.04044
C	2.36385	-2.36076	0.13248
C	2.31581	-0.82126	0.33257
N	0.89366	-0.48131	0.14478
C	-3.95378	-0.03506	0.39377
C	-4.30344	1.17771	-0.48549
C	-3.10281	0.36161	1.62640
C	3.23258	-0.02672	-0.61401
C	4.70415	-0.31349	-0.26315
C	2.86705	1.47029	-0.62546
C	-5.44017	0.94143	-1.48636
C	-5.79055	2.20390	-2.27828
C	-1.97188	1.37755	1.38403
C	-1.03842	1.49330	2.59068
C	2.99493	2.19488	0.71937
C	2.58263	3.66558	0.61823
C	5.72709	0.35862	-1.18426
C	7.16375	-0.06919	-0.87453
H	-3.70552	-2.51397	1.32369
H	-3.54241	-3.38755	-0.22446
H	-3.88546	-1.32586	-1.34614
H	2.85458	-2.65016	-0.80360
H	2.81257	-2.91078	0.96173
H	2.57621	-0.56131	1.36680
H	-4.90153	-0.45065	0.77206
H	-4.59121	2.00995	0.17191
H	-3.40455	1.50502	-1.02143
H	-2.67102	-0.54438	2.07480
H	-3.77833	0.77206	2.38974
H	3.04805	-0.40882	-1.63011
H	4.87301	-1.40040	-0.29351
H	4.89927	-0.01089	0.77538
H	1.83135	1.55777	-0.96948
H	3.48939	1.98160	-1.37093
H	-6.33033	0.58538	-0.94796
H	-5.16875	0.14409	-2.19033
H	-6.60510	2.02067	-2.98794
H	-6.10459	3.01415	-1.60906
H	-4.92445	2.56260	-2.84716
H	-2.40781	2.36030	1.16362
H	-1.38375	1.08839	0.51035
H	-0.26534	2.25113	2.41926
H	-1.58365	1.76728	3.50332
H	-0.52862	0.54036	2.77592
H	4.02662	2.12984	1.09105
H	2.36065	1.69965	1.46474
H	2.67784	4.17714	1.58266
H	3.20417	4.20277	-0.10889
H	1.53944	3.75469	0.29240
H	5.64666	1.44871	-1.09420
H	5.48671	0.11872	-2.22950
H	7.88146	0.42761	-1.53661
H	7.43464	0.18006	0.15873
H	7.28941	-1.15197	-0.99674

L1_55 Ground State

N	-1.36122	-0.03277	-0.81444
C	-0.75030	-1.12350	-0.57456
O	-1.34889	-2.31013	-0.87883
C	-2.60028	-1.94991	-1.51558
C	-2.68756	-0.41030	-1.33886
C	0.58964	-1.22774	0.03905
O	1.16240	-2.46427	-0.01219
C	2.42038	-2.32871	0.69614
C	2.53249	-0.80758	0.98592
N	1.22088	-0.26592	0.58360
C	-3.80473	0.05947	-0.37945
C	-3.92565	1.59410	-0.38223
C	-3.58674	-0.48520	1.04548
C	3.67511	-0.09858	0.22480
C	3.78093	1.37773	0.65204
C	3.51819	-0.24256	-1.30790
C	-4.50224	2.19495	-1.66894
C	-4.64079	3.71749	-1.59031
C	-4.84954	-0.48653	1.91334
C	-4.58699	-1.00837	3.32807
C	4.83260	-0.50803	-2.05789
C	5.89813	0.58337	-1.92146
C	4.33111	1.60209	2.06428
C	4.44914	3.08761	2.41466
H	-3.40359	-2.50017	-1.01907
H	-2.54500	-2.25988	-2.56355

H	-2.82672	0.07699	-2.30886
H	3.21388	-2.71644	0.05203
H	2.36201	-2.93775	1.60324
H	2.66161	-0.63158	2.05859
H	-4.74394	-0.36449	-0.77126
H	-2.93209	2.01709	-0.18765
H	-4.56462	1.90265	0.45513
H	-2.80062	0.10640	1.53160
H	-3.20160	-1.51325	1.00318
H	4.60144	-0.61378	0.52718
H	2.78549	1.83035	0.56346
H	4.42565	1.90802	-0.05841
H	3.03779	0.66127	-1.70349
H	2.83235	-1.06448	-1.54547
H	-3.86632	1.93903	-2.52633
H	-5.48522	1.74547	-1.87054
H	-5.05660	4.13208	-2.51548
H	-5.30112	4.01082	-0.76504
H	-3.66686	4.19092	-1.41834
H	-5.61874	-1.10503	1.42916
H	-5.26722	0.52664	1.97279
H	-5.50166	-1.01250	3.93142
H	-4.19646	-2.03311	3.30423
H	-3.84691	-0.38572	3.84490
H	4.60230	-0.65041	-3.12204
H	5.25157	-1.46301	-1.70833
H	6.78081	0.34461	-2.52545
H	5.51564	1.55449	-2.25811
H	6.23128	0.69908	-0.88417
H	5.31818	1.12441	2.14877
H	3.68845	1.11023	2.80600
H	4.84795	3.23274	3.42491
H	5.11505	3.60555	1.71364
H	3.47073	3.58008	2.36592

L1_56 Ground State

N	-1.56309	-0.00375	-0.67270
C	-0.90363	-1.07543	-0.48035
O	-1.54604	-2.27580	-0.51982
C	-2.92606	-1.96254	-0.83185
C	-2.96683	-0.40867	-0.86791
C	0.54411	-1.14045	-0.19104
O	1.09006	-2.38859	-0.20728
C	2.51065	-2.18183	-0.01112
C	2.63803	-0.66781	0.30966
N	1.28223	-0.13734	0.07100
C	-3.88146	0.25646	0.18539
C	-3.40369	-0.04697	1.61704
C	-5.35936	-0.12121	-0.02496
C	3.69718	0.06942	-0.53059
C	5.10188	-0.53654	-0.32571
C	3.63504	1.58311	-0.26569
C	-4.18370	0.66007	2.73639
C	-4.19173	2.18720	2.61875
C	-5.93059	0.13586	-1.42826
C	-5.83381	1.59708	-1.87698
C	4.60306	2.41666	-1.11094
C	4.40189	3.92084	-0.90977
C	5.71735	-0.34795	1.06634
C	7.09957	-0.99653	1.17809
H	-3.55311	-2.40788	-0.05582
H	-3.16802	-2.42336	-1.79372
H	-3.27588	-0.05888	-1.85824
H	3.01851	-2.46155	-0.94085
H	2.84262	-2.84253	0.79246
H	2.86289	-0.51209	1.37309
H	-3.76990	1.33476	0.02160
H	-2.34890	0.24286	1.68809
H	-3.44225	-1.13106	1.79677
H	-5.96414	0.44221	0.69635
H	-5.50221	-1.18077	0.23277
H	3.42372	-0.09485	-1.58446
H	5.78071	-0.10362	-1.07099
H	5.07101	-1.61168	-0.55391
H	3.82218	1.77867	0.79988
H	2.60827	1.91383	-0.45361
H	-3.72994	0.37650	3.69489
H	-5.21608	0.28926	2.77423
H	-4.66662	2.64728	3.49243
H	-3.17064	2.58027	2.54410
H	-4.73951	2.52405	1.73139
H	-6.98424	-0.17189	-1.42912
H	-5.43388	-0.50824	-2.16632
H	-6.33529	1.74917	-2.83897
H	-6.30623	2.26296	-1.14413
H	-4.79346	1.92035	-1.99220
H	4.46573	2.16619	-2.17258
H	5.64170	2.15668	-0.86780
H	5.10087	4.50549	-1.51845
H	3.38361	4.22105	-1.18373
H	4.55677	4.20095	0.13942
H	5.05591	-0.77215	1.83356
H	5.79900	0.72198	1.29388

H	7.53238	-0.85087	2.17395
H	7.04629	-2.07601	0.99068
H	7.79448	-0.56889	0.44517

L1_57 Ground State

N	-1.71038	-0.69239	-0.96414
C	-1.13985	-1.36671	-0.05033
O	-1.89314	-2.05945	0.84896
C	-3.26687	-1.83680	0.43392
C	-3.15726	-0.76717	-0.68798
C	0.31598	-1.37843	0.19975
O	0.86766	-2.56666	0.56305
C	2.28922	-2.29623	0.69940
C	2.40360	-0.75613	0.53094
N	1.04420	-0.33729	0.14359
C	-3.69101	0.63673	-0.30566
C	-2.86616	1.28757	0.83027
C	-5.19158	0.60294	0.03890
C	3.46204	-0.30439	-0.49109
C	4.86704	-0.62827	0.04889
C	3.26441	1.17052	-0.89168
C	-1.68535	2.13991	0.34090
C	-0.77665	2.60118	1.48113
C	-6.10543	-0.00400	-1.03165
C	-7.58962	0.16045	-0.69438
C	3.37978	2.18927	0.24788
C	3.12885	3.61950	-0.23637
C	6.01509	-0.30512	-0.91242
C	7.37238	-0.77361	-0.38209
H	-3.82719	-1.51128	1.31247
H	-3.67106	-2.78985	0.07963
H	-3.66895	-1.10263	-1.59438
H	2.81124	-2.84807	-0.09025
H	2.60928	-2.66922	1.67414
H	2.62689	-0.28078	1.49479
H	-3.57359	1.25498	-1.20652
H	-3.52856	1.91826	1.43914
H	-2.49333	0.51174	1.51421
H	-5.51001	1.63720	0.22805
H	-5.34560	0.07243	0.99034
H	3.30355	-0.90620	-1.39953
H	4.91554	-1.69901	0.29800
H	5.02765	-0.09467	0.99633
H	2.26993	1.26336	-1.34004
H	3.98749	1.42472	-1.67722
H	-2.08303	3.01166	-0.19865
H	-1.09387	1.56536	-0.37655
H	0.02986	3.24352	1.10915
H	-1.33190	3.16387	2.24288
H	-0.30907	1.73818	1.96927
H	-5.88392	-1.07203	-1.15824
H	-5.89228	0.46851	-2.00081
H	-8.22839	-0.28578	-1.46451
H	-7.83193	-0.32041	0.26125
H	-7.85842	1.22004	-0.60786
H	4.37311	2.13031	0.71331
H	2.65066	1.94816	1.03083
H	3.21455	4.34228	0.58284
H	3.84716	3.90736	-1.01406
H	2.12309	3.71348	-0.66316
H	6.05161	0.77556	-1.09583
H	5.81604	-0.77479	-1.88588
H	8.18165	-0.52633	-1.07795
H	7.60348	-0.30098	0.58038
H	7.38364	-1.85952	-0.22777

L1_58 Ground State

N	-1.25385	-0.49005	-0.24612
C	-0.61076	-0.32172	0.83922
O	-1.24399	-0.50411	2.03127
C	-2.59029	-0.91836	1.68990
C	-2.63756	-0.82367	0.13864
C	0.80704	0.08364	0.92917
O	1.41847	-0.18594	2.11581
C	2.77231	0.31111	1.97139
C	2.84305	0.80469	0.49853
N	1.46856	0.63648	-0.00724
C	-3.63061	0.21556	-0.43176
C	-3.24753	1.64520	-0.00714
C	-5.08713	-0.13111	-0.07625
C	3.85485	0.05898	-0.40073
C	3.49634	-1.43039	-0.54331
C	5.30260	0.26367	0.08555
C	-4.11690	2.76713	-0.59543
C	-4.14340	2.79427	-2.12655
C	-5.55030	-1.53378	-0.48850
C	-7.05178	-1.73873	-0.27181
C	5.75477	1.71973	0.27879
C	5.64671	2.57604	-0.98646
C	4.32067	-2.18823	-1.59032
C	3.81885	-3.61965	-1.79703
H	-3.28512	-0.24764	2.20056
H	-2.73576	-1.93571	2.06437
H	-2.87607	-1.79881	-0.29679

H	3.45498	-0.51060	2.20008
H	2.91857	1.11097	2.70282
H	3.07774	1.87328	0.46522
H	-3.52311	0.14638	-1.52220
H	-2.20634	1.81645	-0.30384
H	-3.27527	1.72195	1.08936
H	-5.74386	0.60133	-0.56169
H	-5.24808	0.00171	1.00436
H	3.75271	0.51195	-1.39575
H	2.43735	-1.50111	-0.81757
H	3.60174	-1.93752	0.42758
H	5.97793	-0.20993	-0.63723
H	5.44583	-0.28359	1.02878
H	-3.72639	3.72450	-0.22672
H	-5.14268	2.69603	-0.21128
H	-4.68938	3.66947	-2.49599
H	-3.12667	2.83387	-2.53561
H	-4.63025	1.90421	-2.54092
H	-5.00055	-2.29793	0.07636
H	-5.30411	-1.70034	-1.54657
H	-7.36556	-2.74732	-0.56259
H	-7.32088	-1.59547	0.78188
H	-7.63605	-1.02228	-0.86170
H	6.79859	1.70965	0.61830
H	5.18484	2.19137	1.09066
H	6.06284	3.57614	-0.82306
H	6.19547	2.11635	-1.81764
H	4.60665	2.69948	-1.30784
H	5.37784	-2.21635	-1.29792
H	4.27895	-1.64277	-2.54359
H	4.41615	-4.15029	-2.54698
H	3.86876	-4.19303	-0.86316
H	2.77496	-3.62530	-2.13241

L1_59 Ground State

N	1.17951	-0.40993	0.48783
C	0.54564	-1.07541	-0.39281
O	1.16368	-2.11136	-1.02751
C	2.46944	-2.21088	-0.40499
C	2.54645	-0.96500	0.51755
C	-0.84618	-0.81284	-0.81152
O	-1.46386	-1.83792	-1.46641
C	-2.78518	-1.33640	-1.79474
C	-2.85529	0.04577	-1.08870
N	-1.48699	0.26239	-0.58301
C	3.57698	0.09576	0.06859
C	3.71049	1.21753	1.11359
C	3.22210	0.66558	-1.31991
C	-3.89532	0.18867	0.05199
C	-4.14568	1.68145	0.34956
C	-3.50006	-0.53912	1.35177
C	4.40056	0.80613	2.41881
C	4.54872	1.97645	3.39445
C	4.38348	1.35451	-2.05197
C	5.49522	0.39599	-2.49054
C	-3.39836	-2.06895	1.30119
C	-3.13360	-2.66596	2.68635
C	-4.94755	2.43165	-0.71992
C	-5.17923	3.89988	-0.35311
H	3.22236	-2.22297	-1.19715
H	2.50771	-3.15637	0.14446
H	2.77399	-1.26553	1.54493
H	-3.52113	-2.05978	-1.44013
H	-2.84893	-1.25988	-2.88429
H	-3.06467	0.82140	-1.83178
H	4.54050	-0.43206	0.00278
H	2.70812	1.60796	1.33017
H	4.27864	2.04754	0.67385
H	2.39187	1.37089	-1.19640
H	2.84059	-0.13407	-1.96963
H	-4.83544	-0.24901	-0.32111
H	-3.17630	2.17405	0.50269
H	-4.68634	1.76341	1.30209
H	-4.24981	-0.27753	2.11133
H	-2.54717	-0.12582	1.70470
H	3.83692	0.00221	2.90981
H	5.39217	0.39004	2.18944
H	5.04574	1.66763	4.32089
H	5.14009	2.78669	2.95070
H	3.56903	2.39042	3.66106
H	4.80979	2.14672	-1.42298
H	3.97989	1.86024	-2.93858
H	6.26953	0.92162	-3.06030
H	5.98620	-0.08055	-1.63451
H	5.09482	-0.40164	-3.12910
H	-2.59726	-2.38381	0.62509
H	-4.33238	-2.48543	0.89632
H	-3.06157	-3.75855	2.64514
H	-2.19358	-2.28345	3.10186
H	-3.93526	-2.40792	3.38912
H	-5.91547	1.93023	-0.86265
H	-4.43390	2.38407	-1.68922
H	-5.76051	4.41977	-1.12285

H	-5.72387	3.98782	0.59479
H	-4.22640	4.42989	-0.23673

L1_60 Ground State

N	1.14794	-0.38953	0.36253
C	0.49693	-1.19449	-0.37766
O	1.05390	-2.38854	-0.72177
C	2.39470	-2.35275	-0.17242
C	2.43581	-1.04238	0.66119
C	-0.85913	-0.94697	-0.91037
O	-1.44652	-2.00939	-1.53073
C	-2.72038	-1.51085	-2.01001
C	-2.82460	-0.08616	-1.40248
N	-1.49282	0.15290	-0.81472
C	3.62866	-0.12455	0.33598
C	4.94479	-0.85461	0.66688
C	3.50152	1.23069	1.07084
C	-3.92714	0.07095	-0.33049
C	-4.07123	1.54135	0.10175
C	-3.66853	-0.84850	0.87863
C	6.23175	-0.11933	0.26685
C	6.40658	0.04295	-1.24596
C	3.82643	2.44951	0.19904
C	3.69219	3.76824	0.96308
C	-4.91064	-1.12113	1.73350
C	-4.60733	-2.01620	2.93746
C	-4.68729	2.46776	-0.95246
C	-4.84566	3.90363	-0.44578
H	3.09774	-2.34055	-1.01272
H	2.54634	-3.26363	0.41029
H	2.45401	-1.26144	1.73866
H	-3.50155	-2.19616	-1.67113
H	-2.69064	-1.51082	-3.10382
H	-2.99149	0.65316	-2.19198
H	3.58299	0.05887	-0.74717
H	4.95474	-1.84207	0.18284
H	4.96311	-1.04579	1.74960
H	4.15186	1.23049	1.95754
H	2.47514	1.34379	1.43440
H	-4.86840	-0.24494	-0.80963
H	-3.07979	1.91339	0.38917
H	-4.69464	1.58813	1.00389
H	-2.88040	-0.40157	1.49781
H	-3.26890	-1.81458	0.54096
H	7.08633	-0.68091	0.66623
H	6.26420	0.86380	0.75260
H	7.36473	0.51817	-1.48343
H	6.38348	-0.93163	-1.74951
H	5.61504	0.65990	-1.68406
H	3.14576	2.45252	-0.66296
H	4.84104	2.36606	-0.21061
H	3.90975	4.62909	0.32085
H	2.67603	3.89097	1.35640
H	4.38326	3.80321	1.81449
H	-5.68180	-1.59329	1.10821
H	-5.34159	-0.17497	2.08503
H	-5.50742	-2.20981	3.53162
H	-4.20240	-2.98398	2.61716
H	-3.86457	-1.54997	3.59585
H	-5.66831	2.07296	-1.25354
H	-4.06874	2.47634	-1.85931
H	-5.28970	4.55290	-1.20866
H	-5.48987	3.93954	0.44126
H	-3.87470	4.32956	-0.16636

L1_61 Ground State

N	1.15770	-0.10887	-0.06660
C	0.43548	-0.88123	-0.77480
O	0.98659	-2.00169	-1.31980
C	2.39681	-1.92422	-0.99655
C	2.50422	-0.71096	-0.03335
C	-0.99894	-0.67307	-1.06289
O	-1.62980	-1.71685	-1.67241
C	-2.98713	-1.26012	-1.89565
C	-3.05503	0.10773	-1.16494
N	-1.65852	0.37637	-0.77354
C	3.59533	0.30596	-0.41627
C	4.99191	-0.35030	-0.44980
C	3.51862	1.54409	0.49282
C	-3.97898	0.12488	0.07487
C	-4.14502	1.56247	0.62269
C	-3.47691	-0.84667	1.15869
C	5.54911	-0.81213	0.90243
C	6.92703	-1.46495	0.76520
C	4.51683	2.65215	0.14335
C	4.30468	3.91174	0.98712
C	-4.54444	-1.21208	2.19457
C	-4.00760	-2.13182	3.29377
C	-5.41457	2.29013	0.15703
C	-5.51559	2.51778	-1.35435
H	2.94427	-1.77063	-1.93316
H	2.69770	-2.87729	-0.55658
H	2.68244	-1.04580	0.99712
H	-3.66854	-2.01295	-1.49087

H	-3.14082	-1.17901	-2.97596
H	-3.37557	0.89650	-1.85162
H	3.36584	0.63248	-1.44249
H	5.69979	0.35837	-0.89735
H	4.97327	-1.21029	-1.13459
H	3.66348	1.24171	1.53987
H	2.49912	1.93938	0.43479
H	-4.96167	-0.23527	-0.27064
H	-3.25524	2.14574	0.35537
H	-4.15997	1.53014	1.71846
H	-2.60831	-0.39801	1.65698
H	-3.11146	-1.77531	0.69865
H	4.85763	-1.52308	1.37414
H	5.61890	0.04261	1.58635
H	7.31820	-1.78572	1.73698
H	6.88388	-2.34655	0.11393
H	7.65048	-0.76676	0.32695
H	4.42131	2.90342	-0.92266
H	5.54583	2.29512	0.28184
H	5.02552	4.69561	0.72864
H	3.29718	4.31827	0.83957
H	4.41798	3.69224	2.05586
H	-5.38814	-1.69892	1.68483
H	-4.95156	-0.29981	2.65036
H	-4.78802	-2.39176	4.01770
H	-3.61815	-3.06596	2.87088
H	-3.18813	-1.65136	3.84160
H	-5.46512	3.26179	0.66592
H	-6.29365	1.72299	0.49538
H	-6.41089	3.09762	-1.60547
H	-4.64454	3.06811	-1.73059
H	-5.57644	1.57199	-1.90521

L1_62 Ground State

N	-1.37298	-0.23559	-0.81870
C	-0.70740	-1.06939	-0.12450
O	-1.34095	-2.13921	0.43076
C	-2.72381	-2.02629	0.01181
C	-2.77346	-0.69423	-0.78965
C	0.73900	-0.97006	0.16158
O	1.31687	-2.09330	0.66547
C	2.71960	-1.76266	0.82534
C	2.82215	-0.27099	0.38868
N	1.44661	0.07103	-0.02298
C	-3.69883	0.39590	-0.20137
C	-3.22458	0.84837	1.19052
C	-5.17274	-0.04887	-0.20327
C	3.84556	0.00545	-0.73761
C	5.28896	0.06595	-0.20336
C	3.49319	1.27700	-1.53731
C	-3.95107	2.07862	1.74616
C	-3.33448	2.57152	3.05783
C	-5.73255	-0.47538	-1.56597
C	-7.24144	-0.73007	-1.52149
C	3.42805	2.57840	-0.72942
C	3.07151	3.77858	-1.61035
C	5.83964	-1.21550	0.43323
C	7.32006	-1.08834	0.80292
H	-3.34522	-2.02941	0.91052
H	-2.96638	-2.90458	-0.59288
H	-3.08048	-0.88099	-1.82340
H	3.29235	-2.43863	0.18511
H	2.98846	-1.94053	1.86934
H	3.07359	0.36660	1.24621
H	-3.60335	1.25768	-0.87740
H	-3.32474	0.02117	1.90921
H	-2.15426	1.07649	1.12729
H	-5.78393	0.78048	0.17273
H	-5.31250	-0.86809	0.51843
H	3.78053	-0.83854	-1.44195
H	5.37096	0.88314	0.52636
H	5.94409	0.34411	-1.04066
H	2.52194	1.12369	-2.01868
H	4.23541	1.38796	-2.34091
H	-3.91713	2.88373	0.99877
H	-5.01277	1.85507	1.90974
H	-3.86237	3.45052	3.44435
H	-3.37378	1.79216	3.82879
H	-2.28190	2.84526	2.91853
H	-5.22769	-1.38451	-1.91782
H	-5.51157	0.30362	-2.30894
H	-7.62484	-1.04246	-2.49907
H	-7.48683	-1.51780	-0.79867
H	-7.78467	0.17398	-1.22120
H	4.38782	2.76792	-0.23085
H	2.67305	2.47456	0.05832
H	3.02359	4.70498	-1.02677
H	3.81415	3.92179	-2.40529
H	2.09602	3.63321	-2.08919
H	5.70669	-2.05762	-0.26021
H	5.27020	-1.46624	1.33757
H	7.69952	-2.00705	1.26365
H	7.93017	-0.88062	-0.08424

H	7.47893	-0.26730	1.51250

L1_63 Ground State

N	1.16730	-0.48244	0.57056
C	0.69680	-0.40868	-0.60937
O	1.49409	-0.72269	-1.67097
C	2.74612	-1.16324	-1.08658
C	2.58510	-0.86179	0.43043
C	-0.67110	0.03031	-0.95127
O	-1.08763	-0.27659	-2.21253
C	-2.40784	0.31157	-2.32752
C	-2.73145	0.80263	-0.89120
N	-1.45707	0.64818	-0.16331
C	3.50105	0.23327	1.03445
C	3.11826	1.67361	0.63510
C	4.99235	-0.06659	0.80266
C	-3.85809	0.01394	-0.18545
C	-4.21886	0.65611	1.16629
C	-3.48463	-1.47202	-0.02032
C	3.28110	2.07945	-0.83668
C	2.93481	3.55527	-1.05448
C	5.47817	-1.41177	1.35579
C	6.99373	-1.58428	1.22753
C	-4.68471	-2.39593	0.21228
C	-4.27065	-3.85830	0.39332
C	-4.94033	2.00497	1.07014
C	-5.31900	2.56247	2.44468
H	3.55377	-0.61955	-1.57725
H	2.85331	-2.23207	-1.29503
H	2.74588	-1.77762	1.00766
H	-3.08998	-0.45754	-2.69844
H	-2.35008	1.12519	-3.05700
H	-2.99646	1.86428	-0.90251
H	3.32514	0.17316	2.11780
H	3.72822	2.35281	1.24801
H	2.07700	1.84253	0.93229
H	5.57367	0.73882	1.27306
H	5.23319	-0.01496	-0.26775
H	-4.73773	0.07762	-0.84691
H	-3.29658	0.76930	1.74980
H	-4.86003	-0.03482	1.72854
H	-2.77474	-1.56597	0.81124
H	-2.94839	-1.82876	-0.91035
H	4.31191	1.89795	-1.16893
H	2.63345	1.46887	-1.47495
H	3.04514	3.84264	-2.10611
H	1.89946	3.76078	-0.75706
H	3.58547	4.20650	-0.45801
H	4.97874	-2.23805	0.83235
H	5.18428	-1.49788	2.41122
H	7.32262	-2.55236	1.62112
H	7.30960	-1.52475	0.17879
H	7.52696	-0.79966	1.77759
H	-5.37517	-2.31104	-0.63903
H	-5.24829	-2.06731	1.09479
H	-5.14052	-4.50632	0.54849
H	-3.73067	-4.22714	-0.48734
H	-3.60730	-3.97403	1.25880
H	-5.84583	1.88940	0.45723
H	-4.30940	2.73755	0.55032
H	-5.83565	3.52509	2.36016
H	-5.98177	1.87216	2.98072
H	-4.42763	2.71330	3.06513

L1_64 Ground State

N	1.25912	-0.07198	-0.05240
C	0.52223	-0.98951	-0.53678
O	1.06238	-2.20973	-0.81057
C	2.48009	-2.06222	-0.54890
C	2.60889	-0.65172	0.08802
C	-0.91989	-0.85245	-0.82359
O	-1.60026	-2.02548	-0.96350
C	-2.97691	-1.64266	-1.21793
C	-2.96336	-0.09018	-1.13655
N	-1.54829	0.25042	-0.89917
C	3.68367	0.24005	-0.56094
C	5.08206	-0.40759	-0.47553
C	3.62672	1.66126	0.02392
C	-3.90687	0.55162	-0.09338
C	-3.88503	-0.07596	1.31521
C	-5.33958	0.57447	-0.66397
C	5.67943	-0.53171	0.93162
C	7.05638	-1.20064	0.91608
C	4.61003	2.64979	-0.61028
C	4.41424	4.07661	-0.09126
C	-6.36797	1.34069	0.17508
C	-7.72215	1.45951	-0.52908
C	-2.51704	-0.28251	1.98060
C	-2.65520	-0.58681	3.47472
H	3.00467	-2.14372	-1.50729
H	2.79250	-2.88108	0.10254
H	2.81753	-0.72707	1.16331
H	-3.60209	-2.12238	-0.46132
H	-3.25315	-2.02267	-2.20484

H	-3.23465	0.33845	-2.10951
H	3.42316	0.30942	-1.62849
H	5.77337	0.17158	-1.10027
H	5.04871	-1.40695	-0.93272
H	3.80149	1.62046	1.10858
H	2.60431	2.03325	-0.09976
H	-3.56073	1.59039	-0.00082
H	-4.48106	0.57641	1.96564
H	-4.42429	-1.03549	1.29992
H	-5.69243	-0.45948	-0.80499
H	-5.30852	1.02275	-1.66743
H	5.76396	0.46224	1.38791
H	5.00521	-1.10733	1.57986
H	7.47631	-1.27913	1.92493
H	6.99966	-2.21284	0.49718
H	7.76359	-0.62939	0.30252
H	4.48497	2.63559	-1.70242
H	5.64404	2.33510	-0.41717
H	5.12426	4.77328	-0.55103
H	3.40126	4.43699	-0.30593
H	4.55673	4.12228	0.99541
H	-5.97658	2.34398	0.39485
H	-6.50826	0.84636	1.14365
H	-8.44701	2.00390	0.08620
H	-7.62634	1.99120	-1.48352
H	-8.14302	0.46943	-0.74336
H	-1.89138	0.60526	1.83374
H	-1.98718	-1.11123	1.49971
H	-1.67786	-0.76211	3.93786
H	-3.13315	0.24572	4.00572
H	-3.26924	-1.48073	3.64257

L1_65 Ground State

N	1.33349	-0.16113	0.03526
C	0.58882	-1.15836	-0.23077
O	1.10384	-2.41769	-0.15806
C	2.51461	-2.23275	0.11474
C	2.65651	-0.71096	0.38747
C	-0.83541	-1.07555	-0.61799
O	-1.46615	-2.27032	-0.78323
C	-2.83306	-1.93755	-1.13120
C	-2.86219	-0.38094	-1.13962
N	-1.48150	0.00594	-0.79894
C	3.78831	-0.02932	-0.40325
C	5.15947	-0.66366	-0.08760
C	3.75066	1.49326	-0.18992
C	-3.88118	0.22890	-0.15620
C	-5.32283	-0.18348	-0.54700
C	-3.69873	1.75409	-0.08246
C	5.68699	-0.44776	1.33630
C	7.04074	-1.12723	1.55852
C	4.79219	2.27439	-0.99701
C	4.62014	3.78889	-0.85475
C	-4.57939	2.46871	0.94715
C	-4.26760	3.96521	1.03391
C	-6.23870	-0.54731	0.63358
C	-5.87286	-1.87305	1.30773
H	3.07000	-2.55681	-0.77255
H	2.78396	-2.86971	0.95977
H	2.81107	-0.51942	1.45769
H	-3.48641	-2.37785	-0.37286
H	-3.05202	-2.39065	-2.10135
H	-3.08371	0.00288	-2.14466
H	3.57967	-0.22116	-1.46722
H	5.89733	-0.27116	-0.79834
H	5.11468	-1.74420	-0.28589
H	3.87575	1.71848	0.87887
H	2.74708	1.84340	-0.45311
H	-3.64375	-0.18835	0.83362
H	-5.30128	-1.04485	-1.22998
H	-5.77590	0.63378	-1.12355
H	-3.89445	2.17910	-1.07918
H	-2.64591	1.96225	0.13525
H	5.78264	0.62627	1.53771
H	4.96523	-0.83142	2.06975
H	7.41089	-0.96203	2.57634
H	6.97058	-2.21026	1.39926
H	7.79367	-0.73989	0.86140
H	4.71478	1.99362	-2.05712
H	5.80604	1.99593	-0.68069
H	5.37175	4.33577	-1.43517
H	3.62972	4.10602	-1.20196
H	4.71642	4.09836	0.19319
H	-4.43428	2.00627	1.93381
H	-5.64013	2.33606	0.69851
H	-4.90224	4.46618	1.77361
H	-3.22197	4.13249	1.31814
H	-4.42875	4.45683	0.06672
H	-7.27309	-0.60743	0.27052
H	-6.22160	0.25682	1.37809
H	-6.55809	-2.10050	2.13173
H	-5.92373	-2.70458	0.59354
H	-4.85835	-1.85300	1.72231

L1_66 Ground State

N	-1.50972	0.39800	-0.48703
C	-0.88941	-0.66949	-0.79772
O	-1.53474	-1.64094	-1.50076
C	-2.86536	-1.11997	-1.74367
C	-2.88192	0.24701	-1.00327
C	0.51299	-0.96990	-0.44112
O	1.00836	-2.13596	-0.94096
C	2.40339	-2.15315	-0.54736
C	2.55558	-0.92235	0.38738
N	1.25556	-0.23408	0.28484
C	-3.91846	0.36818	0.13668
C	-3.64108	-0.63953	1.26531
C	-5.36003	0.26065	-0.39698
C	3.72530	0.00923	0.02144
C	5.05542	-0.75810	0.13079
C	3.70417	1.29261	0.88403
C	-4.48929	-0.43603	2.52596
C	-4.06352	-1.36384	3.66680
C	-5.73486	1.21964	-1.53802
C	-5.56114	2.70015	-1.18646
C	3.95891	2.57715	0.08637
C	3.97932	3.82451	0.97185
C	6.29428	0.02552	-0.31429
C	7.57292	-0.81301	-0.24115
H	-3.58360	-1.84616	-1.35570
H	-2.99970	-1.02818	-2.82507
H	-3.05744	1.06247	-1.71225
H	3.00649	-2.06807	-1.45827
H	2.60830	-3.11280	-0.06866
H	2.68195	-1.23608	1.43375
H	-3.77548	1.37179	0.55853
H	-2.58335	-0.55791	1.54167
H	-3.78904	-1.66642	0.89883
H	-6.04959	0.43780	0.43721
H	-5.54652	-0.77328	-0.72241
H	3.57568	0.29433	-1.03137
H	5.00279	-1.68041	-0.46592
H	5.18976	-1.08006	1.17473
H	4.44681	1.20605	1.69042
H	2.72587	1.38426	1.36660
H	-5.55069	-0.60302	2.30396
H	-4.40340	0.61026	2.85132
H	-4.67682	-1.20793	4.56139
H	-4.15979	-2.41682	3.37481
H	-3.01628	-1.19226	3.94282
H	-6.78271	1.03437	-1.80755
H	-5.15254	0.98608	-2.43952
H	-5.92515	3.34316	-1.99524
H	-6.12115	2.95456	-0.27819
H	-4.51112	2.95666	-1.00785
H	3.17072	2.67593	-0.67204
H	4.90572	2.50037	-0.46347
H	4.13861	4.73416	0.38188
H	3.03185	3.93689	1.51236
H	4.78117	3.76553	1.71842
H	6.41127	0.92021	0.30900
H	6.14588	0.38412	-1.34215
H	8.44831	-0.23730	-0.56140
H	7.75787	-1.16078	0.78252
H	7.50223	-1.69946	-0.88334

L1_67 Ground State

N	1.26510	-0.25674	0.29667
C	0.58683	-1.23973	-0.14310
O	1.15043	-2.47829	-0.18735
C	2.51180	-2.29611	0.27575
C	2.59342	-0.78868	0.64952
C	-0.80925	-1.15828	-0.62087
O	-1.43251	-2.35536	-0.81339
C	-2.74552	-2.02004	-1.32815
C	-2.81570	-0.47366	-1.21273
N	-1.44453	-0.07724	-0.84005
C	3.72709	-0.03377	-0.07171
C	5.08765	-0.55159	0.43452
C	3.56448	1.49345	0.03939
C	-3.83546	0.03974	-0.17106
C	-3.96582	1.57200	-0.22980
C	-3.46877	-0.43455	1.24992
C	6.32138	0.09157	-0.21474
C	6.38809	-0.08785	-1.73409
C	3.64016	2.06861	1.45811
C	3.47964	3.59096	1.46734
C	-4.62455	-0.39649	2.26090
C	-5.72784	-1.42125	1.97859
C	-4.67261	2.11266	-1.47763
C	-4.81320	3.63683	-1.45443
H	3.18235	-2.56894	-0.54592
H	2.67674	-2.97563	1.11511
H	2.72395	-0.66411	1.73207
H	-3.49047	-2.54359	-0.72340
H	-2.80263	-2.37781	-2.36063
H	-3.05081	-0.02950	-2.18500

H	3.63487	-0.28839	-1.13766
H	5.13956	-1.63803	0.27064
H	5.14234	-0.40938	1.52219
H	2.59530	1.76040	-0.39446
H	4.33028	1.97546	-0.58268
H	-4.80284	-0.40081	-0.45640
H	-2.96097	2.00633	-0.15399
H	-4.52028	1.91610	0.65303
H	-2.63936	0.18450	1.61172
H	-3.08212	-1.46244	1.21736
H	7.21761	-0.34997	0.24014
H	6.35461	1.16048	0.03038
H	7.32419	0.31324	-2.13779
H	6.33374	-1.14903	-2.00798
H	5.56374	0.42668	-2.23975
H	4.59704	1.80241	1.92687
H	2.85293	1.62093	2.07733
H	3.52919	3.99490	2.48482
H	4.26764	4.07430	0.87642
H	2.51526	3.88418	1.03609
H	-5.06042	0.61034	2.29832
H	-4.21387	-0.58302	3.26154
H	-6.49905	-1.39765	2.75652
H	-6.22482	-1.23412	1.01999
H	-5.31769	-2.43858	1.94612
H	-5.66777	1.65210	-1.55890
H	-4.12423	1.81906	-2.38215
H	-5.32278	4.00775	-2.35078
H	-5.38919	3.96598	-0.58091
H	-3.83024	4.11994	-1.40304

L1_68 Ground State

N	-1.23275	-0.41527	-0.94905
C	-0.61311	-1.28136	-0.25185
O	-1.16509	-2.51411	-0.06457
C	-2.39060	-2.50187	-0.83924
C	-2.51318	-1.03653	-1.33736
C	0.69164	-1.06407	0.40640
O	1.31600	-2.19036	0.85424
C	2.52389	-1.72041	1.50365
C	2.56384	-0.20293	1.17967
N	1.25198	0.06825	0.56158
C	-3.70541	-0.25787	-0.73903
C	-3.79795	1.12460	-1.40762
C	-3.62622	-0.18368	0.80405
C	3.71153	0.21440	0.23236
C	3.78484	1.74487	0.08918
C	3.57564	-0.46894	-1.14353
C	-4.98718	1.98830	-0.97754
C	-5.05390	3.30767	-1.75147
C	-4.97200	-0.38243	1.51181
C	-4.86138	-0.24627	3.03170
C	4.86545	-0.50514	-1.97687
C	5.95357	-1.41327	-1.39520
C	4.27640	2.48750	1.33652
C	4.37413	3.99906	1.11507
H	-3.20742	-2.81491	-0.18363
H	-2.28174	-3.22647	-1.65170
H	-2.59496	-1.00323	-2.43019
H	3.36819	-2.28272	1.09659
H	2.43287	-1.92992	2.57377
H	2.63761	0.38156	2.10201
H	-4.60617	-0.83131	-1.01161
H	-3.84558	0.98213	-2.49746
H	-2.86247	1.66350	-1.21219
H	-3.18905	0.77952	1.09684
H	-2.93225	-0.94220	1.18833
H	4.63831	-0.13268	0.71393
H	2.79064	2.11237	-0.19469
H	4.45677	1.99261	-0.74286
H	2.78724	0.04755	-1.70361
H	3.22513	-1.50271	-1.01872
H	-4.92196	2.20476	0.09611
H	-5.92213	1.42862	-1.12300
H	-5.90336	3.92020	-1.42908
H	-4.14037	3.89585	-1.60287
H	-5.15909	3.12861	-2.82844
H	-5.36280	-1.37855	1.25854
H	-5.70819	0.33509	1.13082
H	-5.82692	-0.41243	3.52239
H	-4.14744	-0.97120	3.44159
H	-4.51121	0.75473	3.31143
H	5.26351	0.51031	-2.10104
H	4.61357	-0.85403	-2.98660
H	6.82879	-1.45428	-2.05307
H	6.29755	-1.06393	-0.41512
H	5.58207	-2.43825	-1.26996
H	5.26052	2.09368	1.62890
H	3.60502	2.29406	2.18321
H	4.72931	4.51544	2.01391
H	5.06722	4.23337	0.29784
H	3.39691	4.41995	0.85023

L1_69 Ground State

N	1.20504	-0.13829	-0.06744
C	0.49494	-1.10926	-0.48293
O	1.03676	-2.35789	-0.54445
C	2.43119	-2.18167	-0.19253
C	2.52767	-0.70107	0.26507
C	-0.91572	-1.00586	-0.91127
O	-1.54242	-2.19314	-1.14907
C	-2.87278	-1.83513	-1.60171
C	-2.93887	-0.29572	-1.41269
N	-1.55935	0.08318	-1.05280
C	3.67013	0.09213	-0.39563
C	5.04433	-0.54538	-0.10010
C	3.58490	1.57854	-0.01005
C	-3.93678	0.17580	-0.33185
C	-4.00823	1.71283	-0.34181
C	-3.59210	-0.40215	1.06235
C	5.51253	-0.48441	1.35911
C	6.87459	-1.15505	1.55589
C	4.63767	2.46978	-0.67614
C	4.42100	3.95350	-0.36763
C	-4.80556	-0.86019	1.88817
C	-5.45962	-2.13761	1.35227
C	-5.03442	2.33153	0.61183
C	-5.10531	3.85498	0.47653
H	3.02833	-2.38724	-1.08798
H	2.68130	-2.91031	0.58137
H	2.64041	-0.63663	1.35545
H	-3.59509	-2.38686	-0.99545
H	-2.96607	-2.14470	-2.64698
H	-3.19744	0.19955	-2.35608
H	3.50680	0.02098	-1.48220
H	5.79796	-0.05785	-0.73095
H	5.03454	-1.59646	-0.42273
H	3.66070	1.68093	1.08196
H	2.58408	1.93582	-0.27407
H	-4.91965	-0.21053	-0.64292
H	-4.23908	2.04420	-1.36516
H	-3.00944	2.10541	-0.11354
H	-3.02310	0.34965	1.62179
H	-2.91550	-1.26058	0.96242
H	4.77438	-0.96624	2.01414
H	5.57204	0.56092	1.68613
H	7.20202	-1.10074	2.59997
H	6.83918	-2.21364	1.27061
H	7.64247	-0.67308	0.93864
H	4.61039	2.31268	-1.76389
H	5.64479	2.17780	-0.35063
H	4.46701	4.14084	0.71220
H	5.18102	4.57983	-0.84820
H	3.43750	4.28806	-0.71817
H	-5.55318	-0.05977	1.93505
H	-4.48056	-1.03665	2.92183
H	-6.30982	-2.44049	1.97348
H	-5.83349	-2.00569	0.32982
H	-4.74306	-2.96845	1.33898
H	-4.78377	2.07433	1.64843
H	-6.02625	1.89841	0.41815
H	-5.39303	4.14796	-0.54050
H	-4.13162	4.31281	0.68832
H	-5.83662	4.28646	1.16917

L1_70 Ground State

N	-1.60508	-0.99995	-1.14348
C	-1.01463	-1.62894	-0.20985
O	-1.73963	-2.39079	0.65616
C	-3.10929	-2.28889	0.18312
C	-3.04969	-1.19509	-0.91899
C	0.42535	-1.51526	0.10018
O	1.06624	-2.65538	0.47078
C	2.45097	-2.26134	0.67085
C	2.43316	-0.71453	0.52729
N	1.05846	-0.41235	0.08864
C	-3.70822	0.15311	-0.53812
C	-2.99778	0.83476	0.65551
C	-5.21841	-0.03741	-0.30552
C	3.48700	-0.15337	-0.44402
C	4.89284	-0.36213	0.14793
C	3.17559	1.30536	-0.83115
C	-1.88531	1.81044	0.24366
C	-1.06282	2.30768	1.43291
C	-6.02174	1.26518	-0.38918
C	-7.51310	1.06012	-0.11367
C	3.16260	2.31106	0.32567
C	2.80200	3.72149	-0.14731
C	6.04441	0.08171	-0.75950
C	7.41622	-0.27282	-0.18035
H	-3.73565	-2.03099	1.03910
H	-3.40589	-3.26912	-0.20175
H	-3.51282	-1.55268	-1.84522
H	3.05248	-2.75117	-0.10296
H	2.76286	-2.62039	1.65343
H	2.57353	-0.23715	1.50565
H	-3.58785	0.79948	-1.41858

H	-3.73485	1.37562	1.26318
H	-2.57703	0.06964	1.32311
H	-5.38854	-0.50122	0.67723
H	-5.61948	-0.74213	-1.04920
H	3.41808	-0.75041	-1.36670
H	5.02733	-1.42919	0.38064
H	4.96744	0.16395	1.11017
H	2.19299	1.31917	-1.31376
H	3.90063	1.63434	-1.58654
H	-2.34307	2.66207	-0.28009
H	-1.21863	1.31955	-0.47057
H	-0.30565	3.03354	1.11466
H	-1.69342	2.78892	2.19183
H	-0.53609	1.47208	1.90824
H	-5.88619	1.70253	-1.38780
H	-5.61687	1.99756	0.32105
H	-8.06812	2.00154	-0.19157
H	-7.95334	0.35246	-0.82681
H	-7.67636	0.65834	0.89380
H	4.14144	2.33188	0.82396
H	2.43247	1.99384	1.08010
H	2.79713	4.43552	0.68396
H	3.51672	4.08399	-0.89656
H	1.80614	3.73367	-0.60629
H	5.98994	1.16466	-0.92417
H	5.92799	-0.38494	-1.74769
H	8.22700	0.05962	-0.83791
H	7.56456	0.20019	0.79810
H	7.51977	-1.35605	-0.04248

L1_71 Ground State

N	1.22248	-0.16067	0.01296
C	0.49750	-1.01732	-0.58725
O	1.04511	-2.20044	-0.98228
C	2.45547	-2.08710	-0.66985
C	2.56877	-0.75440	0.11968
C	-0.93673	-0.84403	-0.89821
O	-1.57950	-1.96349	-1.33671
C	-2.92838	-1.52976	-1.64057
C	-2.98844	-0.07555	-1.10176
N	-1.58687	0.24305	-0.76999
C	3.65776	0.20006	-0.40467
C	5.05492	-0.45375	-0.35052
C	3.58269	1.55292	0.32285
C	-3.90229	0.11860	0.12946
C	-3.98764	1.59995	0.54126
C	-3.44319	-0.75875	1.31028
C	5.61816	-0.71791	1.05137
C	6.99702	-1.38126	1.00289
C	4.58115	2.60069	-0.17873
C	4.36982	3.96600	0.48067
C	-4.39440	-0.79390	2.51649
C	-5.80584	-1.28838	2.18634
C	-4.46390	2.57866	-0.54283
C	-5.83822	2.24145	-1.12943
H	3.00467	-2.06600	-1.61762
H	2.75044	-2.97291	-0.10338
H	2.75348	-0.94648	1.18482
H	-3.62450	-2.21676	-1.15335
H	-3.06332	-1.58940	-2.72500
H	-3.31984	0.60389	-1.89247
H	3.42496	0.38012	-1.46571
H	5.76010	0.18461	-0.89721
H	5.03453	-1.40242	-0.90596
H	3.72821	1.39953	1.40173
H	2.56338	1.93697	0.21121
H	-4.89958	-0.21765	-0.18707
H	-2.99859	1.91329	0.89607
H	-4.67095	1.68165	1.39617
H	-2.45804	-0.40646	1.63855
H	-3.29806	-1.79156	0.96469
H	4.93000	-1.35569	1.62210
H	5.68852	0.22555	1.60644
H	7.39243	-1.56003	2.00885
H	6.95354	-2.34652	0.48365
H	7.71731	-0.75117	0.46707
H	4.48518	2.70041	-1.26937
H	5.61010	2.26615	0.00790
H	5.09077	4.70575	0.11478
H	3.36237	4.34826	0.27819
H	4.48361	3.89806	1.56955
H	-4.45382	0.19882	2.97927
H	-3.95209	-1.45115	3.27633
H	-6.40945	-1.39548	3.09441
H	-6.33413	-0.59604	1.52118
H	-5.77462	-2.26631	1.68917
H	-3.72147	2.64052	-1.34826
H	-4.50084	3.58189	-0.09901
H	-6.17672	3.02120	-1.82068
H	-5.82557	1.29576	-1.68373
H	-6.59149	2.14697	-0.33702

L1_72 Ground State

N	-1.36103	0.35021	-0.59538

C	-0.75575	-0.73460	-0.87289
O	-1.31789	-1.61231	-1.75186
C	-2.52701	-0.96070	-2.21539
C	-2.64432	0.30314	-1.32201
C	0.53890	-1.15429	-0.29792
O	1.15076	-2.19514	-0.93168
C	2.35255	-2.45279	-0.16269
C	2.39492	-1.30110	0.87778
N	1.09921	-0.61608	0.71028
C	-3.82877	0.27526	-0.32907
C	-3.96702	1.62244	0.40280
C	-3.69958	-0.89489	0.66521
C	3.56882	-0.31437	0.68919
C	3.57060	0.69405	1.85355
C	3.52487	0.36424	-0.70056
C	-4.46423	2.78263	-0.46658
C	-4.62528	4.08022	0.32956
C	-5.01634	-1.28654	1.34390
C	-4.84173	-2.43452	2.34110
C	4.89058	0.51934	-1.38064
C	4.78744	1.19227	-2.75101
C	4.74593	1.67943	1.89609
C	6.10705	1.01796	2.13276
H	-3.35585	-1.66387	-2.10080
H	-2.39654	-0.72662	-3.27633
H	-2.72355	1.20160	-1.94179
H	3.20051	-2.45581	-0.85263
H	2.25421	-3.44269	0.29274
H	2.44380	-1.70112	1.89736
H	-4.73468	0.11419	-0.93632
H	-2.99348	1.87688	0.84030
H	-4.66348	1.50194	1.24246
H	-2.95270	-0.63028	1.42441
H	-3.30255	-1.78313	0.15491
H	4.48124	-0.92707	0.74912
H	3.55440	0.13355	2.80007
H	2.62696	1.25020	1.81243
H	3.04316	1.34595	-0.60689
H	2.88061	-0.20713	-1.38120
H	-3.77021	2.95912	-1.29860
H	-5.42649	2.50811	-0.92225
H	-4.98389	4.89924	-0.30394
H	-5.34196	3.95251	1.15004
H	-3.67037	4.39020	0.77038
H	-5.74664	-1.57464	0.57427
H	-5.44629	-0.41958	1.86159
H	-5.79364	-2.70863	2.80952
H	-4.44144	-3.32842	1.84723
H	-4.14234	-2.15802	3.13915
H	5.34890	-0.47402	-1.49201
H	5.57023	1.09498	-0.74202
H	5.76855	1.28137	-3.23069
H	4.13573	0.62035	-3.42284
H	4.36517	2.20051	-2.66208
H	4.55703	2.39963	2.70285
H	4.77362	2.27016	0.97151
H	6.90399	1.76621	2.20879
H	6.10225	0.43926	3.06482
H	6.37581	0.33259	1.32155

L1_73 Ground State

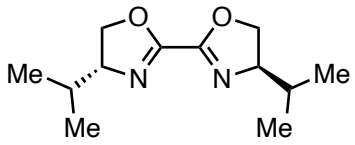
N	1.06796	-0.27520	0.45096
C	0.43543	-1.03577	-0.34978
O	1.02997	-2.17105	-0.80917
C	2.34061	-2.19414	-0.19135
C	2.40167	-0.87520	0.63347
C	-0.93560	-0.79141	-0.84407
O	-1.53975	-1.85657	-1.44376
C	-2.82297	-1.35689	-1.89601
C	-2.91904	0.06022	-1.27094
N	-1.56785	0.30780	-0.73241
C	3.52101	0.08280	0.17982
C	4.90850	-0.57059	0.39615
C	3.38296	1.44186	0.88478
C	-3.98052	0.20089	-0.15714
C	-4.08480	1.65660	0.33635
C	-3.70032	-0.76078	1.01386
C	5.88551	-0.37250	-0.76882
C	7.26511	-0.97372	-0.49366
C	4.38235	2.51128	0.43323
C	4.13032	3.86118	1.11018
C	-4.89053	-0.97491	1.95544
C	-4.57520	-1.96908	3.07587
C	-4.43186	2.71107	-0.72579
C	-5.74410	2.44564	-1.47010
H	3.08533	-2.23977	-0.99142
H	2.40970	-3.10026	0.41637
H	2.53876	-1.08439	1.70252
H	-3.59642	-2.04913	-1.55423
H	-2.81038	-1.34215	-2.99024
H	-3.12424	0.80192	-2.04850
H	3.37373	0.24238	-0.89982
H	4.80112	-1.65167	0.56531

H	5.35348	-0.17601	1.32028
H	3.48831	1.28646	1.96967
H	2.36313	1.80854	0.72760
H	-4.93961	-0.08976	-0.61255
H	-3.12992	1.92382	0.80412
H	-4.84714	1.70102	1.12443
H	-2.84120	-0.38339	1.58289
H	-3.39390	-1.74236	0.62708
H	5.98609	0.69659	-0.99017
H	5.45670	-0.82837	-1.67246
H	7.94022	-0.83653	-1.34555
H	7.73111	-0.50451	0.38138
H	7.19480	-2.04988	-0.29244
H	4.31904	2.63054	-0.65758
H	5.40898	2.18691	0.64781
H	4.84982	4.61818	0.77829
H	3.12331	4.23142	0.88448
H	4.21330	3.77567	2.20056
H	-5.75133	-1.33560	1.37426
H	-5.19939	-0.01964	2.39742
H	-5.43591	-2.11464	3.73820
H	-4.29662	-2.94835	2.66768
H	-3.73655	-1.61682	3.68837
H	-3.60996	2.80492	-1.44670
H	-4.49552	3.68559	-0.22465
H	-5.99402	3.27550	-2.14043
H	-5.69132	1.53654	-2.08040
H	-6.57710	2.32068	-0.76697

L1_74 Ground State

N	1.21652	-0.17848	-0.01173
C	0.52587	-1.10076	-0.55227
O	1.10827	-2.30147	-0.82623
C	2.50785	-2.12633	-0.49456
C	2.56961	-0.73221	0.18634
C	-0.90187	-0.98854	-0.91722
O	-1.47903	-2.13532	-1.37684
C	-2.83901	-1.76571	-1.71752
C	-2.96929	-0.29776	-1.22860
N	-1.60045	0.07130	-0.82294
C	3.65710	0.20039	-0.37842
C	5.06284	-0.42146	-0.23966
C	3.53955	1.60134	0.24507
C	-3.95946	-0.10410	-0.05845
C	-4.10994	1.38974	0.28657
C	-3.55473	-0.94112	1.17847
C	5.58958	-0.57719	1.19232
C	6.97906	-1.21885	1.22840
C	4.53116	2.62908	-0.30889
C	4.27935	4.03457	0.24311
C	-4.73171	-1.61221	1.90301
C	-5.78740	-0.65567	2.46483
C	-4.88420	2.21478	-0.74656
C	-5.03366	3.67997	-0.32909
H	3.07806	-2.16646	-1.42932
H	2.81151	-2.95573	0.14751
H	2.72166	-0.83364	1.26912
H	-3.51459	-2.46158	-1.21315
H	-2.95432	-1.87222	-2.80027
H	-3.26937	0.35466	-2.05491
H	3.45059	0.29749	-1.45560
H	5.77274	0.19038	-0.81004
H	5.07454	-1.40665	-0.72762
H	3.66124	1.53044	1.33541
H	2.51654	1.95585	0.08137
H	-4.93128	-0.47456	-0.42350
H	-3.10614	1.81077	0.42352
H	-4.61799	1.48200	1.25351
H	-3.00191	-0.30035	1.87706
H	-2.85170	-1.73185	0.89028
H	5.62993	0.40374	1.68168
H	4.89500	-1.18526	1.78725
H	7.34816	-1.32043	2.25491
H	6.96484	-2.21850	0.77705
H	7.70487	-0.61551	0.66975
H	4.46034	2.64683	-1.40585
H	5.56097	2.32924	-0.07421
H	4.99574	4.75955	-0.15946
H	3.27051	4.38115	-0.01028
H	4.36754	4.04879	1.33638
H	-4.33177	-2.22338	2.72291
H	-5.21776	-2.31507	1.21057
H	-6.56305	-1.20638	3.00892
H	-5.33919	0.06465	3.15979
H	-6.28379	-0.08657	1.67108
H	-5.87955	1.77033	-0.89277
H	-4.38296	2.17079	-1.72224
H	-5.59319	4.25613	-1.07455
H	-5.56409	3.76450	0.62728

H	-4.05261	4.15378	-0.20570



L2_1 Ground State

N	1.27256	0.48766	0.20938
C	0.57658	-0.56390	0.03691
O	1.15847	-1.78626	0.18494
C	2.55739	-1.51296	0.44468
C	2.63536	0.03630	0.54474
C	-0.85898	-0.58220	-0.31497
O	-1.46292	-1.80130	-0.24049
C	-2.82632	-1.57619	-0.67662
C	-2.92777	-0.03448	-0.83022
N	-1.54109	0.43691	-0.65685
C	3.69196	0.67236	-0.37456
C	5.09815	0.19951	0.01551
C	3.59563	2.20055	-0.34727
C	-3.87123	0.64957	0.18432
C	-4.01419	2.14082	-0.13866
C	-3.40782	0.44303	1.63157
H	3.13622	-1.91416	-0.39434
H	2.84081	-2.03714	1.35995
H	2.84744	0.35396	1.57586
H	-3.49672	-1.99123	0.08036
H	-2.97090	-2.11340	-1.61872
H	-3.26126	0.23369	-1.83972
H	3.47489	0.32766	-1.39664
H	5.34053	0.51041	1.03983
H	5.20185	-0.89076	-0.03711
H	5.85104	0.63488	-0.65030
H	2.59261	2.53213	-0.62550
H	3.81102	2.58345	0.65877
H	4.32200	2.64611	-1.03638
H	-4.85372	0.16894	0.05900
H	-4.40679	2.29317	-1.15108
H	-4.69686	2.62946	0.56550
H	-3.04039	2.63665	-0.07699
H	-3.28542	-0.61701	1.88247
H	-2.44700	0.94034	1.79851
H	-4.13670	0.86690	2.33061

