Catalytic Generation of *ortho*-Quinone Dimethides via Donor/Donor Rhodium Carbenes

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General Information

Chemicals were purchased and used without further purification unless otherwise specified. All reactions using anhydrous solvents were carried out in flame-dried glassware with magnetic stirring. Anhydrous solvent was dispensed from a solvent purification system that passes solvent through two columns of dry neutral alumina. Reactions were monitored by thin layer chromatography (TLC, Merck), and detected by examination under UV light (254 nm and 365 nm). Flash column chromatography was performed using silica gel [230−400 mesh (40−63 μm)]. Extracts were concentrated *in vacuo* using both a rotary evaporator (bath temperatures up to 40 °C) at a pressure of ≥10 torr (diaphragm pump). High vacuum procedures were carried out at room temperature at a pressure of 1 mtorr (diaphragm pump) or ≥1000 mtorr (oil pump). ^{1}H and proton-decoupled ^{13}C spectra were measured at 400, 600 or 800 MHz, and 101, 151 or 201MHz respectively unless otherwise noted. ^{1}H NMR spectra in $CDCl_3$, Acetone-d6, CD_2Cl_2, DMSO-d6, C_6D_6 were referenced at 0 ppm (TMS), 2.05 ppm, 5.32 ppm, 2.50 ppm and 7.16 ppm, respectively. ^{13}C NMR spectra in $CDCl_3$, Acetone-d6, CD_2Cl_2, DMSO-d6, C_6D_6 were referenced at 77.16 ppm, 29.84 ppm, 53.84 ppm, 39.52 ppm and 128.06 ppm, respectively. Multiplicities are given as: s (singlet), d (doublet), t (triplet), q (quartet), p (pentet), m (multiplet), or combinations of these signals. Apparent signals are indicated with *app.* and are used when signals with multiple couplings appear to form a certain peak type. High-resolution mass spectrometry was performed on positive mode, and ESI/OrbitrapTM, ESI/TOF, and CI/TOF techniques were generally used. For some substrates, high-resolution mass spectrometry using the aforementioned techniques was not achieved; low-resolution mass spectrometry using an Advion© ASAP-APCI-MS was achieved and the corresponding data is reported. Melting points were taken on an EZ-melting apparatus and were uncorrected. Infrared spectra were taken on a Bruker Tensor 27 spectrometer. All microwave experiments were run in a Biotage Initiator EXP EU 400W microwave synthesizer 2.0 serial number 11031. NOTE: it is necessary that the MnO_2 used for the oxidation of hydrazones be ~85% pure with an average particle size of 2 microns, appearing as a fine black powder.

Experimental Procedures and Characterization

General Procedure A (acetal synthesis). To a flame-dried round bottom were added aldehyde, diol (1.1-4.0 equiv), *p*-toluenesulfonic acid monohydrate (0.02-0.2 equiv) and toluene or benzene (0.33-1.0 M). The resulting solution was heated under reflux with Dean-Stark trap. Upon full conversion monitored by ^{1}H NMR, the reaction was quenched with 15% NaOH aqueous solution or saturated $NaHCO_3$ aqueous solution and extracted with EtOAc (3 × 20 mL). The combined organic phases were washed with H_2O (1 × 10 mL) and brine (1 × 10 mL). The organic phase was dried over anhydrous Na_2SO_4, filtered and concentrated. The residue was further purified by flash column chromatography to obtain the desired acetal.

General Procedure B (ketone synthesis using Weinreb amide). To a flame-dried round bottom flask were added aryl bromide and THF (0.2-0.25 M). The solution was cooled to -78 °C and *n*-BuLi (in hexane or toluene, 1.1 equiv) was added dropwise. The reaction was kept at -78 °C for 1-2 h and Weinreb amide (1.3-1.5 equiv) in THF was added dropwise. The reaction was then allowed to warm to room temperature overnight. Upon completion monitored by TLC, the reaction was quenched with saturated NH_4Cl aqueous solution and extracted with EtOAc (3 × 10 mL). The combined organic phases were washed with H_2O (1 × 10 mL) and brine (1 × 10 mL). The organic phase was dried over anhydrous Na_2SO_4, filtered and concentrated. The residue was further purified by flash column chromatography to obtain the desired ketone.

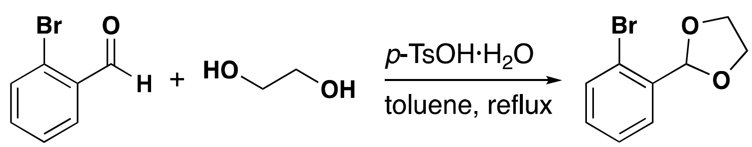
General Procedure C (hydrazone synthesis by microwave reaction). To a flame-dried microwave vial were added ketone and EtOH (0.2-0.33 M). The solution was sparged with Ar for 5 min, followed by the addition of N_2H_4 (13 equiv) and HOAc (1.2 equiv). The vial was heated in a microwave reactor at 160 °C for 3 h. If the poor conversion was observed by TLC, to the reaction were added N_2H_4 (13 equiv) and HOAc (1.2 equiv) again and the reaction was heated in the microwave reactor at 160 °C for another 3 h. Upon full conversion, the reaction was quenched with H_2O and extracted with ether (3 × 10 mL). The combined organic phases were further washed with brine (1 × 10 mL) and dried over anhydrous Na_2SO_4. After filtration and concentration, the residue was purified by flash column chromatography to obtain the desired hydrazone as *Z*/*E* mixture. *Hydrazones were often isolated as a mixture of E/Z isomers. As such*

[1]H NMR peaks have been reported only for selected examples. Due to restricted rotation, the hydrazone NMRs often indicated diastereotopic protons.

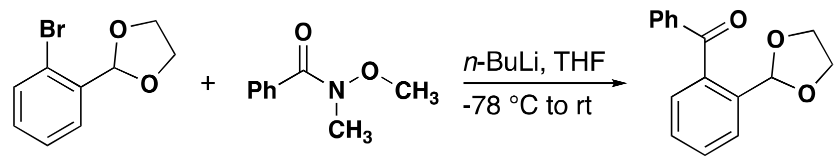
General Procedure D ((Hetero) Diels-Alder reaction). To a flame-dried vial were added hydrazone, dienophile (1.0-1.2 equiv), MnO_2 (8.0 equiv), $Rh_2(MesCO_2)_4$ or Rh_2(*R*-PTAD)$_4$ (0.01 equiv) and DCM (0.017 M). After stirred at room temperature for 5-24 h, the crude reaction was filtered over celite to remove MnO_2, concentrated and further purified by flash column chromatography to obtain the desired product.

General Procedure E ((Hetero) Diels-Alder reaction). To a flame-dried vial were added hydrazone, MnO_2 (8.0 equiv) and DCM (0.017 M). After stirred at room temperature for 2 h, dienophile (1.0-1.2 equiv), $Rh_2(MesCO_2)_4$ (0.01 equiv) were added. After stirred for another 3-22 h, the crude reaction was filtered over celite to remove MnO_2, concentrated and further purified by flash column chromatography to obtain the desired product.

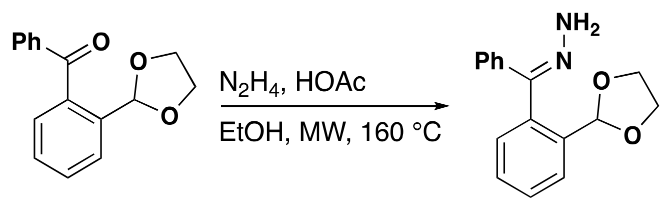
General Procedure F ((Hetero) Diels-Alder reaction at 55 °C). To a flame-dried vial were added hydrazone, MnO_2 (8.0 equiv) and THF (0.017 M). After stirred at room temperature for 1 h, dienophile (1.0-1.2 equiv), $Rh_2(MesCO_2)_4$ or Rh_2(*S*-TCPTTL)$_4$ (0.01 equiv) were added, and the reaction was heated to 55 °C. After stirred for another 12-20 h, the crude reaction was cooled to room temperature and filtered over celite to remove MnO_2, concentrated and further purified by flash column chromatography to obtain the desired product.



2-(2-Bromophenyl)-1,3-dioxolane was synthesized according to General Procedure E, using 2-bromobenzaldehyde (1.17 mL, 10 mmol), ethylene glycol (775.9 mg, 12.5 mmol), *p*-toluenesulfonic acid monohydrate (34.4 mg, 0.18 mmol) and toluene (20 mL). The crude product was purified by flash column chromatography (hexane/EtOAc = 30:1, v/v) to obtain the acetal as a colorless oil (2.16 g, 94%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.60 (d, *J* = 7.7 Hz, 1H), 7.57 (d, *J* = 8.0 Hz, 1H), 7.34 (t, *J* = 7.5 Hz, 1H), 7.22 (t, *J* = 7.4 Hz, 1H), 6.10 (s, 1H), 4.21 – 4.03 (m, 4H). ^{1}H NMR data was consistent with reported literature values.[1]

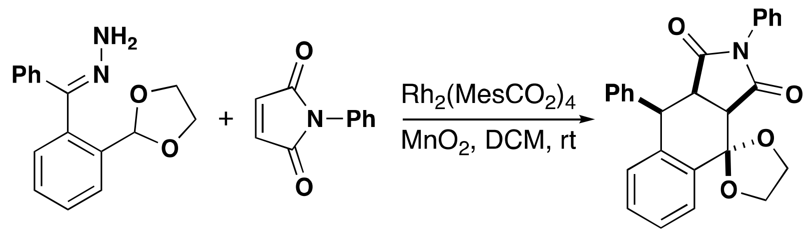


(2-(1,3-Dioxolan-2-yl)phenyl)(phenyl)methanone was synthesized according to General Procedure A, using 2-(2-Bromophenyl)-1,3-dioxolane (687.2 mg, 3 mmol), *n*-BuLi (1.8 M, 1.8 mL, 3.3 mmol), *N*-methoxy-*N*-methylbenzamide (743.4 mg, 4.5 mmol) and THF (20 mL). The crude product was purified by flash column chromatography (hexane/EtOAc = 10:1, v/v) to obtain the ketone as a colorless oil (454.2 mg, 60%). ^{1}H NMR (400 MHz, C_6D_6) δ 7.91 – 7.86 (m, 2H), 7.76 (dd, *J* = 7.8, 1.2 Hz, 1H), 7.15 – 7.06 (m, 3H), 7.04 – 6.94 (m, 3H), 6.24 (s, 1H), 3.44 – 3.34 (m, 2H), 3.28 – 3.19 (m, 2H). ^{1}H NMR data was consistent with reported literature values.[2]



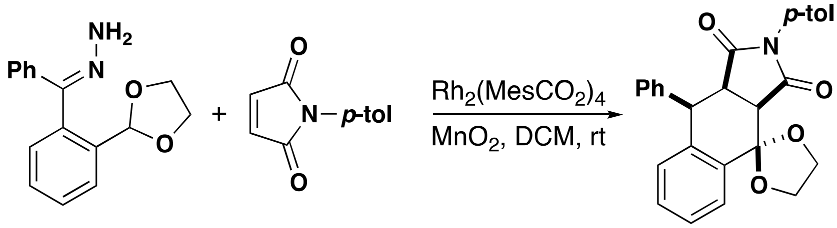
(*E*)-((2-(1,3-Dioxolan-2-yl)phenyl)(phenyl)methylene)hydrazine was synthesized according to General Procedure B, using (2-(1,3-dioxolan-2-yl)phenyl)(phenyl)methanone (254.3 mg, 1 mmol), N_2H_4 (0.41 mL, 13 mmol), HOAc (0.07 mL, 1.2 mmol) and EtOH (4 mL). The crude product was purified by flash column chromatography (hexane/EtOAc = 2:1, v/v) to obtain the hydrazone as a pale yellow solid (195.2 mg, 73%). m.p. 131-133 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.81 – 7.73 (m, 1H), 7.59 – 7.48 (m, 2H), 7.49 – 7.41 (m, 2H), 7.32 – 7.22 (m, 3H), 7.19 – 7.11 (m, 1H), 5.59 (s, 1H), 5.39 (s, 2H), 4.12 – 3.97 (m, 2H), 3.95 – 3.83 (m, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 148.2, 138.3, 136.5, 132.9, 130.7, 129.5, 129.1, 128.3, 128.2, 127.6, 126.1, 101.7, 65.6, 65.5. HRMS (ESI) *m/z* calcd for $C_{16}H_{17}N_2O_2^+$ [M+H]$^+$ 269.1285, found 269.1283.

[4+2] Cycloaddition



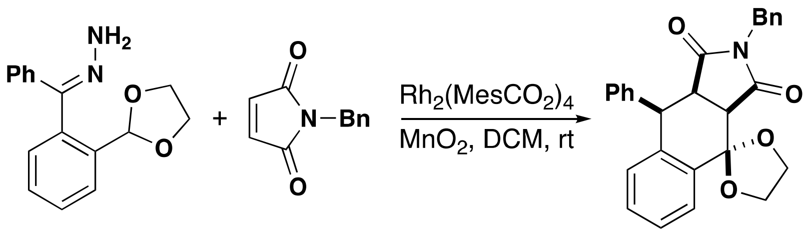
15a

2,9-Diphenyl-9,9a-dihydrospiro[benzo[*f*]isoindole-4,2'-[1,3]dioxolane]-1,3(2*H*,3a*H*)-dione was synthesized according to General Procedure D, using (*E*)-((2-(1,3-dioxolan-2-yl)phenyl)(phenyl)methylene)hydrazine (26.8 mg, 0.1 mmol), 1-phenyl-1*H*-pyrrole-2,5-dione (20.8 mg, 0.12 mmol), MnO_2 (69.6 mg, 0.8 mmol), $Rh_2(MesCO_2)_4$ (0.9 mg, 0.001 mmol) and DCM (6 mL). The crude product was purified by flash column chromatography (hexane/EtOAc = 3:1, v/v) to obtain **15a** as a white solid (22.6 mg, 55%, 87:13 dr). m.p. 150-152 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.70 – 7.62 (m, 1H), 7.62 – 7.52 (m, 2H), 7.42 – 7.23 (m, 8H), 7.22 – 7.13 (m, 1H), 6.93 – 6.80 (m, 2H), 5.02 (d, *J* = 6.3 Hz, 1H), 4.36 (q, *J* = 6.3 Hz, 1H), 4.28 (q, *J* = 6.5 Hz, 1H), 4.21 (q, *J* = 6.4 Hz, 1H), 4.12 (q, *J* = 6.3 Hz, 1H), 3.86 (dd, *J* = 9.2, 6.3 Hz, 1H), 3.74 (d, *J* = 9.1 Hz, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 175.4, 172.8, 138.4, 137.8, 135.7, 131.8, 131.0, 129.6, 129.1, 128.6, 128.2, 128.0, 127.4, 127.2, 126.5, 124.6, 105.1, 66.3, 65.1, 51.3, 45.0, 44.5. IR (neat): 2920, 1707, 1377, 1177, 1062, 730, 693 cm^{-1}. HRMS (ESI) *m/z* calcd for $C_{26}H_{22}NO_4^+$ $[M+H]^+$ 412.1543, found 412.1554.



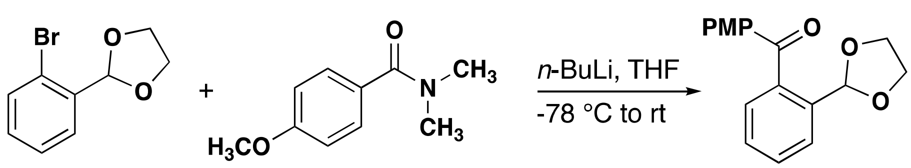
15b

9-Phenyl-2-(*p*-tolyl)-9,9a-dihydrospiro[benzo[*f*]isoindole-4,2'-[1,3]dioxolane]-1,3(2*H*,3a*H*)-dione was synthesized according to General Procedure D, using (*E*)-((2-(1,3-dioxolan-2-yl)phenyl)(phenyl)methylene)hydrazine (26.8 mg, 0.1 mmol), 1-(*p*-tolyl)-1*H*-pyrrole-2,5-dione (22.5 mg, 0.12 mmol), MnO_2 (69.6 mg, 0.8 mmol), $Rh_2(MesCO_2)_4$ (0.9 mg, 0.001 mmol) and DCM (6 mL). The crude product was purified by flash column chromatography (hexane/EtOAc = 2:1, v/v) to obtain **15b** as a white solid (27.3 mg, 64%, 87:13 dr). m.p. 199-201 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.69 – 7.62 (m, 1H), 7.60 – 7.50 (m, 2H), 7.40 – 7.25 (m, 5H), 7.19 – 7.16 (m, 1H), 7.12 (d, *J* = 8.2 Hz, 2H), 6.73 (d, *J* = 8.3 Hz, 2H), 5.01 (d, *J* = 6.3 Hz, 1H), 4.42 – 4.33 (m, 1H), 4.33 – 4.26 (m, 1H), 4.25 – 4.18 (m, 1H), 4.17 – 4.07 (m, 1H), 3.86 (dd, *J* = 9.2, 6.4 Hz, 1H), 3.74 (d, *J* = 9.2 Hz, 1H), 2.30 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 175.6, 173.0, 138.7, 138.4, 137.9, 135.7, 131.0, 129.7, 129.6, 129.2, 128.2, 128.0, 127.4, 127.2, 126.3, 124.6, 105.1, 66.4, 65.1, 51.3, 45.0, 44.5, 21.3. IR (neat): 2902, 1705, 1382, 1179, 1067, 736, 696 cm^{-1}. HRMS (ESI) *m/z* calcd for $C_{27}H_{24}NO_4^+$ [M+H]$^+$ 426.1700, found 426.1713.

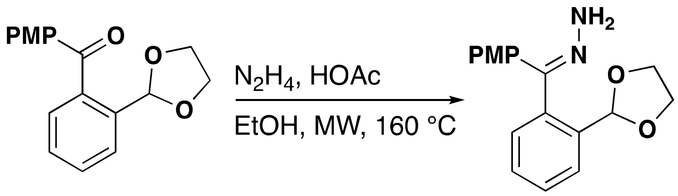


15c

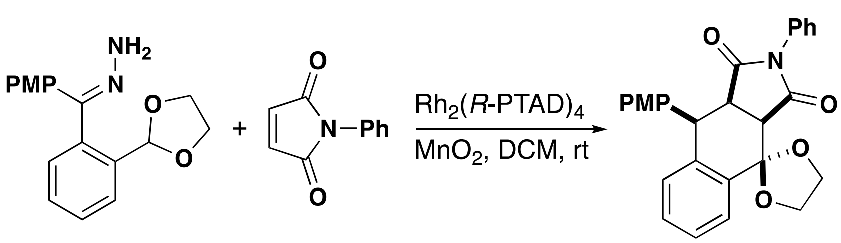
2-Benzyl-9-phenyl-9,9a-dihydrospiro[benzo[*f*]isoindole-4,2'-[1,3]dioxolane]-1,3(2*H*,3a*H*)-dione was synthesized according to General Procedure D, using (*E*)-((2-(1,3-dioxolan-2-yl)phenyl)(phenyl)methylene)hydrazine (26.8 mg, 0.1 mmol), 1-benzyl-1*H*-pyrrole-2,5-dione (22.5 mg, 0.12 mmol), MnO_2 (69.6 mg, 0.8 mmol), $Rh_2(MesCO_2)_4$ (0.9 mg, 0.001 mmol) and DCM (6 mL). The crude product was purified by flash column chromatography (hexane/EtOAc = 2:1, v/v) to obtain **15c** as a white solid (31.2 mg, 73%, 91:9 dr). m.p. 178-180 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.58 – 7.51 (m, 1H), 7.43 – 7.36 (m, 2H), 7.35 – 7.28 (m, 3H), 7.28 – 7.21 (m, 2H), 7.18 – 7.05 (m, 4H), 6.77 (d, *J* = 6.7 Hz, 2H), 4.99 (d, *J* = 6.3 Hz, 1H), 4.51 (d, *J* = 14.4 Hz, 1H), 4.43 (d, *J* = 14.4 Hz, 1H), 4.36 – 4.29 (m, 1H), 4.29 – 4.22 (m, 1H), 4.22 – 4.15 (m, 1H), 4.02 – 3.94 (m, 1H), 3.69 (dd, *J* = 8.7, 6.3 Hz, 1H), 3.59 (d, *J* = 8.8 Hz, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 175.9, 173.3, 137.9, 137.0, 135.5, 131.3, 129.4, 128.5, 128.0, 127.8, 127.46, 127.46, 127.4, 127.0, 124.3, 105.4, 66.4, 64.6, 50.9, 44.6, 44.2, 42.1. IR (neat): 2923, 1701, 1287, 1180, 1016, 695 cm^{-1}. HRMS (ESI) *m/z* calcd for $C_{27}H_{24}NO_4^+$ [M+H]$^+$ 426.1700, found 426.1707.



To a flame-dried round bottom flask were added 2-(2-bromophenyl)-1,3-dioxolane (755.9 mg, 3.3 mmol) and THF (20 mL). The solution was cooled to -78 °C and *n*-BuLi (2.5 M in hexane, 1.5 mL, 1.2 equiv) was added dropwise. The reaction was kept at -78 °C for 15 min and 4-methoxy-*N*,*N*-dimethylbenzamide (585.7 mg, 3 mmol) in THF (10 mL) was then added dropwise. The reaction was allowed to warm to room temperature and stirred overnight. Upon completion monitored by TLC, the reaction was quenched with saturated NH_4Cl aqueous solution and extracted with EtOAc (3 × 10 mL). The combined organic phases were washed with H_2O (1 × 10 mL) and brine (1 × 10 mL). The organic phase was dried over anhydrous Na_2SO_4, filtered and concentrated. The residue was further purified by flash column chromatography (hexane/EtOAc = 3:1, v/v) to obtain the ketone as a clear oil (228.3 mg, 27%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.79 (d, *J* = 8.9 Hz, 2H), 7.69 (dd, *J* = 7.8, 1.3 Hz, 1H), 7.50 (td, *J* = 7.6, 1.4 Hz, 1H), 7.41 (td, *J* = 7.5, 1.3 Hz, 1H), 7.31 (dd, *J* = 7.6, 1.5 Hz, 1H), 6.92 (d, *J* = 8.9 Hz, 2H), 5.99 (s, 1H), 3.95 – 3.91 (m, 2H), 3.91 – 3.88 (m, 2H), 3.87 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 196.4, 163.8, 139.1, 136.7, 132.6, 130.8, 129.8, 128.5, 128.0, 127.1, 113.7, 101.6, 65.3, 55.6. IR (neat): 2898, 1711, 1511, 1377, 1179, 1065, 1027, 736 cm^{-1}. HRMS (ESI) *m/z* calcd for $C_{17}H_{17}O_4^+$ $[M+H]^+$ 285.1121, found 285.1126.



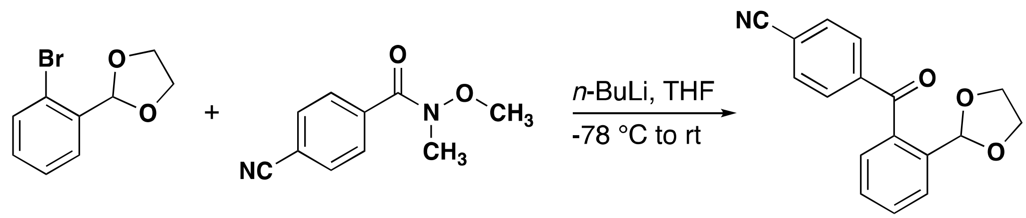
(*E*)-((2-(1,3-Dioxolan-2-yl)phenyl)(4-methoxyphenyl)methylene)hydrazine was synthesized according to General Procedure B, using (2-(1,3-dioxolan-2-yl)phenyl)(4-methoxyphenyl)methanone (200 mg, 0.7 mmol), N_2H_4 (0.29 mL, 9.1 mmol), HOAc (0.05 mL, 0.84 mmol) and EtOH (3 mL). The crude product was purified by flash column chromatography (hexane/EtOAc = 2:1, v/v) to obtain the hydrazone as a pale yellow solid (139.9 mg, 67%). m.p. 80-81 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.79 – 7.72 (m, 1H), 7.56 – 7.48 (m, 2H), 7.39 (d, *J* = 8.9 Hz, 2H), 7.19 – 7.11 (m, 1H), 6.81 (d, *J* = 8.9 Hz, 2H), 5.59 (s, 1H), 5.28 (s, 2H), 4.11 – 3.99 (m, 2H), 3.95 – 3.85 (m, 2H), 3.78 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 159.9, 148.5, 136.4, 133.2, 131.2, 130.7, 129.4, 129.0, 127.6, 113.7, 101.8, 65.7, 65.6, 55.4. HRMS (ESI) *m/z* calcd for $C_{17}H_{19}N_2O_3^+$ $[M+H]^+$ 299.1390, found 299.1391.



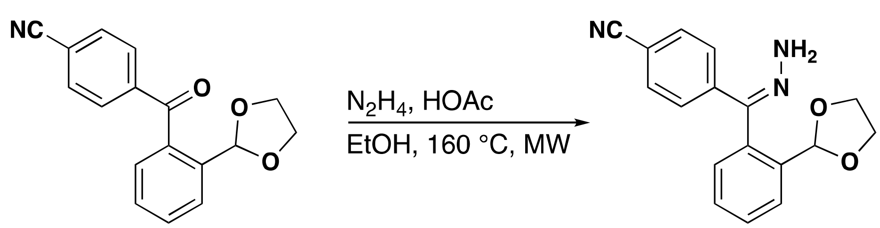
15d

(3a*R*,9*R*,9a*R*)-9-(4-Methoxyphenyl)-2-phenyl-9,9a-dihydrospiro[benzo[*f*]isoindole-4,2'-[1,3]dioxolane]-1,3(2*H*,3a*H*)-dione was synthesized according to General Procedure D, using (*E*)-

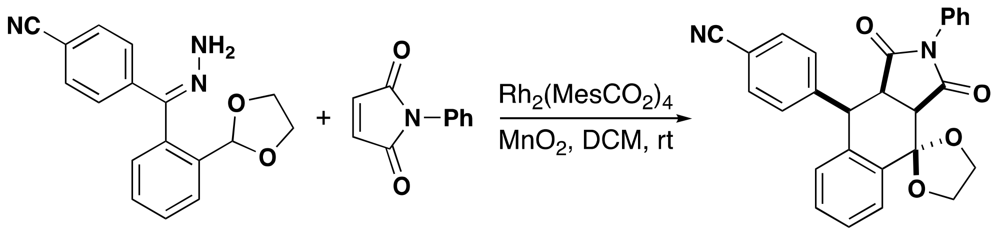
((2-(1,3-dioxolan-2-yl)phenyl)(4-methoxyphenyl)methylene)hydrazine (29.8 mg, 0.1 mmol), 1-phenyl-1*H*-pyrrole-2,5-dione (20.8 mg, 0.12 mmol), MnO_2 (69.6 mg, 0.8 mmol), Rh_2(*R*-PTAD)$_4$ (1.6 mg, 0.001 mmol) and DCM (6 mL). The crude product was purified by flash column chromatography (hexane/EtOAc = 2:1, v/v) to obtain **15d** as a white solid (27.0 mg, 61%, >95:5 dr). m.p. 113-114 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.68 – 7.62 (m, 1H), 7.48 (d, *J* = 8.8 Hz, 2H), 7.37 – 7.27 (m, 5H), 7.20 – 7.14 (m, 1H), 6.92 – 6.83 (m, 4H), 4.97 (d, *J* = 6.3 Hz, 1H), 4.37 (q, *J* = 6.2 Hz, 1H), 4.29 (q, *J* = 6.4 Hz, 1H), 4.22 (q, *J* = 6.4 Hz, 1H), 4.16 – 4.09 (m, 1H), 3.86 – 3.78 (m, 4H), 3.74 (d, *J* = 9.2 Hz, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 175.6, 172.9, 158.9, 138.6, 135.7, 132.2, 131.8, 129.8, 129.6, 129.1, 128.6, 128.0, 127.2, 126.5, 124.6, 113.5, 105.1, 66.4, 65.1, 55.4, 51.3, 45.2, 43.8. HRMS (ESI) *m/z* calcd for $C_{27}H_{24}NO_5^+$ [M+H]$^+$ 442.1649, found 442.1654.



4-(2-(1,3-Dioxolan-2-yl)benzoyl)benzonitrile was synthesized according to General Procedure A, using 2-(2-Bromophenyl)-1,3-dioxolane (229.1 mg, 1 mmol), *n*-BuLi (2.16 M, 0.51 mL, 1.1 mmol), 4-cyano-*N*-methoxy-*N*-methylbenzamide (285.3 mg, 1.5 mmol) and THF (6 mL). The crude product was purified by flash column chromatography (hexane/EtOAc = 5:1, v/v) to obtain the ketone as a white solid (141.0 mg, 51%). m.p. 104-106 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.88 (d, *J* = 8.4 Hz, 2H), 7.74 (d, *J* = 8.4 Hz, 2H), 7.70 (d, *J* = 7.8 Hz, 1H), 7.56 (td, *J* = 7.6, 1.4 Hz, 1H), 7.46 (td, *J* = 7.5, 1.3 Hz, 1H), 7.29 (dd, *J* = 7.6, 1.3 Hz, 1H), 6.00 (s, 1H), 3.90 – 3.79 (m, 4H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 196.2, 141.0, 137.3, 137.2, 132.3, 130.7, 130.3, 128.8, 128.0, 127.5, 118.2, 116.3, 101.7, 65.2. HRMS (ESI) *m/z* calcd for $C_{17}H_{14}NO_3^+$ [M+H]$^+$ 280.0968, found 280.0975.

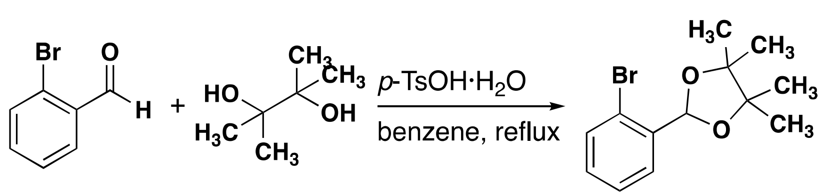


(*E*)-4-((2-(1,3-dioxolan-2-yl)phenyl)(hydrazineylidene)methyl)benzonitrile was synthesized according to General Procedure B, using 4-(2-(1,3-dioxolan-2-yl)benzoyl)benzonitrile (83.8 mg, 0.3 mmol), N_2H_4 (0.12 mL, 3.9 mmol), HOAc (0.02 mL, 0.36 mmol) and EtOH (2 mL). The crude product was purified by flash column chromatography (hexane/EtOAc = 2:1, v/v) to obtain the hydrazone as a yellow oil (34.0 mg, 39%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.79 – 7.74 (m, 1H), 7.60 – 7.49 (m, 6H), 7.17 – 7.09 (m, 1H), 5.91 – 5.14 (m, 3H), 4.08 – 3.84 (m, 4H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 145.6, 142.7, 136.8, 132.1, 131.6, 131.1, 130.0, 129.3, 128.1, 126.4, 119.3, 111.1, 102.0, 65.62, 65.59. HRMS (ESI) *m/z* calcd for $C_{17}H_{16}N_3O_2^+$ $[M+H]^+$ 294.1237, found 294.1245.



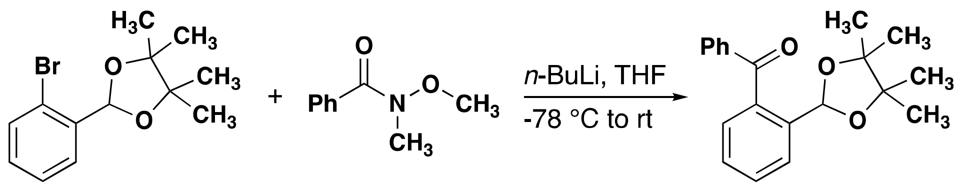
15e

4-((3a*R*,9*R*,9a*R*)-1,3-Dioxo-2-phenyl-1,2,3,3a,9,9a-hexahydrospiro[benzo[*f*]isoindole-4,2'-[1,3]dioxolan]-9-yl)benzonitrile was synthesized according to General Procedure D, using (*E*)-4-((2-(1,3-dioxolan-2-yl)phenyl)(hydrazineylidene)methyl)benzonitrile (29.3 mg, 0.1 mmol), 1-phenyl-1*H*-pyrrole-2,5-dione (20.8 mg, 0.12 mmol), MnO_2 (69.6 mg, 0.8 mmol), $Rh_2(MesCO_2)_4$ (0.9 mg, 0.001 mmol) and DCM (6 mL). The crude product was purified by flash column chromatography (hexane/EtOAc = 1:1, v/v) to obtain **15e** as a white solid (34.3 mg, 79%, 86:14 dr). m.p. 110-111 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.71 (d, *J* = 8.4 Hz, 2H), 7.69 – 7.65 (m, 1H), 7.62 (d, *J* = 8.4 Hz, 2H), 7.39 – 7.28 (m, 5H), 7.11 – 7.04 (m, 1H), 6.93 – 6.82 (m, 2H), 5.09 (d, *J* = 6.5 Hz, 1H), 4.39 – 4.28 (m, 2H), 4.24 – 4.12 (m, 2H), 3.92 (dd, *J* = 9.4, 6.6 Hz, 1H), 3.77 (d, *J* = 9.4 Hz, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 175.2, 172.5, 143.8, 137.1, 135.8, 131.84, 131.81, 131.6, 129.9, 129.2, 128.9, 127.8, 127.7, 126.4, 124.8, 119.0, 111.2, 105.2, 66.3, 65.4, 51.0, 44.3, 44.2. IR (neat): 2974, 2226, 1716, 1383, 1067, 761 cm^{-1}. HRMS (ESI) *m/z* calcd for $C_{27}H_{21}N_2O_4^+$ $[M+H]^+$ 437.1496, found 437.1507.

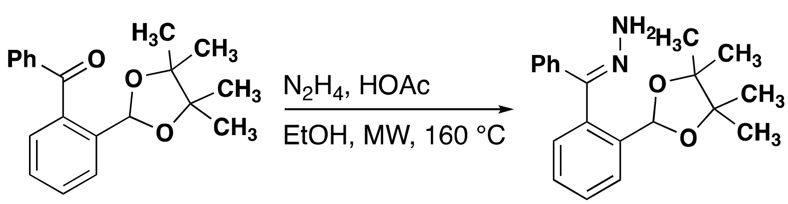


2-(2-Bromophenyl)-4,4,5,5-tetramethyl-1,3-dioxolane was synthesized according to General Procedure C, using 2-bromobenzaldehyde (1.17 mL, 10 mmol), pinacol (4.7 g, 40 mmol), *p*-

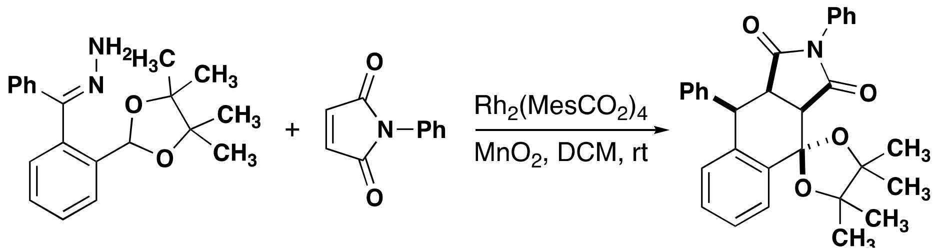
toluenesulfonic acid monohydrate (344.4 mg, 1.8 mmol) and benzene (30 mL). Upon full conversion determined by ^{1}H NMR, the crude product was purified by flash column chromatography (hexane/EtOAc = 30:1, v/v) to obtain the acetal as a pale yellow solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.69 (d, J = 7.8 Hz, 1H), 7.53 (d, J = 7.9 Hz, 1H), 7.32 (t, J = 7.5 Hz, 1H), 7.18 (t, J = 7.7 Hz, 1H), 6.20 (s, 1H), 1.35 (s, 6H), 1.29 (s, 6H). ^{1}H NMR data was consistent with reported literature values.[3]



Phenyl(2-(4,4,5,5-tetramethyl-1,3-dioxolan-2-yl)phenyl)methanone was synthesized according to General Procedure A, using 2-(2-bromophenyl)-4,4,5,5-tetramethyl-1,3-dioxolane (855.5 mg, 3 mmol), *n*-BuLi (1.8 M, 1.8 mL, 3.3 mmol), *N*-methoxy-*N*-methylbenzamide (743.4 mg, 4.5 mmol) and THF (20 mL). The crude product was purified by flash column chromatography (hexane/EtOAc = 15:1, v/v) to obtain the ketone as a colorless oil (296.9 mg, 32%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.79 (d, J = 7.8 Hz, 3H), 7.56 (t, J = 7.5 Hz, 1H), 7.50 (t, J = 7.6 Hz, 1H), 7.43 (t, J = 7.5 Hz, 2H), 7.37 (t, J = 7.4 Hz, 1H), 7.30 (d, J = 7.6 Hz, 1H), 6.11 (s, 1H), 1.15 (s, 6H), 1.11 (s, 6H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 198.2, 139.6, 138.4, 138.2, 133.0, 130.3, 130.1, 128.3, 128.2, 127.7, 126.5, 97.1, 82.8, 24.1, 22.3. HRMS (ESI) m/z calcd for $C_{20}H_{23}O_3^+$ $[M+H]^+$ 311.1642, found 311.1646.

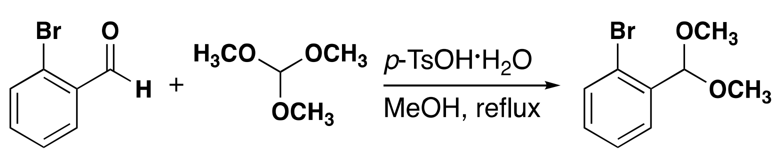


(*E*)-(Phenyl(2-(4,4,5,5-tetramethyl-1,3-dioxolan-2-yl)phenyl)methylene)hydrazine was synthesized according to General Procedure B, using phenyl(2-(4,4,5,5-tetramethyl-1,3-dioxolan-2-yl)phenyl)methanone (290 mg, 0.93 mmol), N_2H_4 (0.38 mL, 12.1 mmol), HOAc (0.06 mL, 1.12 mmol) and EtOH (2.8 mL). The crude product was purified by flash column chromatography (hexane/EtOAc = 5:1, v/v) to obtain the hydrazone as a pale yellow solid (234.4 mg, 78%). m.p. 88-90 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.91 – 7.86 (m, 1H), 7.56 – 7.49 (m, 2H), 7.49 – 7.43 (m, 2H), 7.33 – 7.26 (m, 3H), 7.18 – 7.13 (m, 1H), 5.76 (s, 1H), 5.44 (s, 2H), 1.29 (s, 3H), 1.25 (s, 3H), 1.21 (s, 3H), 1.17 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 148.8, 138.5, 138.1, 133.1, 130.1, 129.4, 129.0, 128.2, 128.1, 126.9, 126.4, 97.5, 82.9, 82.8, 24.7, 24.6, 22.4, 22.3. HRMS (ESI) *m/z* calcd for $C_{20}H_{25}N_2O_2^+$ [M+H]$^+$ 325.1911, found 325.1917.

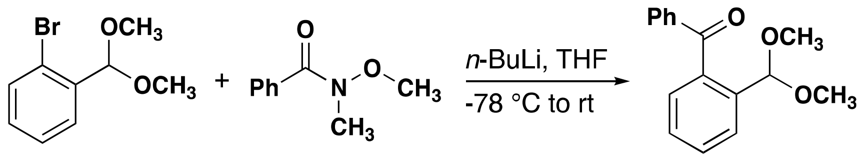


15f

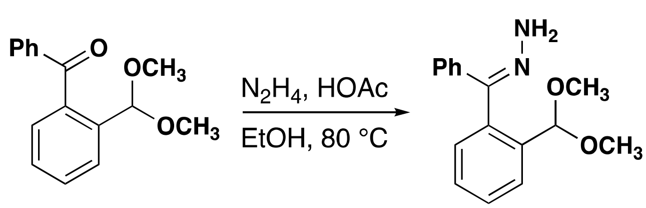
4',4',5',5'-Tetramethyl-2,9-diphenyl-9,9a-dihydrospiro[benzo[*f*]isoindole-4,2'-[1,3]dioxolane]-1,3(2*H*,3a*H*)-dione was synthesized according to General Procedure D, using (*E*)-(phenyl(2-(4,4,5,5-tetramethyl-1,3-dioxolan-2-yl)phenyl)methylene)hydrazine (32.4 mg, 0.1 mmol), 1-phenyl-1*H*-pyrrole-2,5-dione (20.8 mg, 0.12 mmol), MnO_2 (69.6 mg, 0.8 mmol), $Rh_2(MesCO_2)_4$ (0.9 mg, 0.001 mmol) and DCM (6 mL). The crude product was purified by flash column chromatography (hexane/EtOAc = 5:1, v/v) to obtain **15f** as a white solid (29.8 mg, 64%, >95:5 dr). m.p. 202-204 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.79 – 7.72 (m, 1H), 7.68 (d, *J* = 7.3 Hz, 2H), 7.42 (t, *J* = 7.5 Hz, 2H), 7.38 – 7.31 (m, 1H), 7.30 – 7.21 (m, 5H), 7.12 – 7.05 (m, 1H), 6.77 (d, *J* = 6.4 Hz, 2H), 5.23 (d, *J* = 4.3 Hz, 1H), 3.86 (dd, *J* = 8.1, 4.4 Hz, 1H), 3.78 (d, *J* = 8.2 Hz, 1H), 1.57 (s, 3H), 1.45 (s, 3H), 1.33 (s, 3H), 1.06 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 175.6, 172.4, 138.8, 137.9, 137.0, 131.9, 131.2, 128.9, 128.8, 128.4, 128.1, 127.3, 126.6, 126.5, 126.2, 124.6, 103.1, 84.7, 84.0, 55.0, 45.3, 44.0, 25.5, 24.7, 23.7, 23.6. IR (neat): 2975, 1712, 1377, 1119, 1062, 707, 692 cm^{-1}. HRMS (ESI) *m/z* calcd for $C_{30}H_{30}NO_4^+$ [M+H]$^+$ 468.2169, found 468.2170.



To a flame-dried round bottom flask were added 2-bromobenzaldehyde (2.33 mL, 20 mmol), trimethoxymethane (5.5 mL, 50 mmol), *p*-toluenesulfonic acid monohydrate (380.4 mg, 2 mmol) and methanol (40 mL). The reaction was stirred under reflux overnight. After half conversion was observed, another 4 mL of trimethoxymethane was added. The reaction was stirred for another 1 d. Upon full conversion determined by ^{1}H NMR, the reaction was quenched with saturated $NaHCO_3$ aqueous solution. Most of methanol solvent was removed under reduced pressure as well as trimethoxymethane. The mixture was then extracted with EtOAc (3 × 20 mL). The combined organic phases were washed with H_2O (1 × 10 mL) and brine (1 × 10 mL). The organic phase was dried over anhydrous Na_2SO_4, filtered and concentrated. The residue was further purified by flash column chromatography (hexane/EtOAc = 30:1, v/v) to obtain 1-bromo-2-(dimethoxymethyl)benzene as a colorless oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.61 (dd, *J* = 7.7, 1.8 Hz, 1H), 7.56 (dd, *J* = 8.0, 1.2 Hz, 1H), 7.33 (td, *J* = 7.5, 1.3 Hz, 1H), 7.20 (td, *J* = 7.7, 1.8 Hz, 1H), 5.56 (s, 1H), 3.39 (s, 6H). ^{1}H NMR data was consistent with reported literature values.[4]

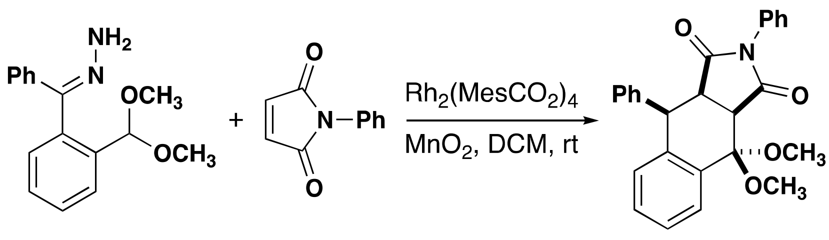


(2-(Dimethoxymethyl)phenyl)(phenyl)methanone was synthesized according to General Procedure A, using 1-bromo-2-(dimethoxymethyl)benzene (2.31 g, 10 mmol), *n*-BuLi (1.8 M, 6.1 mL, 11 mmol), *N*-methoxy-*N*-methylbenzamide (2.15 g, 13 mmol) and THF (60 mL). The crude product was purified by flash column chromatography (hexane/EtOAc = 10:1, v/v) to obtain the ketone as a pale yellow oil (1.50 g, 58%). ^{1}H NMR (400 MHz, Acetone) δ 7.75 (dd, *J* = 8.4, 1.4 Hz, 2H), 7.69 (d, *J* = 7.4 Hz, 1H), 7.66 – 7.61 (m, 1H), 7.58 – 7.45 (m, 4H), 7.33 (dd, *J* = 7.4, 1.4 Hz, 1H), 5.53 (s, 1H), 3.13 (s, 6H). ^{13}C NMR (101 MHz, Acetone) δ 197.5, 139.7, 138.5, 138.0, 133.8, 130.3, 129.3, 128.7, 128.6, 127.7, 101.5, 53.3. HRMS (TOF MS CI$^+$) *m/z* calcd for $C_{16}H_{16}O_3^+$ [M$^+$] 256.1100, found 256.1105.



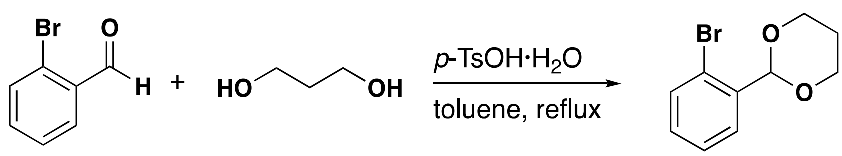
(*E*)-((2-(Dimethoxymethyl)phenyl)(phenyl)methylene)hydrazine was synthesized according to General Procedure B, using (2-(dimethoxymethyl)phenyl)(phenyl)methanone (768.9 mg, 3 mmol), N_2H_4 (1.23 mL, 39 mmol), HOAc (0.2 mL, 3.6 mmol) and EtOH (9 mL). The crude product was purified by flash column chromatography (hexane/EtOAc = 5:1, v/v) to obtain the hydrazone as a yellow solid (627.3 mg, 77%). m.p. 77-79 °C. ^{1}H NMR (599 MHz, $CDCl_3$) δ 7.80 –

7.75 (m, 1H), 7.55 – 7.48 (m, 2H), 7.48 – 7.42 (m, 2H), 7.31 – 7.24 (m, 3H), 7.20 – 7.15 (m, 1H), 5.40 (s, 2H), 5.04 (s, 1H), 3.38 (s, 3H), 3.12 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 148.0, 138.2, 137.6, 132.3, 129.9, 129.3, 129.0, 128.3, 128.2, 126.9, 126.1, 102.8, 55.0, 54.5. HRMS (ESI) *m/z* calcd for $C_{16}H_{19}N_2O_2^+$ $[M+H]^+$ 271.1441, found 271.1444.

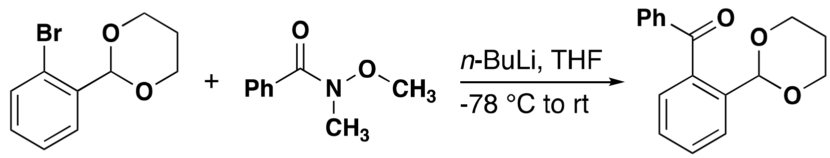


15g

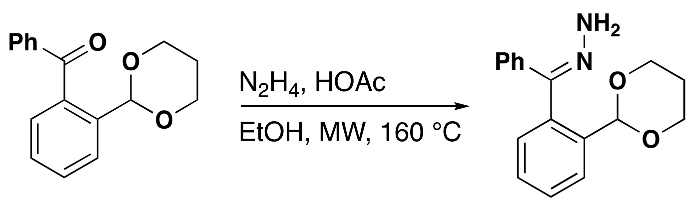
4,4-Dimethoxy-2,9-diphenyl-3a,4,9,9a-tetrahydro-1*H*-benzo[*f*]isoindole-1,3(2*H*)-dione was synthesized according to General Procedure D, using (*E*)-((2-(dimethoxymethyl)phenyl)(phenyl)methylene)hydrazine (27.0 mg, 0.1 mmol), 1-phenyl-1*H*-pyrrole-2,5-dione (20.8 mg, 0.12 mmol), MnO_2 (69.6 mg, 0.8 mmol), $Rh_2(MesCO_2)_4$ (0.9 mg, 0.001 mmol) and DCM (6 mL). The crude product was purified by flash column chromatography (hexane/EtOAc = 2:1, v/v) to obtain **15g** as a white solid (34.5 mg, 84%, >95:5 dr). m.p. 169-171 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.63 – 7.54 (m, 3H), 7.47 (dd, *J* = 7.7, 1.5 Hz, 1H), 7.41 – 7.23 (m, 8H), 7.10 – 6.99 (m, 2H), 5.06 (d, *J* = 6.2 Hz, 1H), 3.88 (d, *J* = 9.0 Hz, 1H), 3.79 (dd, *J* = 9.0, 6.2 Hz, 1H), 3.54 (s, 3H), 3.05 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 174.1, 173.7, 139.7, 136.9, 135.3, 132.0, 129.2, 129.1, 129.0, 128.48, 128.42, 128.38, 127.7, 127.5, 127.2, 126.6, 81.1, 75.6, 57.4, 51.3, 50.0, 44.2. IR (neat): 2922, 1711, 1375, 1153, 1052, 741, 694 cm^{-1}. HRMS (ESI) *m/z* calcd for $C_{26}H_{24}NO_4^+$ $[M+H]^+$ 414.1700, found 414.1706.



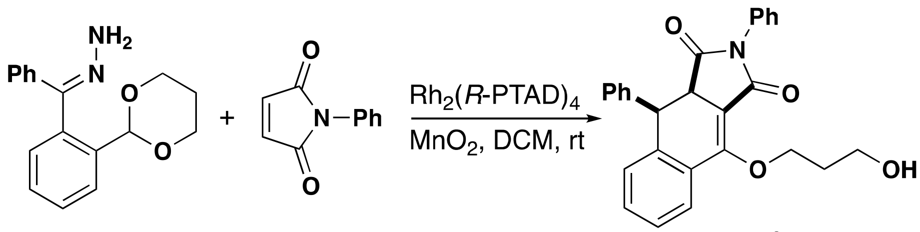
2-(2-Bromophenyl)-1,3-dioxane was synthesized according to General Procedure C, using 2-bromobenzaldehyde (925.1 mg, 5 mmol), propane-1,3-diol (418.5 mg, 5.5 mmol), *p*-toluenesulfonic acid monohydrate (95.1 mg, 0.5 mmol) and toluene (10 mL). The crude product was purified by flash column chromatography (hexane/EtOAc = 30:1, v/v) to obtain the acetal as a white solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.69 (dd, *J* = 7.8, 1.8 Hz, 1H), 7.53 (dd, *J* = 8.0, 1.2 Hz, 1H), 7.34 (td, *J* = 7.6, 1.2 Hz, 1H), 7.19 (td, *J* = 7.7, 1.8 Hz, 1H), 5.76 (s, 1H), 4.28 (dd, *J* = 5.0, 1.3 Hz, 1H), 4.25 (dd, *J* = 5.1, 1.4 Hz, 1H), 4.03 (td, *J* = 12.4, 2.6 Hz, 2H), 2.35 – 2.14 (m, 1H), 1.50 – 1.40 (m, 1H). ^{1}H NMR data was consistent with reported literature values.[5]



(2-(1,3-Dioxan-2-yl)phenyl)(phenyl)methanone was synthesized according to General Procedure A, using 2-(2-bromophenyl)-1,3-dioxane (729.3 mg, 3 mmol), *n*-BuLi (2.5 M, 1.3 mL, 3.3 mmol), *N*-methoxy-*N*-methylbenzamide (743.4 mg, 4.5 mmol) and THF (18 mL). The crude product was purified by flash column chromatography (hexane/EtOAc = 10:1, v/v) to obtain the ketone as a white solid (427.9 mg, 53%). m.p. 76-77 °C. ^{1}H NMR (400 MHz, C_6D_6) δ 8.04 (d, *J* = 7.9 Hz, 1H), 7.94 – 7.86 (m, 2H), 7.24 – 7.16 (m, 1H), 7.14 – 7.01 (m, 4H), 7.00 – 6.92 (m, 1H), 5.94 (s, 1H), 3.74 – 3.62 (m, 2H), 3.32 (td, *J* = 12.2, 2.4 Hz, 2H), 1.79 – 1.61 (m, 1H), 0.56 – 0.43 (m, 1H). ^{13}C NMR (101 MHz, C_6D_6) δ 197.2, 138.8, 138.7, 138.4, 132.60, 132.58, 130.4, 129.8, 128.4, 128.2, 126.5, 98.9, 67.1, 25.8. HRMS (ESI) *m/z* calcd for $C_{17}H_{17}O_3^+$ $[M+H]^+$ 269.1172, found 269.1175.

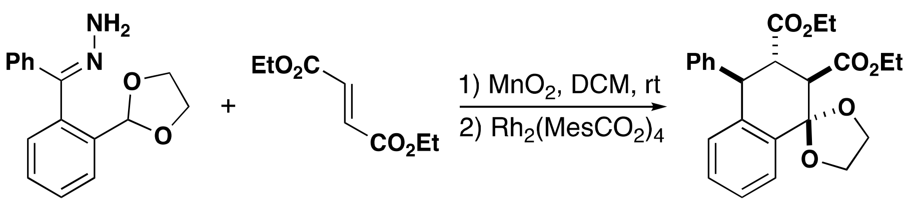


(*E*)-((2-(1,3-Dioxan-2-yl)phenyl)(phenyl)methylene)hydrazine was synthesized according to General Procedure C, using (2-(1,3-dioxan-2-yl)phenyl)(phenyl)methanone (268.3 mg, 1 mmol), N_2H_4 (0.41 mL, 13 mmol), HOAc (0.07 mL, 1.2 mmol) and EtOH (3 mL). The crude product was purified by flash column chromatography (hexane/EtOAc = 3:1, v/v) to obtain the hydrazone as a pale yellow solid (226.8 mg, 80%). m.p. 106-108 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.90 – 7.83 (m, 1H), 7.57 – 7.48 (m, 2H), 7.48 – 7.41 (m, 2H), 7.33 – 7.24 (m, 3H), 7.18 – 7.11 (m, 1H), 6.03 – 4.48 (m, 3H), 4.20 – 4.03 (m, 2H), 3.89 – 3.79 (m, 1H), 3.70 (td, *J* = 12.0, 2.6 Hz, 1H), 2.24 – 2.09 (m, 1H), 1.39 – 1.29 (m, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 148.4, 138.4, 137.4, 131.9, 130.3, 129.6, 128.9, 128.3, 128.2, 127.0, 126.3, 99.8, 67.6, 67.5, 25.8. HRMS (ESI) *m/z* calcd for $C_{17}H_{19}N_2O_2^+$ $[M+H]^+$ 283.1441, found 283.1442.



15h

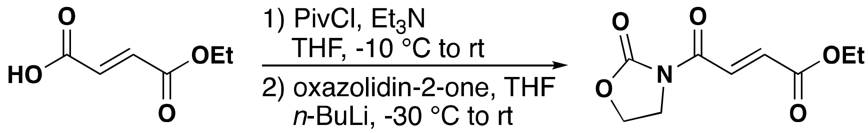
(3a*R*,4*R*)-9-(3-Hydroxypropoxy)-2,4-diphenyl-3a,4-dihydro-1*H*-benzo[*f*]isoindole-1,3(2*H*)-dione was synthesized according to General Procedure G, using (*E*)-((2-(1,3-dioxan-2-yl)phenyl)(phenyl)methylene)hydrazine (28.2 mg, 0.1 mmol), 1-phenyl-1*H*-pyrrole-2,5-dione (20.8 mg, 0.12 mmol), MnO_2 (69.6 mg, 0.8 mmol), Rh_2(*R*-PTAD)$_4$ (1.6 mg, 0.001 mmol) and DCM (6 mL). The crude product was purified by flash column chromatography (hexane/EtOAc = 2:1, v/v) to obtain **15h** as a clear oil (15.3 mg, 36%, >95:5 dr). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.97 – 7.89 (m, 1H), 7.47 – 7.40 (m, 2H), 7.39 – 7.27 (m, 4H), 7.25 – 7.16 (m, 3H), 7.13 – 7.05 (m, 2H), 6.93 – 6.81 (m, 2H), 5.15 (dt, *J* = 10.0, 6.0 Hz, 1H), 4.74 (d, *J* = 6.6 Hz, 1H), 4.49 (dt, *J* = 10.1, 5.7 Hz, 1H), 4.28 (d, *J* = 6.6 Hz, 1H), 4.02 – 3.85 (m, 2H), 2.35 (s, 1H), 2.18 – 2.10 (m, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 173.9, 165.6, 159.8, 140.8, 136.3, 132.3, 132.1, 131.8, 129.4, 129.2, 129.1, 128.6, 128.5, 128.3, 127.7, 126.9, 126.4, 100.1, 73.9, 59.5, 47.6, 44.2, 33.2. IR (neat): 3442, 2925, 1695, 1614, 1377, 741 cm^{-1}. HRMS (ESI) *m/z* calcd for $C_{27}H_{24}NO_4^+$ [M+H]$^+$ 426.1700, found 426.1717.