L2_2 Ground State

N	-1.44525	0.50121	-0.27118
C	-0.72638	-0.54057	-0.13663
O	-1.29941	-1.77082	-0.25194
C	-2.71551	-1.51556	-0.42103
C	-2.81564	0.03024	-0.54218
C	0.72640	-0.54055	0.13674
O	1.29949	-1.77078	0.25190
C	2.71556	-1.51548	0.42120
C	2.81564	0.03034	0.54226
N	1.44521	0.50125	0.27139
C	-3.84118	0.66953	0.40880
C	-5.25537	0.16751	0.09054
C	-3.76992	2.19799	0.34586
C	3.84106	0.66960	-0.40888
C	5.25523	0.16732	-0.09100
C	3.77005	2.19806	-0.34576
H	-3.23238	-1.90549	0.46292
H	-3.05459	-2.05961	-1.30500
H	-3.07319	0.32840	-1.56904
H	3.23259	-1.90547	-0.46262
H	3.05450	-2.05944	1.30529
H	3.07332	0.32855	1.56908
H	-3.57454	0.34975	1.42723
H	-5.54622	0.45066	-0.92922
H	-5.33975	-0.92260	0.17264
H	-5.98571	0.60751	0.77807
H	-2.76040	2.54984	0.57070
H	-4.03697	2.55645	-0.65680
H	-4.47067	2.64762	1.05848
H	3.57414	0.34996	-1.42729
H	5.33941	-0.92281	-0.17320
H	5.98548	0.60724	-0.77868
H	5.54638	0.45034	0.92871
H	2.76054	2.55011	-0.57035
H	4.03737	2.55637	0.65688
H	4.47073	2.64765	-1.05847

L2_3 Ground State

N	1.35223	0.45070	0.58940
C	0.70272	-0.58289	0.22813
O	1.31601	-1.79945	0.23567
C	2.64070	-1.55191	0.76923
C	2.72626	-0.00534	0.87297
C	-0.70274	-0.58289	-0.22814
O	-1.31605	-1.79944	-0.23564
C	-2.64073	-1.55191	-0.76924
C	-2.72628	-0.00533	-0.87298
N	-1.35224	0.45069	-0.58946
C	3.73250	0.64748	-0.10115
C	3.84443	2.15112	0.17299

C	3.36998	0.38194	-1.56746
C	-3.73249	0.64750	0.10116
C	-3.84441	2.15114	-0.17297
C	-3.36992	0.38195	1.56747
H	3.36922	-1.99143	0.08321
H	2.71127	-2.05310	1.73928
H	2.99012	0.30138	1.89192
H	-3.36926	-1.99143	-0.08324
H	-2.71126	-2.05309	-1.73929
H	-2.99017	0.30138	-1.89193
H	4.70695	0.18027	0.10909
H	4.16511	2.34528	1.20344
H	4.57159	2.61796	-0.50075
H	2.87458	2.63630	0.02498
H	2.41878	0.86233	-1.81812
H	4.14131	0.78703	-2.23120
H	3.27369	-0.68802	-1.78546
H	-4.70694	0.18030	-0.10905
H	-4.57155	2.61798	0.50079
H	-2.87455	2.63631	-0.02499
H	-4.16511	2.34529	-1.20341
H	-2.41871	0.86234	1.81810
H	-4.14124	0.78704	2.23123
H	-3.27364	-0.68801	1.78546

L2_4 Ground State

N	1.41410	0.55096	0.19668
C	0.65669	-0.46167	0.05246
O	1.16596	-1.71207	0.23165
C	2.57939	-1.51521	0.48142
C	2.74845	0.02871	0.54313
C	-0.77822	-0.40536	-0.29830
O	-1.44495	-1.59011	-0.21963
C	-2.79957	-1.29517	-0.64112
C	-2.81220	0.24771	-0.83284
N	-1.40613	0.64682	-0.64444
C	3.83928	0.57871	-0.39156
C	5.21578	0.03305	0.00924
C	3.83350	2.11013	-0.40121
C	-3.73203	1.02565	0.13305
C	-3.36032	0.80408	1.60296
C	-5.20490	0.69654	-0.13787
H	3.13065	-1.96999	-0.34884
H	2.83500	-2.03269	1.40861
H	2.98036	0.35869	1.56612
H	-3.47709	-1.65537	0.13666
H	-2.99221	-1.84650	-1.56573
H	-3.10900	0.50613	-1.85656
H	3.60043	0.22293	-1.40495
H	5.47785	0.35324	1.02583
H	5.25492	-1.06239	-0.01755
H	5.99193	0.40732	-0.66693
H	4.07341	2.50377	0.59508
H	4.58340	2.49519	-1.10151
H	2.85119	2.49361	-0.68652
H	-3.56716	2.08618	-0.09708
H	-3.49914	-0.24148	1.90543
H	-2.31710	1.07692	1.78655
H	-3.99345	1.41745	2.25335
H	-5.47133	0.87986	-1.18570
H	-5.43084	-0.35363	0.08708
H	-5.86081	1.31074	0.48854

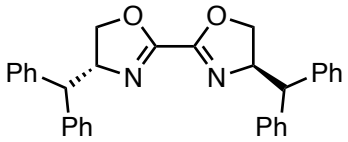
L2_5 Ground State

N	-1.21558	0.63140	-0.58761
C	-0.62822	-0.42672	-0.19221
O	-1.31755	-1.60001	-0.14388
C	-2.63575	-1.28907	-0.65988
C	-2.61634	0.25368	-0.84950
C	0.78048	-0.49951	0.24829
O	1.32138	-1.74978	0.27360
C	2.66542	-1.57024	0.78540
C	2.84253	-0.02961	0.85762
N	1.49414	0.50087	0.58061
C	-3.57104	1.04423	0.07155
C	-3.27763	0.81179	1.55751
C	-5.03362	0.74135	-0.27494
C	3.87304	0.54434	-0.14043
C	4.07647	2.04366	0.10305
C	3.47697	0.27320	-1.59703
H	-3.37041	-1.64245	0.06730
H	-2.76832	-1.83678	-1.59726
H	-2.85693	0.51774	-1.88624
H	3.35757	-2.06449	0.09896
H	2.72002	-2.05630	1.76413
H	3.13651	0.28035	1.86731
H	-3.37689	2.10251	-0.14578
H	-3.44613	-0.23293	1.84762
H	-2.24150	1.06929	1.79538
H	-3.93452	1.43149	2.17762
H	-5.28870	-0.30553	-0.06656
H	-5.70972	1.36452	0.32036
H	-5.24355	0.93314	-1.33404
H	4.82097	0.02455	0.06761

H	4.42105	2.23791	1.12574
H	4.82116	2.45410	-0.58804
H	3.13495	2.58225	-0.04316
H	2.55225	0.80365	-1.84579
H	4.26212	0.61999	-2.27740
H	3.31575	-0.79319	-1.79311

L2_6 Ground State

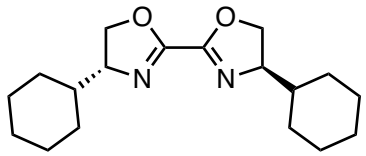
N	1.36087	-0.69702	-0.57722
C	0.70772	0.33311	-0.21254
O	1.32619	1.54599	-0.18435
C	2.66698	1.30172	-0.67771
C	2.73978	-0.24312	-0.83411
C	-0.70765	0.33316	0.21238
O	-1.32603	1.54608	0.18418
C	-2.66691	1.30189	0.67734
C	-2.73971	-0.24293	0.83407
N	-1.36084	-0.69692	0.57713
C	3.72942	-0.95674	0.11246
C	3.40656	-0.71183	1.59026
C	5.17524	-0.57460	-0.22612
C	-3.72951	-0.95674	-0.11219
C	-3.40677	-0.71232	-1.59009
C	-5.17526	-0.57439	0.22642
H	3.37020	1.71236	0.05051
H	2.77995	1.83670	-1.62493
H	3.00630	-0.51430	-1.86265
H	-3.37001	1.71233	-0.05112
H	-2.78009	1.83709	1.62441
H	-3.00608	-0.51388	1.86271
H	3.60055	-2.02887	-0.08452
H	3.50894	0.34693	1.85957
H	2.38522	-1.02623	1.82357
H	4.09274	-1.27788	2.22966
H	5.36576	0.48945	-0.03645
H	5.88055	-1.14480	0.38809
H	5.40750	-0.77431	-1.27907
H	-3.60071	-2.02883	0.08510
H	-3.50912	0.34636	-1.85974
H	-2.38547	-1.02685	-1.82340
H	-4.09305	-1.27853	-2.22926
H	-5.36573	0.48962	0.03644
H	-5.88068	-1.14473	-0.38753
H	-5.40742	-0.77375	1.27947



L3_1 Ground State

N	-1.45309	-0.22565	-0.20304
C	-0.72462	-1.26877	-0.14542
O	-1.28123	-2.48785	-0.36958
C	-2.70242	-2.23436	-0.51280
C	-2.80790	-0.68519	-0.55568
C	0.72458	-1.26880	0.14511
O	1.28113	-2.48791	0.36928
C	2.70235	-2.23448	0.51236
C	2.80787	-0.68533	0.55543
N	1.45309	-0.22571	0.20274
C	-3.89183	-0.12113	0.38854
C	-5.20734	-0.83487	0.10834
C	-4.06566	1.39620	0.32699
C	3.89189	-0.12120	-0.38861
C	5.20740	-0.83487	-0.10822
C	4.06564	1.39613	-0.32704
C	-5.74132	-1.74936	1.02117
C	-6.92868	-2.43003	0.74173
C	-7.59591	-2.20371	-0.46087
C	-7.07340	-1.28824	-1.37834
C	-5.89182	-0.60821	-1.09370
C	-5.13883	1.96816	1.02714
C	-5.35737	3.34271	1.01148
C	-4.50648	4.17783	0.28402
C	-3.43657	3.62147	-0.41306
C	-3.21308	2.24221	-0.39031
C	5.13866	1.96814	-1.02738
C	5.35720	3.34269	-1.01168
C	4.50645	4.17775	-0.28399
C	3.43669	3.62135	0.41328
C	3.21321	2.24209	0.39050
C	5.89177	-0.60803	1.09385
C	7.07334	-1.28799	1.37868
C	7.59596	-2.20356	0.46136
C	6.92884	-2.43006	-0.74126
C	5.74149	-1.74944	-1.02090
H	-3.21078	-2.67269	0.35090
H	-3.04918	-2.73025	-1.42035
H	-3.02658	-0.33881	-1.57395
H	3.21059	-2.67268	-0.35148
H	3.04922	-2.73052	1.41979
H	3.02646	-0.33908	1.57377

H	-3.57648	-0.38593	1.40747
H	3.57672	-0.38601	-1.40760
H	-5.22545	-1.92551	1.96219
H	-7.33018	-3.13392	1.46543
H	-8.51961	-2.73105	-0.68141
H	-7.59197	-1.09993	-2.31436
H	-5.50239	0.12183	-1.79814
H	-5.81640	1.32298	1.57980
H	-6.19525	3.76153	1.56238
H	-4.67600	5.25088	0.26528
H	-2.76139	4.26027	-0.97599
H	-2.34944	1.83637	-0.90163
H	5.81612	1.32299	-1.58022
H	6.19496	3.76156	-1.56273
H	4.67596	5.25081	-0.26522
H	2.76162	4.26011	0.97638
H	2.34968	1.83621	0.90197
H	5.50226	0.12209	1.79816
H	7.59183	-1.09955	2.31471
H	8.51965	-2.73085	0.68205
H	7.33042	-3.13402	-1.46485
H	5.22570	-1.92572	-1.96194



L4_1 Ground State

N	1.18470	-0.15939	0.87980
C	0.63706	-1.19140	0.37411
O	1.24573	-2.40399	0.49592
C	2.42247	-2.15693	1.30545
C	2.47156	-0.61123	1.44358
C	-0.63692	-1.19138	-0.37413
O	-1.24548	-2.40399	-0.49621
C	-2.42238	-2.15683	-1.30549
C	-2.47146	-0.61112	-1.44350
N	-1.18467	-0.15930	-0.87957
C	3.65521	0.05839	0.71671
C	-3.65521	0.05839	-0.71671
C	-3.63211	-0.18345	0.80188
C	-4.82580	0.48514	1.49619
C	-4.87485	1.98778	1.19204
C	-4.89302	2.24382	-0.32040
C	-3.70709	1.56476	-1.01730
C	3.63203	-0.18334	-0.80190
C	4.82566	0.48531	-1.49624
C	4.87466	1.98794	-1.19202
C	4.89290	2.24390	0.32043
C	3.70706	1.56474	1.01738
H	3.28492	-2.58319	0.78706
H	2.28612	-2.67050	2.26193
H	2.50948	-0.31645	2.49903
H	-2.28625	-2.67036	-2.26202
H	-3.28474	-2.58308	-0.78694
H	-2.50926	-0.31625	-2.49894
H	4.57049	-0.40247	1.12415
H	-4.57043	-0.40249	-1.12424
H	-3.62345	-1.25838	1.02414
H	-2.69858	0.22861	1.20550
H	-4.77193	0.31608	2.57874
H	-5.75873	0.01530	1.15094
H	-3.98910	2.47118	1.62857
H	-5.75145	2.44526	1.66741
H	-4.88236	3.32145	-0.52542
H	-5.83239	1.85400	-0.74010
H	-2.76596	2.01774	-0.68123
H	-3.76323	1.72451	-2.10244
H	3.62338	-1.25826	-1.02425
H	2.69847	0.22872	-1.20545
H	4.77174	0.31630	-2.57878
H	5.75862	0.01549	-1.15104
H	3.98887	2.47131	-1.62848
H	5.75121	2.44546	-1.66742
H	4.88221	3.32152	0.52550
H	5.83233	1.85411	0.74006
H	2.76589	2.01771	0.68141
H	3.76327	1.72443	2.10252

L4_2 Ground State

N	1.10770	-0.06771	0.28520
C	0.45244	-1.14405	0.10650
O	1.01141	-2.33652	0.45302
C	2.35023	-2.01371	0.90347
C	2.40765	-0.46065	0.86006
C	-0.91167	-1.22194	-0.45721
O	-1.52011	-2.43614	-0.34926
C	-2.80090	-2.27880	-1.00849
C	-2.87691	-0.76298	-1.33746
N	-1.53312	-0.25418	-1.00309
C	3.58299	0.09913	0.04635
C	-3.96622	0.00570	-0.56288
C	-3.75054	-0.03279	0.95924
C	-4.85314	0.73157	1.70355

C	-4.95340	2.18091	1.21141
C	-5.16402	2.23408	-0.30718
C	-4.06921	1.45921	-1.05162
C	3.48722	1.62438	-0.11011
C	4.66846	2.18606	-0.91099
C	6.01175	1.78866	-0.28561
C	6.11552	0.26695	-0.12174
C	4.93042	-0.29254	0.67680
H	3.05691	-2.48486	0.21197
H	2.48436	-2.44007	1.90007
H	2.46420	-0.04074	1.87432
H	-2.80047	-2.91353	-1.89963
H	-3.57901	-2.62233	-0.32216
H	-3.04827	-0.60666	-2.40931
H	3.52679	-0.35189	-0.95750
H	-4.92115	-0.49810	-0.78748
H	-3.70462	-1.06874	1.31936
H	-2.77718	0.42155	1.18365
H	-4.66206	0.70712	2.78351
H	-5.81790	0.22759	1.54380
H	-4.02411	2.71098	1.46494
H	-5.76723	2.70440	1.72847
H	-5.18900	3.27485	-0.65302
H	-6.14521	1.79936	-0.54974
H	-3.09733	1.94541	-0.90012
H	-4.26304	1.47386	-2.13254
H	2.53418	1.88286	-0.58009
H	3.47769	2.08092	0.89163
H	4.58871	3.27776	-0.98178
H	4.62182	1.80186	-1.94050
H	6.10440	2.26387	0.70202
H	6.84469	2.16274	-0.89376
H	7.05923	-0.00297	0.36820
H	6.13185	-0.20322	-1.11567
H	4.96616	0.10145	1.70398
H	5.01918	-1.38403	0.75801

L4_3 Ground State

N	1.40962	-0.02397	0.42069
C	0.70517	-1.06523	0.22206
O	1.25229	-2.29549	0.42874
C	2.63817	-2.04358	0.76733
C	2.73621	-0.49532	0.85972
C	-0.70491	-1.06516	-0.22181
O	-1.25188	-2.29534	-0.42941
C	-2.63791	-2.04333	-0.76729
C	-2.73595	-0.49506	-0.85930
N	-1.40949	-0.02385	-0.41971
C	3.86632	0.11106	0.01680
C	-3.86637	0.11106	-0.01665
C	-3.80891	1.64614	-0.01363
C	-4.94700	2.25321	0.81610
C	-6.31825	1.76325	0.33327
C	-6.38461	0.23072	0.32356
C	-5.24248	-0.37421	-0.50394
C	3.80867	1.64613	0.01396
C	4.94644	2.25342	-0.81605
C	6.31790	1.76359	-0.33370
C	6.38444	0.23106	-0.32416
C	5.24263	-0.37409	0.50364
H	3.25870	-2.46051	-0.03353
H	2.85885	-2.56489	1.70119
H	2.87604	-0.17181	1.90118
H	-2.85907	-2.56448	-1.70111
H	-3.25808	-2.46034	0.03383
H	-2.87538	-0.17129	-1.90073
H	3.72283	-0.23883	-1.01823
H	-3.72315	-0.23891	1.01838
H	-2.83326	1.97308	0.35690
H	-3.88618	2.00324	-1.05212
H	-4.89760	3.34828	0.77658
H	-4.81435	1.97220	1.87115
H	-6.49670	2.13748	-0.68552
H	-7.11698	2.17392	0.96332
H	-7.35188	-0.10923	-0.06670
H	-6.31455	-0.14051	1.35630
H	-5.36488	-0.08402	-1.55865
H	-5.30130	-1.47030	-0.47297
H	2.83288	1.97299	-0.35623
H	3.88621	2.00312	1.05247
H	4.89691	3.34848	-0.77639
H	4.81350	1.97251	-1.87109
H	6.49662	2.13773	0.68508
H	7.11637	2.17441	-0.96395
H	7.35187	-0.10882	0.06577
H	6.31411	-0.14008	-1.35691
H	5.36531	-0.08397	1.55833
H	5.30159	-1.47017	0.47257

L4_4 Ground State

N	-1.30701	-0.08605	0.28971
C	-0.57342	0.94212	0.13384
O	-1.04470	2.16591	0.50166
C	-2.40603	1.93420	0.94058

C	-2.57704	0.39067	0.86808
C	0.79494	0.93078	-0.42487
O	1.50201	2.08332	-0.26110
C	2.76799	1.85123	-0.92692
C	2.71779	0.35023	-1.32755
N	1.33622	-0.05948	-1.01424
C	-3.78670	-0.06668	0.04078
C	3.72610	-0.56270	-0.60324
C	5.17229	-0.23460	-1.00873
C	6.17715	-1.17363	-0.32784
C	6.01308	-1.15433	1.19742
C	4.57143	-1.48789	1.60204
C	3.56532	-0.54755	0.92501
C	-3.80200	-1.59181	-0.14279
C	-5.01757	-2.05148	-0.95722
C	-6.33101	-1.56821	-0.32895
C	-6.32406	-0.04614	-0.13806
C	-5.10472	0.41116	0.67398
H	-3.07255	2.46846	0.25508
H	-2.51396	2.35108	1.94434
H	-2.66843	-0.04246	1.87420
H	2.82393	2.52384	-1.78775
H	3.56583	2.10239	-0.22465
H	2.87700	0.23445	-2.40645
H	-3.69323	0.39679	-0.95457
H	3.50207	-1.58304	-0.94609
H	5.27696	-0.29122	-2.10053
H	5.40784	0.80226	-0.72489
H	7.20114	-0.89648	-0.60726
H	6.01658	-2.19749	-0.69493
H	6.27207	-0.15413	1.57533
H	6.71408	-1.85732	1.66408
H	4.45880	-1.43669	2.69192
H	4.34590	-2.52409	1.31159
H	3.72126	0.47255	1.30617
H	2.54066	-0.83150	1.18694
H	-2.86835	-1.91095	-0.61439
H	-3.83017	-2.06547	0.85062
H	-5.01734	-3.14467	-1.04734
H	-4.93856	-1.65360	-1.97952
H	-6.46245	-2.05282	0.64968
H	-7.18638	-1.86956	-0.94629
H	-7.24765	0.28336	0.35380
H	-6.30176	0.44150	-1.12343
H	-5.17361	0.00282	1.69384
H	-5.11398	1.50463	0.77438

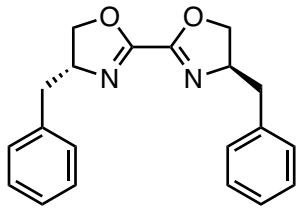
L4_5 Ground State

N	1.00394	-0.18812	-0.80045
C	0.53969	0.90323	-0.33766
O	1.26422	2.04938	-0.46432
C	2.44063	1.67315	-1.22303
C	2.34375	0.12589	-1.33203
C	-0.75346	1.04330	0.36323
O	-1.26532	2.30537	0.40042
C	-2.48640	2.19605	1.17367
C	-2.66226	0.66913	1.39401
N	-1.39912	0.08690	0.90055
C	3.42276	-0.66119	-0.56311
C	-3.87328	0.05320	0.66495
C	-3.78244	0.19955	-0.86322
C	-5.00367	-0.41347	-1.56094
C	-5.18452	-1.88615	-1.17169
C	-5.27197	-2.04688	0.35136
C	-4.05738	-1.42319	1.05059
C	4.81664	-0.44758	-1.17545
C	5.88754	-1.26727	-0.44301
C	5.89170	-0.96216	1.06050
C	4.50232	-1.18190	1.67248
C	3.43023	-0.36042	0.94402
H	3.31723	2.03159	-0.67924
H	2.39030	2.17582	-2.19330
H	2.38293	-0.18933	-2.38158
H	-3.29334	2.65610	0.59785
H	-2.34521	2.75229	2.10522
H	-2.75492	0.43907	2.46212
H	3.15922	-1.72173	-0.68421
H	-4.76031	0.60924	1.01160
H	-3.67959	1.25497	-1.14708
H	-2.87290	-0.30868	-1.20752
H	-4.90142	-0.31570	-2.64877
H	-5.90596	0.14905	-1.27845
H	-4.32750	-2.46401	-1.54632
H	-6.07976	-2.30086	-1.65157
H	-5.35625	-3.10733	0.61932
H	-6.18918	-1.55820	0.71254
H	-3.14615	-1.96939	0.77633
H	-4.16106	-1.51143	2.14039
H	4.80076	-0.70790	-2.24230
H	5.08493	0.61812	-1.11717
H	6.87543	-1.07024	-0.87741
H	5.68509	-2.33744	-0.59340
H	6.19320	0.08449	1.21519

H	6.63787	-1.58251	1.57214
H	4.50993	-0.92731	2.73936
H	4.24367	-2.24850	1.60630
H	3.62900	0.70882	1.10967
H	2.43994	-0.56817	1.36271

L4_6 Ground State

N	1.22332	-0.83137	0.34286
C	0.65477	-0.34455	-0.68694
O	1.27325	-0.42622	-1.89774
C	2.48750	-1.17910	-1.65383
C	2.53595	-1.33136	-0.10806
C	-0.65445	0.34038	-0.68855
O	-1.27275	0.41672	-1.89978
C	-2.48702	1.17070	-1.65939
C	-2.53547	1.33022	-0.11434
N	-1.22306	0.83188	0.33899
C	3.67158	-0.56480	0.59758
C	-3.67149	0.56755	0.59486
C	-5.04836	1.14945	0.23564
C	-6.17944	0.42446	0.97746
C	-6.13467	-1.08753	0.72132
C	-4.76274	-1.66900	1.08584
C	-3.63050	-0.94787	0.34232
C	5.04876	-1.14774	0.24125
C	6.17942	-0.41866	0.97970
C	6.13395	1.09207	0.71634
C	4.76171	1.67461	1.07796
C	3.62989	0.94939	0.33780
H	3.32113	-0.61436	-2.07657
H	2.40101	-2.13612	-2.17672
H	2.61977	-2.38809	0.17250
H	-3.32065	0.60395	-2.07945
H	-2.40058	2.12524	-2.18679
H	-2.61884	2.38831	0.16123
H	3.50816	-0.71720	1.67410
H	-3.50808	0.72502	1.67066
H	-5.07137	2.22389	0.46201
H	-5.21703	1.05401	-0.84768
H	-7.15116	0.83599	0.67773
H	-6.07763	0.61065	2.05626
H	-6.33703	-1.27910	-0.34294
H	-6.92719	-1.59251	1.28728
H	-4.73213	-2.74311	0.86573
H	-4.60352	-1.56602	2.16888
H	-3.72906	-1.14883	-0.73476
H	-2.65750	-1.34352	0.65189
H	5.07228	-2.22108	0.47276
H	5.21749	-1.05740	-0.84249
H	7.15137	-0.83115	0.68204
H	6.07761	-0.59974	2.05937
H	6.33631	1.27865	-0.34881
H	6.92618	1.60013	1.27994
H	4.73060	2.74764	0.85271
H	4.60245	1.57673	2.16146
H	3.72845	1.14522	-0.74024
H	2.65668	1.34605	0.64538



L5_1 Ground State

N	-1.31984	-1.23190	-0.62715
C	-0.71896	-2.24630	-0.14872
O	-1.42758	-3.36644	0.15732
C	-2.78362	-3.07291	-0.28292
C	-2.75681	-1.55031	-0.57268
C	0.72639	-2.24484	0.14980
O	1.43770	-3.36259	-0.15896
C	2.79290	-3.06684	0.28248
C	2.76280	-1.54462	0.57321
N	1.32504	-1.22993	0.62995
C	-3.41269	-0.71280	0.54835
C	3.41450	-0.70497	-0.54873
C	3.22245	0.78431	-0.38081
C	-3.22523	0.77708	0.38053
C	2.00768	1.39282	-0.72852
C	1.82872	2.76389	-0.55655
C	2.85723	3.54889	-0.02965
C	4.06728	2.95254	0.32321
C	4.24556	1.57926	0.14575
C	-2.01261	1.38942	0.72900
C	-1.83785	2.76105	0.55710
C	-2.86848	3.54278	0.02949
C	-4.07641	2.94260	-0.32414
C	-4.25049	1.56879	-0.14675
H	-3.46520	-3.36187	0.52052
H	-2.98606	-3.67718	-1.17292
H	-3.22370	-1.30490	-1.53150
H	2.99568	-3.67114	1.17241
H	3.47562	-3.35415	-0.52054

H	3.23068	-1.29848	1.53134
H	-2.98014	-1.04180	1.50222
H	-4.48157	-0.95951	0.57771
H	4.48412	-0.94826	-0.57947
H	2.98173	-1.03544	-1.50199
H	1.19359	0.78678	-1.11278
H	0.88162	3.21672	-0.83548
H	2.71658	4.61835	0.10182
H	4.87500	3.55416	0.73132
H	5.19402	1.11953	0.41601
H	-1.19690	0.78590	1.11379
H	-0.89239	3.21688	0.83666
H	-2.73112	4.61267	-0.10193
H	-4.88574	3.54168	-0.73283
H	-5.19731	1.10605	-0.41762

L5_2 Ground State

N	1.88389	-0.64863	0.31201
C	0.93809	-1.44732	0.01601
O	1.18905	-2.78230	-0.07600
C	2.60560	-2.92418	0.19523
C	3.09876	-1.47058	0.44384
C	-0.45656	-1.04056	-0.25654
O	-1.36797	-2.05054	-0.27507
C	-2.62869	-1.42105	-0.62104
C	-2.30221	0.09645	-0.62165
N	-0.83867	0.15707	-0.46373
C	4.18211	-1.02173	-0.55617
C	-2.98498	0.88301	0.51563
C	-4.48805	0.90018	0.37435
C	4.77320	0.33553	-0.25320
C	-5.09934	1.68560	-0.61277
C	-6.48235	1.67170	-0.78319
C	-7.28128	0.86846	0.03368
C	-6.68633	0.08464	1.02160
C	-5.30041	0.10219	1.18827
C	4.01640	1.50547	-0.41023
C	4.56960	2.74983	-0.11406
C	5.88569	2.84769	0.34306
C	6.64576	1.69006	0.50467
C	6.08975	0.44475	0.20800
H	3.06992	-3.39196	-0.67885
H	2.72062	-3.58195	1.06068
H	3.49085	-1.34801	1.46009
H	-2.93712	-1.79901	-1.59980
H	-3.37121	-1.71181	0.12546
H	-2.57499	0.55873	-1.57641
H	3.73639	-1.03688	-1.55946
H	4.97888	-1.77644	-0.55058
H	-2.69550	0.43109	1.47159
H	-2.57788	1.89994	0.50645
H	-4.48340	2.31809	-1.24821
H	-6.93824	2.29087	-1.55091
H	-8.35959	0.85822	-0.09713
H	-7.29952	-0.53902	1.66624
H	-4.84247	-0.50362	1.96672
H	2.98636	1.42962	-0.74162
H	3.96955	3.64706	-0.23923
H	6.31453	3.81960	0.57136
H	7.67112	1.75378	0.85896
H	6.68810	-0.45536	0.33222

L5_3 Ground State

N	0.85067	0.69961	-0.22517
C	-0.09395	1.55164	-0.18294
O	-0.00553	2.69289	-0.91680
C	1.26906	2.60620	-1.60420
C	1.88821	1.27173	-1.10062
C	-1.32700	1.38119	0.61094
O	-2.44879	1.93798	0.08562
C	-3.50090	1.63078	1.03720
C	-2.83611	0.62652	2.01272
N	-1.40043	0.71447	1.69376
C	3.20792	1.46745	-0.32883
C	-3.30870	-0.83911	1.83811
C	-3.19140	-1.34497	0.41959
C	3.86144	0.17155	0.09014
C	-4.32554	-1.45274	-0.39474
C	-4.21997	-1.86712	-1.72314
C	-2.97045	-2.17970	-2.25779
C	-1.83270	-2.08160	-1.45440
C	-1.94096	-1.67295	-0.12632
C	3.32767	-0.60112	1.13111
C	3.92572	-1.80587	1.49564
C	5.06534	-2.25923	0.82744
C	5.60280	-1.49904	-0.21054
C	5.00216	-0.29270	-0.57381
H	1.85872	3.48641	-1.33026
H	1.07395	2.62087	-2.67974
H	2.06721	0.57504	-1.92735
H	-3.79935	2.56539	1.52221
H	-4.34160	1.21779	0.47680
H	-2.99469	0.91544	3.05681
H	2.99380	2.09496	0.54605

H	3.89372	2.03559	-0.97016
H	-2.70837	-1.45451	2.51694
H	-4.35087	-0.90375	2.17466
H	-5.30360	-1.21619	0.01913
H	-5.11288	-1.94613	-2.33732
H	-2.88390	-2.50054	-3.29226
H	-0.85408	-2.32217	-1.86026
H	-1.04837	-1.58333	0.48344
H	2.42913	-0.26216	1.63572
H	3.49966	-2.39376	2.30411
H	5.53071	-3.19795	1.11520
H	6.49025	-1.84108	-0.73621
H	5.42751	0.29914	-1.38157

L5_4 Ground State

N	1.42175	-0.86883	-0.38294
C	0.72154	0.17223	-0.16081
O	1.30912	1.39939	-0.20641
C	2.68371	1.15096	-0.59667
C	2.80138	-0.39670	-0.58998
C	-0.72153	0.17223	0.16075
O	-1.30910	1.39938	0.20639
C	-2.68370	1.15095	0.59660
C	-2.80136	-0.39671	0.58993
N	-1.42174	-0.86883	0.38286
C	3.71696	-0.94902	0.52135
C	-3.71698	-0.94904	-0.52137
C	-5.15807	-0.54252	-0.32802
C	5.15806	-0.54251	0.32804
C	-5.73917	0.45910	-1.11431
C	-7.05744	0.86538	-0.89984
C	-7.81589	0.27274	0.10905
C	-7.24906	-0.73012	0.89882
C	-5.93269	-1.13203	0.68067
C	5.73914	0.45913	1.11432
C	7.05741	0.86540	0.89988
C	7.81590	0.27273	-0.10896
C	7.24909	-0.73015	-0.89873
C	5.93271	-1.13205	-0.68061
H	3.33806	1.64597	0.12450
H	2.83972	1.59342	-1.58460
H	3.16238	-0.76962	-1.55458
H	-3.33804	1.64595	-0.12461
H	-2.83976	1.59343	1.58452
H	-3.16234	-0.76962	1.55454
H	3.61355	-2.03955	0.52454
H	3.34435	-0.58925	1.48763
H	-3.61358	-2.03958	-0.52455
H	-3.34440	-0.58929	-1.48767
H	-5.15524	0.91791	-1.90880
H	-7.49099	1.64220	-1.52362
H	-8.84249	0.58555	0.27708
H	-7.83507	-1.20209	1.68270
H	-5.49915	-1.91784	1.29527
H	5.15519	0.91795	1.90879
H	7.49095	1.64223	1.52367
H	8.84250	0.58553	-0.27697
H	7.83512	-1.20213	-1.68258
H	5.49918	-1.91787	-1.29521

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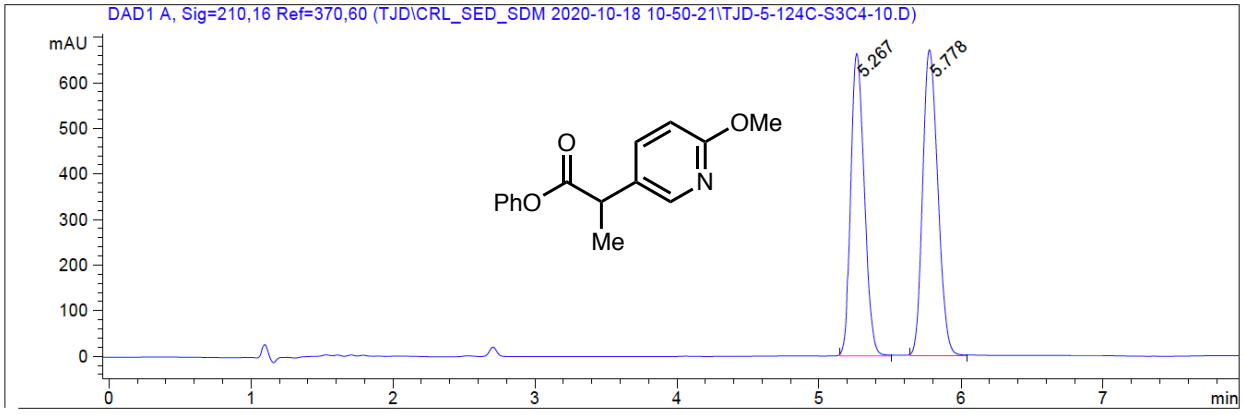
5. Chiral SFC Traces *(Note: Racemic samples made with scalemic ligand or racemized with tBuLi.)*

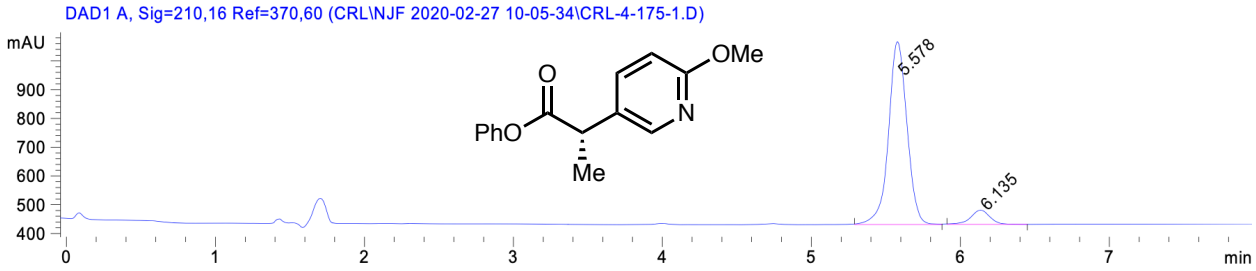
3a: racemic



Signal 1: DAD1 A, Sig=210,16 Ref=370,60

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	5.267	BB	0.1056	4399.58740	661.64484	46.8769
2	5.778	BB	0.1187	4985.82080	670.74689	53.1231

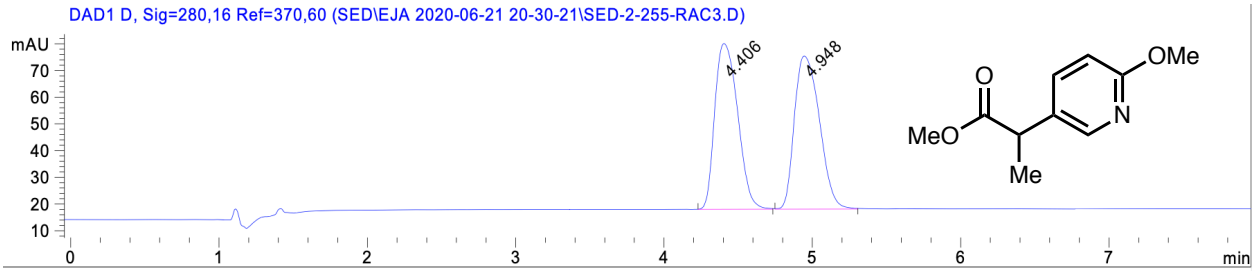
3a: enantioenriched (85% ee)



Signal 1: DAD1 A, Sig=210,16 Ref=370,60

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	5.578	BB	0.1328	5477.42188	633.93433	92.4667
2	6.135	BB	0.1366	446.25061	49.78547	7.5333

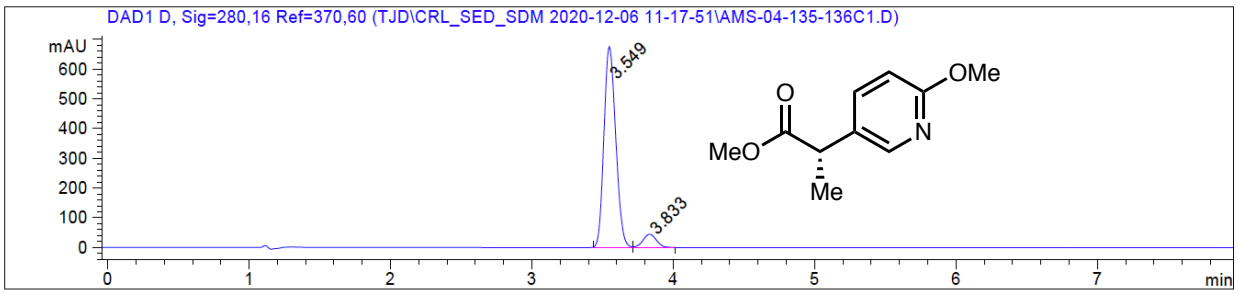
S4: racemic



Signal 3: DAD1 D, Sig=280,16 Ref=370,60

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	4.406	BB	0.1733	666.45874	62.07742	49.7780
2	4.948	BB	0.1890	672.40375	57.26835	50.2220

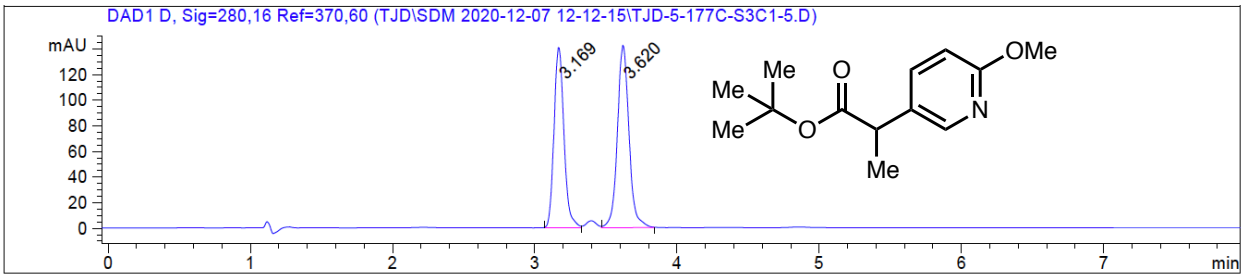
S4: enantioenriched (84% ee)



Signal 3: DAD1 D, Sig=280,16 Ref=370,60

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	3.549	BV	0.0917	3913.79761	674.04877	92.9594
2	3.833	VB	0.1011	296.42624	44.87164	7.0406

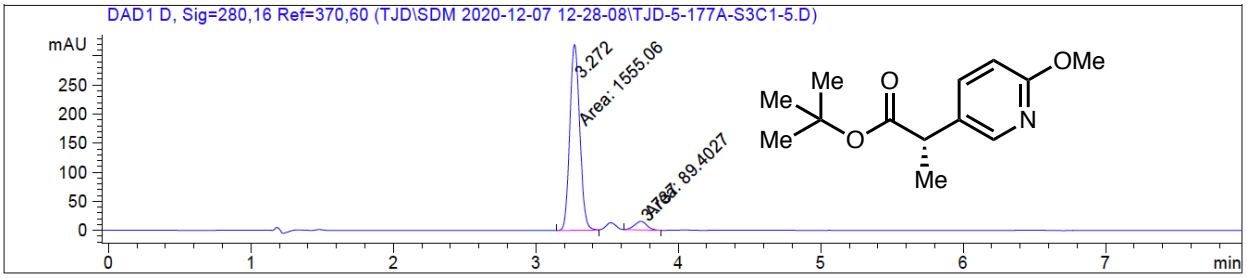
S5: racemic



Signal 3: DAD1 D, Sig=280,16 Ref=370,60

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	3.169	BV	0.0770	684.62677	140.04613	45.8754
2	3.620	VB	0.0905	807.73425	141.75697	54.1246

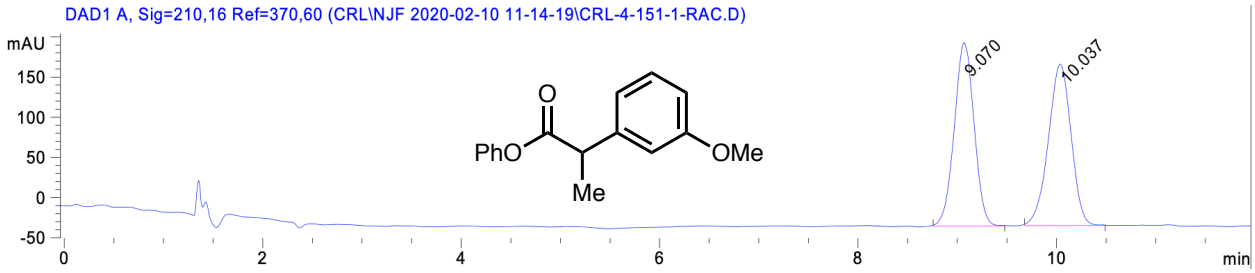
S5: enantioenriched (89% ee)



Signal 3: DAD1 D, Sig=280,16 Ref=370,60

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	3.272	MM	0.0803	1555.05725	322.73770	94.5634
2	3.737	MM	0.1000	89.40274	14.89493	5.4366

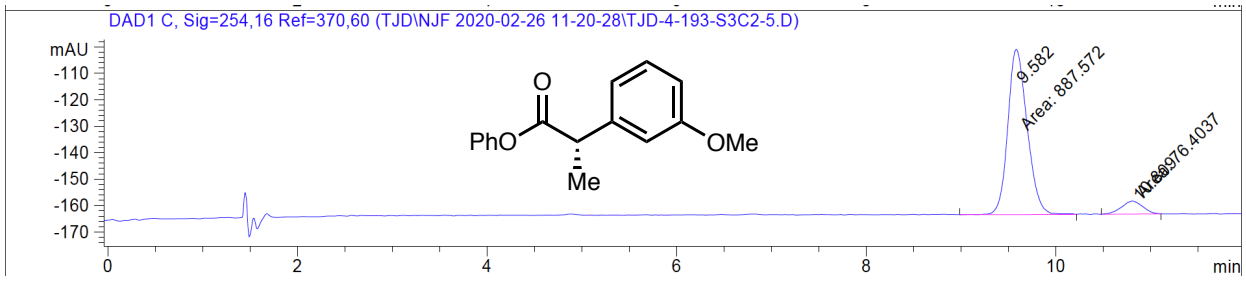
3b: racemic



Signal 1: DAD1 A, Sig=210,16 Ref=370,60

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	9.070	BB	0.2178	3161.34277	227.95787	49.6518
2	10.037	BB	0.2462	3205.68213	200.82071	50.3482

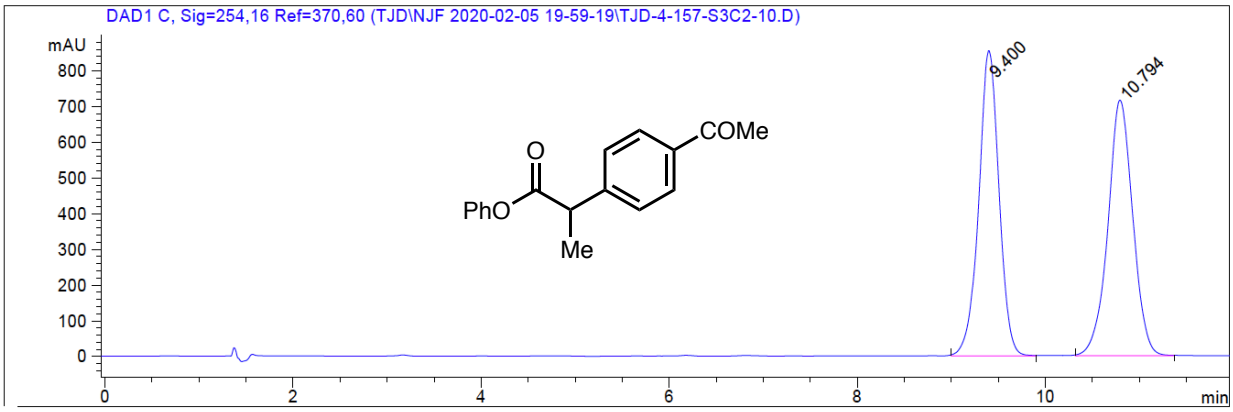
3b: enantioenriched (84% ee)



Signal 2: DAD1 C, Sig=254,16 Ref=370,60

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	9.582	MM	0.2366	887.57214	62.52427	92.0741
2	10.809	MM	0.2580	76.40370	4.93502	7.9259
Totals :				963.97585	67.45928	

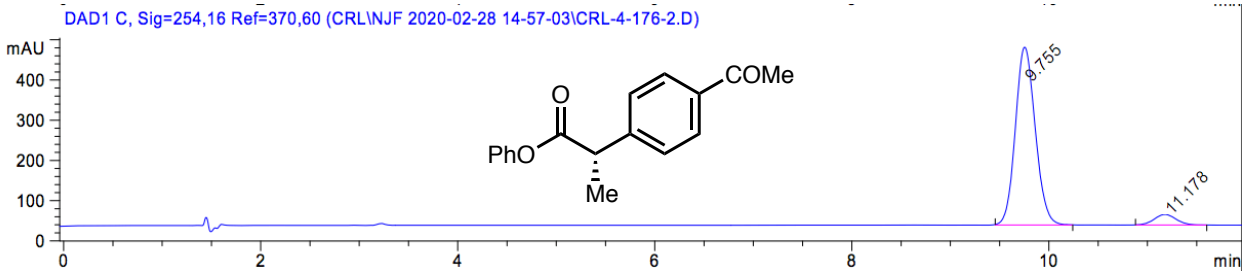
3c: racemic



Signal 1: DAD1 C, Sig=254,16 Ref=370,60

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	9.400	BB	0.2309	1.28069e4	854.31305	49.3412
2	10.794	BB	0.2785	1.31489e4	715.31354	50.6588

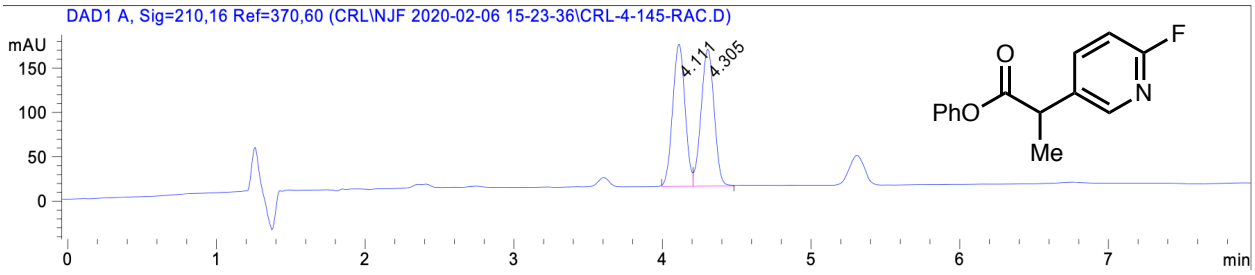
3c: enantioenriched (87% ee)



Signal 2: DAD1 C, Sig=254,16 Ref=370,60

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	9.755	BB	0.2193	6186.69824	442.03229	93.7495
2	11.178	BB	0.2423	412.48062	26.39767	6.2505
Totals :				6599.17886	468.42995	

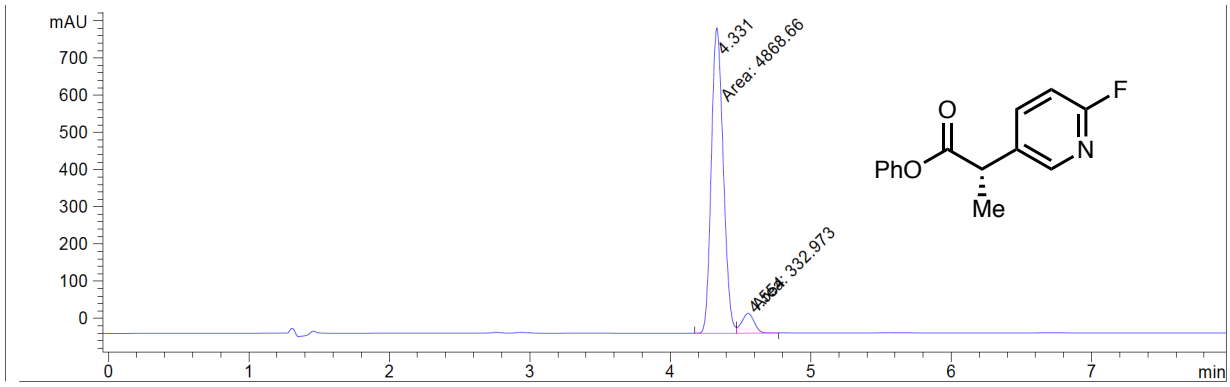
3d: racemic



Signal 1: DAD1 A, Sig=210,16 Ref=370,60

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	4.111	BV	0.0917	926.81171	159.74318	49.6334
2	4.305	VB	0.0954	940.50269	153.77911	50.3666

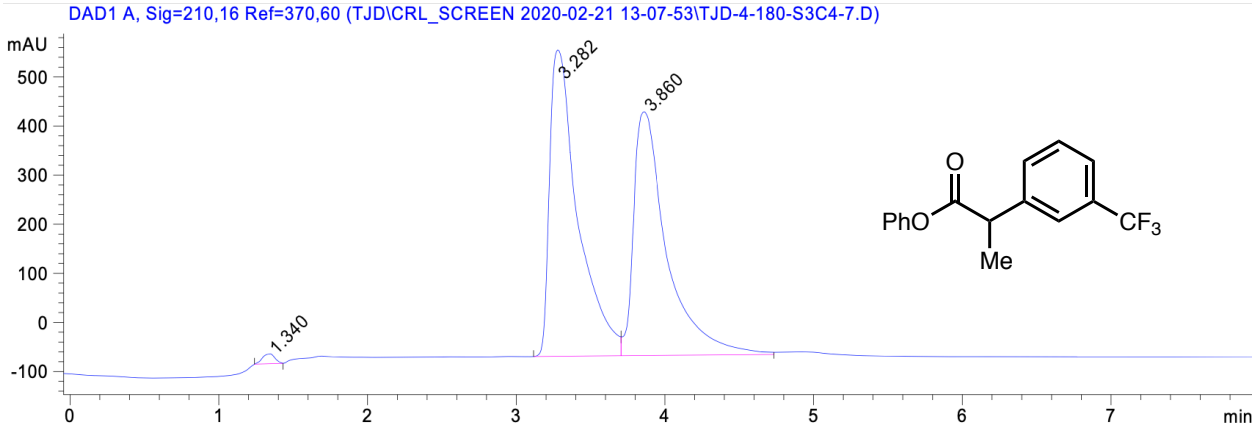
3d: enantioenriched (87% ee)



Signal 1: DAD1 C, Sig=254,16 Ref=370,60

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	4.331	MF	0.0982	4868.65674	826.07782	93.5987
2	4.554	FM	0.1038	332.97314	53.44642	6.4013

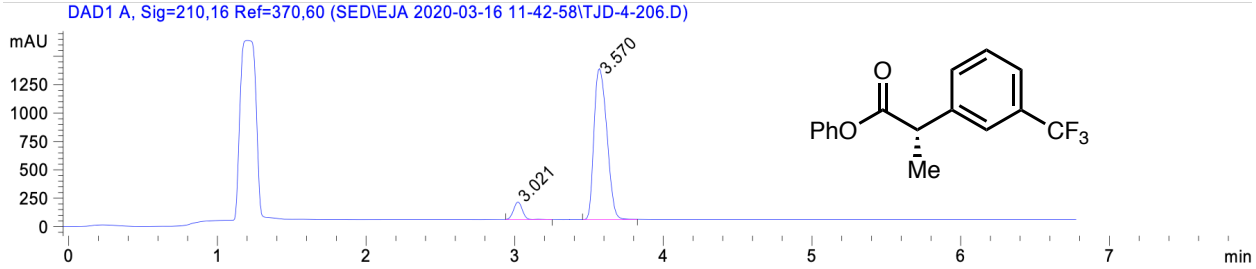
3e: racemic



Signal 1: DAD1 A, Sig=210,16 Ref=370,60

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	1.340	BV	0.0950	117.00625	20.38576	0.7277
2	3.282	BV	0.1938	8219.68555	623.68298	51.1235
3	3.860	VB	0.2298	7741.40479	496.70050	48.1488

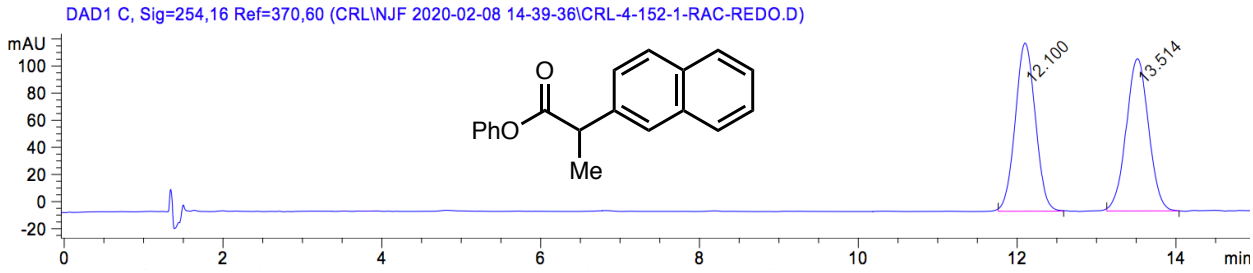
3e: enantioenriched (85% ee)



Signal 1: DAD1 A, Sig=210,16 Ref=370,60

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	3.021	BB	0.0654	648.23724	153.08775	7.4973
2	3.570	BB	0.0987	7997.99707	1320.49683	92.5027

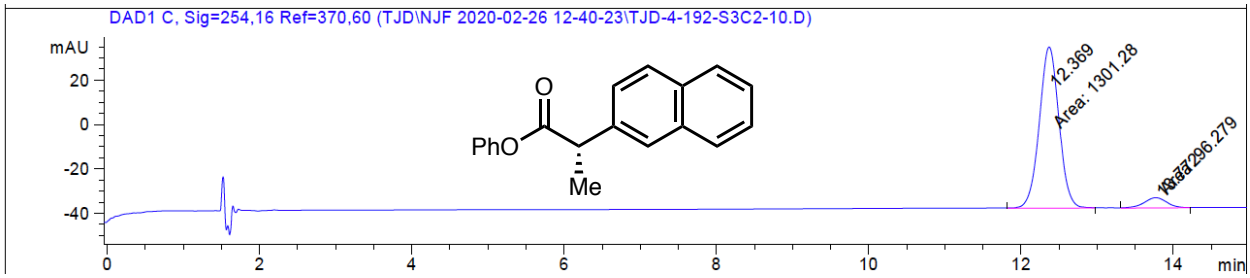
3f: racemic



Signal 2: DAD1 C, Sig=254,16 Ref=370,60

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	12.100	BB	0.2733	2182.32544	124.00195	49.8075
2	13.514	BB	0.3042	2199.19604	112.41534	50.1925

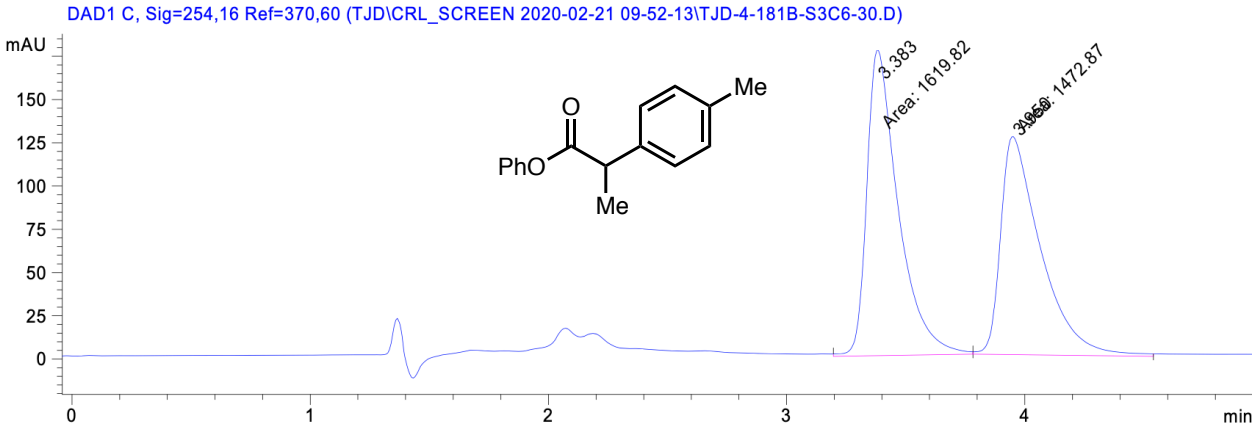
3f: enantioenriched (86% ee)



Signal 2: DAD1 C, Sig=254,16 Ref=370,60

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	12.369	MM	0.2984	1301.28259	72.68660	93.1109
2	13.772	MM	0.3490	96.27898	4.59845	6.8891

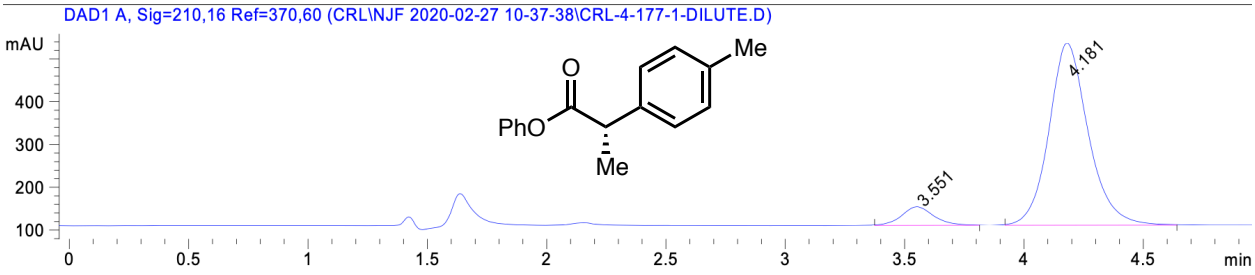
3g: racemic



Signal 1: DAD1 C, Sig=254,16 Ref=370,60

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	3.383	MM	0.1524	1619.82019	177.15884	52.3757
2	3.950	MM	0.1940	1472.87122	126.55457	47.6243

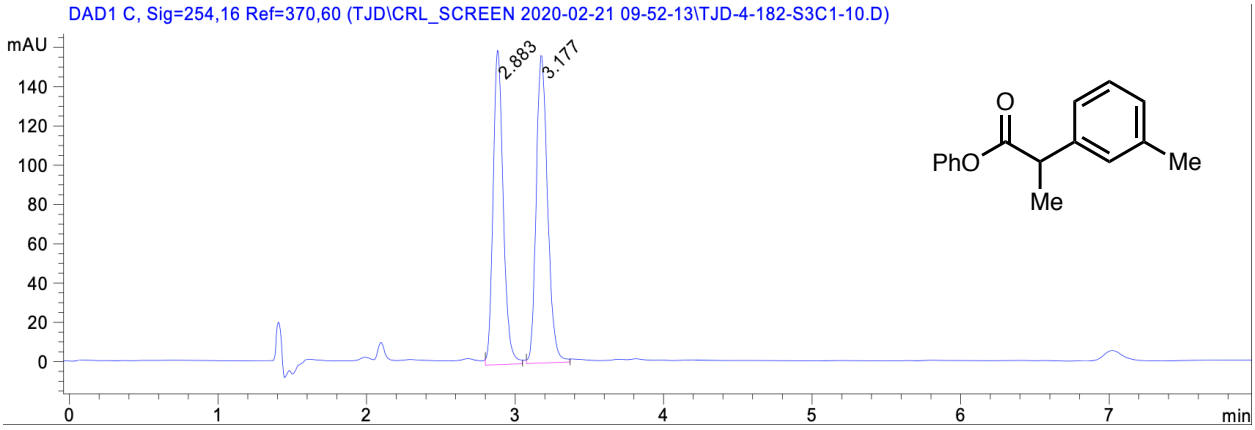
3g: enantioenriched (85% ee)



Signal 1: DAD1 A, Sig=210,16 Ref=370,60

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	3.551	BB	0.1418	409.49893	43.51672	7.7344
2	4.181	BB	0.1741	4885.02783	425.09625	92.2656

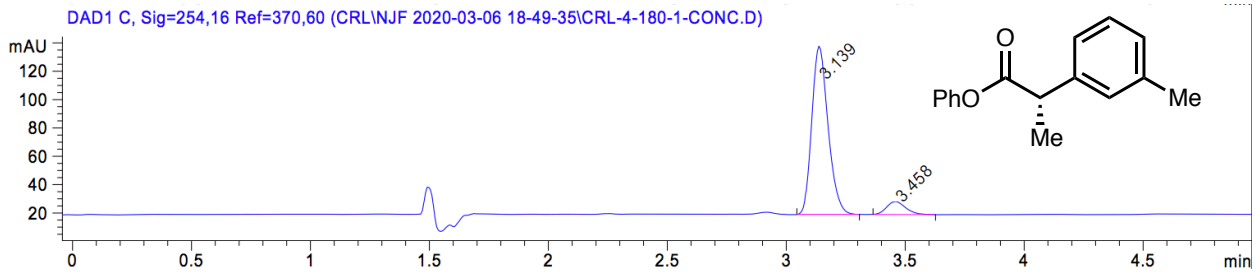
3h: racemic



Signal 1: DAD1 C, Sig=254,16 Ref=370,60

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	2.883	BB	0.0716	760.25134	159.58742	47.6164
2	3.177	BB	0.0868	836.36414	155.34096	52.3836

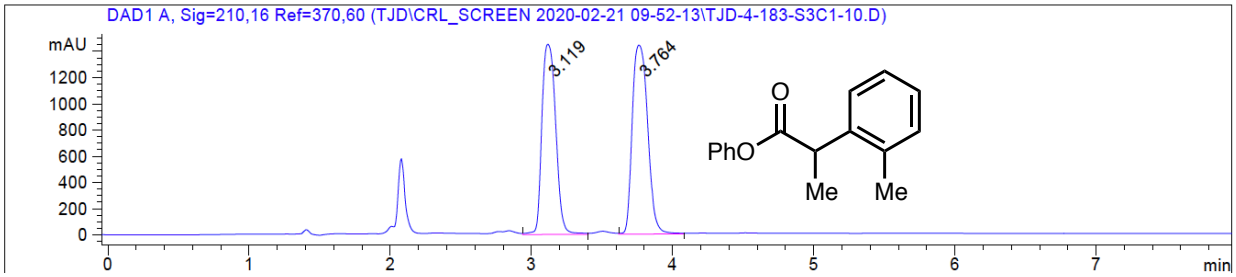
3g: enantioenriched (84% ee)



Signal 2: DAD1 C, Sig=254,16 Ref=370,60

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	3.139	BB	0.0756	562.89771	118.16418	91.8131
2	3.458	BB	0.0882	50.19327	9.11589	8.1869

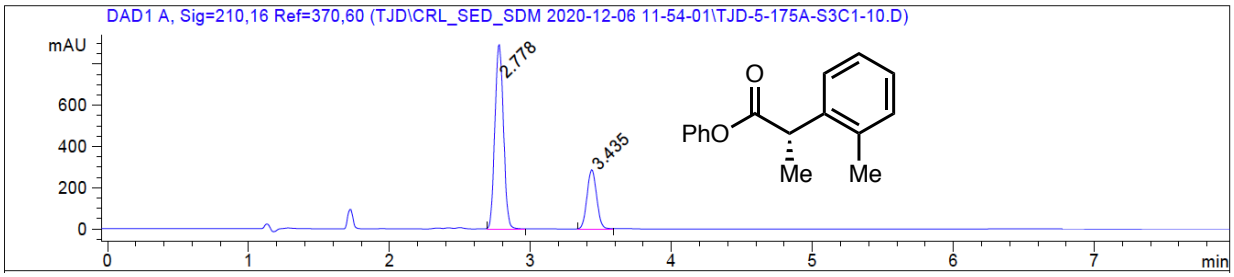
S6: racemic



Signal 1: DAD1 A, Sig=210,16 Ref=370,60

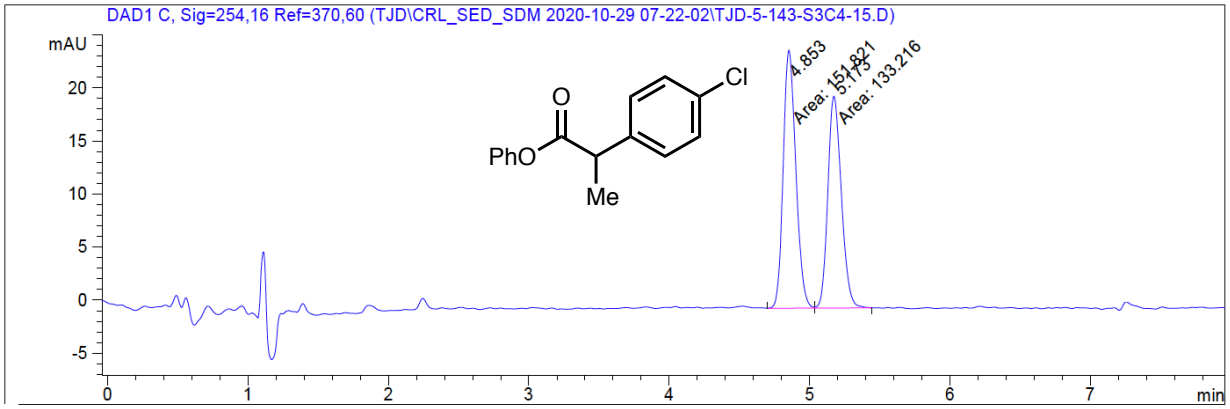
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	3.119	VB	0.1078	9902.10938	1447.56604	47.4210
2	3.764	VB	0.1250	1.09792e4	1439.59082	52.5790

S6: enantioenriched (47% ee)



Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	2.778	BB	0.0695	3782.13501	891.90027	73.4290
2	3.435	BB	0.0758	1368.59949	286.35406	26.5710
Totals :				5150.73450	1178.25433	

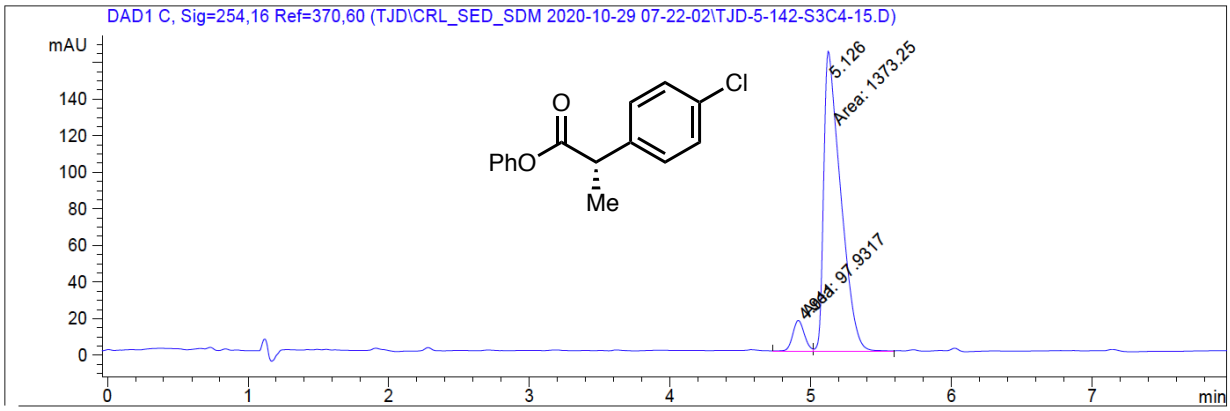
3i: racemic



Signal 1: DAD1 C, Sig=254,16 Ref=370,60

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	4.853	MF	0.1035	151.82059	24.43783	53.2635
2	5.173	FM	0.1107	133.21631	20.05564	46.7365

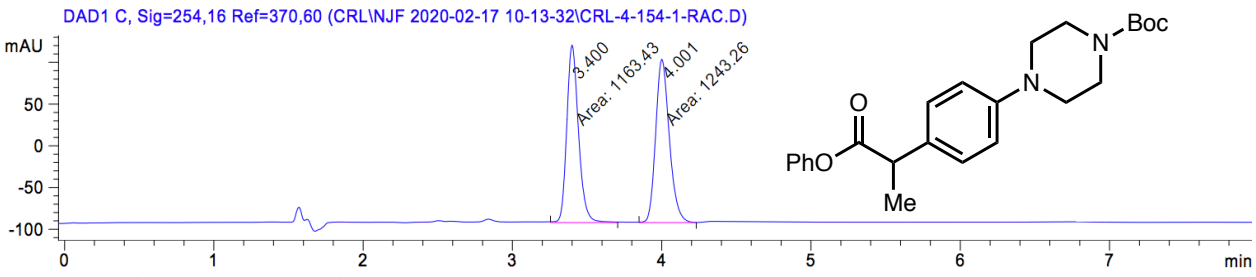
3i: enantioenriched (87% ee)



Signal 1: DAD1 C, Sig=254,16 Ref=370,60

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	4.911	MF	0.0966	97.93172	16.90302	6.6567
2	5.126	FM	0.1395	1373.25208	164.05779	93.3433

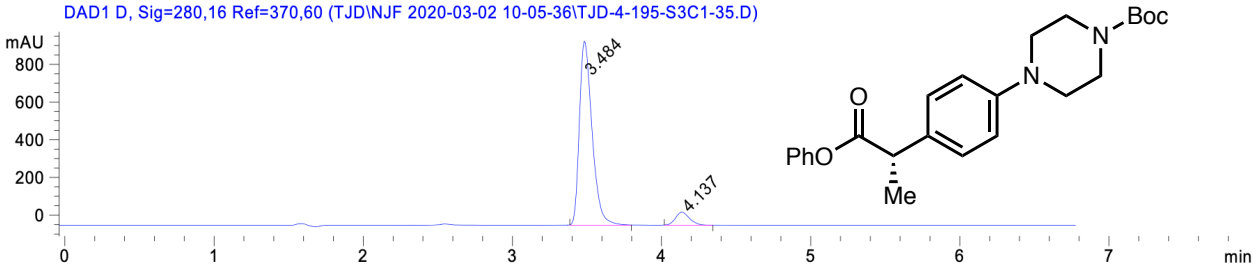
3j: racemic



Signal 2: DAD1 C, Sig=254,16 Ref=370,60

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	3.400	MM	0.0908	1163.42700	213.53700	48.3415
2	4.001	MM	0.1052	1243.25525	196.90825	51.6585

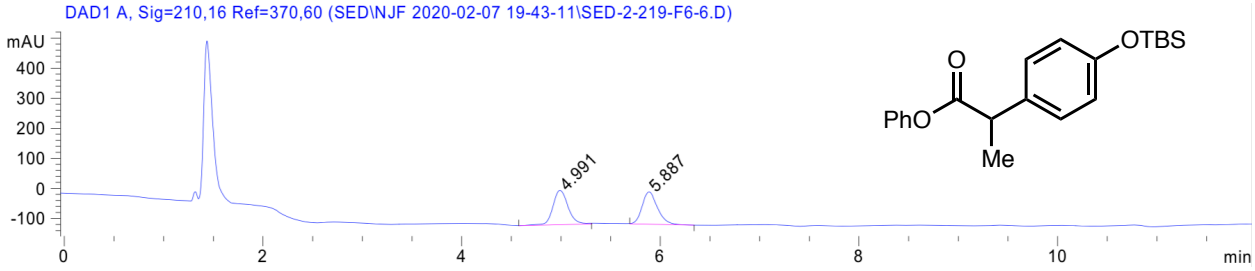
3j: enantioenriched (85% ee)



Signal 3: DAD1 D, Sig=280,16 Ref=370,60

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	3.484	BB	0.0929	5762.43311	976.36920	92.6488
2	4.137	BB	0.1010	457.21939	69.31146	7.3512

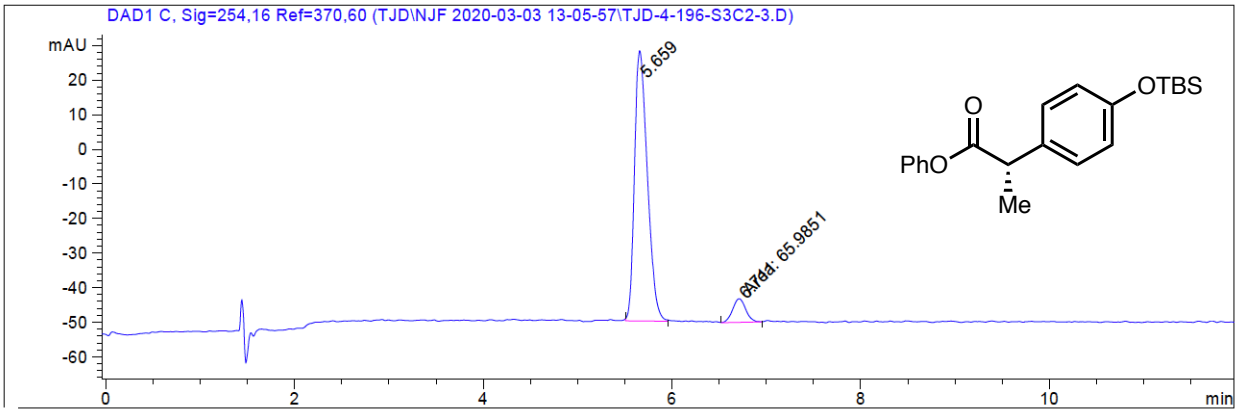
3k: racemic



Signal 1: DAD1 A, Sig=210,16 Ref=370,60

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	4.991	VB	0.1636	1210.89258	114.33277	51.1595
2	5.887	BB	0.1674	1156.00208	107.50758	48.8405

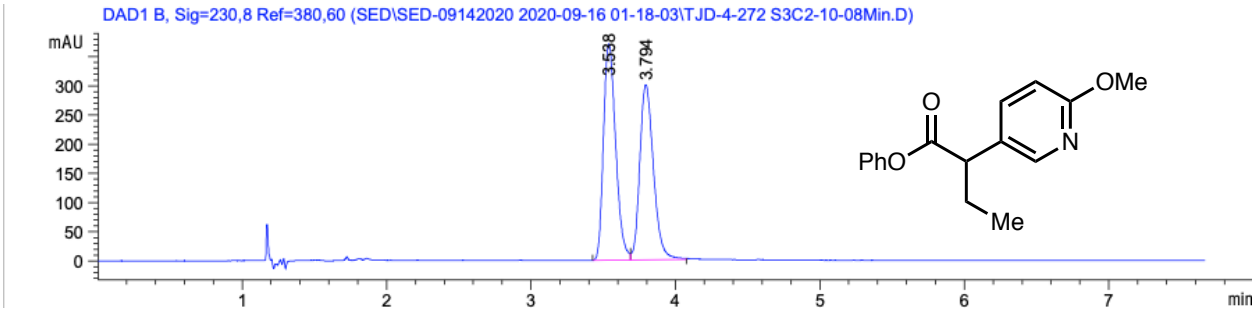
3k: enantioenriched (84% ee)



Signal 1: DAD1 C, Sig=254,16 Ref=370,60

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	5.659	BB	0.1465	741.06787	78.21878	91.8239
2	6.711	MM	0.1607	65.98505	6.84389	8.1761

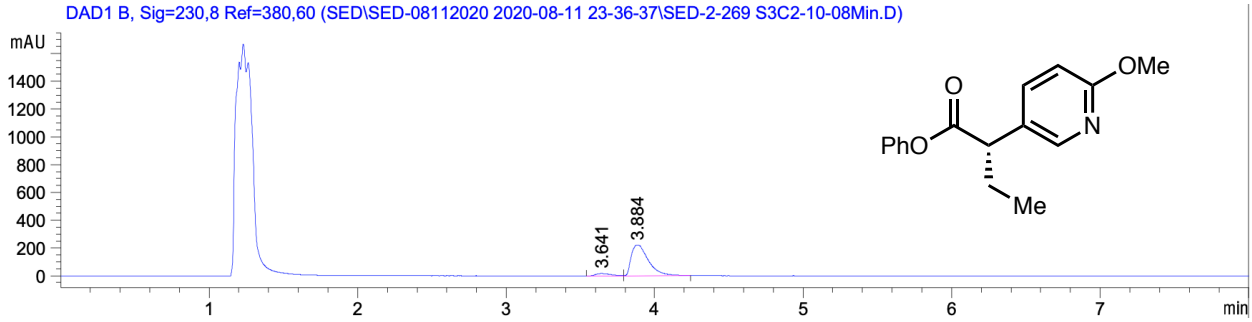
6a: racemic



Signal 2: DAD1 B, Sig=230,8 Ref=380,60

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	3.538	BV	0.0914	2168.98657	370.22299	52.3424
2	3.794	VB	0.1029	1974.85364	299.69391	47.6576

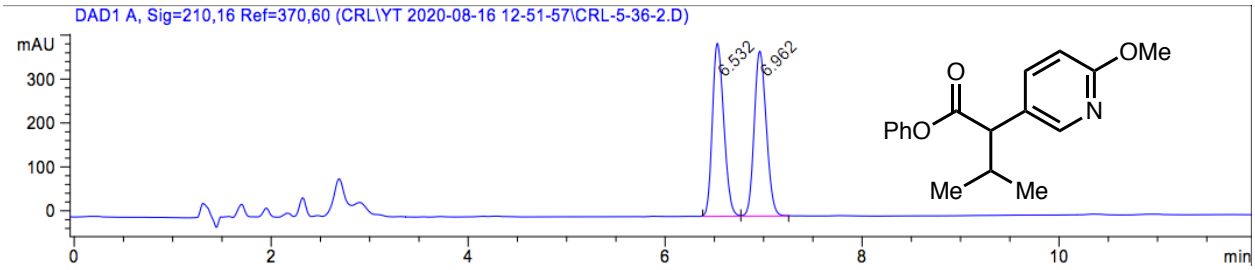
6a: enantioenriched (88% ee)



Signal 2: DAD1 B, Sig=230,8 Ref=380,60

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	3.641	BV	0.1008	117.22110	16.72034	6.0588
2	3.884	VB	0.1291	1817.48889	223.03073	93.9412

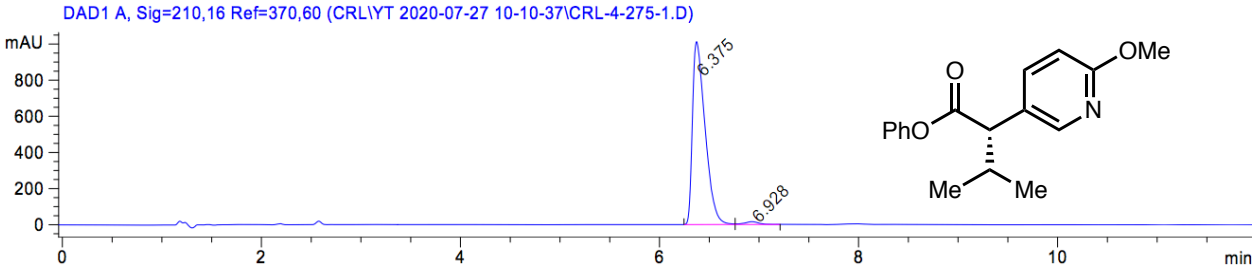
6b: racemic



Signal 2: DAD1 C, Sig=254,16 Ref=370,60

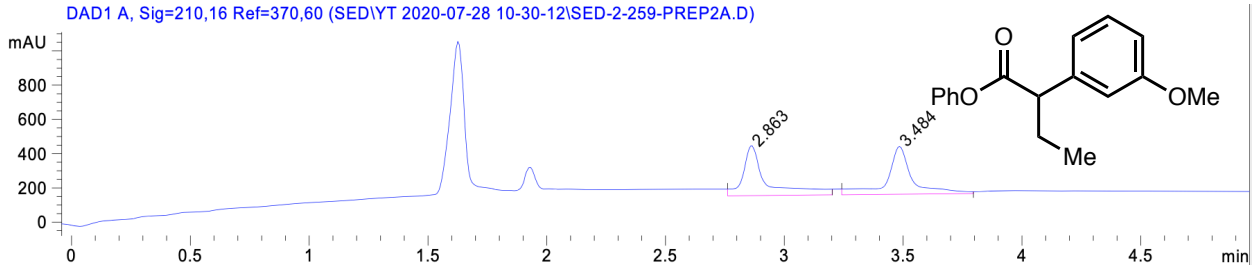
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	6.532	BB	0.1258	477.47354	59.41205	50.2311
2	6.962	BB	0.1342	473.07962	56.19732	49.7689

6b: enantioenriched (96% ee)



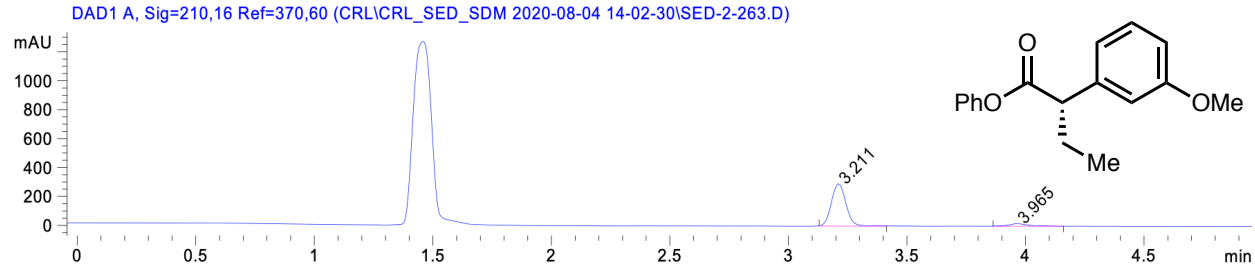
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	6.375	BV	0.1344	8893.69629	1013.02643	98.2261
2	6.928	VB	0.1465	160.61084	15.81807	1.7739

6c: racemic



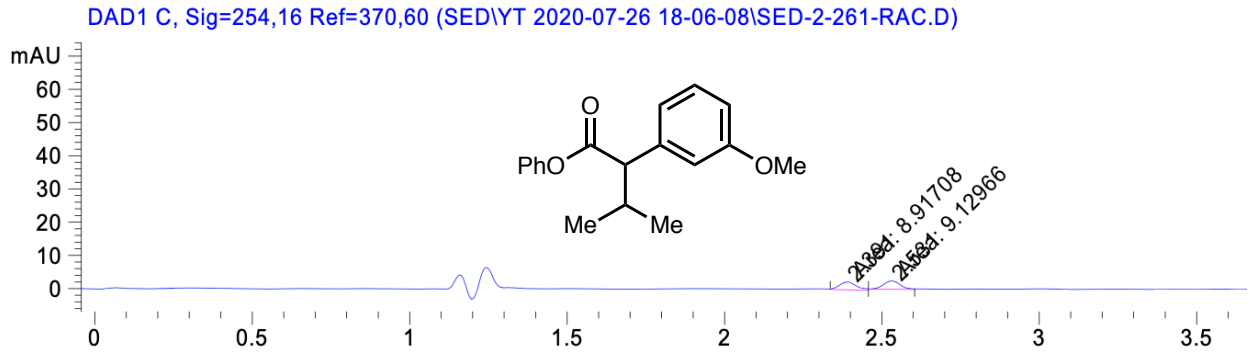
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	2.863	BB	0.0973	2002.59912	287.39008	49.3969
2	3.484	BV	0.1062	2051.50366	277.62616	50.6031

6c: enantioenriched (85% ee)



Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	3.211	BB	0.0700	1246.63501	291.08588	92.4092
2	3.965	BB	0.0851	102.40295	18.36087	7.5908

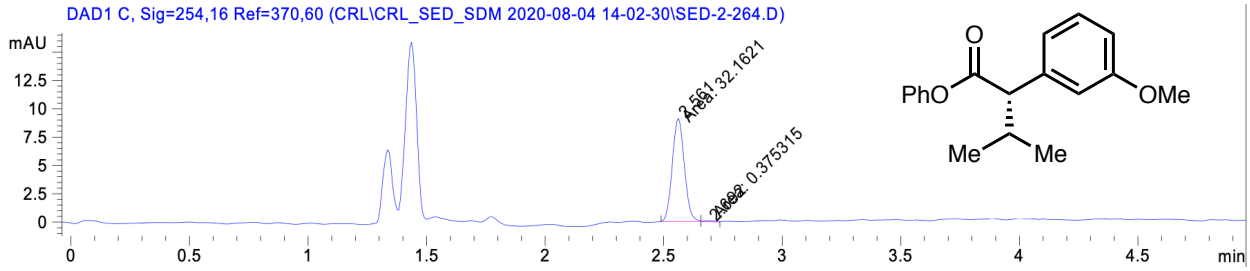
6d: racemic



Signal 2: DAD1 C, Sig=254,16 Ref=370,60

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	2.391	MM	0.0622	8.91708	2.38762	49.4110
2	2.531	MM	0.0591	9.12966	2.57560	50.5890

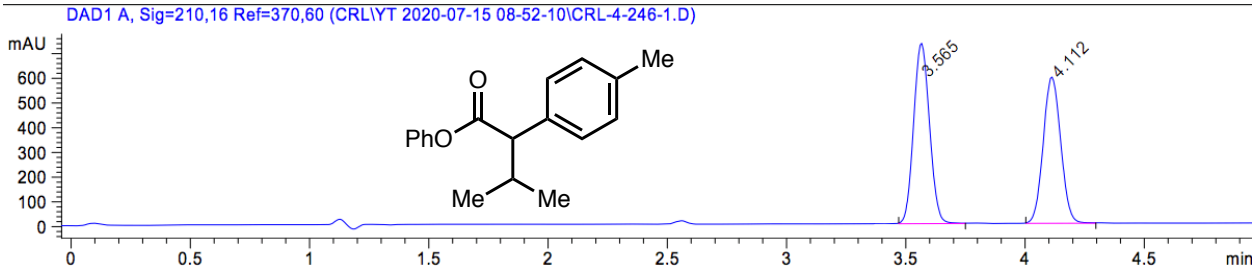
6d: enantioenriched (98% ee)



Signal 2: DAD1 C, Sig=254,16 Ref=370,60

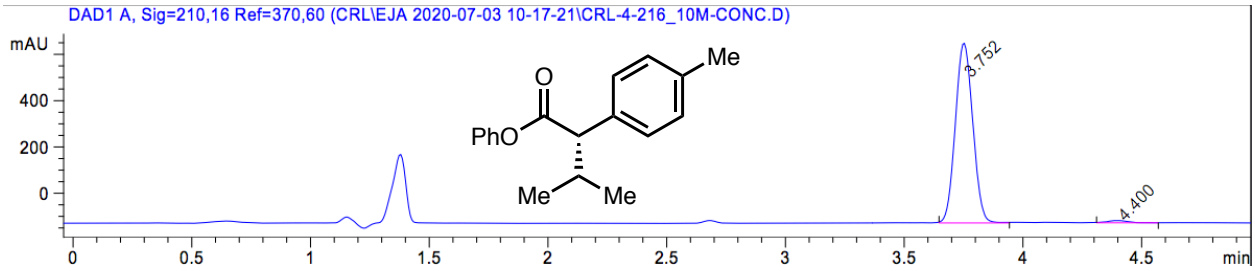
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	2.561	MM	0.0584	32.16210	9.17854	98.8465
2	2.692	MM	0.0596	3.75315e-1	1.04957e-1	1.1535

6e: racemic



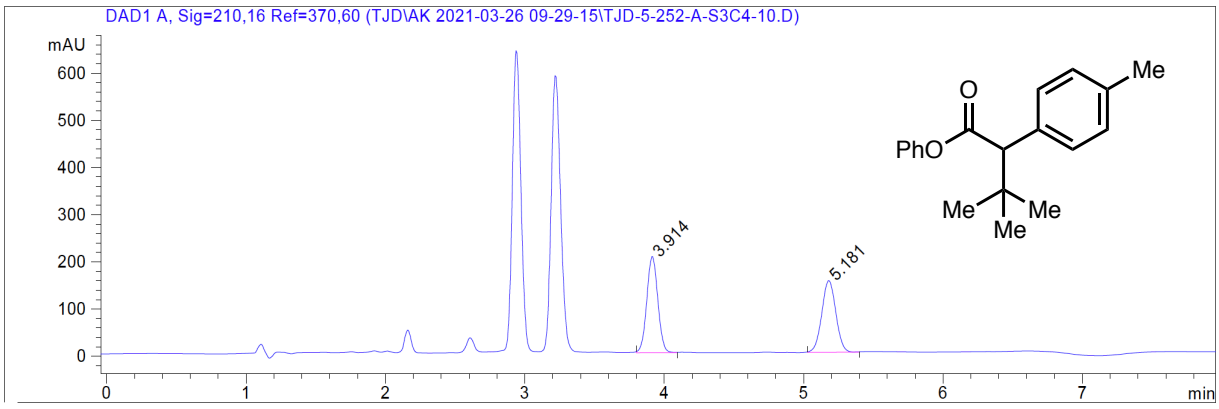
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	3.565	BB	0.0741	3370.06152	726.86560	52.6856
2	4.112	BB	0.0798	3026.49292	590.10248	47.3144

6e: enantioenriched (97% ee)



Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	3.752	BB	0.0840	3964.34082	771.31055	98.5706
2	4.400	BB	0.0911	57.48809	9.99575	1.4294
Totals :				4021.82891	781.30630	

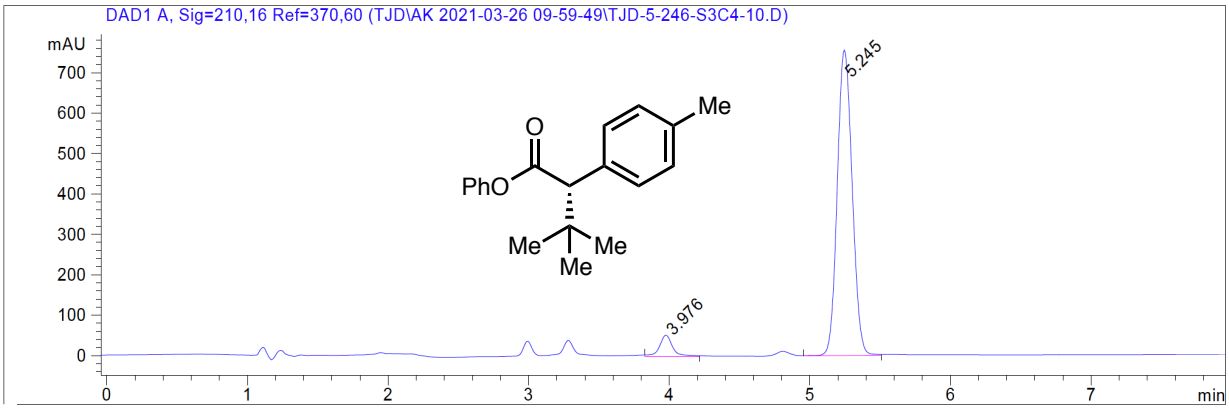
6f: racemic



Signal 1: DAD1 A, Sig=210,16 Ref=370,60

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	3.914	BB	0.0885	1121.01794	202.67258	51.2899
2	5.181	BB	0.1140	1064.63135	151.49474	48.7101

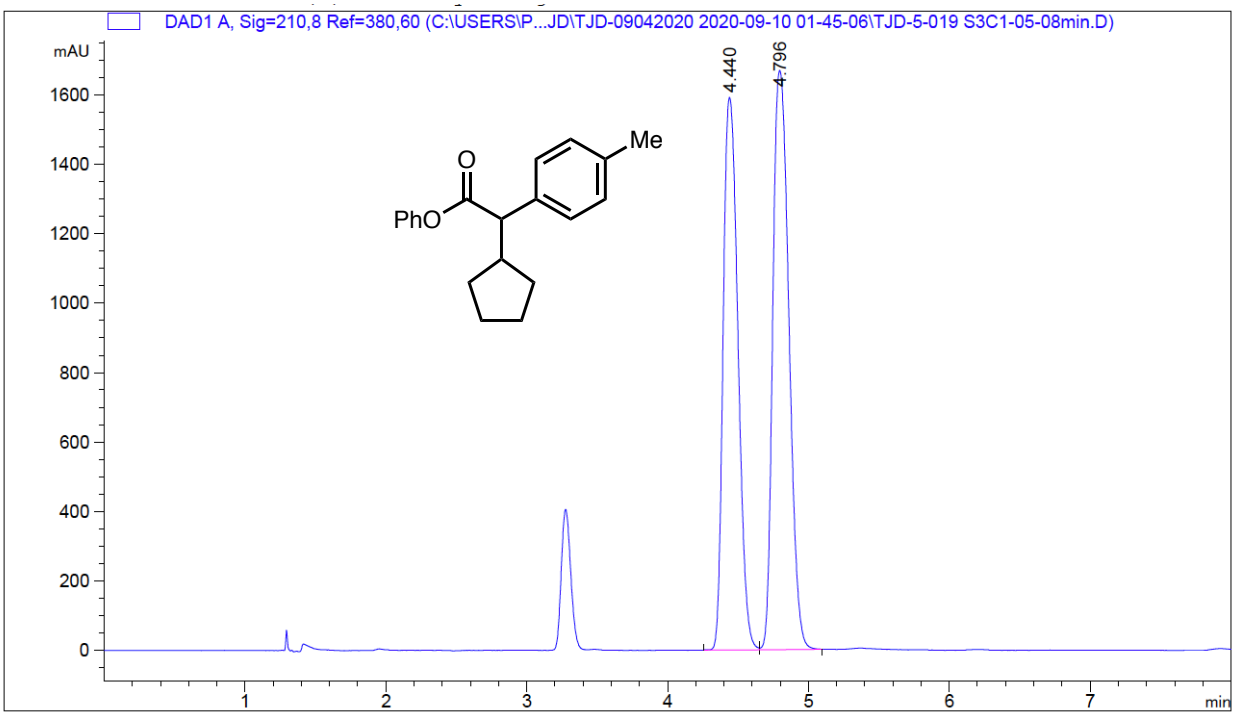
6f: enantioenriched (89% ee)



Signal 1: DAD1 A, Sig=210,16 Ref=370,60

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	3.976	BB	0.0952	334.60458	51.92270	5.6587
2	5.245	VB	0.1182	5578.52588	754.67139	94.3413

6g: racemic

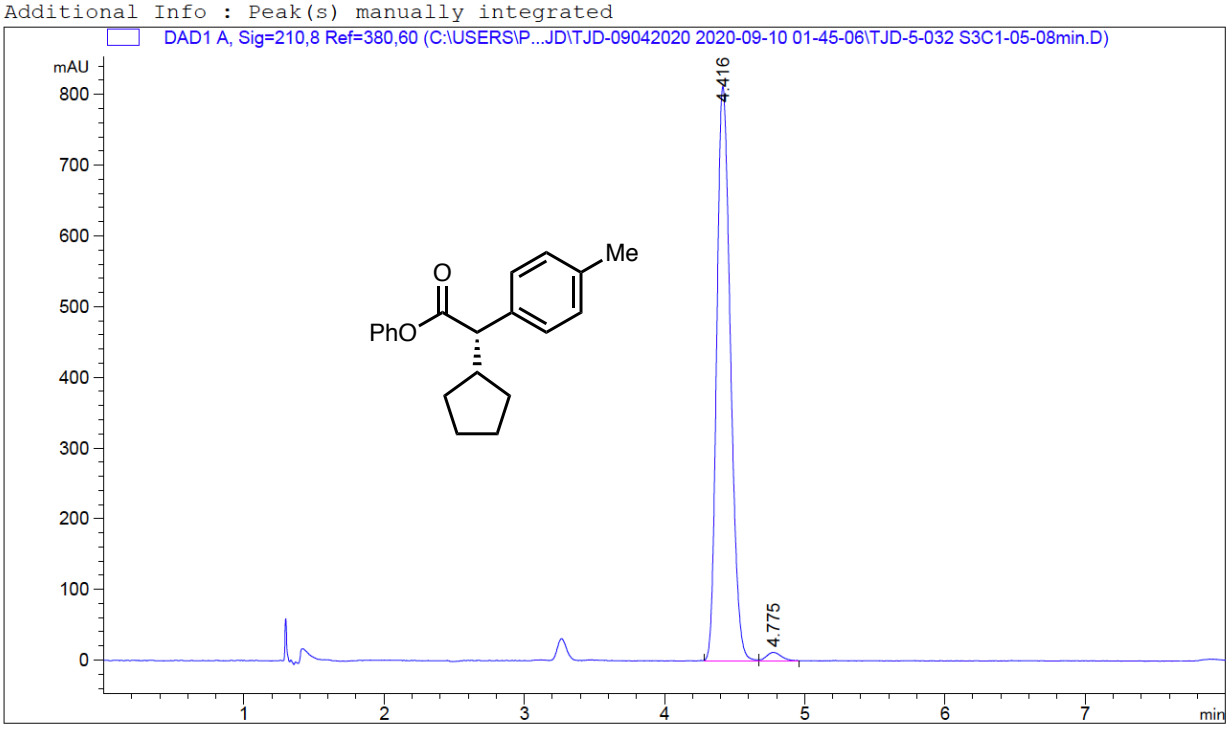


Signal 1: DAD1 A, Sig=210,8 Ref=380,60

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	4.440	BV	0.1160	1.16044e4	1592.55542	46.6413
2	4.796	VB	0.1278	1.32757e4	1669.30603	53.3587

6g: enantioenriched (97% ee)

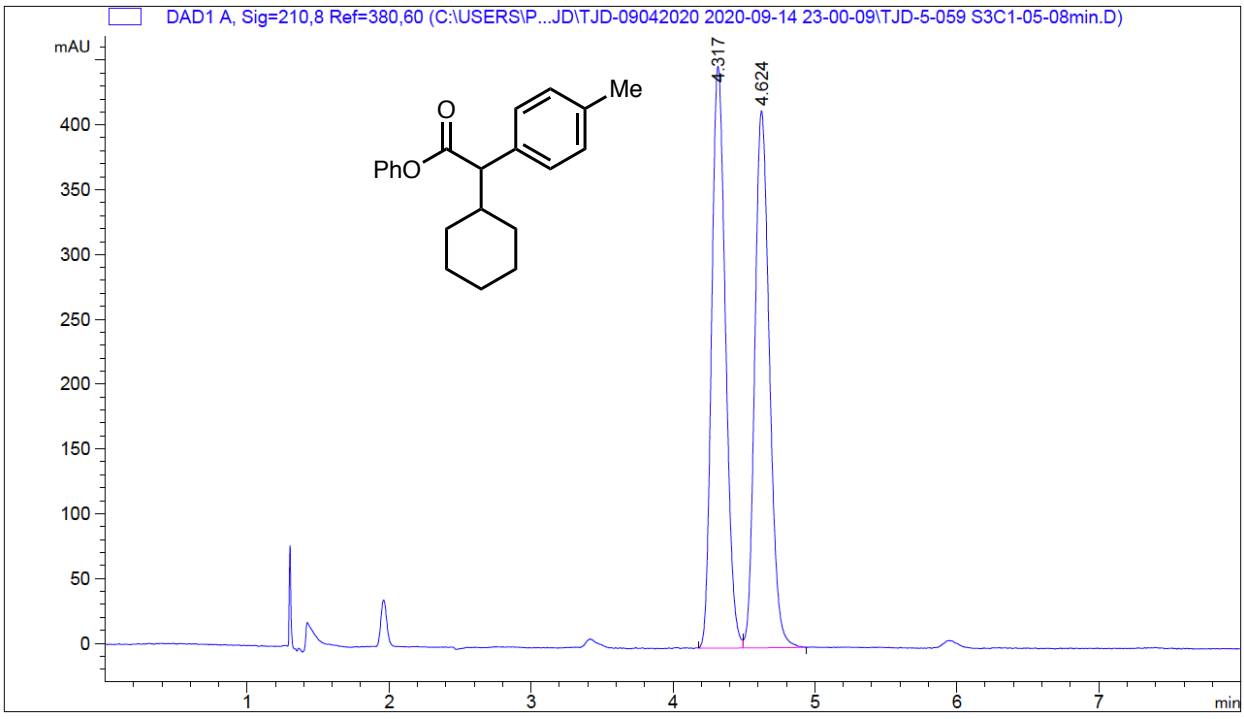
Additional Info : Peak(s) manually integrated



Signal 1: DAD1 A, Sig=210,8 Ref=380,60

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	4.416	BB	0.1053	5520.55078	812.62140	98.4486
2	4.775	BB	0.1129	86.99767	11.95724	1.5514

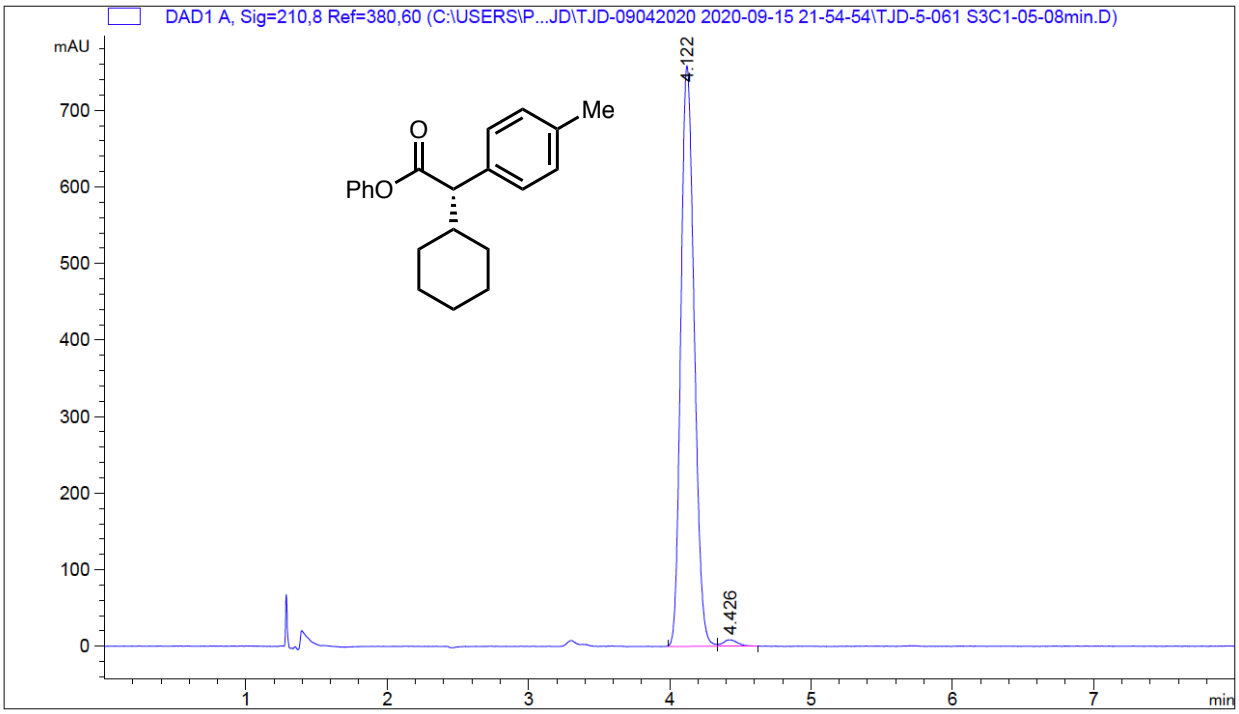
6h: racemic



Signal 1: DAD1 A, Sig=210,8 Ref=380,60

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	4.317	BV	0.1073	3052.68945	449.10693	50.5905
2	4.624	VB	0.1120	2981.42773	414.27054	49.4095

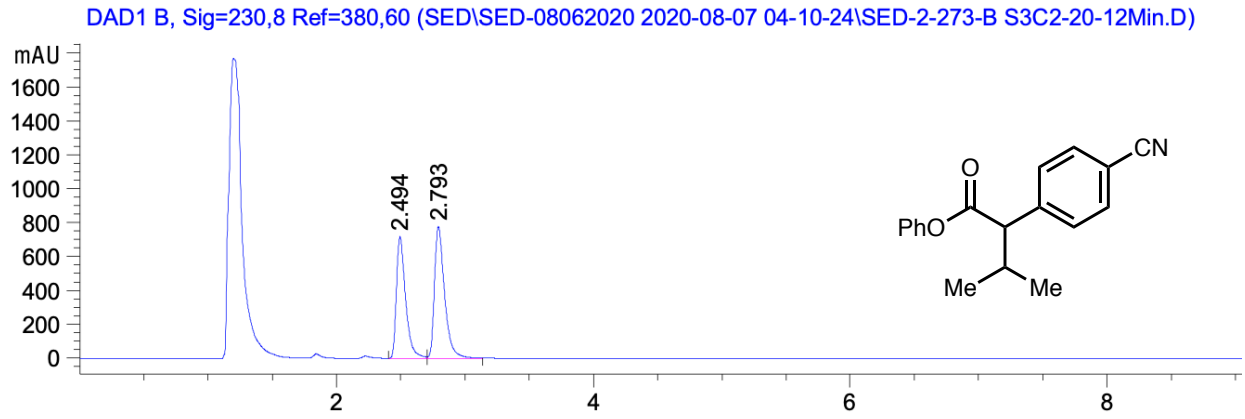
6h: enantioenriched (98% ee)



Signal 1: DAD1 A, Sig=210,8 Ref=380,60

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	4.122	BV	0.1030	5002.38818	758.40417	98.7564
2	4.426	VB	0.1116	62.99316	8.48333	1.2436

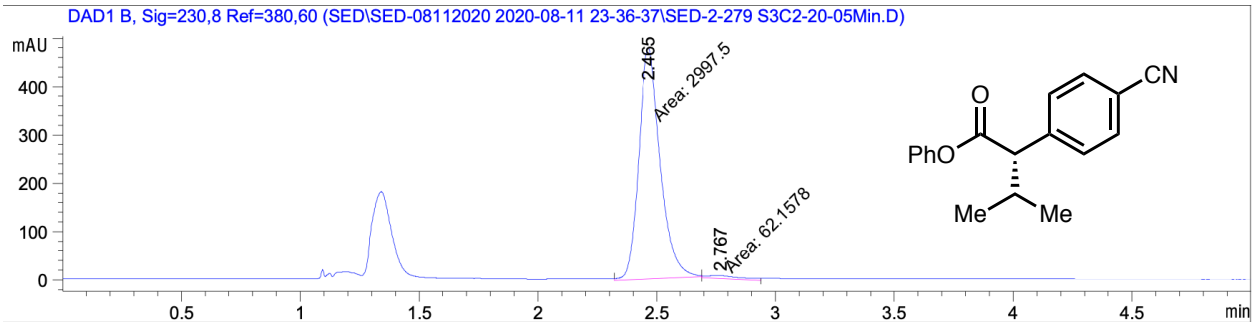
6k: racemic



Signal 1: DAD1 A, Sig=210,8 Ref=380,60

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	2.494	BV	0.0749	1755.62146	354.03247	45.7863
2	2.793	VB	0.0824	2078.76001	382.38654	54.2137

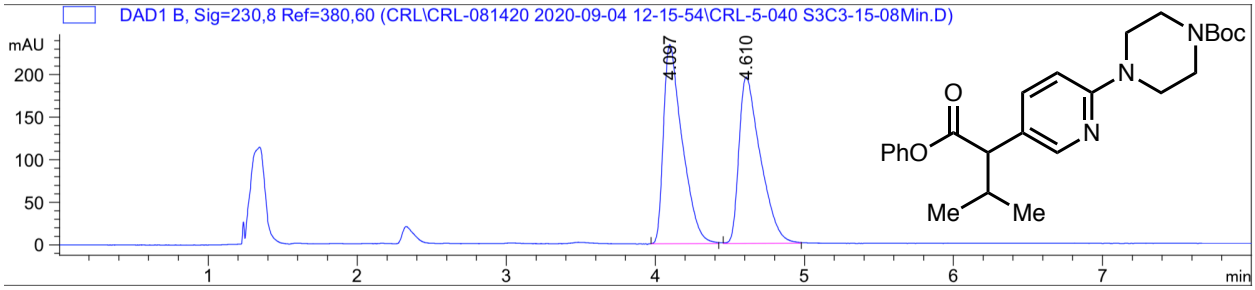
6k: enantioenriched (96% ee)



Signal 2: DAD1 B, Sig=230,8 Ref=380,60

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	2.465	MM	0.1044	2997.49683	478.73755	97.9685
2	2.767	MM	0.1767	62.15777	5.86131	2.0315

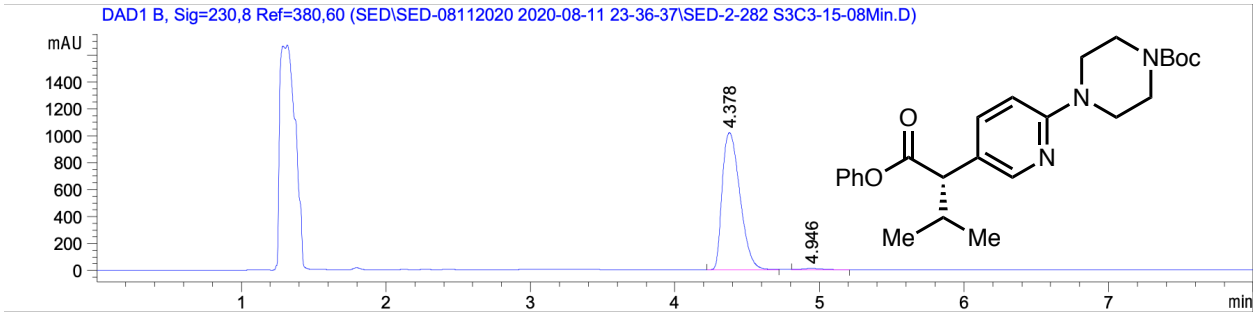
6l: racemic



Signal 2: DAD1 B, Sig=230,8 Ref=380,60

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	4.097	BB	0.1271	2048.80249	234.09145	51.1026
2	4.610	BB	0.1479	1960.39368	195.58250	48.8974

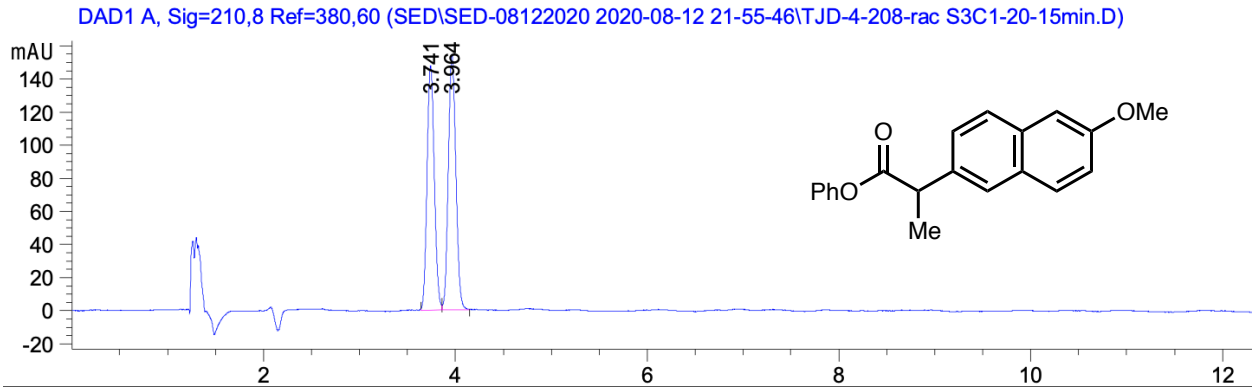
6l: enantioenriched (97% ee)



Signal 2: DAD1 B, Sig=230,8 Ref=380,60

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	4.378	BB	0.1357	8701.73438	1018.52362	98.6089
2	4.946	BB	0.1641	122.75417	11.09463	1.3911

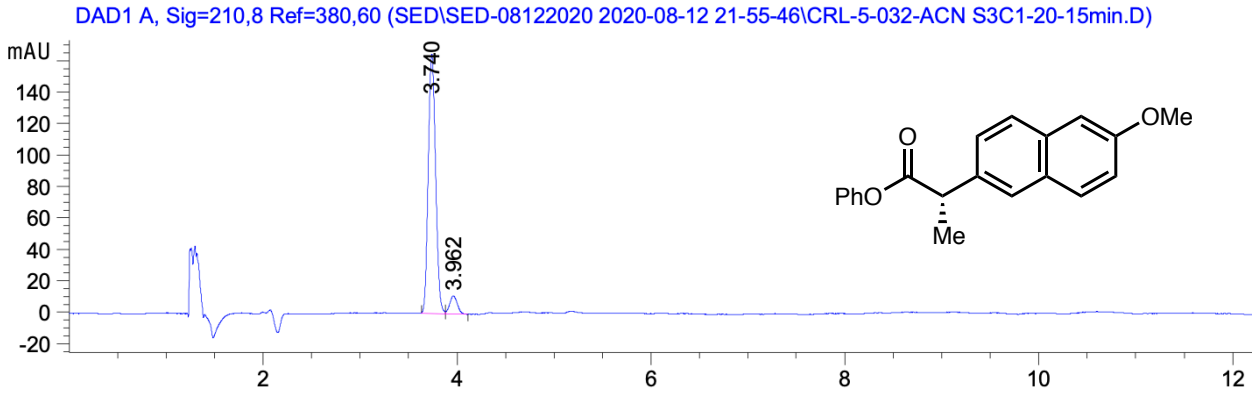
8: racemic



Signal 1: DAD1 A, Sig=210,8 Ref=380,60

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	3.741	BV	0.0827	781.13239	147.68906	48.0866
2	3.964	VB	0.0857	843.29541	154.40327	51.9134