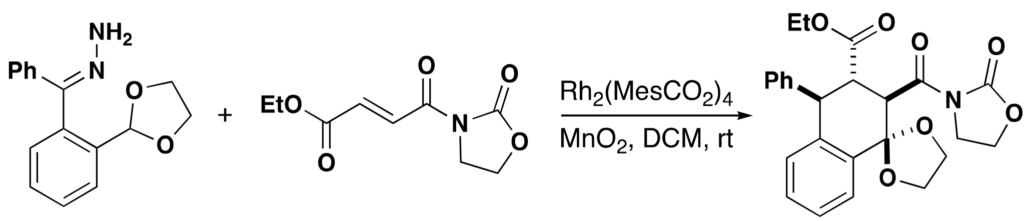
15i

Diethyl (2*R*,3*S*,4*R*)-4-phenyl-3,4-dihydro-2*H*-spiro[naphthalene-1,2'-[1,3]dioxolane]-2,3-dicarboxylate was synthesized according to General Procedure H, using (*E*)-((2-(1,3-dioxolan-2-yl)phenyl)(phenyl)methylene)hydrazine (26.8 mg, 0.1 mmol), diethyl fumarate (0.01 mL, 0.1 mmol), MnO_2 (69.6 mg, 0.8 mmol), $Rh_2(MesCO_2)_4$ (0.9 mg, 0.001 mmol) and DCM (6 mL). The crude product was purified by flash column chromatography (hexane/EtOAc = 4:1, v/v) to obtain **15i** as a yellowish oil (22.7 mg, 55%, >95:5 dr). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.45 (dd, *J* = 7.8, 1.5 Hz, 1H), 7.34 – 7.10 (m, 7H), 6.75 (dt, *J* = 7.8, 1.4 Hz, 1H), 4.41 – 4.35 (m, 1H), 4.25 –

4.09 (m, 6H), 3.91 (qt, *J* = 7.1, 3.7 Hz, 2H), 3.73 (t, *J* = 11.5 Hz, 1H), 3.52 (d, *J* = 11.8 Hz, 1H), 1.28 (t, *J* = 7.1 Hz, 3H), 0.92 (t, *J* = 7.1 Hz, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 173.6, 170.8, 143.1, 138.9, 137.7, 129.5, 129.5, 129.0, 128.6, 127.2, 126.7, 124.5, 107.7, 67.2, 65.1, 61.2, 60.6, 52.5, 50.0, 49.0, 14.3, 13.9. IR (neat): 2979, 2898, 1728, 1448, 1252 cm^{-1}. HRMS (ESI) *m/z* calcd for $C_{24}H_{27}O_6^+$ $[M+H]^+$ 411.1802, found 411.1806.



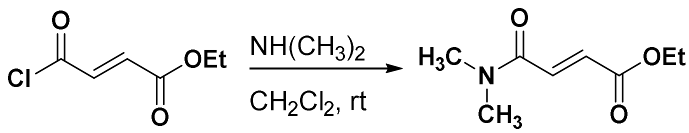
To a round bottom flask were added (*E*)-4-ethoxy-4-oxobut-2-enoic acid (720.7 mg, 5 mmol) and THF (20 mL). Then triethyl amine (0.76 mL, 5.5 mmol) and pivaloyl chloride (0.66 mL,5 mmol) were added at -10 °C. The reaction was then allowed to stir for 3 hours at room temperature. In another flask, oxazolidine-2-one(435.4 mg, 5 mmol) was dissolved in THF (20 mL) and cooled to -30 °C before adding *n*-Buli (2.78 mL, 5 mmol). After stirring for one hour at room temperature, the oxazolidinone solution was cooled to -30 °C and the anhydride solution was added dropwise. After allowing the reaction to stir overnight at room temperature, sodium bicarbonate was added (30 mL), the organic layer was extracted in diethyl ether (3x 50 mL), dried over sodium sulfate and concentrated in vacuo. The crude product was purified by flash column chromatography to obtain ethyl (*E*)-4-oxo-4-(2-oxooxazolidin-3-yl)but-2-enoate as a white powder (835.4 mg, 78%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.15 (d, *J* = 15.6 Hz, 1H), 6.96 (d, *J* = 15.5 Hz, 1H), 4.48 (dd, *J* = 8.5, 7.5 Hz, 2H), 4.28 (q, *J* = 7.1 Hz, 2H), 4.11 (dd, *J* = 8.6, 7.4 Hz, 2H), 1.33 (t, *J* = 7.1 Hz, 3H). ^{1}H NMR data was consistent with reported literature values.[6]



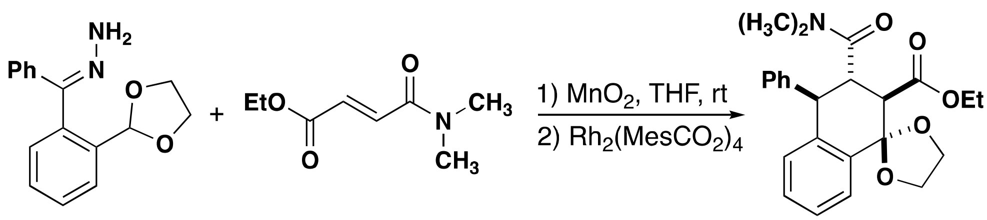
15k

Ethyl (2*R*,3*S*,4*R*)-2-(2-oxooxazolidine-3-carbonyl)-4-phenyl-3,4-dihydro-2*H*-spiro[naphthalene-1,2'-[1,3]dioxolane]-3-carboxylate was synthesized according to General Procedure G, using (*E*)-((2-(1,3-dioxolan-2-yl)phenyl)(phenyl)methylene)hydrazine (26.8 mg, 0.1 mmol), ethyl (*E*)-4-oxo-4-(2-oxooxazolidin-3-yl)but-2-enoate (21.3 mg, 0.1 mmol), MnO_2 (69.6 mg, 0.8 mmol),

$Rh_2(MesCO_2)_4$ (0.9 mg, 0.001 mmol) and DCM (6 mL). The crude product was purified by flash column chromatography (hexane/EtOAc = 1:1, v/v) to obtain **15k** as a white powder (35.0 mg, 77%, >95:5 dr). m.p. 217-218 °C. ^1H NMR (400 MHz, $CDCl_3$) δ 7.41 (dd, *J* = 7.4, 1.9 Hz, 1H), 7.35 – 7.02 (m, 7H), 6.77 (dt, *J* = 7.8, 1.3 Hz, 1H), 5.23 (d, *J* = 10.6 Hz, 1H), 4.49 – 4.24 (m, 4H), 4.19 – 3.79 (m, 8H), 0.95 (t, *J* = 7.1 Hz, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 173.6, 171.7, 153.2, 143.4, 139.3, 137.3, 129.6, 129.4, 129.0, 128.6, 127.0, 126.4, 123.6, 107.9, 67.2, 64.9, 61.7, 60.8, 49.6, 48.4, 48.1, 43.3, 13.9. IR (neat): 2897, 1788, 1724, 1687, 1390, 1371 cm^{-1}. HRMS (ESI) *m/z* calcd for $C_{25}H_{26}NO_7^+$ $[M+H]^+$ 452.1704, found 452.1707.

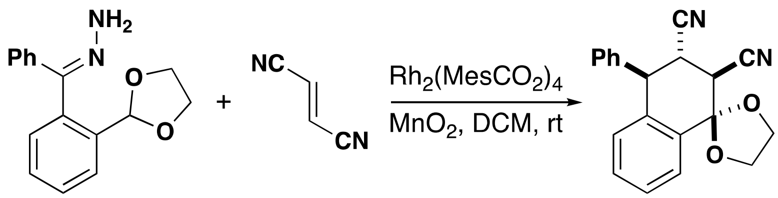


Ethyl (*E*)-4-(dimethylamino)-4-oxobut-2-enoate was synthesized by dissolving ethyl (*E*)-4-chloro-4-oxobut-2-enoate (1.3 g, 8 mmol) in DCM (15 mL). After cooling the solution to 0 °C, dimethyl amine (2 M) in methanol (8 mL, 16 mmol) was added dropwise. The reaction was allowed to stir overnight at room temperature. Sodium bicarbonate (20 mL) was added, and the organic layer was extracted in methylene chloride (3 × 20 mL). The combined organic layers were dried over sodium sulfate and concentrated in vacuo to afford a clear yellow oil (1.26 g, 92 %). ^1H NMR (400 MHz, $CDCl_3$) δ 7.40 (d, *J* = 15.3 Hz, 1H), 6.78 (d, *J* = 15.3 Hz, 1H), 4.26 (q, *J* = 7.2 Hz, 2H), 3.13 (s, 3H), 3.04 (s, 3H), 1.32 (t, *J* = 7.1 Hz, 3H). ^1H NMR data was consistent with reported literature values.[7]



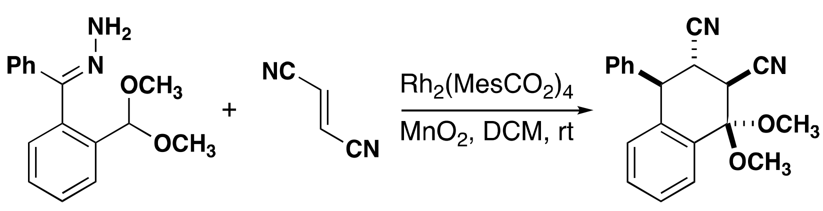
15l

Ethyl (2*R*,3*S*,4*R*)-3-(dimethylcarbamoyl)-4-phenyl-3,4-dihydro-2H-spiro[naphthalene-1,2'-[1,3]dioxolane]-2-carboxylate was synthesized according to General Procedure H, using (*E*)-((2-(1,3-dioxolan-2-yl)phenyl)(phenyl)methylene)hydrazine (26.8 mg, 0.1 mmol), Ethyl (*E*)-4-(dimethylamino)-4-oxobut-2-enoate (17.1 mg, 0.1 mmol), MnO_2 (69.6 mg, 0.8 mmol), $Rh_2(MesCO_2)_4$ (0.9 mg, 0.001 mmol) and THF (6 mL). The crude product was purified by flash column chromatography (hexane/EtOAc = 3:2, v/v) to obtain **15l** as a white powder (31.6 mg, 77%, >95:5 dr). m.p. 168-169 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.46 (dd, *J* = 7.8, 1.6 Hz, 1H), 7.34 – 7.12 (m, 7H), 6.81 (dt, *J* = 7.6, 1.3 Hz, 1H), 4.46 – 4.37 (m, 1H), 4.32 (d, *J* = 10.8 Hz, 1H), 4.23 – 3.96 (m, 6H), 3.65 (d, *J* = 11.8 Hz, 1H), 2.75 (s, 3H), 2.38 (s, 3H), 1.28 (t, *J* = 7.1 Hz, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 173.2, 171.4, 144.3, 139.2, 138.1, 129.8, 129.5, 129.0, 128.6, 127.1, 126.5, 124.5, 108.1, 67.3, 64.8, 61.2, 52.6, 49.4, 46.0, 37.0, 35.7, 14.3. IR (neat): 3442, 2925, 1757, 1695, 1614, 1596, 1566, 1377 cm^{-1}. HRMS (ESI) *m/z* calcd for $C_{24}H_{28}NO_5^+$ [M+H]$^+$ 410.1962, found 410.1963.



15m

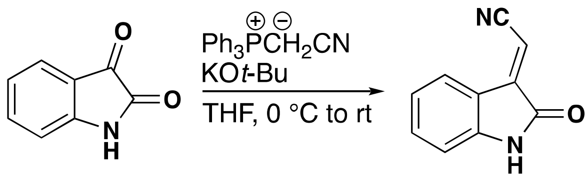
(2*S*,3*S*,4*R*)-4-Phenyl-3,4-dihydro-2*H*-spiro[naphthalene-1,2'-[1,3]dioxolane]-2,3-dicarbonitrile was synthesized according to General Procedure G, using (*E*)-((2-(1,3-dioxolan-2-yl)phenyl)(phenyl)methylene)hydrazine (26.8 mg, 0.1 mmol), fumaronitrile (7.8 mg, 0.1 mmol), MnO_2 (69.6 mg, 0.8 mmol), $Rh_2(MesCO_2)_4$ (0.9 mg, 0.001 mmol) and DCM (6 mL). The crude product was purified by flash column chromatography (hexane/EtOAc = 4:1, v/v) to obtain **15m** as a white solid (20.1 mg, 65%, >95:5 dr). m.p. 209-211 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.46 (dd, *J* = 7.8, 1.5 Hz, 1H), 7.42 – 7.20 (m, 7H), 6.80 (d, *J* = 7.8 Hz, 1H), 4.65 – 4.41 (m, 3H), 4.30 (d, *J* = 11.4 Hz, 1H), 4.26 – 4.15 (m, 1H), 3.79 (t, *J* = 11.9 Hz, 1H), 3.57 (d, *J* = 12.4 Hz, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 141.0, 136.2, 135.5, 130.1, 129.9, 129.4, 129.2, 128.5, 127.7, 124.8, 117.8, 116.4, 105.5, 68.7, 68.5, 66.3, 66.0, 48.6, 41.6, 37.7. IR (neat): 2922, 2853, 2252, 1765, 1453 cm^{-1}. HRMS (ESI) *m/z* calcd for $C_{20}H_{17}N_2O_2^+$ [M+H]$^+$ 317.1285, found 317.1286.



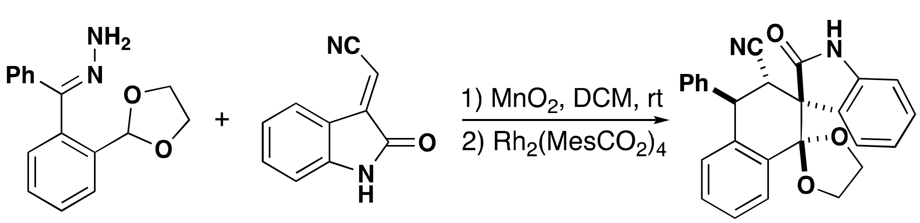
15n

(2*S*,3*S*,4*R*)-1,1-dimethoxy-4-phenyl-1,2,3,4-tetrahydronaphthalene-2,3-dicarbonitrile was synthesized according to General Procedure G, using (*E*)-((2-

(dimethoxymethyl)phenyl)(phenyl)methylene)hydrazine (27.0 mg, 0.1 mmol), fumaronitrile (7.8 mg, 0.1 mmol), MnO_2 (69.6 mg, 0.8 mmol), $Rh_2(MesCO_2)_4$ (0.9 mg, 0.001 mmol) and DCM (6 mL). The crude product was purified by flash column chromatography (hexane/EtOAc = 4:1, v/v) to obtain **15n** as a white solid (29.8 mg, 94%, >95:5 dr). m.p. 226-228 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.58 (d, *J* = 7.9 Hz, 1H), 7.47 (td, *J* = 7.6, 1.4 Hz, 1H), 7.41 – 7.31 (m, 4H), 7.31 – 7.13 (m, 3H), 4.87 (d, *J* = 9.4 Hz, 1H), 3.92 – 3.74 (m, 4H), 3.44 – 3.23 (m, 4H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 140.5, 136.0, 134.8, 129.6, 129.6, 129.2, 128.5, 128.3, 128.1, 127.3, 117.9, 115.3, 81.3, 78.7, 59.8, 51.5, 37.5, 33.7. IR (neat): 2935, 2249, 1488, 1445, 1213 cm^{-1}. HRMS (TOF MS CI$^+$) *m/z* calcd for $C_{20}H_{22}N_3O_2^+$ $[M+NH_4]^+$ 336.1712, found 336.1716.



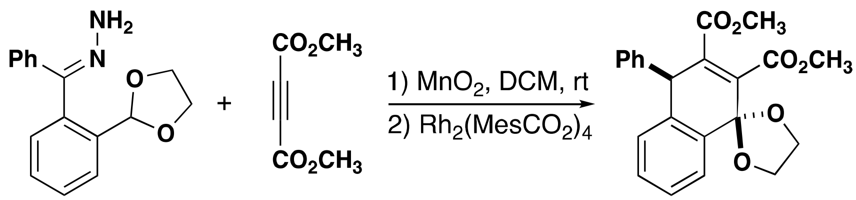
To a flame-dried round bottom flask were added (triphenylphosphoranylidene)acetonitrile (1.1 g, 3.3 mmol) and THF (10 mL). KO*t*-Bu (370.3 mg, 3.3 mmol) was then added. After the mixture was stirred at 0 °C for 30 min, indoline-2,3-dione (441.4 mg, 3 mmol) was added and the reaction was stirred for 1 h at room temperature. After quenched with H_2O, the reaction was extracted with EtOAc (3 × 10 mL). The combined organic phases were washed with brine (1 × 10 mL). The organic phase was dried over anhydrous Na_2SO_4, filtered and concentrated. The residue was further purified by flash column chromatography (hexane/EtOAc = 4:1, v/v) to obtain the product as an orange solid (333.3 mg, 65%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.08 (d, *J* = 7.8 Hz, 1H), 7.88 (s, 1H), 7.40 (td, *J* = 7.8, 1.2 Hz, 1H), 7.12 (td, *J* = 7.7, 1.0 Hz, 1H), 6.89 (d, *J* = 7.9 Hz, 1H), 6.30 (s, 1H). ^{1}H NMR data was consistent with reported literature values.[8]



15o

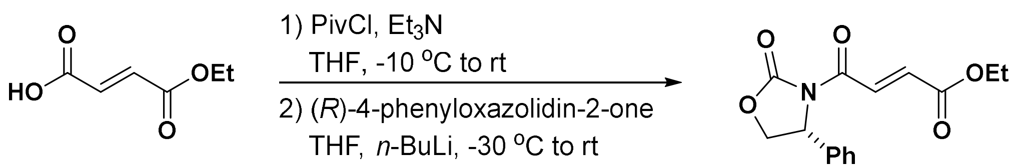
(3*S*,3'*S*,4'*R*)-2-Oxo-4'-phenyl-3',4'-dihydrodispiro[indoline-3,2'-naphthalene-1',2''-[1,3]dioxolane]-3'-carbonitrile was synthesized according to General Procedure H, using (*E*)-((2-(1,3-dioxolan-2-yl)phenyl)(phenyl)methylene)hydrazine (26.8 mg, 0.1 mmol), (*E*)-2-(2-

oxoindolin-3-ylidene)acetonitrile (15 mg, 0.12 mmol), MnO_2 (69.6 mg, 0.8 mmol), $Rh_2(MesCO_2)_4$ (0.9 mg, 0.001 mmol) and DCM (6 mL). The crude product was purified by flash column chromatography (hexane/EtOAc = 1:1, v/v) to obtain **15o** as a pale yellow solid (37.3 mg, 91%, >95:5 dr). m.p. 290-292 °C. ^1H NMR (400 MHz, $CDCl_3$) δ 8.28 (s, 1H), 7.42 – 7.28 (m, 8H), 7.23 (d, *J* = 7.7 Hz, 1H), 7.01 (d, *J* = 7.4 Hz, 1H), 6.95 (d, *J* = 7.8 Hz, 1H), 6.82 (t, *J* = 7.7 Hz, 1H), 6.36 (d, *J* = 7.7 Hz, 1H), 4.50 (d, *J* = 11.0 Hz, 1H), 4.40 (d, *J* = 11.0 Hz, 1H), 4.35 – 4.26 (m, 2H), 4.21 – 4.14 (m, 1H), 4.13 – 4.06 (m, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 175.7, 142.0, 141.9, 137.7, 136.6, 129.9, 129.8, 129.7, 129.4, 129.3, 128.1, 127.6, 125.3, 125.0, 124.4, 122.9, 118.1, 110.5, 108.8, 68.6, 66.0, 57.4, 46.4, 40.9. IR (neat): 3278, 2989, 2870, 1725, 1686, 1471, 756 cm^{-1}. HRMS (ESI) *m/z* calcd for $C_{26}H_{21}N_2O_3^+$ $[M+H]^+$ 409.1547, found 409.1546.

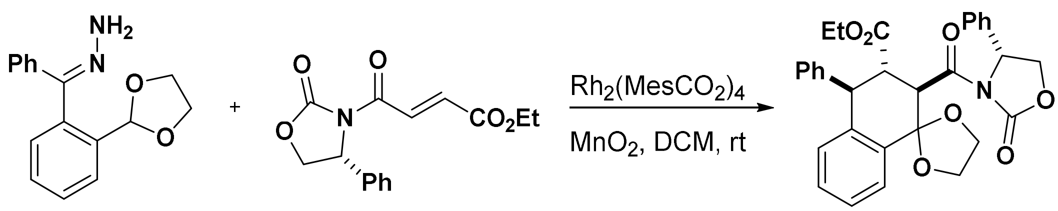


15p

Dimethyl (*R*)-4-phenyl-4*H*-spiro[naphthalene-1,2'-[1,3]dioxolane]-2,3-dicarboxylate was synthesized according to General Procedure H, using (*E*)-((2-(1,3-dioxolan-2-yl)phenyl)(phenyl)methylene)hydrazine (26.8 mg, 0.1 mmol), dimethyl but-2-ynedioate (15 µL, 0.12 mmol), MnO_2 (69.6 mg, 0.8 mmol), $Rh_2(MesCO_2)_4$ (0.9 mg, 0.001 mmol) and DCM (6 mL). The crude product was purified by flash column chromatography (hexane/EtOAc = 4:1, v/v) to obtain **15p** as a clear oil (22.9 mg, 60%). ^1H NMR (400 MHz, $CDCl_3$) δ 7.50 – 7.45 (m, 1H), 7.44 – 7.38 (m, 2H), 7.31 – 7.20 (m, 5H), 7.19 – 7.13 (m, 1H), 5.20 (s, 1H), 4.52 – 4.42 (m, 2H), 4.32 – 4.24 (m, 1H), 4.24 – 4.17 (m, 1H), 3.83 (s, 3H), 3.66 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 167.4, 165.8, 140.3, 139.3, 138.0, 137.0, 135.1, 129.03, 128.95, 128.9, 128.6, 127.19, 127.15, 124.9, 103.8, 68.9, 65.3, 52.63, 52.60, 46.7. IR (neat): 2975, 2857, 1725, 1259, 1070, 756, 701 cm^{-1}. HRMS (ESI) *m/z* calcd for $C_{22}H_{21}O_6^+$ $[M+H]^+$ 381.1333, found 381.1327.

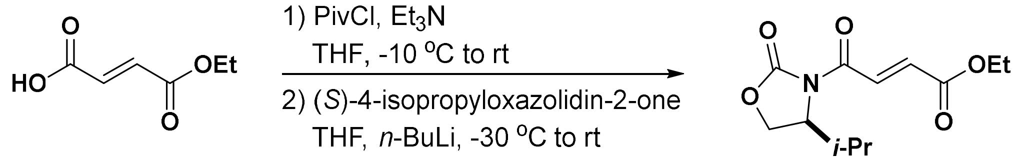


To a round bottom flask were added (*E*)-4-ethoxy-4-oxobut-2-enoic acid (144.3 mg, 1 mmol) and THF (5 mL). Then triethyl amine (0.12 mL, 1.2 mmol) and pivaloyl chloride (144.7 mg,1.2 mmol) were added at -10 °C. The reaction was then allowed to stir for 3 hours at room temperature. In another flask, (R)-4-phenyloxazolidin-2-one (163.2 mg, 1 mmol) was dissolved in THF (5 mL) and cooled to -30 °C before adding *n*-Buli (0.53 mL, 1.2 mmol). After stirring for one hour at room temperature, the oxazolidinone solution was cooled to -30 °C and the anhydride solution was added dropwise. After allowing the reaction to stir overnight at room temperature, sodium bicarbonate was added (30 mL), the organic layer was extracted in diethyl ether (3x 50 mL), dried over sodium sulfate and concentrated in vacuo. The crude product was purified by flash column chromatography to obtain ethyl (R,E)-4-oxo-4-(2-oxo-4-phenyloxazolidin-3-yl)but-2-enoate as a white powder (188.0 mg, 65%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.16 (d, *J* = 15.6 Hz, 1H), 7.47 – 7.29 (m, 5H), 6.86 (d, *J* = 15.6 Hz, 1H), 5.50 (dd, *J* = 8.7, 4.0 Hz, 1H), 4.76 (t, *J* = 8.8 Hz, 1H), 4.35 (dd, *J* = 8.9, 4.0 Hz, 1H), 4.26 (q, *J* = 7.1 Hz, 2H), 1.31 (t, *J* = 7.1 Hz, 3H). ^{1}H NMR data was consistent with reported literature values.[6]

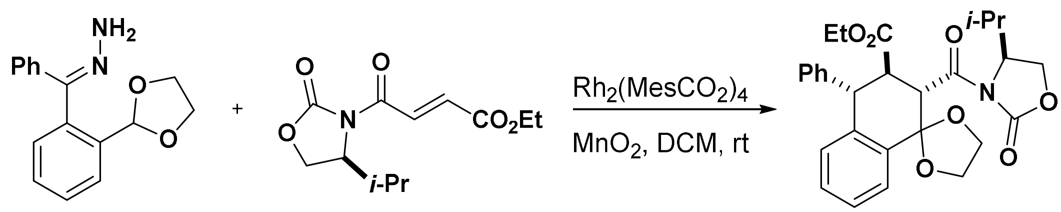


15q

Ethyl (2R,3S,4R)-2-((R)-2-oxo-4-phenyloxazolidine-3-carbonyl)-4-phenyl-3,4-dihydro-2H-spiro[naphthalene-1,2'-[1,3]dioxolane]-3-carboxylate was synthesized according to General Procedure G, using (*E*)-((2-(1,3-dioxolan-2-yl)phenyl)(phenyl)methylene)hydrazine (26.8 mg, 0.1 mmol), ethyl (R,E)-4-oxo-4-(2-oxo-4-phenyloxazolidin-3-yl)but-2-enoate (28.9 mg, 0.1 mmol), MnO_2 (69.6 mg, 0.8 mmol), $Rh_2(MesCO_2)_4$ (0.9 mg, 0.001 mmol) and DCM (6 mL). The crude product was purified by flash column chromatography (hexane/EtOAc = 1:1, v/v) to obtain **15q** as a white powder (26.4 mg, 46%, 78:22 dr). m.p. 235-237 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.41 (dd, *J* = 7.6, 1.6 Hz, 1H), 7.37 – 7.07 (m, 12H), 6.72 (d, *J* = 7.5 Hz, 1H), 5.46 (dd, *J* = 8.3, 2.9 Hz, 1H), 5.31 (d, *J* = 10.2 Hz, 1H), 4.67 (t, *J* = 8.6 Hz, 1H), 4.50 – 4.21 (m, 3H), 4.22 – 3.97 (m, 3H), 3.84 – 3.64 (m, 3H), 0.80 (t, *J* = 7.1 Hz, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 173.17, 170.95, 153.46, 142.83, 139.46, 139.02, 137.22, 129.61, 129.25, 129.12, 129.03, 128.59, 127.09, 126.44, 125.93, 123.53, 107.93, 69.82, 67.06, 65.17, 60.64, 58.32, 49.76, 48.96, 47.99, 13.89. IR (neat): 2899, 1782, 1726, 1689, 1392, 1377 cm^{-1}. HRMS (ESI) *m/z* calcd for $C_{31}H_{30}NO_7^+$ $[M+H]^+$ 528.2017, found 528.2019.



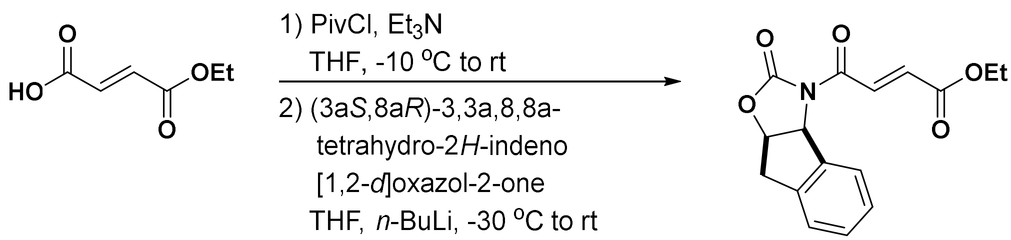
To a round bottom flask were added (*E*)-4-ethoxy-4-oxobut-2-enoic acid (144.3 mg, 1 mmol) and THF (5 mL). Then triethyl amine (0.12 mL, 1.2 mmol) and pivaloyl chloride (144.7 mg,1.2 mmol) were added at -10 °C. The reaction was then allowed to stir for 3 hours at room temperature. In another flask, (S)-4-isopropyloxazolidin-2-one (128.2 mg, 1 mmol) was dissolved in THF (5 mL) and cooled to -30 °C before adding *n*-Buli (0.53 mL, 1.2 mmol). After stirring for one hour at room temperature, the oxazolidinone solution was cooled to -30 °C and the anhydride solution was added dropwise. After allowing the reaction to stir overnight at room temperature, sodium bicarbonate was added (30 mL), the organic layer was extracted in diethyl ether (3x 50 mL), dried over sodium sulfate and concentrated in vacuo. The crude product was purified by flash column chromatography to obtain ethyl (S,E)-4-(4-isopropyl-2-oxooxazolidin-3-yl)-4-oxobut-2-enoate as a clear oil (145.5 mg, 57%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.17 (dd, *J* = 15.6, 1.0 Hz, 1H), 6.93 (dd, *J* = 15.6, 1.1 Hz, 1H), 4.51 (dt, *J* = 7.8, 3.6 Hz, 1H), 4.41 – 4.23 (m, 4H), 2.43 (pd, *J* = 6.9, 3.9 Hz, 1H), 1.33 (td, *J* = 7.1, 1.0 Hz, 3H), 1.02 – 0.93 (m, 3H), 0.92 – 0.87 (m, 3H). ^{1}H NMR data was consistent with reported literature values.[6]



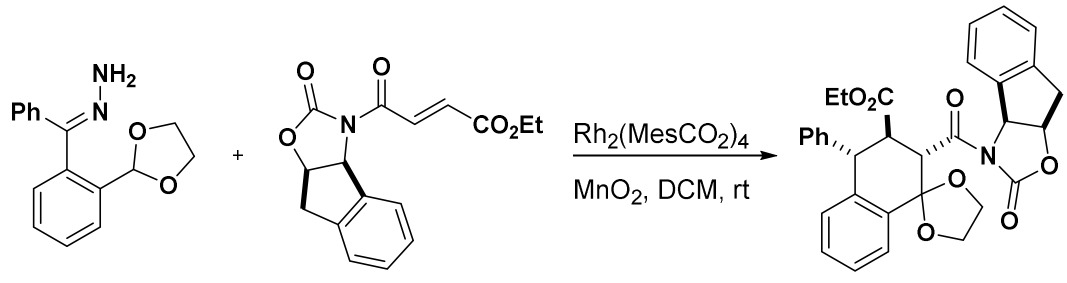
15r

Ethyl (2S,3R,4S)-2-((S)-4-isopropyl-2-oxooxazolidine-3-carbonyl)-4-phenyl-3,4-dihydro-2H-spiro[naphthalene-1,2'-[1,3]dioxolane]-3-carboxylate was synthesized according to General Procedure G, using (*E*)-((2-(1,3-dioxolan-2-yl)phenyl)(phenyl)methylene)hydrazine (26.8 mg, 0.1 mmol), ethyl (S,E)-4-(4-isopropyl-2-oxooxazolidin-3-yl)-4-oxobut-2-enoate (25.5 mg, 0.1 mmol),

MnO_2 (69.6 mg, 0.8 mmol), $Rh_2(MesCO_2)_4$ (0.9 mg, 0.001 mmol) and DCM (6 mL). The crude product was purified by flash column chromatography (hexane/EtOAc = 1:1, v/v) to obtain **15r** as a clear oil (35.0 mg, 71%, 81:19 dr). ^1H NMR (400 MHz, $CDCl_3$) δ 7.40 (dd, *J* = 7.2, 1.9 Hz, 1H), 7.36 – 7.23 (m, 5H), 7.23 – 7.11 (m, 2H), 6.75 (dt, *J* = 7.7, 1.3 Hz, 1H), 5.29 (d, 1H), 4.44 (ddd, *J* = 7.3, 4.1, 2.8 Hz, 1H), 4.36 (d, *J* = 11.2 Hz, 1H), 4.31 – 4.18 (m, 3H), 4.16 – 4.01 (m, 3H), 3.93 (qd, *J* = 7.1, 4.6 Hz, 2H), 3.84 (dd, *J* = 11.3, 10.1 Hz, 1H), 2.32 (pd, *J* = 7.0, 4.1 Hz, 1H), 0.97 (t, *J* = 7.1 Hz, 3H), 0.90 (d, *J* = 7.0 Hz, 6H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 173.35, 171.48, 153.85, 142.95, 139.45, 137.16, 129.60, 129.20, 128.97, 128.57, 127.05, 126.38, 123.48, 107.87, 66.92, 65.06, 63.37, 60.71, 59.44, 49.85, 48.67, 47.91, 28.85, 18.04, 14.95, 13.99. IR (neat): 2895, 1780, 1721, 1675, 1395, 1374 cm^{-1}. HRMS (ESI) *m/z* calcd for $C_{28}H_{32}NO_7^+$ $[M+H]^+$ 494.2173, found 494.2170.

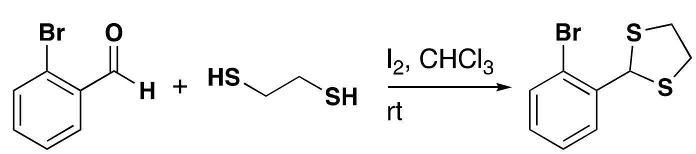


To a round bottom flask were added (*E*)-4-ethoxy-4-oxobut-2-enoic acid (144.3 mg, 1 mmol) and THF (5 mL). Then triethyl amine (0.12 mL, 1.2 mmol) and pivaloyl chloride (144.7 mg,1.2 mmol) were added at -10 °C. The reaction was then allowed to stir for 3 hours at room temperature. In another flask, (3aS,8aR)-3,3a,8,8a-tetrahydro-2H-indeno[1,2-d]oxazol-2-one (175.2 mg, 1 mmol) was dissolved in THF (5 mL) and cooled to -30 °C before adding *n*-Buli (0.53 mL, 1.2 mmol). After stirring for one hour at room temperature, the oxazolidinone solution was cooled to -30 °C and the anhydride solution was added dropwise. After allowing the reaction to stir overnight at room temperature, sodium bicarbonate was added (30 mL), the organic layer was extracted in diethyl ether (3x 50 mL), dried over sodium sulfate and concentrated in vacuo. The crude product was purified by flash column chromatography to obtain ethyl (E)-4-oxo-4-((3aS,8aR)-2-oxo-8,8a-dihydro-2H-indeno[1,2-d]oxazol-3(3aH)-yl)but-2-enoate as a white powder (118.3 mg, 40 %). ^1H NMR (300 MHz, $CDCl_3$) δ 8.14 (d, *J* = 15.6 Hz, 1H), 7.72 – 7.59 (m, 1H), 7.39 – 7.26 (m, 3H), 7.01 (d, *J* = 15.5 Hz, 1H), 6.00 (d, *J* = 6.9 Hz, 1H), 5.35 (ddd, *J* = 7.1, 4.6, 2.7 Hz, 1H), 4.26 (q, *J* = 7.1 Hz, 2H), 3.47 – 3.36 (m, 2H), 1.32 (t, *J* = 7.1 Hz, 3H). ^1H NMR data was consistent with reported literature values.[6]

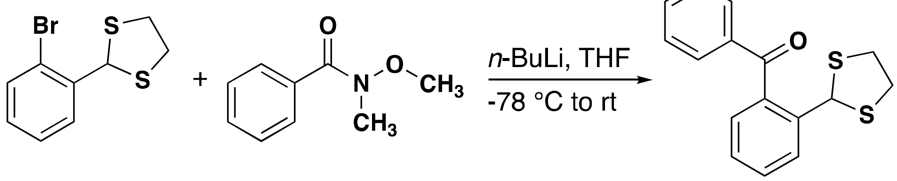


15s

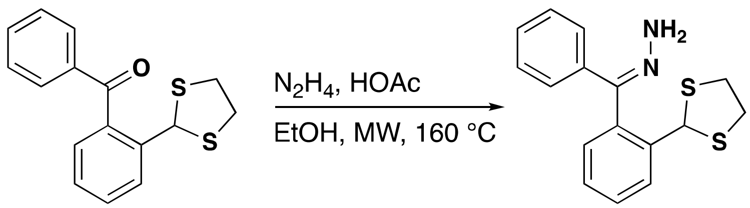
Ethyl (2S,3R,4S)-2-((3aS,8aR)-2-oxo-3,3a,8,8a-tetrahydro-2H-indeno[1,2-d]oxazole-3-carbonyl)-4-phenyl-3,4-dihydro-2H-spiro[naphthalene-1,2'-[1,3]dioxolane]-3-carboxylate was synthesized according to General Procedure G, using (*E*)-((2-(1,3-dioxolan-2-yl)phenyl)(phenyl)methylene)hydrazine (26.8 mg, 0.1 mmol), ethyl (E)-4-oxo-4-((3aS,8aR)-2-oxo-8,8a-dihydro-2H-indeno[1,2-d]oxazol-3(3aH)-yl)but-2-enoate (30.1 mg, 0.1 mmol), MnO_2 (69.6 mg, 0.8 mmol), $Rh_2(MesCO_2)_4$ (0.9 mg, 0.001 mmol) and DCM (6 mL). The crude product was purified by flash column chromatography (hexane/EtOAc = 1:1, v/v) to obtain **15s** as a clear oil (36.0 mg, 67 %, 85:15 dr). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.54 (d, *J* = 7.7 Hz, 1H), 7.42 (dd, *J* = 7.3, 1.9 Hz, 1H), 7.37 – 7.09 (m, 11H), 6.85 – 6.67 (m, 1H), 5.95 (d, *J* = 6.7 Hz, 1H), 5.34 – 5.18 (m, 2H), 4.49 – 4.31 (m, 2H), 4.24 – 4.03 (m, 3H), 3.93 (t, *J* = 10.8 Hz, 1H), 3.81 (ddd, *J* = 40.6, 10.7, 7.1 Hz, 1H), 3.37 (d, *J* = 5.4 Hz, 2H), 0.82 (t, *J* = 7.1 Hz, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 172.81, 172.00, 152.68, 143.15, 139.47, 139.45, 139.14, 137.13, 129.95, 129.57, 129.35, 129.04, 128.60, 128.19, 127.56, 127.06, 126.37, 125.19, 123.44, 107.87, 77.83, 67.07, 65.09, 63.89, 60.73, 49.83, 48.63, 47.77, 37.94. IR (neat): 2893, 1777, 1724, 1676, 1393, 1375 cm^{-1}. HRMS (ESI) *m/z* calcd for $C_{32}H_{30}NO_7^+$ [M+H]$^+$ 540.2017, found 540.2015.



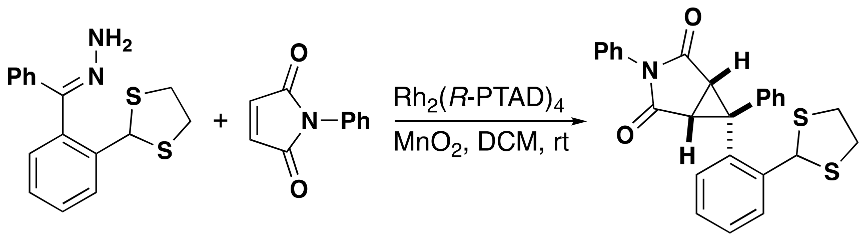
To a flame-dried round bottom flask were added 2-bromobenzaldehyde (0.6 mL, 5 mmol), ethane-1,2-dithiol (0.5 mL, 6 mmol), iodine (126.9 mg, 0.5 mmol) and chloroform (25 mL). The reaction was stirred under room temperature for 18 h. Upon full conversion determined by ^{1}H NMR, the reaction was quenched with 2 N NaOH aqueous solution and extracted with EtOAc (3 × 10 mL). The combined organic phases were washed with H_2O (1 × 10 mL) and brine (1 × 10 mL). The organic phase was dried over anhydrous Na_2SO_4, filtered and concentrated. The residue was further purified by flash column chromatography (hexane/EtOAc = 10:1, v/v) to obtain 2-(2-bromophenyl)-1,3-dithiolane as a colorless oil (quantitive yield). ^{1}H NMR (400 MHz, C_6D_6) δ 7.84 (dd, *J* = 7.9, 1.7 Hz, 1H), 7.25 (dd, *J* = 8.0, 1.3 Hz, 1H), 6.91 (td, *J* = 7.6, 1.3 Hz, 1H), 6.59 (td, *J* = 7.7, 1.7 Hz, 1H), 6.15 (s, 1H), 2.82 – 2.72 (m, 2H), 2.72 – 2.62 (m, 2H). ^{1}H NMR data was consistent with reported literature values.[9]



(2-(1,3-Dithiolan-2-yl)phenyl)(phenyl)methanone was synthesized according to General Procedure B, using 2-(2-bromophenyl)-1,3-dithiolane (1.04 g, 4 mmol), *n*-BuLi (2.5 M, 1.76 mL, 4.4 mmol), *N*-methoxy-*N*-methylbenzamide (0.99 g, 6 mmol) and THF (25 mL). The crude product was purified by flash column chromatography (hexane/EtOAc = 15:1, v/v) to obtain the ketone as a yellow oil (554.2 mg, 48%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.04 (d, *J* = 8.0 Hz, 1H), 7.83 (d, *J* = 8.3 Hz, 2H), 7.60 (t, *J* = 7.4 Hz, 1H), 7.55 – 7.42 (m, 3H), 7.35 – 7.26 (m, 2H), 5.84 (s, 1H), 3.52 – 3.41 (m, 2H), 3.35 – 3.24 (m, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 197.8, 140.5, 138.2, 137.6, 133.6, 131.0, 130.6, 129.5, 128.63, 128.60, 127.2, 52.5, 40.4. HRMS (ESI) *m/z* calcd for $C_{16}H_{15}OS_2^+$ $[M+H]^+$ 287.0559, found 287.0565.

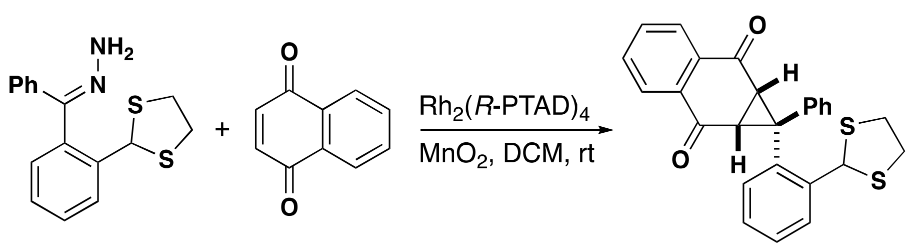


(*E*)-((2-(1,3-Dithiolan-2-yl)phenyl)(phenyl)methylene)hydrazine was synthesized according to General Procedure C, using (2-(1,3-dithiolan-2-yl)phenyl)(phenyl)methanone (344.4 mg, 1.2 mmol), N_2H_4 (0.49 mL, 15.6 mmol), HOAc (0.08 mL, 1.44 mmol) and EtOH (3.6 mL). After the reaction, the precipitated solid was filtered and washed with hexane. The product was then dried on the vacuum and obtained as a white solid (238.7 mg, 66%). m.p. 147-149 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.03 (dd, *J* = 7.9, 1.3 Hz, 1H), 7.54 – 7.37 (m, 4H), 7.36 – 7.27 (m, 3H), 7.08 (dd, *J* = 7.5, 1.4 Hz, 1H), 5.49 (s, 1H), 5.39 (s, 2H), 3.53 – 3.41 (m, 2H), 3.33 – 3.18 (m, 2H). ^{13}C NMR (101 MHz, CD_2Cl_2) δ 147.1, 140.8, 138.4, 132.3, 130.2, 130.0, 129.3, 128.9, 128.6, 128.5, 126.3, 52.4, 40.9, 40.7. HRMS (ESI) *m/z* calcd for $C_{16}H_{17}N_2S_2^+$ [M+H]$^+$ 301.0828, found 301.0832.



16a

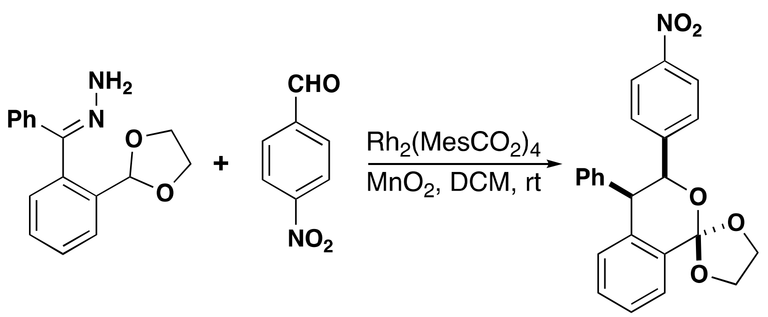
6-(2-(1,3-Dithiolan-2-yl)phenyl)-3,6-diphenyl-3-azabicyclo[3.1.0]hexane-2,4-dione was synthesized according to General Procedure G, using (*E*)-((2-(1,3-dithiolan-2-yl)phenyl)(phenyl)methylene)hydrazine (30.0 mg, 0.1 mmol), 1-phenyl-1*H*-pyrrole-2,5-dione (20.8 mg, 0.12 mmol), MnO_2 (69.6 mg, 0.8 mmol), Rh_2(*R*-PTAD)$_4$ (1.6 mg, 0.001 mmol) and DCM (6 mL). The crude product was purified by flash column chromatography (hexane/EtOAc = 4:1, v/v) to obtain **16a** as a white solid (35.6 mg, 80%, >95:5 dr). m.p. 192-194 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.95 (d, *J* = 8.0 Hz, 1H), 7.51 – 7.41 (m, 2H), 7.37 – 7.28 (m, 3H), 7.28 – 7.20 (m, 4H), 7.09 (d, *J* = 6.8 Hz, 2H), 6.45 – 6.36 (m, 2H), 6.11 (s, 1H), 3.74 (d, *J* = 5.4 Hz, 1H), 3.59 – 3.49 (m, 1H), 3.43 – 3.31 (m, 2H), 3.26 – 3.15 (m, 1H), 3.10 (d, *J* = 5.4 Hz, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 171.8, 171.4, 144.0, 139.6, 132.5, 131.3, 131.2, 130.6, 129.8, 129.09, 129.07, 128.6, 128.5, 128.2, 126.6, 126.4, 50.7, 47.1, 41.1, 40.7, 36.5, 34.6. IR (neat): 2921, 2852, 1707, 1375, 1170 cm^{-1}. HRMS (ESI) *m/z* calcd for $C_{26}H_{22}NO_2S_2^+$ [M+H]$^+$ 444.1086, found 444.1089.



16b

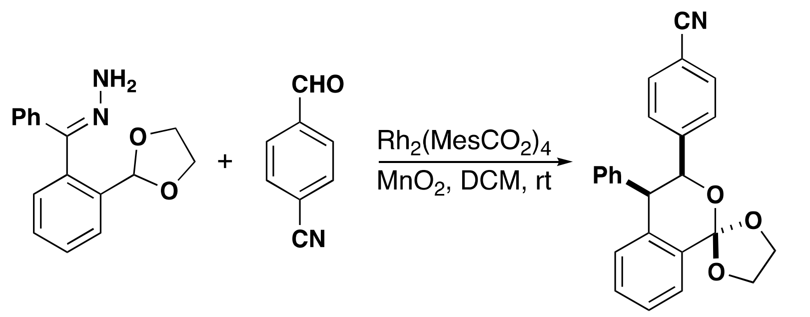
1-(2-(1,3-dithiolan-2-yl)phenyl)-1-phenyl-1a,7a-dihydro-1*H*-cyclopropa[*b*]naphthalene-2,7-dione was synthesized according to General Procedure G, using (*E*)-((2-(1,3-dithiolan-2-

yl)phenyl)(phenyl)methylene)hydrazine (30.0 mg, 0.1 mmol), naphthalene-1,4-dione (19.0 mg, 0.12 mmol), MnO_2 (69.6 mg, 0.8 mmol), Rh_2(*R*-PTAD)$_4$ (1.6 mg, 0.001 mmol) and DCM (6 mL). The crude product was purified by flash column chromatography (hexane/EtOAc = 8:1, v/v) to obtain **7b** as a white solid (30.7 mg, 72%, >95:5 dr). m.p. 167-169 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.85 – 7.76 (m, 2H), 7.54 (dd, *J* = 7.9, 1.4 Hz, 1H), 7.50 – 7.41 (m, 2H), 7.36 – 7.29 (m, 2H), 7.29 – 7.23 (m, 1H), 7.19 – 7.10 (m, 3H), 7.01 (td, *J* = 7.6, 1.4 Hz, 1H), 6.85 (td, *J* = 7.5, 1.4 Hz, 1H), 5.91 (s, 1H), 3.84 (d, *J* = 7.4 Hz, 1H), 3.54 – 3.45 (m, 1H), 3.41 – 3.28 (m, 2H), 3.24 – 3.16 (m, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 192.2, 191.6, 143.0, 141.7, 134.8, 133.9, 133.77, 133.75, 132.6, 131.4, 131.0, 129.0, 128.9, 127.9, 127.5, 126.8, 126.1, 51.2, 45.8, 42.6, 41.0, 40.6, 40.5. IR (neat): 2922, 1672, 1593, 1294, 750, 695 cm^{-1}. HRMS (ESI) *m/z* calcd for $C_{26}H_{21}O_2S_2^+$ $[M+H]^+$ 429.0977, found 429.0973.



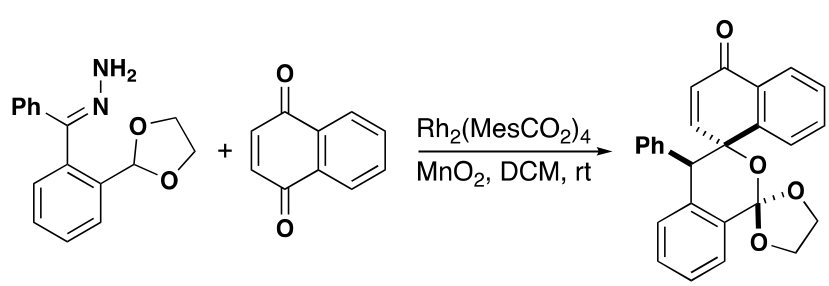
18a

(3*R*,4*S*)-3-(4-Nitrophenyl)-4-phenylspiro[isochromane-1,2'-[1,3]dioxolane] was synthesized according to General Procedure G, using (*E*)-((2-(1,3-dioxolan-2-yl)phenyl)(phenyl)methylene)hydrazine (26.8 mg, 0.1 mmol), 4-nitrobenzaldehyde (18.1 mg, 0.12 mmol), MnO_2 (69.6 mg, 0.8 mmol), $Rh_2(MesCO_2)_4$ (0.9 mg, 0.001 mmol) and DCM (6 mL). The crude product was purified by flash column chromatography (hexane/DCM = 1:1, v/v) to obtain **18a** as a pale yellow solid (26.1 mg, 67%, >95:5 dr). m.p. 198-200 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.02 (d, *J* = 8.8 Hz, 2H), 7.58 (dd, *J* = 7.5, 1.7 Hz, 1H), 7.38 – 7.28 (m, 2H), 7.21 (d, *J* = 8.8 Hz, 2H), 7.11 – 6.98 (m, 4H), 6.82 – 6.70 (m, 2H), 5.73 (d, *J* = 3.4 Hz, 1H), 4.55 – 4.45 (m, 1H), 4.37 (q, *J* = 7.3 Hz, 1H), 4.32 – 4.23 (m, 1H), 4.18 (t, *J* = 7.6 Hz, 1H), 4.14 (d, *J* = 3.5 Hz, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 147.1, 147.1, 139.1, 138.6, 131.8, 130.1, 130.0, 129.3, 128.0, 127.6, 127.0, 126.9, 123.1, 119.4, 75.9, 66.4, 64.4, 50.0. IR (neat): 2910, 1519, 1344, 1011, 764, 711, 697 cm^{-1}. HRMS (ESI) *m/z* calcd for $C_{23}H_{20}NO_5^+$ $[M+H]^+$ 390.1336, found 390.1338.



18b

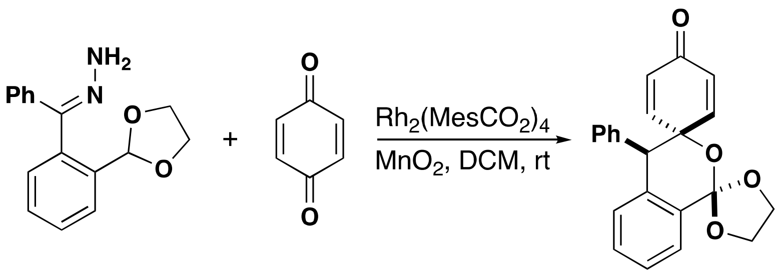
4-((3*R*,4*S*)-4-phenylspiro[isochromane-1,2'-[1,3]dioxolan]-3-yl)benzonitrile was synthesized according to General Procedure H, using (*E*)-((2-(1,3-dioxolan-2-yl)phenyl)(phenyl)methylene)hydrazine (26.8 mg, 0.1 mmol), 4-formylbenzonitrile (15.7 mg, 0.12 mmol), MnO_2 (69.6 mg, 0.8 mmol), $Rh_2(MesCO_2)_4$ (0.9 mg, 0.001 mmol) and DCM (6 mL). The crude product was purified by flash column chromatography (hexane/DCM = 1:3, v/v) to obtain **18b** as a white solid (22.7 mg, 61%, >95:5 dr). m.p. 289-291 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.58 (dd, *J* = 7.6, 1.7 Hz, 1H), 7.45 (d, *J* = 8.3 Hz, 2H), 7.38 – 7.28 (m, 2H), 7.15 (d, *J* = 8.1 Hz, 2H), 7.09 – 6.98 (m, 4H), 6.74 (dd, *J* = 7.5, 2.1 Hz, 2H), 5.67 (d, *J* = 3.4 Hz, 1H), 4.54 – 4.45 (m, 1H), 4.36 (q, *J* = 7.3 Hz, 1H), 4.31 – 4.23 (m, 1H), 4.16 (q, *J* = 7.6 Hz, 1H), 4.10 (d, *J* = 3.5 Hz, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 145.1, 139.2, 138.6, 131.9, 131.7, 130.1, 130.0, 129.3, 127.9, 127.6, 127.0, 126.9, 126.8, 119.4, 119.0, 111.0, 76.0, 66.4, 64.3, 50.0. IR (neat): 2888, 2225, 1068, 1019, 945, 765, 739 cm^{-1}. HRMS (ESI) *m/z* calcd for $C_{24}H_{20}NO_3^+$ $[M+H]^+$ 370.1438, found 370.1437.



18c

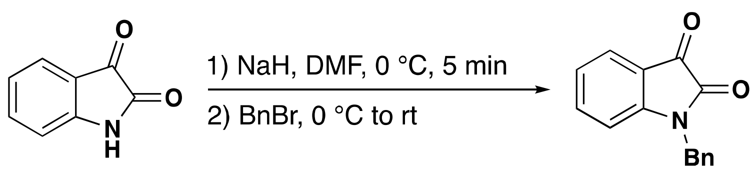
(1*S*,4'*R*)-4'-Phenyl-4*H*-dispiro[naphthalene-1,3'-isochromane-1',2''-[1,3]dioxolan]-4-one was synthesized according to General Procedure G, using (*E*)-((2-(1,3-dioxolan-2-yl)phenyl)(phenyl)methylene)hydrazine (26.8 mg, 0.1 mmol), naphthalene-1,4-dione (19.0 mg, 0.12 mmol), MnO_2 (69.6 mg, 0.8 mmol), $Rh_2(MesCO_2)_4$ (0.9 mg, 0.001 mmol) and DCM (6 mL). The crude product was purified by flash column chromatography (hexane/EtOAc = 5:1, v/v) to obtain **18c** as a white solid (37.5 mg, 95%, >95:5 dr). m.p. 190-192 °C. ^{1}H NMR (400 MHz, CD_2Cl_2)

δ 7.91 (d, *J* = 7.8 Hz, 1H), 7.69 (d, *J* = 7.8 Hz, 1H), 7.61 (d, *J* = 10.5 Hz, 1H), 7.42 (t, *J* = 8.0 Hz, 1H), 7.38 – 7.25 (m, 2H), 7.19 – 6.99 (m, 4H), 6.96 (d, *J* = 7.7 Hz, 1H), 6.72 (d, *J* = 8.0 Hz, 1H), 6.61 (d, *J* = 7.5 Hz, 2H), 6.22 (d, *J* = 10.5 Hz, 1H), 4.50 – 4.40 (m, 1H), 4.40 – 4.23 (m, 3H), 4.17 (s, 1H). ^{13}C NMR (101 MHz, CD_2Cl_2) δ 184.1, 151.5, 143.2, 138.7, 137.2, 133.2, 131.6, 131.0, 130.4, 128.8, 128.2, 128.04, 127.98, 127.9, 127.5, 126.5, 125.9, 119.0, 77.2, 66.2, 65.0, 56.7. IR (neat): 2913, 1668, 1301, 1043, 1005, 948 cm^{-1}. HRMS (ESI) *m/z* calcd for $C_{26}H_{21}O_4^+$ [M+H]$^+$ 397.1434, found 397.1429.