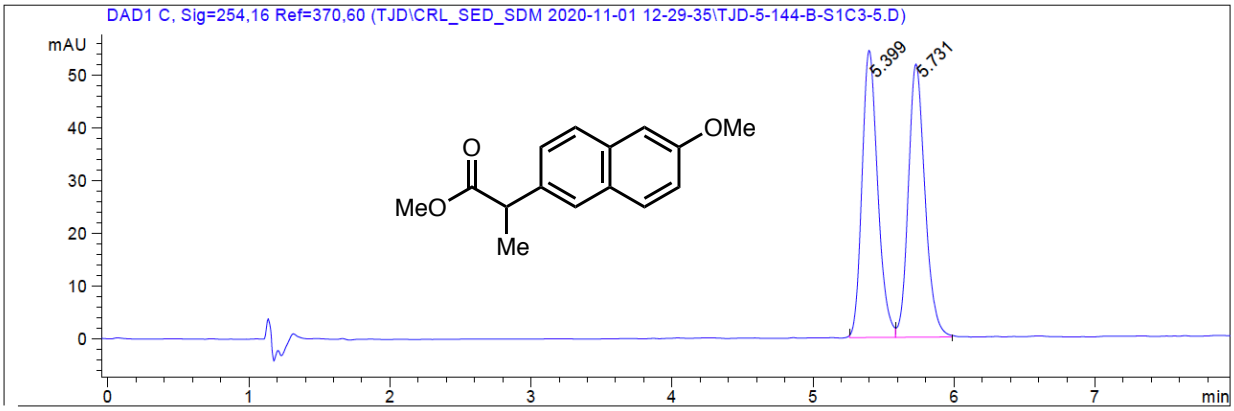
8: enantioenriched (86% ee)



Signal 1: DAD1 A, Sig=210,8 Ref=380,60

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	3.740	BV	0.0836	871.17084	165.12762	93.2478
2	3.962	VB	0.0859	63.08263	11.51540	6.7522

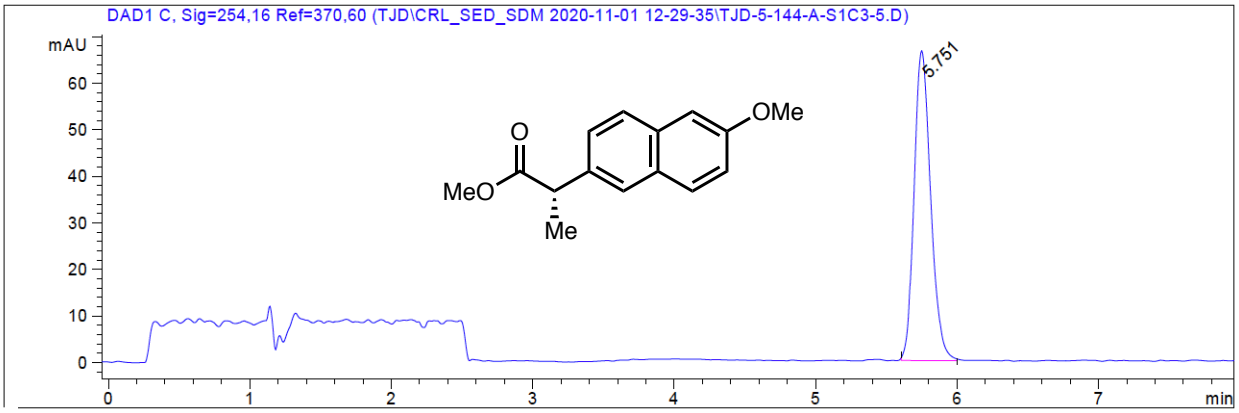
9-OMe: racemic



Signal 1: DAD1 C, Sig=254,16 Ref=370,60

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	5.399	BV	0.1185	421.47626	54.33418	49.6834
2	5.731	VB	0.1283	426.84814	51.69842	50.3166

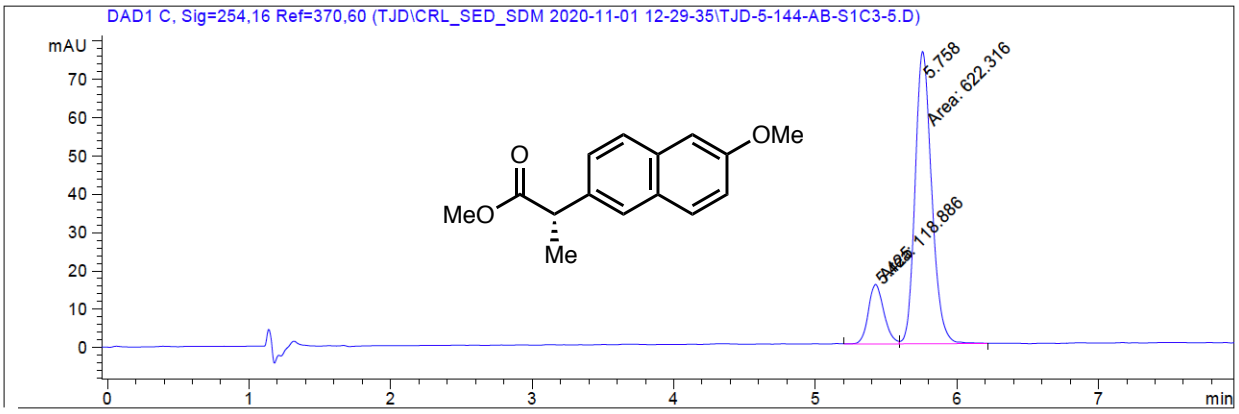
9-OMe: from commercial (*S*)-naproxen



Signal 1: DAD1 C, Sig=254,16 Ref=370,60

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	5.751	BB	0.1272	542.44702	66.49943	100.0000

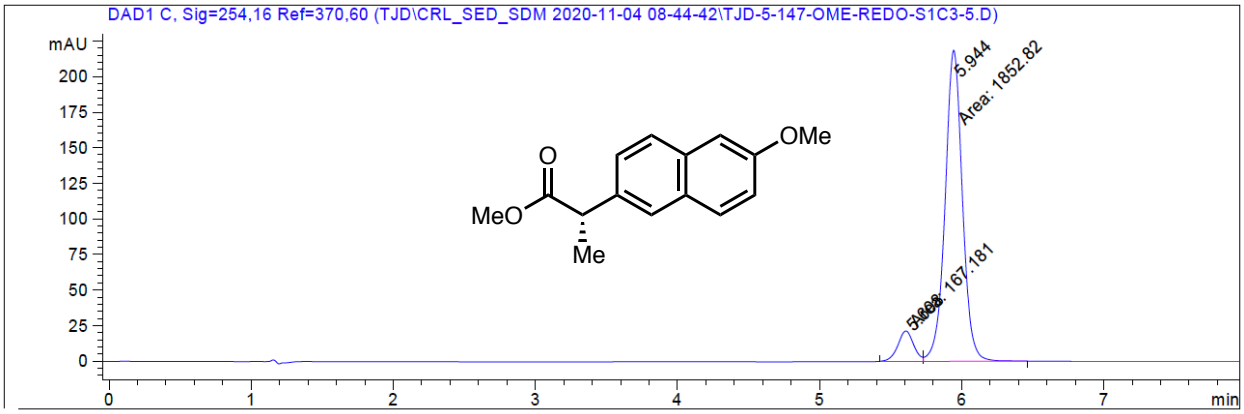
9-OMe: scalemic mixture of racemic **9-OMe** and **9-OMe** derived from (S)-naproxen



Signal 1: DAD1 C, Sig=254,16 Ref=370,60

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	5.425	MF	0.1271	118.88623	15.59370	16.0397
2	5.758	FM	0.1354	622.31573	76.57549	83.9603

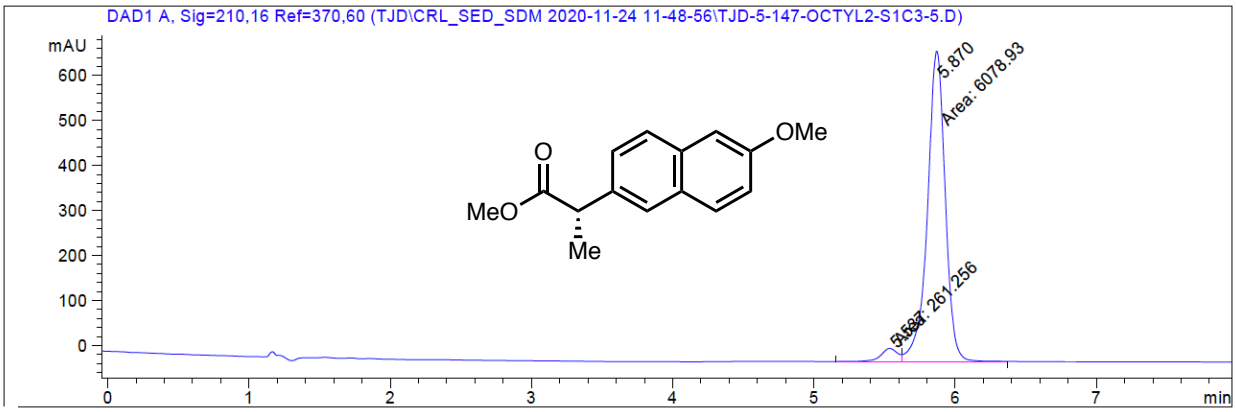
9-OMe: enantioenriched (from coupling) (83% ee)



Signal 1: DAD1 C, Sig=254,16 Ref=370,60

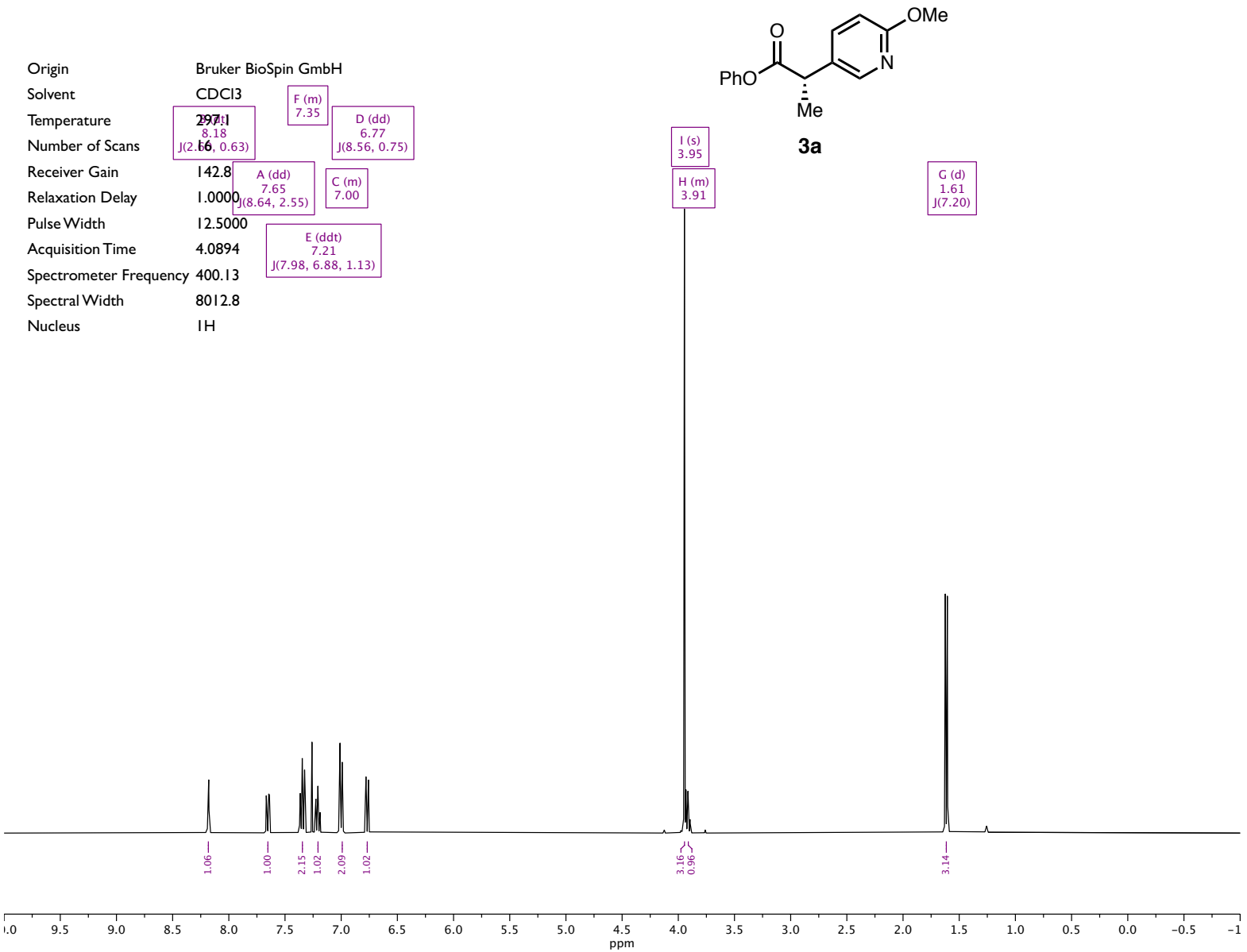
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	5.608	MF	0.1294	167.18143	21.53582	8.2763
2	5.944	FM	0.1408	1852.82397	219.37854	91.7237

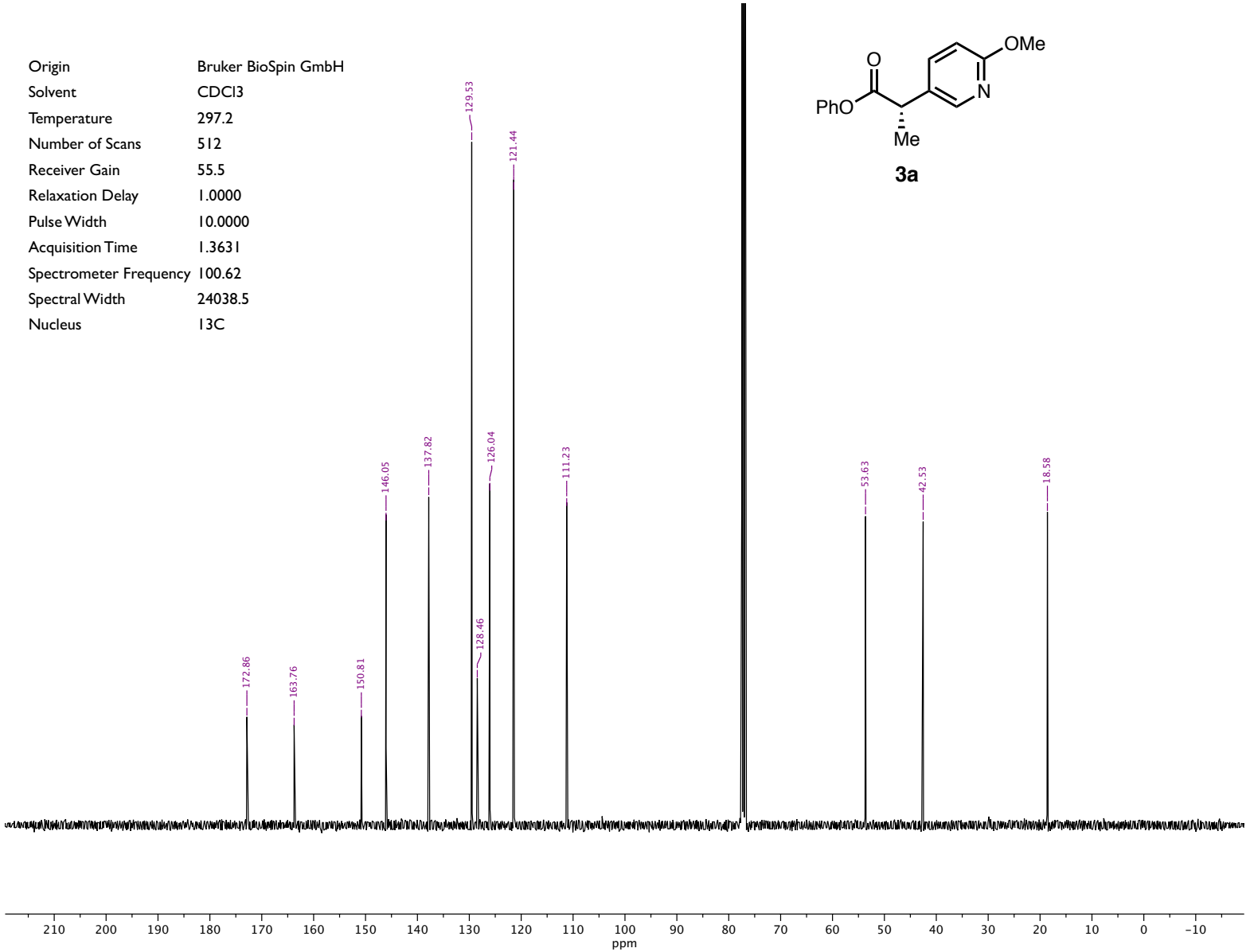
9-OMe: enantioenriched (after recrystallization) (92% ee)

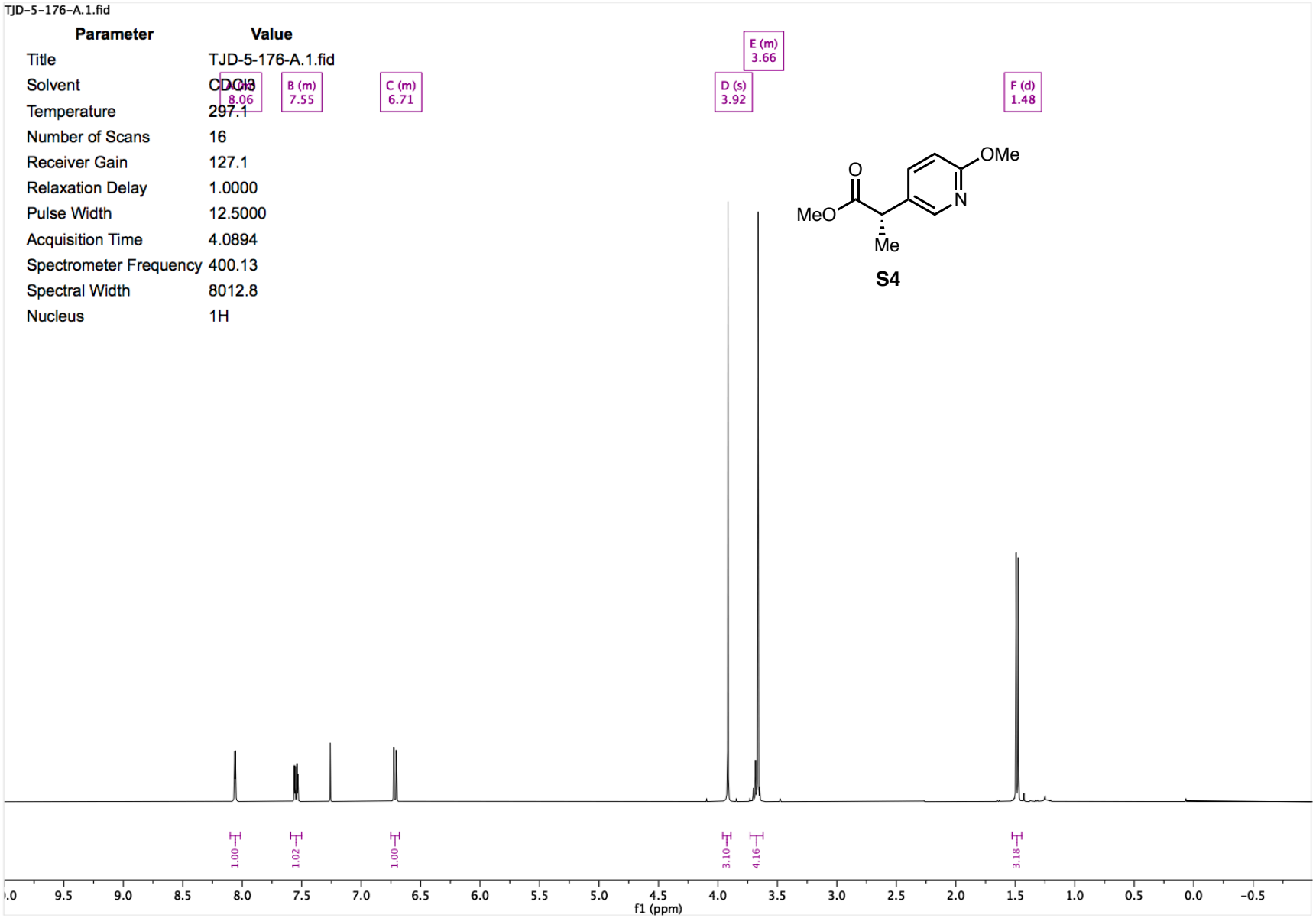


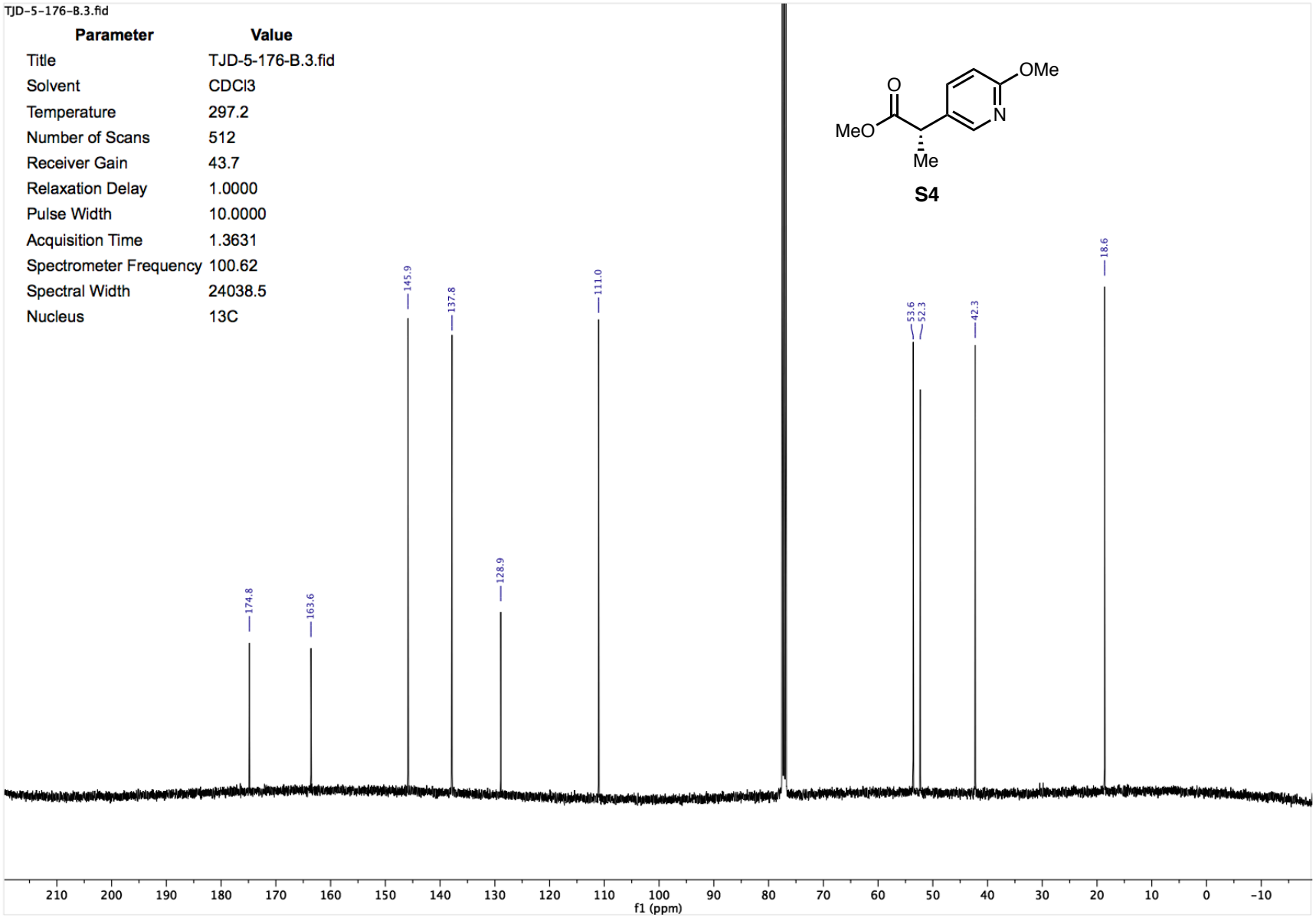
Signal 1: DAD1 A, Sig=210,16 Ref=370,60

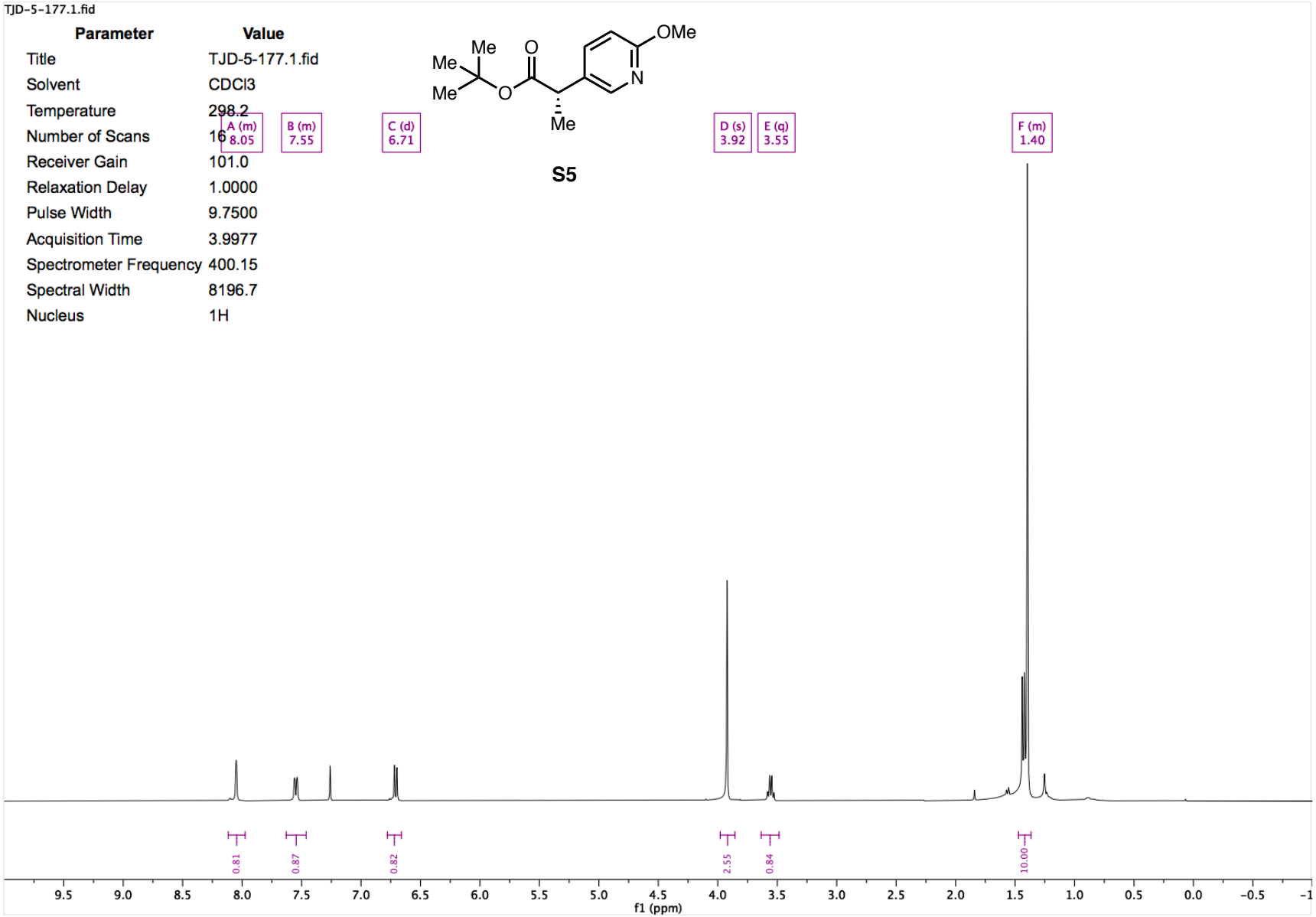
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	5.537	MF	0.1456	261.25620	29.90784	4.1206
2	5.870	FM	0.1463	6078.92725	692.64124	95.8794

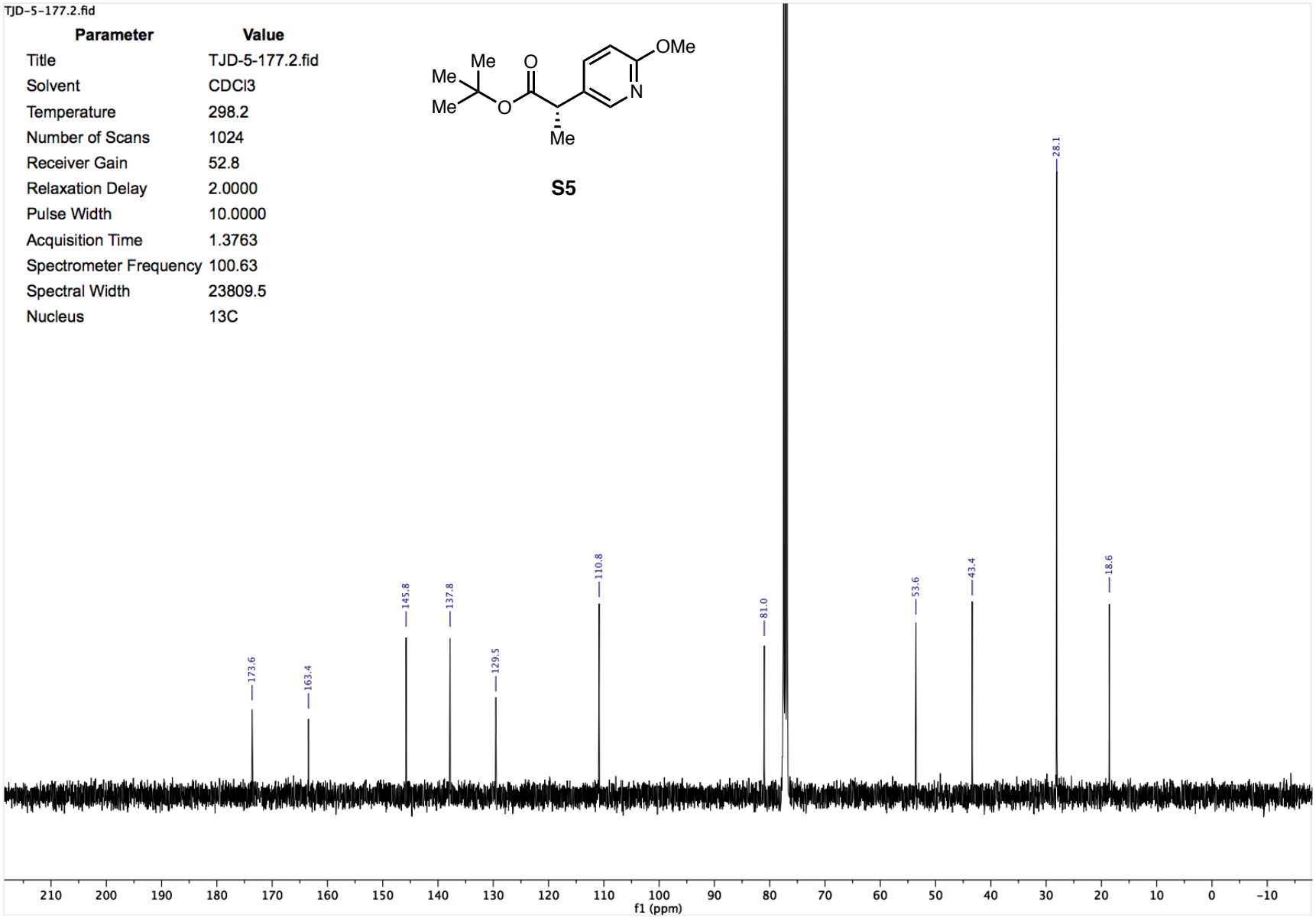

Origin Bruker BioSpin GmbH
Solvent CDCl3
Temperature 297.1
Number of Scans 16
Receiver Gain 142.8
Relaxation Delay 1.0000
Pulse Width 12.5000
Acquisition Time 4.0894
Spectrometer Frequency 400.13
Spectral Width 8012.8
Nucleus 1H
OMe
O
N
PhO
Me
3a
F (m) 7.35
D (dd) 6.77 J(8.56, 0.75)
A (dd) 7.65 J(8.64, 2.55)
C (m) 7.00
E (ddt) 7.21 J(7.98, 6.88, 1.13)
I (s) 3.95
H (m) 3.91
G (d) 1.61 J(7.20)
1.06
1.00
2.15
1.02
2.09
1.02
3.16
0.96
3.14
ppm


Origin Bruker BioSpin GmbH
Solvent CDCl3
Temperature 297.2
Number of Scans 512
Receiver Gain 55.5
Relaxation Delay 1.0000
Pulse Width 10.0000
Acquisition Time 1.3631
Spectrometer Frequency 100.62
Spectral Width 24038.5
Nucleus 13C
OMe
O
PhO
N
Me
3a
129.53
121.44
146.05
137.82
126.04
111.23
53.63
42.53
18.58
172.86
163.76
150.81
128.46
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 −10
ppm

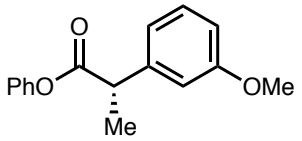

TJD-5-176-A.1.fid
Parameter
Value
Title
TJD-5-176-A.1.fid
Solvent
CDCl3
Temperature
297.1
Number of Scans
16
Receiver Gain
127.1
Relaxation Delay
1.0000
Pulse Width
12.5000
Acquisition Time
4.0894
Spectrometer Frequency
400.13
Spectral Width
8012.8
Nucleus
1H
A (m) 8.06
B (m) 7.55
C (m) 6.71
D (s) 3.92
E (m) 3.66
F (d) 1.48
OMe
O
MeO
N
Me
S4
1.00
1.02
1.00
3.10
4.16
3.18
f1 (ppm)


TJD-5-176-B.3.fid
Parameter Value
Title TJD-5-176-B.3.fid
Solvent CDCl3
Temperature 297.2
Number of Scans 512
Receiver Gain 43.7
Relaxation Delay 1.0000
Pulse Width 10.0000
Acquisition Time 1.3631
Spectrometer Frequency 100.62
Spectral Width 24038.5
Nucleus 13C
OMe
O
MeO
N
Me
S4
174.8
163.6
145.9
137.8
128.9
111.0
53.6
52.3
42.3
18.6
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

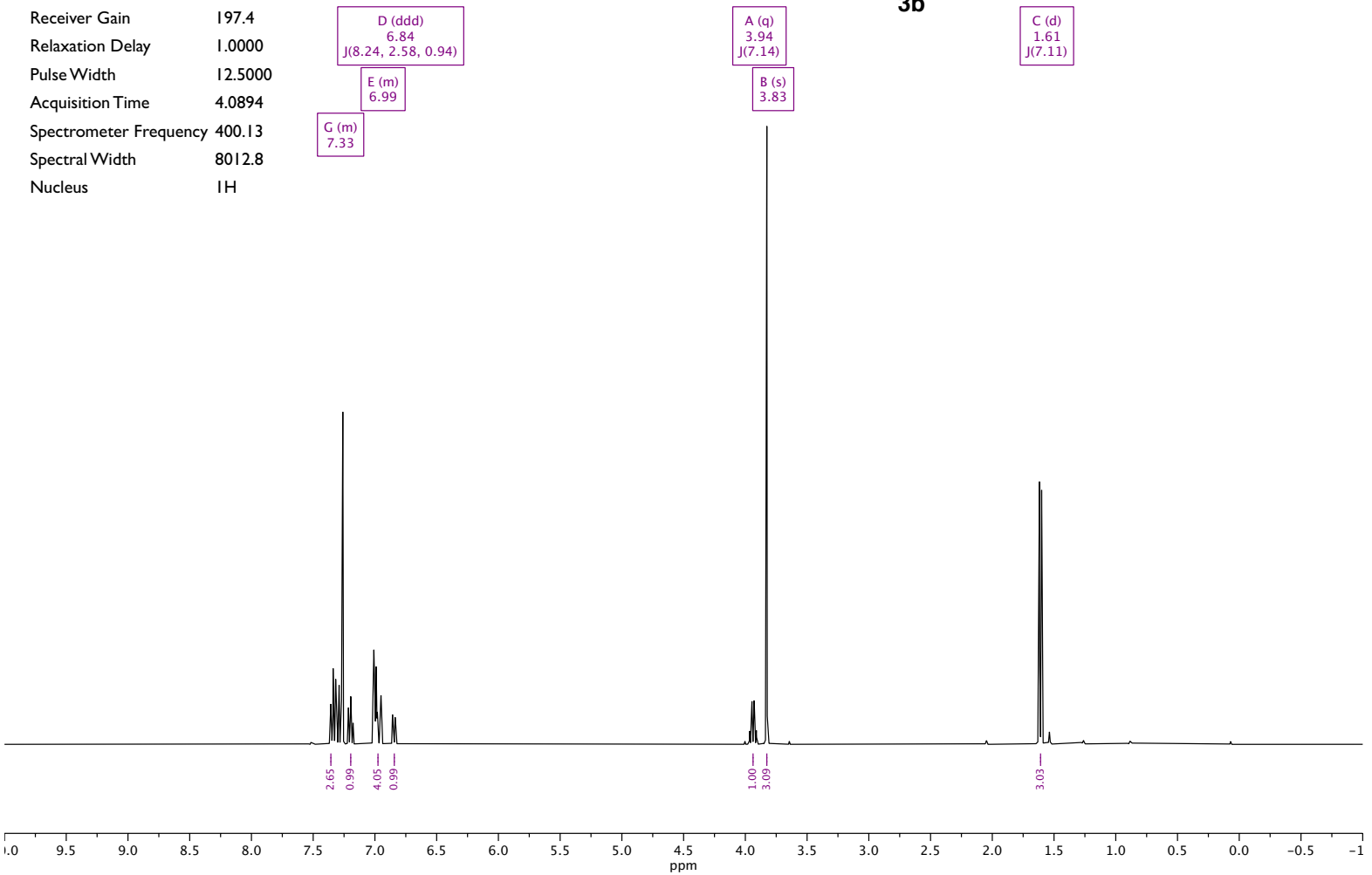

TJD-5-177.1.fid
Parameter Value
Title TJD-5-177.1.fid
Solvent CDCl3
Temperature 298.2
Number of Scans 16
Receiver Gain 101.0
Relaxation Delay 1.0000
Pulse Width 9.7500
Acquisition Time 3.9977
Spectrometer Frequency 400.15
Spectral Width 8196.7
Nucleus 1H
A (m) 8.05
B (m) 7.55
C (d) 6.71
D (s) 3.92
E (q) 3.55
F (m) 1.40
Me
Me
Me
O
O
OMe
N
Me
S5
0.81
0.87
0.82
2.55
0.84
10.00
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1
f1 (ppm)


TJD-5-177.2.fid
Parameter Value
Title TJD-5-177.2.fid
Solvent CDCl3
Temperature 298.2
Number of Scans 1024
Receiver Gain 52.8
Relaxation Delay 2.0000
Pulse Width 10.0000
Acquisition Time 1.3763
Spectrometer Frequency 100.63
Spectral Width 23809.5
Nucleus 13C
Me
Me
Me
O
O
OMe
N
Me
S5
28.1
18.6
43.4
53.6
81.0
110.8
129.5
137.8
145.8
163.4
173.6
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

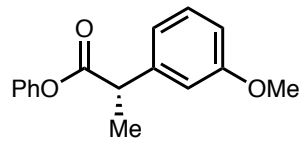
Origin	Bruker BioSpin GmbH
Solvent	CDCl3
Temperature	297.2
Number of Scans	16
Receiver Gain	197.4
Relaxation Delay	1.0000
Pulse Width	12.5000
Acquisition Time	4.0894
Spectrometer Frequency	400.13
Spectral Width	8012.8
Nucleus	1H



3b

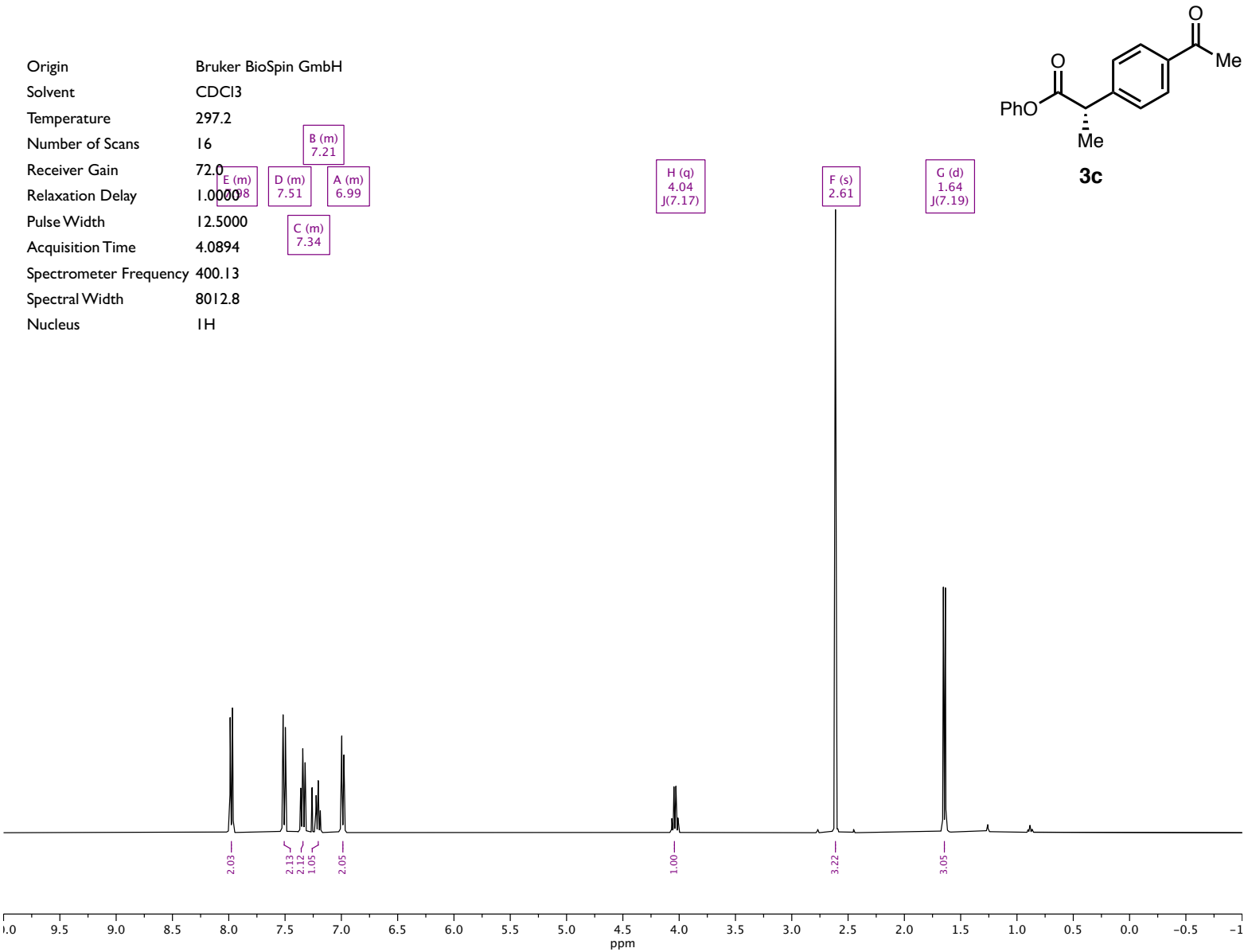


Origin	Bruker BioSpin GmbH
Solvent	CDCl3
Temperature	297.2
Number of Scans	512
Receiver Gain	50.3
Relaxation Delay	1.0000
Pulse Width	10.0000
Acquisition Time	1.3631
Spectrometer Frequency	100.62
Spectral Width	24038.5
Nucleus	13C



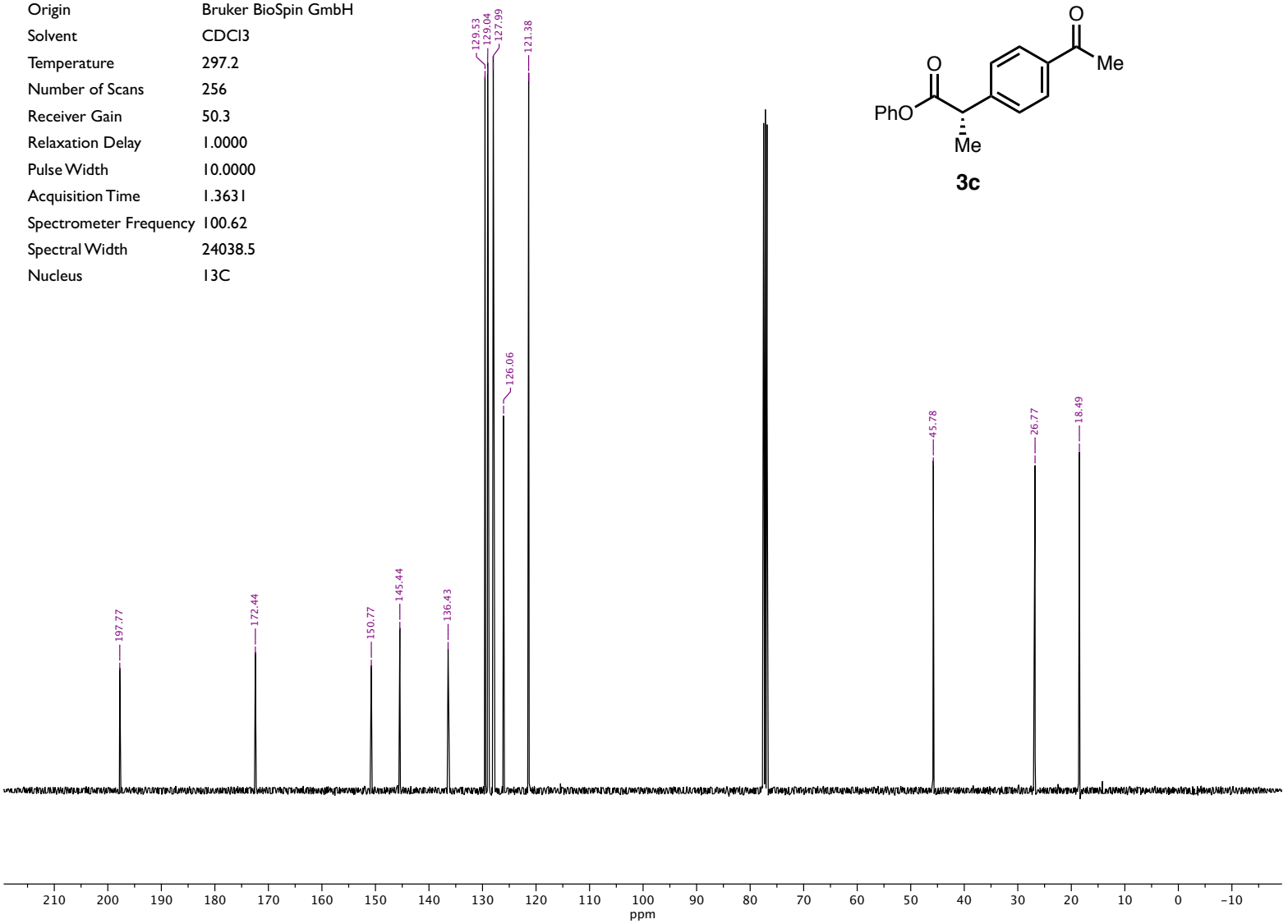
3b

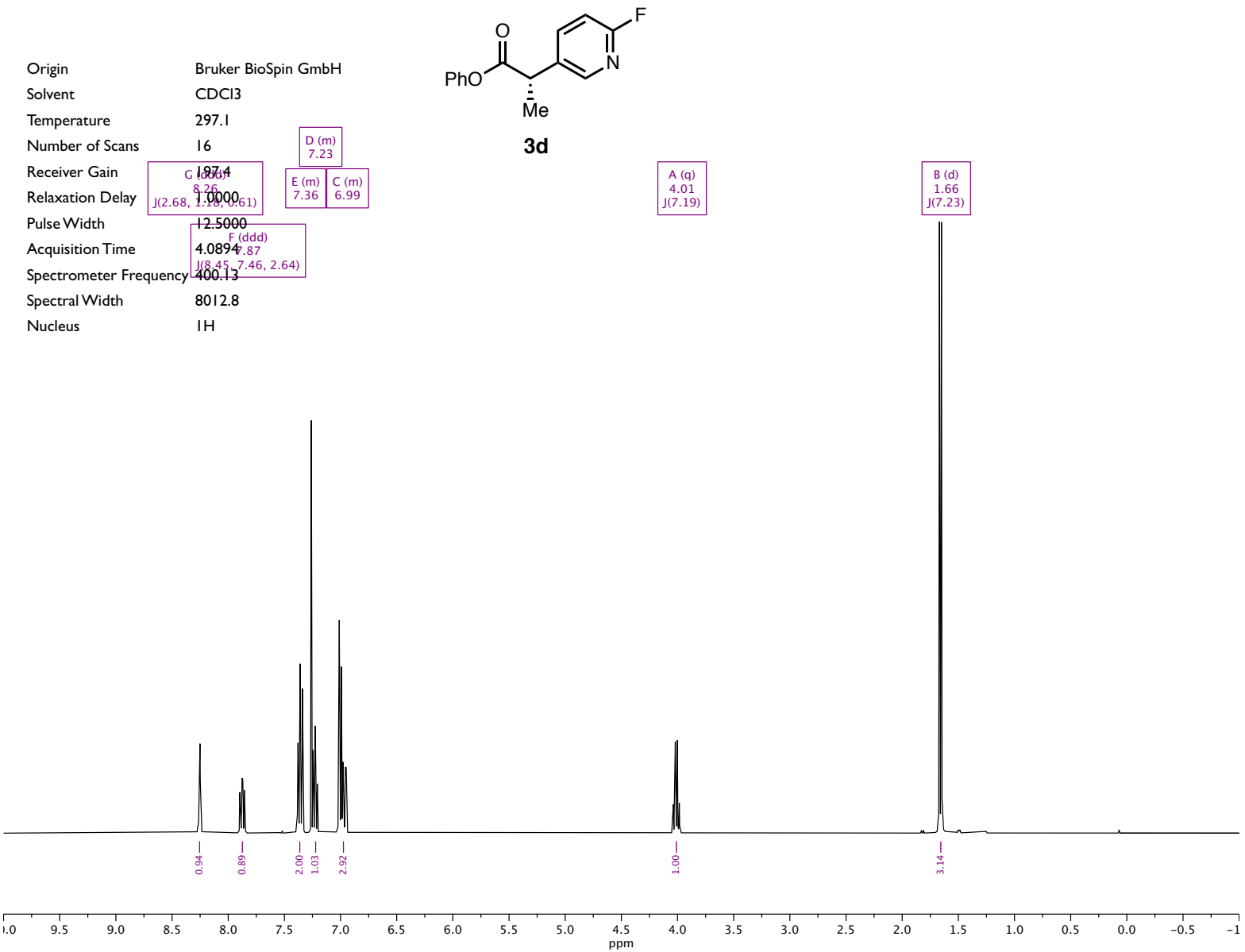
Origin	Bruker BioSpin GmbH
Solvent	CDCl3
Temperature	297.2
Number of Scans	16
Receiver Gain	72.0
Relaxation Delay	1.0000
Pulse Width	12.5000
Acquisition Time	4.0894
Spectrometer Frequency	400.13
Spectral Width	8012.8
Nucleus	1H

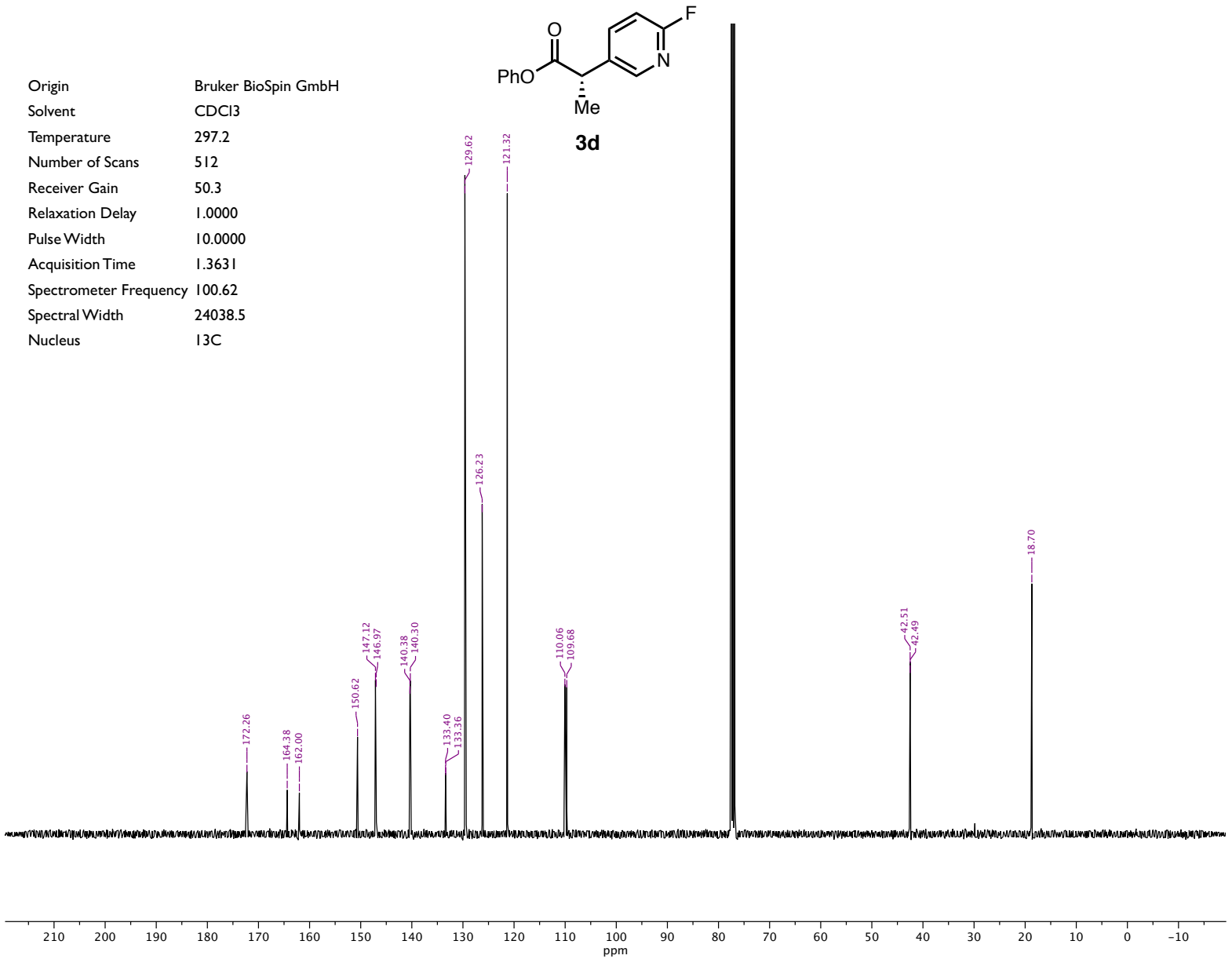


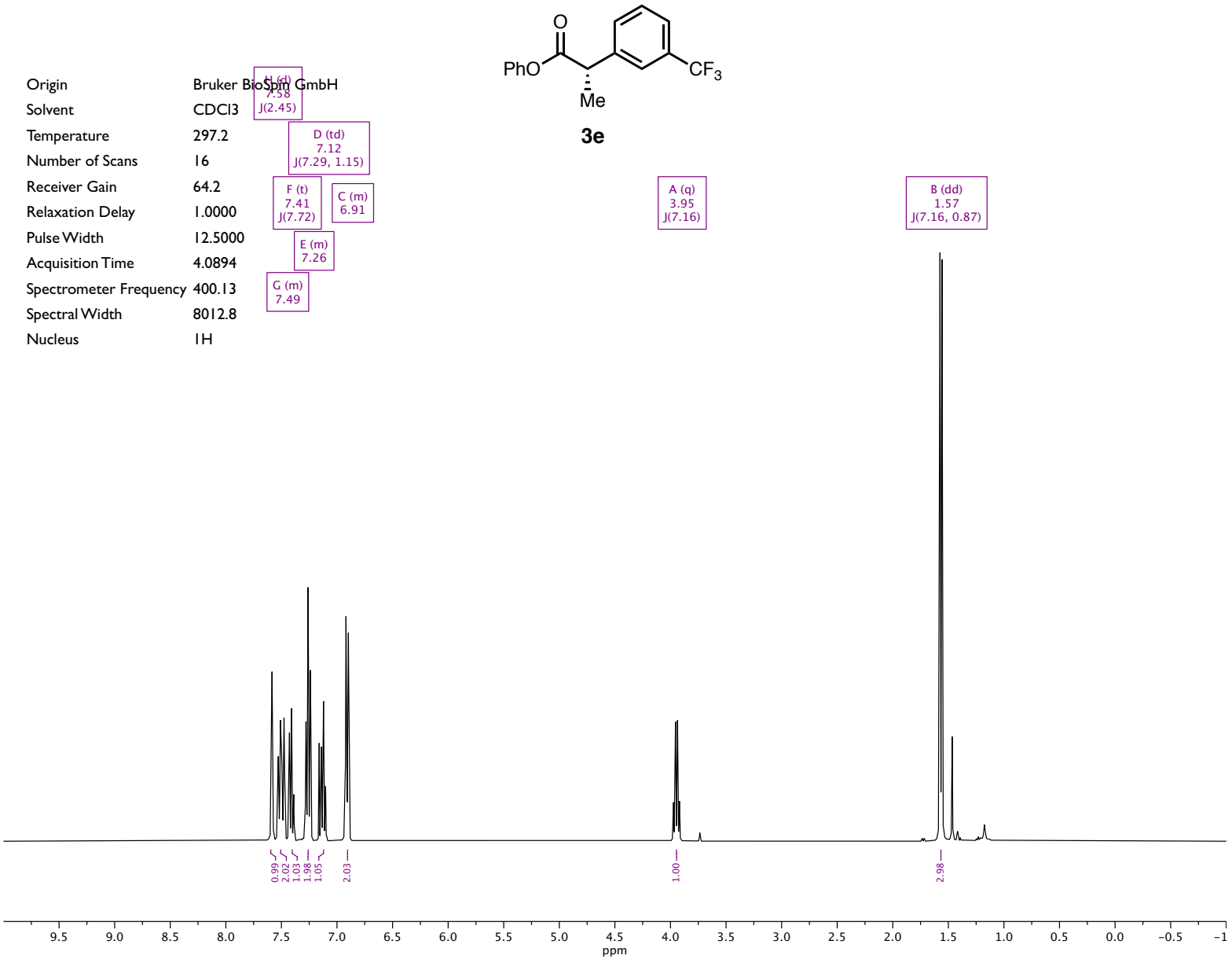
3c

Origin	Bruker BioSpin GmbH
Solvent	CDCl3
Temperature	297.2
Number of Scans	256
Receiver Gain	50.3
Relaxation Delay	1.0000
Pulse Width	10.0000
Acquisition Time	1.3631
Spectrometer Frequency	100.62
Spectral Width	24038.5
Nucleus	13C