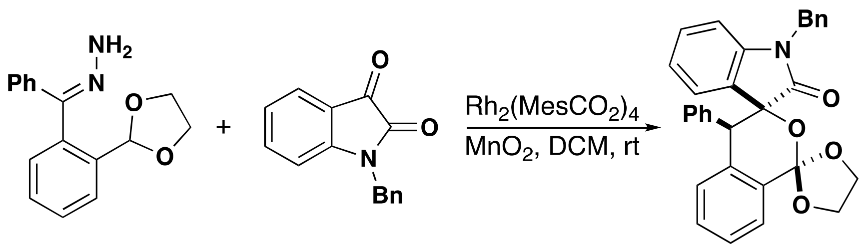


18d

(*S*)-4'-Phenyldispiro[cyclohexane-1,3'-isochromane-1',2''-[1,3]dioxolane]-2,5-dien-4-one was synthesized according to General Procedure G, using (*E*)-((2-(1,3-dioxolan-2-yl)phenyl)(phenyl)methylene)hydrazine (26.8 mg, 0.1 mmol), benzoquinone (13.0 mg, 0.12 mmol), MnO_2 (69.6 mg, 0.8 mmol), $Rh_2(MesCO_2)_4$ (0.9 mg, 0.001 mmol) and DCM (6 mL). The crude product was purified by flash column chromatography (hexane/EtOAc = 7:1, v/v) to obtain **18d** as a white solid (32.5 mg, 94%). m.p. 198-200 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.55 (d, *J* = 7.6 Hz, 1H), 7.39 – 7.20 (m, 6H), 7.19 – 7.10 (m, 2H), 6.96 (d, *J* = 7.6 Hz, 1H), 6.54 (dd, *J* = 10.5, 3.2 Hz, 1H), 6.18 – 6.02 (m, 2H), 4.40 – 4.32 (m, 1H), 4.32 – 4.23 (m, 3H), 4.10 (s, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 185.2, 148.9, 147.8, 138.8, 137.0, 131.5, 130.3, 130.2, 128.79, 128.76, 128.5, 128.3, 127.8, 127.7, 127.2, 117.9, 74.0, 65.7, 64.9, 52.9. IR (neat): 2910, 1669, 1631, 1322, 1004, 949 cm^{-1}. HRMS (ESI) *m/z* calcd for $C_{22}H_{19}O_4^+$ [M+H]$^+$ 347.1278, found 347.1282.

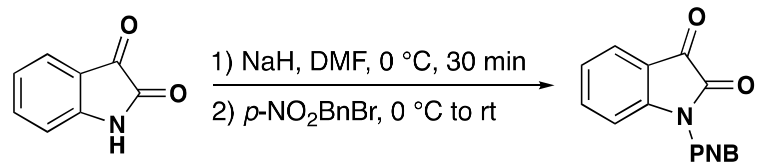


To a flame-dried round bottom flask were added indoline-2,3-dione (441.4 mg, 3 mmol) and DMF (15 mL). NaH (60%, 144 mg, 3.6 mmol) was added at 0 °C. After the mixture was stirred at 0 °C for 5 min, (bromomethyl)benzene (0.39 mL, 3.3 mmol) was added. The reaction was then stirred for another 30 min. After quenched with saturated NH_4Cl aqueous, the reaction was extracted with EtOAc (3 × 10 mL). The combined organic phases were washed with H_2O (1 × 10 mL) and brine (1 × 10 mL). The organic phase was dried over anhydrous Na_2SO_4, filtered and concentrated. The residue was further purified by flash column chromatography (hexane/EtOAc = 3:1, v/v) to obtain the product as an orange solid (632.0 mg, 89%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.61 (d, *J* = 7.5 Hz, 1H), 7.48 (td, *J* = 7.8, 1.4 Hz, 1H), 7.41 – 7.27 (m, 5H), 7.09 (t, *J* = 7.4 Hz, 1H), 6.78 (d, *J* = 7.9 Hz, 1H), 4.93 (s, 2H). ^{1}H NMR data was consistent with reported literature values.[10]

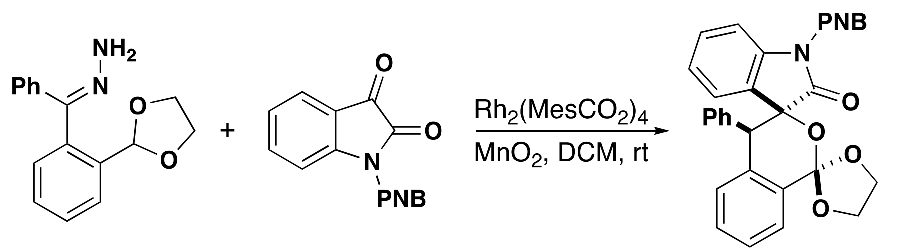


18e

(3*R*,4'*S*)-1-Benzyl-4'-phenyldispiro[indoline-3,3'-isochromane-1',2''-[1,3]dioxolan]-2-one was synthesized according to General Procedure G, using (*E*)-((2-(1,3-dioxolan-2-yl)phenyl)(phenyl)methylene)hydrazine (26.8 mg, 0.1 mmol), 1-benzylindoline-2,3-dione (28.5 mg, 0.12 mmol), MnO_2 (69.6 mg, 0.8 mmol), $Rh_2(MesCO_2)_4$ (0.9 mg, 0.001 mmol) and DCM (6 mL). The crude product was purified by flash column chromatography (DCM/EtOAc = 5:1, v/v) to obtain **18e** as a white solid (45.8 mg, 96%, >95:5 dr). m.p. 178-180 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.69 (dd, *J* = 7.7, 1.4 Hz, 1H), 7.42 (t, *J* = 7.5 Hz, 2H), 7.37 – 7.26 (m, 3H), 7.16 – 7.01 (m, 4H), 6.94 (d, *J* = 7.8 Hz, 2H), 6.78 (td, *J* = 7.6, 1.0 Hz, 1H), 6.62 (dd, *J* = 7.6, 1.3 Hz, 1H), 6.45 (d, *J* = 7.0 Hz, 2H), 6.37 (s, 1H), 6.30 (d, *J* = 7.8 Hz, 1H), 5.20 (s, 1H), 5.04 (d, *J* = 16.0 Hz, 1H), 4.52 – 4.42 (m, 1H), 4.35 – 4.17 (m, 4H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 173.9, 143.2, 136.7, 135.0, 134.5, 133.6, 133.5, 129.9, 129.7, 129.4, 129.1, 128.7, 127.9, 127.7, 127.44, 127.42, 127.2, 126.5, 126.3, 125.5, 122.5, 118.5, 109.5, 81.6, 65.5, 64.7, 50.0, 43.9. IR (neat): 2922, 1726, 1608, 1466, 1364, 1318, 1066, 987, 752 cm^{-1}. HRMS (ESI) *m/z* calcd for $C_{31}H_{26}NO_4^+$ $[M+H]^+$ 476.1856, found 476.1874.

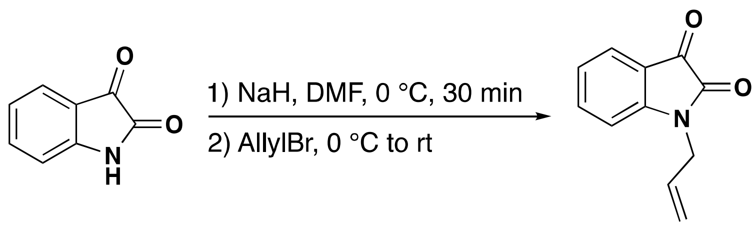


To a flame-dried round bottom flask were added indoline-2,3-dione (735.7 mg, 5 mmol) and DMF (10 mL). NaH (60%, 220 mg, 5.5 mmol) was added at 0 °C. After the mixture was stirred at 0 °C for 30 min, 1-(bromomethyl)-4-nitrobenzene (1.3 g, 6 mmol) was added. The reaction was then allowed to warm to room temperature and stirred overnight. After quenched with H_2O, an orange solid precipitated. It was then collected and washed with H_2O and EtOAc. After dried under reduced pressure, the product was obtained as an orange solid (820.9 mg, 58%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.23 (d, *J* = 8.7 Hz, 2H), 7.67 (dd, *J* = 7.5, 1.4 Hz, 1H), 7.59 – 7.45 (m, 3H), 7.16 (t, *J* = 7.6 Hz, 1H), 6.72 (d, *J* = 7.9 Hz, 1H), 5.04 (s, 2H). ^{1}H NMR data was consistent with reported literature values.[11]

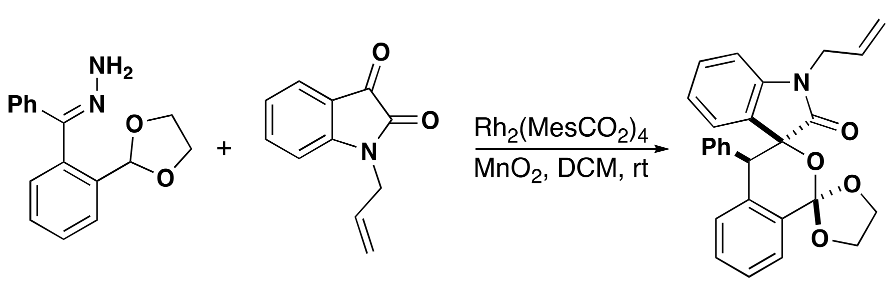


18f

(3*S*,4'*R*)-1-(4-Nitrobenzoyl)-4'-phenyldispiro[indoline-3,3'-isochromane-1',2''-[1,3]dioxolan]-2-one was synthesized according to General Procedure G, using (*E*)-((2-(1,3-dioxolan-2-yl)phenyl)(phenyl)methylene)hydrazine (26.8 mg, 0.1 mmol), 1-(4-nitrobenzyl)indoline-2,3-dione (33.9 mg, 0.12 mmol), MnO_2 (69.6 mg, 0.8 mmol), $Rh_2(MesCO_2)_4$ (0.9 mg, 0.001 mmol) and DCM (6 mL). The crude product was purified by flash column chromatography (DCM) to obtain **18f** as a pale yellow solid (45.6 mg, 88%, >95:5 dr). m.p. 261-263 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.92 (d, *J* = 8.2 Hz, 2H), 7.70 (d, *J* = 7.7 Hz, 1H), 7.53 – 7.30 (m, 5H), 7.08 (t, *J* = 7.7 Hz, 1H), 6.99 (s, 1H), 6.92 (d, *J* = 7.7 Hz, 1H), 6.84 (t, *J* = 7.6 Hz, 1H), 6.65 (d, *J* = 7.5 Hz, 1H), 6.50 (d, *J* = 8.3 Hz, 2H), 6.36 (s, 1H), 6.22 (d, *J* = 7.9 Hz, 1H), 5.32 – 5.09 (m, 2H), 4.58 – 4.41 (m, 1H), 4.41 – 4.16 (m, 4H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 174.0, 147.3, 142.6, 142.5, 136.4, 134.4, 133.6, 130.1, 129.8, 129.5, 129.2, 128.1, 127.9, 127.6, 127.3, 127.2, 126.6, 125.5, 124.0, 123.0, 118.5, 108.9, 81.5, 65.5, 64.8, 50.0, 43.3. IR (neat): 2890, 1729, 1519, 1340, 1066, 751, 709 cm^{-1}. HRMS (ESI) *m/z* calcd for $C_{31}H_{25}N_2O_6^+$ $[M+H]^+$ 521.1707, found 521.1709.



To a flame-dried round bottom flask were added indoline-2,3-dione (735.7 mg, 5 mmol) and DMF (10 mL). NaH (60%, 220 mg, 5.5 mmol) was added at 0 °C. After the mixture was stirred at 0 °C for 30 min, 3-bromoprop-1-ene (0.52 mL, 6 mmol) was added. The reaction was then allowed to warm to room temperature and stirred overnight. After quenched with H_2O, the reaction was extracted with EtOAc (3 × 10 mL). The combined organic phases were washed with H_2O (1 × 10 mL) and brine (1 × 10 mL). The organic phase was dried over anhydrous Na_2SO_4, filtered and concentrated. The residue was further purified by flash column chromatography (hexane/EtOAc = 2:1, v/v) to obtain the product as a red solid (812.1 mg, 87%). ^1H NMR (400 MHz, $CDCl_3$) δ 7.62 (dd, *J* = 7.3, 1.3 Hz, 1H), 7.57 (td, *J* = 7.8, 1.4 Hz, 1H), 7.13 (td, *J* = 7.6, 0.9 Hz, 1H), 6.90 (d, *J* = 7.9 Hz, 1H), 5.85 (ddt, *J* = 17.2, 10.5, 5.4 Hz, 1H), 5.42 – 5.26 (m, 2H), 4.42 – 4.31 (m, 2H). ^1H NMR data was consistent with reported literature values.[12]



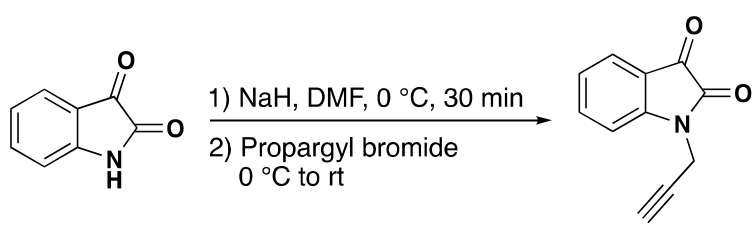
18g

(3*S*,4'*R*)-1-Allyl-4'-phenyldispiro[indoline-3,3'-isochromane-1',2''-[1,3]dioxolan]-2-one was synthesized according to General Procedure G, using (*E*)-((2-(1,3-dioxolan-2-yl)phenyl)(phenyl)methylene)hydrazine (26.8 mg, 0.1 mmol), 1-allylindoline-2,3-dione (22.5 mg, 0.12 mmol), MnO_2 (69.6 mg, 0.8 mmol), $Rh_2(MesCO_2)_4$ (0.9 mg, 0.001 mmol) and DCM (6 mL). The crude product was purified by flash column chromatography (DCM/EtOAc = 15:1, v/v) to obtain **18g** as a pale yellow solid (38.0 mg, 89%, >95:5 dr). m.p. 175-176 °C. ^1H NMR (400 MHz,

CD_2Cl_2) δ 7.66 (dd, *J* = 7.7, 1.4 Hz, 1H), 7.43 (t, *J* = 7.6 Hz, 1H), 7.40 – 7.08 (m, 5H), 6.92 (d, *J* = 7.8 Hz, 2H), 6.80 (td, *J* = 7.6, 1.0 Hz, 1H), 6.67 (dd, *J* = 7.6, 1.3 Hz, 1H), 6.52 (d, *J* = 7.8 Hz, 1H), 6.33 (s, 1H), 5.32 – 5.21 (m, 1H), 4.97 (s, 1H), 4.84 (dd, *J* = 10.4, 1.4 Hz, 1H), 4.44 – 4.33 (m, 2H), 4.33 – 4.16 (m, 4H), 3.79 (ddt, *J* = 16.6, 5.4, 1.7 Hz, 1H). ^{13}C NMR (101 MHz, CD_2Cl_2) δ 173.3, 143.6, 136.9, 134.9, 133.8, 131.07, 131.05, 130.1, 129.9, 128.1, 127.72, 127.65, 127.0, 126.8, 126.3, 122.3, 118.8, 116.8, 109.3, 81.8, 65.6, 65.2, 50.6, 42.4. IR (neat): 2903, 1728, 1609, 1369, 1177, 1063, 1020, 750, 713 cm^{-1}. HRMS (ESI) *m/z* calcd for $C_{27}H_{24}NO_4^+$ $[M+H]^+$ 426.1700, found 426.1706.

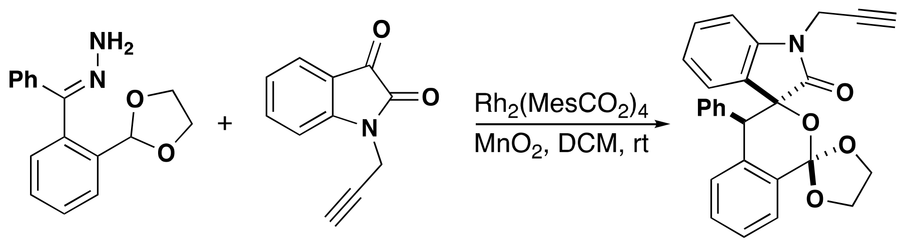
Scale-up reaction

To a flame-dried round bottom flask were added (*E*)-((2-(1,3-dioxolan-2-yl)phenyl)(phenyl)methylene)hydrazine (134.2 mg, 0.5 mmol), 1-allylindoline-2,3-dione (112.3 mg, 0.6 mmol), MnO_2 (347.8 mg, 4.0 mmol), $Rh_2(MesCO_2)_4$ (4.3 mg, 0.005 mmol) and DCM (30 mL). After filtration of MnO_2, the reaction was concentrated. dr was determined as >95:5 by ^1H NMR of residue. After flash column chromatography (DCM/EtOAc = 15:1, v/v), the desired product was obtained as a pale yellow solid (201.1 mg, 95%, >95:5 dr).



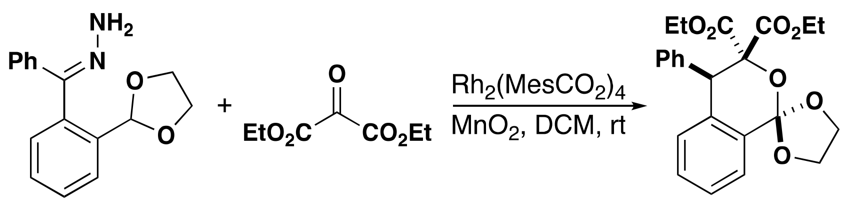
To a flame-dried round bottom flask were added indoline-2,3-dione (735.7 mg, 5 mmol) and DMF (10 mL). NaH (60%, 220 mg, 5.5 mmol) was added at 0 °C. After the mixture was stirred at 0 °C for 30 min, 3-bromoprop-1-yne (80% in toluene, 892.2 mg, 6 mmol) was added. The reaction was then allowed to warm to room temperature and stirred overnight. After quenched with H_2O, the reaction was extracted with EtOAc (3 × 10 mL). The combined organic phases were washed with H_2O (1 × 10 mL) and brine (1 × 10 mL). The organic phase was dried over anhydrous Na_2SO_4, filtered and concentrated. The residue was further purified by flash column chromatography (hexane/EtOAc = 1:1, v/v) to obtain the product as an orange solid (825.3 mg, 89%). ^1H NMR (400 MHz, $CDCl_3$) δ 7.71 – 7.60 (m, 2H), 7.19 (dd, *J* = 7.5, 0.9 Hz, 1H), 7.14 (dd, *J* =

8.3, 0.9 Hz, 1H), 4.54 (d, *J* = 2.6 Hz, 2H), 2.31 (s, 1H). ^{1}H NMR data was consistent with reported literature values.[13]



18h

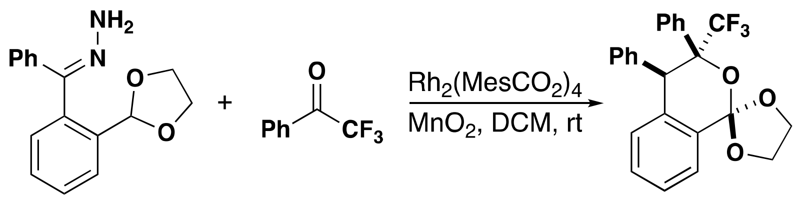
(3*S*,4'*R*)-4'-Phenyl-1-(prop-2-yn-1-yl)dispiro[indoline-3,3'-isochromane-1',2''-[1,3]dioxolan]-2-one was synthesized according to General Procedure G, using (*E*)-((2-(1,3-dioxolan-2-yl)phenyl)(phenyl)methylene)hydrazine (26.8 mg, 0.1 mmol), 1-(prop-2-yn-1-yl)indoline-2,3-dione (22.2 mg, 0.12 mmol), MnO_2 (69.6 mg, 0.8 mmol), $Rh_2(MesCO_2)_4$ (0.9 mg, 0.001 mmol) and DCM (6 mL). The crude product was purified by flash column chromatography (DCM/EtOAc = 5:1, v/v) to obtain **18h** as a white solid (36.4 mg, 86%, >95:5 dr). m.p. 199-201 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.68 (dd, *J* = 7.8, 1.4 Hz, 1H), 7.41 (t, *J* = 7.6 Hz, 1H), 7.32 (td, *J* = 7.6, 1.4 Hz, 1H), 7.29 – 7.15 (m, 3H), 7.12 (t, *J* = 8.0 Hz, 1H), 6.98 (d, *J* = 7.8 Hz, 1H), 6.90 (s, 1H), 6.84 (t, *J* = 7.6 Hz, 1H), 6.72 (d, *J* = 7.8 Hz, 1H), 6.62 (d, *J* = 7.6 Hz, 1H), 6.33 (s, 1H), 5.00 (s, 1H), 4.48 – 4.40 (m, 1H), 4.33 – 4.20 (m, 3H), 4.20 – 4.08 (m, 2H), 1.99 (t, *J* = 2.5 Hz, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 172.9, 141.9, 136.3, 134.3, 133.4, 129.9, 129.7, 127.7, 127.5, 127.4, 126.9, 126.4, 125.7, 122.7, 118.4, 109.0, 81.7, 76.3, 72.1, 65.4, 64.8, 50.3, 29.0. IR (neat): 2891, 1728, 1609, 1466, 1066, 987, 753, 708 cm^{-1}. HRMS (ESI) *m/z* calcd for $C_{27}H_{22}NO_4^+$ [M+H]$^+$ 424.1543, found 424.1548.



18i

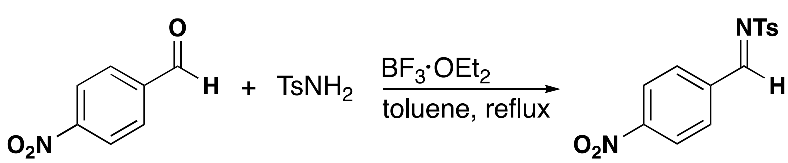
Diethyl (*S*)-4-phenylspiro[isochromane-1,2'-[1,3]dioxolane]-3,3-dicarboxylate was synthesized according to General Procedure H, using (*E*)-((2-(1,3-dioxolan-2-yl)phenyl)(phenyl)methylene)hydrazine (26.8 mg, 0.1 mmol), diethyl 2-oxomalonate (18 µL, 0.12 mmol), MnO_2 (69.6 mg, 0.8 mmol), $Rh_2(MesCO_2)_4$ (0.9 mg, 0.001 mmol) and DCM (6 mL).

The crude product was purified by flash column chromatography (DCM/EtA = 5:1, v/v) to obtain **18i** as a white solid (32.9 mg, 80%). m.p. 149-151 °C. ^1H NMR (400 MHz, CD_2Cl_2) δ 7.45 – 7.40 (m, 1H), 7.34 – 7.26 (m, 2H), 7.26 – 7.12 (m, 5H), 7.10 – 7.02 (m, 1H), 4.72 (s, 1H), 4.60 – 4.50 (m, 1H), 4.36 – 4.18 (m, 4H), 4.16 – 4.07 (m, 1H), 4.04 – 3.93 (m, 1H), 3.89 – 3.78 (m, 1H), 1.25 (t, *J* = 7.0 Hz, 3H), 1.07 (t, *J* = 7.1 Hz, 3H). ^{13}C NMR (101 MHz, CD_2Cl_2) δ 168.7, 166.4, 139.7, 138.2, 130.6, 130.0, 129.8, 129.1, 128.6, 127.8, 127.4, 126.9, 118.6, 83.4, 66.9, 64.6, 62.4, 62.1, 46.7, 14.03, 13.99. IR (neat): 2918, 1774, 1745, 1241, 1066, 1046 cm^{-1}. HRMS (ESI) *m/z* calcd for $C_{23}H_{25}O_7^+$ $[M+H]^+$ 413.1595, found 413.1585.

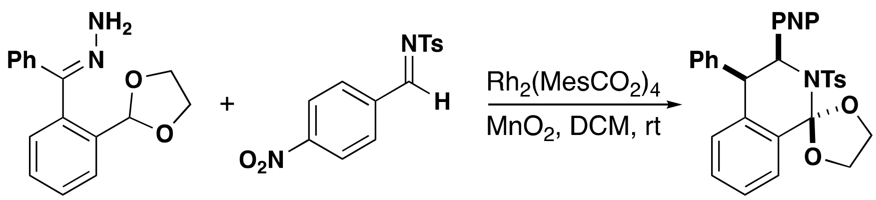


18j

(3*R*,4*S*)-3,4-Diphenyl-3-(trifluoromethyl)spiro[isochromane-1,2'-[1,3]dioxolane] was synthesized according to General Procedure G, using (*E*)-((2-(1,3-dioxolan-2-yl)phenyl)(phenyl)methylene)hydrazine (26.8 mg, 0.1 mmol), 2,2,2-trifluoro-1-phenylethan-1-one (17 µL, 0.12 mmol), MnO_2 (69.6 mg, 0.8 mmol), $Rh_2(MesCO_2)_4$ (0.9 mg, 0.001 mmol) and DCM (6 mL). The crude product was purified by flash column chromatography (DCM/hexane = 1:1, v/v) to obtain **18j** as a white solid (19.6 mg, 48%, >95:5 dr). m.p. 133-135 °C. ^1H NMR (400 MHz, $CDCl_3$) δ 7.59 – 7.52 (m, 1H), 7.45 (d, *J* = 7.5 Hz, 2H), 7.33 – 7.26 (m, 2H), 7.20 – 7.09 (m, 6H), 7.06 – 6.98 (m, 2H), 6.98 – 6.92 (m, 1H), 4.77 (s, 1H), 4.67 – 4.59 (m, 1H), 4.58 – 4.49 (m, 1H), 4.46 – 4.36 (m, 2H). ^{19}F NMR (376 MHz, $CDCl_3$) δ -72.61. ^{13}C NMR (101 MHz, $CDCl_3$) δ 139. 9, 137.0, 136.4, 130.1, 129.9, 129.7, 128.3, 128.2, 128.0, 127.5 (q, $^3J_{C-F}$ = 2 Hz), 127.4, 127.3, 126.8, 126.7, 125.0 (q, $^1J_{C-F}$ = 290 Hz), 118.6, 81.5 (q, $^2J_{C-F}$ = 30 Hz), 65.7, 64.8, 47.3. IR (neat): 2905, 1333, 1240, 1150, 1015, 948, 756, 700, 691 cm^{-1}. HRMS (ESI) *m/z* calcd for $C_{24}H_{20}F_3O_3^+$ $[M+H]^+$ 413.1359, found 413.1363.

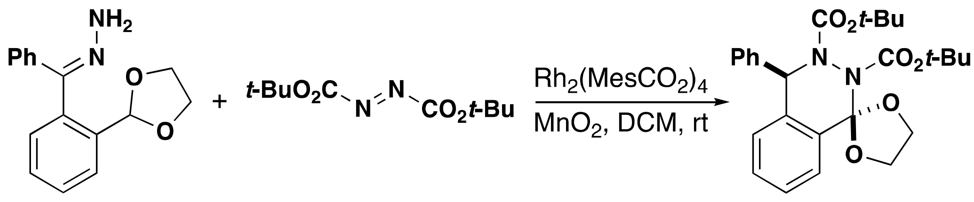


To a flame-dried round bottom flask equipped were added 4-nitrobenzaldehyde (1.96 g, 13 mmol), 4-methylbenzenesulfonamide (1.7 g, 10 mmol) and toluene (30 mL). After $BF_3·OEt_2$ was added at room temperature, the mixture was stirred in refluxing toluene with a Dean-Stark trap overnight. After completion of the reaction monitored by TLC, the reaction was allowed to cool down to room temperature, and solid precipitated. The solid was collected and washed with hexane and DCM. After dried under reduced pressure, the desired product was obtained as a pale yellow solid (2.7 g, 89%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.11 (s, 1H), 8.33 (d, J = 8.8 Hz, 2H), 8.17 – 8.03 (m, 2H), 7.91 (d, J = 8.3 Hz, 2H), 7.38 (d, J = 7.9 Hz, 2H), 2.46 (s, 3H). ^{1}H NMR data was consistent with reported literature values.[14]



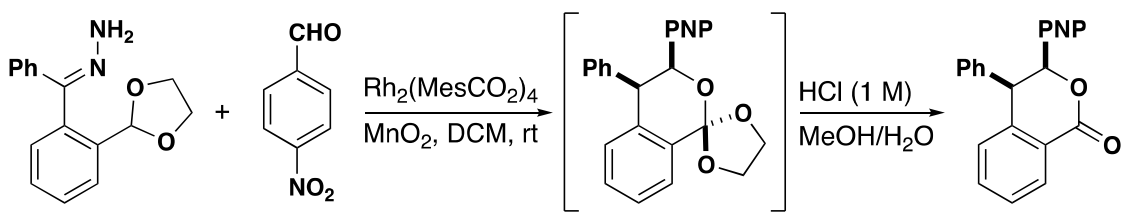
18k

(3*R*,4*S*)-3-(4-Nitrophenyl)-4-phenyl-2-tosyl-3,4-dihydro-2*H*-spiro[isoquinoline-1,2'-[1,3]dioxolane] was synthesized according to General Procedure H, using (*E*)-((2-(1,3-dioxolan-2-yl)phenyl)(phenyl)methylene)hydrazine (26.8 mg, 0.1 mmol), (*E*)-4-methyl-*N*-(4-nitrobenzylidene)benzenesulfonamide (36.5 mg, 0.12 mmol), MnO_2 (69.6 mg, 0.8 mmol), $Rh_2(MesCO_2)_4$ (0.9 mg, 0.001 mmol) and DCM (6 mL). The crude product was purified by flash column chromatography (hexane/DCM = 1:2 to 0:1, v/v) to obtain **18k** as a white solid (41.1 mg, 76%, 90:10 dr). m.p. 111-113 °C. ^{1}H NMR (400 MHz, CD_2Cl_2) δ 7.69 (d, J = 8.8 Hz, 2H), 7.54 (dd, J = 7.8, 1.4 Hz, 1H), 7.41 – 7.33 (m, 1H), 7.33 – 7.25 (m, 3H), 7.25 – 7.15 (m, 3H), 7.01 (d, J = 8.1 Hz, 2H), 6.92 (d, J = 7.7 Hz, 1H), 6.68 (d, J = 7.2 Hz, 2H), 6.54 (d, J = 8.8 Hz, 2H), 5.51 (d, J = 5.5 Hz, 1H), 5.11 (d, J = 5.5 Hz, 1H), 4.74 (dt, J = 8.2, 6.8 Hz, 1H), 4.58 – 4.49 (m, 1H), 4.40 (ddd, J = 7.4, 6.6, 4.2 Hz, 1H), 3.94 (q, J = 7.7 Hz, 1H), 2.30 (s, 3H). ^{13}C NMR (101 MHz, CD_2Cl_2) δ 147.6, 145.7, 143.8, 139.4, 138.2, 135.7, 134.7, 131.6, 130.9, 129.5, 129.1, 128.5, 128.4, 127.74, 127.71, 127.6, 123.5, 122.5, 114.1, 67.6, 64.8, 63.6, 50.2, 21.5. IR (neat): 2917, 1518, 1344, 1166, 1072, 949, 856, 707 cm^{-1}. HRMS (ESI) m/z calcd for $C_{30}H_{27}N_2O_6S^+$ [M+H]$^+$ 543.1584, found 543.1593.



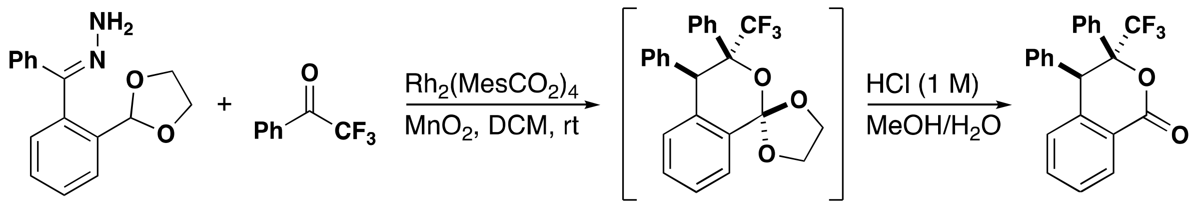
18l

To a flame-dried round bottom flask were added (*E*)-((2-(1,3-dioxolan-2-yl)phenyl)(phenyl)methylene)hydrazine (53.7 mg, 0.2 mmol), di-*tert*-butyl (*E*)-diazene-1,2-dicarboxylate (55.3 mg, 0.24 mmol), MnO_2 (139.1 mg, 1.6 mmol), $Rh_2(MesCO_2)_4$ (1.7 mg, 0.002 mmol) and DCM (12 mL). The reaction was stirred at room temperature for 24 h. After filtration of MnO_2 over celite, the crude product was purified by flash column chromatography (hexane/EtOAc = 5:1, v/v) to obtain **18l** as a white solid (76.6 mg, 82%). m.p. 192-194 °C. ^{1}H NMR (500 MHz, DMSO, 353 K) δ 7.56 (d, *J* = 7.0 Hz, 1H), 7.46 – 7.26 (m, 5H), 7.19 – 7.09 (m, 2H), 7.05 (d, *J* = 7.5 Hz, 1H), 6.39 (s, 1H), 4.53 – 4.44 (m, 1H), 4.34 (s, 1H), 4.27 – 4.14 (m, 2H), 1.45 (s, 9H), 1.05 (s, 9H). ^{13}C NMR (126 MHz, DMSO, 353 K) δ 150.4, 139.1, 135.7, 132.2, 128.64, 128.58, 127.6, 127.1, 127.0, 126.3, 126.2, 110.0, 79.8, 79.1, 67.1, 64.9, 56.4, 27.6, 27.0. IR (neat): 2967, 1729, 1695, 1348, 1128, 1075, 932, 758, 709 cm^{-1}. HRMS (ESI) *m/z* calcd for $C_{26}H_{33}N_2O_6^+$ [M+H]$^+$ 469.2333, found 469.2336.



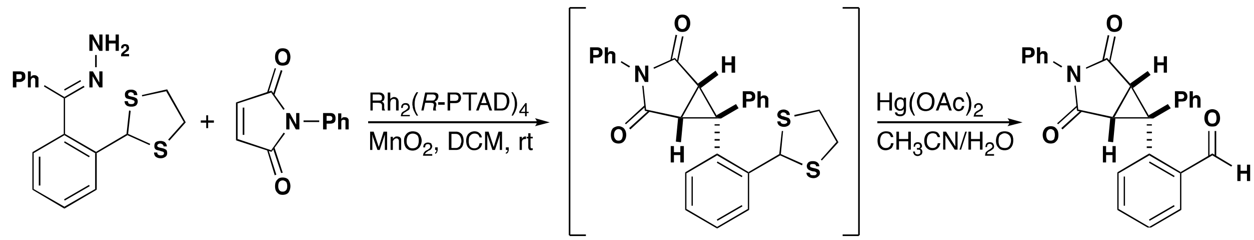
21a

(3*R*,4*S*)-3-(4-Nitrophenyl)-4-phenylisochroman-1-one (**21a**). According to General Procedure G, Diels-Alder reaction was stirred for 24 h using (*E*)-((2-(1,3-dioxolan-2-yl)phenyl)(phenyl)methylene)hydrazine (26.8 mg, 0.1 mmol), 4-nitrobenzaldehyde (18.1 mg, 0.12 mmol), MnO_2 (69.6 mg, 0.8 mmol), $Rh_2(MesCO_2)_4$ (0.9 mg, 0.001 mmol) and DCM (6 mL). After filtrating MnO_2, the solvent was removed under reduced pressure. The residue was dissolved in MeOH (2 mL) and H_2O (0.4 mL). 1 M HCl (0.3 mL) was then added and the reaction was allowed to stir at room temperature for another 24 h. After quenched with sat. $NaHCO_3$ aq., the reaction was extracted with ethyl acetate (3 × 5 mL). The combined organic phase was washed with H_2O (5 mL) and brine (5 mL), respectively. After dried over Na_2SO_4, the product was purified by flash column chromatography (hexane/DCM = 1:5, v/v) as a white solid (17.9 mg, 52%, >95:5 dr). m.p. 220-222 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.31 (d, *J* = 7.9 Hz, 1H), 8.10 (d, *J* = 8.7 Hz, 2H), 7.63 (td, *J* = 7.5, 1.5 Hz, 1H), 7.54 (t, *J* = 7.6 Hz, 1H), 7.29 (t, *J* = 8.7 Hz, 3H), 7.18 – 7.02 (m, 3H), 6.63 (d, *J* = 7.2 Hz, 2H), 6.05 (d, *J* = 3.5 Hz, 1H), 4.38 (d, *J* = 3.5 Hz, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 165.1, 147.7, 144.0, 141.7, 135.1, 134.9, 130.7, 129.3, 128.8, 128.5, 128.4, 127.9, 127.3, 124.9, 123.5, 81.3, 50.2. IR (neat): 2921, 1714, 1520, 1346, 1272, 1122, 1089 cm^{-1}. HRMS (ESI) *m/z* calcd for $C_{21}H_{16}NO_4^+$ $[M+H]^+$ 346.1074, found 346.1076.



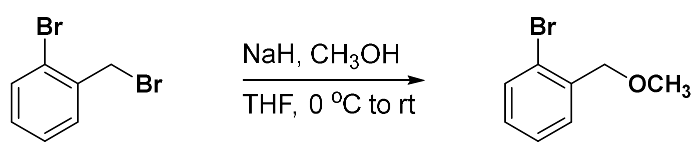
21b

(3*R*,4*S*)-3,4-Diphenyl-3-(trifluoromethyl)isochroman-1-one (**21b**). According to General Procedure G, Diels-Alder reaction was stirred for 24 h using (*E*)-((2-(1,3-dioxolan-2-yl)phenyl)(phenyl)methylene)hydrazine (26.8 mg, 0.1 mmol), 2,2,2-trifluoro-1-phenylethan-1-one (17 µL, 0.12 mmol), MnO_2 (69.6 mg, 0.8 mmol), $Rh_2(MesCO_2)_4$ (0.9 mg, 0.001 mmol) and DCM (6 mL). After filtrating MnO_2, the solvent was removed under reduced pressure. The residue was dissolved in MeOH (2 mL) and H_2O (0.4 mL). 1 M HCl (0.3 mL) was then added and the reaction was allowed to stir at room temperature for another 20 h. After quenched with sat. $NaHCO_3$ aq., the reaction was extracted with ethyl acetate (3 × 5 mL). The combined organic phase was washed with H_2O (5 mL) and brine (5 mL), respectively. After dried over Na_2SO_4, the product was purified by flash column chromatography (hexane/EtOAc = 5:1, v/v) as a white solid (20.5 mg, 56%, >95:5 dr). m.p. 164-166 °C.^{1}H NMR (400 MHz, $CDCl_3$) δ 8.24 (d, *J* = 7.8 Hz, 1H), 7.60 – 7.48 (m, 3H), 7.47 – 7.38 (m, 1H), 7.30 (d, *J* = 7.7 Hz, 1H), 7.25 – 7.13 (m, 3H), 7.08 – 6.96 (m, 3H), 6.96 – 6.85 (m, 2H), 4.91 (s, 1H). ^{19}F NMR (376 MHz, $CDCl_3$) δ -72.89. ^{13}C NMR (201 MHz, $CDCl_3$) δ 162.9, 140.1, 138.3, 135.0, 133.9, 130.2, 128.72, 128.71, 128.3, 128.2, 128.1, 127.4, 126.4, 124.6 (q, $^1J_{C-F}$ = 286 Hz), 123.10, 85.9 (q, $^2J_{C-F}$ = 28 Hz), 47.5. IR (neat): 2921, 1736, 1272, 1237, 1174, 1079, 714 cm^{-1}. HRMS (ESI) *m/z* calcd for $C_{22}H_{16}F_3O_2^+$ $[M+H]^+$ 369.1097, found 369.1101.

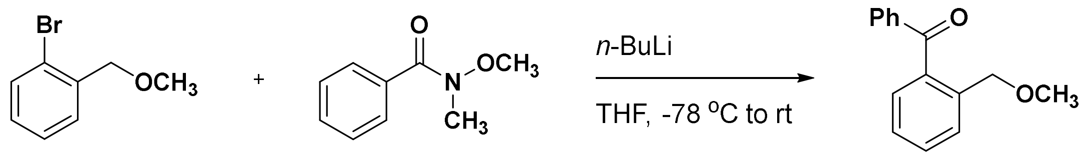


21c

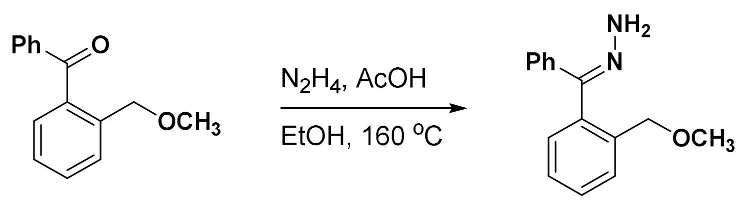
2-((1*R*,5*S*,6*s*)-2,4-dioxo-3,6-diphenyl-3-azabicyclo[3.1.0]hexan-6-yl)benzaldehyde (**21c**). According to General Procedure G, Diels-Alder reaction was stirred for 5 h using (*E*)-((2-(1,3-dithiolan-2-yl)phenyl)(phenyl)methylene)hydrazine (30.0 mg, 0.1 mmol), 1-phenyl-1*H*-pyrrole-2,5-dione (20.8 mg, 0.12 mmol), MnO_2 (69.6 mg, 0.8 mmol), Rh_2(*R*-PTAD)$_4$ (1.6 mg, 0.001 mmol) and DCM (6 mL). After filtrating MnO_2, the solvent was removed under reduced pressure. The residue was dissolved in CH_3CN (1 mL) and H_2O (1 mL). $Hg(OAc)_2$ (79.7 mg, 0.25 mmol) was then added and the reaction was allowed to stir at room temperature for 24 h. After filtration over celite, the product was purified by flash column chromatography (hexane/EtOAc = 3:1, v/v) as a white solid (26.0 mg, 71%, >95:5 dr). m.p. 189-191 °C. ^1H NMR (400 MHz, $CDCl_3$) δ 10.36 (s, 1H), 8.01 (dd, *J* = 7.5, 1.6 Hz, 1H), 7.75 (d, *J* = 7.6 Hz, 1H), 7.66 (td, *J* = 7.5, 1.6 Hz, 1H), 7.59 (t, *J* = 7.5 Hz, 1H), 7.35 – 7.18 (m, 6H), 7.14 (d, *J* = 6.8 Hz, 2H), 6.45 – 6.27 (m, 2H), 3.67 (d, *J* = 5.4 Hz, 1H), 3.24 (d, *J* = 5.3 Hz, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 189.9, 171.8, 171.4, 140.1, 137.2, 135.5, 134.7, 132.1, 131.4, 130.9, 129.5, 129.2, 129.1, 128.7, 128.2, 126.4, 126.2, 46.3, 35.9, 35.5. IR (neat): 2736, 1697, 1495, 1392, 1185, 697 cm^{-1}. HRMS (ESI) *m/z* calcd for $C_{24}H_{18}NO_3^+$ $[M+H]^+$ 368.1281, found 368.1283.



1-bromo-2-(methoxymethyl)benzene. Sodium Hydride 60% in an oil dispersion (1.200 g, 50.0 mmol) was suspended in THF under argon and cooled to 0 °C. Methanol (0.80 mL, 20.0 mmol) was added dropwise and allowed to react for 30 minutes. 2-bromo benzylbromide (2.4993 g, 10.0 mmol) was added in small portions and the reaction was allowed to warm up to room temperature overnight. The reaction was quenched by adding 10 mL of NH_4Cl aq, extracted in diethyl ether (3 x 50 mL), washed with water (2 x 25 mL) and brine (2 x 25 mL), and dried the combined organic layers over Na_2SO_4. Removed solvent by rotatory evaporation and purified by flash column chromatography (hexanes/ EtOAc = 100:0 to 90:10 v/v) to obtain a clear colorless oil (2.0092 g, 100%).^{1}H NMR (400 MHz, $CDCl_3$) δ 7.54 (dd, *J* = 7.9, 1.2 Hz, 1H), 7.46 (dd, *J* = 7.7, 1.7 Hz, 1H), 7.31 (d, *J* = 1.2 Hz, 1H), 7.14 (td, *J* = 7.7, 1.8 Hz, 1H), 4.53 (s, 2H), 3.47 (s, 3H). ^{1}H NMR data was consistent with reported literature values.[15]

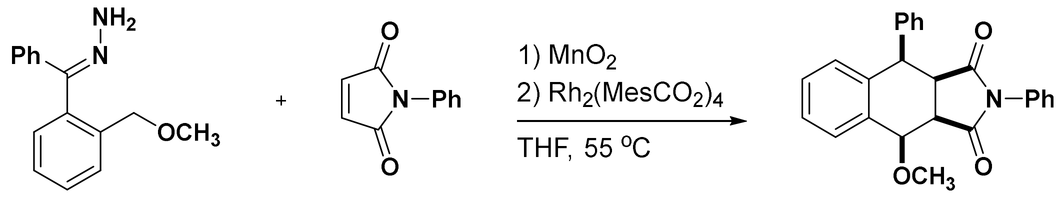


(2-(methoxymethyl)phenyl)(phenyl)methanone was synthesized according to General Procedure A, using 1-bromo-2-(methoxymethyl)benzene (1.0053 g, 5.0 mmol), *n*-BuLi (2.5 M, 2.4 mL, 6.0 mmol), *N*-methoxy-*N*-methylbenzamide (991.1 mg, 6.0 mmol) and THF (20 mL). The crude product was purified by flash column chromatography (hexane/EtOAc = 90:10, v/v) to obtain the ketone as a colorless oil (754.8 mg, 67%).^{1}H NMR (400 MHz, $CDCl_3$) δ 7.86 – 7.74 (m, 2H), 7.62 – 7.42 (m, 5H), 7.40 – 7.30 (m, 2H), 4.54 (s, 2H), 3.25 (s, 3H). ^{1}H NMR data was consistent with reported literature values.[16]

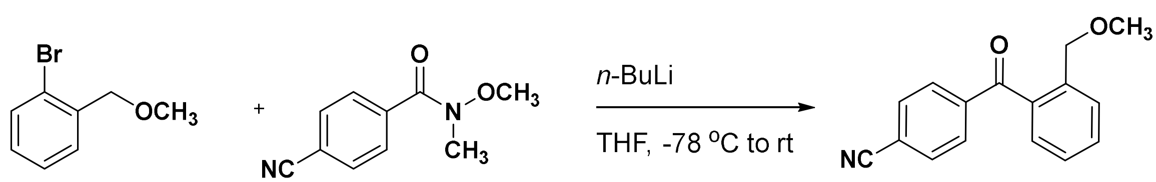


13f

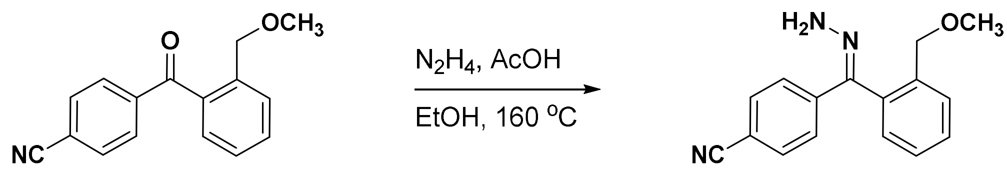
(E)-((2-(methoxymethyl)phenyl)(phenyl)methylene)hydrazine was synthesized according to General Procedure B, using (2-(methoxymethyl)phenyl)(phenyl)methanone (678.8 mg, 3.0 mmol), N_2H_4 (1.17 mL, 39 mmol), HOAc (0.21 mL, 3.6 mmol) and EtOH (6.0 mL). The crude product was purified by flash column chromatography (hexane/EtOAc = 60:40, v/v) to obtain the hydrazone as a pale yellow 0il (720.9 mg, 97%). Compound was isolated as a mixture of isomers; ^{1}H NMR spectral data for this mixture is complex and the mixture was carried on to the next step.



(3aR,4R,9R,9aR)-4-methoxy-2,9-diphenyl-3a,4,9,9a-tetrahydro-1H-benzo[f]isoindole-1,3(2H)-dione was synthesized according to General Procedure F, using (E)-((2-(methoxymethyl)phenyl)(phenyl)methylene)hydrazine (24.0 mg, 0.1 mmol), N-phenyl maleimide (17.3 mg, 0.1 mmol), MnO_2 (69.6 mg, 0.8 mmol), $Rh_2(MesCO_2)_4$ (0.9 mg, 0.001 mmol) and THF (6 mL). The crude product was purified by flash column chromatography (hexane/EtOAc = 70:30, v/v) to obtain **19a** as a yellowish solid (26.3 mg, 69%, >95:5 dr). m.p. 165-166 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.61 – 7.16 (m, 13H), 7.07 – 6.95 (m, 1H), 4.82 (d, *J* = 6.0 Hz, 1H), 4.69 (d, *J* = 7.9 Hz, 1H), 3.87 (dd, *J* = 9.7, 7.9 Hz, 1H), 3.70 (dd, *J* = 9.7, 6.0 Hz, 1H), 3.47 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 175.72, 174.57, 139.55, 138.42, 133.60, 132.00, 130.49, 129.19, 129.08, 128.89, 128.55, 128.02, 127.64, 127.03, 126.94, 126.64, 76.45, 56.90, 45.62, 44.60, 42.79. IR (neat): 2922, 1705, 1317, 1181, 1056, cm^{-1}. HRMS (ESI) *m/z* calcd for C25H21NNaO3+ $[M+Na]^+$ 406.1414, found 406.1416 .

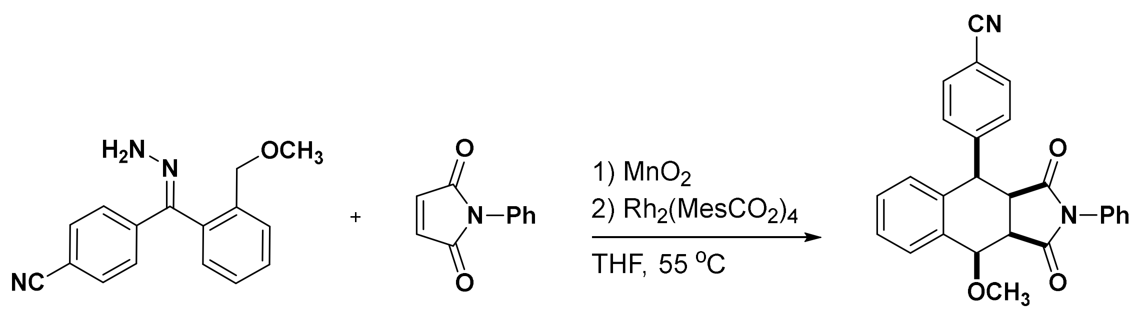


4-(2-(methoxymethyl)benzoyl)benzonitrile was synthesized according to General Procedure A, using 1-bromo-2-(methoxymethyl)benzene (1.0053 g, 5.0 mmol), *n*-BuLi (2.5 M, 2.4 mL, 6.0 mmol), 4-cyano-*N*-methoxy-*N*-methylbenzamide (1.1412 g, 6 mmol) and THF (20 mL). The crude product was purified by flash column chromatography (hexane/EtOAc = 85:15, v/v) to obtain the ketone as a yellowish oil (615.6 mg, 49%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.87 (d, *J* = 8.1 Hz, 2H), 7.76 (d, *J* = 8.0 Hz, 2H), 7.53 (dd, *J* = 3.8, 2.4 Hz, 2H), 7.45 – 7.29 (m, 2H), 4.52 (s, 2H), 3.21 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 196.37, 141.15, 138.47, 136.62, 132.34, 131.24, 130.25, 128.99, 128.73, 127.43, 118.15, 116.18, 72.33, 58.54. HRMS (ESI) *m/z* calcd for C16H14NO2+ $[M+H]^+$ 252.1019, found 252.1021.



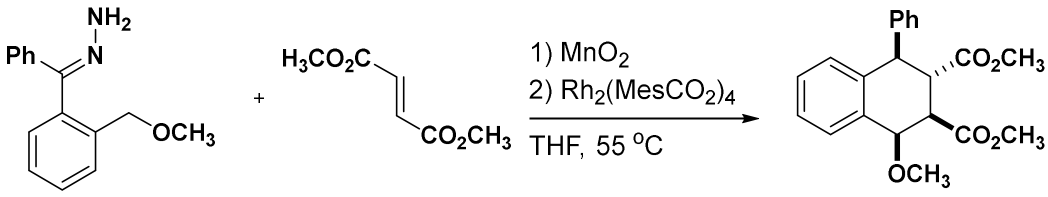
13g

(E)-4-(hydrazineylidene(2-(methoxymethyl)phenyl)methyl)benzonitrile was synthesized according to General Procedure B, using 4-(2-(methoxymethyl)benzoyl)benzonitrile (502.6 mg, 2.0 mmol), N_2H_4 (0.77 mL, 24 mmol), HOAc (0.15 mL, 2.4 mmol) and EtOH (4.0 mL). The crude product was purified by flash column chromatography (hexane/EtOAc = 60:40, v/v) to obtain the hydrazone as a pale yellow 0il (60.8 mg, 11%). Compound was isolated as a mixture of isomers. ^{1}H NMR spectral data for this mixture is complex and the mixture was carried on to the next step.



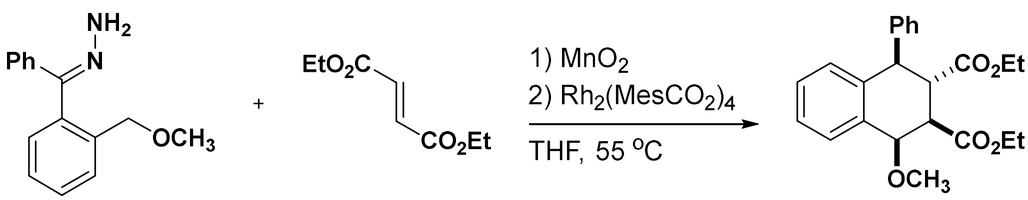
19b

(3aR,4R,9R,9aR)-4-methoxy-2-phenyl-9-(p-tolyl)-3a,4,9,9a-tetrahydro-1H-benzo[f]isoindole-1,3(2H)-dione was synthesized according to General Procedure F, using (E)-4-(hydrazineylidene(2-(methoxymethyl)phenyl)methyl)benzonitrile (26.5 mg, 0.1 mmol), N-phenyl maleimide (17.3 mg, 0.1 mmol), MnO_2 (69.6 mg, 0.8 mmol), $Rh_2(MesCO_2)_4$ (0.9 mg, 0.001 mmol) and THF (6 mL). The crude product was purified by flash column chromatography (hexane/EtOAc = 70:30, v/v) to obtain **19b** as a white solid (31.3 mg, 77%, >95:5 dr). m.p. 160-162 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.62 – 7.48 (m, 4H), 7.49 – 7.30 (m, 6H), 7.15 (dd, *J* = 6.4, 2.5 Hz, 1H), 7.07 (dd, *J* = 8.4, 1.4 Hz, 2H), 4.95 – 4.75 (m, 2H), 3.91 (t, *J* = 9.7 Hz, 1H), 3.60 (dd, *J* = 10.0, 5.3 Hz, 1H), 3.37 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 175.54, 174.54, 146.19, 137.55, 133.22, 131.82, 131.65, 131.23, 129.91, 129.77, 129.23, 129.02, 128.77, 127.43, 126.52, 119.04, 110.72, 76.54, 56.50, 46.21, 44.43, 41.66. IR (neat): 2976, 2225, 1709, 1369, 1061 cm^{-1}. HRMS (ESI) *m/z* calcd for C26H20N2NaO3+ $[M+Na]^+$ 431.1366, found 431.13059.