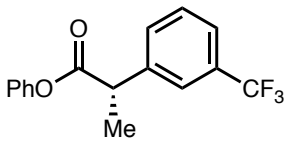



Origin Bruker BioSpin GmbH
Solvent CDCl3
Temperature 297.1
Number of Scans 16
Receiver Gain 197.4
Relaxation Delay 1.0000
Pulse Width 12.5000
Acquisition Time 4.0894
Spectrometer Frequency 400.13
Spectral Width 8012.8
Nucleus 1H
O
F
N
PhO
Me
3d
D (m) 7.23
E (m) 7.36
C (m) 6.99
A (q) 4.01 J(7.19)
B (d) 1.66 J(7.23)
0.94
0.89
2.00
1.03
2.92
1.00
3.14
ppm


Origin Bruker BioSpin GmbH
Solvent CDCl3
Temperature 297.2
Number of Scans 512
Receiver Gain 50.3
Relaxation Delay 1.0000
Pulse Width 10.0000
Acquisition Time 1.3631
Spectrometer Frequency 100.62
Spectral Width 24038.5
Nucleus 13C
O
PhO
F
N
Me
3d
129.62
121.32
126.23
172.26
164.38
162.00
150.62
147.12
146.97
140.38
140.30
133.40
133.36
110.06
109.68
42.51
42.49
18.70
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 −10
ppm

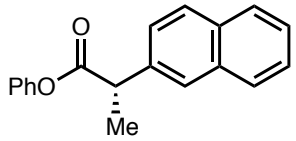

Origin Bruker BioSpin GmbH
Solvent CDCl3
Temperature 297.2
Number of Scans 16
Receiver Gain 64.2
Relaxation Delay 1.0000
Pulse Width 12.5000
Acquisition Time 4.0894
Spectrometer Frequency 400.13
Spectral Width 8012.8
Nucleus 1H
H (dd) 7.58 J(2.45)
D (td) 7.12 J(7.29, 1.15)
F (t) 7.41 J(7.72)
C (m) 6.91
E (m) 7.26
G (m) 7.49
A (q) 3.95 J(7.16)
B (dd) 1.57 J(7.16, 0.87)
PhO
O
CF3
Me
3e
0.99
2.02
1.03
1.98
1.05
2.03
1.00
2.98
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 −0.5 −1
ppm

Origin	Bruker BioSpin GmbH
Solvent	CDCl3
Temperature	297.1
Number of Scans	512
Receiver Gain	50.3
Relaxation Delay	1.0000
Pulse Width	10.0000
Acquisition Time	1.3631
Spectrometer Frequency	100.62
Spectral Width	24038.5
Nucleus	13C

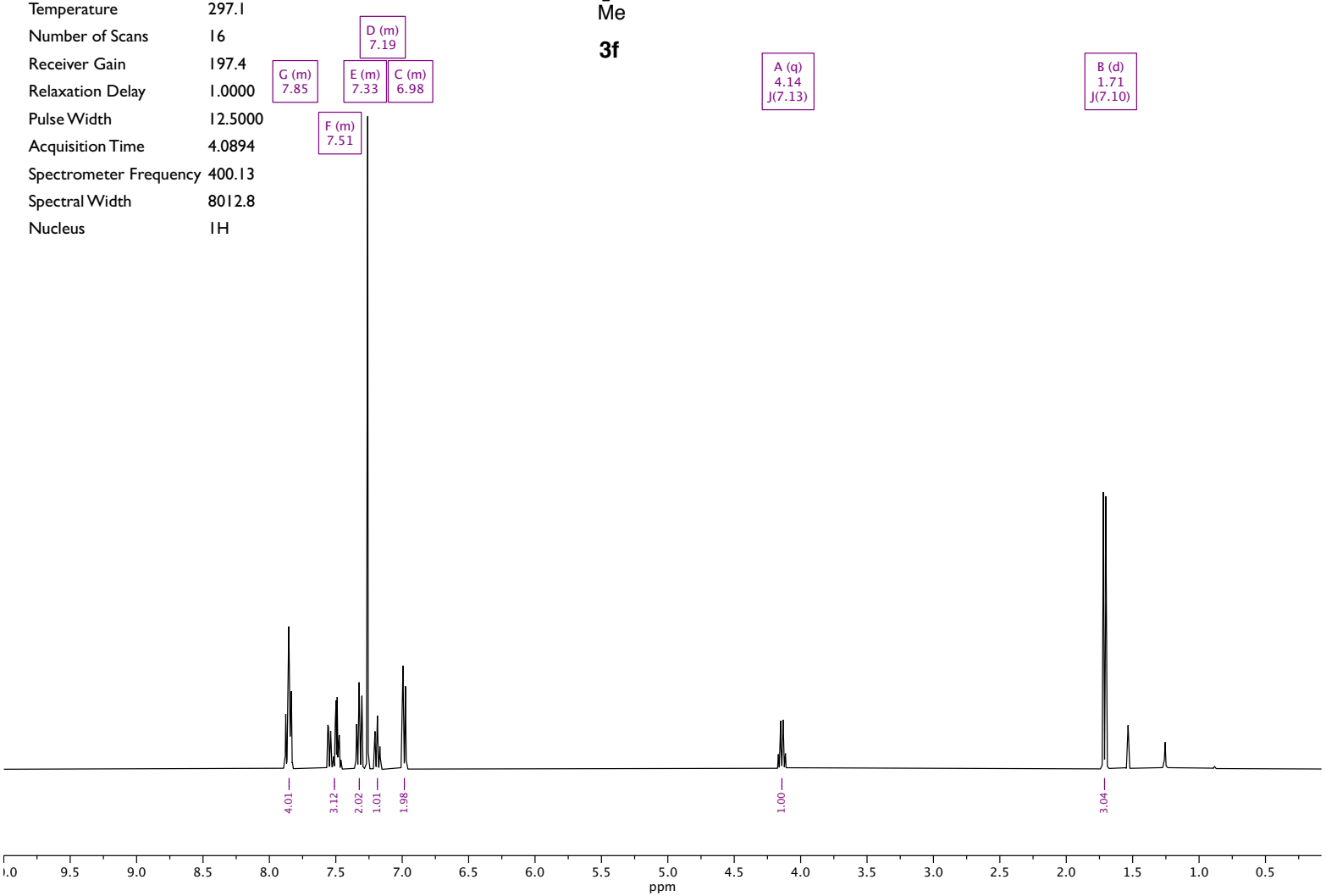


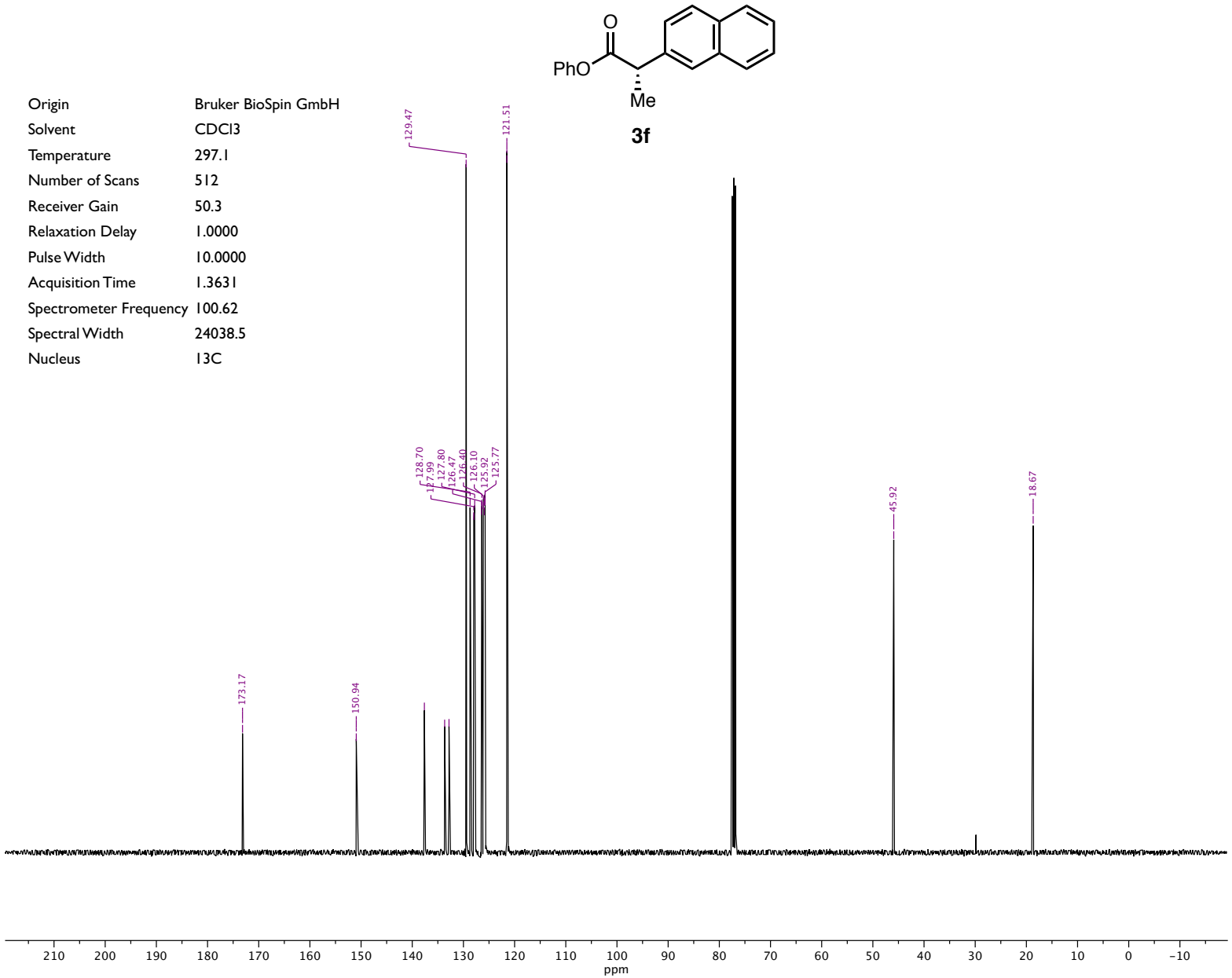
3e

Origin	Bruker BioSpin GmbH
Solvent	CDCl3
Temperature	297.1
Number of Scans	16
Receiver Gain	197.4
Relaxation Delay	1.0000
Pulse Width	12.5000
Acquisition Time	4.0894
Spectrometer Frequency	400.13
Spectral Width	8012.8
Nucleus	1H

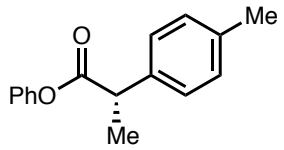


3f

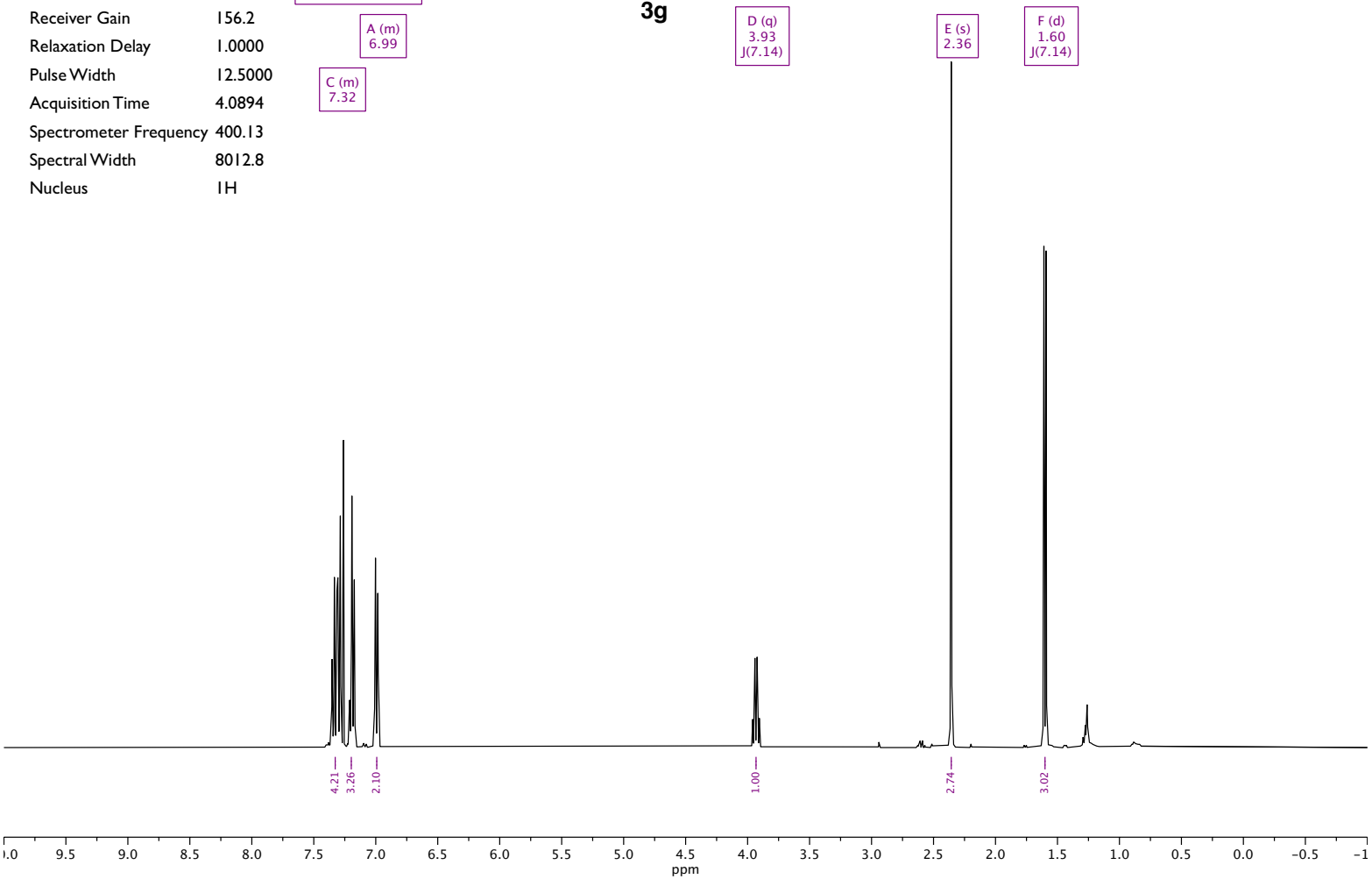



O
PhO
Me
3f
Origin Bruker BioSpin GmbH
Solvent CDCl3
Temperature 297.1
Number of Scans 512
Receiver Gain 50.3
Relaxation Delay 1.0000
Pulse Width 10.0000
Acquisition Time 1.3631
Spectrometer Frequency 100.62
Spectral Width 24038.5
Nucleus 13C
129.47
121.51
128.70
127.99
127.80
126.47
126.40
126.10
125.92
125.77
45.92
18.67
173.17
150.94
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 −10
ppm

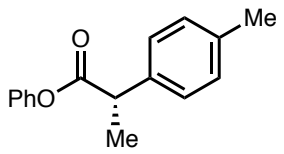
Origin	Bruker BioSpin GmbH
Solvent	CDCl3
Temperature	297.2
Number of Scans	16
Receiver Gain	156.2
Relaxation Delay	1.0000
Pulse Width	12.5000
Acquisition Time	4.0894
Spectrometer Frequency	400.13
Spectral Width	8012.8
Nucleus	1H



3g

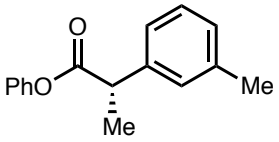


Origin	Bruker BioSpin GmbH
Solvent	CDCl3
Temperature	297.1
Number of Scans	512
Receiver Gain	55.5
Relaxation Delay	1.0000
Pulse Width	10.0000
Acquisition Time	1.3631
Spectrometer Frequency	100.62
Spectral Width	24038.5
Nucleus	13C

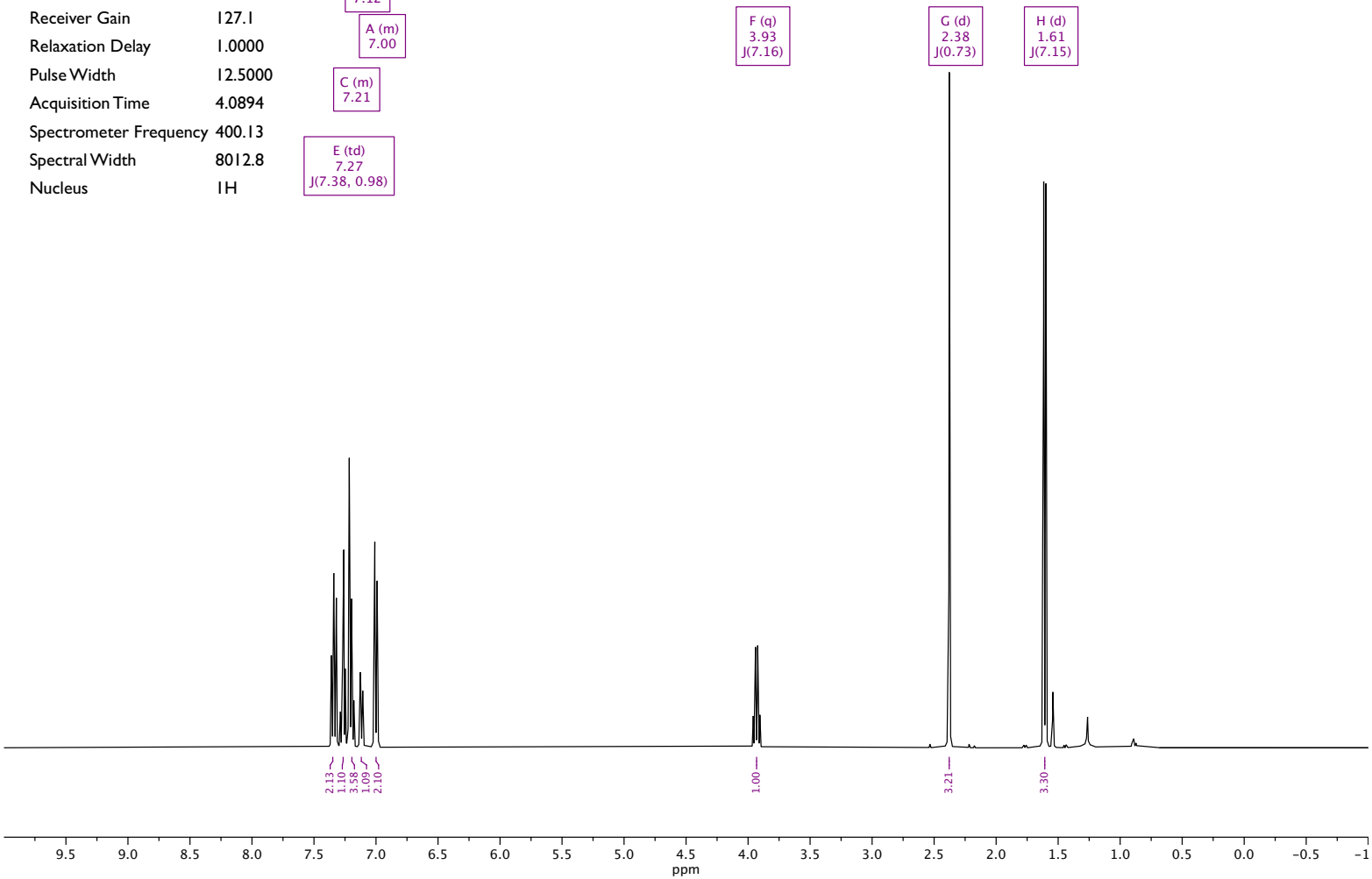


3g

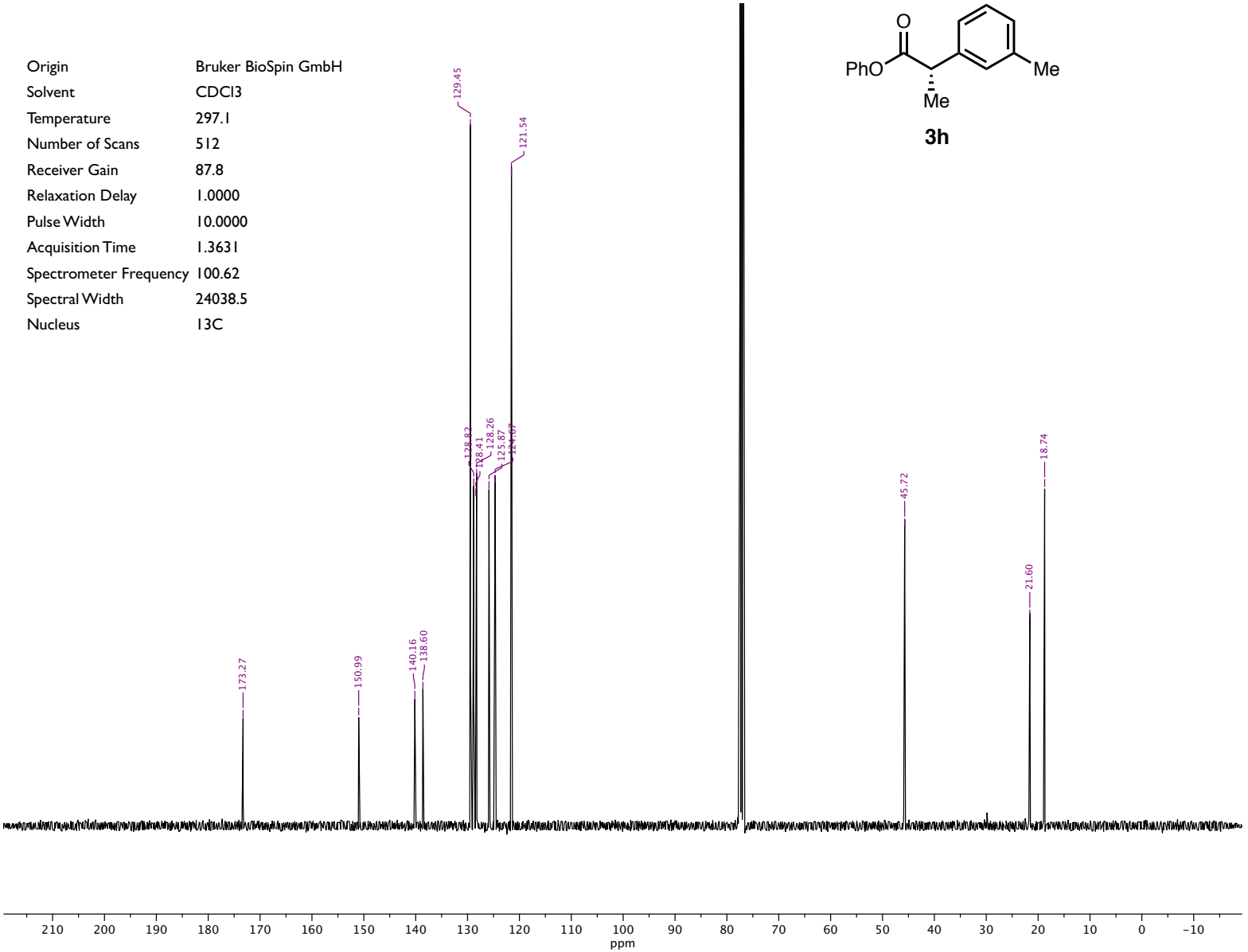
Origin	Bruker BioSpin GmbH
Solvent	CDCl3
Temperature	297.2
Number of Scans	16
Receiver Gain	127.1
Relaxation Delay	1.0000
Pulse Width	12.5000
Acquisition Time	4.0894
Spectrometer Frequency	400.13
Spectral Width	8012.8
Nucleus	1H

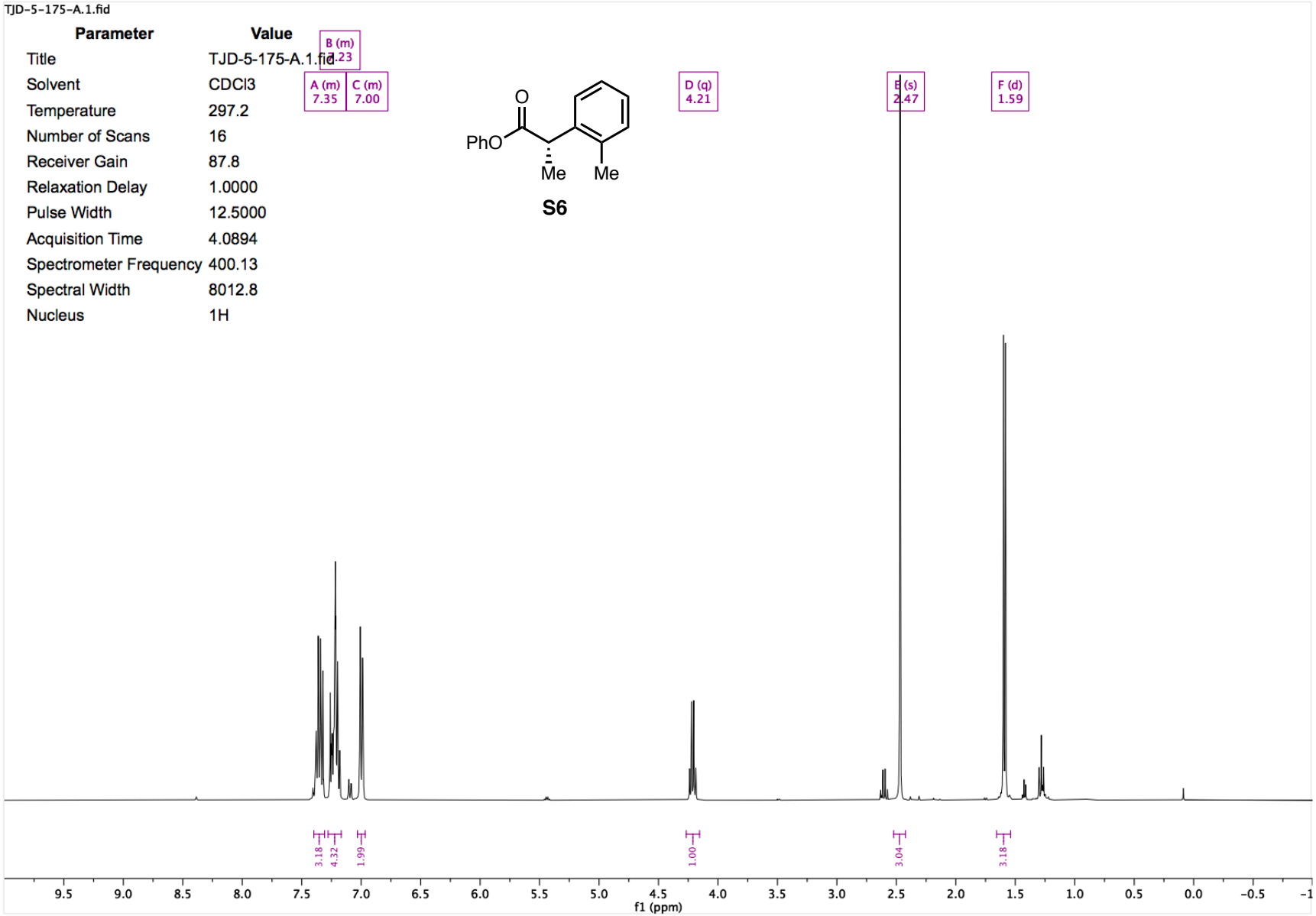


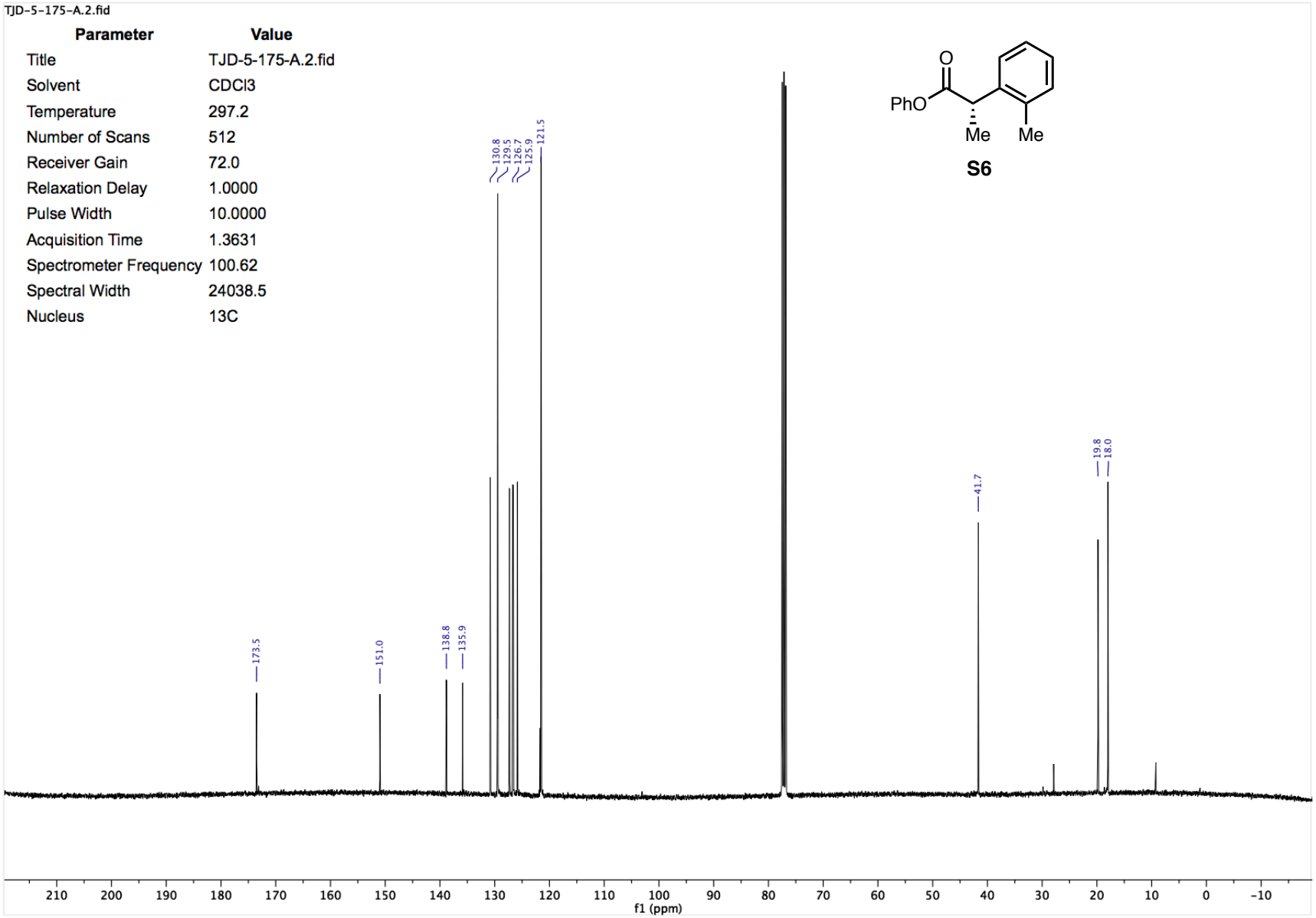
3h

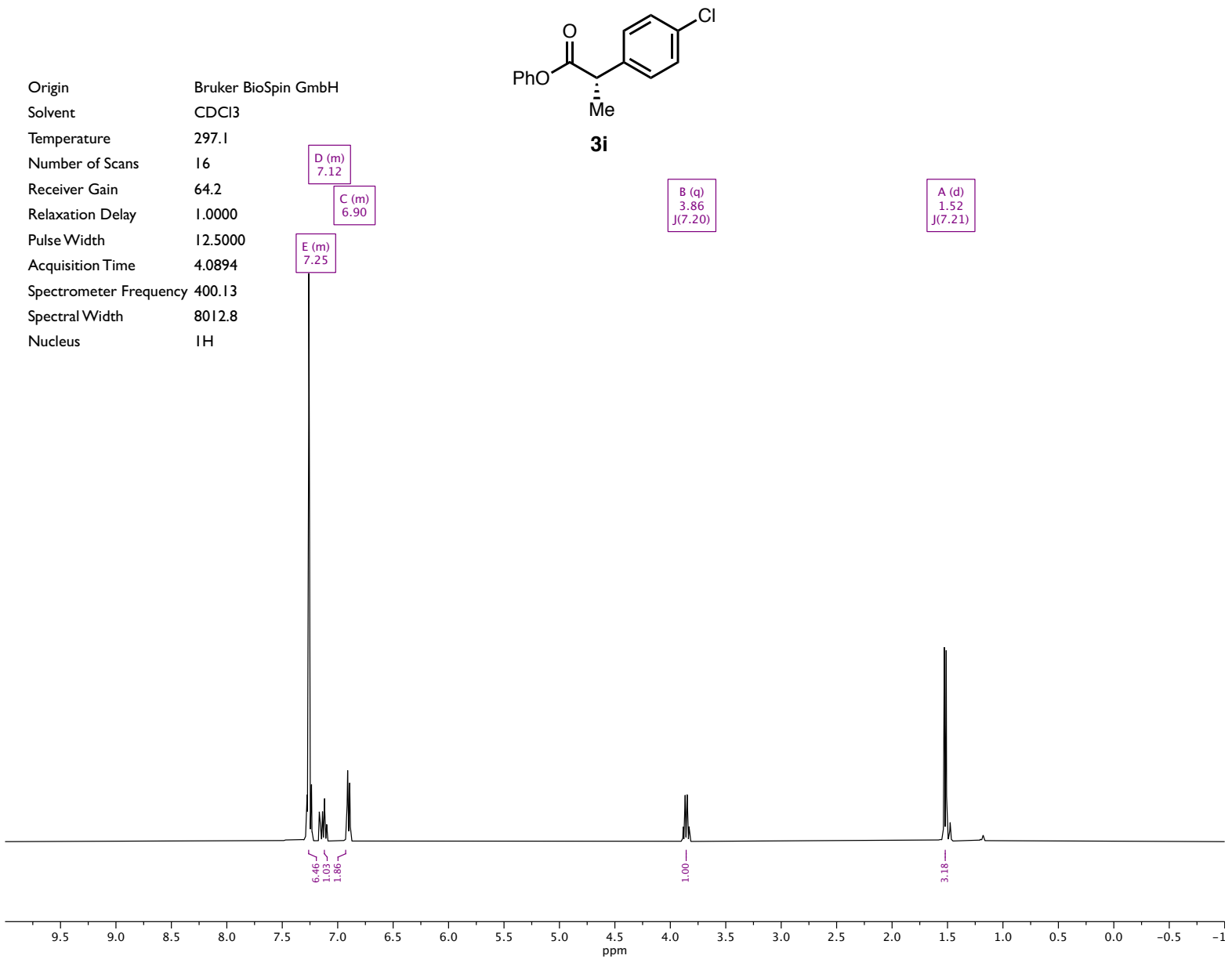


Origin	Bruker BioSpin GmbH
Solvent	CDCl3
Temperature	297.1
Number of Scans	512
Receiver Gain	87.8
Relaxation Delay	1.0000
Pulse Width	10.0000
Acquisition Time	1.3631
Spectrometer Frequency	100.62
Spectral Width	24038.5
Nucleus	13C

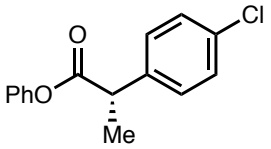



TJD-5-175-A.1.fid
Parameter Value
Title TJD-5-175-A.1.fid
Solvent CDCl3
Temperature 297.2
Number of Scans 16
Receiver Gain 87.8
Relaxation Delay 1.0000
Pulse Width 12.5000
Acquisition Time 4.0894
Spectrometer Frequency 400.13
Spectral Width 8012.8
Nucleus 1H
B (m) 7.23
A (m) 7.35
C (m) 7.00
D (q) 4.21
E (s) 2.47
F (d) 1.59
PhO
Me
Me
S6
3.18
4.32
1.99
1.00
3.04
3.18
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1
f1 (ppm)

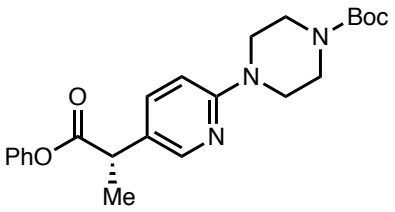

TJD-5-175-A.2.fid
Parameter Value
Title TJD-5-175-A.2.fid
Solvent CDCl3
Temperature 297.2
Number of Scans 512
Receiver Gain 72.0
Relaxation Delay 1.0000
Pulse Width 10.0000
Acquisition Time 1.3631
Spectrometer Frequency 100.62
Spectral Width 24038.5
Nucleus 13C
O
PhO
Me
Me
S6
173.5
151.0
138.8
135.9
130.8
129.5
126.7
125.9
121.5
41.7
19.8
18.0
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)


Origin Bruker BioSpin GmbH
Solvent CDCl3
Temperature 297.1
Number of Scans 16
Receiver Gain 64.2
Relaxation Delay 1.0000
Pulse Width 12.5000
Acquisition Time 4.0894
Spectrometer Frequency 400.13
Spectral Width 8012.8
Nucleus 1H
O
PhO
Cl
Me
3i
D (m) 7.12
C (m) 6.90
E (m) 7.25
B (q) 3.86 J(7.20)
A (d) 1.52 J(7.21)
6.46
1.03
1.86
1.00
3.18
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 −0.5 −1
ppm

Origin	Bruker BioSpin GmbH
Solvent	CDCl3
Temperature	298.1
Number of Scans	1024
Receiver Gain	52.8
Relaxation Delay	2.0000
Pulse Width	10.0000
Acquisition Time	1.3763
Spectrometer Frequency	100.63
Spectral Width	23809.5
Nucleus	13C

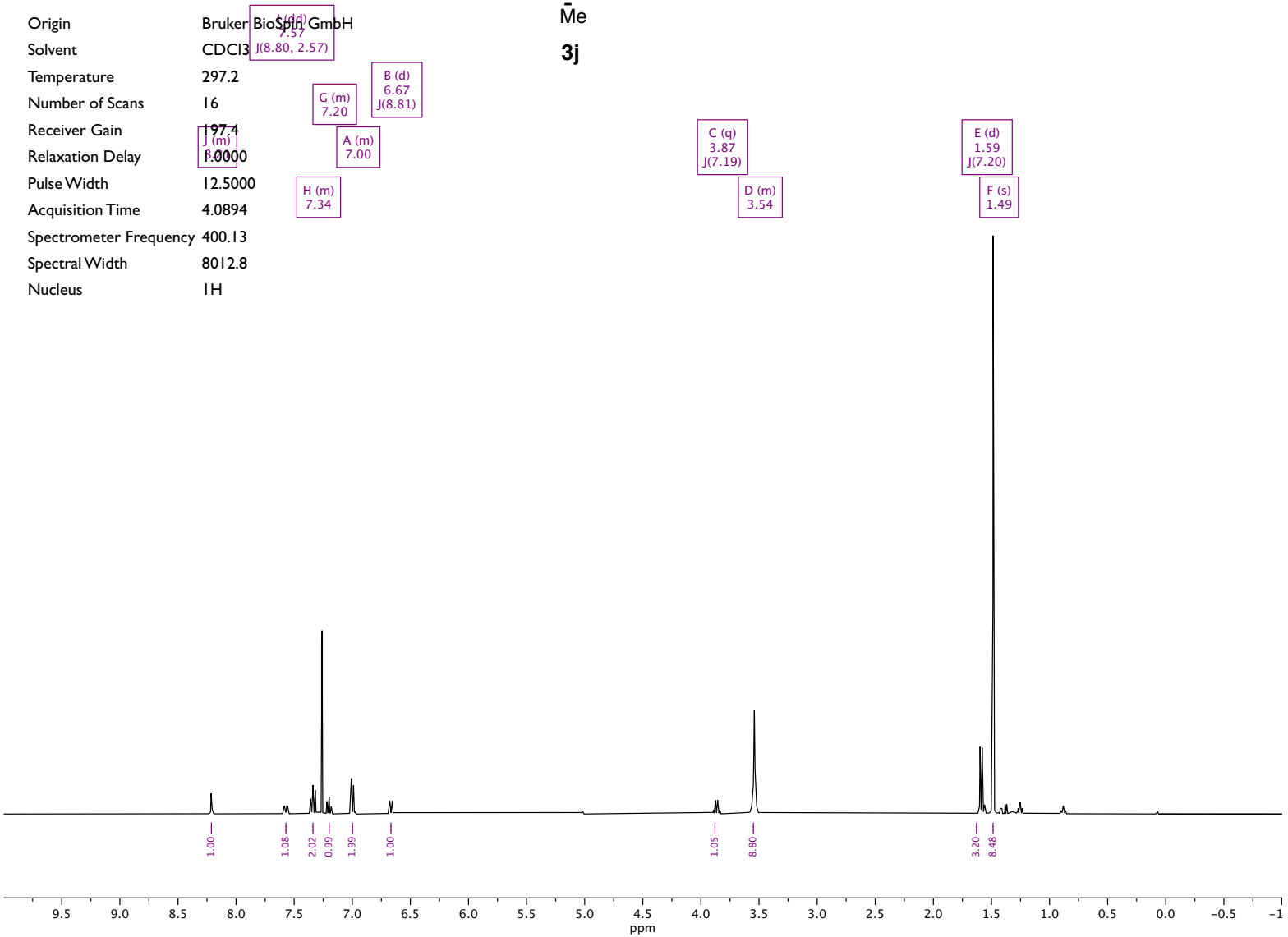


3i

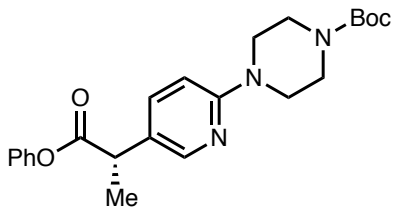


3j

Origin	Bruker BioSpin GmbH
Solvent	CDCl3
Temperature	297.2
Number of Scans	16
Receiver Gain	197.4
Relaxation Delay	1.0000
Pulse Width	12.5000
Acquisition Time	4.0894
Spectrometer Frequency	400.13
Spectral Width	8012.8
Nucleus	1H

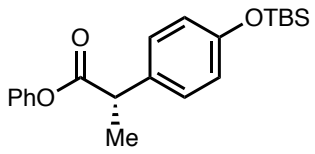


Origin	Bruker BioSpin GmbH
Solvent	CDCl3
Temperature	297.2
Number of Scans	512
Receiver Gain	50.3
Relaxation Delay	1.0000
Pulse Width	10.0000
Acquisition Time	1.3631
Spectrometer Frequency	100.62
Spectral Width	24038.5
Nucleus	13C

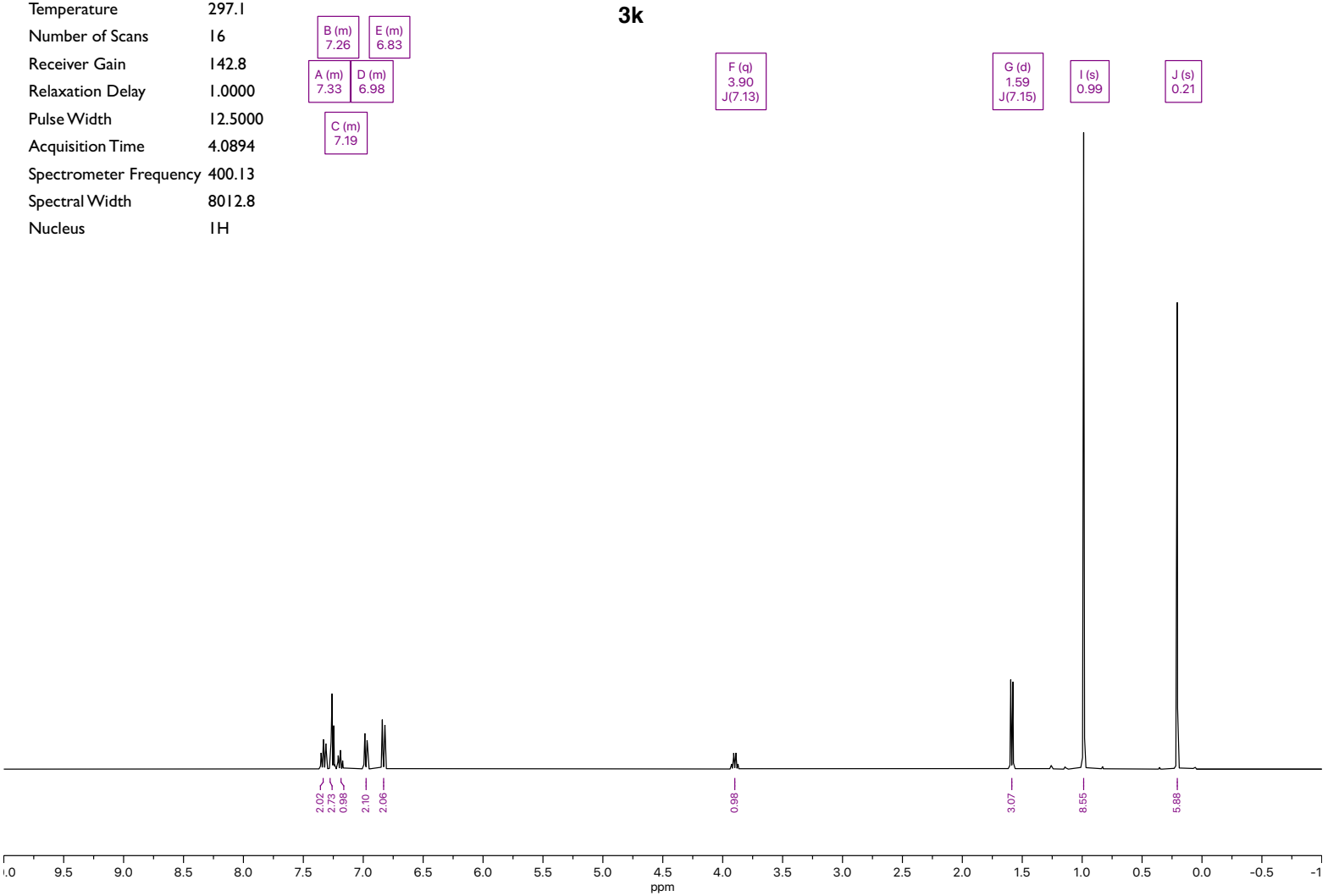


3j

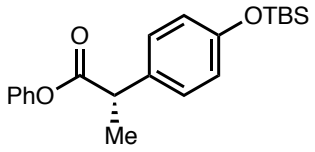
Origin	Bruker BioSpin GmbH
Solvent	CDCl3
Temperature	297.1
Number of Scans	16
Receiver Gain	142.8
Relaxation Delay	1.0000
Pulse Width	12.5000
Acquisition Time	4.0894
Spectrometer Frequency	400.13
Spectral Width	8012.8
Nucleus	1H



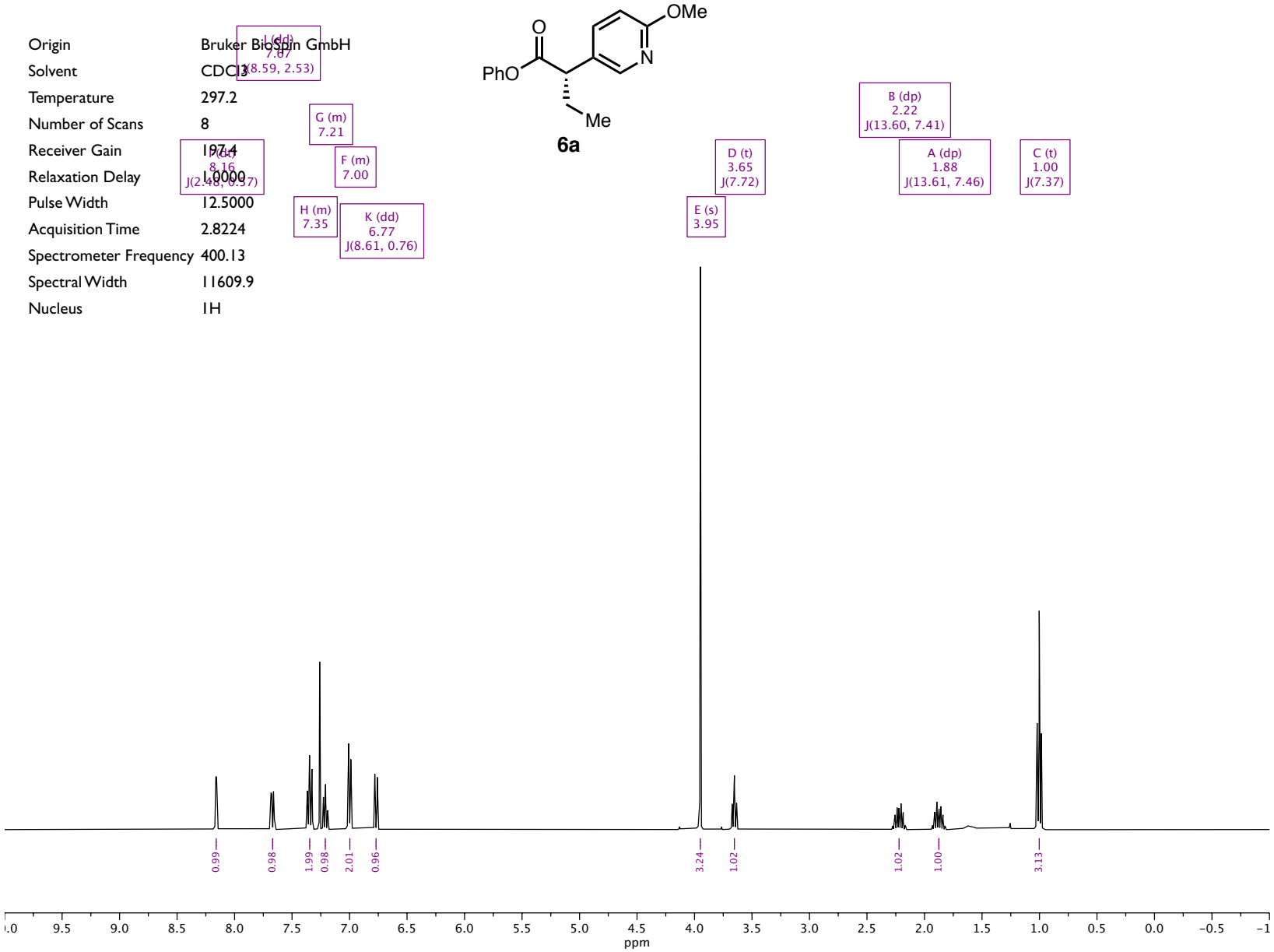
3k

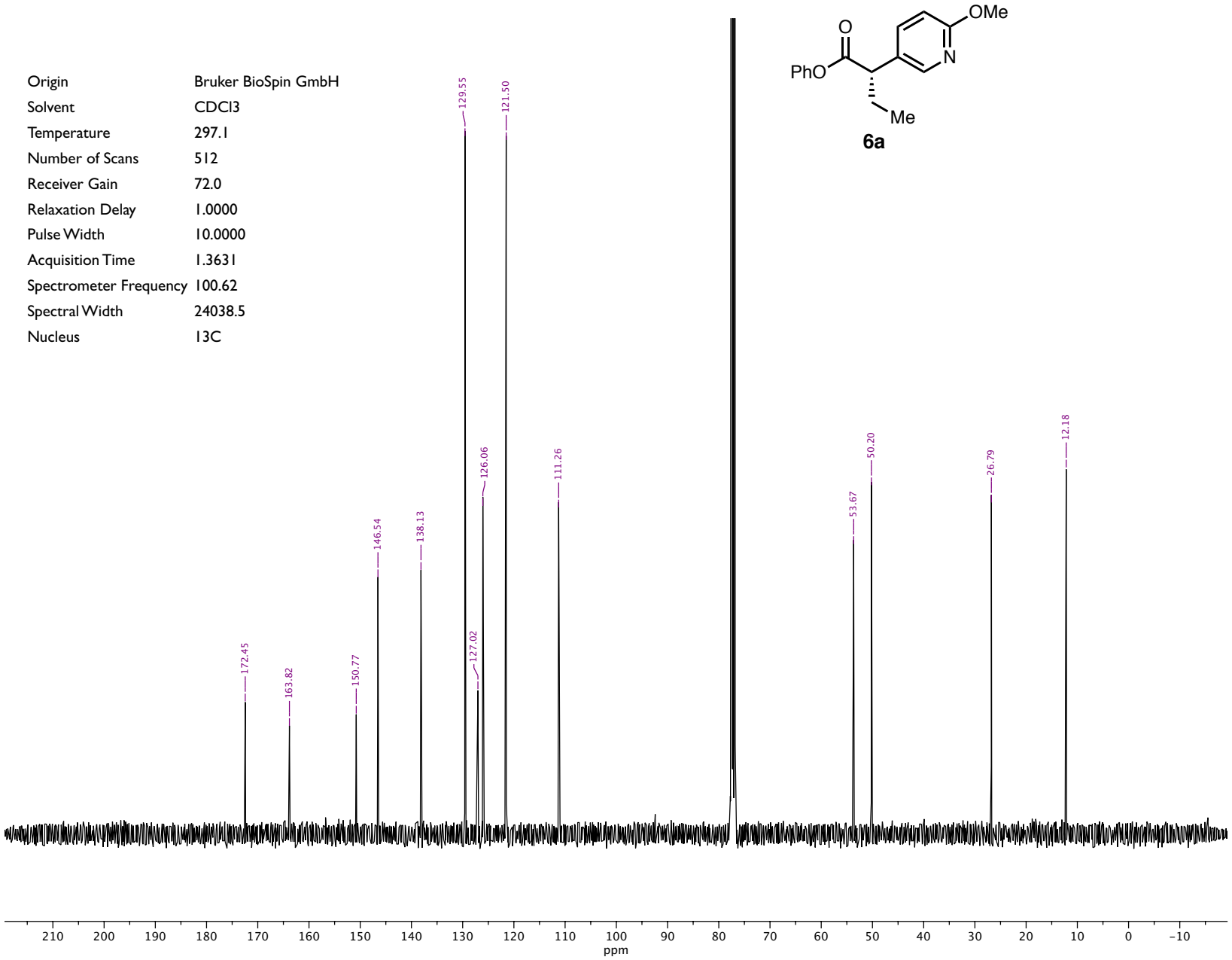


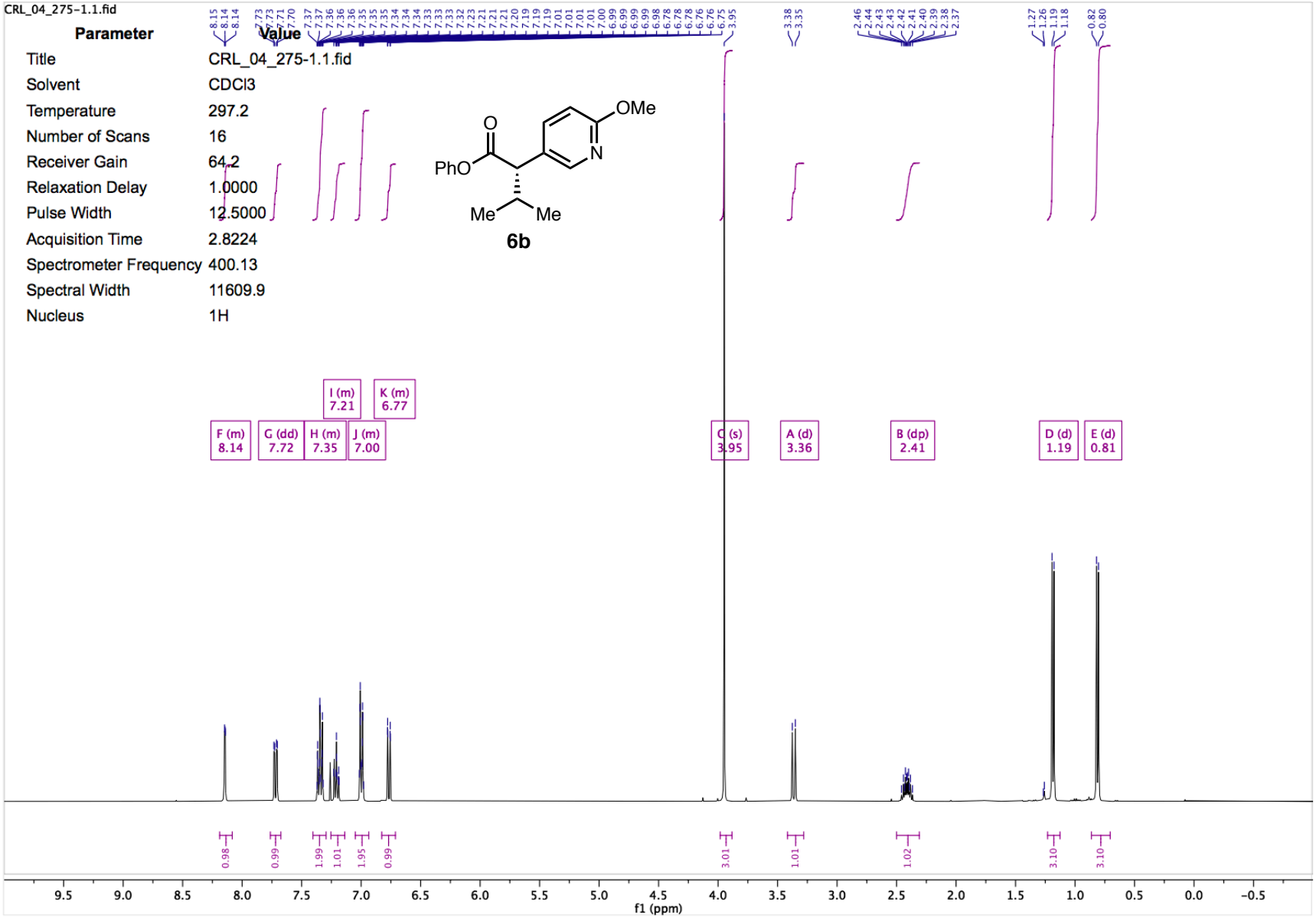
Origin	Bruker BioSpin GmbH
Solvent	CDCl3
Temperature	297.2
Number of Scans	512
Receiver Gain	72.0
Relaxation Delay	1.0000
Pulse Width	10.0000
Acquisition Time	1.3631
Spectrometer Frequency	100.62
Spectral Width	24038.5
Nucleus	13C