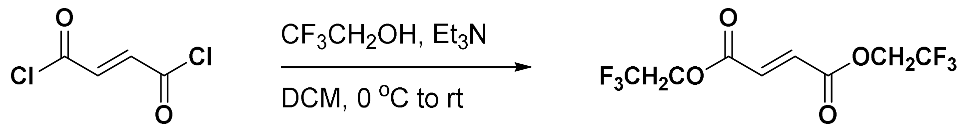
19c

Dimethyl (1R,2R,3S,4R)-1-methoxy-4-phenyl-1,2,3,4-tetrahydronaphthalene-2,3-dicarboxylate was synthesized according to General Procedure F, using (E)-((2-(methoxymethyl)phenyl)(phenyl)methylene)hydrazine (24.0 mg, 0.1 mmol), dimethyl fumarate (14.4 mg, 0.1 mmol), MnO_2 (69.6 mg, 0.8 mmol), $Rh_2(MesCO_2)_4$ (0.9 mg, 0.001 mmol) and THF (6 mL). The crude product was purified by flash column chromatography (hexane/EtOAc = 80:20, v/v) to obtain **19c** as a clear colorless oil (30.8 mg, 87%, >95:5 dr). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.33 – 7.09 (m, 8H), 6.91 – 6.80 (m, 1H), 4.70 (d, *J* = 2.9 Hz, 1H), 4.09 (d, *J* = 11.0 Hz, 1H), 3.76 (s, 3H), 3.61 (dd, *J* = 12.2, 11.0 Hz, 1H), 3.48 (s, 3H), 3.39 (s, 3H), 3.30 (dd, *J* = 12.1, 2.9 Hz, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 175.93, 172.30, 143.77, 138.93, 133.30, 130.30, 129.85, 129.18, 128.65, 127.11, 126.03, 77.63, 57.04, 52.25, 51.68, 50.00, 48.42, 45.92. IR (neat): 2978, 2896 1717, 1375, 1249 cm^{-1}. HRMS (ESI) *m/z* calcd for C21H22NaO5+ $[M+Na]^+$ 377.1365, found 377.1359.

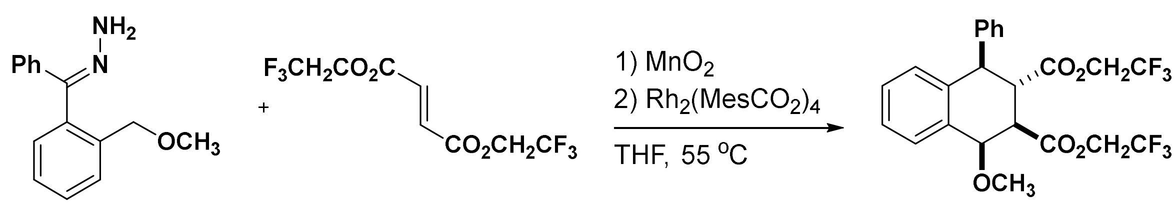


19d

Diethyl (1R,2R,3S,4R)-1-methoxy-4-phenyl-1,2,3,4-tetrahydronaphthalene-2,3-dicarboxylate was synthesized according to General Procedure F, using (E)-((2-(methoxymethyl)phenyl)(phenyl)methylene)hydrazine (24.0 mg, 0.1 mmol), diethyl fumarate (17.2 mg, 0.1 mmol), MnO_2 (69.6 mg, 0.8 mmol), $Rh_2(MesCO_2)_4$ (0.9 mg, 0.001 mmol) and THF (6 mL). The crude product was purified by flash column chromatography (hexane/EtOAc = 80:20, v/v) to obtain **19d** as a clear colorless oil (32.5 mg, 85%, >95:5 dr). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.34 – 7.12 (m, 8H), 6.88 – 6.82 (m, 1H), 4.70 (d, *J* = 2.9 Hz, 1H), 4.30 (dq, *J* = 10.8, 7.1 Hz, 1H), 4.16 (dq, *J* = 10.8, 7.1 Hz, 1H), 4.07 (d, *J* = 11.1 Hz, 1H), 4.02 – 3.86 (m, 2H), 3.58 (dd, *J* = 12.2, 11.1 Hz, 1H), 3.40 (s, 3H), 3.28 (dd, *J* = 12.1, 3.0 Hz, 1H), 1.29 (t, *J* = 7.1 Hz, 3H), 0.92 (t, *J* = 7.1 Hz, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 175.39, 171.85, 143.66, 139.07, 133.38, 130.24, 129.82, 129.40, 129.10, 128.56, 127.04, 125.99, 77.82, 61.05, 60.35, 57.12, 50.14, 48.42, 45.84, 14.32, 13.95. IR (neat): 2980, 2897 1719, 1380, 1250 cm^{-1}. HRMS (ESI) *m/z* calcd for C23H26NaO5+ $[M+Na]^+$ 405.1678, found 405.1673.



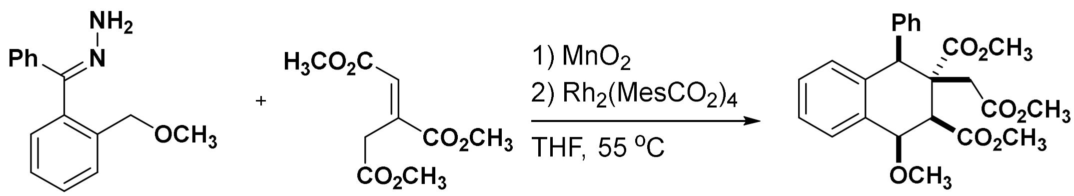
Bis(2,2,2-trifluoroethyl) fumarate was synthesized by dissolving 2,2,2-frifluoroethanol (0.57 mL, 8.0 mmol) in DCM (10 mL). After cooling to 0 °C, triethyl amine (1.59 mL, 12 mmol), and fumaryl chloride (0.42 mL, 4.0 mmol) were added dropwise. The black solution was allowed to warm up to room temperature overnight. Removed excess DCM by rotatory evaporation, dissolved in diethyl ether (50 mL), washed with brine (2 x 20 mL), dried over Na_2SO_4 and removed excess solvent by rotatory evaporation. The crude product was purified by flash column chromatography (hexane/EtOAc = 60:40, v/v) to obtain bis(2,2,2-trifluoroethyl) fumarate as a white solid (923.2 mg, 82%). ^1H NMR (400 MHz, $CDCl_3$) δ 7.01 (s, 2H), 4.61 (d, *J* = 8.2 Hz, 4H). ^1H NMR data was consistent with reported literature values.[17]



19e

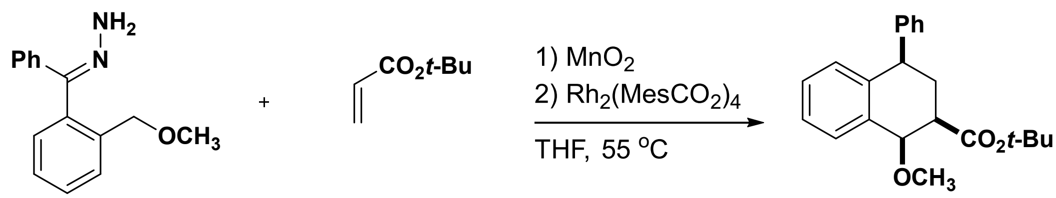
bis(2,2,2-trifluoroethyl) (1R,2R,3S,4R)-1-methoxy-4-phenyl-1,2,3,4-tetrahydronaphthalene-2,3-dicarboxylate was synthesized according to General Procedure F, using (E)-((2-(methoxymethyl)phenyl)(phenyl)methylene)hydrazine (24.0 mg, 0.1 mmol), bis(2,2,2-trifluoroethyl) fumarate (28.0 mg, 0.1 mmol), MnO_2 (69.6 mg, 0.8 mmol), $Rh_2(MesCO_2)_4$ (0.9 mg, 0.001 mmol) and THF (6 mL). The crude product was purified by flash column chromatography (hexane/EtOAc = 80:20, v/v) to obtain **19e** as a clear yellowish oil (36.5 mg, 74%, >95:5 dr). ^1H NMR (400 MHz, $CDCl_3$) δ 7.37 – 7.21 (m, 6H), 7.16 – 7.11 (m, 2H), 6.87 (dd, *J* = 6.2, 2.9 Hz, 1H), 4.82 – 4.68 (m, 2H), 4.38 (dq, *J* = 12.7, 8.4 Hz, 1H), 4.26 (qd, *J* = 8.5, 1.7 Hz, 2H), 4.10 (d, *J* = 11.1

Hz, 1H), 3.77 (t, *J* = 11.6 Hz, 1H), 3.43 (dd, *J* = 12.1, 3.0 Hz, 1H), 3.39 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 173.48, 170.14, 142.63, 138.42, 132.30, 130.33, 129.96, 129.50, 129.08, 128.86, 128.65, 128.27, 128.15, 127.47, 127.37, 127.13, 126.23, 72.69, 61.02, 60.73, 60.65, 60.36, 56.78, 49.74, 48.30, 45.48. ^{19}F NMR (376 MHz, $CDCl_3$) δ -73.67 (t, *J* = 8.5 Hz), -73.77 (t, *J* = 8.3 Hz). IR (neat): 2990, 2905 1708, 1365, 1241 cm^{-1}. HRMS (ESI) *m/z* calcd for C23H20F6NaO5+ [M+Na]$^+$ 513.1113, found 513.1121.



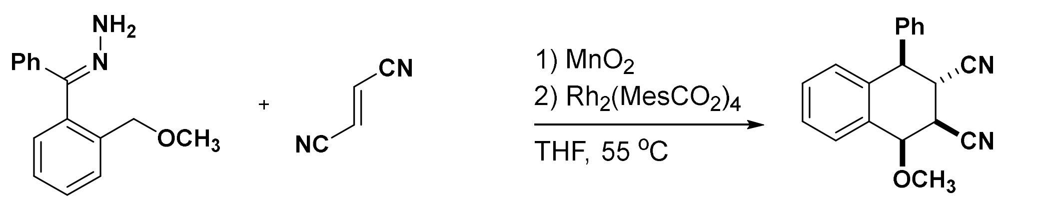
19f

Dimethyl (1R,2S,3R,4R)-4-methoxy-2-(2-methoxy-2-oxoethyl)-1-phenyl-1,2,3,4-tetrahydronaphthalene-2,3-dicarboxylate was synthesized according to General Procedure F, using (E)-((2-(methoxymethyl)phenyl)(phenyl)methylene)hydrazine (24.0 mg, 0.1 mmol), trimethyl (E)-prop-1-ene-1,2,3-tricarboxylate (21.6 mg, 0.1 mmol), MnO_2 (69.6 mg, 0.8 mmol), $Rh_2(MesCO_2)_4$ (0.9 mg, 0.001 mmol) and THF (6 mL). The crude product was purified by flash column chromatography (hexane/EtOAc = 75:25, v/v) to obtain **19f** as a clear colorless oil (20.5 mg, 48%, >95:5 dr). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.50 – 7.45 (m, 1H), 7.35 – 7.23 (m, 4H), 7.15 (ddd, *J* = 10.3, 6.8, 5.1 Hz, 3H), 6.90 – 6.82 (m, 1H), 4.80 (s, 1H), 4.77 (d, *J* = 4.2 Hz, 1H), 3.72 (d, *J* = 7.0 Hz, 4H), 3.69 (s, 3H), 3.65 (s, 3H), 3.52 (s, 3H), 2.91 (d, *J* = 17.2 Hz, 1H), 2.59 (d, *J* = 17.2 Hz, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 174.90, 171.74, 170.88, 139.73, 136.31, 135.88, 131.66, 129.46, 128.27, 127.77, 127.61, 127.37, 126.72, 76.99, 59.26, 53.60, 52.53, 51.98, 51.41, 50.35, 49.17, 37.37. IR (neat): 2978, 2896, 1717, 1705, 1375, 1249 cm^{-1}. HRMS (ESI) *m/z* calcd for C24H26NaO7+ [M+Na]$^+$ 449.1576, found 449.1572.



19g

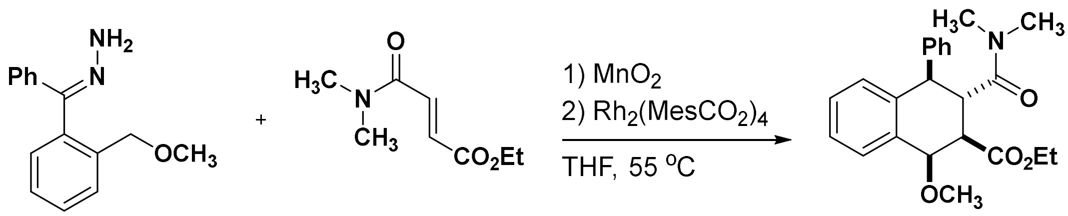
Tert-butyl (1R,2R,4R)-1-methoxy-4-phenyl-1,2,3,4-tetrahydronaphthalene-2-carboxylate was synthesized according to General Procedure F, using (E)-((2-(methoxymethyl)phenyl)(phenyl)methylene)hydrazine (24.0 mg, 0.1 mmol), *t*-butyl acrylate(12.8 mg, 0.1 mmol), MnO_2 (69.6 mg, 0.8 mmol), $Rh_2(MesCO_2)_4$ (0.9 mg, 0.001 mmol) and THF (6 mL). The crude product was purified by flash column chromatography (hexane/EtOAc = 90:10, v/v) to obtain **19g** as a clear colorless oil (10.9 mg, 32%, >95:5 dr). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.33 – 7.17 (m, 8H), 6.88 (dd, *J* = 6.0, 3.1 Hz, 1H), 4.60 (d, *J* = 2.9 Hz, 1H), 3.98 (dd, *J* = 11.6, 6.9 Hz, 1H), 3.45 (s, 3H), 2.85 – 2.72 (m, 1H), 2.47 – 2.24 (m, 2H), 1.50 (s, 9H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 172.09, 146.74, 140.65, 135.01, 130.41, 130.11, 129.04, 128.65, 128.62, 126.49, 125.63, 80.63, 78.28, 57.28, 46.59, 46.35, 29.85, 29.29, 28.31. IR (neat): 2975, 2899, 1705, 1378, 1245 cm^{-1}. HRMS (ESI) *m/*z calcd for C22H26NaO3+ $[M+Na]^+$ 361.1780, found 361.1783.



19h

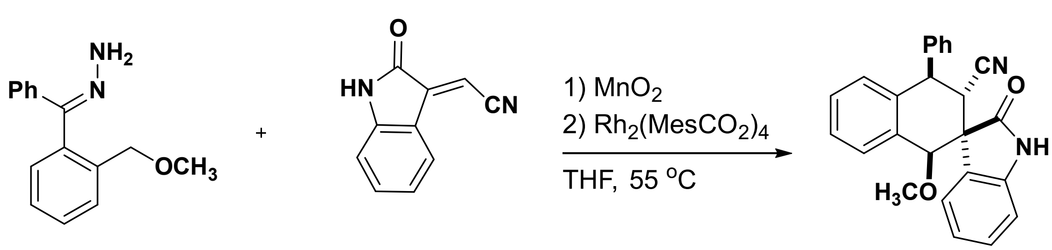
(1R,2S,3S,4R)-1-methoxy-4-phenyl-1,2,3,4-tetrahydronaphthalene-2,3-dicarbonitrile was synthesized according to General Procedure F, using (E)-((2-(methoxymethyl)phenyl)(phenyl)methylene)hydrazine (24.0 mg, 0.1 mmol), fumaronitrile(7.8 mg, 0.1 mmol), MnO_2 (69.6 mg, 0.8 mmol), $Rh_2(MesCO_2)_4$ (0.9 mg, 0.001 mmol) and THF (6 mL). The crude product was purified by flash column chromatography (hexane/EtOAc = 80:20, v/v) to obtain **19h** mixture of diastereomers as a white powder (17.1 mg, 59%, 82:18 dr). m.p. 195-197 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.53 (d, *J* = 7.9 Hz, 0H), 7.43 – 7.31 (m, 4H), 7.30 – 7.25 (m, 3H), 7.24 – 7.20 (m, 2H), 7.16 – 7.12 (m, 1H), 6.98 (d, *J* = 7.8 Hz, 0H), 6.89 (dt, *J* = 4.6, 2.1 Hz, 1H), 4.82 (d, *J* = 8.2 Hz, 0H), 4.55 (d, *J* = 2.5 Hz, 1H), 4.27 (d, *J* = 11.2 Hz, 1H), 3.84 (dd, *J* = 12.2, 11.1

Hz, 1H), 3.79 (s, 1H), 3.56 (s, 3H), 3.44 (dd, J = 10.7, 8.2 Hz, 0H), 3.37 (dd, J = 12.2, 2.3 Hz, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 141.13, 137.89, 135.78, 134.16, 133.39, 131.02, 130.36, 130.02, 129.97, 129.55, 129.20, 129.12, 128.84, 128.70, 128.33, 128.23, 128.11, 128.07, 126.88, 118.53, 117.00, 116.47, 78.28, 75.21, 59.02, 57.46, 48.45, 44.91, 36.20, 34.63, 34.02, 31.12. IR (neat): 2921, 2881, 2260, 1251, 978 cm^{-1}. HRMS (ESI) m/z calcd for C19H17N2O+ $[M+H]^+$ 289.1335, found 289.1341.



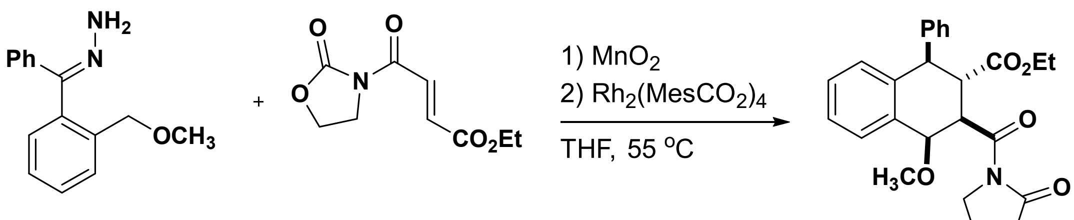
19i

Ethyl (1R,2R,3S,4R)-3-(dimethylcarbamoyl)-1-methoxy-4-phenyl-1,2,3,4-tetrahydronaphthalene-2-carboxylate was synthesized according to General Procedure F, using (E)-((2-(methoxymethyl)phenyl)(phenyl)methylene)hydrazine (24.0 mg, 0.1 mmol), ethyl (E)-4-(dimethylamino)-4-oxobut-2-enoate (17.1 mg, 0.1 mmol), MnO_2 (69.6 mg, 0.8 mmol), $Rh_2(MesCO_2)_4$ (0.9 mg, 0.001 mmol) and THF (6 mL). The crude product was purified by flash column chromatography (hexane/EtOAc = 70:30, v/v) to obtain **19i** as a colorless oil(36.2 mg, 95%, >95:5 dr). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.32 – 7.12 (m, 8H), 6.88 (dd, J = 5.5, 3.6 Hz, 1H), 4.67 (d, J = 2.9 Hz, 1H), 4.31 – 4.20 (m, 2H), 4.11 (dq, J = 10.8, 7.1 Hz, 1H), 3.85 (dd, J = 11.8, 10.5 Hz, 1H), 3.41 (s, 4H), 2.82 (s, 3H), 2.37 (s, 3H), 1.28 (t, J = 7.2 Hz, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 174.93, 172.38, 144.85, 139.55, 133.46, 130.43, 129.82, 129.43, 129.06, 128.52, 126.95, 125.68, 78.32, 60.80, 56.99, 49.92, 48.83, 41.60, 36.96, 35.76, 14.34. IR (neat): 3428, 2920, 1715, 1675, 1553, 1052 cm^{-1}. HRMS (ESI) m/z calcd for C23H28NO4+ $[M+H]^+$ 382.2013, found 382.2015.



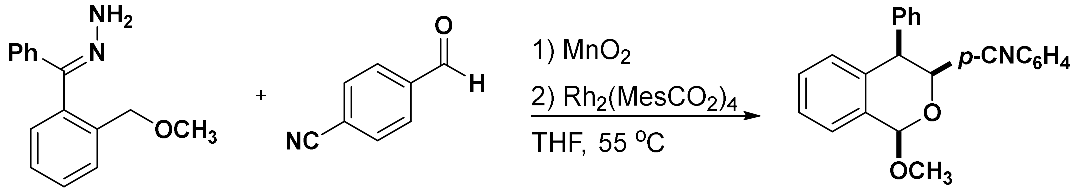
19i

(1'S,3S,3'S,4'R)-1'-methoxy-2-oxo-4'-phenyl-3',4'-dihydro-1'H-spiro[indoline-3,2'-naphthalene]-3'-carbonitrile was synthesized according to General Procedure F, using (E)-((2-(methoxymethyl)phenyl)(phenyl)methylene)hydrazine (24.0 mg, 0.1 mmol), (E)-2-(2-oxoindolin-3-ylidene)acetonitrile (17.0 mg, 0.1 mmol), MnO_2 (69.6 mg, 0.8 mmol), $Rh_2(MesCO_2)_4$ (0.9 mg, 0.001 mmol) and THF (6 mL). The crude product was purified by flash column chromatography (hexane/EtOAc = 70:30, v/v) to obtain **19j** as a white powder (25.3 mg, 67%, >95:5 dr). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.63 (d, *J* = 7.7 Hz, 1H), 7.48 (s, 1H), 7.40 (t, *J* = 7.5 Hz, 1H), 7.28 – 7.18 (m, 2H), 7.13 (ddd, *J* = 7.8, 5.9, 1.8 Hz, 2H), 6.98 (d, *J* = 7.7 Hz, 1H), 6.91 – 6.81 (m, 2H), 6.60 (d, *J* = 7.8 Hz, 1H), 6.27 (d, *J* = 9.9 Hz, 1H), 4.83 (d, *J* = 6.1 Hz, 1H), 4.46 (s, 1H), 4.05 (d, *J* = 6.1 Hz, 1H), 3.83 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 178.02, 141.14, 136.15, 135.20, 134.97, 129.39, 128.81, 128.72, 128.68, 128.48, 127.80, 127.55, 126.18, 122.19, 116.72, 109.74, 75.07, 61.23, 54.99, 52.35, 39.88. IR (neat): 3282, 2990, 2245, 1708, 1375 cm^{-1}. HRMS (ESI) *m/*z calcd for C25H21N2O2+ $[M+H]^+$ 381.1598, found 381.1606.



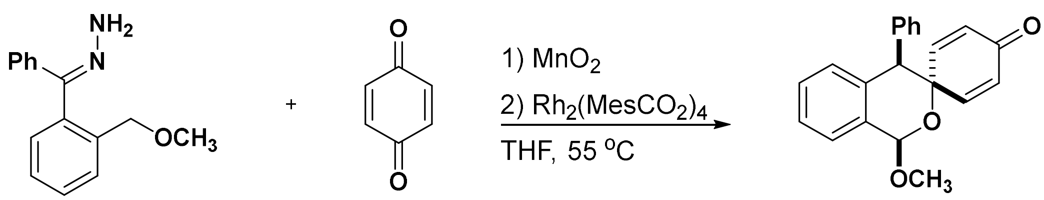
19k

Ethyl (1R,2S,3R,4R)-4-methoxy-3-(2-oxooxazolidine-3-carbonyl)-1-phenyl-1,2,3,4-tetrahydronaphthalene-2-carboxylate was synthesized according to General Procedure F, using (E)-((2-(methoxymethyl)phenyl)(phenyl)methylene)hydrazine (24.0 mg, 0.1 mmol), ethyl (E)-4-oxo-4-(2-oxooxazolidin-3-yl)but-2-enoate (21.3 mg, 0.1 mmol), MnO_2 (69.6 mg, 0.8 mmol), $Rh_2(MesCO_2)_4$ (0.9 mg, 0.001 mmol) and THF (6 mL). The crude product was purified by flash column chromatography (hexane/EtOAc = 60:40, v/v) to obtain **19k** as a clear oil (26.9 mg, 65%, >95:5 dr, 72:28 rr. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.35 – 7.23 (m, 4H), 7.21 – 7.15 (m, 4H), 6.84 (dd, *J* = 5.4, 3.7 Hz, 1H), 4.78 (d, *J* = 2.7 Hz, 1H), 4.47 (t, *J* = 8.1 Hz, 2H), 4.40 (dd, *J* = 11.9, 2.6 Hz, 1H), 4.20 – 3.99 (m, 3H), 3.89 (qd, *J* = 7.1, 5.5 Hz, 2H), 3.80 (t, *J* = 11.5 Hz, 1H), 3.35 (s, 3H), 0.89 (t, *J* = 7.1 Hz, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 175.34, 172.01, 153.54, 143.79, 139.13, 133.08, 130.26, 130.20, 129.45, 129.13, 128.53, 127.00, 125.97, 77.03, 62.45, 60.42, 56.84, 49.94, 48.13, 45.84, 42.91, 13.87. IR (neat): 2889, 1781, 1675, 1353, 1252 cm^{-1}. HRMS (ESI) *m/z* calcd for C24H25NNaO6 [M+Na]$^+$ 446.1580, found 446.1568.



20a

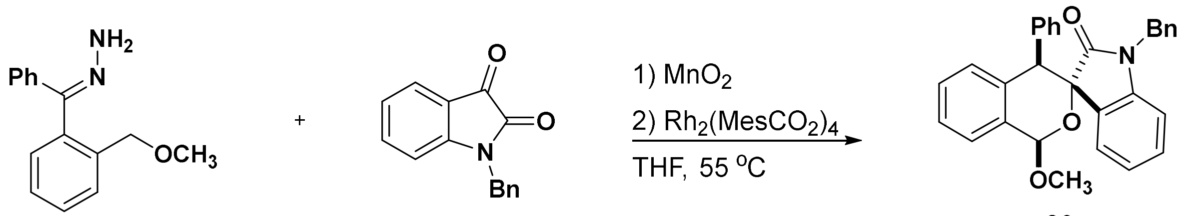
4-((1R,3S,4R)-1-methoxy-4-phenylisochroman-3-yl)benzonitrile was synthesized according to General Procedure F, using (E)-((2-(methoxymethyl)phenyl)(phenyl)methylene)hydrazine (24.0 mg, 0.1 mmol), 4-cyanobenzaldehyde (13.1 mg, 0.1 mmol), MnO_2 (69.6 mg, 0.8 mmol), $Rh_2(MesCO_2)_4$ (0.9 mg, 0.001 mmol) and THF (6 mL). The crude product was purified by flash column chromatography (hexane/EtOAc = 90:10, v/v) to obtain **20a** as a white powder (23.0 mg, 67%, 77:23 dr). m.p. 280-282 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.55 – 7.50 (m, 1H), 7.45 (d, *J* = 8.4 Hz, 2H), 7.38 – 7.22 (m, 4H), 7.20 – 7.13 (m, 2H), 7.03 (tt, *J* = 4.6, 1.1 Hz, 5H), 6.82 – 6.73 (m, 2H), 5.90 (s, 1H), 5.31 (d, *J* = 3.5 Hz, 1H), 4.13 (d, *J* = 3.4 Hz, 1H), 3.77 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 145.41, 139.62, 137.81, 134.28, 131.72, 130.15, 129.83, 128.90, 127.75, 127.45, 126.76, 126.67, 125.92, 110.89, 101.77, 76.53, 56.61, 50.23. IR (neat): 2872, 2213, 1275, 1153, 1052 cm^{-1}. HRMS (ESI) *m/z* calcd for C23H20NO2+ [M+H]$^+$ 342.1489, found 342.1483.



20b

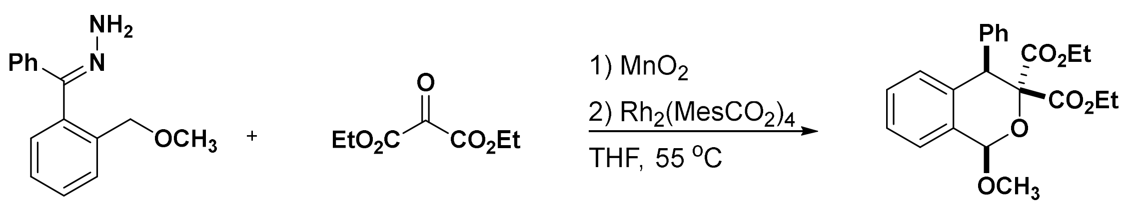
(1'R,4'R)-1'-methoxy-4'-phenylspiro[cyclohexane-1,3'-isochromane]-2,5-dien-4-one was synthesized according to General Procedure F, using (E)-((2-(methoxymethyl)phenyl)(phenyl)methylene)hydrazine (24.0 mg, 0.1 mmol), benzoquinone (10.8 mg, 0.1 mmol), MnO_2 (69.6 mg, 0.8 mmol), $Rh_2(MesCO_2)_4$ (0.9 mg, 0.001 mmol) and THF (6 mL). The crude product was purified by flash column chromatography (hexane/EtOAc = 90:10, v/v) to obtain **20b** as a clear oil (22.5 mg, 71%, >95:5 dr. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.43 (dd, *J* = 7.7, 1.5 Hz, 1H), 7.38 – 7.29 (m, 2H), 7.28 – 7.17 (m, 5H), 7.12 – 7.05 (m, 2H), 6.98 – 6.83 (m, 2H), 6.07 (ddd, *J* = 14.7, 10.3, 2.0 Hz, 2H), 5.76 (s, 1H), 4.44 (s, 1H), 3.55 (s, 3H). ^{13}C NMR (101

MHz, $CDCl_3$) δ 185.64, 148.70, 146.39, 136.81, 134.47, 132.92, 130.04, 129.21, 128.97, 128.58, 128.10, 128.04, 127.51, 127.26, 97.85, 72.21, 55.99, 53.71. IR (neat): 2902, 1660, 1315, 1253, 1052 cm^{-1}. HRMS (ESI) *m/z* calcd for C21H19O3+ $[M+H]^+$ 319.1329, found 319.1318.



20c

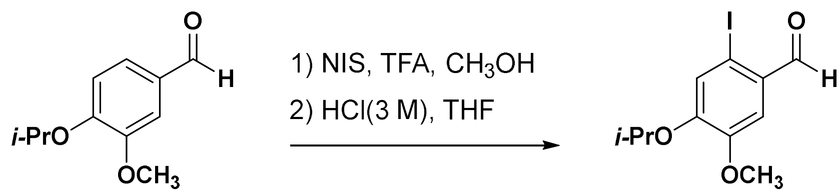
(1'R,3S,4'R)-1-benzyl-1'-methoxy-4'-phenylspiro[indoline-3,3'-isochroman]-2-one was synthesized according to General Procedure F, using (E)-((2-(methoxymethyl)phenyl)(phenyl)methylene)hydrazine (24.0 mg, 0.1 mmol), 1-benzylindoline-2,3-dione (23.7 mg, 0.1 mmol), MnO_2 (69.6 mg, 0.8 mmol), $Rh_2(MesCO_2)_4$ (0.9 mg, 0.001 mmol) and THF (6 mL). The crude product was purified by flash column chromatography (hexane/EtOAc = 80:20, v/v) to obtain **20c** as a yellowish solid (42.4 mg, 95%, >95:5 dr). m.p. 165-166 °C . ^1H NMR (400 MHz, $CDCl_3$) δ 7.56 (d, *J* = 7.7 Hz, 1H), 7.61 – 7.09 (m, 5H), 7.19 – 6.97 (m, 5H), 6.96 – 6.83 (m, 1H), 6.78 (td, *J* = 7.6, 1.0 Hz, 1H), 6.55 – 6.45 (m, 2H), 6.30 (d, *J* = 7.8 Hz, 1H), 6.01 (s, 1H), 5.07 (d, *J* = 16.1 Hz, 1H), 4.92 (s, 1H), 4.37 (d, *J* = 16.1 Hz, 1H), 3.44 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 174.62, 143.29, 135.39, 135.12, 134.89, 134.00, 129.61, 128.66, 128.63, 128.26, 128.13, 127.87, 127.70, 127.33, 127.19, 127.00, 126.92, 126.43, 122.12, 109.18, 98.31, 78.60, 55.94, 51.43, 43.86. IR (neat): 2920, 1721, 1605, 1453, 1352 cm^{-1}. HRMS (ESI) *m/z* calcd for C30H26NO3+ $[M+H]^+$ 448.1907, found 448.1922.



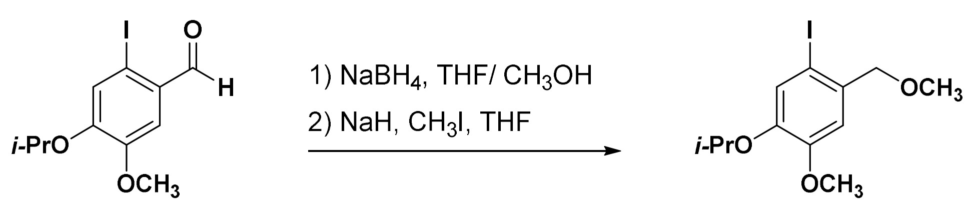
20d

Diethyl (1R,4R)-1-methoxy-4-phenylisochromane-3,3-dicarboxylate was synthesized according to General Procedure F, using (E)-((2-(methoxymethyl)phenyl)(phenyl)methylene)hydrazine (24.0 mg, 0.1 mmol), diethyl ketomalonate(8.7 mg, 0.1 mmol), MnO_2 (69.6 mg, 0.8 mmol),

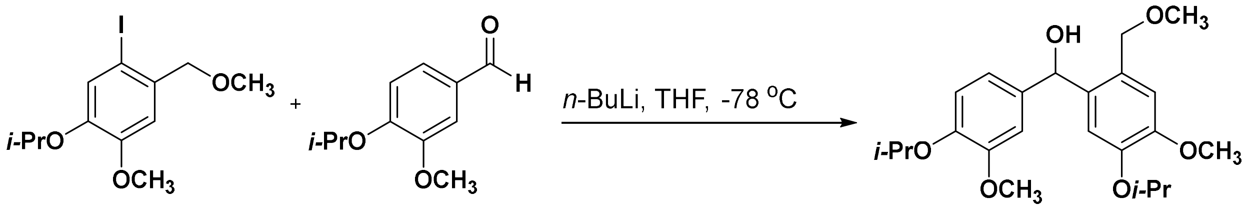
$Rh_2(MesCO_2)_4$ (0.9 mg, 0.001 mmol) and THF (6 mL). The crude product was purified by flash column chromatography (hexane/EtOAc = 90:10, v/v) to obtain **20d** as a clear oil(31.8 mg, 83%, >95:5 dr. ^1H NMR (400 MHz, $CDCl_3$) δ 7.42 – 7.29 (m, 3H), 7.28 – 7.16 (m, 5H), 7.06 (dd, *J* = 7.2, 1.9 Hz, 1H), 5.81 (d, *J* = 1.1 Hz, 1H), 4.84 (s, 1H), 4.22 (q, *J* = 7.1 Hz, 2H), 4.07 – 3.87 (m, 2H), 3.80 (s, 3H), 1.20 (t, *J* = 7.1 Hz, 3H), 1.02 (t, *J* = 7.1 Hz, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 167.94, 166.25, 139.55, 136.02, 131.80, 130.09, 129.45, 129.16, 128.30, 128.26, 127.40, 127.29, 126.03, 99.01, 84.19, 62.50, 62.01, 56.90, 47.48, 14.14, 13.87. IR (neat): 2920, 1761, 1755, 1253, 1052, cm^{-1}. HRMS (ESI) *m/z* calcd for : C22H24NaO6 $[M+H]^+$ 407.1471, found 407.1460.



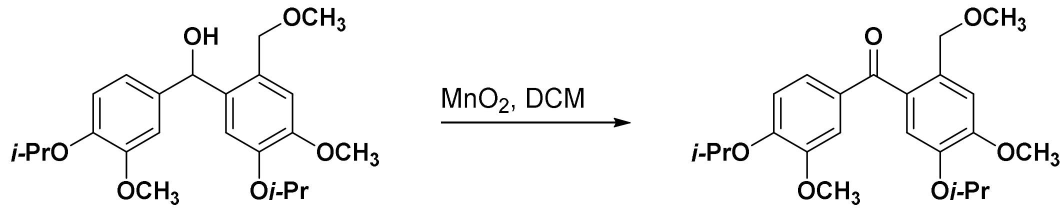
2-iodo-4-isopropoxy-5-methoxybenzaldehyde was synthesized by suspending 4-isopropoxy-3-methoxybenzaldehyde (1.9423 g, 10.0 mmol) and *n*-iodosuccinimide (4.3988 g, 20 mmol) in methanol (25 mL). After cooling to 0 °C, trifluoroacetic acid(0.15 mL, 0.2 mmol) was added dropwise. The reaction was allowed to warm up to room temperature overnight. A saturated solution of sodium thiosulfate (15 mL) was added to quench the reaction. The organic layer was extracted in diethyl ether (3 x 50 mL), washed with $NaHCO_3$(aq) (2 x 25 mL) and brine (2 x 25 mL). The combined organic layers were dried over Na_2SO_4 and concentrated in vacuo. The resulting oil was dissolved in THF (25 mL), 3 M HCl (10 mL) was added dropwise and the resulting suspension was stirred for 2 hours. $NaHCO_3$(aq) (20 mL) was added in small aliquots, the organic layer was extracted in diethyl ether (3 x 50 mL), washed with brine (2 x 25 mL) and dried over Na_2SO_4. The excess solvent was removed by rotatory evaporation to afford 2-iodo-4-isopropoxy-5-methoxybenzaldehyde as a white powder (3.1957 g, 99%). ^1H NMR (300 MHz, $CDCl_3$) δ 9.87 (s, 1H), 7.33 (s, 1H), 7.10 (s, 1H), 4.69 (p, *J* = 6.1 Hz, 1H), 3.91 (s, 3H), 1.45 (d, *J* = 6.1 Hz, 6H). ^1H NMR data was consistent with reported literature values.[18]



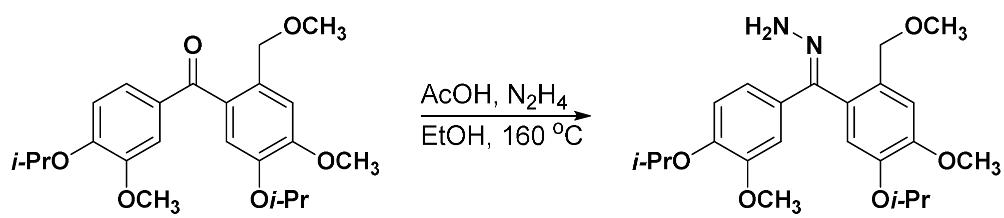
1-iodo-5-isopropoxy-4-methoxy-2-(methoxymethyl)benzene was synthesized by dissolving 2-iodo-4-isopropoxy-5-methoxybenzaldehyde (1.6007 g, 5.0 mmol) in 20 mL (THF/ CH_3OH= 7:3 v/v), followed by cooling to 0 °C and addition of sodium borohydride(0.2270 g, 1.2 mmol). After 2 hours, NH_4Cl(aq) (10 mL) was added, and the organic layer was extracted in diethyl ether (3x 25 mL), washed with brine (2 x 20 mL) and dried over Na_2SO_4. After removing excess solvent, the crude alcohol was dissolved in THF (20 mL), cooled to 0 °C, and sodium hydride (60% in an oil dispersion) (0.1800g, 7.5 mmol) was added in small portions. Iodomethane (0.47 mL, 7.5 mmol) was added dropwise as soon as bubbling stopped and the reaction was allowed to warm up to room temperature overnight. 10 mL of water were added and the organic layer was extracted in diethyl ether (3 x 25 mL), washed with brine (2x 20 mL) and dried over Na_2SO_4. Excess solvent was removed by rotatory evaporation and the resulting crude was purified by flash column chromatography (hexane/EtOAc = 98:2, v/v) to afford 1-iodo-5-isopropoxy-4-methoxy-2-(methoxymethyl)benzene as a yellowish oil (1.5453 g, 92%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.27 (s, 1H), 6.97 (s, 1H), 4.49 (dt, *J* = 12.3, 6.1 Hz, 1H), 4.38 (s, 2H), 3.85 (s, 3H), 3.46 (s, 3H), 1.35 (d, *J* = 6.1 Hz, 6H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 150.98, 147.40, 133.43, 125.96, 112.47, 85.96, 78.27, 72.12, 58.60, 56.14, 22.12. C12H18IO3+ $[M+H]^+$ 337.0295, found 337.0287.



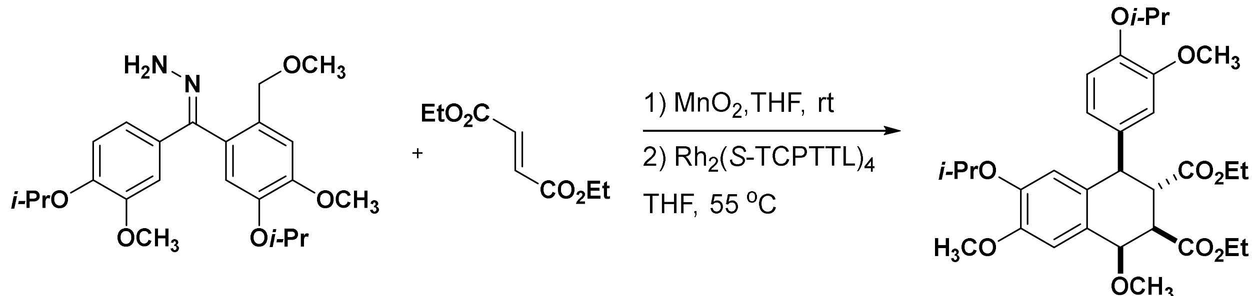
(4-isopropoxy-3-methoxyphenyl)(5-isopropoxy-4-methoxy-2-(methoxymethyl)phenyl)methanol was synthesized according to General Procedure A, using 1-iodo-5-isopropoxy-4-methoxy-2-(methoxymethyl)benzene (1.3447 g, 4.0 mmol), *n*-BuLi (2.25 M, 2.0 mL, 4.4 mmol), 4-isopropoxy-3-methoxybenzaldehyde (854.6 mg, 4.4 mmol) and THF (20 mL). The crude product was purified by flash column chromatography (hexane/EtOAc = 60:40, v/v) to obtain the ketone as a yellowish oil (1.0864 mg, 67%). Compound was isolated as a mixture of rotamers; ^{1}H NMR spectral data for this mixture is complex and the mixture was carried on to the next step.



(4-isopropoxy-3-methoxyphenyl)(5-isopropoxy-4-methoxy-2-(methoxymethyl)phenyl)methanone was synthesized by suspending (4-isopropoxy-3-methoxyphenyl)(5-isopropoxy-4-methoxy-2-(methoxymethyl)phenyl)methanol (2.1967 g, 5.43 mmol), and manganese dioxide (4.7214 g, 54.3 mmol) in DCM (20 mL). After stirring for 48 hours, the mixture was filtered over celites, and the excess solvent was removed by rotatory evaporation to afford the ketone as a white powder (2.0315 g, 93 %). m.p. 221-222 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.48 (d, *J* = 2.0 Hz, 1H), 7.34 – 7.24 (m, 1H), 7.13 (s, 1H), 6.95 (s, 1H), 6.86 (d, *J* = 8.4 Hz, 1H), 4.73 – 4.60 (m, 1H), 4.52 (s, 2H), 4.45 (p, *J* = 6.1 Hz, 1H), 3.94 (s, 3H), 3.90 (s, 3H), 3.32 (s, 3H), 1.42 (d, *J* = 6.0 Hz, 6H), 1.33 (d, *J* = 6.0 Hz, 6H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 195.91, 152.44, 151.95, 149.92, 145.26, 132.61, 130.91, 129.97, 125.57, 117.44, 112.67, 112.41, 111.79, 71.96, 71.91, 71.38, 58.54, 56.19, 22.16, 22.08. C23H31O6+ $[M+H]^+$ 403.2115, found 403.2107.

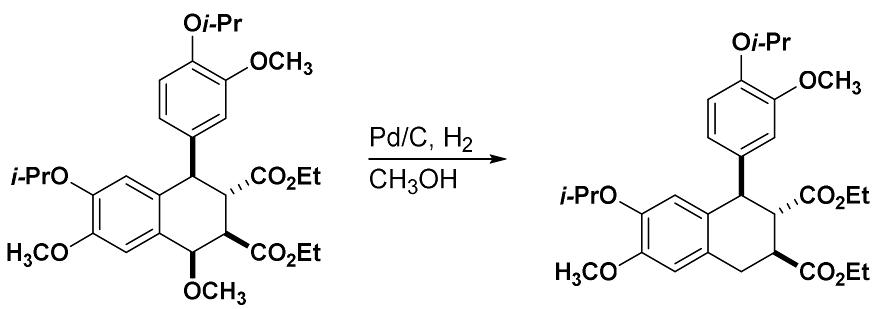


(E)-((4-isopropoxy-3-methoxyphenyl)(5-isopropoxy-4-methoxy-2-(methoxymethyl)phenyl)methylene)hydrazine was synthesized according to General Procedure B, using (4-isopropoxy-3-methoxyphenyl)(5-isopropoxy-4-methoxy-2-(methoxymethyl)phenyl)methanone (805.0 mg, 2.0 mmol), N_2H_4 (0.77 mL, 24 mmol), HOAc (0.15 mL, 2.4 mmol) and EtOH (4.0 mL). The crude product was purified by flash column chromatography (hexane/EtOAc = 50:50, v/v) to obtain the hydrazone as a pale yellow 0il (822.9 mg, 99%). Compound was isolated as a mixture of isomers. ^{1}H NMR spectral data for this mixture is complex and the mixture was carried on to the next step.

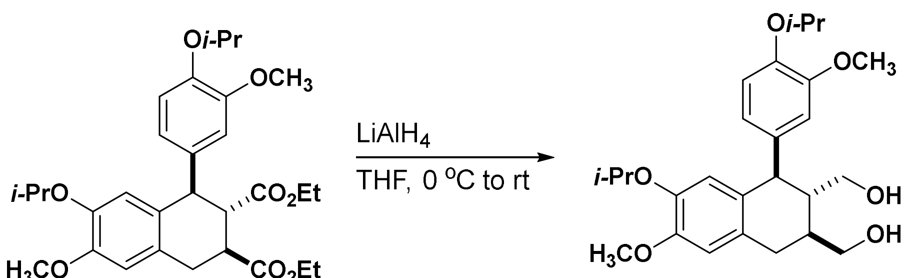


23

Diethyl (1R,2R,3S,4R)-6-isopropoxy-4-(4-isopropoxy-3-methoxyphenyl)-1,7-dimethoxy-1,2,3,4-tetrahydronaphthalene-2,3-dicarboxylate was synthesized according to General Procedure F, using (E)-((4-isopropoxy-3-methoxyphenyl)(5-isopropoxy-4-methoxy-2-(methoxymethyl)phenyl)methylene)hydrazine (222.1 mg, 0.5 mmol), diethyl fumarate (129.1 mg, 0.5 mmol), MnO_2 (347.8 mg, 4.0 mmol), Rh_2(*S*-TCPTTL)$_4$ (9.9 mg, 0.005 mmol) and THF (10 mL). The crude product was purified by flash column chromatography (hexane/EtOAc = 80:20, v/v) to obtain **23** as a clear oil (206.0 mg, 74%, >95:5 dr). ^{1}H NMR (400 MHz, $CDCl_3$) δ 6.82 (d, *J* = 7.9 Hz, 1H), 6.76 (s, 1H), 6.67 (dd, *J* = 8.1, 2.1 Hz, 1H), 6.63 (d, *J* = 2.1 Hz, 1H), 6.33 (s, 1H), 4.64 (d, *J* = 3.1 Hz, 1H), 4.56 – 4.43 (m, 1H), 4.36 – 4.10 (m, 3H), 4.01 – 3.86 (m, 6H), 3.76 (s, 3H), 3.52 – 3.44 (m, 1H), 3.43 (s, 3H), 3.25 (dd, *J* = 12.1, 3.1 Hz, 1H), 1.35 (dd, *J* = 6.1, 4.0 Hz, 7H), 1.29 (t, *J* = 7.1 Hz, 3H), 1.23 (d, *J* = 6.1 Hz, 3H), 1.12 (d, *J* = 6.0 Hz, 3H), 0.96 (t, *J* = 7.1 Hz, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 175.59, 171.95, 150.76, 148.39, 147.78, 146.21, 136.74, 131.48, 126.16, 121.72, 116.42, 116.31, 112.87, 112.69, 77.77, 71.69, 71.10, 61.01, 60.32, 57.44, 56.26, 56.08, 49.67, 48.85, 45.84, 22.20, 22.12, 22.07, 21.65, 14.32, 14.04. IR (neat): 2982, 2890, 1715, 1252, 1240 cm^{-1}. HRMS (ESI) *m/*z calcd for C31H42NaO9+ [M+Na]$^+$ 581.2727, found 581.2731.

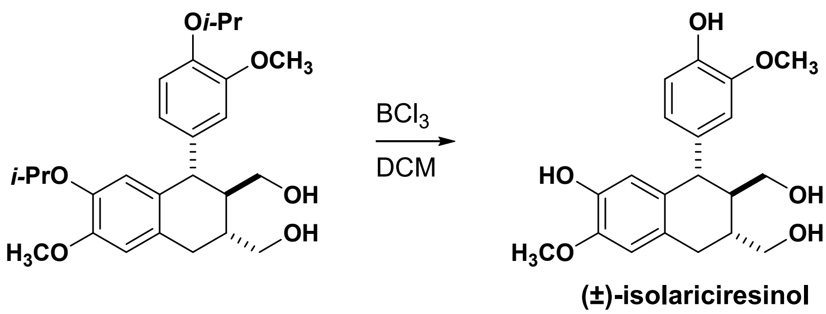


Diethyl (1R,2S,3S)-7-isopropoxy-1-(4-isopropoxy-3-methoxyphenyl)-6-methoxy-1,2,3,4-tetrahydronaphthalene-2,3-dicarboxylate was synthesized by suspending **23** (129.0 mg, 0.23 mmol) and 10 % Pd/C (150.0 mg, 0.14 mmol) in methanol (25 mL). Purged with hydrogen gas for 10 minutes and allowed to stir overnight under a hydrogen. Filtered over pad of celites and removed excess solvent by rotatory evaporation to obtain product as a clear oil (119.0 mg, 98%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 6.82 (d, *J* = 8.1 Hz, 1H), 6.65 (dd, *J* = 8.1, 2.1 Hz, 1H), 6.60 (s, 2H), 6.25 (s, 1H), 4.50 (p, *J* = 6.1 Hz, 1H), 4.24 – 4.07 (m, 4H), 3.92 (ddp, *J* = 14.1, 7.0, 3.5 Hz, 2H), 3.83 (s, 3H), 3.76 (s, 3H), 3.27 – 2.97 (m, 4H), 1.35 (dd, *J* = 6.1, 4.3 Hz, 6H), 1.26 (t, *J* = 7.1 Hz, 3H), 1.20 (d, *J* = 6.1 Hz, 3H), 1.11 (d, *J* = 6.0 Hz, 3H), 0.95 (t, *J* = 7.1 Hz, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 174.45, 173.99, 150.70, 149.22, 146.27, 145.68, 136.25, 130.14, 126.71, 121.82, 117.08, 116.29, 112.79, 111.40, 71.69, 71.39, 61.04, 60.44, 56.13, 56.08, 51.53, 49.24, 43.51, 32.15, 22.23, 22.15, 21.71, 14.30, 14.06. IR (neat): 2978, 2887, 1725, 1249, 1049 cm^{-1}. HRMS (ESI) *m/z* calcd for C30H40NaO8+ $[M+Na]^+$ 551.2621, found 551.2618.



24

((1R,2S,3S)-7-isopropoxy-1-(4-isopropoxy-3-methoxyphenyl)-6-methoxy-1,2,3,4-tetrahydronaphthalene-2,3-diyl)dimethanol was synthesized by suspending lithium aluminum hydride (34.2 mg, 0.90 mmol) in THF (5 mL); after cooling down to 0 °C, diethyl (1R,2S,3S)-7-isopropoxy-1-(4-isopropoxy-3-methoxyphenyl)-6-methoxy-1,2,3,4-tetrahydronaphthalene-2,3-dicarboxylate (119.0 mg, 0.23 mmol) dissolved in THF (5 mL) was added dropwise. The reaction was allowed to stir at room temperature for 2 hours. After cooling down to 0 °C, water (0.05mL) was added, followed by 15% NaOH (0.05 mL) and water (0.15 mL) to quench any leftover hydride. The suspension was filtered over celites and the excess solvent was removed by rotatory evaporation to afford **24** as a white powder (101.1 mg, 99%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 6.82 (d, *J* = 8.1 Hz, 1H), 6.67 (dd, *J* = 8.2, 2.0 Hz, 1H), 6.63 – 6.56 (m, 2H), 6.21 (s, 1H), 4.53 – 4.45 (m, 1H), 4.15 (p, *J* = 6.1 Hz, 1H), 3.88 – 3.67 (m, 10H), 3.70 – 3.60 (m, 1H), 3.50 (dd, *J* = 11.1, 5.3 Hz, 1H), 2.84 – 2.66 (m, 2H), 1.35 (dd, *J* = 6.1, 2.7 Hz, 6H), 1.19 (d, *J* = 6.1 Hz, 3H), 1.10 (d, *J* = 6.1 Hz, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 150.69, 148.72, 145.81, 145.17, 138.66, 132.12, 128.87, 121.99, 118.13, 116.26, 112.98, 111.50, 71.68, 71.39, 66.52, 62.94, 62.83, 56.15, 56.01, 48.19, 48.11, 40.12, 33.33, 29.98, 22.23, 22.20, 22.10, 21.71. IR (neat): 3289, 2980, 2879, 1249, 1219 cm^{-1}. HRMS (ESI) *m/z* calcd for C26H36NaO6+ $[M+Na]^+$ 467.2410, found 467.2406.



(±)-Isolariciresinol was synthesized by dissolving **24** (44.5 mg, 0.1 mmol) in DCM (2 mL), and cooling down to -78 °C before adding boron trichloride (1 M, 0.3 mL, 0.3 mmol). Although a white precipitate started forming almost immediately, the reaction was allowed to stir for 4 hours at room temperature to allow completion. The white precipitated was collected by vacuum filtrating and washed with cold DCM to afford (±)-isolariciresinol as a white powder (34.5 mg, 96%). ^1H NMR (400 MHz, MeOD) δ 6.62 (d, *J* = 8.0 Hz, 1H), 6.57 – 6.52 (m, 2H), 6.49 (dd, *J* = 8.0, 1.9 Hz, 1H), 6.06 (d, *J* = 0.9 Hz, 1H), 3.71 – 3.50 (m, 10H), 3.28 (dd, *J* = 11.2, 4.1 Hz, 1H), 2.65 (d, *J* = 7.7 Hz, 2H), 1.97 – 1.81 (m, 1H), 1.65 (tt, *J* = 10.0, 3.7 Hz, 1H). ^1H NMR data was consistent with reported literature values.[19]

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Computational Methods

Computational Details for Mechanistic Study.

Density functional theory optimization and frequency calculations were carried out in Gaussian 16[1] at the B3LYP-D3/Def2SVP level of theory[2] in solvent—dichloromethane modeled with the SMD[3] implicit solvent model. Electronic energies were subsequently corrected with single-point calculations at the SMD(DCM)-B3LYP-D3/Def2TZVPP level. Intrinsic reaction coordinate calculations[4] were used to further characterize the transition state structures. B3LYP-D3 has repeatedly been proven to be a reliable functional for Rh-catalyzed reaction mechanisms.[5,6]

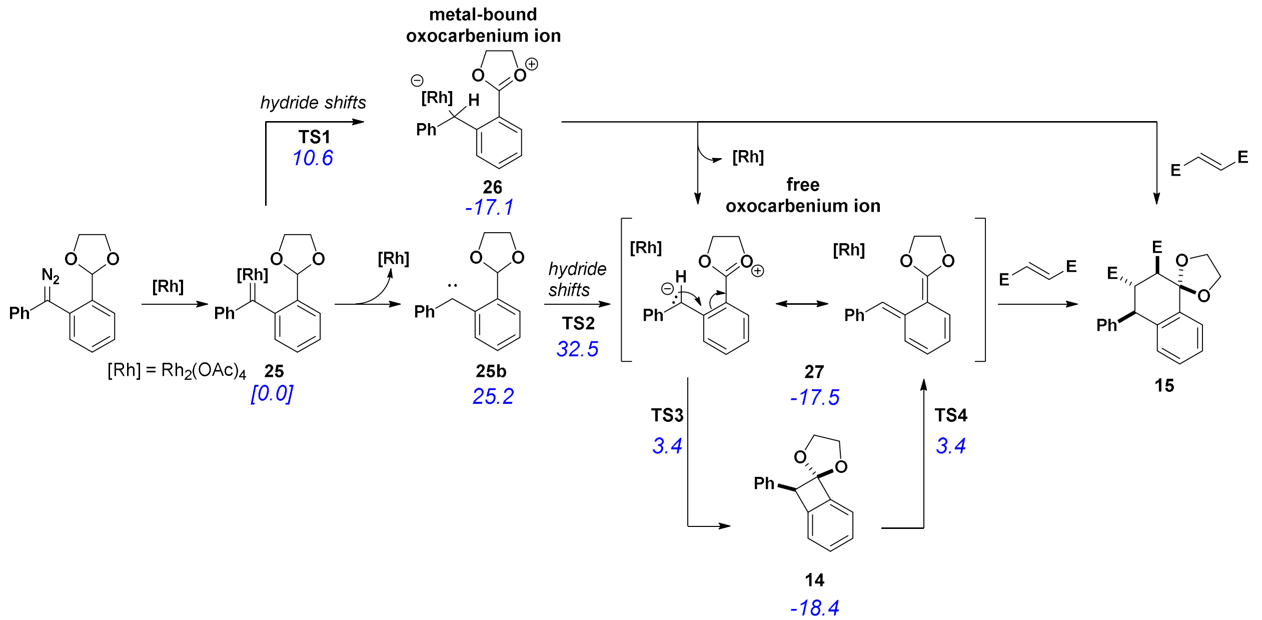


Figure CS1. The mechanism of diene formation from Rh-carbene intermediate. Relative free energies (blue, kcal mol^{-1}) reported at the SMD(DCM)-B3LYP-D3/Def2-TZVPP//SMD(DCM)-B3LYP-D3/Def2-SVP level of theory.

Computational Results of Mechanistic Study. The mechanism for formation of diene (Figure CS1) was investigated with density functional theory calculations at the SMD(DCM)-B3LYP-D3/Def2TZVPP//B3LYP-D3/Def2SVP level of theory. Our calculations predict that the hydride shift event is facile to the ylide intermediate and occurs with the metal bound to the substrate. We tried to find a hydride shift transition state structure free of metal-catalyst, but the TSS and free carbene are too high in energy to be relevant (32 and 25 kcal/mol, respectively). At this stage, loss of Rh-catalyst reveals a metal-free ortho-quinodimethane (o-QDM) which acts as the diene in the Diels-Alder step. From the o-QDM, either direct Diels-Alder or formation of a benzocyclobutane intermediate can occur. Our calculations weigh against benzocyclobutane formation being likely, as the barrier to form that intermediate is ~20 kcal/mol and the benzocyclobutane is only slightly more exergonic (~ 1 kcal/mol). Formation of the Diels-Alder adduct product directly from the o-QDM intermediate is more likely. In sum, hydride shifts with metal-catalyst bound and benzocyclobutane formation is unlikely before forming the DA-adduct.

The structures for Figure 1 of the main text and Figure S1 can be found on the ioChem-BD[6]database for ease of access of coordinates: see the following DOI—https://doi.org/10.19061/iochem-bd-6-122. Energies and lowest vibrational frequencies for these structures are in **Table S0** below.

Table S0. Energies and lowest vibrational frequencies for computed structures for mechanistic study. Free energies were computed at the B3LYP-D3/def2SVP level and electronic energies were computed at the B3LYP-D3/def2TZVPP, both in SMD solvent (dichloromethane).

Structure	Free Energy Correction (Hartree)	Electronic Energy (Hartree)	Lowest Frequency (cm^{-1})
25	0.397437	-1904.657208	16.7337
25b	0.214056	-768.7931436	26.6014
26	0.400483	-1904.687438	22.79
27	0.216283	-768.8635941	29.4769
TS1	0.393071	-1904.635919	-790.1915
TS2	0.211486	-768.7790327	-486.2878
TS3	0.215534	-768.8295676	-259.5939
14	0.217063	-768.8657967	32.2568
TSS_{DA}	0.355746	-1359.613052	-298.8251
15a	0.360889	-1359.683688	23.345
Maleimide	0.113265	-590.7457677	58.9609
Rh catalyst	0.156699	-1135.79711	39.4094

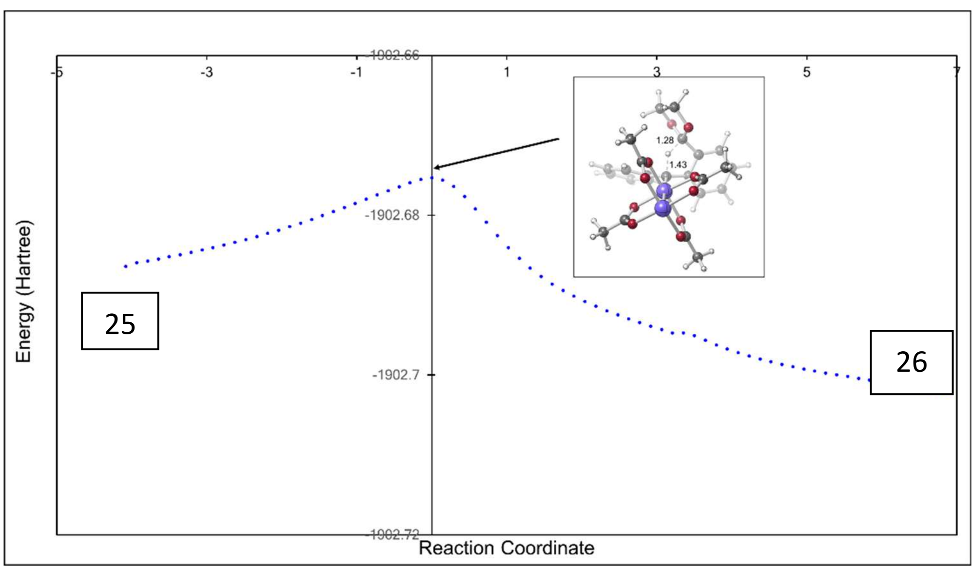


Figure CS2. IRC plot for hydride shift step (TS1).

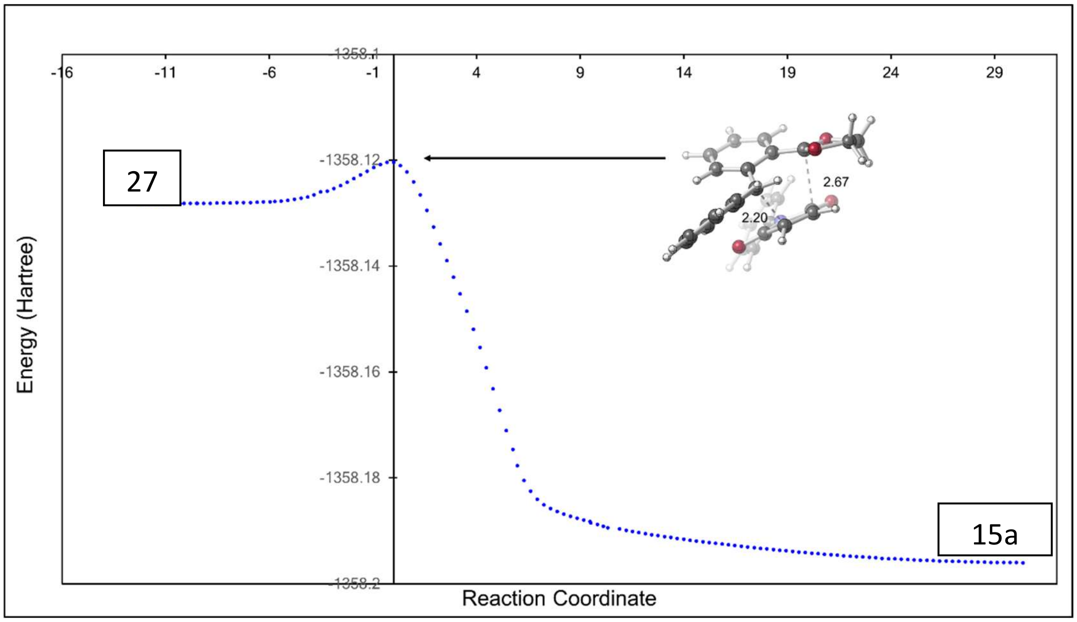


Figure CS3. IRC plot for Diels-Alder step with maleimide (TS_{DA}).

Computational Details for NMR Study.

Computed chemical shifts or coupling constants were produced for the diastereomers that may arise from the methodology described in the manuscript to provide stereochemical information for products **15o, 16a, 18c and 18o.**

All significantly contributing conformers were located by calculating a conformational distribution for each molecule using *Spartan18*[7] software with molecular mechanics (MMFF) using the default parameters. All conformers found to be > 3.0 kcal/mol than the lowest energy conformer were deemed statistically insignificant in their contributions to the computed chemical shifts and coupling constants of the molecule.

Computed chemical shifts and coupling constants were determined using *Gaussian16*[1] on all energetically relevant conformers. Geometry optimizations for computed chemical shifts were conducted at the B3LYP/6-31+G(d,p) level of theory in gas phase unless otherwise indicated. Computed chemical shifts were then determined from the optimized structure using the GIAO method at the B3LYP/6-311+G(2d,p) level of theory in chloroform or dichloromethane (SCRF). Computed coupling constants were obtained on structures optimized in the gas-phase at B3LYP/6-31G(d) level of theory. Subsequently, NMR single-point calculation in gas-phase was performed using the procedure published by Bally and Rablen on ^{1}H-^{1}H coupling constants on the optimized structure using the following command in the route section before the molecule specifications:[8]

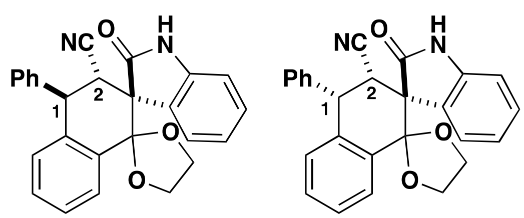
```
#n B3LYP/6-31G(d,p) nmr=(fconly,readatoms) iop(3/10=1100000)
```

Then at the end of the molecule specifications, separated by a blank line, "atoms=H" (without quotation marks) was added in.

Computed chemical shifts and coupling constants were empirically scaled using the appropriate scaling factors, compiled by Rablen *et al.*, and made available on the http://cheshirenmr.info website. Empirical scaling using such methods were shown to reduce systematic error resulting from a variety of sources and is all delineated in this review.[9]

Where multiple conformations were considered, computed free energies at the indicated level of theory (see below) were used to calculate the relative % population of each conformer based on a Boltzmann-weighted average of the computed energies at a relatively high level of theory. These relative populations were then used as weighing factors for the computed chemical shifts of each conformer.

15o



A **B**

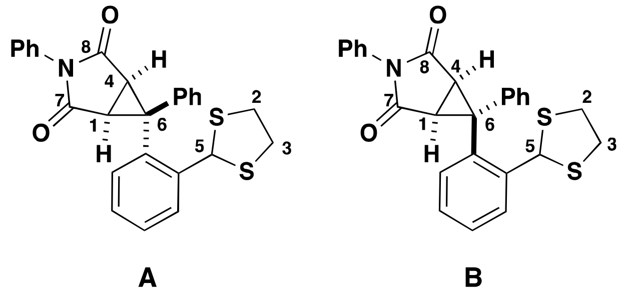
Coupling constants between hydrogens at C1 and C2 were calculated for diastereomers **A** and **B** using the methods described above and scaled by a factor of 0.9117 as recommended by Bally and Rablen.[7] The experimental H1-H2 coupling constant observed by ^{1}H NMR is 11.0 Hz.

Table 1. Coupling constants for both diastereomers of **15o**

	Computed Fermi Contact Terms (H1-H2)	Scaled Computed H1-H2 *J* Values (Hz)	Experimental H1-H2 *J* Value (Hz)	Standard Deviation (Hz)
A	11.4942	10.5229401	11.0	0.4770599
B	6.59437	6.03	11.0	4.97

Computed *J* value for **A** was significantly closer to the experimental *J* value observed and we concluded that **A** depicted the correct relative stereochemistry of **15o.**

<u>16a</u>



^{1}H and ^{13}C chemical shifts were computed for two conformers of diastereomers **A** and **B** (4 structures total). The computed chemical shifts of each conformer were averaged according to their relative populations derived from their relative free energies and then scaled using the procedure described in the computational NMR methods section using $CHCl_3$ as implicit solvent whenever indicated. Computed ^{1}H and ^{13}C chemical shifts for **A** and **B** were compared with all the assignable observed chemical shifts for 8**a** (measured in $CDCl_3$). Computed chemical shifts of chemically equivalent atoms were averaged prior to comparison with experimental shifts.

Computed ^{1}H chemical shifts for diastereomer **B** more consistently matched with the experimental data than computed chemical shifts for diastereomer **A**. Computed ^{13}C chemical for **A** and **B** closely correlated to experimental data. Closer examination of H1 and C1 revealed a greater variation between the two sets of computed data for diastereomers **A** and **B**. Based on these observations, we concluded that **A** depicted the correct relative stereochemistry of **16a**.

Table 2. Computed ^{1}H chemical shifts for **A**

H #	Scaled Computed Chemical Shifts	Experimental Chemical Shifts
1	3.041776706	3.1
2	3.42388724	3.205
2’	3.428787092	3.37
3	3.552485163	3.37
3’	3.699354599	3.49
4	3.19764095	3.74
5	6.86772997	6.11

Table 3. Computed ^{1}H chemical shifts for **B**

H #	Scaled Computed Chemical Shifts	Experimental Chemical Shifts
1	2.67397997	3.1
2	3.23418954	3.205
2’	3.28869158	3.37
3	3.300871662	3.37
3’	3.492539874	3.49
4	3.440008346	3.74
5	6.318824184	6.11

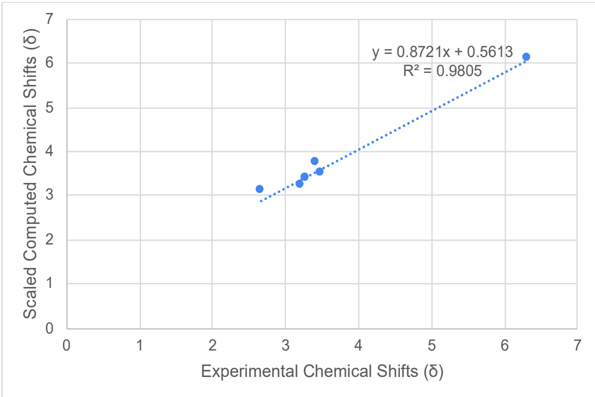


Figure 1. Correlation graph for computed [1]H chemical shift of **A** and experimental [1]H shifts.

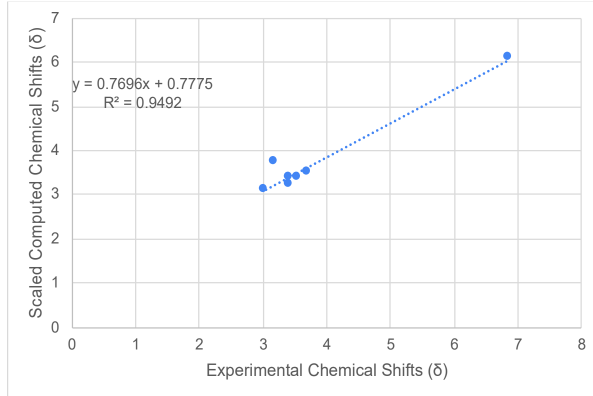


Figure 2. Correlation graph for computed [1]H chemical shift of **B** and experimental [1]H shift

Table 4. Computed ^{13}C chemical shifts for **A**

C #	Scaled Computed Chemical Shifts	Experimental Chemical Shifts
1	35.17669166	34.6
4	35.59417671	36.5
2	46.04838189	40.7
3	46.69335864	41.1
6	52.7711341	47.1
5	66.70339945	50.7
7	170.7508133	171.4
8	170.8872582	171.8

Table 5. Computed ^{13}C chemical shifts for **B**

C #	Scaled Computed Chemical Shifts	Experimental Chemical Shifts
1	33.91432571	34.6
4	36.4932049	36.5
2	46.32365949	40.7
3	48.19341369	41.1
6	52.89329506	47.1
5	62.4061118	50.7
7	170.7599886	171.4
8	170.980298	171.8

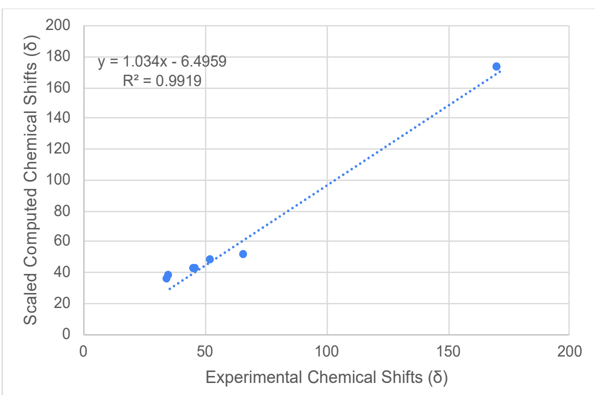


Figure 3. Correlation graph for computed ^{13}C chemical shift of **A** and experimental ^{13}C shifts.

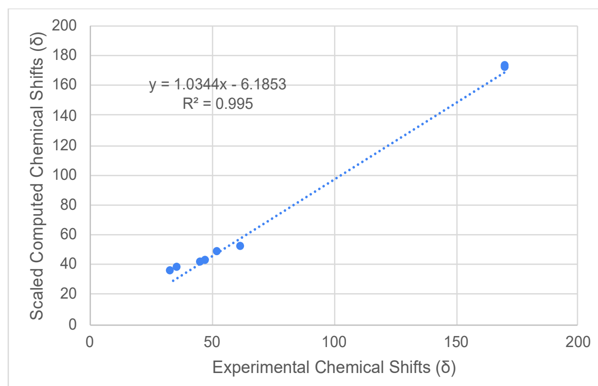
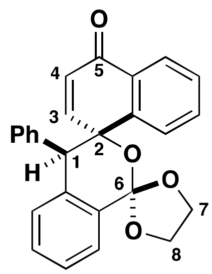
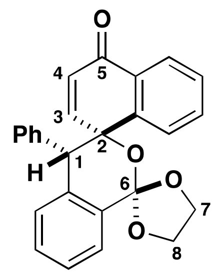


Figure 4. Correlation graph for computed ^{13}C chemical shift of **B** and experimental ^{13}C shifts.

18c



A



B

^{1}H and ^{13}C chemical shifts were computed for diastereomers **A** and **B** and scaled using the procedure described in the computational NMR methods section using CH_2Cl_2 as implicit solvent whenever indicated. Computed ^{1}H and ^{13}C chemical shifts for **A** and **B** were compared with all the assignable observed chemical shifts for **18c** (measured in CD_2Cl_2). Computed chemical shifts of chemically equivalent atoms were averaged prior to comparison with experimental shifts.

Computed chemical shifts for diastereomer **B** more consistently matched with the experimental data than computed chemical shifts for diastereomer **A**. Based off of the computed NMR shifts, combined with a crystal structure obtained of the major product, we concluded that **B** depicted the correct relative stereochemistry of **18c**.

Table 6. Computed ^{1}H chemical shifts for **A**

H #	Scaled Computed Chemical Shifts	Experimental Chemical Shifts
1	3.965696958	4.17
7	4.26760163	4.315
7’	4.217568464	4.315
8	4.269307306	4.315
8’	4.308916896	4.45
4	6.173220885	6.22
3	7.9385009	7.61

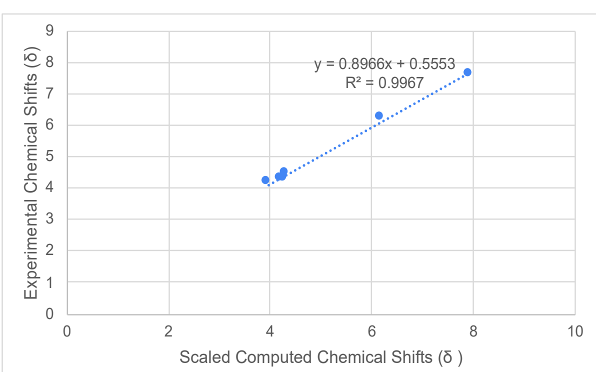


Figure 5. Correlation graph for computed ^{1}H chemical shift of **A** and experimental ^{1}H shifts.

Table 7. Computed ^{1}H chemical shifts for **B**

H #	Scaled Computed Chemical Shifts	Experimental Chemical Shifts
1	4.98227992	4.17
7	4.107173316	4.315
7’	4.171894248	4.315
8	4.18857197	4.315
8’	4.18838245	4.45
4	6.212451436	6.22
3	7.840993083	7.61

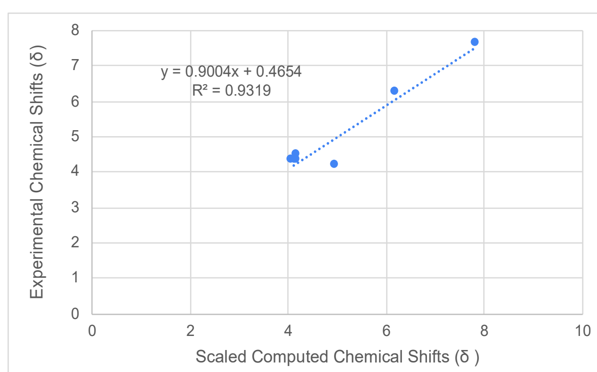


Figure 6. Correlation graph for computed ^{1}H chemical shift of **B** and experimental ^{1}H shifts.

Table 8. Computed ^{13}C chemical shifts for **A**

C #	Scaled Computed Chemical Shifts	Experimental Chemical Shifts
1	61.56270895	56.7
7	63.9852899	65
8	65.79940778	66.2
2	79.97163053	77.2
6	122.0081192	119
5	180.5719744	184.1

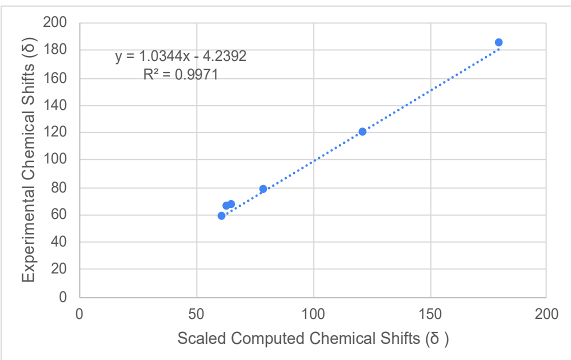


Figure 7. Correlation graph for computed ^{13}C chemical shift of **A** and experimental ^{13}C shifts.

Table 9. Computed ^{13}C chemical shifts for **B**

C #	Scaled Computed Chemical Shifts	Experimental Chemical Shifts
1	61.29238705	56.7
7	63.5524883	65
8	65.78870952	66.2
2	80.54169453	77.2
6	121.6880313	119
5	179.7580476	184.1

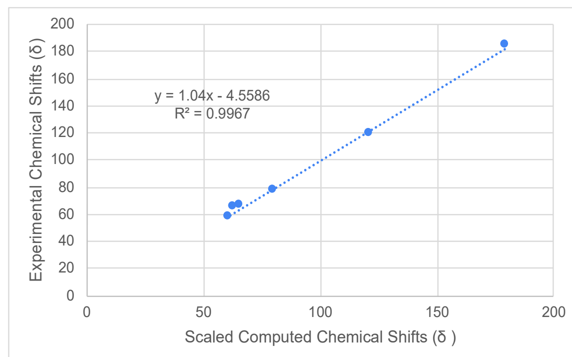
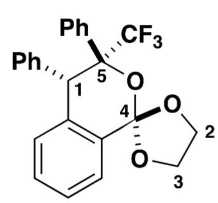
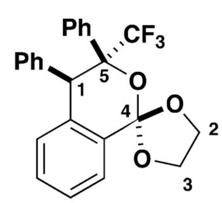


Figure 8. Correlation graph for computed ^{13}C chemical shift of **B** and experimental ^{13}C shifts.

<u>18j</u>



A



B

^{1}H and ^{13}C chemical shifts were computed for diastereomers **A** and **B** and scaled using the procedure described in the computational NMR methods section using $CHCl_3$ as implicit solvent whenever indicated. Computed ^{1}H and ^{13}C chemical shifts for **A** and **B** were compared with all the assignable observed chemical shifts for **18j** (measured in $CDCl_3$)**.** Computed chemical shifts of chemically equivalent atoms were averaged prior to comparison with experimental shifts.

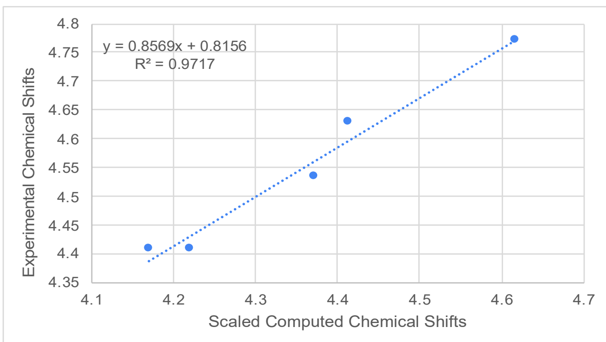
Computed chemical shifts for diastereomer **B** more consistently matched with the experimental data than computed chemical shifts for diastereomer **A**. From this, we concluded that **B** depicted the correct relative stereochemistry of **18j**.

Table 10. Computed ^{1}H chemical shifts for **A**

H #	Scaled Computed Chemical Shifts	Experimental Chemical Shifts
2	4.09523368	4.41
2'	4.141876855	4.41
3	4.216431751	4.535
3'	4.254821958	4.63
1	4.265949555	4.77

Table 11. Computed ^{1}H chemical shifts for **B**

H #	Scaled Computed Chemical Shifts	Experimental Chemical Shifts
2	4.170623145	4.41
2'	4.221439169	4.41
3	4.371939911	4.535
3'	4.414781157	4.63
1	4.617859792	4.77



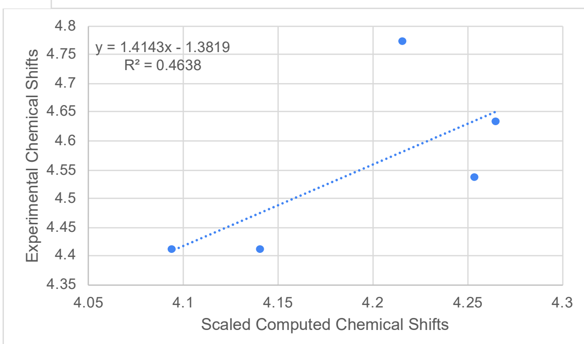


Figure 9. Correlation graph for computed ^{1}H chemical shift of **A** and experimental ^{1}H shifts.

Figure 10. Correlation graph for computed ^{1}H chemical shift of **B** and experimental ^{1}H shifts.

C #	Scaled Computed Chemical Shifts	Experimental Chemical Shifts
1	49.66261744	47.3
2	63.50033216	64.8
3	64.94581	65.7
5	82.82575686	81.5
4	120.9058556	118.6

Table 12. Computed ^{13}C chemical shifts for **A**

C #	Scaled Computed Chemical Shifts	Experimental Chemical Shifts
1	56.91705419	47.3
2	63.25415204	64.8
3	65.10154693	65.7

Table 13. Computed ^{13}C chemical shifts for **B**

5	82.76368985	81.5
4	120.5818544	118.6

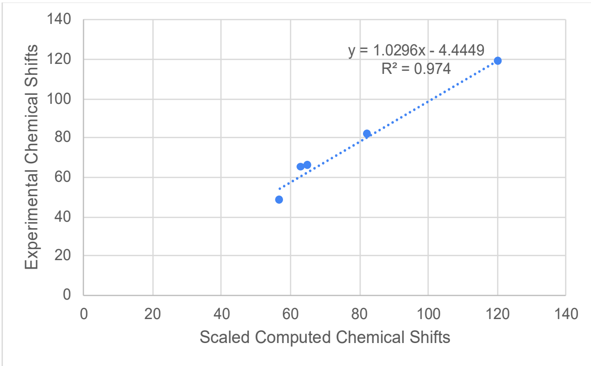


Figure 11. Correlation graph for computed ^{13}C chemical shift of **A** and experimental ^{13}C shifts.

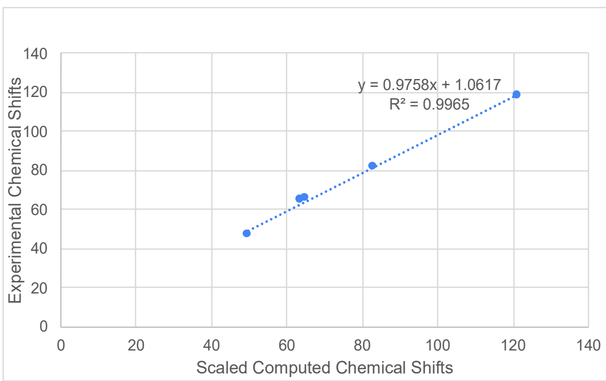


Figure 12. Correlation graph for computed ^{13}C chemical shift of **B** and experimental ^{13}C shifts.

<u>Computed Coordinates, Energies and Coupling Constants</u>

<u>15o</u>

<u>A</u>

G16 optfreq B3LYP/6-31G(d) gas-phase
Sum of electronic and thermal Free Energies = –1337.620496 hartrees

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.347710	4.076467	0.384380
2	6	0	0.188559	3.330958	0.165501
3	6	0	0.275236	1.967159	-0.111709
4	6	0	1.523408	1.322276	-0.146810
5	6	0	2.676922	2.080644	0.067057
6	6	0	2.590960	3.450185	0.328117
7	1	0	1.276718	5.139109	0.600125
8	1	0	-0.789049	3.796500	0.221217
9	1	0	3.649322	1.601835	0.030964
10	1	0	3.500051	4.022600	0.492550
11	6	0	1.549010	-0.163605	-0.489503
12	6	0	-0.951897	1.132137	-0.422969
13	6	0	0.418436	-0.938053	0.296185
14	1	0	0.788615	-1.054761	1.319729
15	6	0	-0.973100	-0.195312	0.412461
16	8	0	-2.144000	1.870342	-0.193216
17	8	0	-0.964252	0.759342	-1.804689
18	6	0	-2.864860	1.992645	-1.424743
19	1	0	-3.282179	3.002077	-1.483798
20	1	0	-3.674770	1.254976	-1.459054
21	6	0	-1.793667	1.707500	-2.474205
22	1	0	-1.223166	2.610886	-2.730225
23	1	0	-2.172359	1.240789	-3.386350
24	6	0	-2.236428	-0.986479	0.111624
25	6	0	-3.081040	-0.934443	1.233320
26	6	0	-2.666189	-1.647095	-1.032943
27	6	0	-4.337154	-1.527236	1.246204
28	6	0	-3.928968	-2.256800	-1.038366
29	1	0	-2.027578	-1.702570	-1.906340
30	6	0	-4.751421	-2.194575	0.087361
31	1	0	-4.975497	-1.477410	2.123734
32	1	0	-4.263685	-2.787282	-1.924778
33	1	0	-5.727084	-2.672596	0.071127
34	7	0	-2.447454	-0.225182	2.260622
35	1	0	-2.800412	-0.110992	3.200595
36	6	0	-1.183064	0.186920	1.912270
37	8	0	-0.370896	0.710044	2.650484
38	6	0	0.295754	-2.286718	-0.268534
39	7	0	0.234415	-3.349543	-0.731745
40	6	0	2.888019	-0.850863	-0.267190
41	6	0	3.465813	-0.925862	1.009967
42	6	0	3.561859	-1.442234	-1.341356
43	6	0	4.684005	-1.575796	1.203351
44	1	0	2.965156	-0.460413	1.855987
45	6	0	4.782363	-2.093233	-1.151063

46	1	0	3.123097	-1.399592	-2.335288
47	6	0	5.346555	-2.162454	0.122362
48	1	0	5.116338	-1.623746	2.199310
49	1	0	5.287394	-2.549390	-1.998265
50	1	0	6.294925	-2.670953	0.273742
51	1	0	1.297686	-0.250601	-1.552355

G16 #n B3LYP/6-31G(d,p) nmr=(fconly,readatoms) iop(3/10=1100000) gas-phase

Fermi Contact (FC) contribution to J (Hz):

	1	2	3	4	5
1	0.000000D+00				
2	0.000000D+00	0.000000D+00			
3	0.000000D+00	0.000000D+00	0.000000D+00		
4	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00	
5	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00
6	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00
7	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00
8	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00
9	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00
10	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00
11	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00
12	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00
13	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00
14	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00
15	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00
16	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00
17	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00
18	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00
19	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00
20	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00
21	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00
22	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00
23	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00
24	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00
25	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00
26	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00
27	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00
28	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00
29	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00
30	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00
31	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00
32	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00
33	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00
34	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00
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39	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00
40	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00
41	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00
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46	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00

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50	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00
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	6	7	8	9	10
6	0.000000D+00				
7	0.000000D+00	0.385007D+12			
8	0.000000D+00	0.845315D+01	0.385007D+12		
9	0.000000D+00	0.118222D+01	0.537317D+00	0.385007D+12	
10	0.000000D+00	0.823168D+01	0.140169D+01	0.861700D+01	0.385007D+12
11	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00
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14	0.000000D+00	0.363274D-01	-0.280402D-01	0.705272D-01	-0.337568D-01
15	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00
16	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00
17	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00
18	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00
19	0.000000D+00	0.112965D-01	0.216535D-01	-0.274826D-02	0.197495D-03
20	0.000000D+00	-0.385085D-02	-0.602761D-02	0.222678D-01	0.167905D-02
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22	0.000000D+00	-0.170575D-02	0.966473D-01	-0.159056D-01	0.116193D-01
23	0.000000D+00	0.184771D-01	0.673136D-01	-0.177794D-02	-0.212891D-01
24	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00
25	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00
26	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00
27	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00
28	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00
29	0.000000D+00	-0.117408D-02	0.385642D-02	-0.152091D-02	0.271715D-02
30	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00
31	0.000000D+00	0.427281D-02	-0.197356D-02	0.110548D-02	-0.300704D-02
32	0.000000D+00	0.210828D-02	-0.918428D-03	0.720785D-03	-0.177694D-02
33	0.000000D+00	-0.393470D-02	0.124204D-02	-0.103342D-02	0.275225D-02
34	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00
35	0.000000D+00	-0.848253D-03	0.999866D-03	-0.108844D-02	0.605094D-03
36	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00
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45	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00
46	0.000000D+00	-0.117366D-02	0.246950D-02	0.189836D-01	-0.554449D-02
47	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00
48	0.000000D+00	-0.242325D-02	0.648777D-02	-0.278203D-01	0.590953D-02
49	0.000000D+00	-0.212290D-03	0.131209D-01	-0.669994D-02	0.267277D-02
50	0.000000D+00	-0.209571D-02	-0.741966D-02	0.131933D-01	-0.427931D-02
51	0.000000D+00	-0.121335D+01	0.534733D+00	-0.151249D+01	0.635427D+00
	11	12	13	14	15
11	0.000000D+00				
12	0.000000D+00	0.000000D+00			
13	0.000000D+00	0.000000D+00	0.000000D+00		
14	0.000000D+00	0.000000D+00	0.000000D+00	0.385007D+12	
15	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00

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20	0.000000D+00	0.000000D+00	0.000000D+00	-0.842895D-02	0.000000D+00
21	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00
22	0.000000D+00	0.000000D+00	0.000000D+00	-0.792530D-03	0.000000D+00
23	0.000000D+00	0.000000D+00	0.000000D+00	-0.615270D-02	0.000000D+00
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31	0.000000D+00	0.000000D+00	0.000000D+00	-0.152216D-02	0.000000D+00
32	0.000000D+00	0.000000D+00	0.000000D+00	0.572179D-02	0.000000D+00
33	0.000000D+00	0.000000D+00	0.000000D+00	0.133304D-01	0.000000D+00
34	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00
35	0.000000D+00	0.000000D+00	0.000000D+00	0.517560D+00	0.000000D+00
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42	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00
43	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00
44	0.000000D+00	0.000000D+00	0.000000D+00	-0.452777D+00	0.000000D+00
45	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00
46	0.000000D+00	0.000000D+00	0.000000D+00	-0.333775D-02	0.000000D+00
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	16	17	18	19	20
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18	0.000000D+00	0.000000D+00	0.000000D+00		
19	0.000000D+00	0.000000D+00	0.000000D+00	0.385007D+12	
20	0.000000D+00	0.000000D+00	0.000000D+00	-0.725690D+01	0.385007D+12
21	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00
22	0.000000D+00	0.000000D+00	0.000000D+00	0.625127D+01	0.117318D+02
23	0.000000D+00	0.000000D+00	0.000000D+00	0.828558D+00	0.599350D+01
24	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00
25	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00
26	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00
27	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00
28	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00
29	0.000000D+00	0.000000D+00	0.000000D+00	0.335058D-01	0.422173D-01
30	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00
31	0.000000D+00	0.000000D+00	0.000000D+00	-0.504935D-02	-0.400904D-02
32	0.000000D+00	0.000000D+00	0.000000D+00	-0.709870D-02	-0.502213D-02
33	0.000000D+00	0.000000D+00	0.000000D+00	0.186555D-02	0.550792D-03
34	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00
35	0.000000D+00	0.000000D+00	0.000000D+00	-0.261856D-03	0.112882D-02
36	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00

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37  0.000000D+00  0.000000D+00  0.000000D+00  0.000000D+00  0.000000D+00
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51  0.000000D+00  0.000000D+00  0.000000D+00 -0.501085D-02 -0.509139D-02
         21            22            23            24            25
21  0.000000D+00
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23  0.000000D+00 -0.841417D+01  0.385007D+12
24  0.000000D+00  0.000000D+00  0.000000D+00  0.000000D+00
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32  0.000000D+00 -0.117328D-02  0.867300D-03  0.000000D+00  0.000000D+00
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48  0.000000D+00 -0.176699D-03 -0.345239D-03  0.000000D+00  0.000000D+00
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         26            27            28            29            30
26  0.000000D+00
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50	0.000000D+00	0.000000D+00	0.000000D+00	0.649667D-03	0.000000D+00
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	31	32	33	34	35
31	0.385007D+12				
32	0.106875D+01	0.385007D+12			
33	0.858406D+01	0.846453D+01	0.385007D+12		
34	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00	
35	0.160719D+00	0.641355D-01	-0.826281D-01	0.000000D+00	0.385007D+12
36	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00
37	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00
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39	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00
40	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00
41	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00
42	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00
43	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00
44	-0.127944D-02	-0.357341D-03	0.892362D-03	0.000000D+00	0.316180D-02
45	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00
46	-0.818946D-03	-0.297859D-03	0.670710D-03	0.000000D+00	-0.334750D-03
47	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00
48	0.575315D-03	0.159231D-03	-0.389687D-03	0.000000D+00	0.539560D-03
49	0.120881D-02	0.314354D-03	-0.738882D-03	0.000000D+00	0.131287D-02
50	-0.124058D-02	-0.366278D-03	0.902297D-03	0.000000D+00	-0.136856D-02
51	0.362024D-02	0.333765D-03	-0.944969D-03	0.000000D+00	-0.218797D-01

	36	37	38	39	40
36	0.000000D+00				
37	0.000000D+00	0.000000D+00			
38	0.000000D+00	0.000000D+00	0.000000D+00		
39	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00	
40	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00
41	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00
42	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00
43	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00
44	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00
45	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00
46	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00
47	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00
48	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00
49	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00
50	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00
51	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00

	41	42	43	44	45
41	0.000000D+00				
42	0.000000D+00	0.000000D+00			

```
 43  0.000000D+00  0.000000D+00  0.000000D+00
 44  0.000000D+00  0.000000D+00  0.000000D+00  0.385007D+12
 45  0.000000D+00  0.000000D+00  0.000000D+00  0.000000D+00  0.000000D+00
 46  0.000000D+00  0.000000D+00  0.000000D+00  0.193672D+01  0.000000D+00
 47  0.000000D+00  0.000000D+00  0.000000D+00  0.000000D+00  0.000000D+00
 48  0.000000D+00  0.000000D+00  0.000000D+00  0.872652D+01  0.000000D+00
 49  0.000000D+00  0.000000D+00  0.000000D+00  0.624231D+00  0.000000D+00
 50  0.000000D+00  0.000000D+00  0.000000D+00  0.117119D+01  0.000000D+00
 51  0.000000D+00  0.000000D+00  0.000000D+00 -0.308743D+00  0.000000D+00
             46            47            48            49            50
 46  0.385007D+12
 47  0.000000D+00  0.000000D+00
 48  0.590820D+00  0.000000D+00  0.385007D+12
 49  0.841662D+01  0.000000D+00  0.139217D+01  0.385007D+12
 50  0.119046D+01  0.000000D+00  0.815287D+01  0.833866D+01  0.385007D+12
 51 -0.469505D+00  0.000000D+00  0.436658D+00  0.855333D-01 -0.514197D-01
             51
 51  0.385007D+12
```

B

G16 optfreq B3LYP/6-31G(d) gas-phase
HF = -1337.617752

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.503978	4.060092	0.198196
2	6	0	0.330761	3.327887	0.047386
3	6	0	0.337614	1.927685	0.101397
4	6	0	1.545180	1.246933	0.339479
5	6	0	2.718303	1.999410	0.496489
6	6	0	2.706850	3.389108	0.417740
7	1	0	1.476899	5.145511	0.154480
8	1	0	-0.613236	3.843405	-0.088925
9	1	0	3.652699	1.483316	0.692432
10	1	0	3.632515	3.944707	0.542242
11	6	0	1.584963	-0.255253	0.605902
12	1	0	1.486284	-0.347214	1.692785
13	6	0	-0.965034	1.189398	-0.199113
14	6	0	0.328787	-1.007600	0.052610
15	1	0	0.293076	-1.983415	0.554215
16	6	0	-1.005992	-0.257304	0.387548
17	8	0	-2.078018	1.933591	0.289144
18	8	0	-1.135564	1.086609	-1.614611
19	6	0	-2.999550	2.155115	-0.783454
20	1	0	-3.447790	3.143632	-0.647754
21	1	0	-3.785471	1.390937	-0.777922
22	6	0	-2.110119	2.044763	-2.018668
23	1	0	-1.632533	3.001987	-2.268349
24	1	0	-2.621758	1.654689	-2.902189
25	6	0	-2.257748	-1.027937	-0.016720
26	6	0	-3.016397	-1.302624	1.133732
27	6	0	-2.722243	-1.463805	-1.253959
28	6	0	-4.221686	-1.991958	1.087183
29	6	0	-3.936207	-2.163560	-1.321199
30	1	0	-2.151981	-1.269763	-2.153751

31	6	0	-4.675134	-2.420575	-0.165785
32	1	0	-4.791693	-2.192799	1.989876
33	1	0	-4.300092	-2.509334	-2.284214
34	1	0	-5.614032	-2.963396	-0.232956
35	7	0	-2.356475	-0.791906	2.255372
36	1	0	-2.697074	-0.823731	3.206355
37	6	0	-1.176253	-0.158939	1.940914
38	8	0	-0.425295	0.357442	2.747021
39	6	0	0.440852	-1.313203	-1.383553
40	7	0	0.548585	-1.605634	-2.501648
41	6	0	2.876823	-0.965721	0.220166
42	6	0	3.464487	-1.853128	1.131446
43	6	0	3.489535	-0.787492	-1.029059
44	6	0	4.628475	-2.551960	0.807184
45	1	0	3.007216	-1.994480	2.108790
46	6	0	4.653743	-1.482534	-1.354903
47	1	0	3.054322	-0.101275	-1.748655
48	6	0	5.226628	-2.367989	-0.439479
49	1	0	5.068423	-3.233435	1.530601
50	1	0	5.112390	-1.332815	-2.328624
51	1	0	6.134396	-2.907755	-0.695818

G16 #n B3LYP/6-31G(d,p) nmr=(fconly,readatoms) iop(3/10=1100000) gas-phase

Fermi Contact (FC) contribution to J (Hz):

	1	2	3	4	5
1	0.000000D+00				
2	0.000000D+00	0.000000D+00			
3	0.000000D+00	0.000000D+00	0.000000D+00		
4	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00	
5	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00
6	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00
7	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00
8	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00
9	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00
10	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00
11	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00
12	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00
13	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00
14	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00
15	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00
16	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00
17	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00
18	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00
19	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00
20	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00
21	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00
22	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00
23	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00
24	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00
25	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00
26	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00
27	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00
28	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00

29	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00
30	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00
31	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00
32	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00
33	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00
34	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00
35	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00
36	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00
37	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00
38	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00
39	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00
40	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00
41	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00
42	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00
43	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00
44	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00
45	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00
46	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00
47	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00
48	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00
49	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00
50	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00
51	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00

	6	7	8	9	10
6	0.000000D+00				
7	0.000000D+00	0.385007D+12			
8	0.000000D+00	0.875205D+01	0.385007D+12		
9	0.000000D+00	0.127996D+01	0.528908D+00	0.385007D+12	
10	0.000000D+00	0.805253D+01	0.138538D+01	0.876728D+01	0.385007D+12
11	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00
12	0.000000D+00	-0.131015D+01	0.604200D+00	-0.153043D+01	0.611313D+00
13	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00
14	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00
15	0.000000D+00	0.290702D-01	-0.378154D-01	0.133801D+00	0.762594D-01
16	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00
17	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00
18	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00
19	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00
20	0.000000D+00	0.782513D-02	0.333513D-01	0.152578D-02	-0.596040D-02
21	0.000000D+00	-0.576173D-02	0.319033D-01	0.176376D-01	-0.423441D-02
22	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00
23	0.000000D+00	-0.274344D-02	-0.347489D-01	-0.405250D-02	0.191819D-02
24	0.000000D+00	0.188973D-01	0.162515D+00	0.280042D-01	-0.538932D-01
25	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00
26	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00
27	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00
28	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00
29	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00
30	0.000000D+00	0.868179D-03	0.192528D-02	-0.878644D-03	0.956784D-03
31	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00
32	0.000000D+00	0.469988D-02	0.481328D-03	-0.119924D-03	-0.588132D-03
33	0.000000D+00	0.158531D-02	0.116440D-03	0.219251D-03	-0.540120D-03
34	0.000000D+00	-0.312531D-02	-0.849245D-04	-0.179513D-03	0.744490D-03

35	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00
36	0.000000D+00	0.328092D-04	-0.105441D-02	0.324493D-03	-0.115185D-02
37	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00
38	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00
39	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00
40	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00
41	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00
42	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00
43	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00
44	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00
45	0.000000D+00	0.194002D-02	0.670134D-02	0.210627D-01	-0.754920D-02
46	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00
47	0.000000D+00	0.746896D-02	-0.743137D-02	0.260444D+00	-0.268660D-01
48	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00
49	0.000000D+00	-0.258385D-02	0.136200D-01	-0.111076D-01	0.478707D-02
50	0.000000D+00	-0.640661D-02	0.580564D-02	-0.321592D-01	0.864858D-02
51	0.000000D+00	-0.174603D-02	-0.305519D-02	0.959397D-02	-0.542876D-02

	11	12	13	14	15
11	0.000000D+00				
12	0.000000D+00	0.385007D+12			
13	0.000000D+00	0.000000D+00	0.000000D+00		
14	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00	
15	0.000000D+00	0.659437D+01	0.000000D+00	0.000000D+00	0.385007D+12
16	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00
17	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00
18	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00
19	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00
20	0.000000D+00	0.942687D-02	0.000000D+00	0.000000D+00	0.168942D+00
21	0.000000D+00	0.928524D-02	0.000000D+00	0.000000D+00	-0.122611D-01
22	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00
23	0.000000D+00	-0.107135D-01	0.000000D+00	0.000000D+00	0.181106D-01
24	0.000000D+00	0.816233D-01	0.000000D+00	0.000000D+00	-0.850254D-02
25	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00
26	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00
27	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00
28	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00
29	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00
30	0.000000D+00	0.832890D-02	0.000000D+00	0.000000D+00	0.724035D-01
31	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00
32	0.000000D+00	-0.774056D-03	0.000000D+00	0.000000D+00	-0.449199D-02
33	0.000000D+00	0.289920D-03	0.000000D+00	0.000000D+00	-0.137021D-01
34	0.000000D+00	-0.266581D-02	0.000000D+00	0.000000D+00	0.305917D-01
35	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00
36	0.000000D+00	0.817424D-03	0.000000D+00	0.000000D+00	0.183725D+00
37	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00
38	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00
39	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00
40	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00
41	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00
42	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00
43	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00
44	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00
45	0.000000D+00	-0.591945D+00	0.000000D+00	0.000000D+00	0.372165D-01

46	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00
47	0.000000D+00	-0.387348D+00	0.000000D+00	0.000000D+00	0.498423D-01
48	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00
49	0.000000D+00	0.156078D+00	0.000000D+00	0.000000D+00	-0.190120D-01
50	0.000000D+00	0.388191D+00	0.000000D+00	0.000000D+00	-0.214399D-01
51	0.000000D+00	-0.169819D+00	0.000000D+00	0.000000D+00	0.311086D-01

	16	17	18	19	20
16	0.000000D+00				
17	0.000000D+00	0.000000D+00			
18	0.000000D+00	0.000000D+00	0.000000D+00		
19	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00	
20	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00	0.385007D+12
21	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00	-0.748150D+01
22	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00
23	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00	0.638367D+01
24	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00	0.955258D+00
25	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00
26	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00
27	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00
28	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00
29	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00
30	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00	0.100054D-01
31	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00
32	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00	0.168946D-02
33	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00	0.942408D-03
34	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00	-0.853703D-02
35	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00
36	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00	-0.283413D-02
37	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00
38	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00
39	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00
40	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00
41	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00
42	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00
43	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00
44	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00
45	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00	-0.292086D-03
46	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00
47	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00	-0.290578D-03
48	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00
49	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00	0.941213D-04
50	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00	0.191685D-03
51	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00	-0.367218D-03

	21	22	23	24	25
21	0.385007D+12				
22	0.000000D+00	0.000000D+00			
23	0.116536D+02	0.000000D+00	0.385007D+12		
24	0.620044D+01	0.000000D+00	-0.846732D+01	0.385007D+12	
25	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00
26	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00
27	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00
28	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00
29	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00

30	0.294068D-01	0.000000D+00	-0.251421D-01	0.222130D-01	0.000000D+00
31	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00
32	0.938784D-03	0.000000D+00	0.923682D-03	-0.720655D-03	0.000000D+00
33	-0.133582D-02	0.000000D+00	0.512310D-03	0.167094D-02	0.000000D+00
34	-0.601258D-02	0.000000D+00	-0.257432D-04	0.641178D-03	0.000000D+00
35	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00
36	-0.451014D-02	0.000000D+00	0.921734D-02	0.308608D-02	0.000000D+00
37	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00
38	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00
39	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00
40	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00
41	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00
42	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00
43	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00
44	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00
45	0.229231D-04	0.000000D+00	-0.106410D-03	-0.827058D-05	0.000000D+00
46	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00
47	-0.505888D-04	0.000000D+00	0.374321D-03	0.120753D-02	0.000000D+00
48	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00
49	-0.110781D-04	0.000000D+00	0.607043D-04	0.893252D-04	0.000000D+00
50	0.177321D-04	0.000000D+00	0.555760D-04	0.329599D-03	0.000000D+00
51	0.332069D-04	0.000000D+00	0.210575D-05	0.304484D-03	0.000000D+00

	26	27	28	29	30
26	0.000000D+00				
27	0.000000D+00	0.000000D+00			
28	0.000000D+00	0.000000D+00	0.000000D+00		
29	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00	
30	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00	0.385007D+12
31	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00
32	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00	0.593364D+00
33	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00	0.862782D+01
34	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00	0.122358D+01
35	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00
36	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00	0.741845D+00
37	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00
38	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00
39	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00
40	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00
41	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00
42	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00
43	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00
44	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00
45	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00	0.112382D-02
46	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00
47	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00	0.205672D-02
48	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00
49	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00	-0.652379D-03
50	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00	-0.361157D-03
51	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00	0.816757D-03

	31	32	33	34	35
31	0.000000D+00				
32	0.000000D+00	0.385007D+12			
33	0.000000D+00	0.108942D+01	0.385007D+12		

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34  0.000000D+00  0.857654D+01  0.845181D+01  0.385007D+12
35  0.000000D+00  0.000000D+00  0.000000D+00  0.000000D+00  0.000000D+00
36  0.000000D+00  0.171302D+00  0.757629D-01 -0.864912D-01  0.000000D+00
37  0.000000D+00  0.000000D+00  0.000000D+00  0.000000D+00  0.000000D+00
38  0.000000D+00  0.000000D+00  0.000000D+00  0.000000D+00  0.000000D+00
39  0.000000D+00  0.000000D+00  0.000000D+00  0.000000D+00  0.000000D+00
40  0.000000D+00  0.000000D+00  0.000000D+00  0.000000D+00  0.000000D+00
41  0.000000D+00  0.000000D+00  0.000000D+00  0.000000D+00  0.000000D+00
42  0.000000D+00  0.000000D+00  0.000000D+00  0.000000D+00  0.000000D+00
43  0.000000D+00  0.000000D+00  0.000000D+00  0.000000D+00  0.000000D+00
44  0.000000D+00  0.000000D+00  0.000000D+00  0.000000D+00  0.000000D+00
45  0.000000D+00 -0.691348D-03 -0.532684D-03  0.903175D-03  0.000000D+00
46  0.000000D+00  0.000000D+00  0.000000D+00  0.000000D+00  0.000000D+00
47  0.000000D+00 -0.856007D-03 -0.696059D-03  0.103041D-02  0.000000D+00
48  0.000000D+00  0.000000D+00  0.000000D+00  0.000000D+00  0.000000D+00
49  0.000000D+00  0.110755D-02  0.592726D-03 -0.114517D-02  0.000000D+00
50  0.000000D+00  0.977992D-03  0.381569D-03 -0.842073D-03  0.000000D+00
51  0.000000D+00 -0.148430D-02 -0.712125D-03  0.131299D-02  0.000000D+00
          36            37            38            39            40
36  0.385007D+12
37  0.000000D+00  0.000000D+00
38  0.000000D+00  0.000000D+00  0.000000D+00
39  0.000000D+00  0.000000D+00  0.000000D+00  0.000000D+00
40  0.000000D+00  0.000000D+00  0.000000D+00  0.000000D+00  0.000000D+00
41  0.000000D+00  0.000000D+00  0.000000D+00  0.000000D+00  0.000000D+00
42  0.000000D+00  0.000000D+00  0.000000D+00  0.000000D+00  0.000000D+00
43  0.000000D+00  0.000000D+00  0.000000D+00  0.000000D+00  0.000000D+00
44  0.000000D+00  0.000000D+00  0.000000D+00  0.000000D+00  0.000000D+00
45 -0.196894D-04  0.000000D+00  0.000000D+00  0.000000D+00  0.000000D+00
46  0.000000D+00  0.000000D+00  0.000000D+00  0.000000D+00  0.000000D+00
47 -0.128644D-03  0.000000D+00  0.000000D+00  0.000000D+00  0.000000D+00
48  0.000000D+00  0.000000D+00  0.000000D+00  0.000000D+00  0.000000D+00
49 -0.312275D-04  0.000000D+00  0.000000D+00  0.000000D+00  0.000000D+00
50 -0.129662D-03  0.000000D+00  0.000000D+00  0.000000D+00  0.000000D+00
51  0.125305D-03  0.000000D+00  0.000000D+00  0.000000D+00  0.000000D+00
          41            42            43            44            45
41  0.000000D+00
42  0.000000D+00  0.000000D+00
43  0.000000D+00  0.000000D+00  0.000000D+00
44  0.000000D+00  0.000000D+00  0.000000D+00  0.000000D+00
45  0.000000D+00  0.000000D+00  0.000000D+00  0.000000D+00  0.385007D+12
46  0.000000D+00  0.000000D+00  0.000000D+00  0.000000D+00  0.000000D+00
47  0.000000D+00  0.000000D+00  0.000000D+00  0.000000D+00  0.195875D+01
48  0.000000D+00  0.000000D+00  0.000000D+00  0.000000D+00  0.000000D+00
49  0.000000D+00  0.000000D+00  0.000000D+00  0.000000D+00  0.839360D+01
50  0.000000D+00  0.000000D+00  0.000000D+00  0.000000D+00  0.585367D+00
51  0.000000D+00  0.000000D+00  0.000000D+00  0.000000D+00  0.120281D+01
          46            47            48            49            50
46  0.000000D+00
47  0.000000D+00  0.385007D+12
48  0.000000D+00  0.000000D+00  0.000000D+00
49  0.000000D+00  0.629729D+00  0.000000D+00  0.385007D+12
50  0.000000D+00  0.882030D+01  0.000000D+00  0.141821D+01  0.385007D+12
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51 0.000000D+00 0.116232D+01 0.000000D+00 0.828814D+01 0.818140D+01
51
51 0.385007D+12

18c

A (Conformer 1)