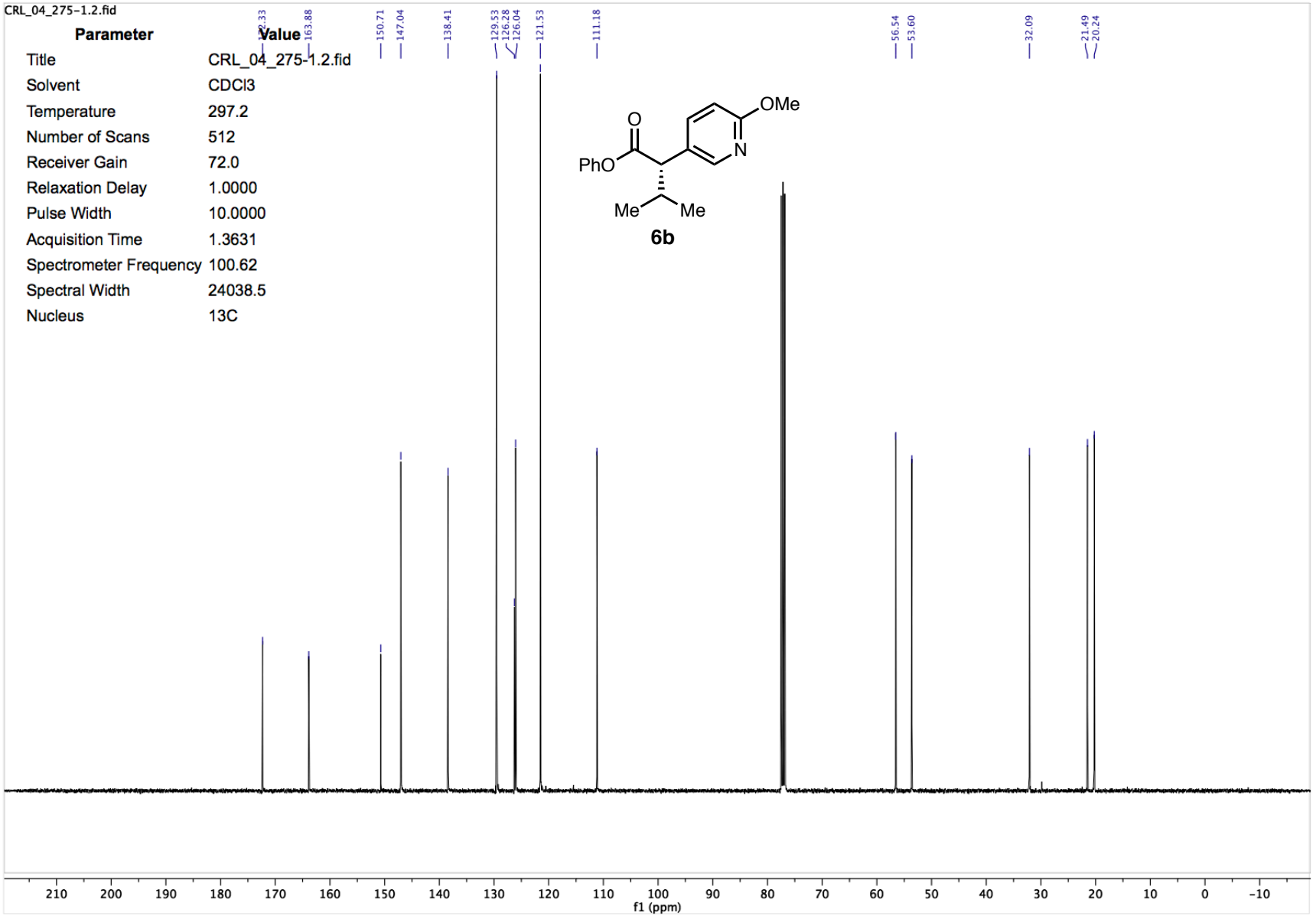


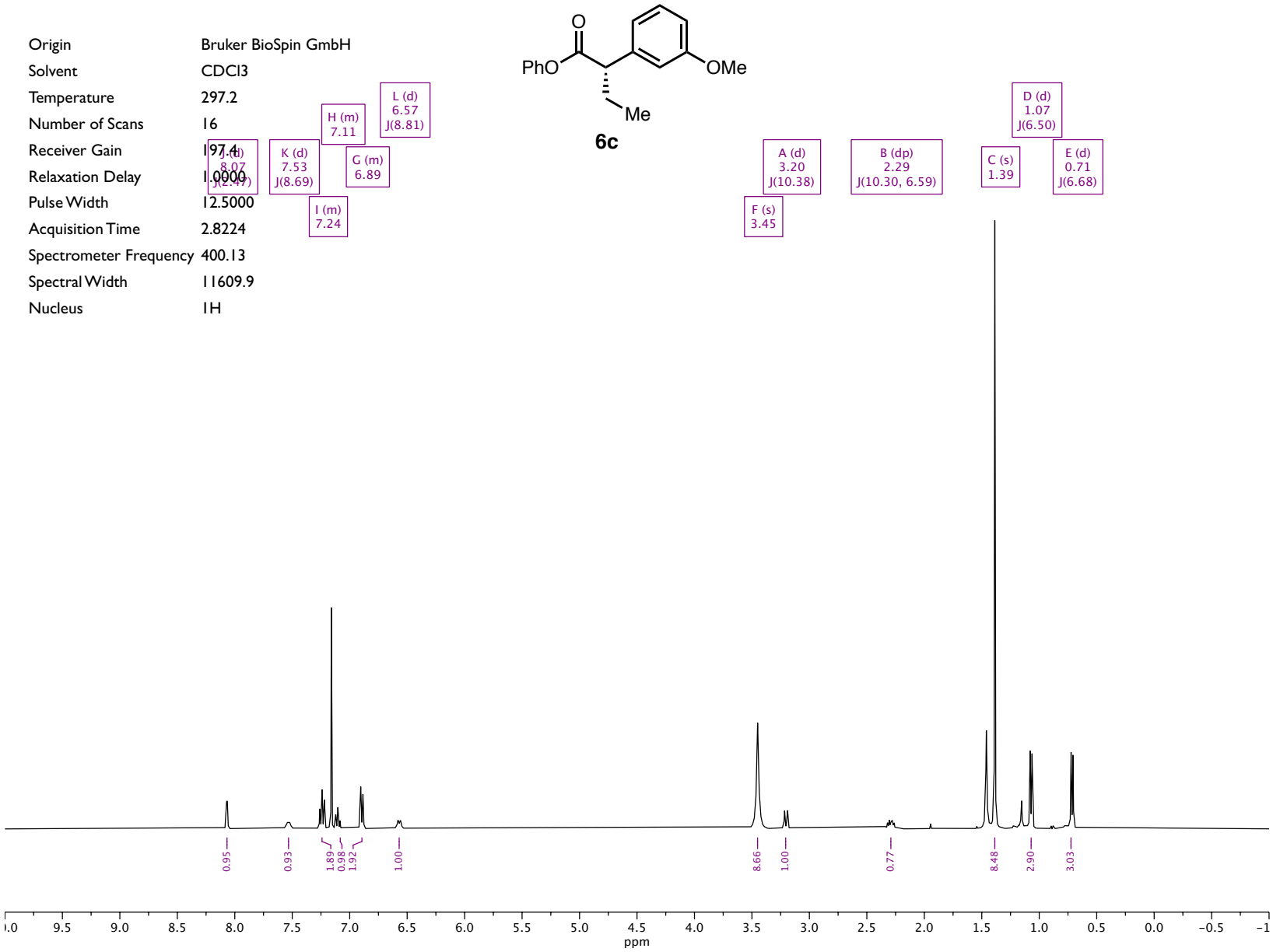
3k

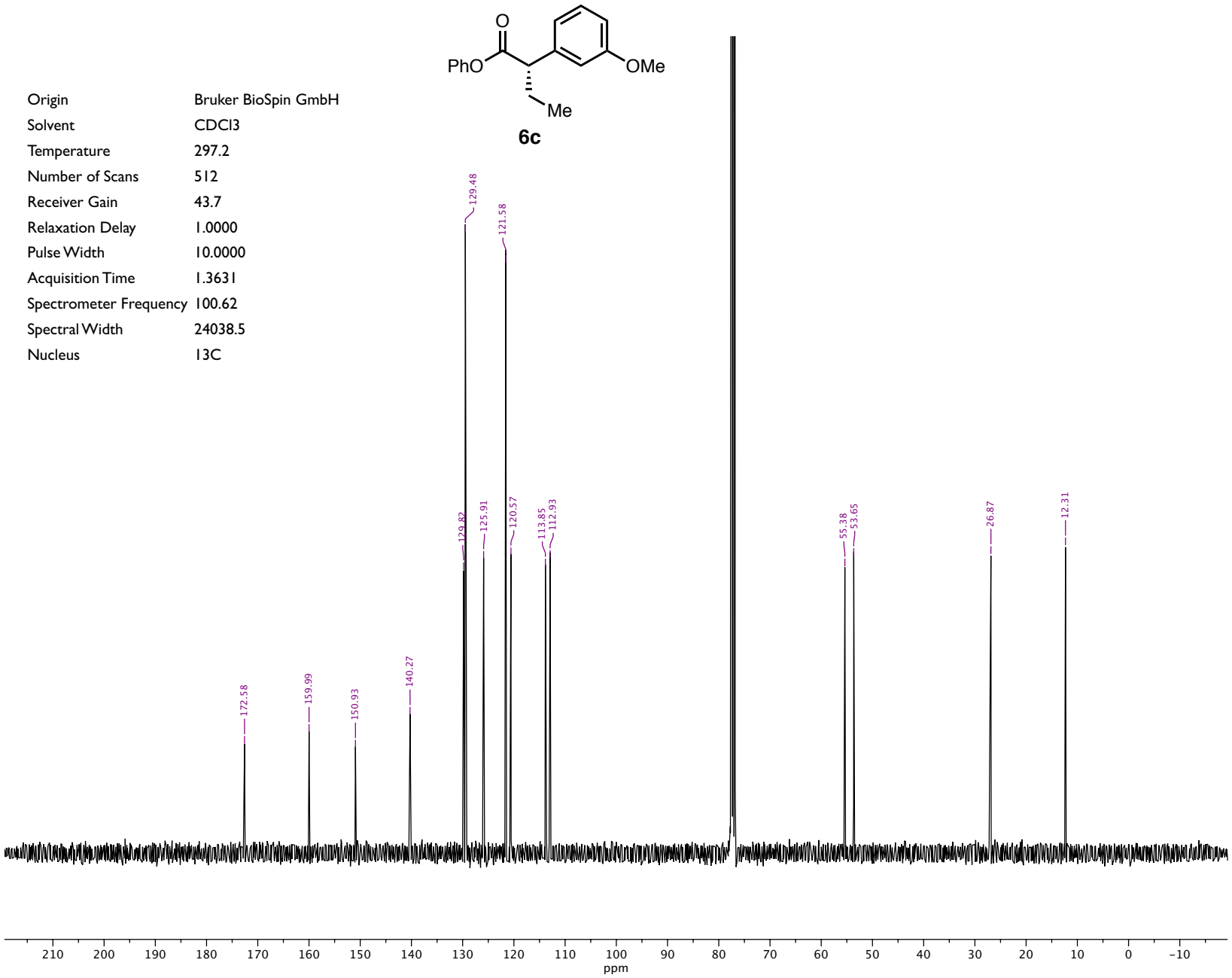

Origin Bruker BioSpin GmbH
Solvent CDCl3
Temperature 297.2
Number of Scans 8
Receiver Gain 197.4
Relaxation Delay 1.0000
Pulse Width 12.5000
Acquisition Time 2.8224
Spectrometer Frequency 400.13
Spectral Width 11609.9
Nucleus 1H
OMe
O
N
PhO
Me
6a
I (dd) 7.87 J(8.59, 2.53)
G (m) 7.21
F (m) 7.00
H (m) 7.35
K (dd) 6.77 J(8.61, 0.76)
E (s) 3.95
D (t) 3.65 J(7.72)
B (dp) 2.22 J(13.60, 7.41)
A (dp) 1.88 J(13.61, 7.46)
C (t) 1.00 J(7.37)
0.99
0.98
1.99
0.98
2.01
0.96
3.24
1.02
1.02
1.00
3.13
ppm

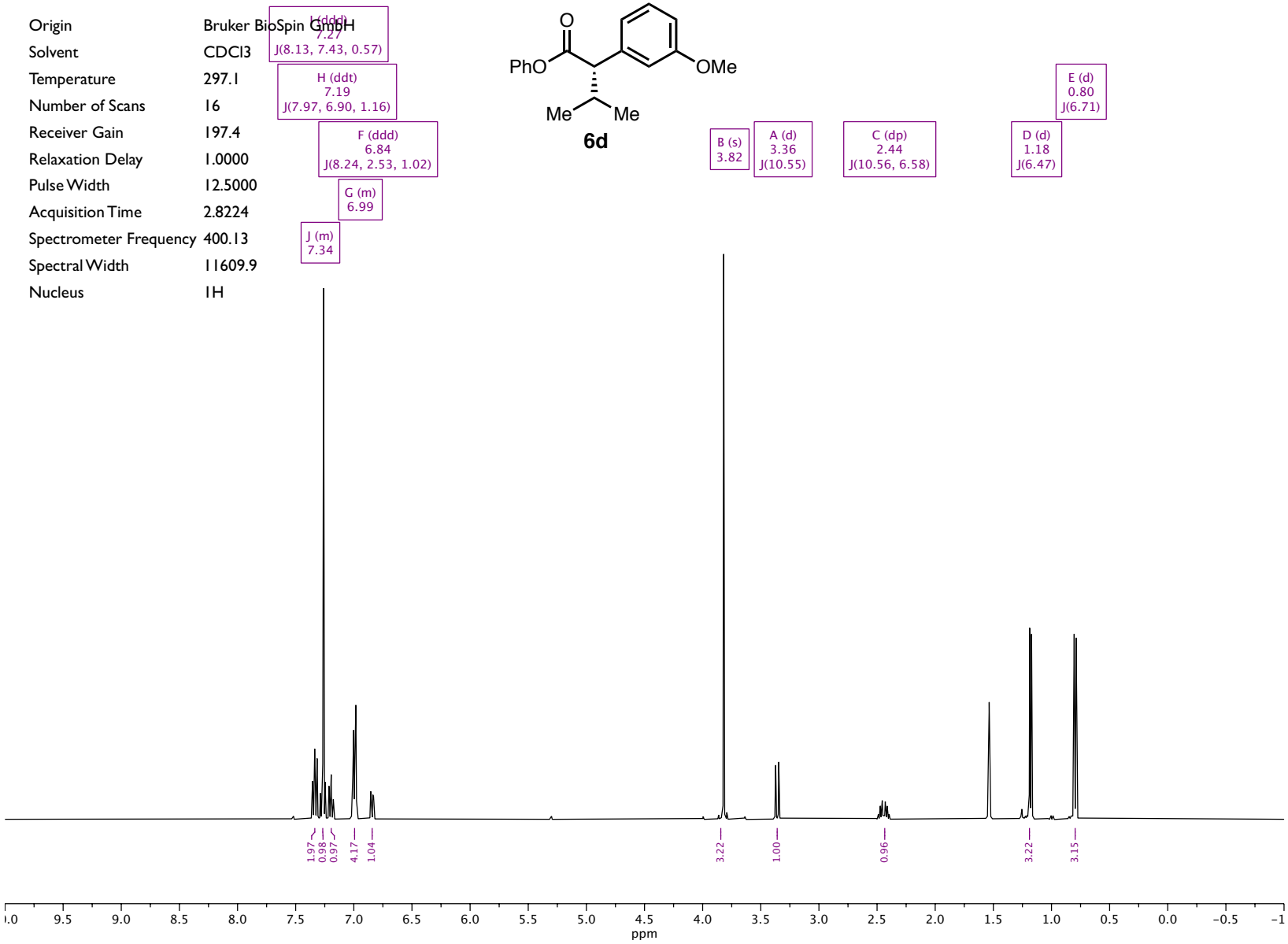

Origin Bruker BioSpin GmbH
Solvent CDCl3
Temperature 297.1
Number of Scans 512
Receiver Gain 72.0
Relaxation Delay 1.0000
Pulse Width 10.0000
Acquisition Time 1.3631
Spectrometer Frequency 100.62
Spectral Width 24038.5
Nucleus 13C
OMe
O
N
PhO
Me
6a
129.55
121.50
126.06
111.26
146.54
138.13
172.45
163.82
150.77
127.02
53.67
50.20
26.79
12.18
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 −10
ppm

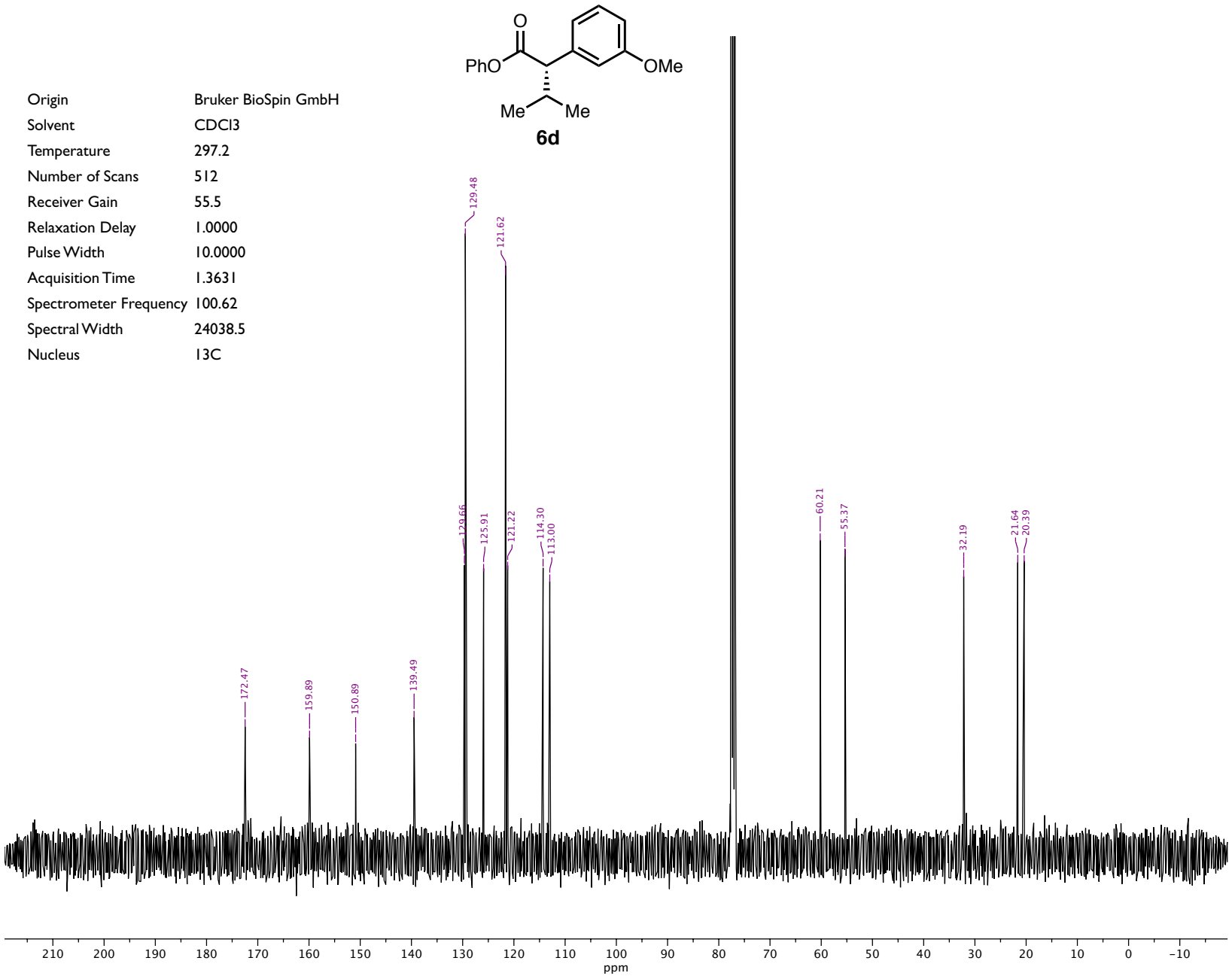

CRL_04_275-1.1.fid
Parameter
Value
Title
CRL_04_275-1.1.fid
Solvent
CDCl3
Temperature
297.2
Number of Scans
16
Receiver Gain
64.2
Relaxation Delay
1.0000
Pulse Width
12.5000
Acquisition Time
2.8224
Spectrometer Frequency
400.13
Spectral Width
11609.9
Nucleus
1H
OMe
O
PhO
N
Me
Me
6b
F (m) 8.14
G (dd) 7.72
H (m) 7.35
I (m) 7.21
J (m) 7.00
K (m) 6.77
C (s) 3.95
A (d) 3.36
B (dp) 2.41
D (d) 1.19
E (d) 0.81
0.98
0.99
1.99
1.01
1.95
0.99
3.01
1.01
1.02
3.10
3.10
f1 (ppm)

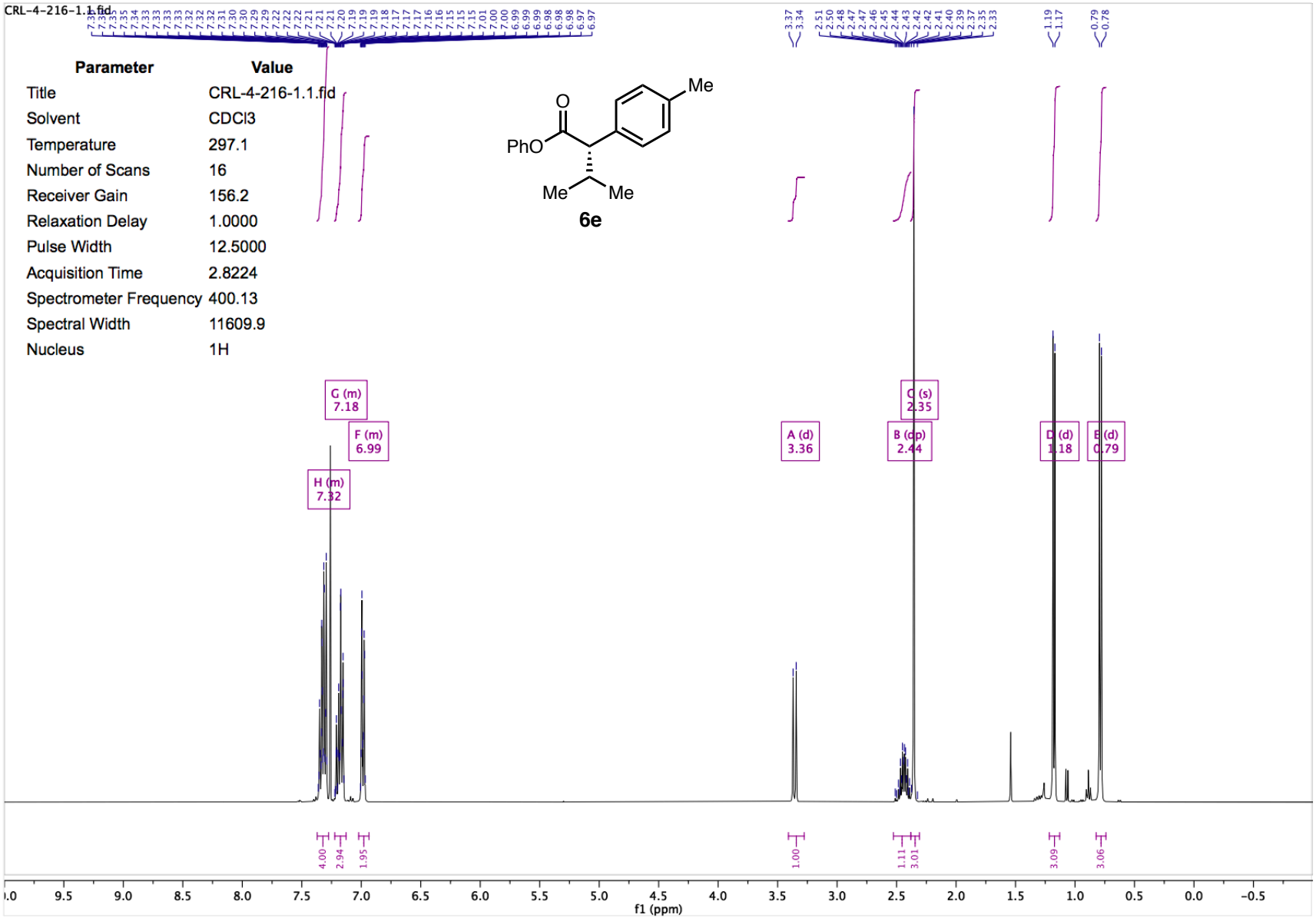

CRL_04_275-1.2.fid
Parameter Value
Title CRL_04_275-1.2.fid
Solvent CDCl3
Temperature 297.2
Number of Scans 512
Receiver Gain 72.0
Relaxation Delay 1.0000
Pulse Width 10.0000
Acquisition Time 1.3631
Spectrometer Frequency 100.62
Spectral Width 24038.5
Nucleus 13C
168.33
163.88
150.71
147.04
138.41
129.53
126.28
126.04
121.53
111.18
56.54
53.60
32.09
21.49
20.24
OMe
O
N
PhO
Me
Me
6b
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

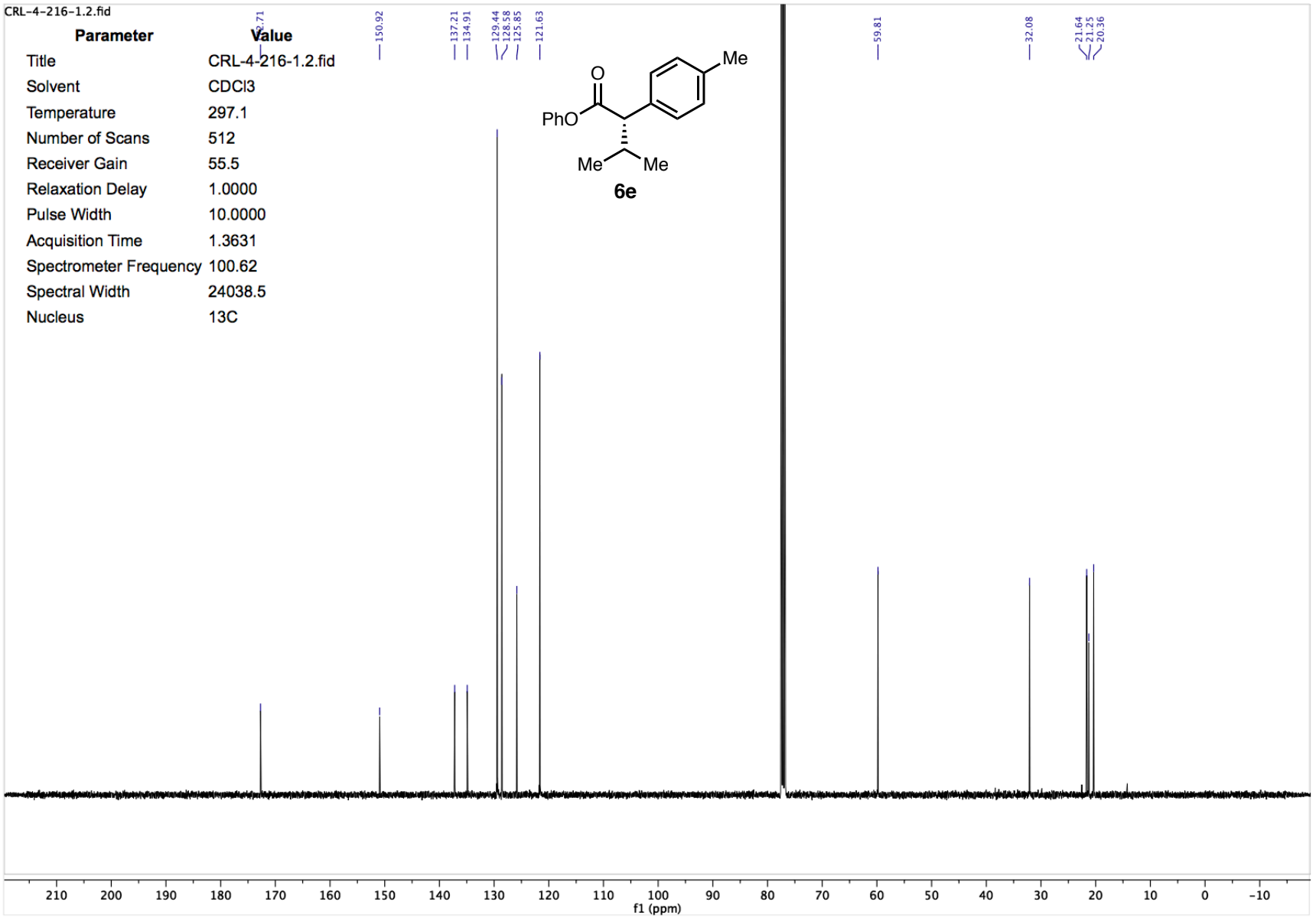

Origin Bruker BioSpin GmbH
Solvent CDCl3
Temperature 297.2
Number of Scans 16
Receiver Gain 197.4
Relaxation Delay 1.0000
Pulse Width 12.5000
Acquisition Time 2.8224
Spectrometer Frequency 400.13
Spectral Width 11609.9
Nucleus 1H
O
PhO
OMe
Me
6c
L (d) 6.57 J(8.81)
H (m) 7.11
K (d) 7.53 J(8.69)
G (m) 6.89
I (m) 7.24
A (d) 3.20 J(10.38)
F (s) 3.45
B (dp) 2.29 J(10.30, 6.59)
C (s) 1.39
D (d) 1.07 J(6.50)
E (d) 0.71 J(6.68)
0.95
0.93
1.89
0.98
1.92
1.00
8.66
1.00
0.77
8.48
2.90
3.03
ppm

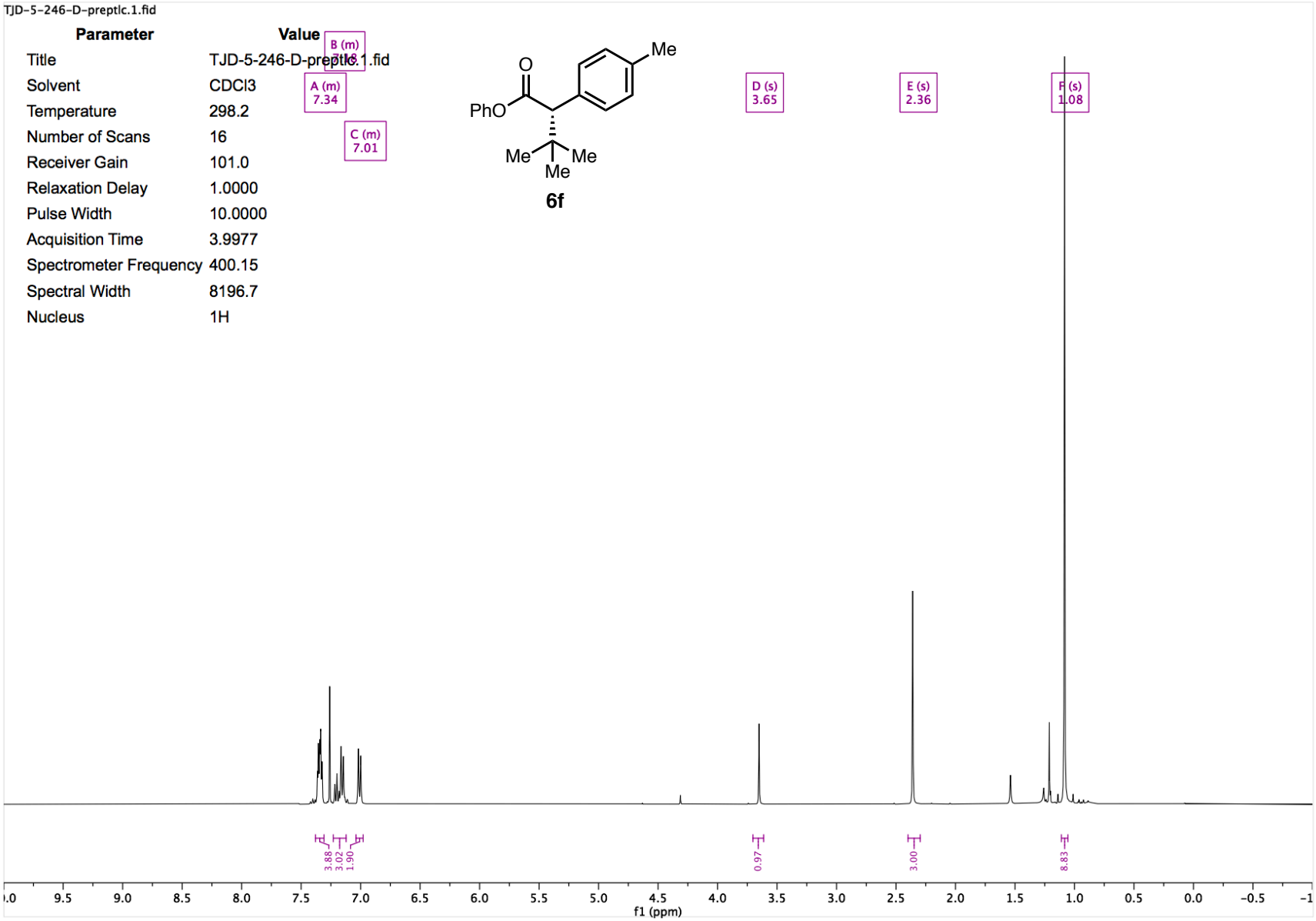

O
PhO
OMe
Me
6c
Origin Bruker BioSpin GmbH
Solvent CDCl3
Temperature 297.2
Number of Scans 512
Receiver Gain 43.7
Relaxation Delay 1.0000
Pulse Width 10.0000
Acquisition Time 1.3631
Spectrometer Frequency 100.62
Spectral Width 24038.5
Nucleus 13C
129.48
121.58
129.82
125.91
120.57
113.85
112.93
55.38
53.65
26.87
12.31
172.58
159.99
150.93
140.27
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 −10
ppm

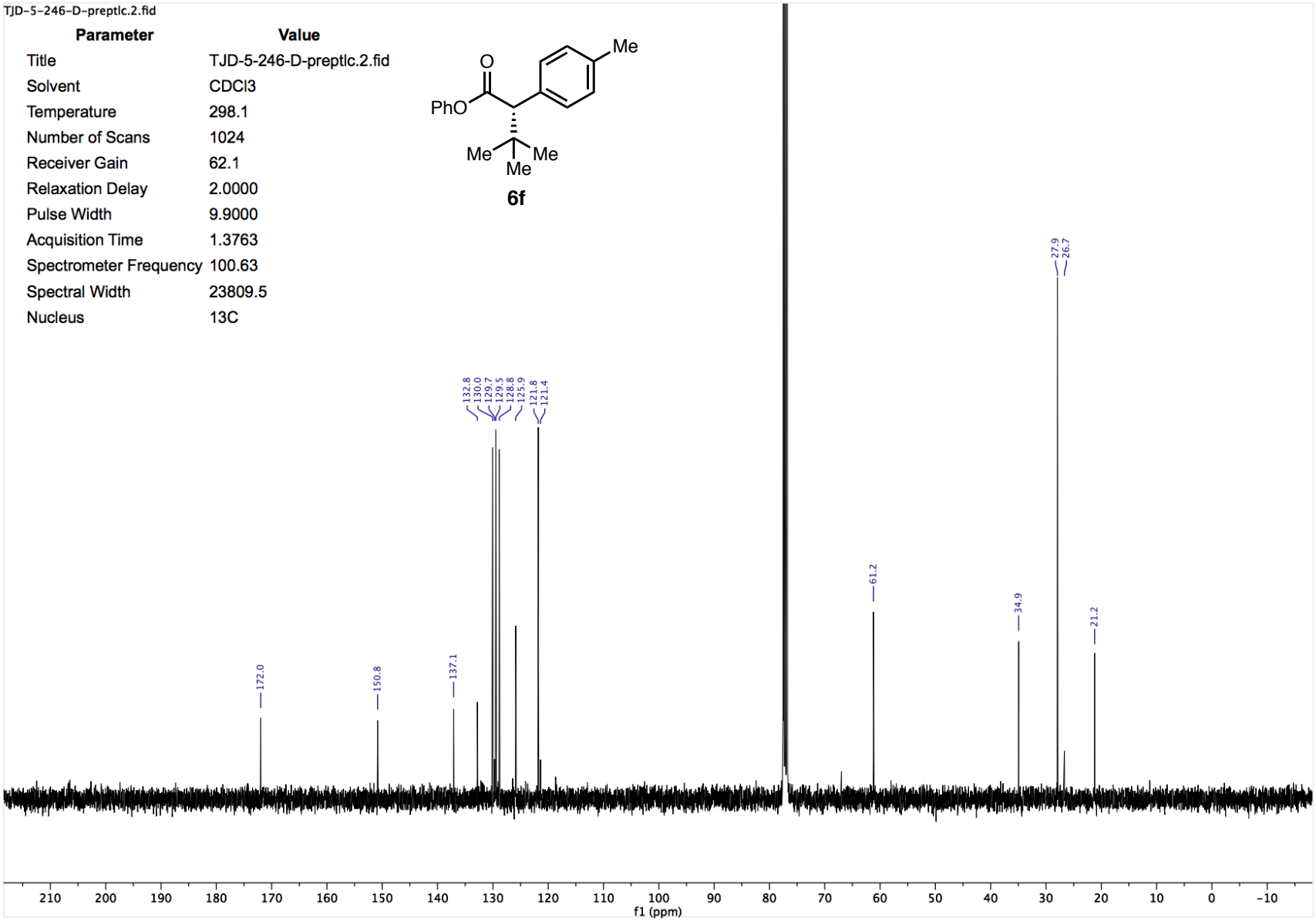

Origin Bruker BioSpin GmbH
Solvent CDCl3
Temperature 297.1
Number of Scans 16
Receiver Gain 197.4
Relaxation Delay 1.0000
Pulse Width 12.5000
Acquisition Time 2.8224
Spectrometer Frequency 400.13
Spectral Width 11609.9
Nucleus 1H
I (ddd) 7.27 J(8.13, 7.43, 0.57)
H (ddt) 7.19 J(7.97, 6.90, 1.16)
F (ddd) 6.84 J(8.24, 2.53, 1.02)
G (m) 6.99
J (m) 7.34
O
PhO
OMe
Me
Me
6d
B (s) 3.82
A (d) 3.36 J(10.55)
C (dp) 2.44 J(10.56, 6.58)
D (d) 1.18 J(6.47)
E (d) 0.80 J(6.71)
1.97
0.98
0.97
4.17
1.04
3.22
1.00
0.96
3.22
3.15
ppm

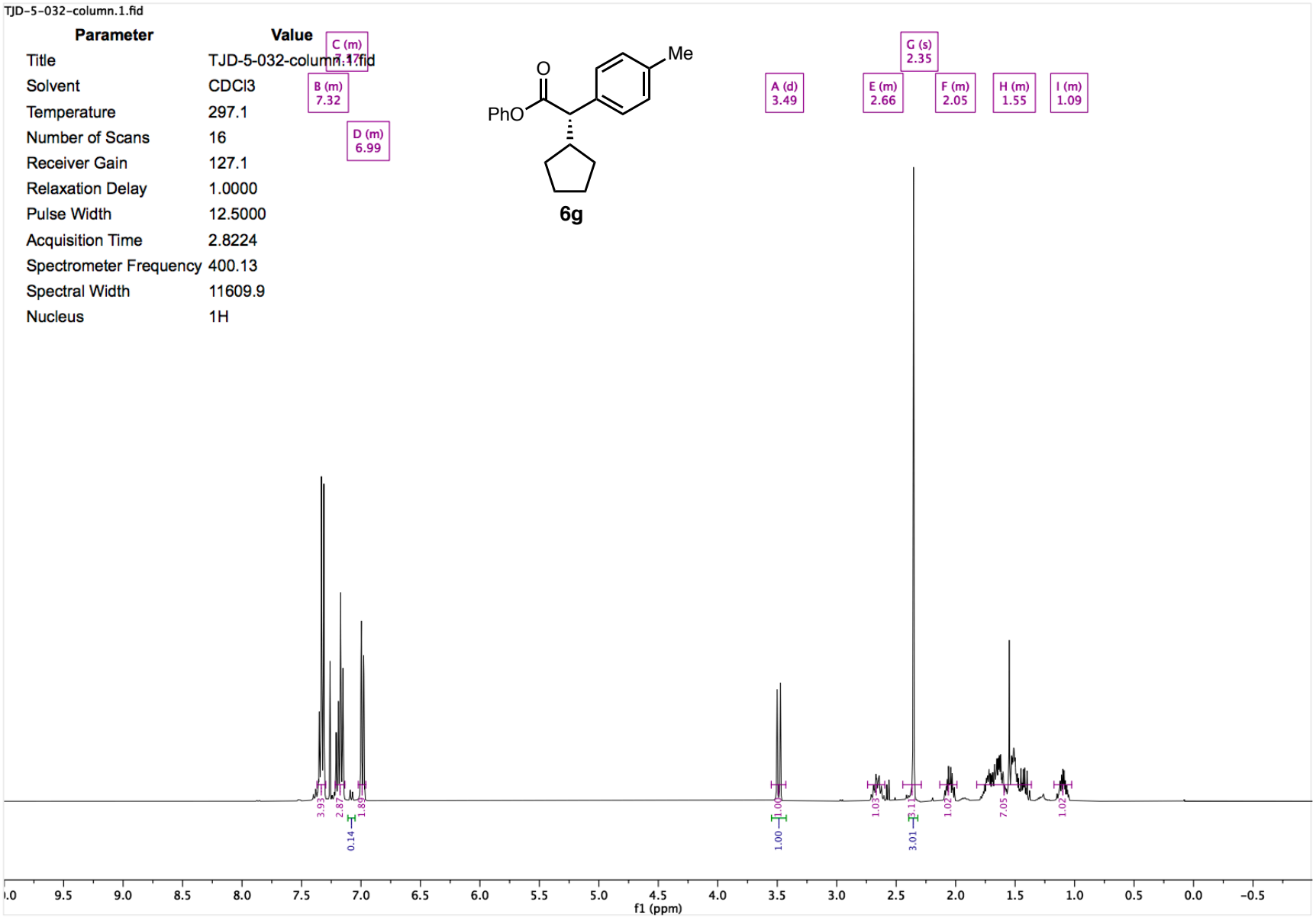

O
PhO
OMe
Me
Me
6d
Origin Bruker BioSpin GmbH
Solvent CDCl3
Temperature 297.2
Number of Scans 512
Receiver Gain 55.5
Relaxation Delay 1.0000
Pulse Width 10.0000
Acquisition Time 1.3631
Spectrometer Frequency 100.62
Spectral Width 24038.5
Nucleus 13C
129.48
121.62
129.66
125.91
121.22
114.30
113.00
60.21
55.37
32.19
21.64
20.39
172.47
159.89
150.89
139.49
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 −10
ppm

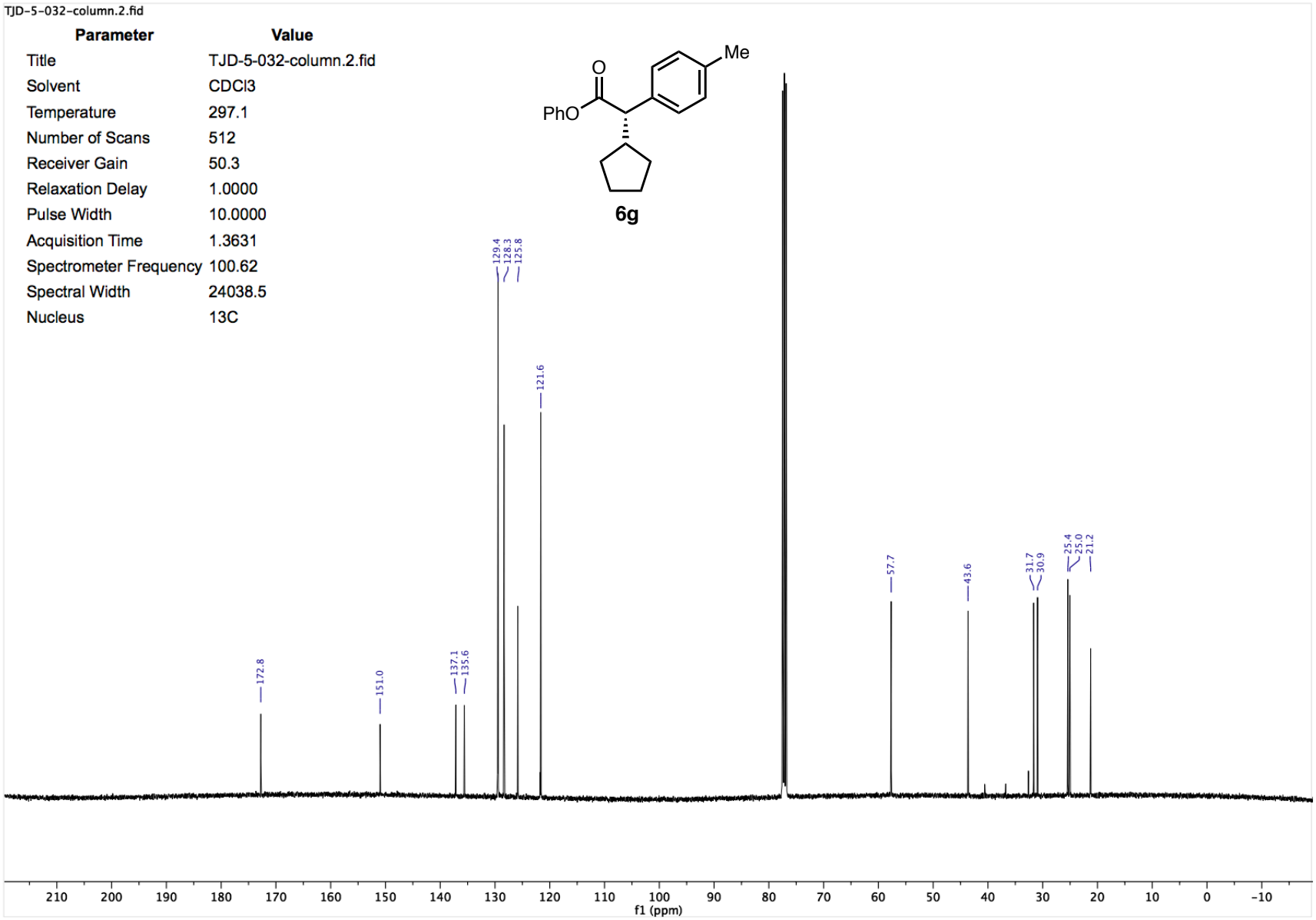

CRL-4-216-1.1.fid
Parameter Value
Title CRL-4-216-1.1.fid
Solvent CDCl3
Temperature 297.1
Number of Scans 16
Receiver Gain 156.2
Relaxation Delay 1.0000
Pulse Width 12.5000
Acquisition Time 2.8224
Spectrometer Frequency 400.13
Spectral Width 11609.9
Nucleus 1H
PhO
Me
Me
Me
6e
G (m) 7.18
F (m) 6.99
H (m) 7.32
A (d) 3.36
C (s) 2.35
B (dq) 2.44
D (d) 1.18
E (d) 0.79
4.00
2.94
1.95
1.00
1.11
3.01
3.09
3.06
f1 (ppm)

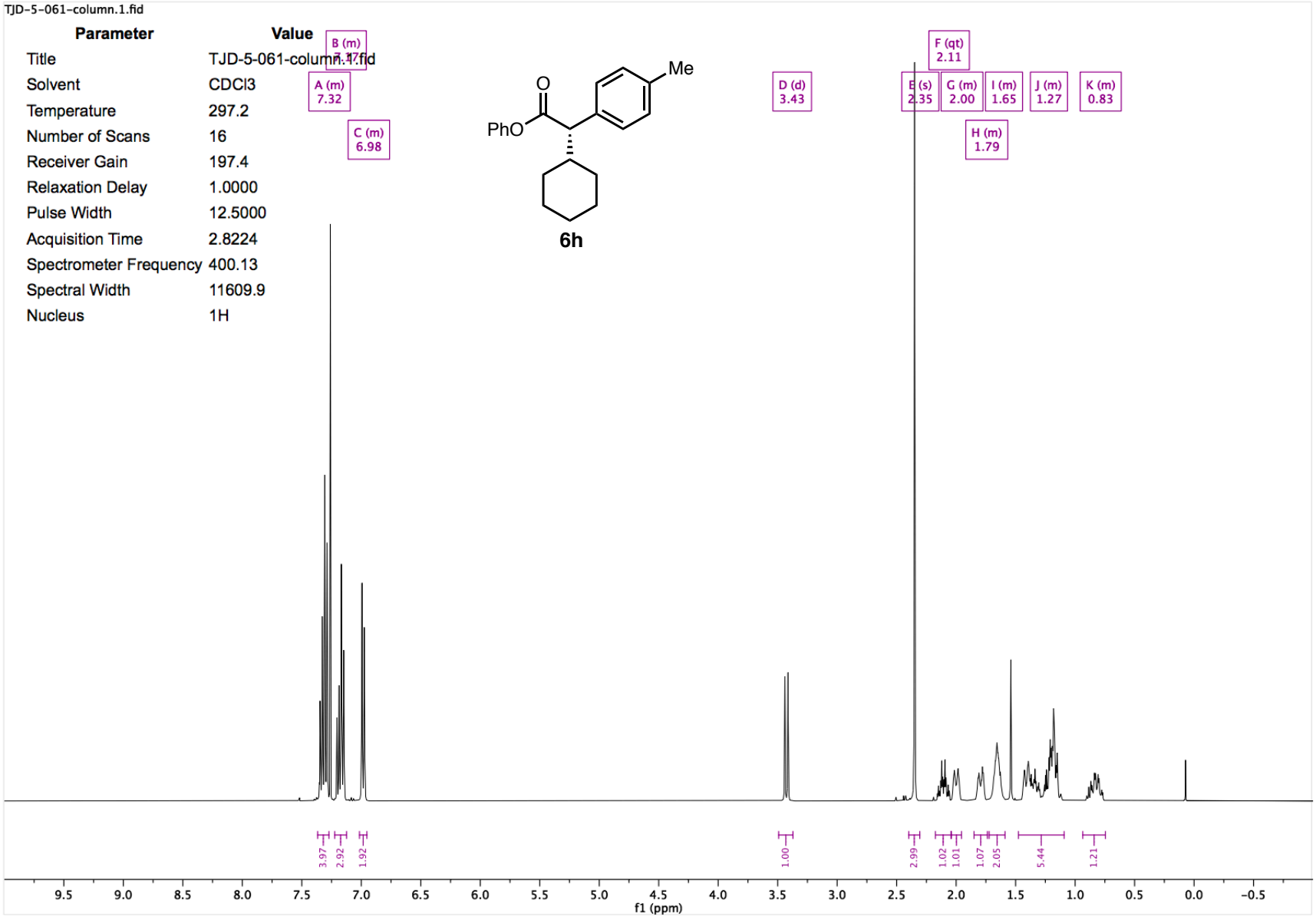

CRL-4-216-1.2.fid
Parameter Value
Title CRL-4-216-1.2.fid
Solvent CDCl3
Temperature 297.1
Number of Scans 512
Receiver Gain 55.5
Relaxation Delay 1.0000
Pulse Width 10.0000
Acquisition Time 1.3631
Spectrometer Frequency 100.62
Spectral Width 24038.5
Nucleus 13C
150.92
137.21
134.91
129.44
128.58
125.85
121.63
59.81
32.08
21.64
21.25
20.36
O
PhO
Me
Me
Me
6e
f1 (ppm)

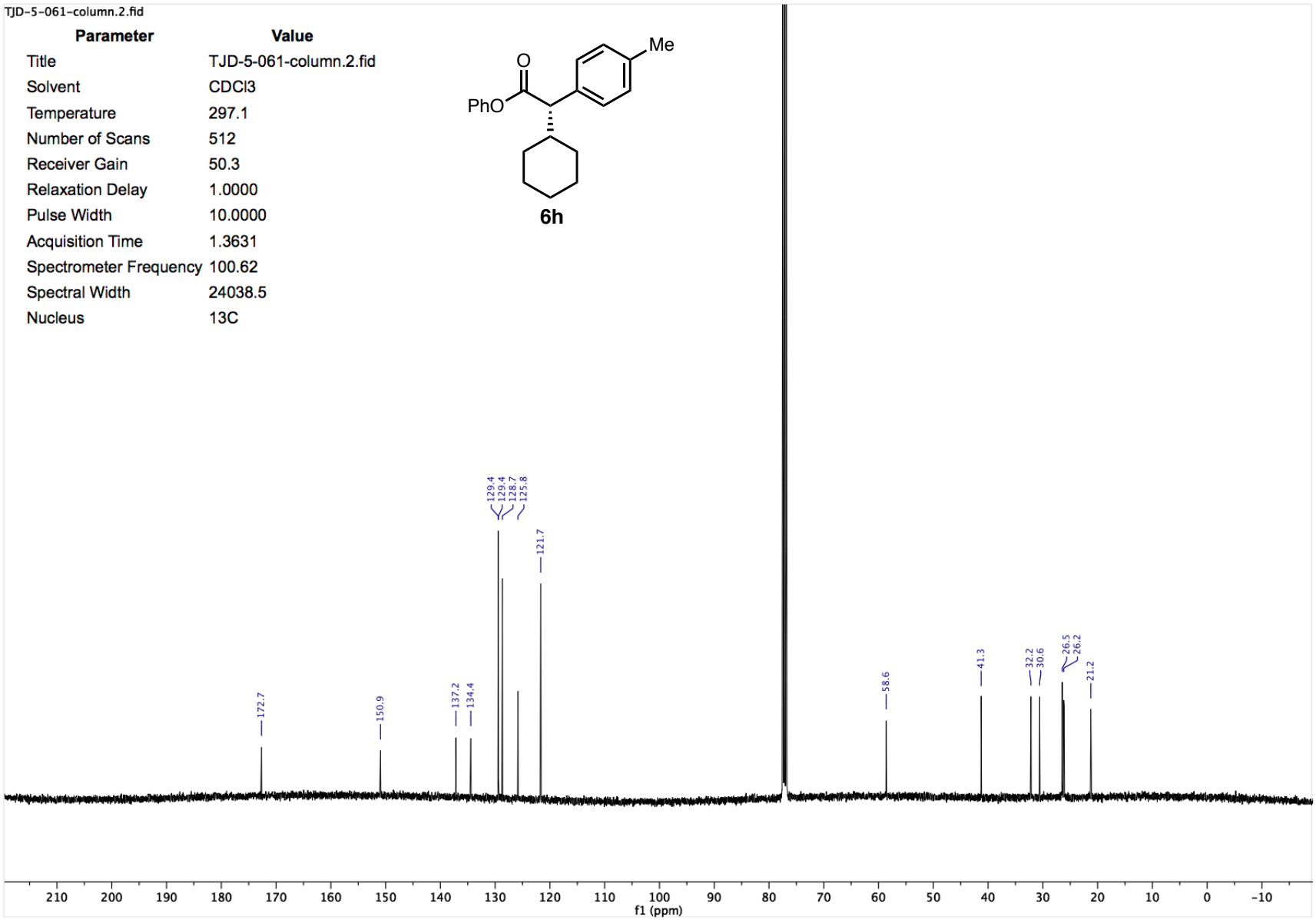

TJD-5-246-D-preptlc.1.fid
Parameter
Value
Title
TJD-5-246-D-preptlc.1.fid
Solvent
CDCl3
Temperature
298.2
Number of Scans
16
Receiver Gain
101.0
Relaxation Delay
1.0000
Pulse Width
10.0000
Acquisition Time
3.9977
Spectrometer Frequency
400.15
Spectral Width
8196.7
Nucleus
1H
B (m) 7.18
A (m) 7.34
C (m) 7.01
D (s) 3.65
E (s) 2.36
F (s) 1.08
PhO
O
Me
Me
Me
Me
6f
3.88
3.02
1.90
0.97
3.00
8.83
f1 (ppm)