G16 optfreq B3LYP/6-31G(d,p) gas-phase

Sum of electronic and thermal Free Energies= -2004.673046

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.655430	1.504604	-0.520464
2	6	0	-4.188843	2.727035	-0.656605
3	6	0	-2.823593	0.732265	-0.339570
4	6	0	-1.788634	2.881736	-0.759567
5	6	0	-3.035468	3.493809	-0.828329
6	6	0	-4.075109	1.363244	-0.415718
7	1	0	-0.891837	3.478903	-0.893810
8	1	0	-3.105384	4.561076	-1.015718
9	1	0	-4.965647	0.759847	-0.273907
10	1	0	-5.170080	3.188745	-0.708613
11	6	0	-0.245892	0.942740	-0.415557
12	6	0	0.121607	-0.180031	-1.383335
13	6	0	0.643179	1.206688	-1.632296
14	1	0	-0.646746	-0.649267	-1.986936
15	1	0	0.282654	1.848625	-2.426713
16	6	0	0.341468	1.016947	0.981409
17	6	0	1.332988	1.249156	3.601544
18	6	0	1.016356	2.175522	1.390575
19	6	0	0.172009	-0.025223	1.902873
20	6	0	0.665418	0.090708	3.203356
21	6	0	1.509627	2.290608	2.689725
22	1	0	1.172922	2.983678	0.682730
23	1	0	-0.339798	-0.936182	1.611136
24	1	0	0.524709	-0.727225	3.903630
25	1	0	2.036792	3.192540	2.986036
26	1	0	1.717211	1.337857	4.613329
27	6	0	-2.774120	-0.761040	-0.092420
28	16	0	-3.628011	-1.284912	1.490307
29	6	0	-4.403319	-2.825125	0.830099
30	6	0	-3.721581	-3.217836	-0.481403
31	16	0	-3.532135	-1.701647	-1.486613
32	1	0	-1.745548	-1.096645	-0.004788
33	1	0	-4.284673	-3.610532	1.582174
34	1	0	-5.468724	-2.643997	0.671856
35	1	0	-4.330800	-3.924557	-1.052266
36	1	0	-2.740512	-3.666141	-0.300543
37	6	0	1.309627	-1.019934	-1.008346
38	6	0	2.129975	1.136816	-1.427954

39	7	0	2.442791	-0.178654	-1.016692
40	8	0	1.310147	-2.204250	-0.748773
41	8	0	2.931267	2.029426	-1.602028
42	6	0	3.751992	-0.602388	-0.626350
43	6	0	6.303428	-1.430804	0.137461
44	6	0	4.859906	-0.239262	-1.398174
45	6	0	3.914558	-1.377038	0.526632
46	6	0	5.191247	-1.792848	0.899257
47	6	0	6.133217	-0.651229	-1.006988
48	1	0	4.724385	0.368966	-2.283275
49	1	0	3.050104	-1.651006	1.118164
50	1	0	5.315137	-2.397851	1.792375
51	1	0	6.993019	-0.363496	-1.604441
52	1	0	7.296617	-1.753934	0.434608

A (Conformer 2)

G16 optfreq B3LYP/6-31G(d,p) gas-phase

Sum of electronic and thermal Free Energies= -2004.672525

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.651554	1.503822	-0.500488
2	6	0	4.174275	2.751882	-0.611021
3	6	0	2.826236	0.738896	-0.332154
4	6	0	1.773354	2.886424	-0.715697
5	6	0	3.014027	3.511520	-0.769036
6	6	0	4.072537	1.382282	-0.401907
7	1	0	0.871323	3.477121	-0.843183
8	1	0	3.074325	4.582460	-0.937849
9	1	0	4.969082	0.781502	-0.289829
10	1	0	5.151510	3.222779	-0.655287
11	6	0	0.244203	0.934625	-0.407449
12	6	0	-0.634976	1.195033	-1.632647
13	6	0	-0.115447	-0.190828	-1.374870
14	1	0	-0.266381	1.834678	-2.425218
15	1	0	0.653846	-0.663457	-1.974368
16	6	0	-0.356061	1.008723	0.983883
17	6	0	-1.374016	1.233241	3.594196
18	6	0	-0.176186	-0.026562	1.910733
19	6	0	-1.053849	2.157253	1.382660
20	6	0	-1.560206	2.268418	2.677188
21	6	0	-0.683013	0.085003	3.206235
22	1	0	0.356119	-0.927460	1.625107
23	1	0	-1.218709	2.959918	0.670496
24	1	0	-2.105213	3.162244	2.965655
25	1	0	-0.534363	-0.727599	3.911100
26	1	0	-1.768757	1.318825	4.602201
27	6	0	2.795252	-0.756379	-0.096506

28	16	0	3.597293	-1.700619	-1.503916
29	6	0	4.376774	-3.022490	-0.477780
30	6	0	3.774817	-2.998230	0.928756
31	16	0	3.634816	-1.254738	1.466097
32	1	0	1.770977	-1.112171	-0.036259
33	1	0	4.193257	-3.985623	-0.962390
34	1	0	5.453311	-2.842324	-0.441415
35	1	0	4.416617	-3.518658	1.645477
36	1	0	2.786906	-3.467755	0.939959
37	6	0	-2.123593	1.125809	-1.442827
38	6	0	-1.307109	-1.028894	-1.004520
39	7	0	-2.440087	-0.187608	-1.028555
40	8	0	-2.923318	2.017526	-1.628601
41	8	0	-1.310310	-2.211012	-0.736306
42	6	0	-3.752697	-0.608878	-0.647079
43	6	0	-6.310953	-1.431731	0.099436
44	6	0	-3.925808	-1.374447	0.510399
45	6	0	-4.853385	-0.251959	-1.431962
46	6	0	-6.130239	-0.661078	-1.049441
47	6	0	-5.205864	-1.787587	0.874366
48	1	0	-3.066805	-1.643496	1.112078
49	1	0	-4.709627	0.349265	-2.320569
50	1	0	-6.984479	-0.378206	-1.657104
51	1	0	-5.338002	-2.385621	1.770993
52	1	0	-7.306815	-1.752758	0.389827

B (Conformer 1)

G16 optfreq B3LYP/6-31G(d,p) gas-phase

Sum of electronic and thermal Free Energies= -2004.669255

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.033234	-1.948922	-0.314231
2	6	0	-4.638316	-3.008403	-0.386096
3	6	0	-2.461874	-2.865614	0.657885
4	6	0	-2.932594	-1.566874	-1.315890
5	6	0	-4.226403	-2.092399	-1.351596
6	6	0	-3.750136	-3.393215	0.621170
7	1	0	-2.634305	-0.846717	-2.071054
8	1	0	-4.909904	-1.778270	-2.134608
9	1	0	-4.061087	-4.105431	1.379792
10	1	0	-5.643547	-3.418029	-0.414254
11	6	0	-0.619501	-1.395098	-0.237074
12	6	0	0.455425	-2.379203	-0.711103
13	6	0	0.086541	-1.206095	-1.576290
14	1	0	0.168093	-3.400771	-0.928662
15	1	0	-0.472779	-1.294092	-2.499315
16	6	0	-0.370482	-0.509911	0.971941

17	6	0	-0.036643	0.934276	3.364227
18	6	0	0.204310	-1.103615	2.107954
19	6	0	-0.782822	0.840771	1.042805
20	6	0	-0.606798	1.536522	2.248443
21	6	0	0.377080	-0.395301	3.292983
22	1	0	0.535631	-2.135252	2.053178
23	1	0	-0.922584	2.572996	2.297065
24	1	0	0.832697	-0.880025	4.150966
25	1	0	0.087159	1.501597	4.281738
26	6	0	1.874009	-2.147025	-0.274463
27	6	0	1.291853	-0.309119	-1.604706
28	7	0	2.277741	-0.891417	-0.777873
29	8	0	2.566789	-2.905012	0.371144
30	8	0	1.416351	0.717549	-2.235529
31	6	0	3.540111	-0.279783	-0.494943
32	6	0	5.996915	0.920535	0.059880
33	6	0	3.596590	1.088558	-0.209456
34	6	0	4.707639	-1.049798	-0.505376
35	6	0	5.931006	-0.444429	-0.220521
36	6	0	4.827580	1.682630	0.061166
37	1	0	2.689745	1.680110	-0.210219
38	1	0	4.653500	-2.109362	-0.718338
39	1	0	6.835273	-1.045555	-0.223467
40	1	0	4.868744	2.745800	0.277666
41	1	0	6.953057	1.387862	0.275627
42	1	0	-1.779473	-3.164995	1.447514
43	6	0	-1.430881	1.547332	-0.133797
44	1	0	-1.317946	0.951275	-1.035639
45	16	0	-3.284226	1.794102	0.078059
46	16	0	-0.651773	3.196238	-0.452126
47	6	0	-3.307721	3.618583	-0.135314
48	1	0	-4.282948	3.876726	-0.560055
49	1	0	-3.200524	4.115171	0.832225
50	6	0	-2.169710	4.003697	-1.072927
51	1	0	-2.378511	3.689832	-2.099276
52	1	0	-1.985260	5.082712	-1.063629

B (Conformer 2)

G16 optfreq B3LYP/6-31G(d,p) gas-phase

Sum of electronic and thermal Free Energies= -2004.671956

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.072066	-1.959067	-0.275817
2	6	0	4.684136	-3.004273	-0.301373
3	6	0	2.962133	-1.633930	-1.305411
4	6	0	2.514287	-2.810657	0.748161
5	6	0	3.806010	-3.330983	0.734682

6	6	0	4.258800	-2.152705	-1.318730
7	1	0	1.839837	-3.064575	1.560203
8	1	0	4.127324	-3.992286	1.533991
9	1	0	4.934662	-1.883699	-2.124901
10	1	0	5.691944	-3.408362	-0.311734
11	6	0	0.654442	-1.414635	-0.222004
12	6	0	-0.049867	-1.249480	-1.564465
13	6	0	-0.412462	-2.415072	-0.687421
14	1	0	0.505880	-1.342409	-2.489098
15	1	0	-0.113085	-3.436006	-0.890875
16	6	0	0.380387	-0.497203	0.956617
17	6	0	-0.065171	1.048734	3.264831
18	6	0	-0.214961	-1.053089	2.101860
19	6	0	0.765603	0.861865	0.978624
20	6	0	0.528116	1.610285	2.140915
21	6	0	-0.439996	-0.295096	3.246078
22	1	0	-0.523535	-2.093159	2.083989
23	1	0	0.819621	2.655208	2.152385
24	1	0	-0.909819	-0.750162	4.112566
25	1	0	-0.236126	1.655897	4.148621
26	6	0	-1.255855	-0.351949	-1.589288
27	6	0	-1.835013	-2.191720	-0.260607
28	7	0	-2.243004	-0.939885	-0.771769
29	8	0	-1.376080	0.684781	-2.205927
30	8	0	-2.528554	-2.949777	0.383487
31	6	0	-3.505262	-0.329652	-0.484921
32	6	0	-5.962577	0.863077	0.077337
33	6	0	-4.674388	-1.095493	-0.527718
34	6	0	-3.558790	1.030234	-0.161936
35	6	0	-4.790855	1.620837	0.111950
36	6	0	-5.898824	-0.494204	-0.238960
37	1	0	-4.620569	-2.149138	-0.769457
38	1	0	-2.649295	1.617473	-0.132810
39	1	0	-4.831042	2.677707	0.357513
40	1	0	-6.805089	-1.091635	-0.267083
41	1	0	-6.919365	1.327885	0.295723
42	1	0	2.654112	-0.963365	-2.101404
43	6	0	1.443266	1.531203	-0.203812
44	1	0	1.426286	0.872526	-1.067811
45	16	0	0.613459	3.097465	-0.795384
46	16	0	3.220861	1.916988	0.200006
47	6	0	1.959799	4.256637	-0.342808
48	1	0	1.835683	5.142270	-0.974027
49	1	0	1.885625	4.557708	0.705720
50	6	0	3.283971	3.555580	-0.616909
51	1	0	3.453863	3.444743	-1.690925
52	1	0	4.128094	4.095845	-0.175884

<u>18c</u>

A

G16 optfreq B3LYP/6-31G(d,p) gas-phase

Sum of electronic and thermal Free Energies= -1303.366173

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	0.771008	3.488874	-0.727764
2	6	0	1.619969	2.846899	-0.521371
3	6	0	3.807210	1.216898	0.009152
4	6	0	1.423573	1.462318	-0.414917
5	6	0	2.884993	3.407423	-0.361838
6	6	0	3.985358	2.592463	-0.088808
7	6	0	2.539821	0.651777	-0.162567
8	1	0	3.010081	4.482834	-0.449040
9	1	0	4.972492	3.025610	0.040554
10	1	0	4.648688	0.563163	0.210606
11	6	0	2.412528	-0.852570	-0.076438
12	6	0	0.053501	0.828974	-0.652628
13	1	0	0.016470	0.569799	-1.717886
14	8	0	1.117267	-1.334723	-0.375236
15	6	0	-0.034557	-0.575986	0.067434
16	8	0	3.273176	-1.486847	-0.986591
17	8	0	2.826859	-1.291303	1.204570
18	6	0	3.718330	-2.718561	-0.401846
19	1	0	3.324795	-3.570754	-0.964770
20	1	0	4.812327	-2.736787	-0.443293
21	6	0	3.175627	-2.668184	1.041183
22	1	0	2.292494	-3.304476	1.164034
23	1	0	3.917742	-2.921119	1.801154
24	6	0	-1.234911	-1.355538	-0.456874
25	6	0	-3.473967	-2.701630	-1.500213
26	6	0	-1.241805	-1.804431	-1.783339
27	6	0	-2.353574	-1.614883	0.352197
28	6	0	-3.468922	-2.279290	-0.177228
29	6	0	-2.349854	-2.472198	-2.300557
30	1	0	-0.364005	-1.649395	-2.401361
31	1	0	-4.311768	-2.456298	0.482500
32	1	0	-2.335035	-2.818415	-3.330089
33	1	0	-4.338658	-3.217350	-1.907048
34	6	0	-0.042928	-0.430628	1.571603
35	1	0	0.866959	-0.044706	2.018216
36	6	0	-1.097779	-0.718326	2.344081
37	1	0	-1.075856	-0.564667	3.419080
38	6	0	-2.358979	-1.255475	1.799062
39	8	0	-3.339366	-1.435401	2.514667
40	6	0	-1.138122	1.734749	-0.378994
41	6	0	-3.392259	3.363954	0.076388
42	6	0	-1.277574	2.451793	0.819399
43	6	0	-2.146928	1.856569	-1.343969
44	6	0	-3.264860	2.661248	-1.121238
45	6	0	-2.392928	3.257549	1.045205

46	1	0	-0.503771	2.389251	1.577218
47	1	0	-2.058384	1.308738	-2.278045
48	1	0	-4.033603	2.738005	-1.884586
49	1	0	-2.480527	3.802963	1.980346
50	1	0	-4.260708	3.991449	0.253598

B

G16 optfreq B3LYP/6-31G(d,p) gas-phase

Sum of electronic and thermal Free Energies= -1303.365951

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.554749	0.575017	-1.225573
2	6	0	-4.325483	0.584840	-1.687113
3	6	0	-2.419763	-0.113671	-0.368808
4	6	0	-2.095523	1.269592	-2.316163
5	6	0	-3.467189	1.276409	-2.547896
6	6	0	-3.799945	-0.108914	-0.603197
7	1	0	-1.428159	1.809031	-2.982742
8	1	0	-3.868755	1.817009	-3.399953
9	1	0	-4.450064	-0.655106	0.071398
10	1	0	-5.396615	0.586581	-1.864380
11	6	0	-0.055358	0.595027	-0.969617
12	1	0	0.456010	0.545613	-1.936294
13	6	0	-1.888888	-0.885303	0.819993
14	8	0	-0.483941	-0.818817	0.976915
15	6	0	0.345920	-0.729249	-0.198201
16	8	0	-2.433186	-0.394278	2.020523
17	8	0	-2.311707	-2.232173	0.737786
18	6	0	-2.590194	-1.495156	2.927357
19	1	0	-1.920187	-1.380261	3.785059
20	1	0	-3.626683	-1.497714	3.279978
21	6	0	-2.245553	-2.734115	2.075263
22	1	0	-1.239791	-3.108576	2.294021
23	1	0	-2.967923	-3.547647	2.166649
24	6	0	0.374990	1.897491	-0.299602
25	6	0	1.203489	4.323303	0.862955
26	6	0	1.463185	2.609570	-0.820384
27	6	0	-0.299789	2.424028	0.812047
28	6	0	0.116209	3.623489	1.389713
29	6	0	1.876272	3.812315	-0.246749
30	1	0	1.996553	2.215222	-1.681591
31	1	0	-1.148760	1.896271	1.233090
32	1	0	-0.416889	4.015325	2.251353
33	1	0	2.721447	4.348324	-0.668912
34	1	0	1.520005	5.260701	1.311091
35	6	0	1.785268	-0.679991	0.297485
36	6	0	4.466376	-0.455171	1.122936

37	6	0	2.109416	-0.019025	1.487276
38	6	0	2.820205	-1.259347	-0.460461
39	6	0	4.154272	-1.131493	-0.049736
40	6	0	3.437145	0.087135	1.898025
41	1	0	1.317457	0.407772	2.088921
42	1	0	4.919756	-1.592646	-0.664936
43	1	0	3.668697	0.599466	2.827397
44	1	0	5.500031	-0.361603	1.442462
45	6	0	0.119694	-1.892821	-1.147312
46	1	0	-0.908396	-2.200281	-1.300885
47	6	0	1.105958	-2.471180	-1.844236
48	1	0	0.908502	-3.244873	-2.580382
49	6	0	2.523664	-2.108129	-1.650111
50	8	0	3.404584	-2.539795	-2.387560

18j

A

G16 optfreq B3LYP/6-31G(d,p) gas-phase

Sum of electronic and thermal Free Energies= -1450.876562

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	-0.323028	3.366759	-1.134171
2	6	0	0.667158	2.953352	-0.980879
3	6	0	3.214513	1.919594	-0.591333
4	6	0	0.805736	1.590623	-0.679408
5	6	0	1.779792	3.785183	-1.080145
6	6	0	3.061794	3.271360	-0.877938
7	6	0	2.098233	1.083233	-0.503609
8	1	0	1.643043	4.837148	-1.313462
9	1	0	3.931972	3.916746	-0.948757
10	1	0	4.200384	1.494191	-0.439116
11	6	0	2.327796	-0.379855	-0.224422
12	8	0	1.140850	-1.162274	-0.293427
13	6	0	-0.130560	-0.675375	0.130577
14	6	0	-0.416662	0.666262	-0.645838
15	8	0	3.186444	-0.953476	-1.179696
16	8	0	2.966034	-0.549916	1.016522
17	6	0	3.587784	-1.835402	0.954441
18	1	0	2.872697	-2.614532	1.238465
19	1	0	4.429749	-1.837160	1.649326
20	6	0	3.998441	-1.939641	-0.525337
21	1	0	5.050118	-1.681678	-0.690656
22	1	0	3.803220	-2.930044	-0.948131
23	6	0	-1.133871	-1.773561	-0.287252
24	6	0	-2.929738	-3.759551	-1.173656
25	6	0	-0.706141	-2.803702	-1.137619

26	6	0	-2.482412	-1.749321	0.102813
27	6	0	-3.366953	-2.735520	-0.335127
28	6	0	-1.594888	-3.786192	-1.574118
29	1	0	0.327005	-2.831686	-1.456365
30	1	0	-2.853956	-0.968368	0.749825
31	1	0	-4.404141	-2.696325	-0.015212
32	1	0	-1.236891	-4.574655	-2.230018
33	1	0	-3.621256	-4.525858	-1.511767
34	6	0	-0.085703	-0.542470	1.683601
35	9	0	-1.305524	-0.379988	2.244169
36	9	0	0.452137	-1.647646	2.229693
37	9	0	0.651503	0.517803	2.081550
38	1	0	-0.538248	0.299709	-1.672952
39	6	0	-1.714397	1.387095	-0.294459
40	6	0	-4.125730	2.733174	0.263592
41	6	0	-2.800153	1.316814	-1.177160
42	6	0	-1.853333	2.157961	0.870542
43	6	0	-3.047950	2.820173	1.147674
44	6	0	-3.997173	1.980810	-0.903041
45	1	0	-2.708094	0.731994	-2.088177
46	1	0	-1.021710	2.244604	1.560395
47	1	0	-3.135311	3.409219	2.056041
48	1	0	-4.824379	1.910602	-1.603356
49	1	0	-5.054341	3.252871	0.480799

B

G16 optfreq B3LYP/6-31G(d,p) gas-phase

Sum of electronic and thermal Free Energies= -1450.881990

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	-4.246487	0.385193	0.724374
2	6	0	-3.560238	0.953540	0.106221
3	6	0	-3.999398	2.067618	-0.599793
4	1	0	-5.036811	2.380578	-0.532469
5	6	0	-3.098302	2.778012	-1.398439
6	1	0	-3.432299	3.646908	-1.957888
7	6	0	-1.770505	2.371154	-1.479594
8	1	0	-1.068946	2.927651	-2.095033
9	6	0	-1.317561	1.251043	-0.770604
10	6	0	0.152530	0.853658	-0.841271
11	6	0	-2.224540	0.546168	0.023760
12	6	0	0.341444	-0.655569	-0.489889
13	8	0	-0.407473	-0.983561	0.675684
14	6	0	-1.795633	-0.677974	0.795104
15	8	0	-2.011329	-0.504114	2.175482
16	8	0	-2.570470	-1.790034	0.425296
17	6	0	1.801474	-1.029345	-0.181927

18	6	0	2.834110	-0.686061	-1.065780
19	1	0	2.616265	-0.143637	-1.977834
20	6	0	4.152964	-1.042022	-0.790740
21	1	0	4.938038	-0.763831	-1.487671
22	6	0	4.463884	-1.748783	0.371253
23	1	0	5.492181	-2.024746	0.585686
24	6	0	3.442504	-2.095202	1.253843
25	1	0	3.670193	-2.644834	2.162674
26	6	0	2.121030	-1.740649	0.979246
27	1	0	1.333001	-2.007187	1.670789
28	6	0	-0.129088	-1.558295	-1.673513
29	6	0	0.987902	1.802230	0.020603
30	6	0	1.914127	2.655110	-0.591005
31	1	0	2.054836	2.608704	-1.668235
32	6	0	2.661684	3.563149	0.160630
33	1	0	3.374405	4.215820	-0.335414
34	6	0	2.493139	3.627992	1.542807
35	1	0	3.072819	4.332090	2.132589
36	6	0	1.570271	2.782854	2.162676
37	1	0	1.429580	2.828488	3.238856
38	6	0	0.818499	1.881241	1.410823
39	1	0	0.099201	1.238797	1.907110
40	1	0	0.482359	0.982942	-1.876979
41	6	0	-2.363099	-1.775718	2.740459
42	6	0	-2.474407	-2.707141	1.517189
43	1	0	-1.594764	-2.102330	3.448179
44	1	0	-3.312963	-1.659727	3.272633
45	1	0	-1.588373	-3.340931	1.402465
46	1	0	-3.371708	-3.328973	1.515048
47	9	0	-0.042710	-2.857696	-1.341238
48	9	0	-1.395090	-1.318680	-2.061503
49	9	0	0.645235	-1.358220	-2.769805

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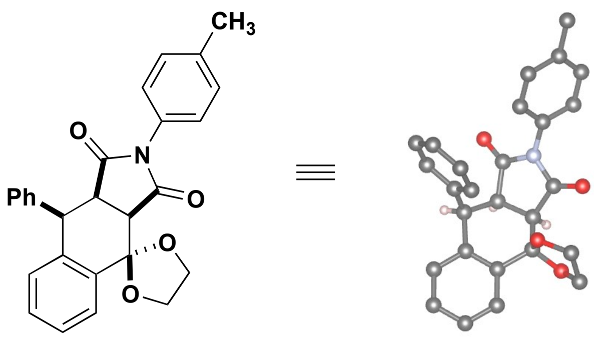
X-ray Structure Data



CCDC 2087127

Table 1. Crystal data and structure refinement for [$C_{27}H_{23}NO_4$].

Identification code	JF2923FMI (MG-3-185-1-2)	
Empirical formula	C27 H23 N O4	
Formula weight	425.46	
Temperature	90(2) K	
Wavelength	1.54178 Å	
Crystal system	Orthorhombic	
Space group	$Pna2_1$	
Unit cell dimensions	a = 9.6342(6) Å	⟨= 90°.
	b = 21.7612(13) Å	®= 90°.
	c = 9.6649(6) Å	© = 90°.
Volume	2026.3(2) $Å^3$	
Z	4	
Density (calculated)	1.395 Mg/m^3	

Absorption coefficient	0.756 mm^{-1}
F(000)	896
Crystal size	0.547 x 0.446 x 0.106 mm^3
Crystal color and habit	Colorless Plate
Diffractometer	Bruker APEX-II CCD
Theta range for data collection	4.063 to 69.555°.
Index ranges	-11<=h<=11, -26<=k<=26, -11<=l<=11
Reflections collected	9041
Independent reflections	3667 [R(int) = 0.0189]
Observed reflections (I > 2sigma(I))	3659
Completeness to theta = 67.679°	99.6 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.8184 and 0.6917
Solution method	SHELXT (Sheldrick, 2014)
Refinement method	SHELXL-2018/3 (Sheldrick, 2018) Full-matrix least-squares on F^2
Data / restraints / parameters	3667 / 7 / 382
Goodness-of-fit on F^2	1.072
Final R indices [I>2sigma(I)]	R1 = 0.0297, wR2 = 0.0776
R indices (all data)	R1 = 0.0297, wR2 = 0.0776
Absolute structure parameters	Flack = 0.04(10), Parson's = 0.12(3), Hooft = 0.06(7)
Extinction coefficient	0.0036(5)
Largest diff. peak and hole	0.213 and -0.156 e.$Å^{-3}$

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for JF2923FMI. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
C(1)	4508(2)	5792(1)	6564(2)	16(1)
N(1)	3178(2)	5959(1)	6143(2)	16(1)
O(1)	4974(2)	5890(1)	7702(2)	22(1)
C(2)	5194(2)	5449(1)	5371(2)	15(1)
C(3)	4140(2)	5476(1)	4182(2)	15(1)
C(4)	2829(2)	5726(1)	4837(2)	16(1)
O(4)	1684(2)	5741(1)	4338(2)	21(1)
C(5)	6702(2)	5656(1)	5092(2)	15(1)
O(5)	6956(2)	6268(1)	5554(2)	17(1)
C(6)	7057(2)	5641(1)	3553(2)	15(1)

O(6)	7578(2)	5265(1)	5884(2)	18(1)
C(7)	6065(2)	5792(1)	2557(2)	14(1)
C(8)	4537(2)	5871(1)	2898(2)	15(1)
C(9)	8435(2)	5546(1)	3153(2)	18(1)
C(10)	8835(2)	5613(1)	1783(2)	19(1)
C(11)	7861(2)	5782(1)	794(2)	19(1)
C(12)	6489(2)	5869(1)	1180(2)	16(1)
C(13)	2268(2)	6344(1)	6927(2)	16(1)
C(14)	1895(2)	6911(1)	6373(2)	19(1)
C(15)	1034(2)	7301(1)	7112(2)	20(1)
C(16)	531(2)	7134(1)	8419(2)	18(1)
C(17)	926(2)	6566(1)	8953(2)	18(1)
C(18)	1788(2)	6170(1)	8228(2)	18(1)
C(19)	-423(3)	7555(1)	9198(2)	26(1)
C(20)	7889(2)	6255(1)	6718(3)	25(1)
C(21)	8588(2)	5636(1)	6588(2)	24(1)
C(22)	4082(2)	6542(1)	2943(2)	15(1)
C(23)	4771(2)	6993(1)	3706(2)	18(1)
C(24)	4309(2)	7600(1)	3668(2)	20(1)
C(25)	3167(2)	7761(1)	2886(2)	21(1)
C(26)	2469(2)	7316(1)	2132(2)	22(1)
C(27)	2927(2)	6711(1)	2162(2)	19(1)

Table 3. Bond lengths [Å] and angles [°] for JF2923FMI.

C(1)-O(1)	1.208(3)
C(1)-N(1)	1.392(3)
C(1)-C(2)	1.524(3)
N(1)-C(4)	1.401(3)
N(1)-C(13)	1.429(3)
C(2)-C(3)	1.534(3)
C(2)-C(5)	1.545(3)
C(2)-H(2)	1.01(3)
C(3)-C(4)	1.515(3)
C(3)-C(8)	1.557(3)

C(3)-H(3)	1.00(3)
C(4)-O(4)	1.204(3)
C(5)-O(6)	1.421(2)
C(5)-O(5)	1.427(2)
C(5)-C(6)	1.527(3)
O(5)-C(20)	1.440(3)
C(6)-C(7)	1.395(3)
C(6)-C(9)	1.398(3)
O(6)-C(21)	1.436(3)
C(7)-C(12)	1.402(3)
C(7)-C(8)	1.518(3)
C(8)-C(22)	1.527(3)
C(8)-H(8)	0.98(3)
C(9)-C(10)	1.387(3)
C(9)-H(9)	0.98(3)
C(10)-C(11)	1.389(3)
C(10)-H(10)	0.97(3)
C(11)-C(12)	1.386(3)
C(11)-H(11)	0.95(3)
C(12)-H(12)	0.97(3)
C(13)-C(18)	1.393(3)
C(13)-C(14)	1.393(3)
C(14)-C(15)	1.384(3)
C(14)-H(14)	0.95(3)
C(15)-C(16)	1.400(3)
C(15)-H(15)	0.97(3)
C(16)-C(17)	1.394(3)
C(16)-C(19)	1.500(3)
C(17)-C(18)	1.387(3)
C(17)-H(17)	0.95(3)
C(18)-H(18)	0.95(3)
C(19)-H(19A)	0.96(2)
C(19)-H(19B)	0.95(2)
C(19)-H(19C)	0.95(2)
C(20)-C(21)	1.511(3)
C(20)-H(20A)	1.03(3)

C(20)-H(20B)	1.00(3)
C(21)-H(21A)	1.00(3)
C(21)-H(21B)	0.95(3)
C(22)-C(27)	1.394(3)
C(22)-C(23)	1.394(3)
C(23)-C(24)	1.394(3)
C(23)-H(23)	0.98(3)
C(24)-C(25)	1.381(3)
C(24)-H(24)	0.98(3)
C(25)-C(26)	1.386(3)
C(25)-H(25)	0.97(3)
C(26)-C(27)	1.389(3)
C(26)-H(26)	0.94(3)
C(27)-H(27)	1.01(3)

O(1)-C(1)-N(1)	124.2(2)
O(1)-C(1)-C(2)	127.94(19)
N(1)-C(1)-C(2)	107.82(17)
C(1)-N(1)-C(4)	112.95(17)
C(1)-N(1)-C(13)	124.22(17)
C(4)-N(1)-C(13)	122.80(16)
C(1)-C(2)-C(3)	105.12(16)
C(1)-C(2)-C(5)	113.43(17)
C(3)-C(2)-C(5)	118.71(17)
C(1)-C(2)-H(2)	105.4(15)
C(3)-C(2)-H(2)	108.2(14)
C(5)-C(2)-H(2)	105.2(14)
C(4)-C(3)-C(2)	104.65(16)
C(4)-C(3)-C(8)	109.86(16)
C(2)-C(3)-C(8)	117.09(16)
C(4)-C(3)-H(3)	107.7(15)
C(2)-C(3)-H(3)	110.2(15)
C(8)-C(3)-H(3)	107.1(15)
O(4)-C(4)-N(1)	124.88(19)
O(4)-C(4)-C(3)	127.30(19)
N(1)-C(4)-C(3)	107.80(17)

O(6)-C(5)-O(5)	106.76(15)
O(6)-C(5)-C(6)	112.31(16)
O(5)-C(5)-C(6)	106.64(16)
O(6)-C(5)-C(2)	106.87(16)
O(5)-C(5)-C(2)	112.20(16)
C(6)-C(5)-C(2)	112.02(17)
C(5)-O(5)-C(20)	109.42(15)
C(7)-C(6)-C(9)	119.68(19)
C(7)-C(6)-C(5)	120.90(18)
C(9)-C(6)-C(5)	118.99(18)
C(5)-O(6)-C(21)	108.76(15)
C(6)-C(7)-C(12)	118.91(19)
C(6)-C(7)-C(8)	122.74(18)
C(12)-C(7)-C(8)	118.35(18)
C(7)-C(8)-C(22)	113.11(16)
C(7)-C(8)-C(3)	110.45(16)
C(22)-C(8)-C(3)	115.79(16)
C(7)-C(8)-H(8)	105.0(15)
C(22)-C(8)-H(8)	105.2(14)
C(3)-C(8)-H(8)	106.4(14)
C(10)-C(9)-C(6)	120.7(2)
C(10)-C(9)-H(9)	119.6(16)
C(6)-C(9)-H(9)	119.6(15)
C(9)-C(10)-C(11)	119.82(19)
C(9)-C(10)-H(10)	117.8(16)
C(11)-C(10)-H(10)	122.4(16)
C(12)-C(11)-C(10)	119.7(2)
C(12)-C(11)-H(11)	121.0(17)
C(10)-C(11)-H(11)	119.3(17)
C(11)-C(12)-C(7)	121.1(2)
C(11)-C(12)-H(12)	121.3(16)
C(7)-C(12)-H(12)	117.6(16)
C(18)-C(13)-C(14)	120.16(19)
C(18)-C(13)-N(1)	121.50(18)
C(14)-C(13)-N(1)	118.31(18)
C(15)-C(14)-C(13)	119.9(2)

C(15)-C(14)-H(14)	119.7(16)
C(13)-C(14)-H(14)	120.4(16)
C(14)-C(15)-C(16)	121.0(2)
C(14)-C(15)-H(15)	122.2(16)
C(16)-C(15)-H(15)	116.8(16)
C(17)-C(16)-C(15)	117.99(19)
C(17)-C(16)-C(19)	121.51(19)
C(15)-C(16)-C(19)	120.5(2)
C(18)-C(17)-C(16)	121.8(2)
C(18)-C(17)-H(17)	119.7(16)
C(16)-C(17)-H(17)	118.4(16)
C(17)-C(18)-C(13)	119.1(2)
C(17)-C(18)-H(18)	117.4(17)
C(13)-C(18)-H(18)	123.4(17)
C(16)-C(19)-H(19A)	110(2)
C(16)-C(19)-H(19B)	115(3)
H(19A)-C(19)-H(19B)	106.0(19)
C(16)-C(19)-H(19C)	112(2)
H(19A)-C(19)-H(19C)	106.5(19)
H(19B)-C(19)-H(19C)	107(2)
O(5)-C(20)-C(21)	103.39(17)
O(5)-C(20)-H(20A)	108.9(16)
C(21)-C(20)-H(20A)	112.8(15)
O(5)-C(20)-H(20B)	106.9(16)
C(21)-C(20)-H(20B)	115.9(15)
H(20A)-C(20)-H(20B)	108(2)
O(6)-C(21)-C(20)	103.79(17)
O(6)-C(21)-H(21A)	109.8(18)
C(20)-C(21)-H(21A)	111.6(18)
O(6)-C(21)-H(21B)	107.0(18)
C(20)-C(21)-H(21B)	113.4(18)
H(21A)-C(21)-H(21B)	111(3)
C(27)-C(22)-C(23)	118.78(18)
C(27)-C(22)-C(8)	117.76(17)
C(23)-C(22)-C(8)	123.45(18)
C(24)-C(23)-C(22)	120.0(2)

C(24)-C(23)-H(23)	119.5(16)
C(22)-C(23)-H(23)	120.5(16)
C(25)-C(24)-C(23)	120.6(2)
C(25)-C(24)-H(24)	121.7(18)
C(23)-C(24)-H(24)	117.6(18)
C(24)-C(25)-C(26)	119.74(19)
C(24)-C(25)-H(25)	120.3(16)
C(26)-C(25)-H(25)	120.0(16)
C(25)-C(26)-C(27)	119.9(2)
C(25)-C(26)-H(26)	121.3(16)
C(27)-C(26)-H(26)	118.7(16)
C(26)-C(27)-C(22)	120.9(2)
C(26)-C(27)-H(27)	117.9(14)
C(22)-C(27)-H(27)	121.2(14)

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($Å^2$x 10^3) for JF2923FMI. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2 a^{*2}U^{11} + ... + 2 h k a^* b^* U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
C(1)	16(1)	16(1)	17(1)	4(1)	2(1)	-2(1)
N(1)	15(1)	19(1)	16(1)	0(1)	0(1)	1(1)
O(1)	20(1)	30(1)	15(1)	1(1)	-1(1)	2(1)
C(2)	16(1)	13(1)	16(1)	2(1)	1(1)	1(1)
C(3)	15(1)	13(1)	17(1)	0(1)	0(1)	-2(1)
C(4)	17(1)	15(1)	16(1)	3(1)	1(1)	-2(1)
O(4)	14(1)	29(1)	20(1)	0(1)	-1(1)	-2(1)
C(5)	15(1)	12(1)	18(1)	2(1)	-1(1)	1(1)
O(5)	19(1)	15(1)	17(1)	-1(1)	-4(1)	-2(1)
C(6)	16(1)	10(1)	18(1)	-1(1)	1(1)	-1(1)
O(6)	16(1)	18(1)	20(1)	4(1)	-4(1)	3(1)
C(7)	15(1)	9(1)	18(1)	-2(1)	1(1)	-2(1)
C(8)	16(1)	14(1)	14(1)	-1(1)	-2(1)	-1(1)
C(9)	16(1)	14(1)	22(1)	1(1)	-1(1)	0(1)
C(10)	16(1)	18(1)	24(1)	-2(1)	4(1)	-1(1)

C(11)	23(1)	17(1)	18(1)	-1(1)	3(1)	-3(1)
C(12)	18(1)	13(1)	18(1)	-1(1)	-1(1)	-2(1)
C(13)	13(1)	19(1)	17(1)	-1(1)	0(1)	-1(1)
C(14)	18(1)	21(1)	18(1)	2(1)	1(1)	0(1)
C(15)	20(1)	19(1)	20(1)	1(1)	-2(1)	0(1)
C(16)	14(1)	23(1)	19(1)	-4(1)	-2(1)	-1(1)
C(17)	17(1)	24(1)	15(1)	0(1)	1(1)	-3(1)
C(18)	16(1)	19(1)	18(1)	2(1)	-1(1)	-1(1)
C(19)	24(1)	31(1)	22(1)	-3(1)	0(1)	7(1)
C(20)	25(1)	28(1)	22(1)	-2(1)	-8(1)	-3(1)
C(21)	21(1)	31(1)	20(1)	-1(1)	-5(1)	2(1)
C(22)	16(1)	16(1)	13(1)	1(1)	3(1)	0(1)
C(23)	17(1)	17(1)	19(1)	-1(1)	0(1)	2(1)
C(24)	24(1)	16(1)	20(1)	-1(1)	2(1)	-1(1)
C(25)	25(1)	17(1)	22(1)	3(1)	5(1)	5(1)
C(26)	20(1)	26(1)	20(1)	3(1)	-2(1)	7(1)
C(27)	18(1)	20(1)	18(1)	-1(1)	-1(1)	1(1)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (Å^{2}x 10 ^{3}) for JF2923FMI.

	x	y	z	U(eq)
H(2)	5270(20)	5009(12)	5690(30)	18(6)
H(3)	3930(30)	5052(12)	3840(30)	20(6)
H(8)	4040(30)	5692(11)	2110(30)	13(6)
H(9)	9120(30)	5415(12)	3850(30)	18(6)
H(10)	9810(30)	5543(11)	1560(30)	15(6)
H(11)	8150(30)	5835(12)	-140(30)	21(6)
H(12)	5790(30)	5990(12)	510(30)	20(6)
H(14)	2220(30)	7031(12)	5490(30)	19(6)
H(15)	760(20)	7701(12)	6760(30)	18(6)
H(17)	580(30)	6447(12)	9830(30)	22(6)
H(18)	1990(30)	5782(13)	8640(30)	21(7)

H(19A)	-1350(30)	7513(16)	8850(30)	60(11)
H(19B)	-200(40)	7980(12)	9130(40)	90(16)
H(19C)	-460(30)	7458(16)	10160(30)	60(11)
H(20A)	7320(30)	6298(12)	7620(30)	21(7)
H(20B)	8510(30)	6620(13)	6630(30)	22(6)
H(21A)	9460(30)	5662(14)	6020(30)	32(8)
H(21B)	8760(30)	5446(14)	7450(30)	28(7)
H(23)	5570(30)	6886(12)	4270(30)	23(6)
H(24)	4800(30)	7901(14)	4250(30)	34(8)
H(25)	2860(30)	8187(13)	2850(30)	22(6)
H(26)	1710(30)	7416(12)	1570(30)	20(6)
H(27)	2390(30)	6396(12)	1600(30)	16(6)

Table 6. Torsion angles [°] for JF2923FMI.

O(1)-C(1)-N(1)-C(4)	-172.52(18)
C(2)-C(1)-N(1)-C(4)	4.9(2)
O(1)-C(1)-N(1)-C(13)	9.4(3)
C(2)-C(1)-N(1)-C(13)	-173.11(17)
O(1)-C(1)-C(2)-C(3)	-179.00(19)
N(1)-C(1)-C(2)-C(3)	3.7(2)
O(1)-C(1)-C(2)-C(5)	-47.8(3)
N(1)-C(1)-C(2)-C(5)	134.91(17)
C(1)-C(2)-C(3)-C(4)	-9.98(19)
C(5)-C(2)-C(3)-C(4)	-138.11(17)
C(1)-C(2)-C(3)-C(8)	111.90(18)
C(5)-C(2)-C(3)-C(8)	-16.2(3)
C(1)-N(1)-C(4)-O(4)	169.80(19)
C(13)-N(1)-C(4)-O(4)	-12.1(3)
C(1)-N(1)-C(4)-C(3)	-11.6(2)
C(13)-N(1)-C(4)-C(3)	166.45(17)
C(2)-C(3)-C(4)-O(4)	-168.4(2)
C(8)-C(3)-C(4)-O(4)	65.1(3)
C(2)-C(3)-C(4)-N(1)	13.10(19)
C(8)-C(3)-C(4)-N(1)	-113.39(17)

C(1)-C(2)-C(5)-O(6)	91.78(19)
C(3)-C(2)-C(5)-O(6)	-144.07(17)
C(1)-C(2)-C(5)-O(5)	-24.9(2)
C(3)-C(2)-C(5)-O(5)	99.2(2)
C(1)-C(2)-C(5)-C(6)	-144.82(17)
C(3)-C(2)-C(5)-C(6)	-20.7(2)
O(6)-C(5)-O(5)-C(20)	-5.3(2)
C(6)-C(5)-O(5)-C(20)	-125.55(17)
C(2)-C(5)-O(5)-C(20)	111.46(19)
O(6)-C(5)-C(6)-C(7)	155.77(17)
O(5)-C(5)-C(6)-C(7)	-87.6(2)
C(2)-C(5)-C(6)-C(7)	35.5(2)
O(6)-C(5)-C(6)-C(9)	-31.8(2)
O(5)-C(5)-C(6)-C(9)	84.8(2)
C(2)-C(5)-C(6)-C(9)	-152.07(17)
O(5)-C(5)-O(6)-C(21)	-13.3(2)
C(6)-C(5)-O(6)-C(21)	103.19(19)
C(2)-C(5)-O(6)-C(21)	-133.59(18)
C(9)-C(6)-C(7)-C(12)	-2.5(3)
C(5)-C(6)-C(7)-C(12)	169.87(17)
C(9)-C(6)-C(7)-C(8)	176.78(17)
C(5)-C(6)-C(7)-C(8)	-10.8(3)
C(6)-C(7)-C(8)-C(22)	104.3(2)
C(12)-C(7)-C(8)-C(22)	-76.4(2)
C(6)-C(7)-C(8)-C(3)	-27.3(2)
C(12)-C(7)-C(8)-C(3)	151.96(17)
C(4)-C(3)-C(8)-C(7)	158.79(16)
C(2)-C(3)-C(8)-C(7)	39.7(2)
C(4)-C(3)-C(8)-C(22)	28.6(2)
C(2)-C(3)-C(8)-C(22)	-90.5(2)
C(7)-C(6)-C(9)-C(10)	1.5(3)
C(5)-C(6)-C(9)-C(10)	-171.04(18)
C(6)-C(9)-C(10)-C(11)	0.5(3)
C(9)-C(10)-C(11)-C(12)	-1.4(3)
C(10)-C(11)-C(12)-C(7)	0.4(3)
C(6)-C(7)-C(12)-C(11)	1.6(3)

C(8)-C(7)-C(12)-C(11)	-177.72(18)
C(1)-N(1)-C(13)-C(18)	-62.7(3)
C(4)-N(1)-C(13)-C(18)	119.4(2)
C(1)-N(1)-C(13)-C(14)	115.6(2)
C(4)-N(1)-C(13)-C(14)	-62.3(3)
C(18)-C(13)-C(14)-C(15)	-0.6(3)
N(1)-C(13)-C(14)-C(15)	-178.97(18)
C(13)-C(14)-C(15)-C(16)	0.2(3)
C(14)-C(15)-C(16)-C(17)	0.1(3)
C(14)-C(15)-C(16)-C(19)	-178.8(2)
C(15)-C(16)-C(17)-C(18)	-0.1(3)
C(19)-C(16)-C(17)-C(18)	178.8(2)
C(16)-C(17)-C(18)-C(13)	-0.2(3)
C(14)-C(13)-C(18)-C(17)	0.6(3)
N(1)-C(13)-C(18)-C(17)	178.90(18)
C(5)-O(5)-C(20)-C(21)	20.5(2)
C(5)-O(6)-C(21)-C(20)	25.6(2)
O(5)-C(20)-C(21)-O(6)	-27.6(2)
C(7)-C(8)-C(22)-C(27)	128.21(19)
C(3)-C(8)-C(22)-C(27)	-102.9(2)
C(7)-C(8)-C(22)-C(23)	-51.0(3)
C(3)-C(8)-C(22)-C(23)	78.0(2)
C(27)-C(22)-C(23)-C(24)	-0.6(3)
C(8)-C(22)-C(23)-C(24)	178.53(19)
C(22)-C(23)-C(24)-C(25)	0.4(3)
C(23)-C(24)-C(25)-C(26)	0.1(3)
C(24)-C(25)-C(26)-C(27)	-0.4(3)
C(25)-C(26)-C(27)-C(22)	0.1(3)
C(23)-C(22)-C(27)-C(26)	0.4(3)
C(8)-C(22)-C(27)-C(26)	-178.80(19)

Symmetry transformations used to generate equivalent atoms:

Table 7. Hydrogen bonds for JF2923FMI [Å and °].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)

C(3)-H(3)...O(1)#1	1.00(3)	2.55(3)	3.408(2)	143(2)
C(20)-H(20A)...O(1)	1.03(3)	2.43(3)	3.070(3)	119(2)

Symmetry transformations used to generate equivalent atoms:

#1 -x+1,-y+1,z-1/2

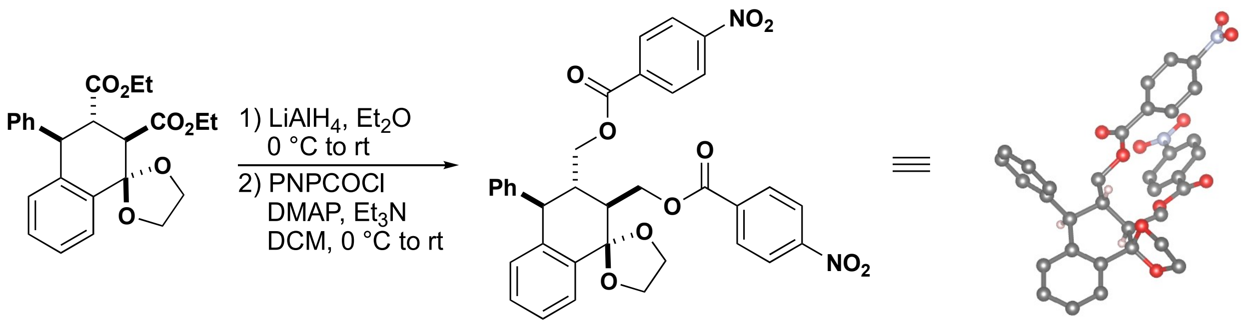


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Table 1. Crystal data and structure refinement for [$C_{34}H_{28}N_2O_{10}$].

Identification code	JF2954FMI_MO_190K (MG-4-130)	
Empirical formula	C34 H28 N2 O10	
Formula weight	624.58	
Temperature	190(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P-1	
Unit cell dimensions	a = 11.3403(4) Å	〈= 75.4010(15)°.
	b = 11.8742(4) Å	®= 71.3610(15)°.
	c = 12.8266(5) Å	© = 62.6841(13)°.
Volume	1442.67(9) Å^3	
Z	2	
Density (calculated)	1.438 Mg/m^3	
Absorption coefficient	0.107 mm^{-1}	
F(000)	652	
Crystal size	0.285 x 0.246 x 0.162 mm^3	
Crystal color and habit	Colorless Block	
Diffractometer	Bruker Photon100 CMOS	
Theta range for data collection	2.081 to 27.500°.	
Index ranges	-14<=h<=14, -15<=k<=15, -16<=l<=16	

Reflections collected	11871
Independent reflections	6538 [R(int) = 0.0135]
Observed reflections (I > 2sigma(I))	5790
Completeness to theta = 25.242°	98.3 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	1.0102 and 0.9609
Solution method	SHELXT (Sheldrick, 2014)
Refinement method	SHELXL-2017/1 (Sheldrick, 2017) Full-matrix least-squares on F^2
Data / restraints / parameters	6538 / 0 / 528
Goodness-of-fit on F^2	1.069
Final R indices [I>2sigma(I)]	R1 = 0.0370, wR2 = 0.0974
R indices (all data)	R1 = 0.0426, wR2 = 0.1012
Extinction coefficient	0.0112(17)
Largest diff. peak and hole	0.370 and -0.313 e.$Å^{-3}$

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for JF2954FMI_MO_190K. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
C(1)	2987(1)	4220(1)	922(1)	14(1)
C(2)	1953(1)	5466(1)	1429(1)	14(1)
C(3)	1852(1)	6586(1)	500(1)	14(1)
O(3)	3176(1)	6604(1)	99(1)	16(1)
C(4)	1362(1)	6449(1)	-419(1)	15(1)
O(4)	947(1)	7774(1)	921(1)	17(1)
C(5)	594(1)	7539(1)	-1050(1)	20(1)
C(6)	169(1)	7422(1)	-1902(1)	22(1)
C(7)	485(1)	6212(1)	-2124(1)	21(1)
C(8)	1221(1)	5131(1)	-1489(1)	18(1)
C(9)	1677(1)	5233(1)	-634(1)	15(1)
C(10)	2461(1)	4004(1)	39(1)	14(1)
C(11)	3291(1)	3022(1)	1764(1)	15(1)
O(11)	4270(1)	2948(1)	2318(1)	16(1)
C(12)	4647(1)	1918(1)	3076(1)	16(1)
O(12)	4218(1)	1104(1)	3297(1)	25(1)
C(13)	5653(1)	1903(1)	3610(1)	16(1)
C(14)	6049(1)	2910(1)	3386(1)	21(1)
C(15)	7001(1)	2846(1)	3889(1)	23(1)
C(16)	7538(1)	1761(1)	4608(1)	21(1)
N(16)	8606(1)	1656(1)	5096(1)	26(1)
O(16)	8843(1)	881(1)	5924(1)	36(1)
C(17)	7147(1)	760(1)	4866(1)	21(1)
O(17)	9225(1)	2333(1)	4636(1)	38(1)
C(18)	6196(1)	837(1)	4356(1)	19(1)
C(19)	2317(1)	5697(1)	2378(1)	16(1)
O(19)	1924(1)	4903(1)	3366(1)	16(1)
C(20)	2428(1)	4792(1)	4221(1)	17(1)
O(20)	3057(1)	5377(1)	4231(1)	28(1)
C(21)	2157(1)	3818(1)	5147(1)	16(1)
C(22)	1283(1)	3278(1)	5174(1)	18(1)

C(23)	1113(1)	2337(1)	6026(1)	18(1)
C(24)	1838(1)	1958(1)	6834(1)	18(1)
N(24)	1715(1)	917(1)	7717(1)	20(1)
O(24)	1106(1)	333(1)	7626(1)	25(1)
C(25)	2710(1)	2478(1)	6834(1)	21(1)
O(25)	2246(1)	685(1)	8487(1)	33(1)
C(26)	2867(1)	3422(1)	5978(1)	21(1)
C(27)	2937(1)	7926(1)	-228(1)	19(1)
C(28)	1661(1)	8592(1)	634(1)	20(1)
C(29)	3629(1)	3051(1)	-717(1)	14(1)
C(30)	3789(1)	1794(1)	-592(1)	17(1)
C(31)	4874(1)	924(1)	-1281(1)	21(1)
C(32)	5798(1)	1307(1)	-2104(1)	22(1)
C(33)	5640(1)	2568(1)	-2248(1)	22(1)
C(34)	4569(1)	3430(1)	-1554(1)	18(1)

Table 3. Bond lengths [Å] and angles [°] for JF2954FMI_MO_190K.

C(1)-C(11)	1.5243(16)
C(1)-C(2)	1.5470(16)
C(1)-C(10)	1.5558(16)
C(1)-H(1)	0.999(16)
C(2)-C(19)	1.5232(16)
C(2)-C(3)	1.5329(15)
C(2)-H(2)	0.973(15)
C(3)-O(4)	1.4269(14)
C(3)-O(3)	1.4324(14)
C(3)-C(4)	1.5247(16)
O(3)-C(27)	1.4359(14)
C(4)-C(9)	1.3971(17)
C(4)-C(5)	1.4059(17)
O(4)-C(28)	1.4437(15)
C(5)-C(6)	1.3869(19)
C(5)-H(5)	0.965(17)
C(6)-C(7)	1.394(2)
C(6)-H(6)	0.977(19)
C(7)-C(8)	1.3894(18)
C(7)-H(7)	0.980(17)
C(8)-C(9)	1.4048(17)
C(8)-H(8)	0.963(16)
C(9)-C(10)	1.5261(16)
C(10)-C(29)	1.5272(16)
C(10)-H(10)	0.986(15)
C(11)-O(11)	1.4587(14)
C(11)-H(11A)	0.991(15)
C(11)-H(11B)	0.972(17)
O(11)-C(12)	1.3452(14)
C(12)-O(12)	1.2073(16)
C(12)-C(13)	1.4990(17)
C(13)-C(18)	1.3950(17)
C(13)-C(14)	1.3962(18)
C(14)-C(15)	1.3902(19)

C(14)-H(14)	0.957(19)
C(15)-C(16)	1.3859(19)
C(15)-H(15)	0.968(17)
C(16)-C(17)	1.3818(19)
C(16)-N(16)	1.4772(16)
N(16)-O(17)	1.2255(16)
N(16)-O(16)	1.2286(16)
C(17)-C(18)	1.3895(18)
C(17)-H(17)	0.950(18)
C(18)-H(18)	0.969(16)
C(19)-O(19)	1.4540(13)
C(19)-H(19A)	0.979(15)
C(19)-H(19B)	0.971(16)
O(19)-C(20)	1.3427(15)
C(20)-O(20)	1.2075(16)
C(20)-C(21)	1.4967(16)
C(21)-C(22)	1.3948(18)
C(21)-C(26)	1.3982(17)
C(22)-C(23)	1.3884(17)
C(22)-H(22)	0.944(18)
C(23)-C(24)	1.3863(18)
C(23)-H(23)	0.946(17)
C(24)-C(25)	1.3863(18)
C(24)-N(24)	1.4771(15)
N(24)-O(24)	1.2254(15)
N(24)-O(25)	1.2274(15)
C(25)-C(26)	1.3900(17)
C(25)-H(25)	0.950(19)
C(26)-H(26)	0.989(18)
C(27)-C(28)	1.5195(17)
C(27)-H(27A)	0.992(16)
C(27)-H(27B)	0.958(17)
C(28)-H(28A)	1.005(17)
C(28)-H(28B)	0.987(18)
C(29)-C(30)	1.3909(17)
C(29)-C(34)	1.3991(17)

C(30)-C(31)	1.4002(18)
C(30)-H(30)	0.975(16)
C(31)-C(32)	1.3813(19)
C(31)-H(31)	0.995(17)
C(32)-C(33)	1.3931(19)
C(32)-H(32)	0.979(17)
C(33)-C(34)	1.3941(18)
C(33)-H(33)	0.961(19)
C(34)-H(34)	0.992(16)

C(11)-C(1)-C(2)	114.31(9)
C(11)-C(1)-C(10)	107.44(9)
C(2)-C(1)-C(10)	110.59(9)
C(11)-C(1)-H(1)	106.6(9)
C(2)-C(1)-H(1)	108.4(9)
C(10)-C(1)-H(1)	109.3(9)
C(19)-C(2)-C(3)	109.28(9)
C(19)-C(2)-C(1)	114.43(10)
C(3)-C(2)-C(1)	107.93(9)
C(19)-C(2)-H(2)	108.8(9)
C(3)-C(2)-H(2)	106.0(9)
C(1)-C(2)-H(2)	110.1(9)
O(4)-C(3)-O(3)	106.44(9)
O(4)-C(3)-C(4)	109.61(9)
O(3)-C(3)-C(4)	111.76(9)
O(4)-C(3)-C(2)	110.85(9)
O(3)-C(3)-C(2)	107.31(9)
C(4)-C(3)-C(2)	110.78(10)
C(3)-O(3)-C(27)	105.74(9)
C(9)-C(4)-C(5)	119.91(11)
C(9)-C(4)-C(3)	119.77(10)
C(5)-C(4)-C(3)	120.31(11)
C(3)-O(4)-C(28)	108.94(9)
C(6)-C(5)-C(4)	120.68(12)
C(6)-C(5)-H(5)	120.0(10)
C(4)-C(5)-H(5)	119.3(10)

C(5)-C(6)-C(7)	119.66(12)
C(5)-C(6)-H(6)	119.7(11)
C(7)-C(6)-H(6)	120.6(11)
C(8)-C(7)-C(6)	119.91(12)
C(8)-C(7)-H(7)	120.0(10)
C(6)-C(7)-H(7)	120.0(10)
C(7)-C(8)-C(9)	121.10(12)
C(7)-C(8)-H(8)	119.6(9)
C(9)-C(8)-H(8)	119.3(9)
C(4)-C(9)-C(8)	118.72(11)
C(4)-C(9)-C(10)	123.11(10)
C(8)-C(9)-C(10)	118.15(11)
C(9)-C(10)-C(29)	111.21(9)
C(9)-C(10)-C(1)	114.00(10)
C(29)-C(10)-C(1)	110.79(9)
C(9)-C(10)-H(10)	106.0(8)
C(29)-C(10)-H(10)	106.4(8)
C(1)-C(10)-H(10)	108.0(8)
O(11)-C(11)-C(1)	108.87(9)
O(11)-C(11)-H(11A)	108.8(9)
C(1)-C(11)-H(11A)	112.7(9)
O(11)-C(11)-H(11B)	107.7(10)
C(1)-C(11)-H(11B)	111.0(10)
H(11A)-C(11)-H(11B)	107.7(13)
C(12)-O(11)-C(11)	115.12(9)
O(12)-C(12)-O(11)	123.50(11)
O(12)-C(12)-C(13)	124.21(11)
O(11)-C(12)-C(13)	112.29(10)
C(18)-C(13)-C(14)	120.04(12)
C(18)-C(13)-C(12)	117.75(11)
C(14)-C(13)-C(12)	122.21(11)
C(15)-C(14)-C(13)	120.20(12)
C(15)-C(14)-H(14)	121.2(11)
C(13)-C(14)-H(14)	118.6(11)
C(16)-C(15)-C(14)	118.13(13)
C(16)-C(15)-H(15)	121.2(10)

C(14)-C(15)-H(15)	120.7(10)
C(17)-C(16)-C(15)	123.12(12)
C(17)-C(16)-N(16)	118.52(12)
C(15)-C(16)-N(16)	118.34(12)
O(17)-N(16)-O(16)	123.73(12)
O(17)-N(16)-C(16)	117.81(11)
O(16)-N(16)-C(16)	118.45(12)
C(16)-C(17)-C(18)	118.07(12)
C(16)-C(17)-H(17)	120.8(10)
C(18)-C(17)-H(17)	121.1(10)
C(17)-C(18)-C(13)	120.42(12)
C(17)-C(18)-H(18)	120.2(9)
C(13)-C(18)-H(18)	119.4(9)
O(19)-C(19)-C(2)	107.30(9)
O(19)-C(19)-H(19A)	108.1(8)
C(2)-C(19)-H(19A)	112.1(8)
O(19)-C(19)-H(19B)	108.5(9)
C(2)-C(19)-H(19B)	111.7(9)
H(19A)-C(19)-H(19B)	109.0(12)
C(20)-O(19)-C(19)	114.62(9)
O(20)-C(20)-O(19)	124.22(11)
O(20)-C(20)-C(21)	123.94(11)
O(19)-C(20)-C(21)	111.80(10)
C(22)-C(21)-C(26)	120.40(11)
C(22)-C(21)-C(20)	122.48(11)
C(26)-C(21)-C(20)	117.06(11)
C(23)-C(22)-C(21)	120.32(12)
C(23)-C(22)-H(22)	120.1(10)
C(21)-C(22)-H(22)	119.6(10)
C(24)-C(23)-C(22)	117.93(12)
C(24)-C(23)-H(23)	121.0(10)
C(22)-C(23)-H(23)	121.1(10)
C(25)-C(24)-C(23)	123.26(11)
C(25)-C(24)-N(24)	118.20(11)
C(23)-C(24)-N(24)	118.51(11)
O(24)-N(24)-O(25)	124.45(11)

O(24)-N(24)-C(24)	118.03(11)
O(25)-N(24)-C(24)	117.51(11)
C(24)-C(25)-C(26)	118.16(12)
C(24)-C(25)-H(25)	119.1(11)
C(26)-C(25)-H(25)	122.7(11)
C(25)-C(26)-C(21)	119.94(12)
C(25)-C(26)-H(26)	120.1(10)
C(21)-C(26)-H(26)	119.9(10)
O(3)-C(27)-C(28)	102.76(9)
O(3)-C(27)-H(27A)	109.5(9)
C(28)-C(27)-H(27A)	112.0(9)
O(3)-C(27)-H(27B)	107.8(10)
C(28)-C(27)-H(27B)	114.4(10)
H(27A)-C(27)-H(27B)	110.1(13)
O(4)-C(28)-C(27)	103.40(10)
O(4)-C(28)-H(28A)	108.0(9)
C(27)-C(28)-H(28A)	112.5(10)
O(4)-C(28)-H(28B)	109.5(10)
C(27)-C(28)-H(28B)	113.5(10)
H(28A)-C(28)-H(28B)	109.7(14)
C(30)-C(29)-C(34)	118.49(11)
C(30)-C(29)-C(10)	121.30(10)
C(34)-C(29)-C(10)	120.22(11)
C(29)-C(30)-C(31)	120.79(12)
C(29)-C(30)-H(30)	120.7(9)
C(31)-C(30)-H(30)	118.5(9)
C(32)-C(31)-C(30)	120.27(12)
C(32)-C(31)-H(31)	120.2(10)
C(30)-C(31)-H(31)	119.4(10)
C(31)-C(32)-C(33)	119.56(12)
C(31)-C(32)-H(32)	120.2(10)
C(33)-C(32)-H(32)	120.2(10)
C(32)-C(33)-C(34)	120.16(12)
C(32)-C(33)-H(33)	121.4(11)
C(34)-C(33)-H(33)	118.4(11)
C(33)-C(34)-C(29)	120.71(12)

C(33)-C(34)-H(34)	121.0(9)
C(29)-C(34)-H(34)	118.3(9)

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($Å^2 x 10^3$) for JF2954FMI_MO_190K. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2 a^{*2}U^{11} + ... + 2 h k a^* b^* U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
C(1)	16(1)	13(1)	12(1)	0(1)	-5(1)	-5(1)
C(2)	15(1)	13(1)	12(1)	0(1)	-2(1)	-6(1)
C(3)	14(1)	13(1)	14(1)	-1(1)	-1(1)	-4(1)
O(3)	15(1)	13(1)	18(1)	1(1)	-2(1)	-5(1)
C(4)	14(1)	17(1)	13(1)	0(1)	-2(1)	-5(1)
O(4)	16(1)	13(1)	19(1)	-4(1)	0(1)	-5(1)
C(5)	20(1)	16(1)	19(1)	1(1)	-6(1)	-5(1)
C(6)	19(1)	23(1)	19(1)	4(1)	-8(1)	-5(1)
C(7)	18(1)	29(1)	16(1)	0(1)	-6(1)	-10(1)
C(8)	18(1)	21(1)	16(1)	-1(1)	-5(1)	-8(1)
C(9)	13(1)	17(1)	12(1)	0(1)	-3(1)	-6(1)
C(10)	15(1)	13(1)	13(1)	0(1)	-4(1)	-6(1)
C(11)	18(1)	14(1)	15(1)	1(1)	-7(1)	-7(1)
O(11)	17(1)	16(1)	15(1)	3(1)	-8(1)	-7(1)
C(12)	18(1)	14(1)	12(1)	-1(1)	-4(1)	-4(1)
O(12)	37(1)	21(1)	26(1)	7(1)	-18(1)	-16(1)
C(13)	14(1)	18(1)	12(1)	-2(1)	-2(1)	-4(1)
C(14)	20(1)	22(1)	20(1)	2(1)	-7(1)	-9(1)
C(15)	23(1)	26(1)	24(1)	0(1)	-7(1)	-13(1)
C(16)	16(1)	31(1)	15(1)	-4(1)	-3(1)	-9(1)
N(16)	21(1)	41(1)	18(1)	-4(1)	-6(1)	-14(1)
O(16)	31(1)	58(1)	21(1)	6(1)	-14(1)	-21(1)
C(17)	18(1)	24(1)	15(1)	0(1)	-6(1)	-5(1)
O(17)	36(1)	58(1)	32(1)	4(1)	-15(1)	-32(1)
C(18)	19(1)	18(1)	16(1)	-1(1)	-4(1)	-5(1)
C(19)	21(1)	16(1)	11(1)	0(1)	-3(1)	-10(1)
O(19)	21(1)	19(1)	10(1)	1(1)	-3(1)	-10(1)
C(20)	22(1)	15(1)	13(1)	-3(1)	-4(1)	-7(1)
O(20)	47(1)	32(1)	19(1)	4(1)	-13(1)	-28(1)
C(21)	21(1)	15(1)	12(1)	-2(1)	-2(1)	-7(1)
C(22)	18(1)	19(1)	14(1)	-2(1)	-4(1)	-6(1)

C(23)	18(1)	19(1)	18(1)	-3(1)	-2(1)	-9(1)
C(24)	19(1)	15(1)	14(1)	1(1)	-1(1)	-6(1)
N(24)	20(1)	18(1)	18(1)	0(1)	0(1)	-7(1)
O(24)	30(1)	22(1)	23(1)	-3(1)	1(1)	-15(1)
C(25)	27(1)	24(1)	15(1)	1(1)	-8(1)	-12(1)
O(25)	36(1)	37(1)	27(1)	16(1)	-17(1)	-21(1)
C(26)	28(1)	23(1)	16(1)	0(1)	-7(1)	-15(1)
C(27)	19(1)	14(1)	21(1)	2(1)	-2(1)	-8(1)
C(28)	21(1)	15(1)	23(1)	-2(1)	-2(1)	-8(1)
C(29)	16(1)	16(1)	12(1)	-1(1)	-6(1)	-6(1)
C(30)	23(1)	17(1)	13(1)	1(1)	-6(1)	-9(1)
C(31)	28(1)	14(1)	19(1)	-1(1)	-10(1)	-5(1)
C(32)	22(1)	22(1)	18(1)	-8(1)	-5(1)	-3(1)
C(33)	21(1)	26(1)	18(1)	-5(1)	-2(1)	-11(1)
C(34)	20(1)	18(1)	18(1)	-3(1)	-4(1)	-9(1)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for JF2954FMI_MO_190K.

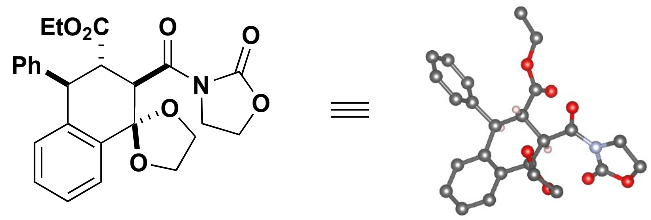
	x	y	z	U(eq)
H(1)	3874(16)	4295(15)	561(13)	18(4)
H(2)	1045(15)	5471(14)	1689(12)	14(3)
H(5)	378(17)	8375(16)	-893(14)	24(4)
H(6)	-347(18)	8190(18)	-2344(15)	33(5)
H(7)	218(17)	6122(16)	-2743(14)	24(4)
H(8)	1426(16)	4297(15)	-1638(13)	18(4)
H(10)	1812(15)	3612(14)	431(12)	13(3)
H(11A)	2462(15)	3012(14)	2332(12)	15(3)
H(11B)	3701(17)	2257(16)	1401(14)	23(4)
H(14)	5642(19)	3643(18)	2889(15)	33(5)
H(15)	7275(17)	3542(17)	3741(14)	27(4)
H(17)	7558(17)	20(17)	5346(14)	27(4)
H(18)	5908(16)	147(15)	4511(13)	18(4)
H(19A)	3298(15)	5455(14)	2241(12)	12(3)
H(19B)	1824(16)	6583(15)	2518(12)	17(4)
H(22)	802(17)	3560(16)	4612(14)	26(4)
H(23)	541(17)	1948(16)	6043(14)	25(4)
H(25)	3196(19)	2160(17)	7402(15)	34(5)
H(26)	3506(18)	3791(17)	5941(14)	30(4)
H(27A)	2782(16)	8191(15)	-987(13)	19(4)
H(27B)	3731(17)	8012(16)	-214(13)	24(4)
H(28A)	1876(17)	8627(16)	1324(14)	25(4)
H(28B)	1072(18)	9457(17)	349(14)	29(4)
H(30)	3131(16)	1507(15)	-38(13)	21(4)
H(31)	4950(17)	38(17)	-1194(14)	27(4)
H(32)	6532(17)	708(16)	-2606(14)	24(4)
H(33)	6267(19)	2861(17)	-2813(15)	33(5)
H(34)	4442(16)	4330(16)	-1650(13)	21(4)

Table 6. Torsion angles [°] for JF2954FMI_MO_190K.

C(11)-C(1)-C(2)-C(19)	53.30(13)
C(10)-C(1)-C(2)-C(19)	174.69(9)
C(11)-C(1)-C(2)-C(3)	175.18(9)
C(10)-C(1)-C(2)-C(3)	-63.42(12)
C(19)-C(2)-C(3)-O(4)	-52.91(12)
C(1)-C(2)-C(3)-O(4)	-177.91(9)
C(19)-C(2)-C(3)-O(3)	62.94(11)
C(1)-C(2)-C(3)-O(3)	-62.07(12)
C(19)-C(2)-C(3)-C(4)	-174.81(9)
C(1)-C(2)-C(3)-C(4)	60.18(12)
O(4)-C(3)-O(3)-C(27)	-28.40(11)
C(4)-C(3)-O(3)-C(27)	91.24(11)
C(2)-C(3)-O(3)-C(27)	-147.12(10)
O(4)-C(3)-C(4)-C(9)	-152.94(10)
O(3)-C(3)-C(4)-C(9)	89.30(12)
C(2)-C(3)-C(4)-C(9)	-30.31(14)
O(4)-C(3)-C(4)-C(5)	27.06(14)
O(3)-C(3)-C(4)-C(5)	-90.70(13)
C(2)-C(3)-C(4)-C(5)	149.70(11)
O(3)-C(3)-O(4)-C(28)	8.37(12)
C(4)-C(3)-O(4)-C(28)	-112.66(10)
C(2)-C(3)-O(4)-C(28)	124.75(10)
C(9)-C(4)-C(5)-C(6)	-1.34(18)
C(3)-C(4)-C(5)-C(6)	178.65(11)
C(4)-C(5)-C(6)-C(7)	1.10(19)
C(5)-C(6)-C(7)-C(8)	0.10(19)
C(6)-C(7)-C(8)-C(9)	-1.06(19)
C(5)-C(4)-C(9)-C(8)	0.39(17)
C(3)-C(4)-C(9)-C(8)	-179.61(10)
C(5)-C(4)-C(9)-C(10)	-177.80(11)
C(3)-C(4)-C(9)-C(10)	2.21(17)
C(7)-C(8)-C(9)-C(4)	0.81(17)
C(7)-C(8)-C(9)-C(10)	179.08(11)
C(4)-C(9)-C(10)-C(29)	-131.08(11)

C(8)-C(9)-C(10)-C(29)	50.73(14)
C(4)-C(9)-C(10)-C(1)	-4.96(15)
C(8)-C(9)-C(10)-C(1)	176.85(10)
C(11)-C(1)-C(10)-C(9)	160.84(10)
C(2)-C(1)-C(10)-C(9)	35.47(13)
C(11)-C(1)-C(10)-C(29)	-72.82(11)
C(2)-C(1)-C(10)-C(29)	161.81(9)
C(2)-C(1)-C(11)-O(11)	-79.72(12)
C(10)-C(1)-C(11)-O(11)	157.17(9)
C(1)-C(11)-O(11)-C(12)	-179.02(9)
C(11)-O(11)-C(12)-O(12)	-0.16(17)
C(11)-O(11)-C(12)-C(13)	179.92(9)
O(12)-C(12)-C(13)-C(18)	4.49(18)
O(11)-C(12)-C(13)-C(18)	-175.59(10)
O(12)-C(12)-C(13)-C(14)	-175.39(12)
O(11)-C(12)-C(13)-C(14)	4.53(16)
C(18)-C(13)-C(14)-C(15)	1.05(19)
C(12)-C(13)-C(14)-C(15)	-179.07(12)
C(13)-C(14)-C(15)-C(16)	0.2(2)
C(14)-C(15)-C(16)-C(17)	-1.6(2)
C(14)-C(15)-C(16)-N(16)	176.62(12)
C(17)-C(16)-N(16)-O(17)	159.12(13)
C(15)-C(16)-N(16)-O(17)	-19.22(19)
C(17)-C(16)-N(16)-O(16)	-19.53(18)
C(15)-C(16)-N(16)-O(16)	162.14(13)
C(15)-C(16)-C(17)-C(18)	1.73(19)
N(16)-C(16)-C(17)-C(18)	-176.52(11)
C(16)-C(17)-C(18)-C(13)	-0.39(18)
C(14)-C(13)-C(18)-C(17)	-0.96(18)
C(12)-C(13)-C(18)-C(17)	179.16(11)
C(3)-C(2)-C(19)-O(19)	159.73(9)
C(1)-C(2)-C(19)-O(19)	-79.13(12)
C(2)-C(19)-O(19)-C(20)	166.88(10)
C(19)-O(19)-C(20)-O(20)	6.30(17)
C(19)-O(19)-C(20)-C(21)	-171.71(10)
O(20)-C(20)-C(21)-C(22)	171.60(13)

O(19)-C(20)-C(21)-C(22)	-10.38(16)
O(20)-C(20)-C(21)-C(26)	-10.95(19)
O(19)-C(20)-C(21)-C(26)	167.08(11)
C(26)-C(21)-C(22)-C(23)	-0.26(19)
C(20)-C(21)-C(22)-C(23)	177.11(11)
C(21)-C(22)-C(23)-C(24)	-0.24(18)
C(22)-C(23)-C(24)-C(25)	0.54(19)
C(22)-C(23)-C(24)-N(24)	-177.28(11)
C(25)-C(24)-N(24)-O(24)	-169.54(11)
C(23)-C(24)-N(24)-O(24)	8.39(17)
C(25)-C(24)-N(24)-O(25)	9.57(17)
C(23)-C(24)-N(24)-O(25)	-172.49(12)
C(23)-C(24)-C(25)-C(26)	-0.3(2)
N(24)-C(24)-C(25)-C(26)	177.50(11)
C(24)-C(25)-C(26)-C(21)	-0.2(2)
C(22)-C(21)-C(26)-C(25)	0.48(19)
C(20)-C(21)-C(26)-C(25)	-177.03(12)
C(3)-O(3)-C(27)-C(28)	36.02(12)
C(3)-O(4)-C(28)-C(27)	13.52(13)
O(3)-C(27)-C(28)-O(4)	-30.13(12)
C(9)-C(10)-C(29)-C(30)	-128.79(12)
C(1)-C(10)-C(29)-C(30)	103.33(12)
C(9)-C(10)-C(29)-C(34)	51.41(14)
C(1)-C(10)-C(29)-C(34)	-76.47(13)
C(34)-C(29)-C(30)-C(31)	0.60(18)
C(10)-C(29)-C(30)-C(31)	-179.20(11)
C(29)-C(30)-C(31)-C(32)	-0.49(19)
C(30)-C(31)-C(32)-C(33)	-0.3(2)
C(31)-C(32)-C(33)-C(34)	1.0(2)
C(32)-C(33)-C(34)-C(29)	-0.9(2)
C(30)-C(29)-C(34)-C(33)	0.11(18)
C(10)-C(29)-C(34)-C(33)	179.91(11)



CCDC 2087133

Table 1. Crystal data and structure refinement for $[C_{25}H_{25}NO_7]_2[C_4H_8O_2]_{0.5}$.

Identification code	JF3005FMI (JMR-1-159-B)	
Empirical formula	C52 H54 N2 O15	
Formula weight	946.97	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P-1	
Unit cell dimensions	a = 9.7429(7) Å	〈= 67.1270(15)°.
	b = 14.3116(10) Å	®= 81.5420(16)°.
	c = 18.0645(12) Å	© = 80.5606(17)°.
Volume	2279.7(3) Å^3	
Z	2	
Density (calculated)	1.380 Mg/m^3	
Absorption coefficient	0.102 mm^{-1}	
F(000)	1000	
Crystal size	0.596 x 0.577 x 0.232 mm^3	
Crystal color and habit	Colourless Block	
Diffractometer	Bruker Photon100 CMOS	
Theta range for data collection	2.128 to 30.684°.	
Index ranges	-13<=h<=13, -20<=k<=20, -25<=l<=25	
Reflections collected	28137	
Independent reflections	14103 [R(int) = 0.0169]	
Observed reflections (I > 2sigma(I))	12151	
Completeness to theta = 25.242°	100.0 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.9660 and 0.8837	
Solution method	SHELXT (Sheldrick, 2014)	
Refinement method	SHELXL-2017/1 (Sheldrick, 2017) Full-matrix least-squares on F^2	
Data / restraints / parameters	14103 / 0 / 652	

Goodness-of-fit on F^2	1.037
Final R indices [I>2sigma(I)]	R1 = 0.0483, wR2 = 0.1297
R indices (all data)	R1 = 0.0554, wR2 = 0.1365
Extinction coefficient	0.0239(14)
Largest diff. peak and hole	0.534 and -0.351 e.$Å^{-3}$

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for JF3005FMI. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
C(1)	7446(1)	6940(1)	1558(1)	18(1)
O(1)	6181(1)	7609(1)	1363(1)	20(1)
C(2)	8461(1)	7047(1)	797(1)	18(1)
O(2)	8087(1)	7261(1)	2072(1)	20(1)
C(3)	9753(1)	6271(1)	1054(1)	18(1)
C(4)	9371(1)	5165(1)	1340(1)	19(1)
C(5)	8024(1)	5028(1)	1898(1)	22(1)
C(6)	7116(1)	5846(1)	1996(1)	20(1)
C(7)	5906(1)	5661(1)	2533(1)	26(1)
C(8)	5601(1)	4673(1)	2975(1)	36(1)
C(9)	6482(2)	3854(1)	2870(1)	41(1)
C(10)	7669(1)	4033(1)	2329(1)	33(1)
C(11)	6044(1)	8325(1)	1755(1)	21(1)
C(12)	6993(1)	7801(1)	2430(1)	21(1)
C(13)	8871(1)	8125(1)	434(1)	19(1)
N(13)	7926(1)	8916(1)	-2(1)	20(1)
O(13)	9957(1)	8330(1)	560(1)	26(1)
C(14)	6790(1)	8864(1)	-369(1)	22(1)
O(14)	6412(1)	8136(1)	-417(1)	27(1)
C(15)	6822(1)	10560(1)	-574(1)	30(1)
O(15)	6131(1)	9819(1)	-701(1)	27(1)
C(16)	8134(1)	9971(1)	-170(1)	23(1)
C(17)	10914(1)	6438(1)	372(1)	21(1)
O(17)	10730(1)	6628(1)	-322(1)	30(1)
C(18)	13372(1)	6342(1)	52(1)	30(1)
O(18)	12167(1)	6309(1)	641(1)	23(1)
C(19)	14654(1)	6020(1)	508(1)	35(1)
C(20)	10598(1)	4414(1)	1729(1)	20(1)
C(21)	11512(1)	3905(1)	1302(1)	24(1)
C(22)	12694(1)	3272(1)	1640(1)	29(1)
C(23)	12958(1)	3140(1)	2409(1)	35(1)

C(24)	12036(2)	3629(1)	2847(1)	34(1)
C(25)	10866(1)	4261(1)	2508(1)	26(1)
C(31)	1800(1)	7851(1)	3111(1)	18(1)
O(31)	716(1)	7229(1)	3255(1)	22(1)
C(32)	2453(1)	7637(1)	3897(1)	18(1)
O(32)	2852(1)	7579(1)	2559(1)	20(1)
C(33)	3609(1)	8330(1)	3681(1)	18(1)
C(34)	2940(1)	9452(1)	3456(1)	18(1)
C(35)	1851(1)	9723(1)	2856(1)	19(1)
C(36)	1254(1)	8977(1)	2729(1)	19(1)
C(37)	200(1)	9268(1)	2205(1)	24(1)
C(38)	-256(1)	10297(1)	1807(1)	28(1)
C(39)	340(1)	11042(1)	1921(1)	28(1)
C(40)	1380(1)	10754(1)	2446(1)	25(1)
C(41)	1194(1)	6482(1)	2897(1)	22(1)
C(42)	2227(1)	7013(1)	2214(1)	22(1)
C(43)	3054(1)	6526(1)	4260(1)	20(1)
N(43)	2241(1)	5821(1)	4834(1)	22(1)
O(43)	4236(1)	6228(1)	4057(1)	26(1)
C(44)	896(1)	5977(1)	5196(1)	24(1)
O(44)	108(1)	6746(1)	5068(1)	35(1)
C(45)	1766(1)	4308(1)	5862(1)	29(1)
O(45)	560(1)	5071(1)	5752(1)	26(1)
C(46)	2780(1)	4734(1)	5133(1)	29(1)
C(47)	4510(1)	8063(1)	4369(1)	20(1)
O(47)	4066(1)	7853(1)	5067(1)	28(1)
C(48)	6813(1)	8153(1)	4631(1)	27(1)
O(48)	5853(1)	8143(1)	4090(1)	24(1)
C(49)	8072(1)	8603(1)	4098(1)	35(1)
C(50)	4078(1)	10159(1)	3182(1)	20(1)
C(51)	4538(1)	10481(1)	3732(1)	23(1)
C(52)	5659(1)	11056(1)	3512(1)	27(1)
C(53)	6326(1)	11323(1)	2736(1)	29(1)
C(54)	5858(1)	11024(1)	2181(1)	27(1)
C(55)	4744(1)	10444(1)	2400(1)	22(1)
C(61)	10864(3)	8464(2)	6037(2)	33(1)

O(61)	8559(2)	9066(2)	5602(1)	34(1)
C(62)	9781(3)	9168(2)	5511(2)	27(1)
O(62)	10328(2)	9962(2)	4918(1)	35(1)
C(63)	9374(3)	10696(2)	4352(2)	40(1)
C(64)	10021(6)	11666(3)	3958(2)	54(1)

Table 3. Bond lengths [Å] and angles [°] for JF3005FMI.

C(1)-O(1)	1.4274(11)
C(1)-O(2)	1.4358(12)
C(1)-C(6)	1.5189(14)
C(1)-C(2)	1.5424(14)
O(1)-C(11)	1.4354(13)
C(2)-C(13)	1.5194(14)
C(2)-C(3)	1.5317(14)
C(2)-H(2)	1.0000
O(2)-C(12)	1.4372(12)
C(3)-C(17)	1.5172(14)
C(3)-C(4)	1.5533(14)
C(3)-H(3)	1.0000
C(4)-C(5)	1.5217(15)
C(4)-C(20)	1.5220(14)
C(4)-H(4)	1.0000
C(5)-C(6)	1.4006(14)
C(5)-C(10)	1.4054(15)
C(6)-C(7)	1.4021(15)
C(7)-C(8)	1.3845(17)
C(7)-H(7)	0.9500
C(8)-C(9)	1.3933(19)
C(8)-H(8)	0.9500
C(9)-C(10)	1.3886(19)
C(9)-H(9)	0.9500
C(10)-H(10)	0.9500
C(11)-C(12)	1.5149(15)
C(11)-H(11A)	0.9900
C(11)-H(11B)	0.9900
C(12)-H(12A)	0.9900
C(12)-H(12B)	0.9900
C(13)-O(13)	1.2178(13)
C(13)-N(13)	1.3883(13)
N(13)-C(14)	1.3971(14)
N(13)-C(16)	1.4619(14)

C(14)-O(14)	1.1964(14)
C(14)-O(15)	1.3526(13)
C(15)-O(15)	1.4491(15)
C(15)-C(16)	1.5234(16)
C(15)-H(15A)	0.9900
C(15)-H(15B)	0.9900
C(16)-H(16A)	0.9900
C(16)-H(16B)	0.9900
C(17)-O(17)	1.2101(14)
C(17)-O(18)	1.3379(13)
C(18)-O(18)	1.4569(13)
C(18)-C(19)	1.5070(18)
C(18)-H(18A)	0.9900
C(18)-H(18B)	0.9900
C(19)-H(19A)	0.9800
C(19)-H(19B)	0.9800
C(19)-H(19C)	0.9800
C(20)-C(21)	1.3927(15)
C(20)-C(25)	1.3960(15)
C(21)-C(22)	1.3981(16)
C(21)-H(21)	0.9500
C(22)-C(23)	1.385(2)
C(22)-H(22)	0.9500
C(23)-C(24)	1.392(2)
C(23)-H(23)	0.9500
C(24)-C(25)	1.3895(17)
C(24)-H(24)	0.9500
C(25)-H(25)	0.9500
C(31)-O(31)	1.4218(12)
C(31)-O(32)	1.4373(12)
C(31)-C(36)	1.5226(14)
C(31)-C(32)	1.5432(14)
O(31)-C(41)	1.4370(13)
C(32)-C(43)	1.5154(14)
C(32)-C(33)	1.5304(14)
C(32)-H(32)	1.0000

O(32)-C(42)	1.4432(13)
C(33)-C(47)	1.5180(14)
C(33)-C(34)	1.5488(14)
C(33)-H(33)	1.0000
C(34)-C(50)	1.5210(14)
C(34)-C(35)	1.5261(14)
C(34)-H(34)	1.0000
C(35)-C(36)	1.4013(14)
C(35)-C(40)	1.4015(14)
C(36)-C(37)	1.4007(14)
C(37)-C(38)	1.3921(16)
C(37)-H(37)	0.9500
C(38)-C(39)	1.3878(18)
C(38)-H(38)	0.9500
C(39)-C(40)	1.3914(16)
C(39)-H(39)	0.9500
C(40)-H(40)	0.9500
C(41)-C(42)	1.5058(15)
C(41)-H(41A)	0.9900
C(41)-H(41B)	0.9900
C(42)-H(42A)	0.9900
C(42)-H(42B)	0.9900
C(43)-O(43)	1.2168(13)
C(43)-N(43)	1.3889(13)
N(43)-C(44)	1.4003(14)
N(43)-C(46)	1.4672(14)
C(44)-O(44)	1.1960(14)
C(44)-O(45)	1.3512(13)
C(45)-O(45)	1.4468(14)
C(45)-C(46)	1.5081(17)
C(45)-H(45A)	0.9900
C(45)-H(45B)	0.9900
C(46)-H(46A)	0.9900
C(46)-H(46B)	0.9900
C(47)-O(47)	1.2064(13)
C(47)-O(48)	1.3380(13)

C(48)-O(48)	1.4547(13)
C(48)-C(49)	1.5082(18)
C(48)-H(48A)	0.9900
C(48)-H(48B)	0.9900
C(49)-H(49A)	0.9800
C(49)-H(49B)	0.9800
C(49)-H(49C)	0.9800
C(50)-C(55)	1.3968(15)
C(50)-C(51)	1.3979(15)
C(51)-C(52)	1.3932(16)
C(51)-H(51)	0.9500
C(52)-C(53)	1.3895(18)
C(52)-H(52)	0.9500
C(53)-C(54)	1.3889(18)
C(53)-H(53)	0.9500
C(54)-C(55)	1.3921(15)
C(54)-H(54)	0.9500
C(55)-H(55)	0.9500
C(61)-C(62)	1.494(4)
C(61)-H(61A)	0.9800
C(61)-H(61B)	0.9800
C(61)-H(61C)	0.9800
O(61)-C(62)	1.203(3)
C(62)-O(62)	1.345(3)
O(62)-C(63)	1.461(4)
C(63)-C(64)	1.489(5)
C(63)-H(63A)	0.9900
C(63)-H(63B)	0.9900
C(64)-H(64A)	0.9800
C(64)-H(64B)	0.9800
C(64)-H(64C)	0.9800

O(1)-C(1)-O(2)	106.15(7)
O(1)-C(1)-C(6)	109.81(8)
O(2)-C(1)-C(6)	110.50(8)
O(1)-C(1)-C(2)	111.27(8)

O(2)-C(1)-C(2)	107.89(8)
C(6)-C(1)-C(2)	111.10(8)
C(1)-O(1)-C(11)	109.09(7)
C(13)-C(2)-C(3)	110.15(8)
C(13)-C(2)-C(1)	108.75(8)
C(3)-C(2)-C(1)	107.81(8)
C(13)-C(2)-H(2)	110.0
C(3)-C(2)-H(2)	110.0
C(1)-C(2)-H(2)	110.0
C(1)-O(2)-C(12)	106.77(7)
C(17)-C(3)-C(2)	111.56(8)
C(17)-C(3)-C(4)	109.43(8)
C(2)-C(3)-C(4)	110.44(8)
C(17)-C(3)-H(3)	108.4
C(2)-C(3)-H(3)	108.4
C(4)-C(3)-H(3)	108.4
C(5)-C(4)-C(20)	112.62(9)
C(5)-C(4)-C(3)	111.30(8)
C(20)-C(4)-C(3)	109.24(8)
C(5)-C(4)-H(4)	107.8
C(20)-C(4)-H(4)	107.8
C(3)-C(4)-H(4)	107.8
C(6)-C(5)-C(10)	118.42(10)
C(6)-C(5)-C(4)	123.17(9)
C(10)-C(5)-C(4)	118.41(10)
C(5)-C(6)-C(7)	120.03(10)
C(5)-C(6)-C(1)	121.21(9)
C(7)-C(6)-C(1)	118.71(9)
C(8)-C(7)-C(6)	120.70(11)
C(8)-C(7)-H(7)	119.6
C(6)-C(7)-H(7)	119.6
C(7)-C(8)-C(9)	119.75(12)
C(7)-C(8)-H(8)	120.1
C(9)-C(8)-H(8)	120.1
C(10)-C(9)-C(8)	119.85(12)
C(10)-C(9)-H(9)	120.1

C(8)-C(9)-H(9)	120.1
C(9)-C(10)-C(5)	121.18(11)
C(9)-C(10)-H(10)	119.4
C(5)-C(10)-H(10)	119.4
O(1)-C(11)-C(12)	103.14(8)
O(1)-C(11)-H(11A)	111.1
C(12)-C(11)-H(11A)	111.1
O(1)-C(11)-H(11B)	111.1
C(12)-C(11)-H(11B)	111.1
H(11A)-C(11)-H(11B)	109.1
O(2)-C(12)-C(11)	102.09(8)
O(2)-C(12)-H(12A)	111.4
C(11)-C(12)-H(12A)	111.4
O(2)-C(12)-H(12B)	111.4
C(11)-C(12)-H(12B)	111.4
H(12A)-C(12)-H(12B)	109.2
O(13)-C(13)-N(13)	118.69(9)
O(13)-C(13)-C(2)	122.20(9)
N(13)-C(13)-C(2)	118.89(9)
C(13)-N(13)-C(14)	128.60(9)
C(13)-N(13)-C(16)	119.32(9)
C(14)-N(13)-C(16)	111.94(8)
O(14)-C(14)-O(15)	122.52(10)
O(14)-C(14)-N(13)	129.26(10)
O(15)-C(14)-N(13)	108.21(9)
O(15)-C(15)-C(16)	105.84(9)
O(15)-C(15)-H(15A)	110.6
C(16)-C(15)-H(15A)	110.6
O(15)-C(15)-H(15B)	110.6
C(16)-C(15)-H(15B)	110.6
H(15A)-C(15)-H(15B)	108.7
C(14)-O(15)-C(15)	111.36(9)
N(13)-C(16)-C(15)	101.80(9)
N(13)-C(16)-H(16A)	111.4
C(15)-C(16)-H(16A)	111.4
N(13)-C(16)-H(16B)	111.4

C(15)-C(16)-H(16B)	111.4
H(16A)-C(16)-H(16B)	109.3
O(17)-C(17)-O(18)	124.34(10)
O(17)-C(17)-C(3)	124.06(10)
O(18)-C(17)-C(3)	111.55(9)
O(18)-C(18)-C(19)	107.03(10)
O(18)-C(18)-H(18A)	110.3
C(19)-C(18)-H(18A)	110.3
O(18)-C(18)-H(18B)	110.3
C(19)-C(18)-H(18B)	110.3
H(18A)-C(18)-H(18B)	108.6
C(17)-O(18)-C(18)	116.23(9)
C(18)-C(19)-H(19A)	109.5
C(18)-C(19)-H(19B)	109.5
H(19A)-C(19)-H(19B)	109.5
C(18)-C(19)-H(19C)	109.5
H(19A)-C(19)-H(19C)	109.5
H(19B)-C(19)-H(19C)	109.5
C(21)-C(20)-C(25)	118.78(10)
C(21)-C(20)-C(4)	120.82(9)
C(25)-C(20)-C(4)	120.32(9)
C(20)-C(21)-C(22)	120.66(11)
C(20)-C(21)-H(21)	119.7
C(22)-C(21)-H(21)	119.7
C(23)-C(22)-C(21)	119.91(11)
C(23)-C(22)-H(22)	120.0
C(21)-C(22)-H(22)	120.0
C(22)-C(23)-C(24)	119.88(11)
C(22)-C(23)-H(23)	120.1
C(24)-C(23)-H(23)	120.1
C(25)-C(24)-C(23)	120.08(12)
C(25)-C(24)-H(24)	120.0
C(23)-C(24)-H(24)	120.0
C(24)-C(25)-C(20)	120.67(11)
C(24)-C(25)-H(25)	119.7
C(20)-C(25)-H(25)	119.7

O(31)-C(31)-O(32)	106.46(8)
O(31)-C(31)-C(36)	110.66(8)
O(32)-C(31)-C(36)	109.40(8)
O(31)-C(31)-C(32)	111.04(8)
O(32)-C(31)-C(32)	108.72(8)
C(36)-C(31)-C(32)	110.45(8)
C(31)-O(31)-C(41)	108.31(8)
C(43)-C(32)-C(33)	110.20(8)
C(43)-C(32)-C(31)	110.63(8)
C(33)-C(32)-C(31)	107.16(8)
C(43)-C(32)-H(32)	109.6
C(33)-C(32)-H(32)	109.6
C(31)-C(32)-H(32)	109.6
C(31)-O(32)-C(42)	107.33(7)
C(47)-C(33)-C(32)	112.49(8)
C(47)-C(33)-C(34)	108.71(8)
C(32)-C(33)-C(34)	109.15(8)
C(47)-C(33)-H(33)	108.8
C(32)-C(33)-H(33)	108.8
C(34)-C(33)-H(33)	108.8
C(50)-C(34)-C(35)	114.30(8)
C(50)-C(34)-C(33)	109.84(8)
C(35)-C(34)-C(33)	111.41(8)
C(50)-C(34)-H(34)	107.0
C(35)-C(34)-H(34)	107.0
C(33)-C(34)-H(34)	107.0
C(36)-C(35)-C(40)	118.75(10)
C(36)-C(35)-C(34)	122.39(9)
C(40)-C(35)-C(34)	118.79(9)
C(37)-C(36)-C(35)	119.95(10)
C(37)-C(36)-C(31)	119.10(9)
C(35)-C(36)-C(31)	120.83(9)
C(38)-C(37)-C(36)	120.32(11)
C(38)-C(37)-H(37)	119.8
C(36)-C(37)-H(37)	119.8
C(39)-C(38)-C(37)	120.17(10)

C(39)-C(38)-H(38)	119.9
C(37)-C(38)-H(38)	119.9
C(38)-C(39)-C(40)	119.59(10)
C(38)-C(39)-H(39)	120.2
C(40)-C(39)-H(39)	120.2
C(39)-C(40)-C(35)	121.21(11)
C(39)-C(40)-H(40)	119.4
C(35)-C(40)-H(40)	119.4
O(31)-C(41)-C(42)	102.74(8)
O(31)-C(41)-H(41A)	111.2
C(42)-C(41)-H(41A)	111.2
O(31)-C(41)-H(41B)	111.2
C(42)-C(41)-H(41B)	111.2
H(41A)-C(41)-H(41B)	109.1
O(32)-C(42)-C(41)	101.85(8)
O(32)-C(42)-H(42A)	111.4
C(41)-C(42)-H(42A)	111.4
O(32)-C(42)-H(42B)	111.4
C(41)-C(42)-H(42B)	111.4
H(42A)-C(42)-H(42B)	109.3
O(43)-C(43)-N(43)	118.55(9)
O(43)-C(43)-C(32)	121.71(9)
N(43)-C(43)-C(32)	119.74(9)
C(43)-N(43)-C(44)	129.51(9)
C(43)-N(43)-C(46)	119.65(9)
C(44)-N(43)-C(46)	110.84(9)
O(44)-C(44)-O(45)	122.17(10)
O(44)-C(44)-N(43)	129.46(10)
O(45)-C(44)-N(43)	108.36(9)
O(45)-C(45)-C(46)	105.44(9)
O(45)-C(45)-H(45A)	110.7
C(46)-C(45)-H(45A)	110.7
O(45)-C(45)-H(45B)	110.7
C(46)-C(45)-H(45B)	110.7
H(45A)-C(45)-H(45B)	108.8
C(44)-O(45)-C(45)	110.28(9)

N(43)-C(46)-C(45)	101.44(9)
N(43)-C(46)-H(46A)	111.5
C(45)-C(46)-H(46A)	111.5
N(43)-C(46)-H(46B)	111.5
C(45)-C(46)-H(46B)	111.5
H(46A)-C(46)-H(46B)	109.3
O(47)-C(47)-O(48)	124.70(10)
O(47)-C(47)-C(33)	124.58(10)
O(48)-C(47)-C(33)	110.63(9)
O(48)-C(48)-C(49)	105.85(10)
O(48)-C(48)-H(48A)	110.6
C(49)-C(48)-H(48A)	110.6
O(48)-C(48)-H(48B)	110.6
C(49)-C(48)-H(48B)	110.6
H(48A)-C(48)-H(48B)	108.7
C(47)-O(48)-C(48)	117.97(9)
C(48)-C(49)-H(49A)	109.5
C(48)-C(49)-H(49B)	109.5
H(49A)-C(49)-H(49B)	109.5
C(48)-C(49)-H(49C)	109.5
H(49A)-C(49)-H(49C)	109.5
H(49B)-C(49)-H(49C)	109.5
C(55)-C(50)-C(51)	118.72(10)
C(55)-C(50)-C(34)	121.20(9)
C(51)-C(50)-C(34)	119.95(9)
C(52)-C(51)-C(50)	120.81(11)
C(52)-C(51)-H(51)	119.6
C(50)-C(51)-H(51)	119.6
C(53)-C(52)-C(51)	119.95(11)
C(53)-C(52)-H(52)	120.0
C(51)-C(52)-H(52)	120.0
C(54)-C(53)-C(52)	119.63(11)
C(54)-C(53)-H(53)	120.2
C(52)-C(53)-H(53)	120.2
C(53)-C(54)-C(55)	120.53(11)
C(53)-C(54)-H(54)	119.7

C(55)-C(54)-H(54)	119.7
C(54)-C(55)-C(50)	120.33(10)
C(54)-C(55)-H(55)	119.8
C(50)-C(55)-H(55)	119.8
C(62)-C(61)-H(61A)	109.5
C(62)-C(61)-H(61B)	109.5
H(61A)-C(61)-H(61B)	109.5
C(62)-C(61)-H(61C)	109.5
H(61A)-C(61)-H(61C)	109.5
H(61B)-C(61)-H(61C)	109.5
O(61)-C(62)-O(62)	122.8(2)
O(61)-C(62)-C(61)	125.4(2)
O(62)-C(62)-C(61)	111.8(2)
C(62)-O(62)-C(63)	116.9(2)
O(62)-C(63)-C(64)	107.6(3)
O(62)-C(63)-H(63A)	110.2
C(64)-C(63)-H(63A)	110.2
O(62)-C(63)-H(63B)	110.2
C(64)-C(63)-H(63B)	110.2
H(63A)-C(63)-H(63B)	108.5
C(63)-C(64)-H(64A)	109.5
C(63)-C(64)-H(64B)	109.5
H(64A)-C(64)-H(64B)	109.5
C(63)-C(64)-H(64C)	109.5
H(64A)-C(64)-H(64C)	109.5
H(64B)-C(64)-H(64C)	109.5

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($Å^2$x 10^3) for JF3005FMI. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2 a^{*2}U^{11} + ... + 2 h k a^* b^* U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
C(1)	16(1)	17(1)	20(1)	-6(1)	-4(1)	-1(1)
O(1)	17(1)	19(1)	24(1)	-9(1)	-6(1)	2(1)
C(2)	18(1)	16(1)	19(1)	-5(1)	-4(1)	-1(1)
O(2)	18(1)	22(1)	22(1)	-10(1)	-5(1)	-1(1)
C(3)	17(1)	17(1)	19(1)	-5(1)	-3(1)	-1(1)
C(4)	20(1)	16(1)	22(1)	-7(1)	-4(1)	-1(1)
C(5)	21(1)	18(1)	27(1)	-7(1)	-2(1)	-3(1)
C(6)	19(1)	17(1)	23(1)	-5(1)	-3(1)	-2(1)
C(7)	21(1)	22(1)	31(1)	-8(1)	2(1)	-4(1)
C(8)	28(1)	26(1)	45(1)	-8(1)	9(1)	-9(1)
C(9)	36(1)	21(1)	56(1)	-6(1)	10(1)	-9(1)
C(10)	29(1)	18(1)	46(1)	-9(1)	4(1)	-4(1)
C(11)	22(1)	18(1)	21(1)	-7(1)	-2(1)	1(1)
C(12)	21(1)	21(1)	21(1)	-9(1)	-2(1)	0(1)
C(13)	20(1)	17(1)	18(1)	-4(1)	-3(1)	-1(1)
N(13)	20(1)	17(1)	20(1)	-3(1)	-4(1)	-1(1)
O(13)	23(1)	21(1)	31(1)	-4(1)	-8(1)	-4(1)
C(14)	23(1)	22(1)	17(1)	-4(1)	-4(1)	0(1)
O(14)	31(1)	26(1)	26(1)	-10(1)	-10(1)	-2(1)
C(15)	25(1)	18(1)	38(1)	-2(1)	-7(1)	-1(1)
O(15)	28(1)	22(1)	26(1)	-4(1)	-10(1)	2(1)
C(16)	25(1)	16(1)	24(1)	-3(1)	-3(1)	-2(1)
C(17)	20(1)	19(1)	22(1)	-7(1)	-2(1)	-1(1)
O(17)	27(1)	40(1)	21(1)	-9(1)	-3(1)	-1(1)
C(18)	21(1)	36(1)	29(1)	-11(1)	3(1)	-2(1)
O(18)	17(1)	27(1)	24(1)	-8(1)	-1(1)	-2(1)
C(19)	20(1)	44(1)	42(1)	-17(1)	0(1)	-4(1)
C(20)	22(1)	14(1)	23(1)	-6(1)	-4(1)	0(1)
C(21)	26(1)	20(1)	26(1)	-10(1)	-3(1)	1(1)
C(22)	26(1)	21(1)	38(1)	-11(1)	-2(1)	3(1)
C(23)	33(1)	24(1)	44(1)	-8(1)	-15(1)	6(1)

C(24)	42(1)	28(1)	31(1)	-8(1)	-17(1)	4(1)
C(25)	33(1)	21(1)	24(1)	-9(1)	-6(1)	1(1)
C(31)	17(1)	18(1)	20(1)	-6(1)	0(1)	-4(1)
O(31)	20(1)	22(1)	27(1)	-11(1)	2(1)	-9(1)
C(32)	19(1)	16(1)	18(1)	-4(1)	-2(1)	-2(1)
O(32)	18(1)	23(1)	21(1)	-10(1)	1(1)	-6(1)
C(33)	18(1)	16(1)	18(1)	-5(1)	-3(1)	-2(1)
C(34)	20(1)	16(1)	19(1)	-5(1)	-2(1)	-2(1)
C(35)	18(1)	18(1)	19(1)	-4(1)	-1(1)	-2(1)
C(36)	17(1)	19(1)	18(1)	-4(1)	-1(1)	-2(1)
C(37)	19(1)	27(1)	23(1)	-7(1)	-4(1)	-3(1)
C(38)	20(1)	32(1)	25(1)	-5(1)	-5(1)	1(1)
C(39)	24(1)	23(1)	27(1)	-2(1)	-4(1)	3(1)
C(40)	24(1)	18(1)	28(1)	-4(1)	-3(1)	-1(1)
C(41)	24(1)	20(1)	23(1)	-9(1)	-2(1)	-6(1)
C(42)	24(1)	24(1)	21(1)	-10(1)	-2(1)	-6(1)
C(43)	23(1)	17(1)	18(1)	-4(1)	-2(1)	-2(1)
N(43)	22(1)	16(1)	22(1)	-2(1)	-1(1)	-1(1)
O(43)	24(1)	21(1)	28(1)	-5(1)	1(1)	1(1)
C(44)	26(1)	20(1)	19(1)	-2(1)	2(1)	-3(1)
O(44)	34(1)	24(1)	33(1)	-2(1)	10(1)	2(1)
C(45)	26(1)	20(1)	32(1)	2(1)	-4(1)	-3(1)
O(45)	28(1)	20(1)	23(1)	0(1)	1(1)	-4(1)
C(46)	28(1)	16(1)	32(1)	0(1)	1(1)	1(1)
C(47)	22(1)	18(1)	21(1)	-7(1)	-5(1)	0(1)
O(47)	30(1)	35(1)	18(1)	-7(1)	-3(1)	-4(1)
C(48)	24(1)	33(1)	26(1)	-13(1)	-10(1)	1(1)
O(48)	20(1)	31(1)	23(1)	-12(1)	-6(1)	0(1)
C(49)	24(1)	40(1)	38(1)	-8(1)	-11(1)	-2(1)
C(50)	21(1)	16(1)	22(1)	-5(1)	-3(1)	-2(1)
C(51)	27(1)	19(1)	24(1)	-8(1)	-4(1)	-3(1)
C(52)	28(1)	23(1)	35(1)	-12(1)	-8(1)	-4(1)
C(53)	23(1)	22(1)	41(1)	-10(1)	-2(1)	-6(1)
C(54)	25(1)	22(1)	29(1)	-6(1)	2(1)	-4(1)
C(55)	23(1)	19(1)	22(1)	-6(1)	-2(1)	-2(1)
C(61)	27(1)	33(1)	34(1)	-11(1)	-3(1)	1(1)

O(61)	27(1)	42(1)	35(1)	-16(1)	-1(1)	-4(1)
C(62)	26(1)	30(1)	28(1)	-16(1)	-1(1)	0(1)
O(62)	30(1)	35(1)	32(1)	-6(1)	-1(1)	-3(1)
C(63)	40(2)	41(2)	32(1)	-7(1)	-8(1)	4(1)
C(64)	95(3)	33(2)	36(2)	-14(1)	-19(2)	0(2)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (Å^{2}x 10^3) for JF3005FMI.

	x	y	z	U(eq)
H(2)	8003	6907	396	22
H(3)	10103	6356	1515	22
H(4)	9217	5040	853	23
H(7)	5290	6219	2593	31
H(8)	4793	4554	3349	43
H(9)	6271	3175	3168	49
H(10)	8251	3472	2249	39
H(11A)	5066	8445	1972	25
H(11B)	6356	8985	1380	25
H(12A)	7362	8304	2577	25
H(12B)	6502	7326	2915	25
H(15A)	6207	10872	-223	36
H(15B)	7068	11109	-1095	36
H(16A)	8989	10166	-537	27
H(16B)	8191	10080	333	27
H(18A)	13398	7042	-359	36
H(18B)	13322	5872	-223	36
H(19A)	14706	6503	764	53
H(19B)	15489	6012	134	53
H(19C)	14601	5335	924	53
H(21)	11329	3988	776	29
H(22)	13316	2933	1342	35
H(23)	13767	2717	2637	42
H(24)	12207	3529	3379	41
H(25)	10241	4594	2810	31
H(32)	1724	7805	4293	22
H(33)	4217	8263	3203	21
H(34)	2436	9515	3961	22
H(37)	-206	8761	2121	28
H(38)	-978	10489	1457	33

H(39)	40	11744	1642	33
H(40)	1778	11265	2528	30
H(41A)	414	6314	2694	26
H(41B)	1650	5848	3287	26
H(42A)	2931	6515	2067	27
H(42B)	1753	7474	1731	27
H(45A)	1502	3653	5894	35
H(45B)	2182	4191	6363	35
H(46A)	3747	4623	5284	35
H(46B)	2753	4429	4729	35
H(48A)	7084	7451	5011	32
H(48B)	6376	8575	4945	32
H(49A)	8520	8157	3813	53
H(49B)	8736	8665	4430	53
H(49C)	7776	9280	3704	53
H(51)	4079	10307	4261	28
H(52)	5968	11264	3893	33
H(53)	7098	11708	2586	35
H(54)	6301	11218	1647	32
H(55)	4436	10240	2017	26
H(61A)	10446	7866	6432	49
H(61B)	11224	8821	6320	49
H(61C)	11632	8243	5703	49
H(63A)	8459	10814	4643	49
H(63B)	9225	10433	3942	49
H(64A)	10015	11981	4353	81
H(64B)	9487	12134	3511	81
H(64C)	10986	11521	3751	81

Table 6. Torsion angles [°] for JF3005FMI.