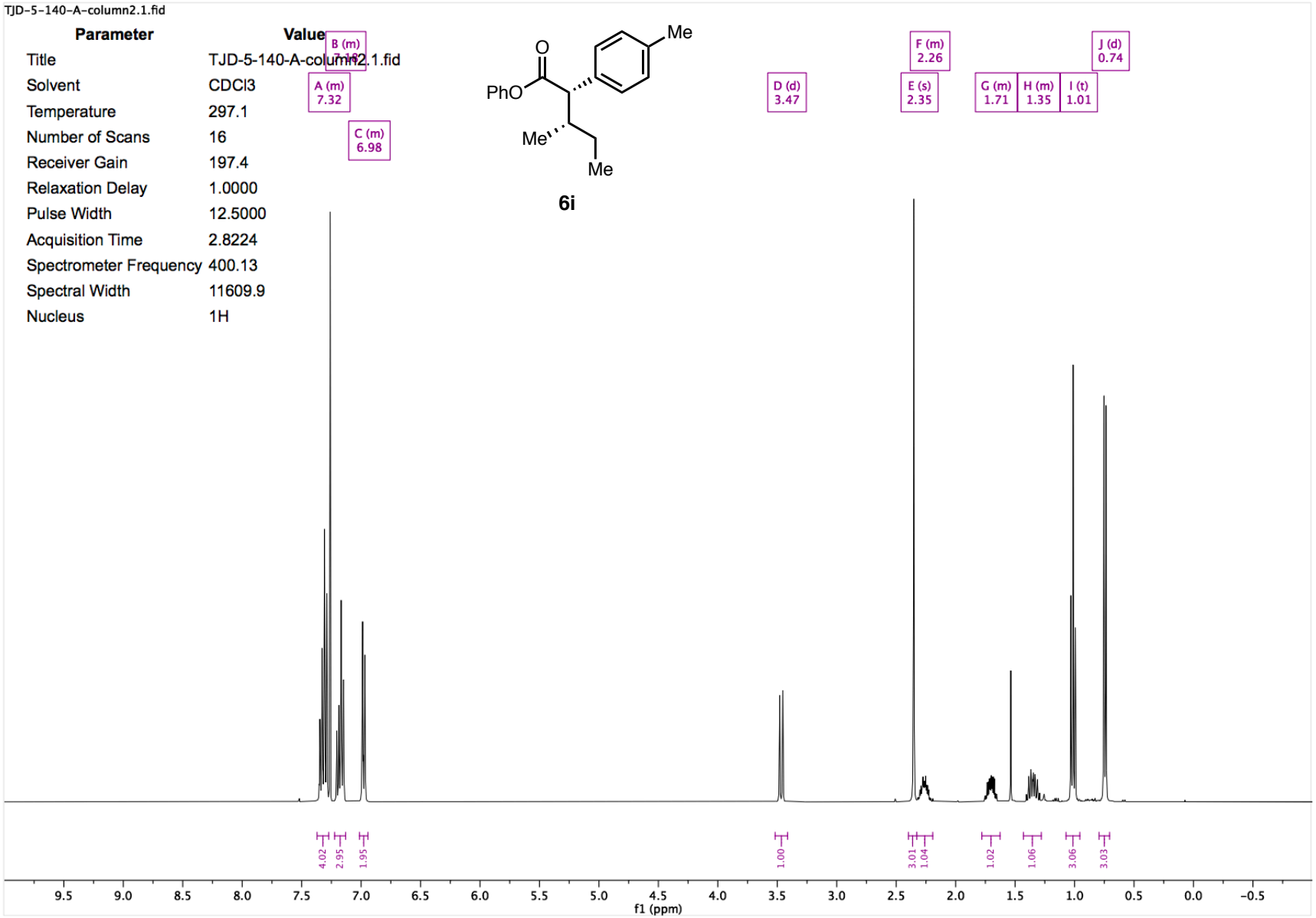

TJD-5-246-D-preptlc.2.fid
Parameter Value
Title TJD-5-246-D-preptlc.2.fid
Solvent CDCl3
Temperature 298.1
Number of Scans 1024
Receiver Gain 62.1
Relaxation Delay 2.0000
Pulse Width 9.9000
Acquisition Time 1.3763
Spectrometer Frequency 100.63
Spectral Width 23809.5
Nucleus 13C
O
PhO
Me
Me
Me
Me
6f
132.8
130.0
129.7
129.5
128.8
125.9
121.8
121.4
172.0
150.8
137.1
61.2
34.9
27.9
26.7
21.2
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

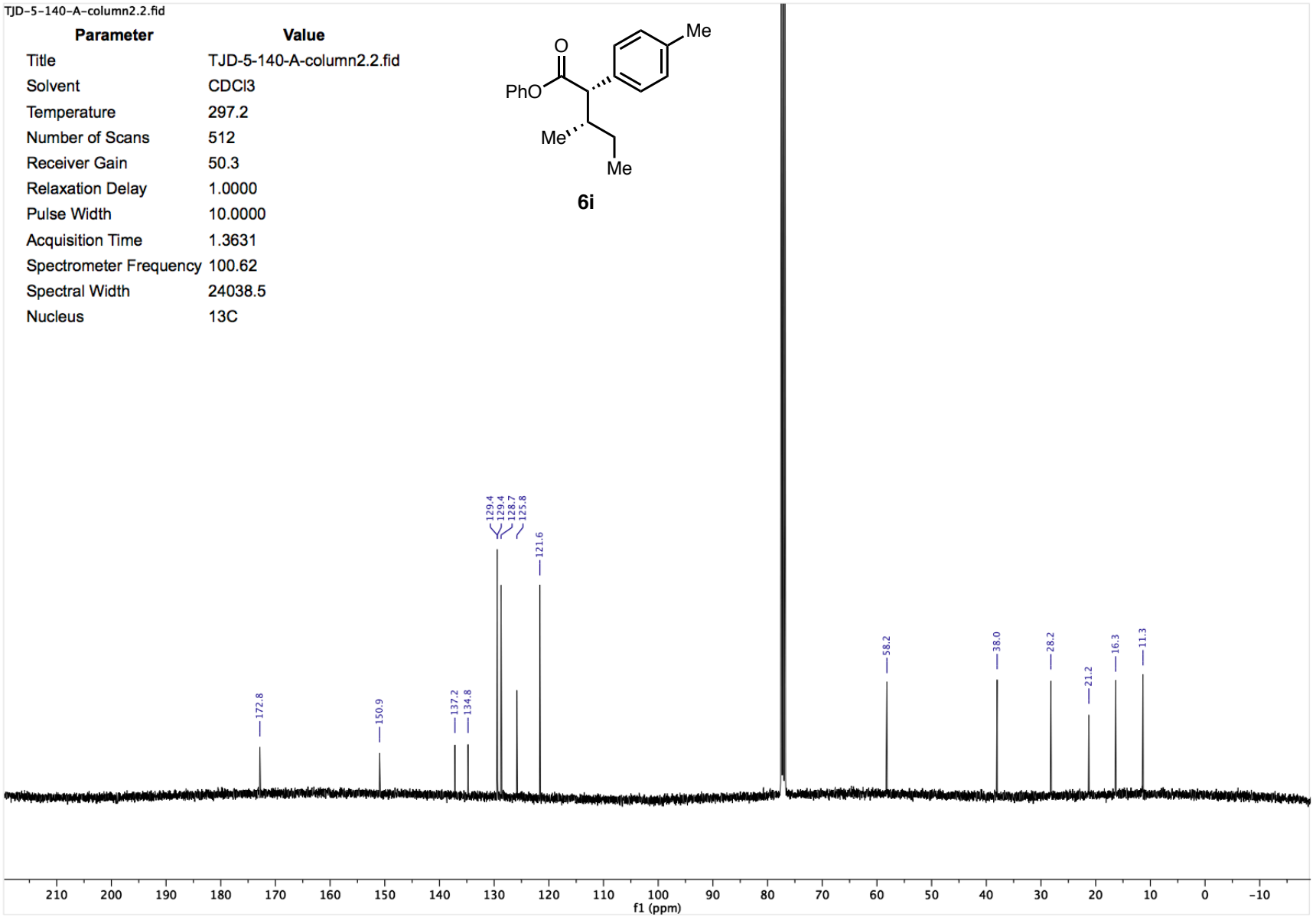

TJD-5-032-column.1.fid
Parameter
Value
Title
TJD-5-032-column.1.fid
Solvent
CDCl3
Temperature
297.1
Number of Scans
16
Receiver Gain
127.1
Relaxation Delay
1.0000
Pulse Width
12.5000
Acquisition Time
2.8224
Spectrometer Frequency
400.13
Spectral Width
11609.9
Nucleus
1H
C (m) 7.17
B (m) 7.32
D (m) 6.99
A (d) 3.49
E (m) 2.66
G (s) 2.35
F (m) 2.05
H (m) 1.55
I (m) 1.09
O
PhO
Me
6g
f1 (ppm)

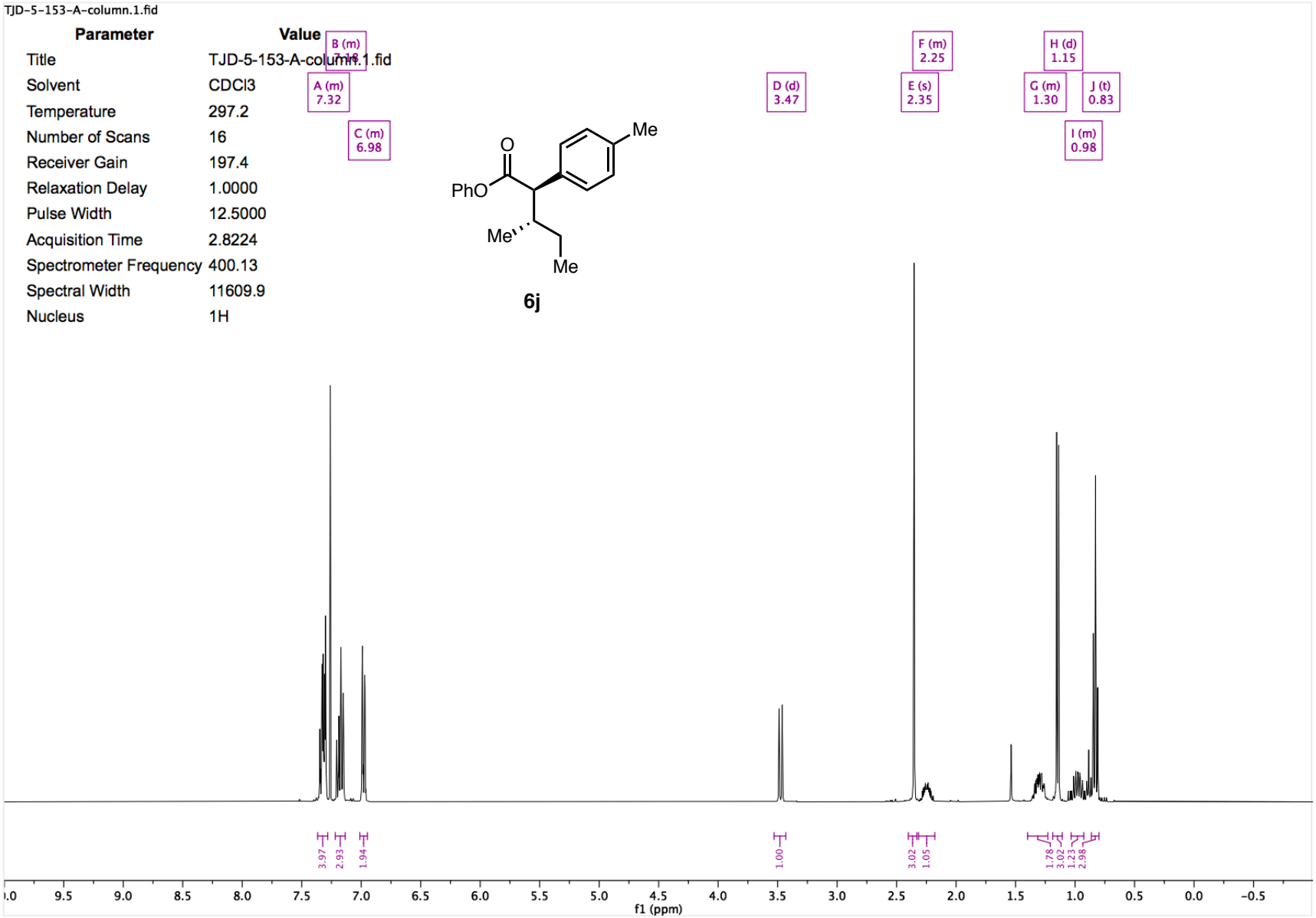

TJD-5-032-column.2.fid
Parameter Value
Title TJD-5-032-column.2.fid
Solvent CDCl3
Temperature 297.1
Number of Scans 512
Receiver Gain 50.3
Relaxation Delay 1.0000
Pulse Width 10.0000
Acquisition Time 1.3631
Spectrometer Frequency 100.62
Spectral Width 24038.5
Nucleus 13C
O
PhO
Me
6g
129.4
128.3
125.8
121.6
172.8
151.0
137.1
135.6
57.7
43.6
31.7
30.9
25.4
25.0
21.2
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

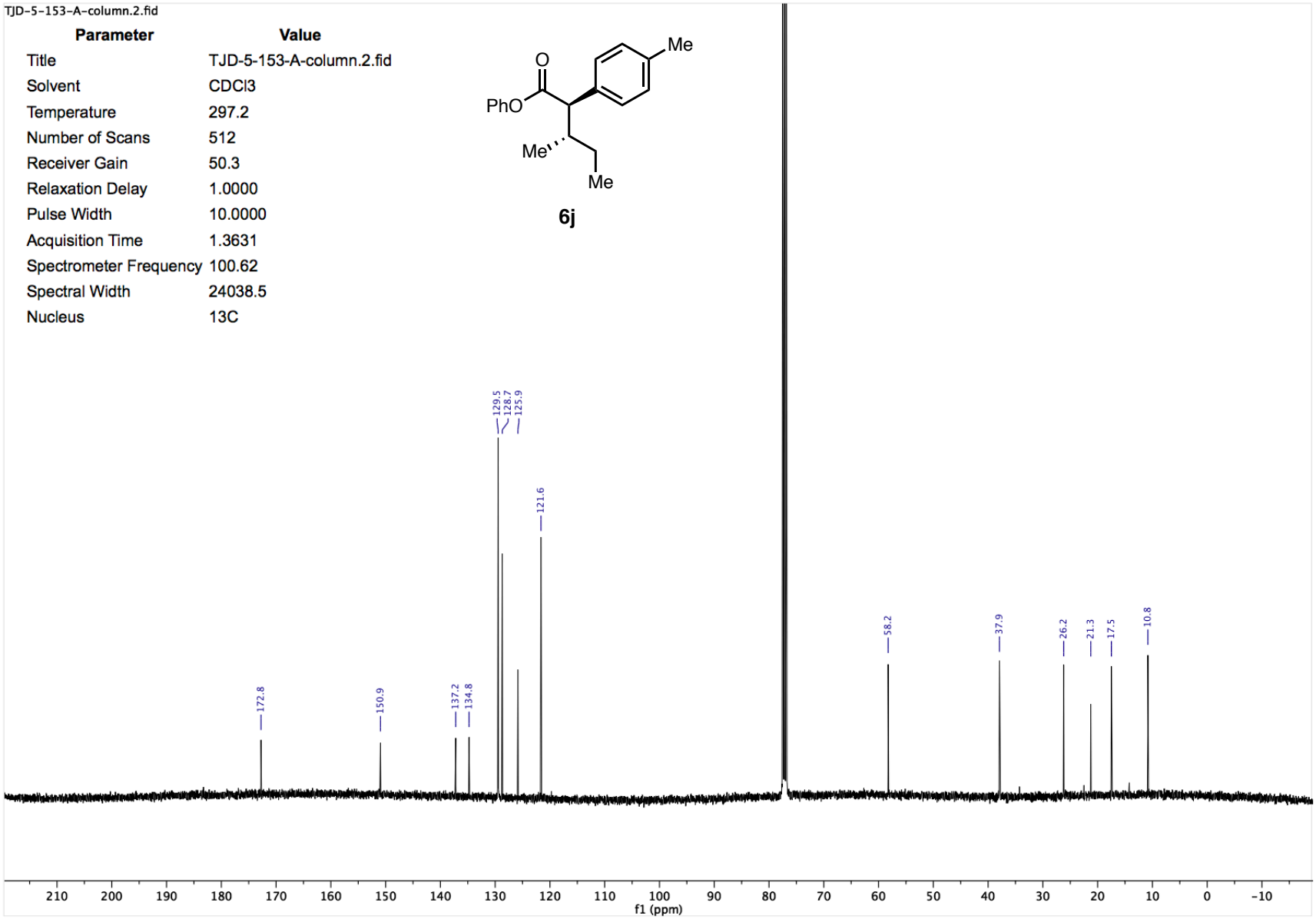

TJD-5-061-column.1.fid
Parameter
Value
Title
TJD-5-061-column.1.fid
Solvent
CDCl3
Temperature
297.2
Number of Scans
16
Receiver Gain
197.4
Relaxation Delay
1.0000
Pulse Width
12.5000
Acquisition Time
2.8224
Spectrometer Frequency
400.13
Spectral Width
11609.9
Nucleus
1H
B (m)
A (m) 7.32
C (m) 6.98
D (d) 3.43
F (qt) 2.11
E (s) 2.35
G (m) 2.00
I (m) 1.65
J (m) 1.27
K (m) 0.83
H (m) 1.79
O
PhO
Me
6h
3.97
2.92
1.92
1.00
2.99
1.02
1.01
1.07
2.05
5.44
1.21
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)

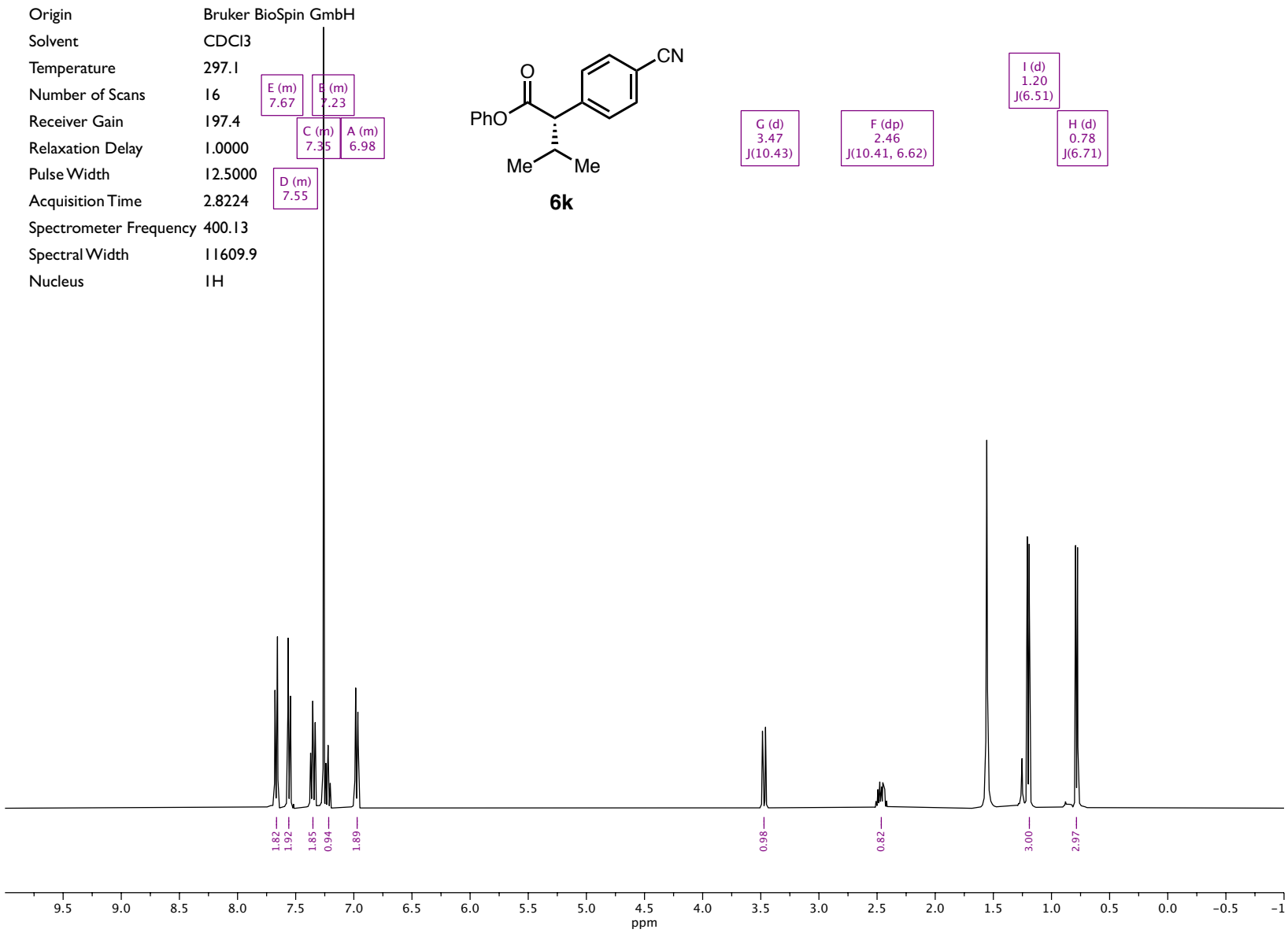

TJD-5-061-column.2.fid
Parameter
Value
Title
TJD-5-061-column.2.fid
Solvent
CDCl3
Temperature
297.1
Number of Scans
512
Receiver Gain
50.3
Relaxation Delay
1.0000
Pulse Width
10.0000
Acquisition Time
1.3631
Spectrometer Frequency
100.62
Spectral Width
24038.5
Nucleus
13C
Me
O
PhO
6h
172.7
150.9
137.2
134.4
129.4
129.4
128.7
125.8
121.7
58.6
41.3
32.2
30.6
26.5
26.2
21.2
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)


TJD-5-140-A-column2.1.fid
Parameter
Value
Title
TJD-5-140-A-column2.1.fid
Solvent
CDCl3
Temperature
297.1
Number of Scans
16
Receiver Gain
197.4
Relaxation Delay
1.0000
Pulse Width
12.5000
Acquisition Time
2.8224
Spectrometer Frequency
400.13
Spectral Width
11609.9
Nucleus
1H
B (m)
7.18
A (m)
7.32
C (m)
6.98
D (d)
3.47
F (m)
2.26
E (s)
2.35
G (m)
1.71
H (m)
1.35
I (t)
1.01
J (d)
0.74
PhO
O
Me
Me
Me
6i
4.02
2.95
1.95
1.00
3.01
1.04
1.02
1.06
3.06
3.03
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)

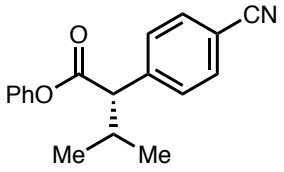

TJD-5-140-A-column2.2.fid
Parameter Value
Title TJD-5-140-A-column2.2.fid
Solvent CDCl3
Temperature 297.2
Number of Scans 512
Receiver Gain 50.3
Relaxation Delay 1.0000
Pulse Width 10.0000
Acquisition Time 1.3631
Spectrometer Frequency 100.62
Spectral Width 24038.5
Nucleus 13C
O
PhO
Me
Me
Me
6i
172.8
150.9
137.2
134.8
129.4
129.4
128.7
125.8
121.6
58.2
38.0
28.2
21.2
16.3
11.3
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)


TJD-5-153-A-column.1.fid
Parameter
Value
Title
TJD-5-153-A-column.1.fid
Solvent
CDCl3
Temperature
297.2
Number of Scans
16
Receiver Gain
197.4
Relaxation Delay
1.0000
Pulse Width
12.5000
Acquisition Time
2.8224
Spectrometer Frequency
400.13
Spectral Width
11609.9
Nucleus
1H
B (m) 7.18
A (m) 7.32
C (m) 6.98
D (d) 3.47
F (m) 2.25
E (s) 2.35
H (d) 1.15
G (m) 1.30
J (t) 0.83
I (m) 0.98
O
PhO
Me
Me
Me
6j
3.97
2.93
1.94
1.00
3.02
1.05
1.78
3.02
1.23
2.98
f1 (ppm)


TJD-5-153-A-column.2.fid
Parameter Value
Title TJD-5-153-A-column.2.fid
Solvent CDCl3
Temperature 297.2
Number of Scans 512
Receiver Gain 50.3
Relaxation Delay 1.0000
Pulse Width 10.0000
Acquisition Time 1.3631
Spectrometer Frequency 100.62
Spectral Width 24038.5
Nucleus 13C
O
PhO
Me
Me
Me
6j
172.8
150.9
137.2
134.8
129.5
128.7
125.9
121.6
58.2
37.9
26.2
21.3
17.5
10.8
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

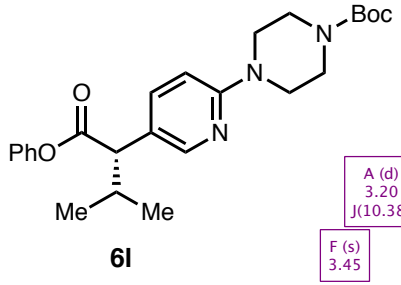

Origin Bruker BioSpin GmbH
Solvent CDCl3
Temperature 297.1
Number of Scans 16
Receiver Gain 197.4
Relaxation Delay 1.0000
Pulse Width 12.5000
Acquisition Time 2.8224
Spectrometer Frequency 400.13
Spectral Width 11609.9
Nucleus 1H
E (m) 7.67
B (m) 7.23
C (m) 7.35
A (m) 6.98
D (m) 7.55
O
PhO
CN
Me
Me
6k
G (d) 3.47 J(10.43)
F (dp) 2.46 J(10.41, 6.62)
I (d) 1.20 J(6.51)
H (d) 0.78 J(6.71)
1.82
1.92
1.85
0.94
1.89
0.98
0.82
3.00
2.97
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 −0.5 −1
ppm

Origin	Bruker BioSpin GmbH
Solvent	CDCl3
Temperature	297.1
Number of Scans	512
Receiver Gain	55.5
Relaxation Delay	1.0000
Pulse Width	10.0000
Acquisition Time	1.3631
Spectrometer Frequency	100.62
Spectral Width	24038.5
Nucleus	13C

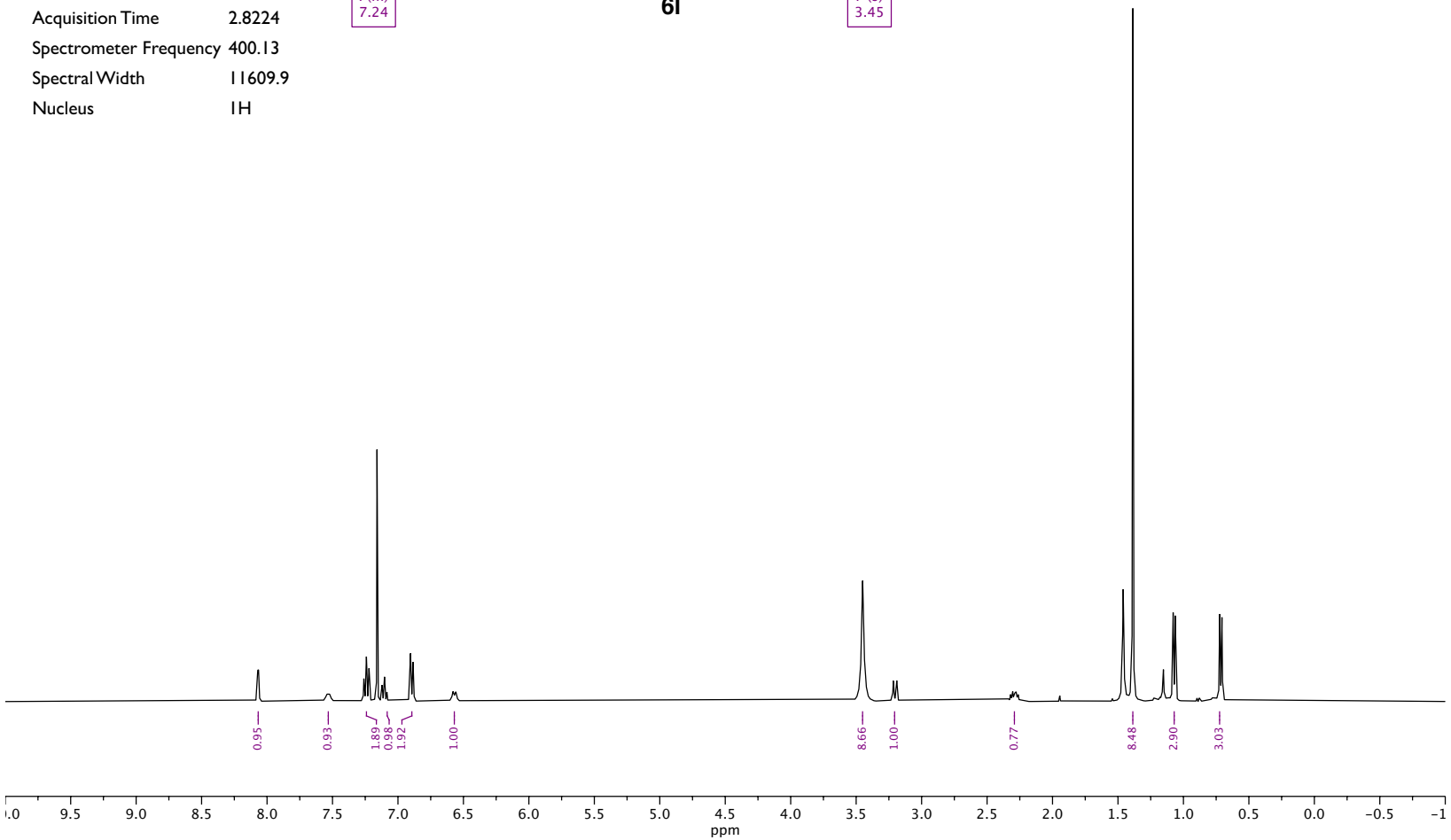


6k

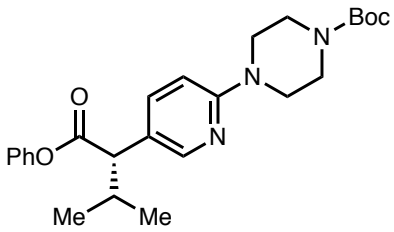
Origin	Bruker BioSpin GmbH
Solvent	CDCl3
Temperature	297.2
Number of Scans	16
Receiver Gain	197.4
Relaxation Delay	1.0000
Pulse Width	12.5000
Acquisition Time	2.8224
Spectrometer Frequency	400.13
Spectral Width	11609.9
Nucleus	1H



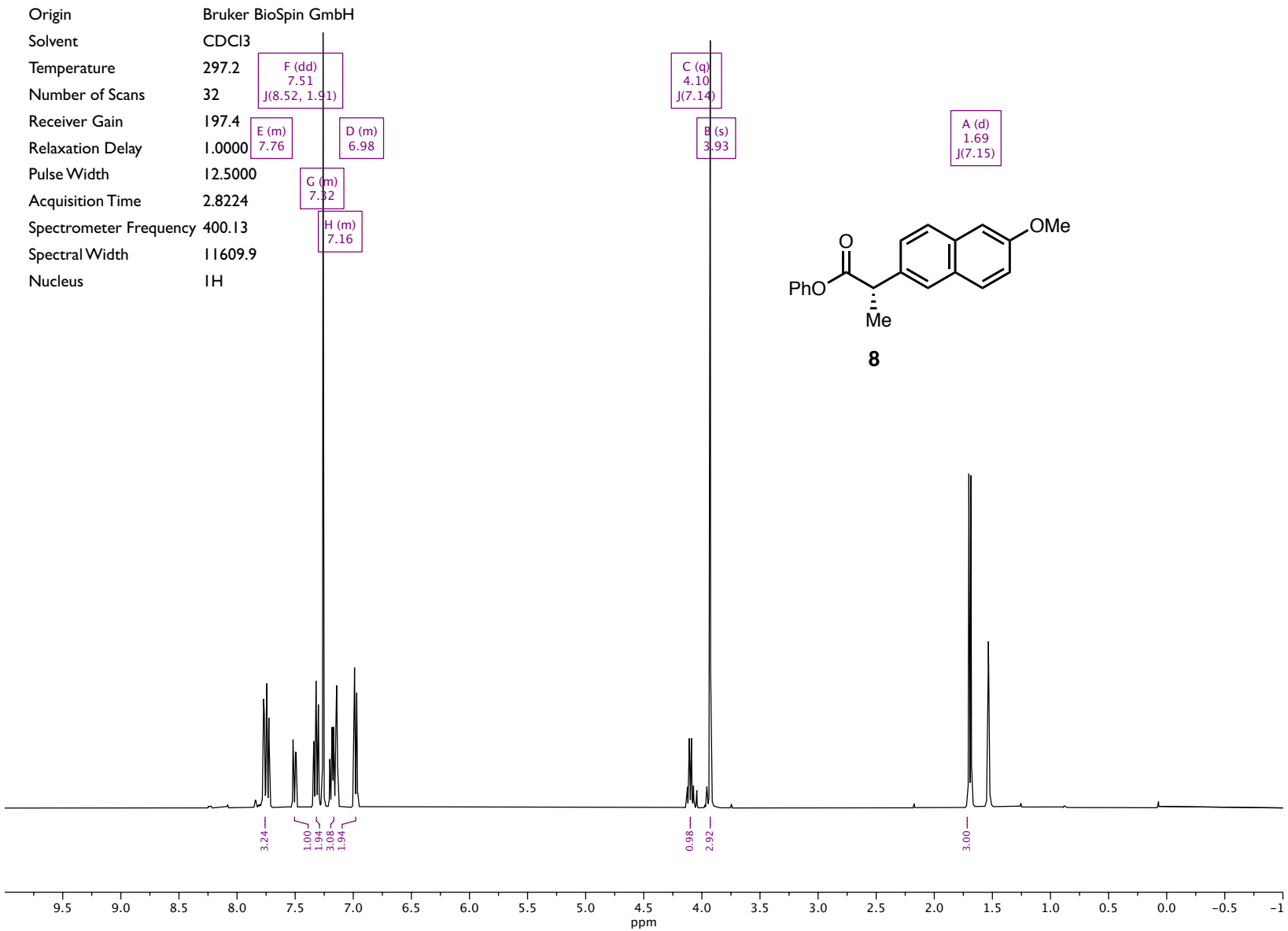
6l

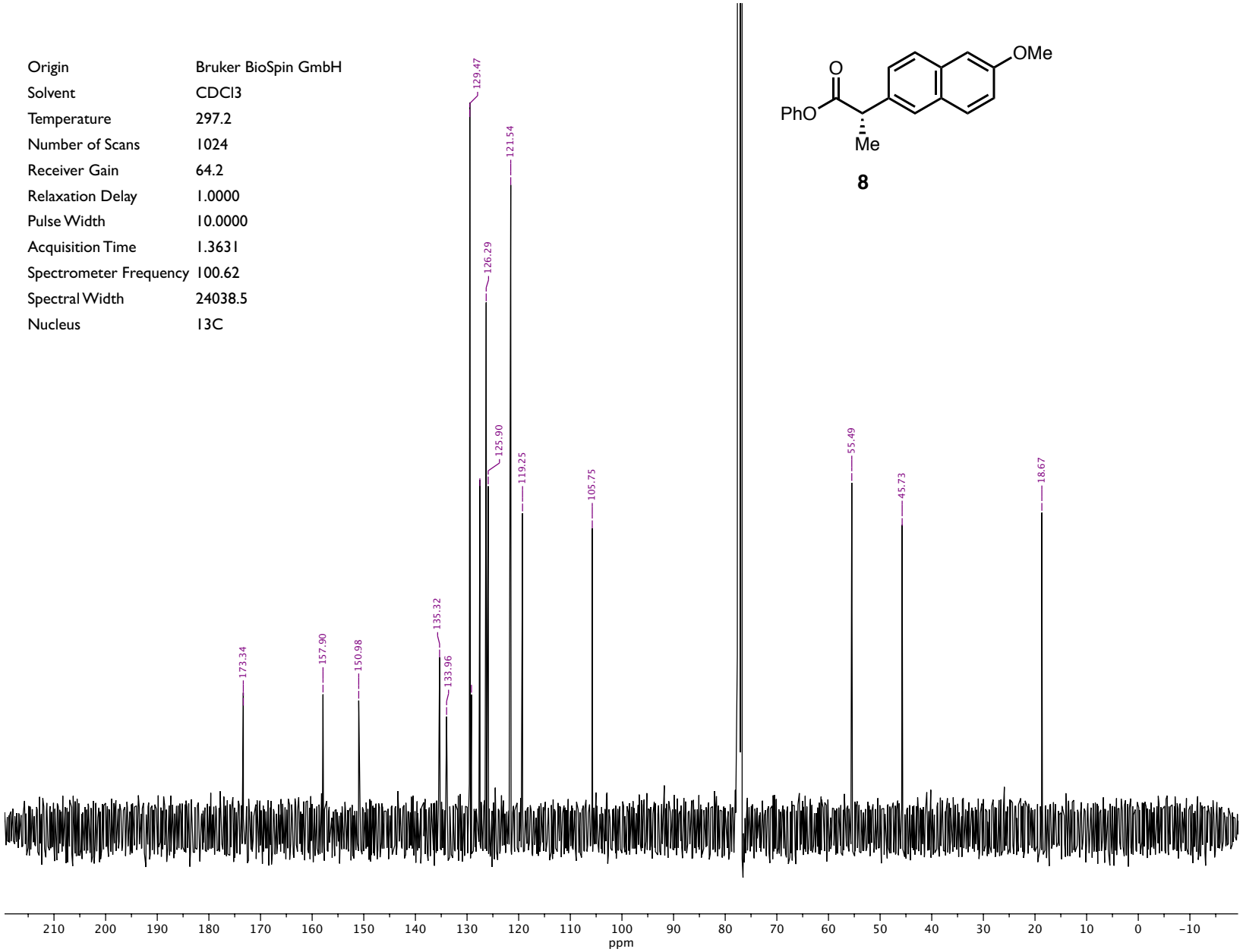


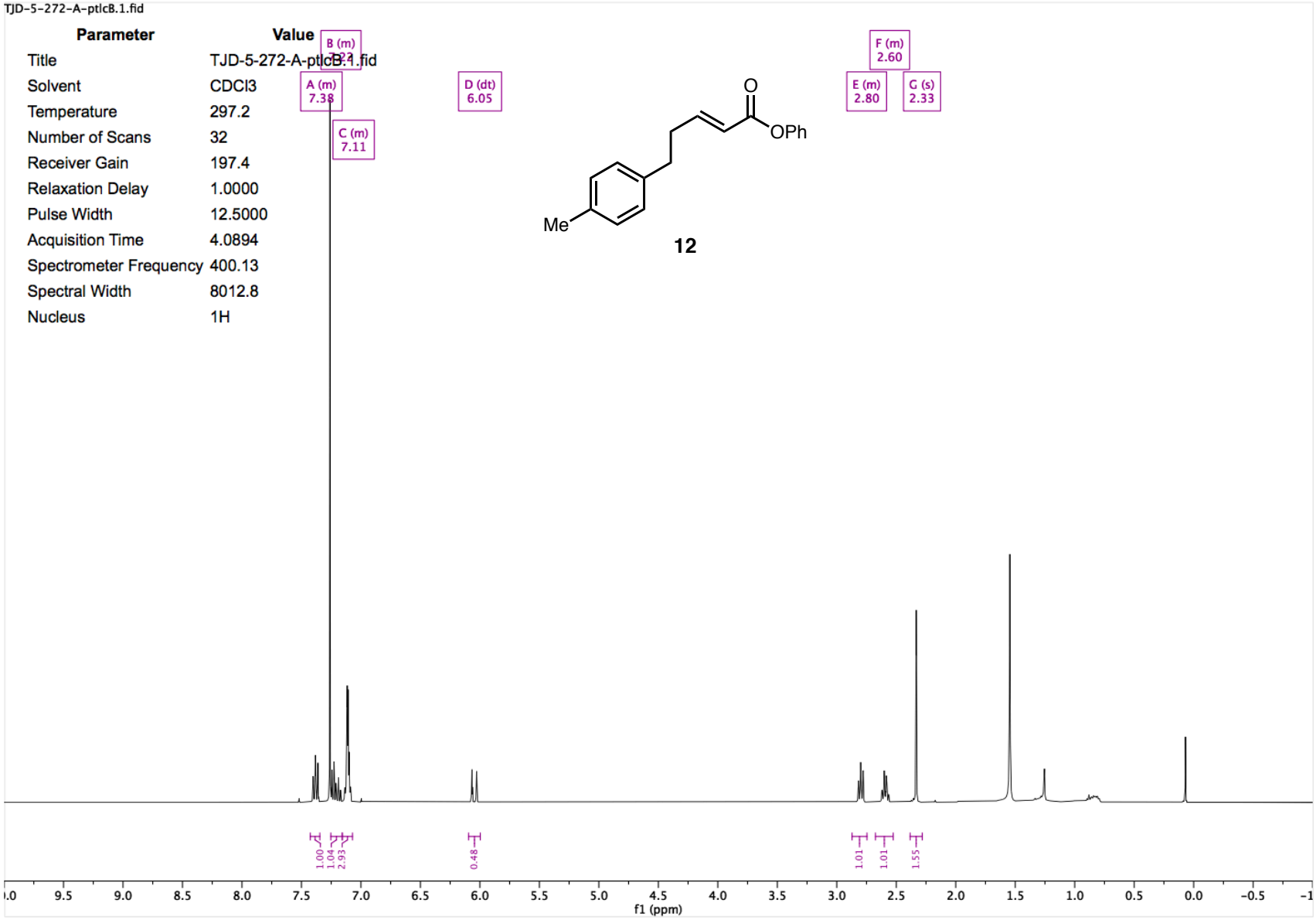
Origin	Bruker BioSpin GmbH
Solvent	CDCl3
Temperature	297.1
Number of Scans	512
Receiver Gain	87.8
Relaxation Delay	1.0000
Pulse Width	10.0000
Acquisition Time	1.3631
Spectrometer Frequency	100.62
Spectral Width	24038.5
Nucleus	13C

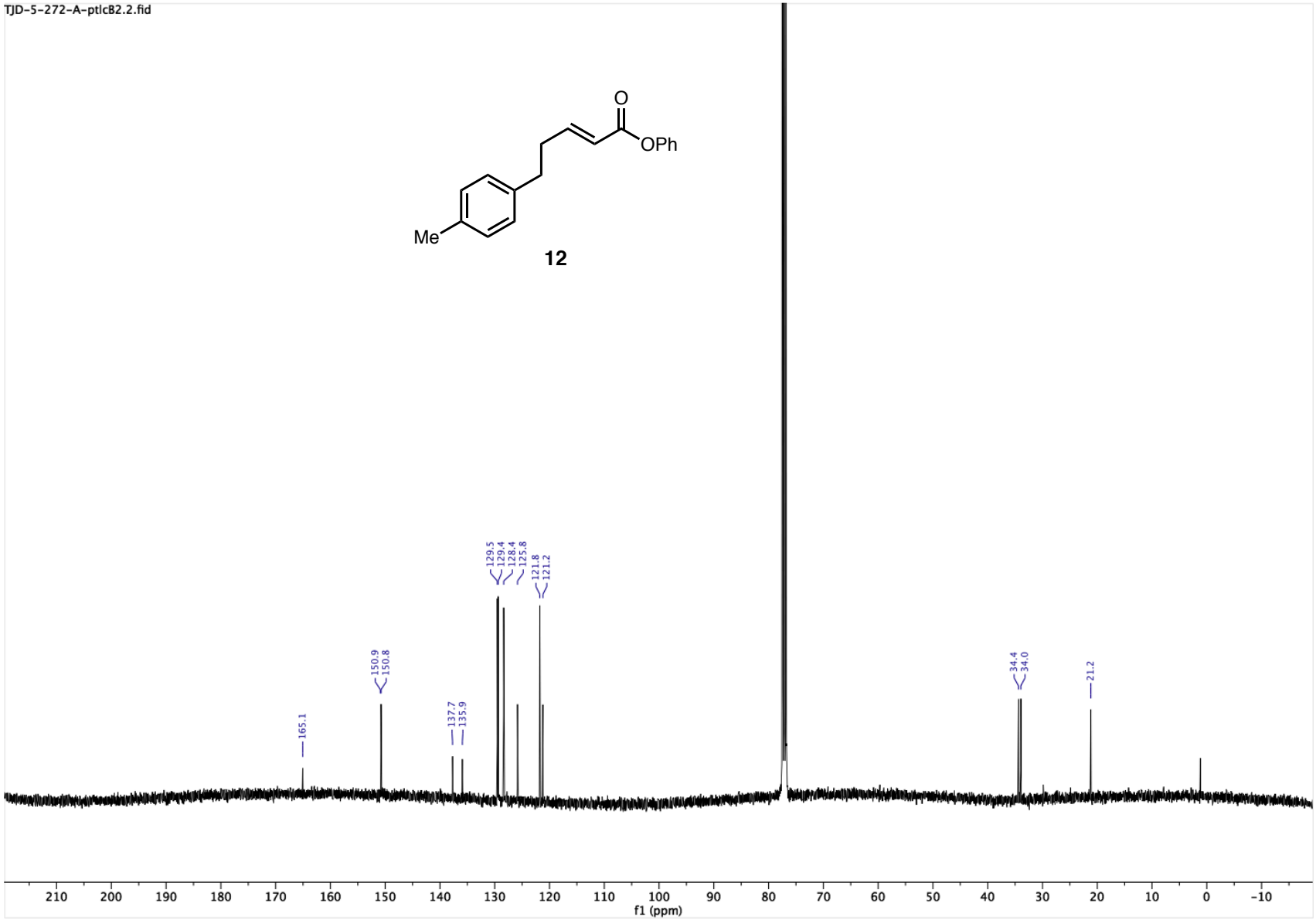


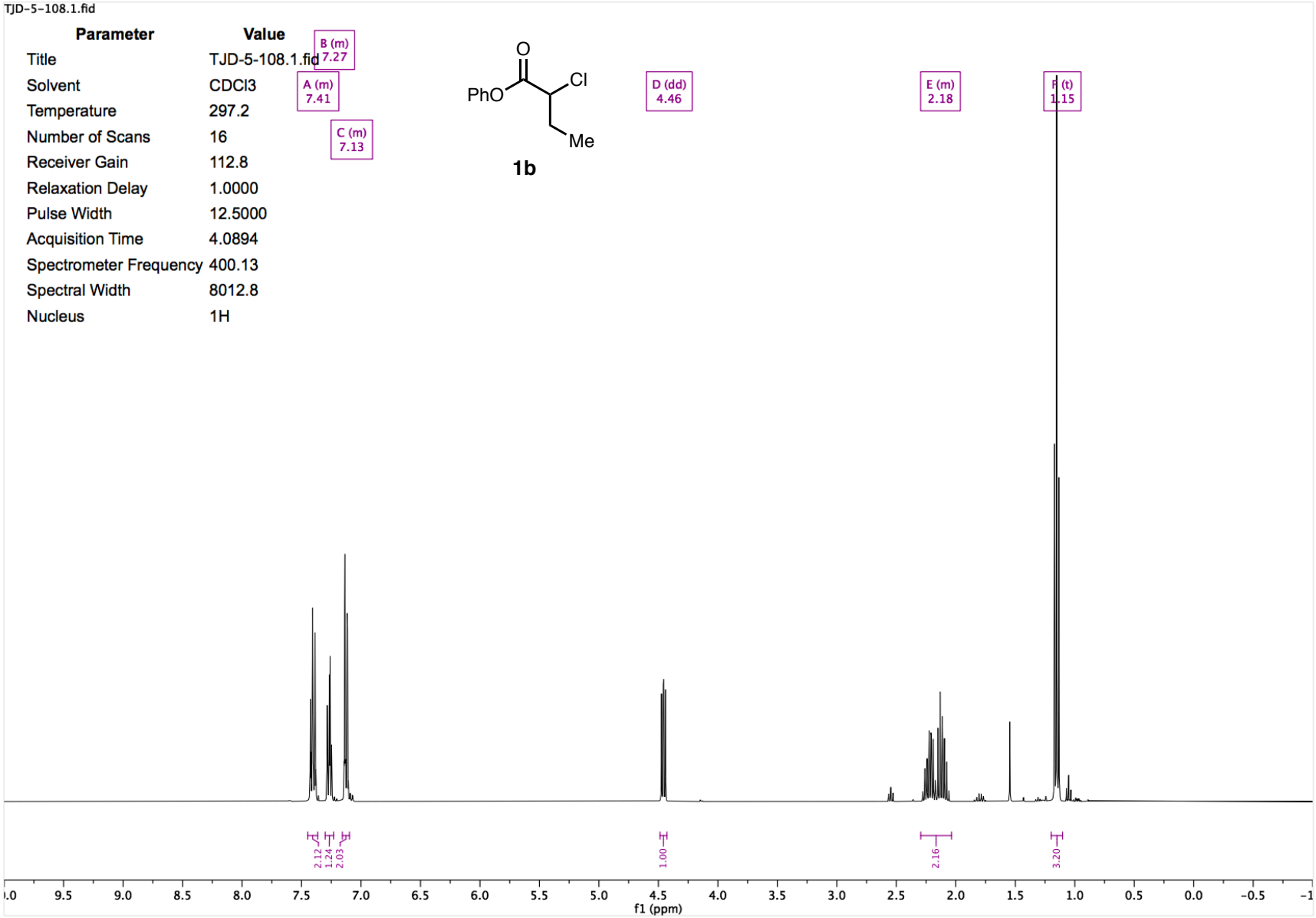
6l

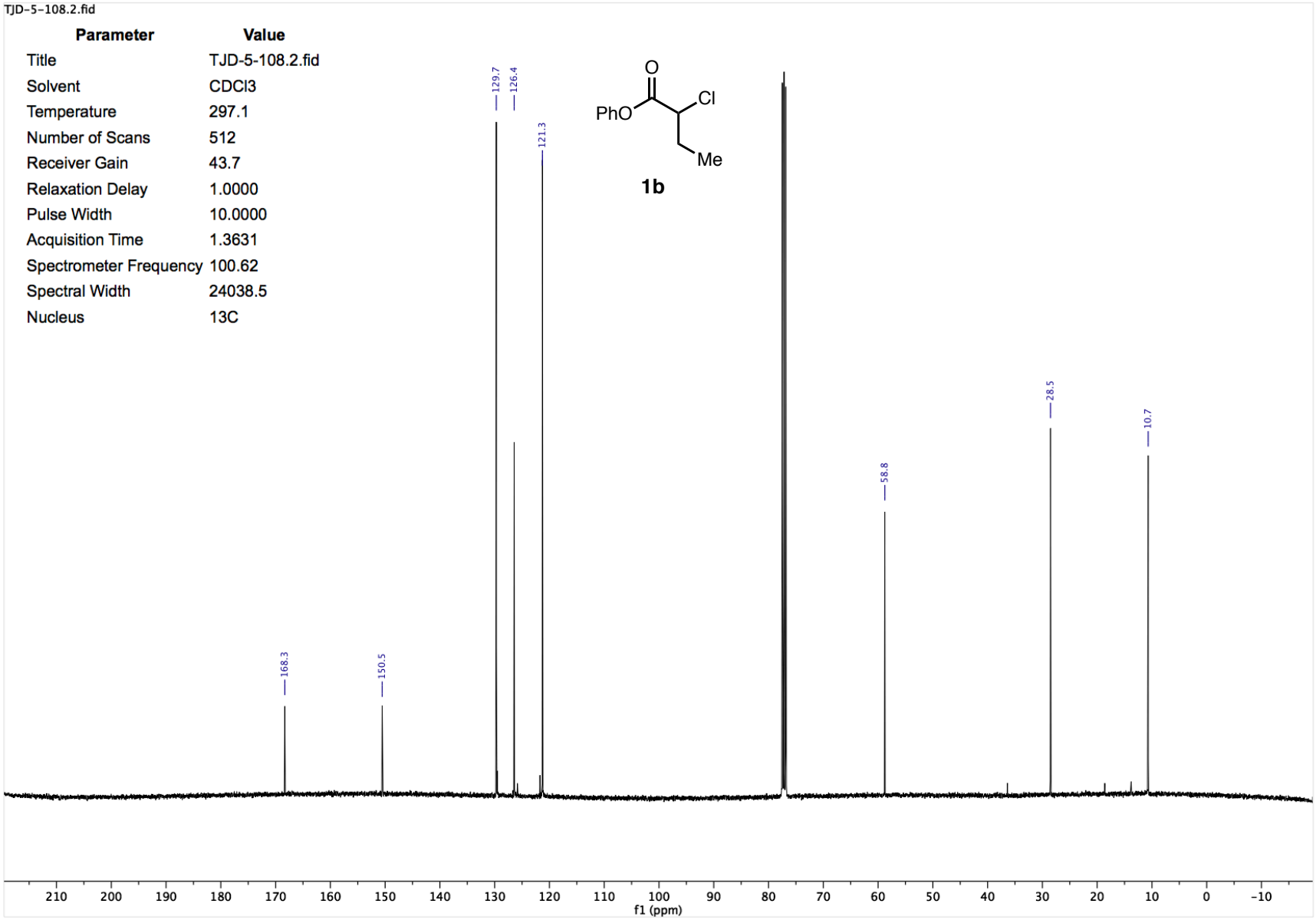

Origin Bruker BioSpin GmbH
Solvent CDCl3
Temperature 297.2
Number of Scans 32
Receiver Gain 197.4
Relaxation Delay 1.0000
Pulse Width 12.5000
Acquisition Time 2.8224
Spectrometer Frequency 400.13
Spectral Width 11609.9
Nucleus 1H
F (dd) 7.51 J(8.52, 1.91)
E (m) 7.76
D (m) 6.98
G (m) 7.32
H (m) 7.16
C (q) 4.10 J(7.14)
B (s) 3.93
A (d) 1.69 J(7.15)
O
PhO
OMe
Me
8
3.24
1.00
1.94
3.08
1.94
0.98
2.92
3.00
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 −0.5 −1
ppm

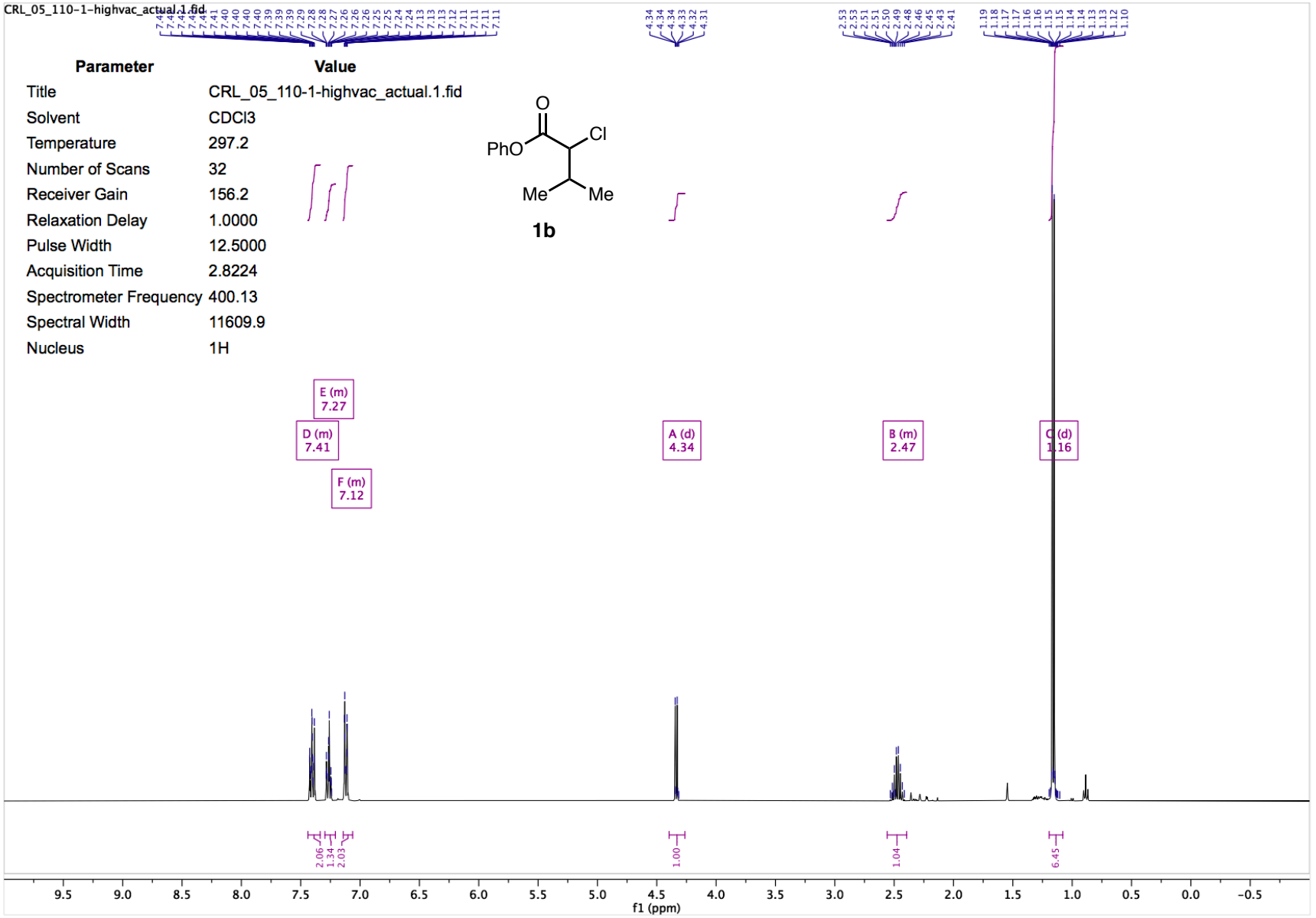

Origin Bruker BioSpin GmbH
Solvent CDCl3
Temperature 297.2
Number of Scans 1024
Receiver Gain 64.2
Relaxation Delay 1.0000
Pulse Width 10.0000
Acquisition Time 1.3631
Spectrometer Frequency 100.62
Spectral Width 24038.5
Nucleus 13C
129.47
126.29
125.90
121.54
119.25
105.75
55.49
45.73
18.67
173.34
157.90
150.98
135.32
133.96
OMe
O
PhO
Me
8
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 −10
ppm

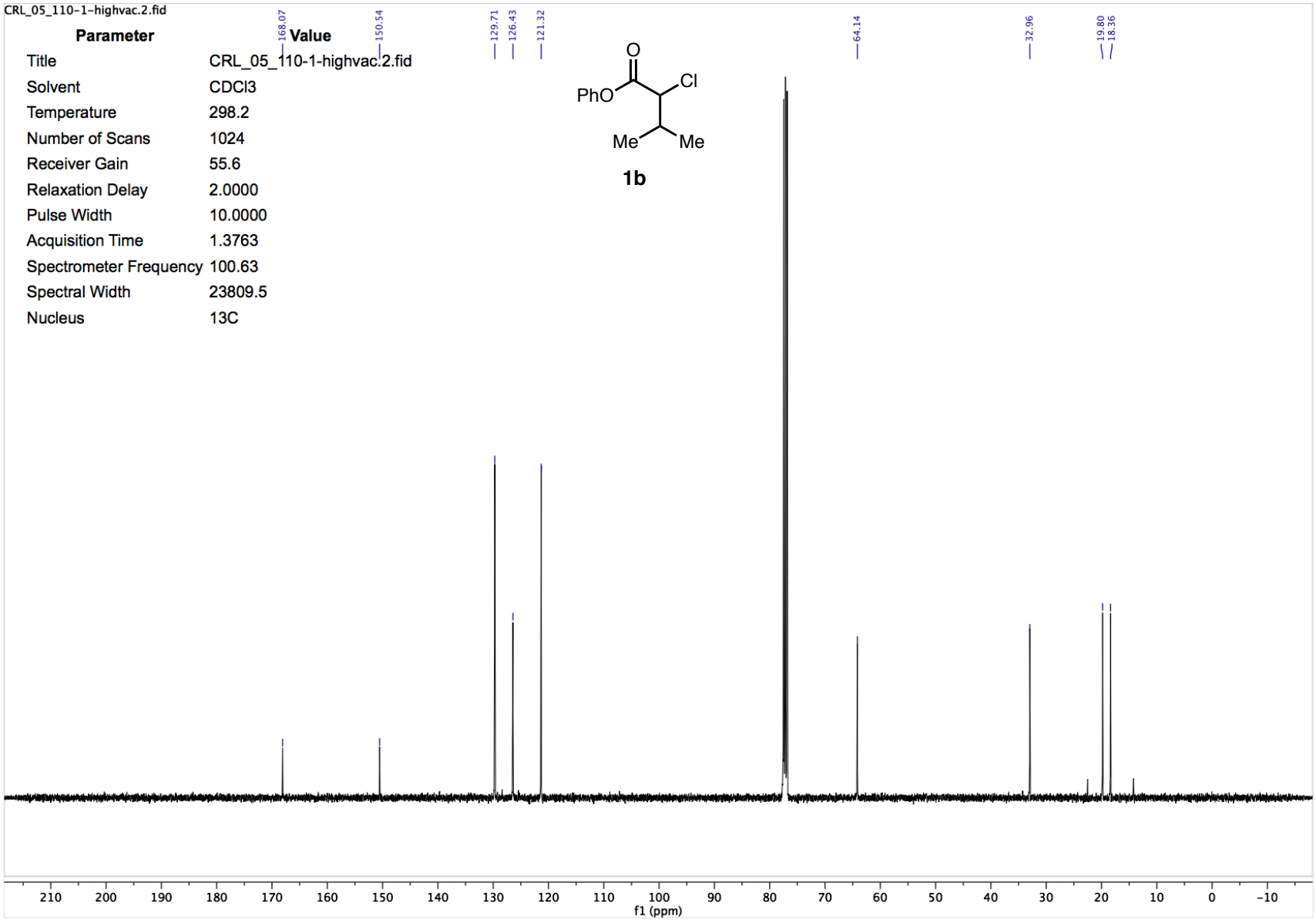

TJD-5-272-A-ptlcB.1.fid
Parameter Value
Title TJD-5-272-A-ptlcB.1.fid
Solvent CDCl3
Temperature 297.2
Number of Scans 32
Receiver Gain 197.4
Relaxation Delay 1.0000
Pulse Width 12.5000
Acquisition Time 4.0894
Spectrometer Frequency 400.13
Spectral Width 8012.8
Nucleus 1H
B (m) 7.22
A (m) 7.38
C (m) 7.11
D (dt) 6.05
F (m) 2.60
E (m) 2.80
G (s) 2.33
O
OPh
Me
12
1.00
1.04
2.93
0.48
1.01
1.01
1.55
f1 (ppm)

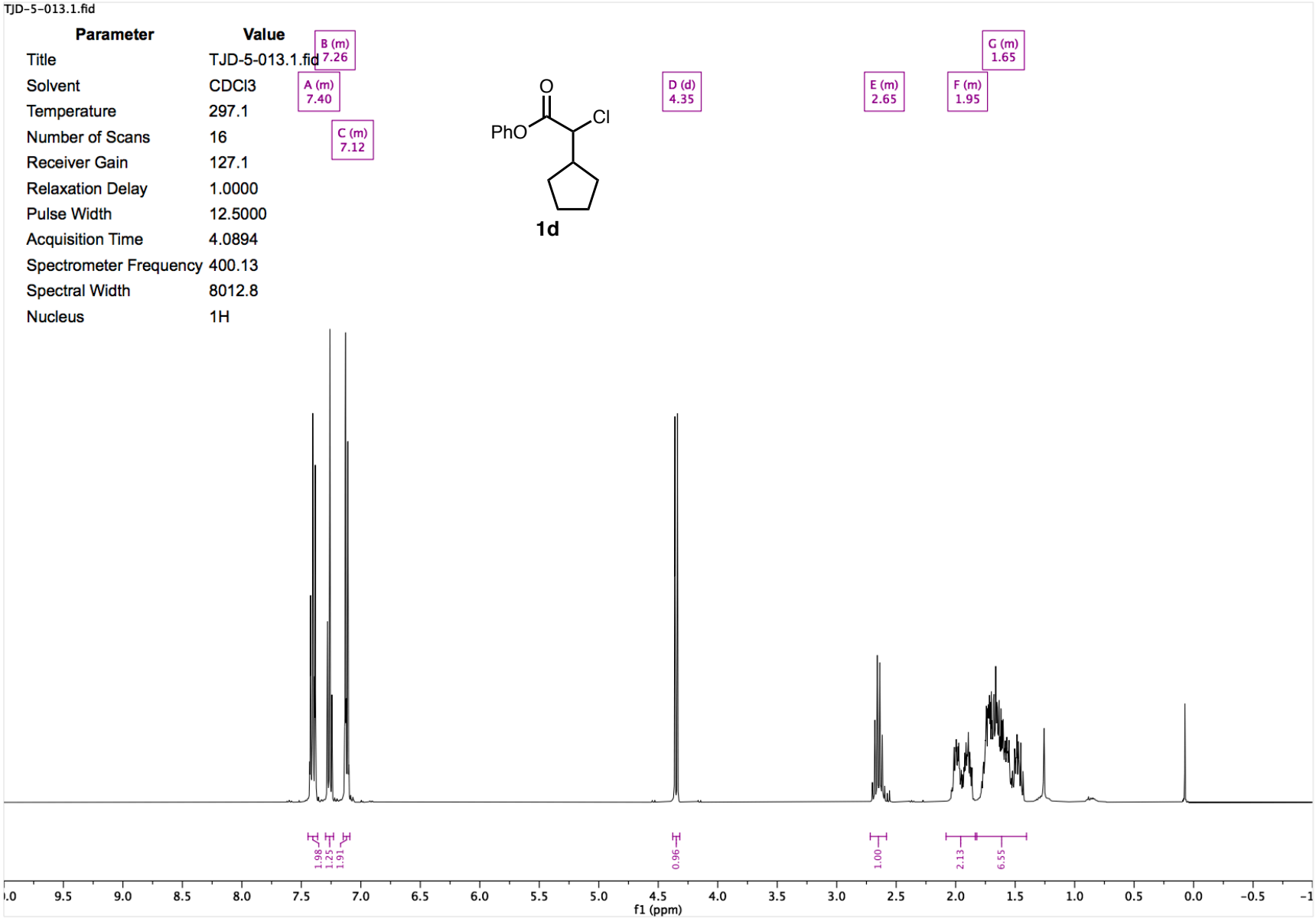

TJD-5-272-A-ptlcB2.2.fid
O
OPh
Me
12
165.1
150.9
150.8
137.7
135.9
129.5
129.4
128.4
125.8
121.8
121.2
34.4
34.0
21.2
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

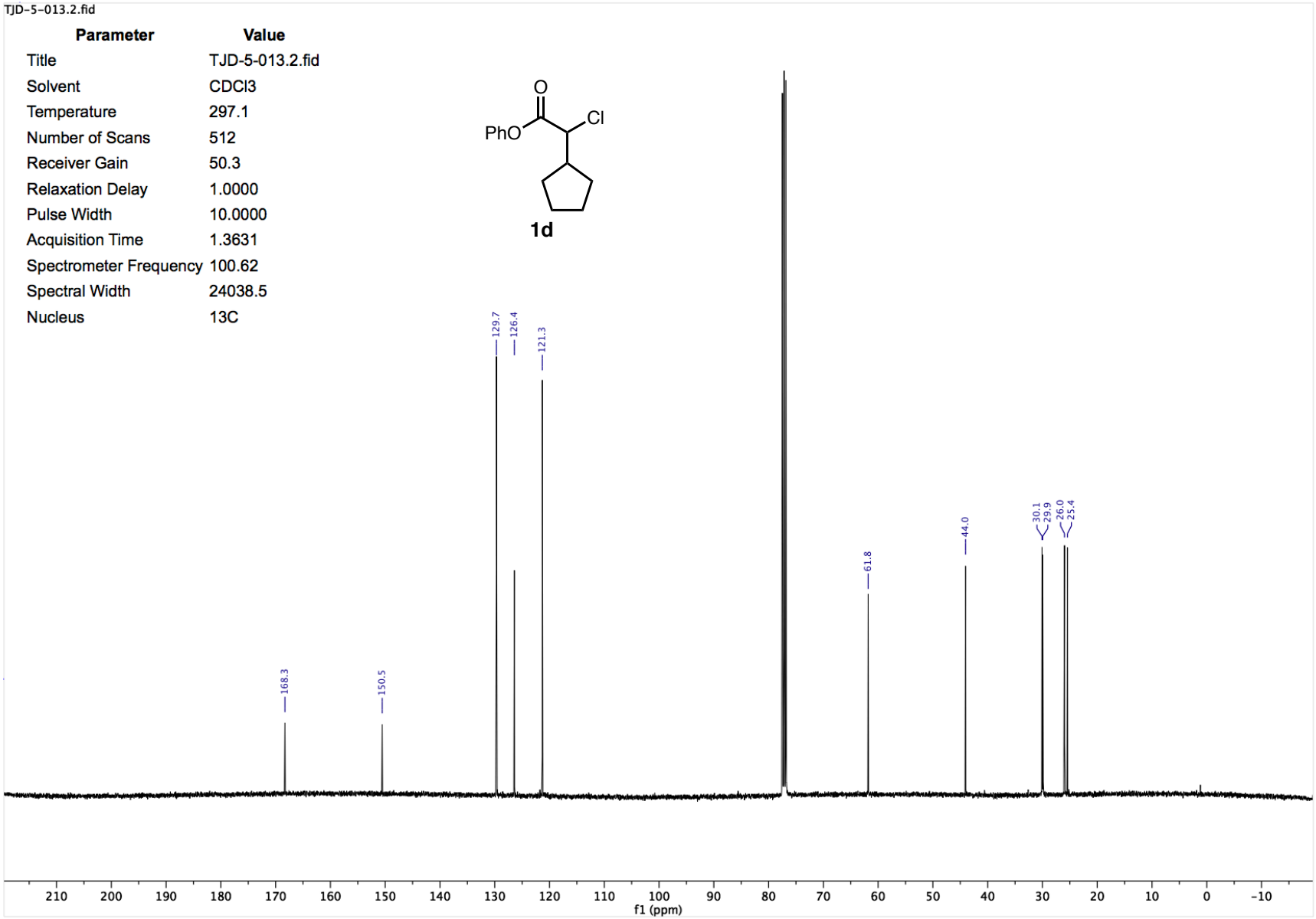

TJD-5-108.1.fid
Parameter Value
Title TJD-5-108.1.fid
Solvent CDCl3
Temperature 297.2
Number of Scans 16
Receiver Gain 112.8
Relaxation Delay 1.0000
Pulse Width 12.5000
Acquisition Time 4.0894
Spectrometer Frequency 400.13
Spectral Width 8012.8
Nucleus 1H
B (m) 7.27
A (m) 7.41
C (m) 7.13
PhO
Cl
Me
1b
D (dd) 4.46
E (m) 2.18
F (t) 1.15
2.12
1.24
2.03
1.00
2.16
3.20
f1 (ppm)

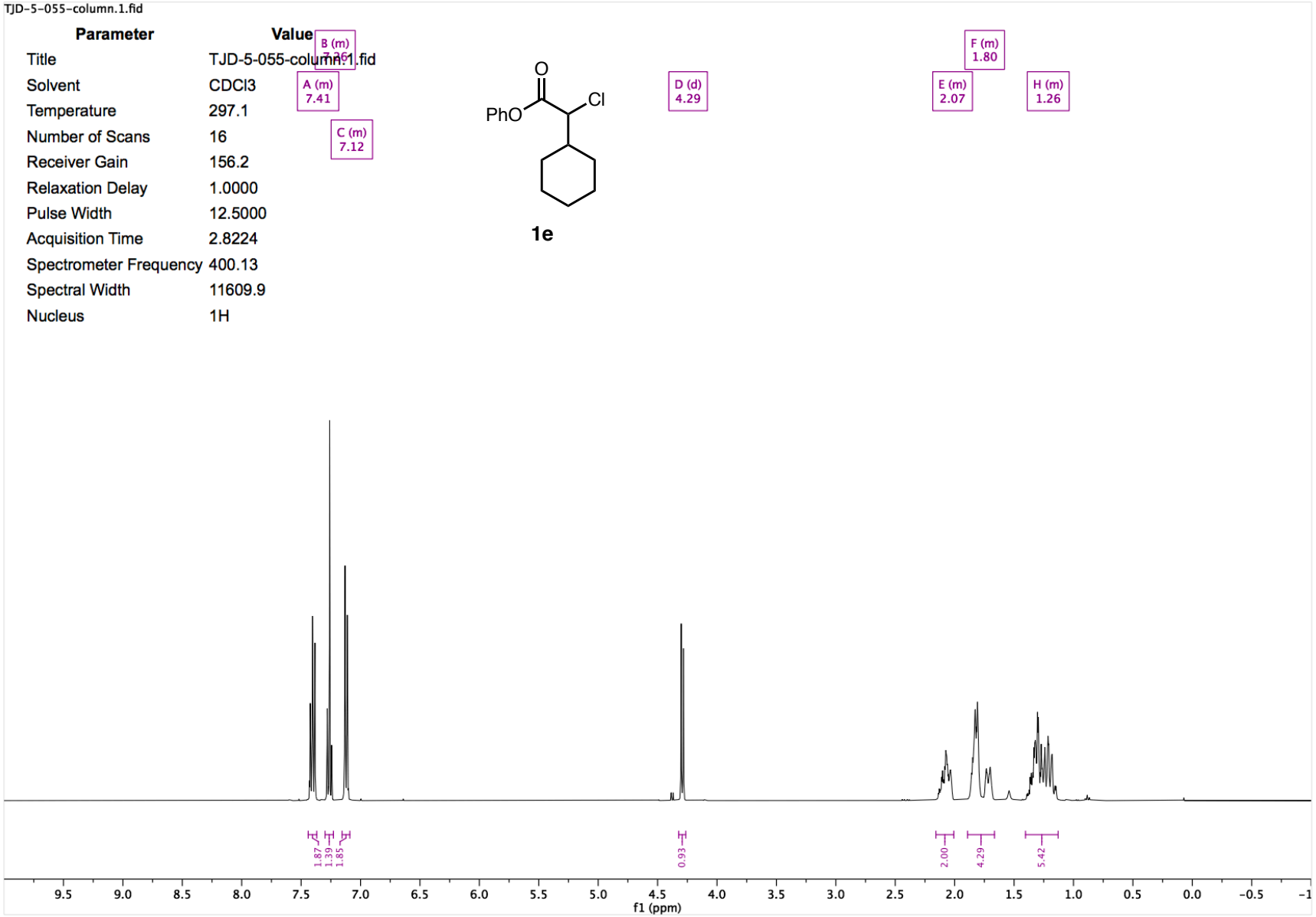

TJD-5-108.2.fid
Parameter Value
Title TJD-5-108.2.fid
Solvent CDCl3
Temperature 297.1
Number of Scans 512
Receiver Gain 43.7
Relaxation Delay 1.0000
Pulse Width 10.0000
Acquisition Time 1.3631
Spectrometer Frequency 100.62
Spectral Width 24038.5
Nucleus 13C
129.7
126.4
121.3
168.3
150.5
58.8
28.5
10.7
O
PhO
Cl
Me
1b
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

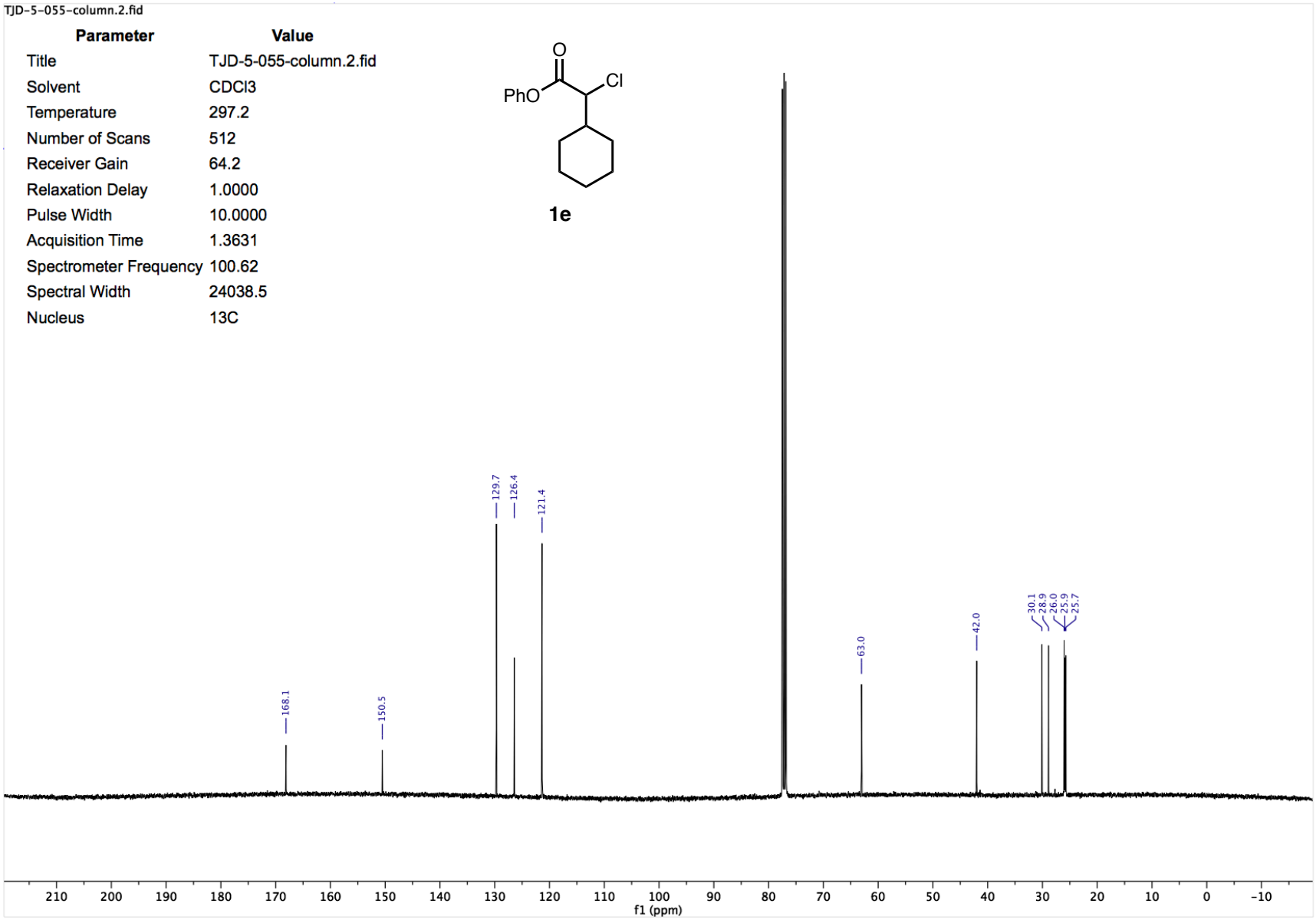

CRL_05_110-1-highvac_actual.1.fid
Parameter
Value
Title
CRL_05_110-1-highvac_actual.1.fid
Solvent
CDCl3
Temperature
297.2
Number of Scans
32
Receiver Gain
156.2
Relaxation Delay
1.0000
Pulse Width
12.5000
Acquisition Time
2.8224
Spectrometer Frequency
400.13
Spectral Width
11609.9
Nucleus
1H
PhO
O
Cl
Me
Me
1b
E (m) 7.27
D (m) 7.41
F (m) 7.12
A (d) 4.34
B (m) 2.47
C (d) 1.16
2.06
1.34
2.03
1.00
1.04
6.45
f1 (ppm)

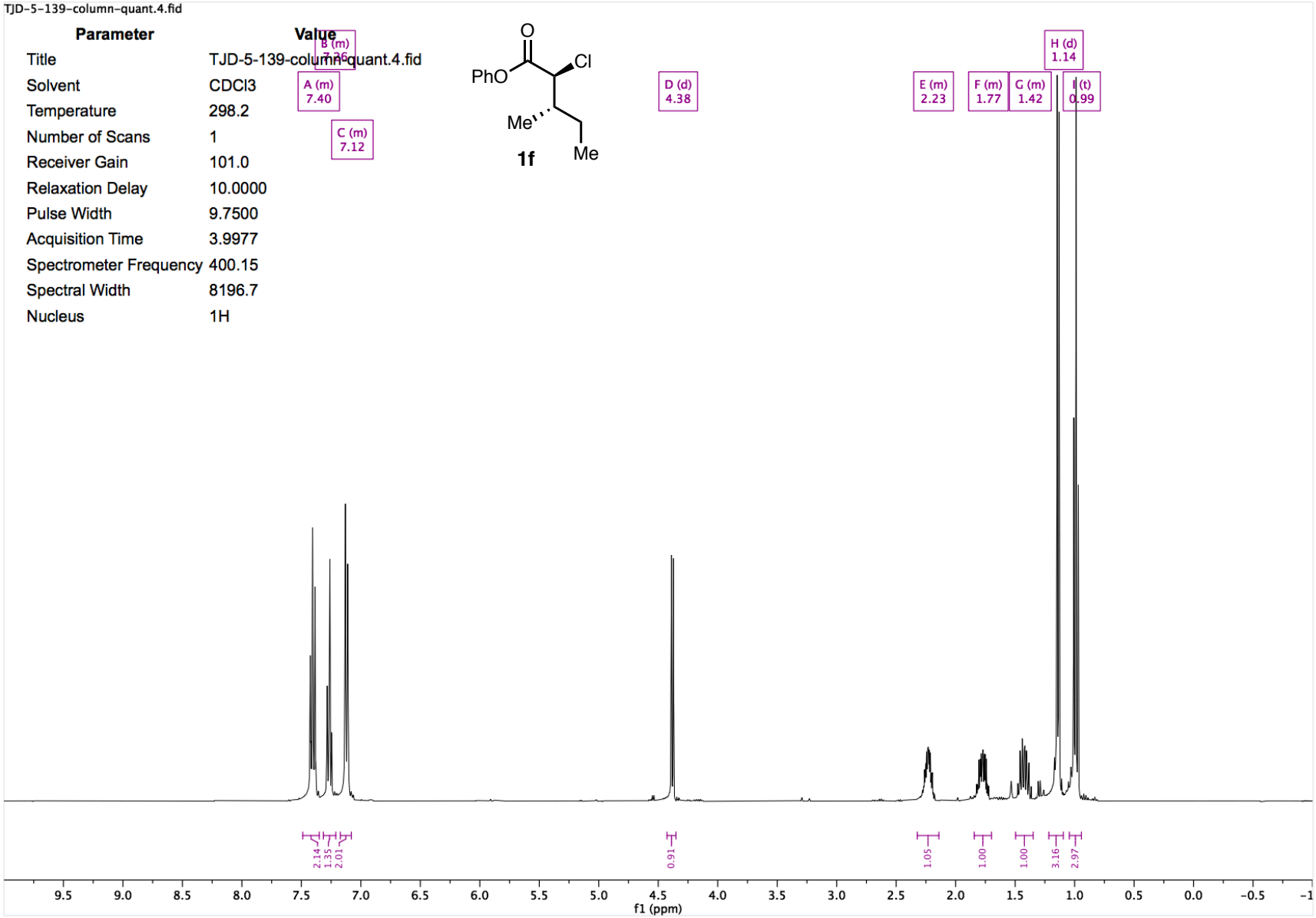

CRL_05_110-1-highvac.2.fid
Parameter
Value
Title
CRL_05_110-1-highvac.2.fid
Solvent
CDCl3
Temperature
298.2
Number of Scans
1024
Receiver Gain
55.6
Relaxation Delay
2.0000
Pulse Width
10.0000
Acquisition Time
1.3763
Spectrometer Frequency
100.63
Spectral Width
23809.5
Nucleus
13C
168.07
150.54
129.71
126.43
121.32
64.14
32.96
19.80
18.36
O
PhO
Cl
Me
Me
1b
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)


TJD-5-013.1.fid
Parameter Value
Title TJD-5-013.1.fid
Solvent CDCl3
Temperature 297.1
Number of Scans 16
Receiver Gain 127.1
Relaxation Delay 1.0000
Pulse Width 12.5000
Acquisition Time 4.0894
Spectrometer Frequency 400.13
Spectral Width 8012.8
Nucleus 1H
B (m) 7.26
A (m) 7.40
C (m) 7.12
D (d) 4.35
E (m) 2.65
F (m) 1.95
G (m) 1.65
PhO
Cl
O
1d
1.98
1.25
1.91
0.96
1.00
2.13
6.55
f1 (ppm)


TJD-5-013.2.fid
Parameter Value
Title TJD-5-013.2.fid
Solvent CDCl3
Temperature 297.1
Number of Scans 512
Receiver Gain 50.3
Relaxation Delay 1.0000
Pulse Width 10.0000
Acquisition Time 1.3631
Spectrometer Frequency 100.62
Spectral Width 24038.5
Nucleus 13C
O
PhO
Cl
1d
168.3
150.5
129.7
126.4
121.3
61.8
44.0
30.1
29.9
26.0
25.4
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

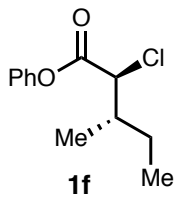

TJD-5-055-column.1.fid
Parameter
Value
Title
TJD-5-055-column.1.fid
Solvent
CDCl3
Temperature
297.1
Number of Scans
16
Receiver Gain
156.2
Relaxation Delay
1.0000
Pulse Width
12.5000
Acquisition Time
2.8224
Spectrometer Frequency
400.13
Spectral Width
11609.9
Nucleus
1H
B (m)
7.26
A (m)
7.41
C (m)
7.12
D (d)
4.29
F (m)
1.80
E (m)
2.07
H (m)
1.26
O
PhO
Cl
1e
1.87
1.39
1.85
0.93
2.00
4.29
5.42
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
-1
f1 (ppm)


TJD-5-055-column.2.fid
Parameter Value
Title TJD-5-055-column.2.fid
Solvent CDCl3
Temperature 297.2
Number of Scans 512
Receiver Gain 64.2
Relaxation Delay 1.0000
Pulse Width 10.0000
Acquisition Time 1.3631
Spectrometer Frequency 100.62
Spectral Width 24038.5
Nucleus 13C
O
PhO
Cl
1e
168.1
150.5
129.7
126.4
121.4
63.0
42.0
30.1
28.9
26.0
25.9
25.7
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

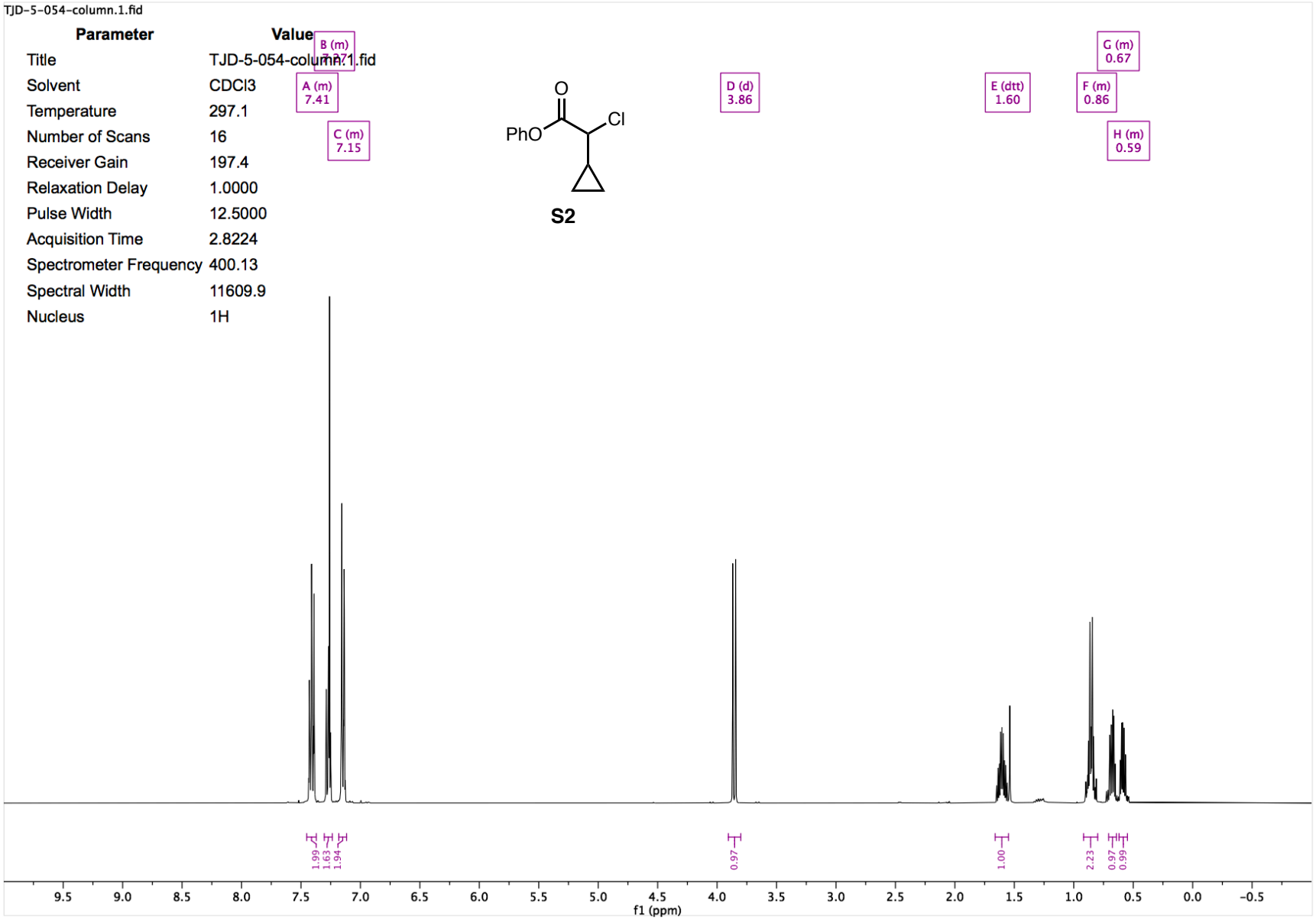

TJD-5-139-column-quant.4.fid
Parameter
Value
Title
TJD-5-139-column-quant.4.fid
Solvent
CDCl3
Temperature
298.2
Number of Scans
1
Receiver Gain
101.0
Relaxation Delay
10.0000
Pulse Width
9.7500
Acquisition Time
3.9977
Spectrometer Frequency
400.15
Spectral Width
8196.7
Nucleus
1H
B (m) 7.36
A (m) 7.40
C (m) 7.12
D (d) 4.38
E (m) 2.23
F (m) 1.77
G (m) 1.42
H (d) 1.14
I (t) 0.99
PhO
Cl
Me
Me
1f
2.14
1.35
2.01
0.91
1.05
1.00
1.00
3.16
2.97
f1 (ppm)

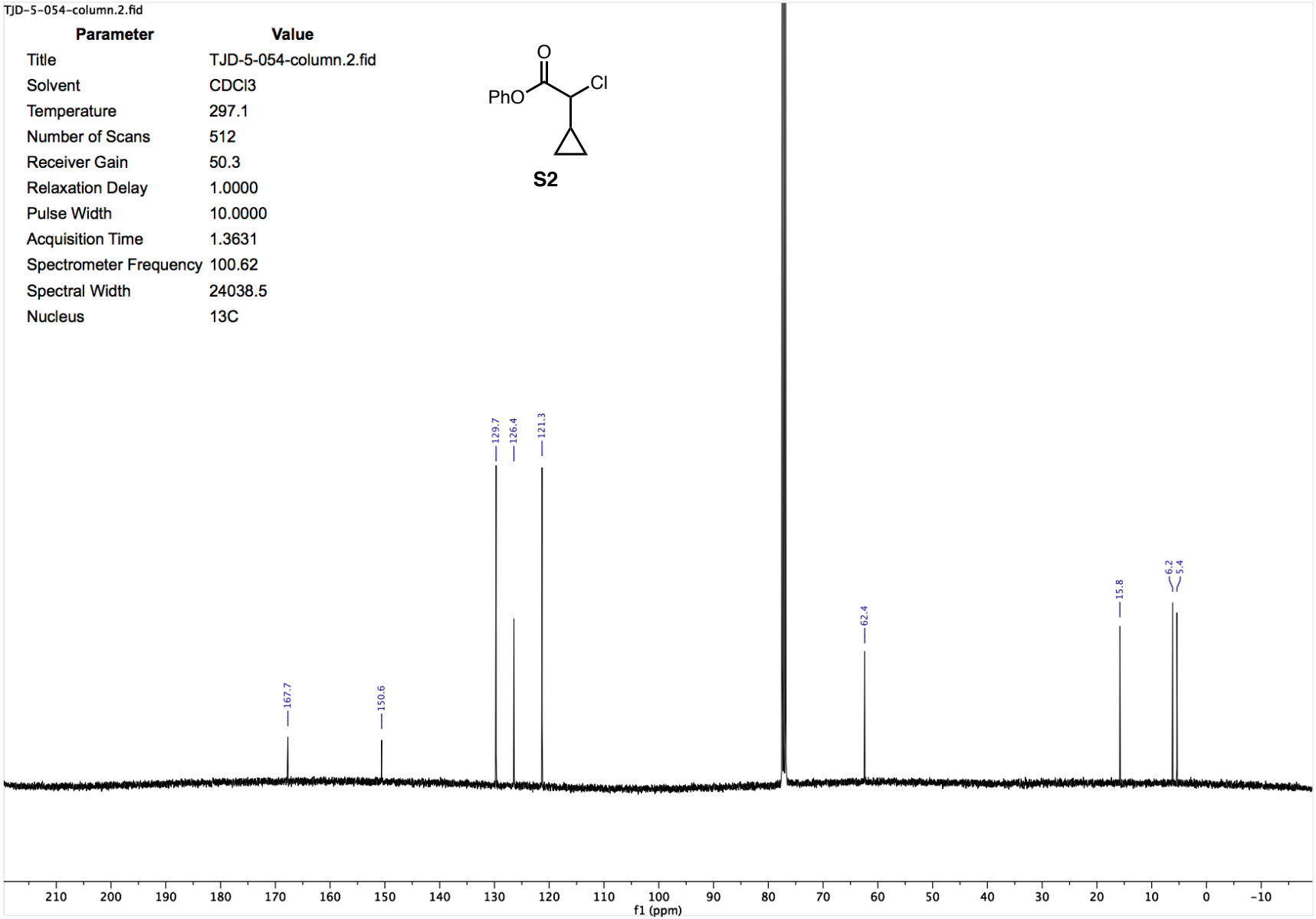
TJD-5-139-column-carbon.6.fid

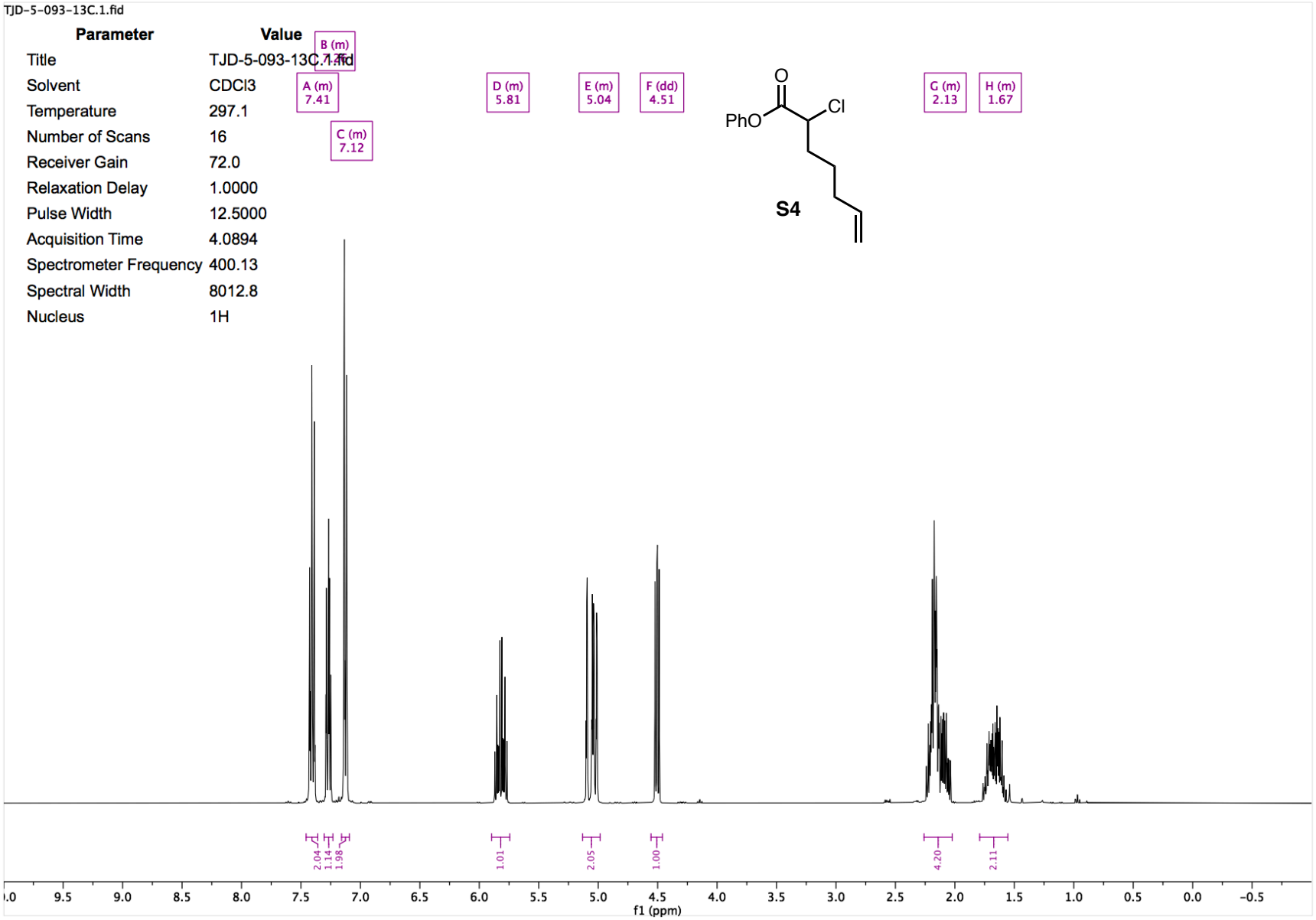
Parameter	Value
Title	TJD-5-139-column-carbon.6.fid
Solvent	CDCl3
Temperature	298.2
Number of Scans	256
Receiver Gain	58.7
Relaxation Delay	2.0000
Pulse Width	10.0000
Acquisition Time	1.3763
Spectrometer Frequency	100.63
Spectral Width	23809.5
Nucleus	13C



1f

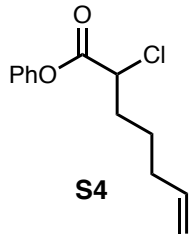

TJD-5-054-column.1.fid
Parameter
Value
Title
TJD-5-054-column.1.fid
Solvent
CDCl3
Temperature
297.1
Number of Scans
16
Receiver Gain
197.4
Relaxation Delay
1.0000
Pulse Width
12.5000
Acquisition Time
2.8224
Spectrometer Frequency
400.13
Spectral Width
11609.9
Nucleus
1H
B (m)
7.37
A (m)
7.41
C (m)
7.15
D (d)
3.86
E (dtt)
1.60
F (m)
0.86
G (m)
0.67
H (m)
0.59
O
PhO
Cl
S2
1.99
1.63
1.94
0.97
1.00
2.23
0.97
0.99
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)


TJD-5-054-column.2.fid
Parameter Value
Title TJD-5-054-column.2.fid
Solvent CDCl3
Temperature 297.1
Number of Scans 512
Receiver Gain 50.3
Relaxation Delay 1.0000
Pulse Width 10.0000
Acquisition Time 1.3631
Spectrometer Frequency 100.62
Spectral Width 24038.5
Nucleus 13C
O
PhO
Cl
S2
167.7
150.6
129.7
126.4
121.3
62.4
15.8
6.2
5.4
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

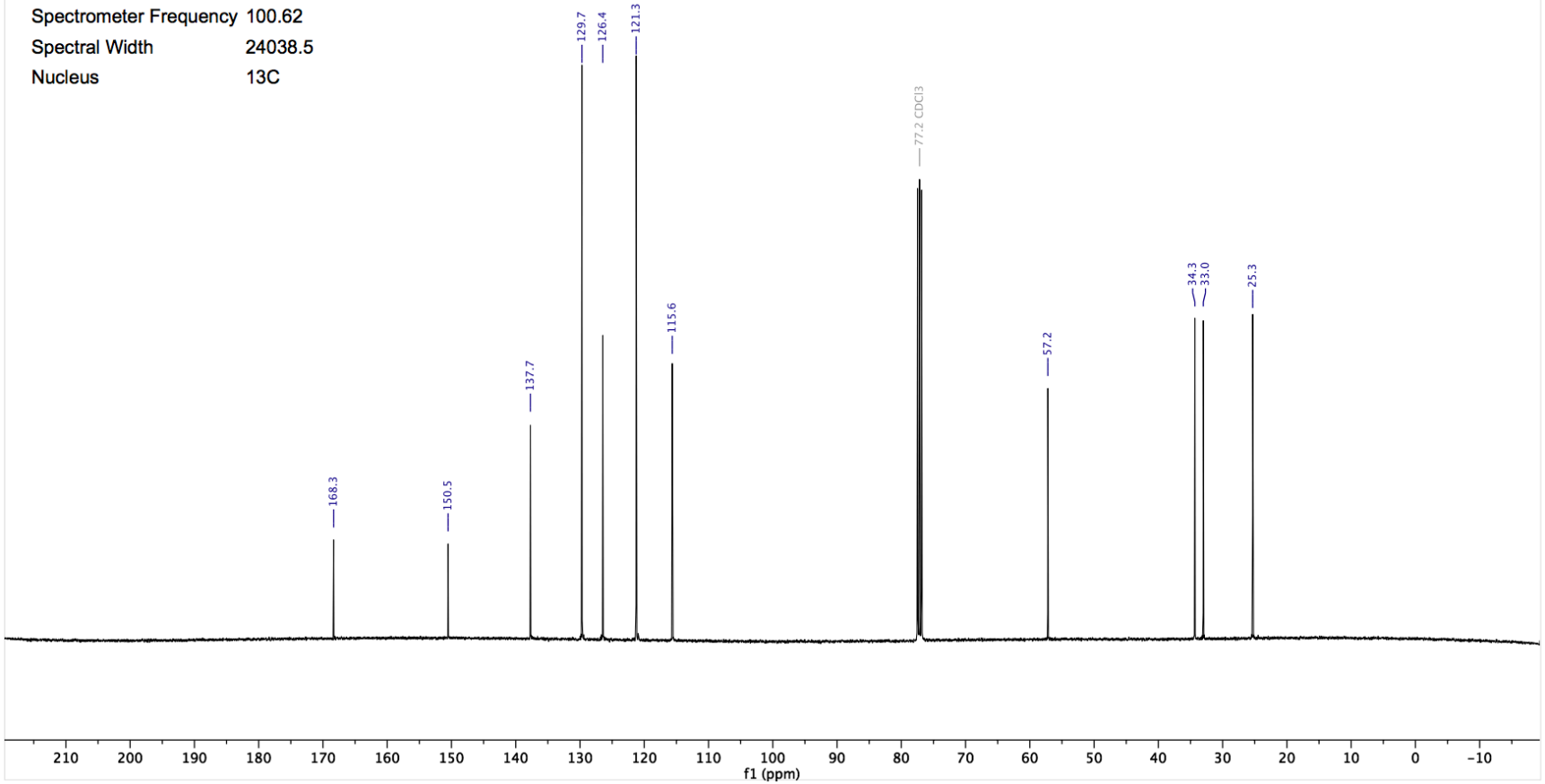

TJD-5-093-13C.1.fid
Parameter
Value
Title
TJD-5-093-13C.1.fid
Solvent
CDCl3
Temperature
297.1
Number of Scans
16
Receiver Gain
72.0
Relaxation Delay
1.0000
Pulse Width
12.5000
Acquisition Time
4.0894
Spectrometer Frequency
400.13
Spectral Width
8012.8
Nucleus
1H
A (m) 7.41
B (m) 7.35
C (m) 7.12
D (m) 5.81
E (m) 5.04
F (dd) 4.51
G (m) 2.13
H (m) 1.67
PhO
O
Cl
S4
2.04
1.14
1.98
1.01
2.05
1.00
4.20
2.11
f1 (ppm)

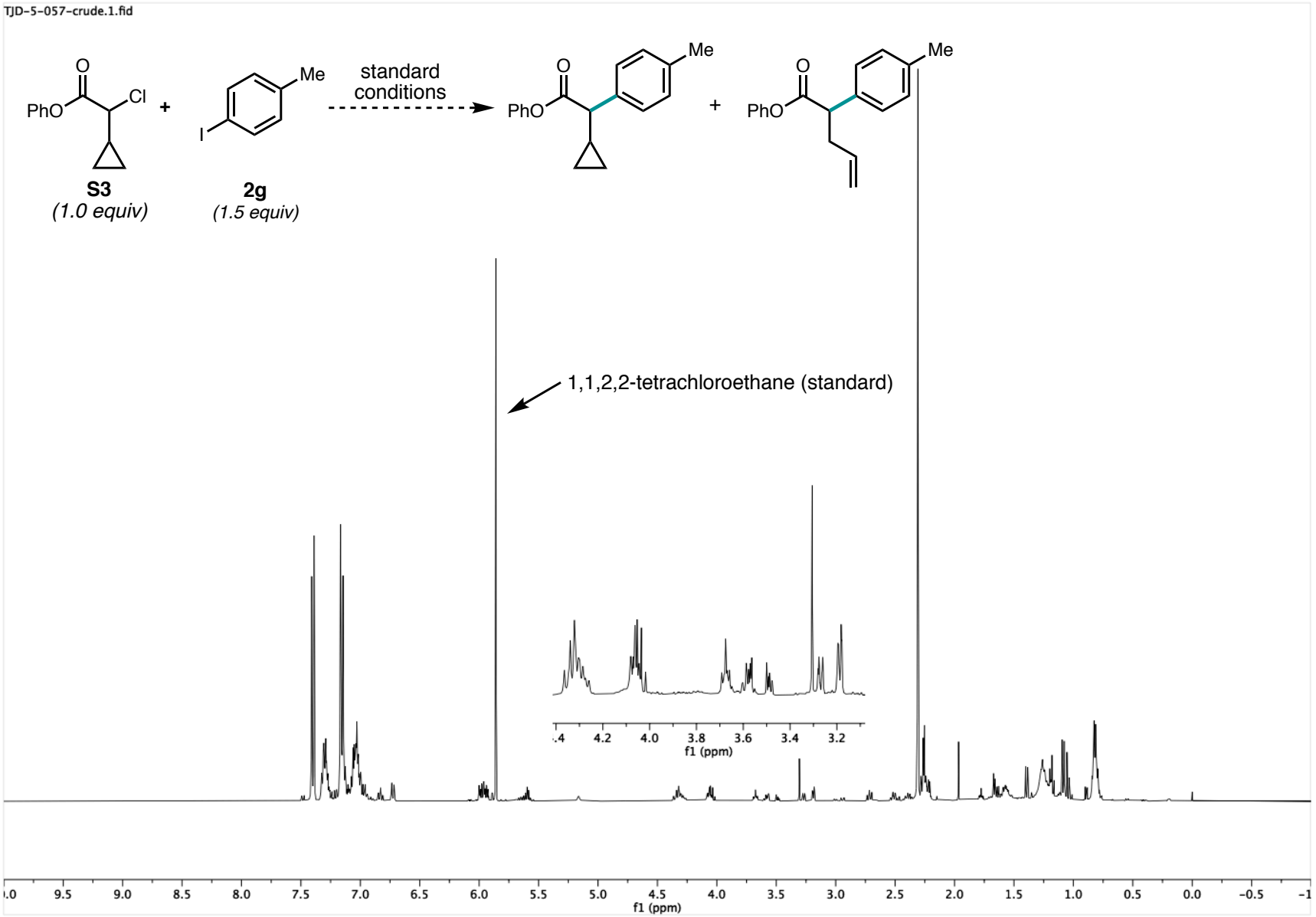
TJD-5-093-13C.2.fid

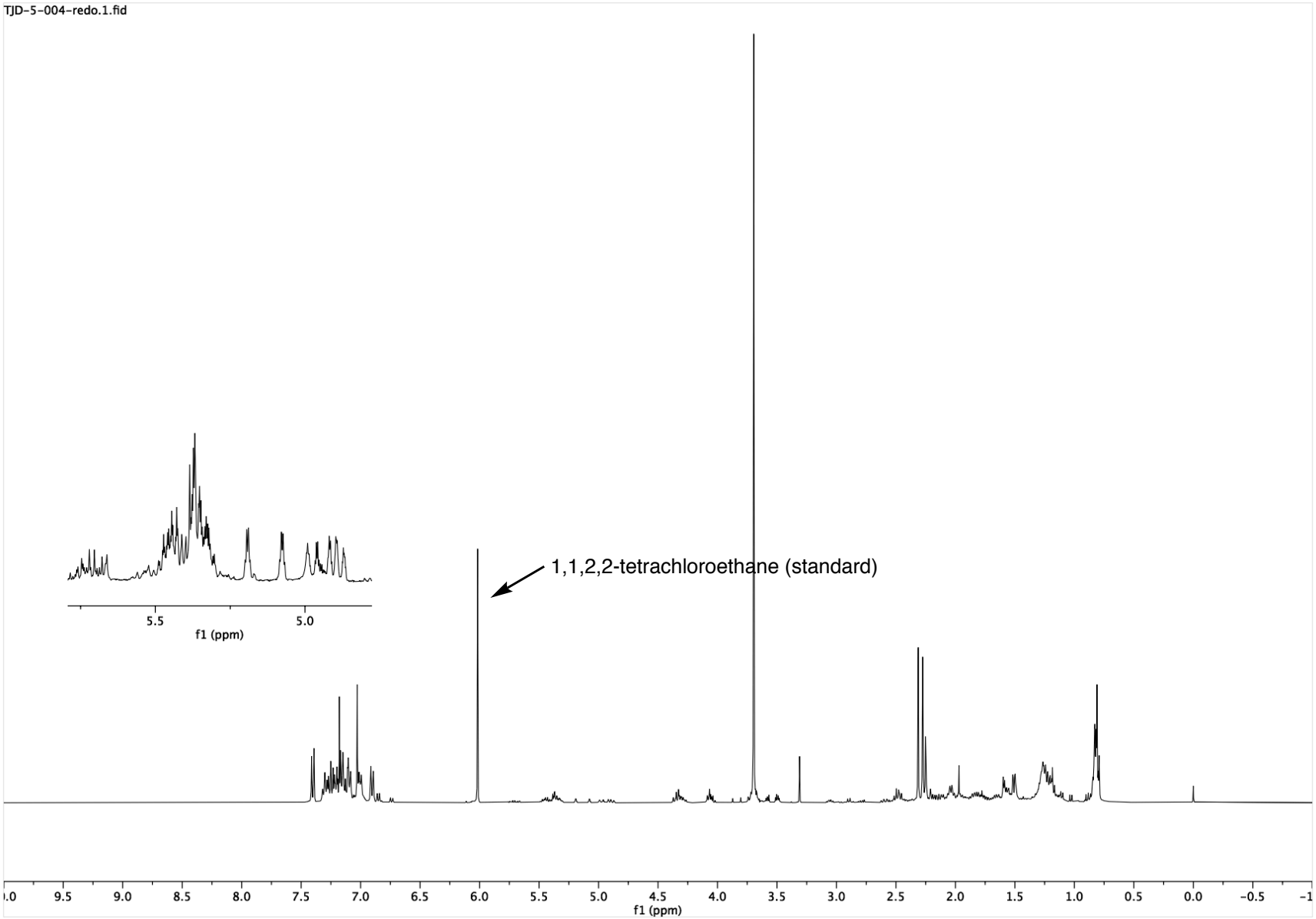
Parameter	Value
Title	TJD-5-093-13C.2.fid
Solvent	CDCl3
Temperature	297.2
Number of Scans	512
Receiver Gain	64.2
Relaxation Delay	1.0000
Pulse Width	10.0000
Acquisition Time	1.3631
Spectrometer Frequency	100.62
Spectral Width	24038.5
Nucleus	13C



S4




TJD-5-057-crude.1.fid
PhO
O
Cl
S3
(1.0 equiv)
+
I
Me
2g
(1.5 equiv)
standard
conditions
PhO
O
Me
+
PhO
O
Me
1,1,2,2-tetrachloroethane (standard)
f1 (ppm)
f1 (ppm)


TJD-5-004-redo.1.fid
1,1,2,2-tetrachloroethane (standard)
5.5
5.0
f1 (ppm)
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)