O(2)-C(1)-O(1)-C(11)	-0.34(10)
C(6)-C(1)-O(1)-C(11)	119.12(9)
C(2)-C(1)-O(1)-C(11)	-117.46(9)
O(1)-C(1)-C(2)-C(13)	63.18(10)
O(2)-C(1)-C(2)-C(13)	-52.87(10)
C(6)-C(1)-C(2)-C(13)	-174.14(8)
O(1)-C(1)-C(2)-C(3)	-177.41(8)
O(2)-C(1)-C(2)-C(3)	66.54(10)
C(6)-C(1)-C(2)-C(3)	-54.72(10)
O(1)-C(1)-O(2)-C(12)	22.74(10)
C(6)-C(1)-O(2)-C(12)	-96.26(9)
C(2)-C(1)-O(2)-C(12)	142.10(8)
C(13)-C(2)-C(3)-C(17)	-51.99(11)
C(1)-C(2)-C(3)-C(17)	-170.51(8)
C(13)-C(2)-C(3)-C(4)	-173.94(8)
C(1)-C(2)-C(3)-C(4)	67.54(10)
C(17)-C(3)-C(4)-C(5)	-168.26(8)
C(2)-C(3)-C(4)-C(5)	-45.07(11)
C(17)-C(3)-C(4)-C(20)	66.75(10)
C(2)-C(3)-C(4)-C(20)	-170.06(8)
C(20)-C(4)-C(5)-C(6)	135.37(11)
C(3)-C(4)-C(5)-C(6)	12.30(14)
C(20)-C(4)-C(5)-C(10)	-45.17(14)
C(3)-C(4)-C(5)-C(10)	-168.24(11)
C(10)-C(5)-C(6)-C(7)	1.79(17)
C(4)-C(5)-C(6)-C(7)	-178.75(10)
C(10)-C(5)-C(6)-C(1)	179.10(11)
C(4)-C(5)-C(6)-C(1)	-1.44(16)
O(1)-C(1)-C(6)-C(5)	146.52(10)
O(2)-C(1)-C(6)-C(5)	-96.73(11)
C(2)-C(1)-C(6)-C(5)	22.99(13)
O(1)-C(1)-C(6)-C(7)	-36.14(13)
O(2)-C(1)-C(6)-C(7)	80.62(12)
C(2)-C(1)-C(6)-C(7)	-159.66(10)

C(5)-C(6)-C(7)-C(8)	0.59(18)
C(1)-C(6)-C(7)-C(8)	-176.79(11)
C(6)-C(7)-C(8)-C(9)	-1.9(2)
C(7)-C(8)-C(9)-C(10)	0.7(2)
C(8)-C(9)-C(10)-C(5)	1.7(2)
C(6)-C(5)-C(10)-C(9)	-3.0(2)
C(4)-C(5)-C(10)-C(9)	177.55(13)
C(1)-O(1)-C(11)-C(12)	-20.61(10)
C(1)-O(2)-C(12)-C(11)	-34.67(10)
O(1)-C(11)-C(12)-O(2)	33.42(10)
C(3)-C(2)-C(13)-O(13)	-20.07(14)
C(1)-C(2)-C(13)-O(13)	97.87(11)
C(3)-C(2)-C(13)-N(13)	165.32(9)
C(1)-C(2)-C(13)-N(13)	-76.74(11)
O(13)-C(13)-N(13)-C(14)	164.46(10)
C(2)-C(13)-N(13)-C(14)	-20.74(16)
O(13)-C(13)-N(13)-C(16)	-10.91(15)
C(2)-C(13)-N(13)-C(16)	163.89(9)
C(13)-N(13)-C(14)-O(14)	-3.16(19)
C(16)-N(13)-C(14)-O(14)	172.48(11)
C(13)-N(13)-C(14)-O(15)	177.75(10)
C(16)-N(13)-C(14)-O(15)	-6.60(12)
O(14)-C(14)-O(15)-C(15)	-178.50(11)
N(13)-C(14)-O(15)-C(15)	0.66(12)
C(16)-C(15)-O(15)-C(14)	5.09(13)
C(13)-N(13)-C(16)-C(15)	-174.70(9)
C(14)-N(13)-C(16)-C(15)	9.20(12)
O(15)-C(15)-C(16)-N(13)	-8.27(12)
C(2)-C(3)-C(17)-O(17)	-42.28(14)
C(4)-C(3)-C(17)-O(17)	80.24(13)
C(2)-C(3)-C(17)-O(18)	140.13(9)
C(4)-C(3)-C(17)-O(18)	-97.35(10)
O(17)-C(17)-O(18)-C(18)	-3.94(16)
C(3)-C(17)-O(18)-C(18)	173.64(9)
C(19)-C(18)-O(18)-C(17)	-171.34(10)
C(5)-C(4)-C(20)-C(21)	135.63(10)

C(3)-C(4)-C(20)-C(21)	-100.15(11)
C(5)-C(4)-C(20)-C(25)	-47.49(13)
C(3)-C(4)-C(20)-C(25)	76.73(12)
C(25)-C(20)-C(21)-C(22)	-1.58(17)
C(4)-C(20)-C(21)-C(22)	175.35(10)
C(20)-C(21)-C(22)-C(23)	0.61(18)
C(21)-C(22)-C(23)-C(24)	0.8(2)
C(22)-C(23)-C(24)-C(25)	-1.1(2)
C(23)-C(24)-C(25)-C(20)	0.1(2)
C(21)-C(20)-C(25)-C(24)	1.22(18)
C(4)-C(20)-C(25)-C(24)	-175.72(11)
O(32)-C(31)-O(31)-C(41)	8.66(10)
C(36)-C(31)-O(31)-C(41)	127.45(9)
C(32)-C(31)-O(31)-C(41)	-109.52(9)
O(31)-C(31)-C(32)-C(43)	59.31(10)
O(32)-C(31)-C(32)-C(43)	-57.48(10)
C(36)-C(31)-C(32)-C(43)	-177.53(8)
O(31)-C(31)-C(32)-C(33)	179.47(8)
O(32)-C(31)-C(32)-C(33)	62.67(10)
C(36)-C(31)-C(32)-C(33)	-57.37(10)
O(31)-C(31)-O(32)-C(42)	15.37(10)
C(36)-C(31)-O(32)-C(42)	-104.24(9)
C(32)-C(31)-O(32)-C(42)	135.06(8)
C(43)-C(32)-C(33)-C(47)	-49.28(11)
C(31)-C(32)-C(33)-C(47)	-169.71(8)
C(43)-C(32)-C(33)-C(34)	-170.02(8)
C(31)-C(32)-C(33)-C(34)	69.54(10)
C(47)-C(33)-C(34)-C(50)	60.91(10)
C(32)-C(33)-C(34)-C(50)	-176.07(8)
C(47)-C(33)-C(34)-C(35)	-171.41(8)
C(32)-C(33)-C(34)-C(35)	-48.38(11)
C(50)-C(34)-C(35)-C(36)	143.12(10)
C(33)-C(34)-C(35)-C(36)	17.88(13)
C(50)-C(34)-C(35)-C(40)	-40.12(13)
C(33)-C(34)-C(35)-C(40)	-165.36(9)
C(40)-C(35)-C(36)-C(37)	-0.45(15)

C(34)-C(35)-C(36)-C(37)	176.31(9)
C(40)-C(35)-C(36)-C(31)	175.50(9)
C(34)-C(35)-C(36)-C(31)	-7.74(15)
O(31)-C(31)-C(36)-C(37)	-33.14(12)
O(32)-C(31)-C(36)-C(37)	83.85(11)
C(32)-C(31)-C(36)-C(37)	-156.51(9)
O(31)-C(31)-C(36)-C(35)	150.88(9)
O(32)-C(31)-C(36)-C(35)	-92.13(11)
C(32)-C(31)-C(36)-C(35)	27.51(12)
C(35)-C(36)-C(37)-C(38)	0.16(16)
C(31)-C(36)-C(37)-C(38)	-175.85(10)
C(36)-C(37)-C(38)-C(39)	0.62(17)
C(37)-C(38)-C(39)-C(40)	-1.09(18)
C(38)-C(39)-C(40)-C(35)	0.80(18)
C(36)-C(35)-C(40)-C(39)	-0.03(16)
C(34)-C(35)-C(40)-C(39)	-176.91(10)
C(31)-O(31)-C(41)-C(42)	-27.89(10)
C(31)-O(32)-C(42)-C(41)	-31.74(10)
O(31)-C(41)-C(42)-O(32)	35.95(10)
C(33)-C(32)-C(43)-O(43)	-31.99(14)
C(31)-C(32)-C(43)-O(43)	86.33(12)
C(33)-C(32)-C(43)-N(43)	148.72(9)
C(31)-C(32)-C(43)-N(43)	-92.95(11)
O(43)-C(43)-N(43)-C(44)	176.28(11)
C(32)-C(43)-N(43)-C(44)	-4.41(17)
O(43)-C(43)-N(43)-C(46)	-4.65(16)
C(32)-C(43)-N(43)-C(46)	174.66(10)
C(43)-N(43)-C(44)-O(44)	3.9(2)
C(46)-N(43)-C(44)-O(44)	-175.20(14)
C(43)-N(43)-C(44)-O(45)	-176.69(10)
C(46)-N(43)-C(44)-O(45)	4.17(13)
O(44)-C(44)-O(45)-C(45)	-171.88(12)
N(43)-C(44)-O(45)-C(45)	8.70(13)
C(46)-C(45)-O(45)-C(44)	-17.60(14)
C(43)-N(43)-C(46)-C(45)	166.54(10)
C(44)-N(43)-C(46)-C(45)	-14.23(13)

O(45)-C(45)-C(46)-N(43)	18.43(13)
C(32)-C(33)-C(47)-O(47)	-42.27(14)
C(34)-C(33)-C(47)-O(47)	78.72(13)
C(32)-C(33)-C(47)-O(48)	140.87(9)
C(34)-C(33)-C(47)-O(48)	-98.14(10)
O(47)-C(47)-O(48)-C(48)	-11.07(16)
C(33)-C(47)-O(48)-C(48)	165.79(9)
C(49)-C(48)-O(48)-C(47)	-161.02(10)
C(35)-C(34)-C(50)-C(55)	-45.90(13)
C(33)-C(34)-C(50)-C(55)	80.16(12)
C(35)-C(34)-C(50)-C(51)	138.33(10)
C(33)-C(34)-C(50)-C(51)	-95.61(11)
C(55)-C(50)-C(51)-C(52)	-1.47(16)
C(34)-C(50)-C(51)-C(52)	174.40(10)
C(50)-C(51)-C(52)-C(53)	0.66(17)
C(51)-C(52)-C(53)-C(54)	0.70(18)
C(52)-C(53)-C(54)-C(55)	-1.24(18)
C(53)-C(54)-C(55)-C(50)	0.42(17)
C(51)-C(50)-C(55)-C(54)	0.93(16)
C(34)-C(50)-C(55)-C(54)	-174.89(10)
O(61)-C(62)-O(62)-C(63)	-2.5(4)
C(61)-C(62)-O(62)-C(63)	178.8(2)
C(62)-O(62)-C(63)-C(64)	159.5(3)

Symmetry transformations used to generate equivalent atoms:

Table 7. Hydrogen bonds for JF3005FMI [Å and °].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
C(2)-H(2)...O(14)	1.00	2.33	2.9721(13)	121.2
C(11)-H(11A)...O(32)	0.99	2.55	3.3876(13)	142.4
C(15)-H(15B)...O(32)#1	0.99	2.58	3.5456(15)	165.0
C(16)-H(16A)...O(13)#2	0.99	2.52	3.1041(14)	117.8
C(32)-H(32)...O(44)	1.00	2.28	2.9582(13)	123.6
C(41)-H(41A)...O(2)#3	0.99	2.61	3.3991(13)	137.0
C(45)-H(45A)...O(31)#4	0.99	2.65	3.3334(14)	126.1
C(46)-H(46A)...O(43)#5	0.99	2.35	3.2956(15)	158.7
C(49)-H(49A)...O(31)#6	0.98	2.61	3.5122(17)	152.4
C(49)-H(49B)...O(61)	0.98	2.38	3.150(2)	135.4
C(61)-H(61C)...O(47)#6	0.98	2.55	3.501(3)	162.5
C(64)-H(64A)...O(44)#7	0.98	2.41	3.351(3)	161.1

Symmetry transformations used to generate equivalent atoms:

#1 -x+1,-y+2,-z   #2 -x+2,-y+2,-z   #3 x-1,y,z

#4 -x,-y+1,-z+1   #5 -x+1,-y+1,-z+1   #6 x+1,y,z

#7 -x+1,-y+2,-z+1

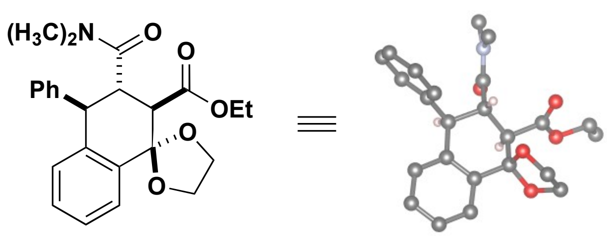


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Table 1. Crystal data and structure refinement for [$C_{24}H_{27}NO_5$].

Identification code	JF3023FMI (JMR-II-14)
Empirical formula	C24 H27 N O5
Formula weight	409.46
Temperature	100(2) K
Wavelength	0.71073 Å
Crystal system	Monoclinic
Space group	$P2_1/c$

Unit cell dimensions	a = 11.2062(10) Å	〈= 90°.
	b = 11.4773(11) Å	®= 94.0553(18)°.
	c = 16.2488(15) Å	© = 90°.
Volume	2084.6(3) $Å^3$	
Z	4	
Density (calculated)	1.305 Mg/m^3	
Absorption coefficient	0.091 mm^{-1}	
F(000)	872	
Crystal size	0.539 x 0.352 x 0.200 mm^3	
Crystal color and habit	Colorless Block	
Diffractometer	Bruker Photon100 CMOS	
Theta range for data collection	2.174 to 27.499°.	
Index ranges	-14<=h<=14, -14<=k<=14, -21<=l<=21	
Reflections collected	18508	
Independent reflections	4785 [R(int) = 0.0244]	
Observed reflections (I > 2sigma(I))	4254	
Completeness to theta = 25.242°	100.0 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.9825 and 0.8832	
Solution method	SHELXT (Sheldrick, 2014)	
Refinement method	SHELXL-2017/1 (Sheldrick, 2017) Full-matrix least-squares on F^2	
Data / restraints / parameters	4785 / 0 / 380	
Goodness-of-fit on F^2	1.047	
Final R indices [I>2sigma(I)]	R1 = 0.0462, wR2 = 0.1216	
R indices (all data)	R1 = 0.0515, wR2 = 0.1275	
Extinction coefficient	0.025(2)	
Largest diff. peak and hole	0.353 and -0.290 e.$Å^{-3}$	

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for JF3023FMI. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
C(1)	6070(1)	3119(1)	3280(1)	21(1)
O(1)	6521(1)	1954(1)	3378(1)	26(1)
C(2)	6193(1)	3514(1)	2385(1)	20(1)
O(2)	4850(1)	3086(1)	3462(1)	26(1)
C(3)	7520(1)	3507(1)	2208(1)	20(1)
C(4)	8232(1)	4387(1)	2772(1)	21(1)
C(5)	7826(1)	4442(1)	3648(1)	20(1)
C(6)	6768(1)	3926(1)	3876(1)	21(1)
C(7)	6387(1)	4114(1)	4664(1)	27(1)
C(8)	7056(1)	4788(1)	5232(1)	30(1)
C(9)	8130(1)	5272(1)	5019(1)	28(1)
C(10)	8503(1)	5103(1)	4233(1)	24(1)
C(11)	5669(1)	1301(1)	3813(1)	33(1)
C(12)	4504(1)	1886(1)	3535(1)	31(1)
C(13)	5491(1)	2717(1)	1782(1)	24(1)
O(13)	5857(1)	1809(1)	1538(1)	36(1)
C(14)	3667(1)	2452(1)	974(1)	35(1)
O(14)	4412(1)	3161(1)	1551(1)	28(1)
C(15)	2721(1)	3228(1)	571(1)	33(1)
C(16)	7643(1)	3892(1)	1314(1)	24(1)
N(16)	8431(1)	3344(1)	859(1)	25(1)
O(16)	7047(1)	4725(1)	1044(1)	38(1)
C(17)	8630(2)	3785(2)	37(1)	35(1)
C(18)	9128(1)	2317(1)	1104(1)	33(1)
C(19)	9572(1)	4166(1)	2770(1)	22(1)
C(20)	10309(1)	4946(1)	2396(1)	28(1)
C(21)	11544(1)	4749(1)	2403(1)	34(1)
C(22)	12036(1)	3761(2)	2768(1)	33(1)
C(23)	11305(1)	2962(1)	3137(1)	30(1)
C(24)	10079(1)	3171(1)	3141(1)	25(1)

Table 3. Bond lengths [Å] and angles [°] for JF3023FMI.

C(1)-O(2)	1.4199(14)
C(1)-O(1)	1.4349(15)
C(1)-C(6)	1.5170(17)
C(1)-C(2)	1.5377(18)
O(1)-C(11)	1.4372(17)
C(2)-C(13)	1.5182(17)
C(2)-C(3)	1.5350(16)
C(2)-H(2)	0.952(17)
O(2)-C(12)	1.4371(17)
C(3)-C(16)	1.5339(18)
C(3)-C(4)	1.5471(17)
C(3)-H(3)	0.956(16)
C(4)-C(19)	1.5227(16)
C(4)-C(5)	1.5252(17)
C(4)-H(4)	0.962(16)
C(5)-C(10)	1.3979(18)
C(5)-C(6)	1.3979(17)
C(6)-C(7)	1.3951(19)
C(7)-C(8)	1.384(2)
C(7)-H(7)	0.950(18)
C(8)-C(9)	1.391(2)
C(8)-H(8)	0.994(19)
C(9)-C(10)	1.386(2)
C(9)-H(9)	0.974(19)
C(10)-H(10)	0.952(17)
C(11)-C(12)	1.509(2)
C(11)-H(11A)	1.010(19)
C(11)-H(11B)	0.965(19)
C(12)-H(12A)	0.986(17)
C(12)-H(12B)	0.943(19)
C(13)-O(13)	1.1980(17)
C(13)-O(14)	1.3408(15)
C(14)-O(14)	1.4586(17)
C(14)-C(15)	1.499(2)

C(14)-H(14A)	0.96(2)
C(14)-H(14B)	0.99(2)
C(15)-H(15A)	1.04(2)
C(15)-H(15B)	1.03(2)
C(15)-H(15C)	1.00(2)
C(16)-O(16)	1.2298(17)
C(16)-N(16)	1.3464(17)
N(16)-C(18)	1.4535(18)
N(16)-C(17)	1.4607(18)
C(17)-H(17A)	1.02(2)
C(17)-H(17B)	1.001(18)
C(17)-H(17C)	0.96(3)
C(18)-H(18A)	0.99(2)
C(18)-H(18B)	0.99(2)
C(18)-H(18C)	0.95(2)
C(19)-C(20)	1.3878(19)
C(19)-C(24)	1.3937(19)
C(20)-C(21)	1.4011(19)
C(20)-H(20)	0.966(17)
C(21)-C(22)	1.377(2)
C(21)-H(21)	0.95(2)
C(22)-C(23)	1.393(2)
C(22)-H(22)	0.96(2)
C(23)-C(24)	1.3955(18)
C(23)-H(23)	0.99(2)
C(24)-H(24)	1.010(17)

O(2)-C(1)-O(1)	106.76(9)
O(2)-C(1)-C(6)	110.16(10)
O(1)-C(1)-C(6)	109.63(10)
O(2)-C(1)-C(2)	110.92(10)
O(1)-C(1)-C(2)	108.99(10)
C(6)-C(1)-C(2)	110.31(10)
C(1)-O(1)-C(11)	107.46(10)
C(13)-C(2)-C(3)	109.89(10)
C(13)-C(2)-C(1)	110.84(10)

C(3)-C(2)-C(1)	109.23(10)
C(13)-C(2)-H(2)	108.5(10)
C(3)-C(2)-H(2)	111.6(10)
C(1)-C(2)-H(2)	106.7(10)
C(1)-O(2)-C(12)	108.17(10)
C(16)-C(3)-C(2)	109.23(10)
C(16)-C(3)-C(4)	107.25(10)
C(2)-C(3)-C(4)	110.56(10)
C(16)-C(3)-H(3)	112.8(9)
C(2)-C(3)-H(3)	107.3(9)
C(4)-C(3)-H(3)	109.7(9)
C(19)-C(4)-C(5)	111.65(10)
C(19)-C(4)-C(3)	110.91(10)
C(5)-C(4)-C(3)	113.85(10)
C(19)-C(4)-H(4)	105.3(9)
C(5)-C(4)-H(4)	107.2(9)
C(3)-C(4)-H(4)	107.4(9)
C(10)-C(5)-C(6)	118.62(12)
C(10)-C(5)-C(4)	118.24(11)
C(6)-C(5)-C(4)	123.00(11)
C(7)-C(6)-C(5)	119.91(12)
C(7)-C(6)-C(1)	120.18(11)
C(5)-C(6)-C(1)	119.85(11)
C(8)-C(7)-C(6)	120.79(12)
C(8)-C(7)-H(7)	120.7(11)
C(6)-C(7)-H(7)	118.5(11)
C(7)-C(8)-C(9)	119.68(13)
C(7)-C(8)-H(8)	117.4(11)
C(9)-C(8)-H(8)	122.9(11)
C(10)-C(9)-C(8)	119.70(13)
C(10)-C(9)-H(9)	121.8(10)
C(8)-C(9)-H(9)	118.5(10)
C(9)-C(10)-C(5)	121.25(12)
C(9)-C(10)-H(10)	119.8(10)
C(5)-C(10)-H(10)	119.0(10)
O(1)-C(11)-C(12)	102.18(11)

O(1)-C(11)-H(11A)	110.5(11)
C(12)-C(11)-H(11A)	109.1(11)
O(1)-C(11)-H(11B)	108.0(11)
C(12)-C(11)-H(11B)	112.4(11)
H(11A)-C(11)-H(11B)	114.0(15)
O(2)-C(12)-C(11)	102.64(11)
O(2)-C(12)-H(12A)	112.8(10)
C(11)-C(12)-H(12A)	110.3(10)
O(2)-C(12)-H(12B)	108.6(11)
C(11)-C(12)-H(12B)	114.8(11)
H(12A)-C(12)-H(12B)	107.7(15)
O(13)-C(13)-O(14)	124.09(12)
O(13)-C(13)-C(2)	124.32(12)
O(14)-C(13)-C(2)	111.59(11)
O(14)-C(14)-C(15)	107.72(12)
O(14)-C(14)-H(14A)	107.7(13)
C(15)-C(14)-H(14A)	112.8(13)
O(14)-C(14)-H(14B)	108.3(12)
C(15)-C(14)-H(14B)	112.8(12)
H(14A)-C(14)-H(14B)	107.3(18)
C(13)-O(14)-C(14)	115.61(11)
C(14)-C(15)-H(15A)	110.5(12)
C(14)-C(15)-H(15B)	106.7(12)
H(15A)-C(15)-H(15B)	110.4(16)
C(14)-C(15)-H(15C)	109.1(12)
H(15A)-C(15)-H(15C)	111.2(17)
H(15B)-C(15)-H(15C)	108.9(17)
O(16)-C(16)-N(16)	121.91(12)
O(16)-C(16)-C(3)	118.59(11)
N(16)-C(16)-C(3)	119.44(11)
C(16)-N(16)-C(18)	126.04(12)
C(16)-N(16)-C(17)	119.28(12)
C(18)-N(16)-C(17)	114.68(11)
N(16)-C(17)-H(17A)	111.4(12)
N(16)-C(17)-H(17B)	107.4(10)
H(17A)-C(17)-H(17B)	107.6(16)

N(16)-C(17)-H(17C)	110.9(15)
H(17A)-C(17)-H(17C)	113.1(19)
H(17B)-C(17)-H(17C)	106.2(18)
N(16)-C(18)-H(18A)	111.5(14)
N(16)-C(18)-H(18B)	107.6(11)
H(18A)-C(18)-H(18B)	107.5(17)
N(16)-C(18)-H(18C)	110.6(12)
H(18A)-C(18)-H(18C)	111.3(19)
H(18B)-C(18)-H(18C)	108.2(17)
C(20)-C(19)-C(24)	118.81(12)
C(20)-C(19)-C(4)	120.74(12)
C(24)-C(19)-C(4)	120.45(11)
C(19)-C(20)-C(21)	120.67(14)
C(19)-C(20)-H(20)	119.9(10)
C(21)-C(20)-H(20)	119.4(10)
C(22)-C(21)-C(20)	120.13(14)
C(22)-C(21)-H(21)	121.9(12)
C(20)-C(21)-H(21)	118.0(12)
C(21)-C(22)-C(23)	119.82(13)
C(21)-C(22)-H(22)	119.9(12)
C(23)-C(22)-H(22)	120.2(12)
C(22)-C(23)-C(24)	119.93(14)
C(22)-C(23)-H(23)	120.8(11)
C(24)-C(23)-H(23)	119.3(11)
C(19)-C(24)-C(23)	120.62(13)
C(19)-C(24)-H(24)	118.6(9)
C(23)-C(24)-H(24)	120.7(10)

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($Å^2$x 10^3) for JF3023FMI. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2 a^{*2}U^{11} + ... + 2 h k a^* b^* U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
C(1)	16(1)	22(1)	26(1)	0(1)	2(1)	0(1)
O(1)	23(1)	21(1)	32(1)	3(1)	2(1)	0(1)
C(2)	16(1)	21(1)	24(1)	-1(1)	0(1)	1(1)
O(2)	16(1)	27(1)	34(1)	0(1)	4(1)	-3(1)
C(3)	17(1)	22(1)	22(1)	0(1)	1(1)	2(1)
C(4)	17(1)	21(1)	24(1)	0(1)	2(1)	0(1)
C(5)	17(1)	21(1)	23(1)	0(1)	2(1)	3(1)
C(6)	17(1)	22(1)	24(1)	1(1)	0(1)	2(1)
C(7)	23(1)	31(1)	28(1)	0(1)	5(1)	-2(1)
C(8)	31(1)	35(1)	23(1)	-2(1)	3(1)	1(1)
C(9)	26(1)	29(1)	27(1)	-5(1)	-4(1)	1(1)
C(10)	19(1)	26(1)	28(1)	-2(1)	0(1)	-1(1)
C(11)	29(1)	29(1)	40(1)	8(1)	2(1)	-5(1)
C(12)	25(1)	30(1)	40(1)	5(1)	2(1)	-8(1)
C(13)	19(1)	27(1)	26(1)	-1(1)	0(1)	-1(1)
O(13)	30(1)	34(1)	44(1)	-14(1)	-7(1)	7(1)
C(14)	30(1)	30(1)	44(1)	-6(1)	-14(1)	-2(1)
O(14)	20(1)	27(1)	35(1)	-5(1)	-6(1)	0(1)
C(15)	29(1)	38(1)	31(1)	-2(1)	-4(1)	2(1)
C(16)	21(1)	28(1)	24(1)	-1(1)	1(1)	1(1)
N(16)	22(1)	29(1)	24(1)	-1(1)	3(1)	2(1)
O(16)	42(1)	43(1)	30(1)	10(1)	8(1)	20(1)
C(17)	35(1)	44(1)	27(1)	2(1)	8(1)	8(1)
C(18)	34(1)	33(1)	32(1)	-2(1)	4(1)	11(1)
C(19)	18(1)	25(1)	24(1)	-5(1)	2(1)	-1(1)
C(20)	24(1)	27(1)	34(1)	-4(1)	8(1)	-3(1)
C(21)	24(1)	38(1)	42(1)	-9(1)	13(1)	-9(1)
C(22)	16(1)	48(1)	35(1)	-15(1)	3(1)	0(1)
C(23)	22(1)	38(1)	29(1)	-8(1)	-2(1)	6(1)
C(24)	20(1)	30(1)	25(1)	-2(1)	1(1)	1(1)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for JF3023FMI.

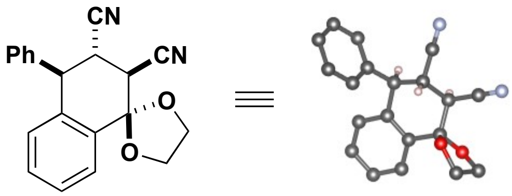
	x	y	z	U(eq)
H(2)	5860(14)	4276(15)	2337(10)	25(4)
H(3)	7816(13)	2736(14)	2316(9)	18(3)
H(4)	8109(14)	5147(14)	2533(9)	20(4)
H(7)	5647(16)	3786(16)	4798(11)	32(4)
H(8)	6753(16)	4876(16)	5789(12)	37(5)
H(9)	8586(16)	5748(16)	5426(11)	34(4)
H(10)	9224(15)	5456(15)	4080(10)	29(4)
H(11A)	5824(16)	1407(17)	4428(12)	37(5)
H(11B)	5699(16)	501(17)	3634(11)	35(4)
H(12A)	4177(15)	1551(15)	3007(11)	27(4)
H(12B)	3905(17)	1837(16)	3912(12)	35(5)
H(14A)	3343(19)	1828(19)	1280(13)	48(6)
H(14B)	4188(19)	2099(18)	574(13)	47(5)
H(15A)	2195(19)	3577(19)	1008(13)	51(6)
H(15B)	2210(18)	2716(18)	158(13)	49(5)
H(15C)	3113(19)	3854(19)	260(13)	51(6)
H(17A)	8294(19)	3232(19)	-411(13)	49(6)
H(17B)	9516(16)	3830(16)	-6(11)	34(5)
H(17C)	8330(20)	4570(20)	-33(15)	66(7)
H(18A)	9920(20)	2530(20)	1367(14)	62(7)
H(18B)	9263(18)	1869(17)	596(13)	43(5)
H(18C)	8699(19)	1837(18)	1455(13)	45(5)
H(20)	9974(15)	5644(15)	2140(10)	26(4)
H(21)	12018(18)	5313(18)	2148(12)	43(5)
H(22)	12886(19)	3631(18)	2776(12)	45(5)
H(23)	11649(17)	2254(17)	3413(12)	38(5)
H(24)	9542(15)	2610(15)	3421(10)	28(4)

Table 6. Torsion angles [°] for JF3023FMI.

O(2)-C(1)-O(1)-C(11)	-14.21(14)
C(6)-C(1)-O(1)-C(11)	105.10(12)
C(2)-C(1)-O(1)-C(11)	-134.08(11)
O(2)-C(1)-C(2)-C(13)	-57.31(13)
O(1)-C(1)-C(2)-C(13)	59.95(12)
C(6)-C(1)-C(2)-C(13)	-179.64(10)
O(2)-C(1)-C(2)-C(3)	-178.53(10)
O(1)-C(1)-C(2)-C(3)	-61.27(12)
C(6)-C(1)-C(2)-C(3)	59.13(13)
O(1)-C(1)-O(2)-C(12)	-9.46(14)
C(6)-C(1)-O(2)-C(12)	-128.43(11)
C(2)-C(1)-O(2)-C(12)	109.15(12)
C(13)-C(2)-C(3)-C(16)	57.79(13)
C(1)-C(2)-C(3)-C(16)	179.59(10)
C(13)-C(2)-C(3)-C(4)	175.59(10)
C(1)-C(2)-C(3)-C(4)	-62.61(13)
C(16)-C(3)-C(4)-C(19)	-76.07(12)
C(2)-C(3)-C(4)-C(19)	164.93(10)
C(16)-C(3)-C(4)-C(5)	157.01(10)
C(2)-C(3)-C(4)-C(5)	38.01(14)
C(19)-C(4)-C(5)-C(10)	45.88(15)
C(3)-C(4)-C(5)-C(10)	172.41(11)
C(19)-C(4)-C(5)-C(6)	-138.49(12)
C(3)-C(4)-C(5)-C(6)	-11.95(16)
C(10)-C(5)-C(6)-C(7)	2.40(18)
C(4)-C(5)-C(6)-C(7)	-173.21(12)
C(10)-C(5)-C(6)-C(1)	-174.78(11)
C(4)-C(5)-C(6)-C(1)	9.60(18)
O(2)-C(1)-C(6)-C(7)	27.11(16)
O(1)-C(1)-C(6)-C(7)	-90.09(14)
C(2)-C(1)-C(6)-C(7)	149.89(12)
O(2)-C(1)-C(6)-C(5)	-155.71(11)
O(1)-C(1)-C(6)-C(5)	87.09(14)
C(2)-C(1)-C(6)-C(5)	-32.93(15)

C(5)-C(6)-C(7)-C(8)	-1.3(2)
C(1)-C(6)-C(7)-C(8)	175.85(13)
C(6)-C(7)-C(8)-C(9)	-0.8(2)
C(7)-C(8)-C(9)-C(10)	1.9(2)
C(8)-C(9)-C(10)-C(5)	-0.7(2)
C(6)-C(5)-C(10)-C(9)	-1.39(19)
C(4)-C(5)-C(10)-C(9)	174.44(12)
C(1)-O(1)-C(11)-C(12)	30.65(14)
C(1)-O(2)-C(12)-C(11)	27.88(15)
O(1)-C(11)-C(12)-O(2)	-35.35(15)
C(3)-C(2)-C(13)-O(13)	37.35(18)
C(1)-C(2)-C(13)-O(13)	-83.48(16)
C(3)-C(2)-C(13)-O(14)	-142.17(11)
C(1)-C(2)-C(13)-O(14)	97.00(12)
O(13)-C(13)-O(14)-C(14)	0.8(2)
C(2)-C(13)-O(14)-C(14)	-179.65(12)
C(15)-C(14)-O(14)-C(13)	-160.98(13)
C(2)-C(3)-C(16)-O(16)	43.26(16)
C(4)-C(3)-C(16)-O(16)	-76.59(15)
C(2)-C(3)-C(16)-N(16)	-139.52(12)
C(4)-C(3)-C(16)-N(16)	100.63(13)
O(16)-C(16)-N(16)-C(18)	-176.50(14)
C(3)-C(16)-N(16)-C(18)	6.4(2)
O(16)-C(16)-N(16)-C(17)	3.1(2)
C(3)-C(16)-N(16)-C(17)	-174.04(12)
C(5)-C(4)-C(19)-C(20)	-121.68(13)
C(3)-C(4)-C(19)-C(20)	110.19(14)
C(5)-C(4)-C(19)-C(24)	58.60(15)
C(3)-C(4)-C(19)-C(24)	-69.52(15)
C(24)-C(19)-C(20)-C(21)	-1.1(2)
C(4)-C(19)-C(20)-C(21)	179.22(13)
C(19)-C(20)-C(21)-C(22)	1.4(2)
C(20)-C(21)-C(22)-C(23)	-0.6(2)
C(21)-C(22)-C(23)-C(24)	-0.5(2)
C(20)-C(19)-C(24)-C(23)	0.0(2)
C(4)-C(19)-C(24)-C(23)	179.69(12)

C(22)-C(23)-C(24)-C(19)	0.8(2)



CCDC 2087135

Table 1. Crystal data and structure refinement for [$C_{20}H_{16}N_2O_2$].

Identification code	JF3006F2MI (JMR-1-156)	
Empirical formula	C20 H16 N2 O2	
Formula weight	316.35	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	$P2_1/n$	
Unit cell dimensions	a = 12.6220(11) Å	〈= 90°.
	b = 9.9052(9) Å	®= 96.220(3)°.
	c = 13.1752(11) Å	© = 90°.
Volume	1637.5(2) $Å^3$	
Z	4	
Density (calculated)	1.283 Mg/m^3	
Absorption coefficient	0.084 mm^{-1}	
F(000)	664	
Crystal size	0.339 x 0.228 x 0.197 mm^3	
Crystal color and habit	Colorless Block	
Diffractometer	Bruker Photon100 CMOS	
Theta range for data collection	2.366 to 27.522°.	
Index ranges	-16<=h<=16, -12<=k<=12, -17<=l<=17	
Reflections collected	14062	
Independent reflections	3764 [R(int) = 0.0279]	
Observed reflections (I > 2sigma(I))	3371	
Completeness to theta = 25.242°	99.9 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.9804 and 0.8651	
Solution method	SHELXT (Sheldrick, 2014)	
Refinement method	SHELXL-2017/1 (Sheldrick, 2017) Full-matrix least-squares on F^2	

Data / restraints / parameters	3764 / 0 / 218
Goodness-of-fit on F^2	1.030
Final R indices [I>2sigma(I)]	R1 = 0.0459, wR2 = 0.1176
R indices (all data)	R1 = 0.0506, wR2 = 0.1223
Extinction coefficient	0.058(4)
Largest diff. peak and hole	0.390 and -0.301 e.Å^{-3}

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for JF3006F2MI. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
C(1)	6528(1)	7185(1)	5949(1)	19(1)
O(1)	5807(1)	7010(1)	5045(1)	22(1)
C(2)	7016(1)	5794(1)	6240(1)	18(1)
O(2)	7338(1)	8080(1)	5703(1)	23(1)
C(3)	6119(1)	4872(1)	6547(1)	19(1)
C(4)	5790(1)	5373(1)	7581(1)	19(1)
C(5)	5610(1)	6900(1)	7561(1)	19(1)
C(6)	5974(1)	7748(1)	6826(1)	19(1)
C(7)	5835(1)	9145(1)	6888(1)	22(1)
C(8)	5330(1)	9702(1)	7673(1)	24(1)
C(9)	4968(1)	8865(1)	8409(1)	25(1)
C(10)	5108(1)	7477(1)	8351(1)	23(1)
C(11)	5985(1)	8106(1)	4367(1)	27(1)
C(12)	7161(1)	8388(2)	4626(1)	30(1)
C(13)	7536(1)	5247(1)	5384(1)	22(1)
N(13)	7943(1)	4817(1)	4725(1)	29(1)
C(14)	6458(1)	3446(1)	6617(1)	21(1)
N(14)	6713(1)	2339(1)	6660(1)	27(1)
C(15)	4828(1)	4591(1)	7860(1)	20(1)
C(16)	3817(1)	4849(1)	7363(1)	24(1)
C(17)	2937(1)	4127(1)	7613(1)	28(1)
C(18)	3067(1)	3127(2)	8358(1)	30(1)
C(19)	4071(1)	2850(2)	8846(1)	31(1)
C(20)	4951(1)	3584(1)	8601(1)	26(1)

Table 3. Bond lengths [Å] and angles [°] for JF3006F2MI.

C(1)-O(2)	1.4176(14)
C(1)-O(1)	1.4287(15)
C(1)-C(6)	1.5197(17)
C(1)-C(2)	1.5406(16)
O(1)-C(11)	1.4384(15)
C(2)-C(13)	1.4683(17)
C(2)-C(3)	1.5428(16)
C(2)-H(2)	1.0000
O(2)-C(12)	1.4445(16)
C(3)-C(14)	1.4762(17)
C(3)-C(4)	1.5476(16)
C(3)-H(3)	1.0000
C(4)-C(15)	1.5177(16)
C(4)-C(5)	1.5292(16)
C(4)-H(4)	1.0000
C(5)-C(10)	1.3975(17)
C(5)-C(6)	1.3978(17)
C(6)-C(7)	1.3984(17)
C(7)-C(8)	1.3874(18)
C(7)-H(7)	0.9500
C(8)-C(9)	1.390(2)
C(8)-H(8)	0.9500
C(9)-C(10)	1.3886(19)
C(9)-H(9)	0.9500
C(10)-H(10)	0.9500
C(11)-C(12)	1.512(2)
C(11)-H(11A)	0.9900
C(11)-H(11B)	0.9900
C(12)-H(12A)	0.9900
C(12)-H(12B)	0.9900
C(13)-N(13)	1.1393(17)
C(14)-N(14)	1.1416(17)
C(15)-C(16)	1.3931(18)
C(15)-C(20)	1.3932(17)

C(16)-C(17)	1.3902(18)
C(16)-H(16)	0.9500
C(17)-C(18)	1.392(2)
C(17)-H(17)	0.9500
C(18)-C(19)	1.385(2)
C(18)-H(18)	0.9500
C(19)-C(20)	1.3941(19)
C(19)-H(19)	0.9500
C(20)-H(20)	0.9500

O(2)-C(1)-O(1)	107.14(9)
O(2)-C(1)-C(6)	110.28(10)
O(1)-C(1)-C(6)	112.05(10)
O(2)-C(1)-C(2)	109.71(9)
O(1)-C(1)-C(2)	107.49(9)
C(6)-C(1)-C(2)	110.08(10)
C(1)-O(1)-C(11)	107.32(9)
C(13)-C(2)-C(1)	109.81(10)
C(13)-C(2)-C(3)	112.65(10)
C(1)-C(2)-C(3)	108.05(9)
C(13)-C(2)-H(2)	108.8
C(1)-C(2)-H(2)	108.8
C(3)-C(2)-H(2)	108.8
C(1)-O(2)-C(12)	108.52(9)
C(14)-C(3)-C(2)	111.50(10)
C(14)-C(3)-C(4)	110.83(10)
C(2)-C(3)-C(4)	108.39(9)
C(14)-C(3)-H(3)	108.7
C(2)-C(3)-H(3)	108.7
C(4)-C(3)-H(3)	108.7
C(15)-C(4)-C(5)	112.81(10)
C(15)-C(4)-C(3)	110.31(10)
C(5)-C(4)-C(3)	110.87(10)
C(15)-C(4)-H(4)	107.5
C(5)-C(4)-H(4)	107.5
C(3)-C(4)-H(4)	107.5

C(10)-C(5)-C(6)	118.65(11)
C(10)-C(5)-C(4)	118.11(11)
C(6)-C(5)-C(4)	123.15(11)
C(5)-C(6)-C(7)	120.11(11)
C(5)-C(6)-C(1)	121.28(11)
C(7)-C(6)-C(1)	118.61(11)
C(8)-C(7)-C(6)	120.54(12)
C(8)-C(7)-H(7)	119.7
C(6)-C(7)-H(7)	119.7
C(7)-C(8)-C(9)	119.63(12)
C(7)-C(8)-H(8)	120.2
C(9)-C(8)-H(8)	120.2
C(10)-C(9)-C(8)	119.96(12)
C(10)-C(9)-H(9)	120.0
C(8)-C(9)-H(9)	120.0
C(9)-C(10)-C(5)	121.10(12)
C(9)-C(10)-H(10)	119.4
C(5)-C(10)-H(10)	119.4
O(1)-C(11)-C(12)	102.39(10)
O(1)-C(11)-H(11A)	111.3
C(12)-C(11)-H(11A)	111.3
O(1)-C(11)-H(11B)	111.3
C(12)-C(11)-H(11B)	111.3
H(11A)-C(11)-H(11B)	109.2
O(2)-C(12)-C(11)	103.08(10)
O(2)-C(12)-H(12A)	111.1
C(11)-C(12)-H(12A)	111.1
O(2)-C(12)-H(12B)	111.1
C(11)-C(12)-H(12B)	111.1
H(12A)-C(12)-H(12B)	109.1
N(13)-C(13)-C(2)	179.59(14)
N(14)-C(14)-C(3)	179.13(14)
C(16)-C(15)-C(20)	119.20(12)
C(16)-C(15)-C(4)	120.53(11)
C(20)-C(15)-C(4)	120.25(11)
C(17)-C(16)-C(15)	120.59(12)

C(17)-C(16)-H(16)	119.7
C(15)-C(16)-H(16)	119.7
C(16)-C(17)-C(18)	119.81(13)
C(16)-C(17)-H(17)	120.1
C(18)-C(17)-H(17)	120.1
C(19)-C(18)-C(17)	120.01(13)
C(19)-C(18)-H(18)	120.0
C(17)-C(18)-H(18)	120.0
C(18)-C(19)-C(20)	120.09(13)
C(18)-C(19)-H(19)	120.0
C(20)-C(19)-H(19)	120.0
C(15)-C(20)-C(19)	120.29(13)
C(15)-C(20)-H(20)	119.9
C(19)-C(20)-H(20)	119.9

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($Å^2$x 10^3) for JF3006F2MI. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2 a^{*2}U^{11} + ... + 2 h k a^* b^* U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
C(1)	18(1)	17(1)	21(1)	2(1)	2(1)	-1(1)
O(1)	22(1)	23(1)	19(1)	3(1)	-1(1)	-1(1)
C(2)	18(1)	18(1)	20(1)	1(1)	2(1)	0(1)
O(2)	22(1)	23(1)	24(1)	4(1)	4(1)	-4(1)
C(3)	19(1)	18(1)	20(1)	1(1)	2(1)	0(1)
C(4)	19(1)	18(1)	19(1)	1(1)	3(1)	0(1)
C(5)	17(1)	20(1)	20(1)	-1(1)	0(1)	-1(1)
C(6)	16(1)	19(1)	20(1)	-1(1)	0(1)	0(1)
C(7)	21(1)	19(1)	25(1)	1(1)	0(1)	0(1)
C(8)	23(1)	20(1)	30(1)	-4(1)	-1(1)	2(1)
C(9)	21(1)	29(1)	26(1)	-7(1)	2(1)	2(1)
C(10)	22(1)	26(1)	23(1)	-1(1)	4(1)	-2(1)
C(11)	33(1)	24(1)	24(1)	7(1)	0(1)	2(1)
C(12)	34(1)	32(1)	25(1)	8(1)	6(1)	-5(1)
C(13)	20(1)	20(1)	25(1)	3(1)	2(1)	2(1)
N(13)	31(1)	28(1)	28(1)	2(1)	9(1)	6(1)
C(14)	21(1)	21(1)	22(1)	1(1)	3(1)	-2(1)
N(14)	28(1)	20(1)	32(1)	2(1)	2(1)	0(1)
C(15)	21(1)	20(1)	19(1)	-1(1)	4(1)	-2(1)
C(16)	23(1)	25(1)	24(1)	2(1)	2(1)	-1(1)
C(17)	21(1)	32(1)	29(1)	-3(1)	3(1)	-3(1)
C(18)	29(1)	32(1)	30(1)	-3(1)	10(1)	-12(1)
C(19)	36(1)	29(1)	29(1)	7(1)	4(1)	-9(1)
C(20)	26(1)	26(1)	25(1)	4(1)	1(1)	-4(1)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for JF3006F2MI.

	x	y	z	U(eq)
H(2)	7563	5906	6842	22
H(3)	5491	4949	6018	22
H(4)	6395	5180	8116	22
H(7)	6088	9717	6388	26
H(8)	5231	10651	7708	29
H(9)	4626	9241	8951	30
H(10)	4858	6911	8856	28
H(11A)	5549	8904	4504	33
H(11B)	5822	7836	3644	33
H(12A)	7597	7800	4228	36
H(12B)	7329	9344	4494	36
H(16)	3729	5525	6849	29
H(17)	2249	4316	7276	33
H(18)	2467	2634	8531	36
H(19)	4160	2160	9349	37
H(20)	5638	3396	8941	31

Table 6. Torsion angles [°] for JF3006F2MI.

O(2)-C(1)-O(1)-C(11)	-18.16(12)
C(6)-C(1)-O(1)-C(11)	102.93(11)
C(2)-C(1)-O(1)-C(11)	-136.01(10)
O(2)-C(1)-C(2)-C(13)	-59.23(12)
O(1)-C(1)-C(2)-C(13)	56.94(12)
C(6)-C(1)-C(2)-C(13)	179.23(10)
O(2)-C(1)-C(2)-C(3)	177.55(9)
O(1)-C(1)-C(2)-C(3)	-66.28(11)
C(6)-C(1)-C(2)-C(3)	56.01(12)
O(1)-C(1)-O(2)-C(12)	-3.91(13)
C(6)-C(1)-O(2)-C(12)	-126.11(11)
C(2)-C(1)-O(2)-C(12)	112.48(11)
C(13)-C(2)-C(3)-C(14)	45.92(13)
C(1)-C(2)-C(3)-C(14)	167.40(10)
C(13)-C(2)-C(3)-C(4)	168.19(10)
C(1)-C(2)-C(3)-C(4)	-70.33(12)
C(14)-C(3)-C(4)-C(15)	-63.40(13)
C(2)-C(3)-C(4)-C(15)	173.92(9)
C(14)-C(3)-C(4)-C(5)	170.90(10)
C(2)-C(3)-C(4)-C(5)	48.23(12)
C(15)-C(4)-C(5)-C(10)	43.21(15)
C(3)-C(4)-C(5)-C(10)	167.50(10)
C(15)-C(4)-C(5)-C(6)	-140.37(12)
C(3)-C(4)-C(5)-C(6)	-16.09(16)
C(10)-C(5)-C(6)-C(7)	0.04(17)
C(4)-C(5)-C(6)-C(7)	-176.35(11)
C(10)-C(5)-C(6)-C(1)	179.94(11)
C(4)-C(5)-C(6)-C(1)	3.54(17)
O(2)-C(1)-C(6)-C(5)	-144.73(11)
O(1)-C(1)-C(6)-C(5)	96.01(13)
C(2)-C(1)-C(6)-C(5)	-23.54(15)
O(2)-C(1)-C(6)-C(7)	35.17(15)
O(1)-C(1)-C(6)-C(7)	-84.09(13)
C(2)-C(1)-C(6)-C(7)	156.36(11)

C(5)-C(6)-C(7)-C(8)	-0.41(18)
C(1)-C(6)-C(7)-C(8)	179.69(11)
C(6)-C(7)-C(8)-C(9)	0.60(19)
C(7)-C(8)-C(9)-C(10)	-0.43(19)
C(8)-C(9)-C(10)-C(5)	0.06(19)
C(6)-C(5)-C(10)-C(9)	0.13(18)
C(4)-C(5)-C(10)-C(9)	176.71(11)
C(1)-O(1)-C(11)-C(12)	31.57(13)
C(1)-O(2)-C(12)-C(11)	22.95(13)
O(1)-C(11)-C(12)-O(2)	-32.89(13)
C(5)-C(4)-C(15)-C(16)	49.73(15)
C(3)-C(4)-C(15)-C(16)	-74.85(14)
C(5)-C(4)-C(15)-C(20)	-131.68(12)
C(3)-C(4)-C(15)-C(20)	103.73(13)
C(20)-C(15)-C(16)-C(17)	0.94(19)
C(4)-C(15)-C(16)-C(17)	179.55(12)
C(15)-C(16)-C(17)-C(18)	-0.7(2)
C(16)-C(17)-C(18)-C(19)	-0.2(2)
C(17)-C(18)-C(19)-C(20)	0.7(2)
C(16)-C(15)-C(20)-C(19)	-0.4(2)
C(4)-C(15)-C(20)-C(19)	-178.97(12)
C(18)-C(19)-C(20)-C(15)	-0.5(2)

Symmetry transformations used to generate equivalent atoms:

Table 7. Hydrogen bonds for JF3006F2MI [Å and °].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
C(2)-H(2)...N(14)#1	1.00	2.52	3.4071(17)	147.6

Symmetry transformations used to generate equivalent atoms:

#1 -x+3/2,y+1/2,-z+3/2

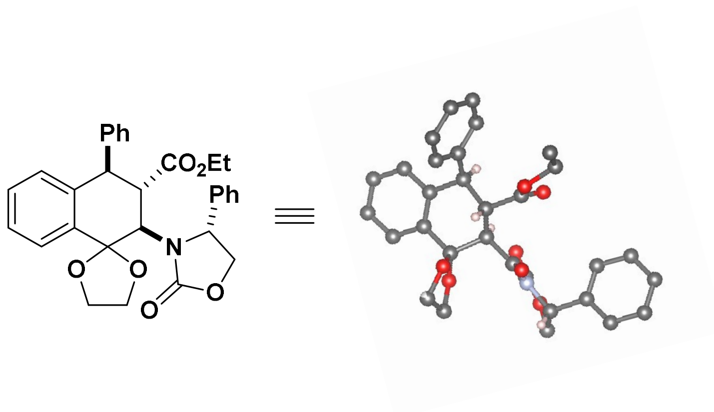


Table 1. Crystal data and structure refinement for [$C_{31}H_{29}NO_7$].

Identification code	(EJ-I-26B) JF3084MOFMI Reference Molecule in CCDC : 2145030
Empirical formula	C31 H29 N O7
Formula weight	527.55
Temperature	90(2) K
Wavelength	0.71073 Å
Crystal system	Orthorhombic
Space group	$P2_12_12_1$
Unit cell dimensions	a = 11.0370(5) Å a= 90°.
	b = 13.7529(7) Å b= 90°.
	c = 17.5560(9) Å g = 90°.
Volume	2664.8(2) Å3
Z	4
Density (calculated)	1.315 Mg/m3
Absorption coefficient	0.093 mm-1
F(000)	1112
Crystal size	0.707 x 0.516 x 0.458 mm3
Crystal color and habit	Colorless Block
Diffractometer	Bruker APEX-II CCD
Theta range for data collection	2.180 to 30.565°.
Index ranges	-15<=h<=10, -19<=k<=19, -23<=l<=25
Reflections collected	16241
Independent reflections	8163 [R(int) = 0.0156]
Observed reflections (I > 2sigma(I))	7591
Completeness to theta = 25.242°	99.9 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.9633 and 0.9122

Solution method SHELXT (Sheldrick, 2014)

Refinement method SHELXL-2018/3 (Sheldrick, 2018) Full-matrix least-squares on F2

Data / restraints / parameters 8163 / 8 / 465

Goodness-of-fit on F2 1.023

Final R indices [I>2sigma(I)] R1 = 0.0339, wR2 = 0.0851

R indices (all data) R1 = 0.0374, wR2 = 0.0877

Absolute structure parameter 0.4(2)

Largest diff. peak and hole 0.309 and -0.188 e.Å-3

Table 2. Atomic coordinates (x 104) and equivalent isotropic displacement parameters (Å2x 103) for JF3084MOFMI. U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
C(1)	6971(1)	3069(1)	3463(1)	14(1)
C(2)	7704(1)	2141(1)	3282(1)	16(1)
O(2)	8872(1)	2184(1)	3618(1)	22(1)
C(3)	7797(1)	2007(1)	2425(1)	17(1)
O(3)	7091(1)	1326(1)	3616(1)	19(1)
C(4)	6902(1)	2372(1)	1940(1)	18(1)
C(5)	5840(1)	2985(1)	2228(1)	16(1)
C(6)	5718(1)	2930(1)	3108(1)	14(1)
C(7)	8938(2)	1455(1)	4200(1)	30(1)
C(8)	7998(2)	732(1)	3954(1)	24(1)
C(8B)	7714(9)	1020(8)	4318(6)	30(2)
C(9)	8775(1)	1481(1)	2125(1)	22(1)
C(10)	8862(2)	1315(1)	1347(1)	26(1)
C(11)	7983(2)	1682(1)	864(1)	27(1)
C(12)	7014(1)	2210(1)	1157(1)	23(1)
C(13)	6895(1)	3215(1)	4315(1)	16(1)
N(13)	7828(1)	3722(1)	4679(1)	16(1)
O(13)	6086(1)	2873(1)	4701(1)	21(1)
C(14)	8720(1)	4319(1)	4358(1)	17(1)
O(14)	8808(1)	4601(1)	3713(1)	20(1)
C(15)	9194(1)	4081(1)	5611(1)	23(1)
O(15)	9489(1)	4600(1)	4911(1)	22(1)
C(16)	7854(1)	3817(1)	5510(1)	18(1)
C(17)	7002(1)	4602(1)	5798(1)	17(1)
C(18)	6816(2)	4680(1)	6583(1)	26(1)
C(19)	6070(2)	5409(2)	6871(1)	31(1)
C(20)	5510(2)	6062(1)	6387(1)	30(1)
C(21)	5677(2)	5983(1)	5607(1)	26(1)
C(22)	6424(1)	5253(1)	5314(1)	20(1)
C(23)	4644(1)	2708(1)	1860(1)	17(1)
C(24)	4271(1)	1737(1)	1859(1)	20(1)

C(25)	3141(2)	1471(1)	1578(1)	24(1)
C(26)	2372(2)	2176(1)	1282(1)	27(1)
C(27)	2739(2)	3139(1)	1268(1)	28(1)
C(28)	3870(2)	3407(1)	1558(1)	23(1)
C(29)	4841(1)	3706(1)	3368(1)	18(1)
O(29)	5120(1)	4546(1)	3470(1)	28(1)
C(30)	2759(2)	4087(1)	3526(1)	29(1)
O(30)	3715(1)	3358(1)	3437(1)	21(1)
C(31)	1568(2)	3566(2)	3418(2)	38(1)

Table 3. Bond lengths [Å] and angles [°] for JF3084MOFMI.

C(1)-C(13)	1.513(2)	C(11)-H(11)	0.98(3)
C(1)-C(6)	1.5290(18)	C(12)-H(12)	0.97(2)
C(1)-C(2)	1.5443(19)	C(13)-O(13)	1.2158(18)
C(1)-H(1)	0.93(2)	C(13)-N(13)	1.3974(18)
C(2)-O(2)	1.4189(17)	N(13)-C(14)	1.4001(18)
C(2)-O(3)	1.4348(17)	N(13)-C(16)	1.4669(18)
C(2)-C(3)	1.519(2)	C(14)-O(14)	1.2002(19)
O(2)-C(7)	1.434(2)	C(14)-O(15)	1.3472(18)
C(3)-C(4)	1.397(2)	C(15)-O(15)	1.458(2)
C(3)-C(9)	1.402(2)	C(15)-C(16)	1.532(2)
O(3)-C(8)	1.421(2)	C(15)-H(15A)	0.96(2)
O(3)-C(8B)	1.473(9)	C(15)-H(15B)	0.96(2)
C(4)-C(12)	1.399(2)	C(16)-C(17)	1.518(2)
C(4)-C(5)	1.529(2)	C(16)-H(16)	0.98(2)
C(5)-C(23)	1.519(2)	C(17)-C(22)	1.389(2)
C(5)-C(6)	1.552(2)	C(17)-C(18)	1.397(2)
C(5)-H(5)	0.99(2)	C(18)-C(19)	1.392(3)
C(6)-C(29)	1.5115(19)	C(18)-H(18)	1.01(3)
C(6)-H(6)	0.96(2)	C(19)-C(20)	1.382(3)
C(7)-C(8B)	1.491(10)	C(19)-H(19)	0.96(3)
C(7)-C(8)	1.501(3)	C(20)-C(21)	1.385(3)
C(7)-H(7A)	0.9900	C(20)-H(20)	0.97(3)
C(7)-H(7B)	0.9900	C(21)-C(22)	1.397(2)
C(7)-H(7C)	0.9900	C(21)-H(21)	0.97(2)
C(7)-H(7D)	0.9900	C(22)-H(22)	0.91(2)
C(8)-H(8A)	0.9900	C(23)-C(28)	1.392(2)
C(8)-H(8B)	0.9900	C(23)-C(24)	1.397(2)
C(8B)-H(8B1)	0.9900	C(24)-C(25)	1.390(2)
C(8B)-H(8B2)	0.9900	C(24)-H(24)	0.96(2)
C(9)-C(10)	1.389(2)	C(25)-C(26)	1.390(2)
C(9)-H(9)	0.98(2)	C(25)-H(25)	0.95(2)
C(10)-C(11)	1.384(3)	C(26)-C(27)	1.386(3)
C(10)-H(10)	0.93(2)	C(26)-H(26)	0.98(2)
C(11)-C(12)	1.391(2)	C(27)-C(28)	1.398(2)

C(27)-H(27)	0.98(3)	C(23)-C(5)-H(5)	109.3(11)
C(28)-H(28)	0.96(2)	C(4)-C(5)-H(5)	106.2(12)
C(29)-O(29)	1.2096(19)	C(6)-C(5)-H(5)	107.1(11)
C(29)-O(30)	1.3370(18)	C(29)-C(6)-C(1)	111.54(11)
C(30)-O(30)	1.4638(18)	C(29)-C(6)-C(5)	108.75(11)
C(30)-C(31)	1.510(3)	C(1)-C(6)-C(5)	108.70(11)
C(30)-H(30A)	0.96(3)	C(29)-C(6)-H(6)	109.7(12)
C(30)-H(30B)	0.97(3)	C(1)-C(6)-H(6)	109.6(12)
C(31)-H(31A)	1.04(3)	C(5)-C(6)-H(6)	108.5(11)
C(31)-H(31B)	1.00(3)	O(2)-C(7)-C(8B)	109.4(4)
C(31)-H(31C)	0.96(3)	O(2)-C(7)-C(8)	102.82(14)
		O(2)-C(7)-H(7A)	111.2
C(13)-C(1)-C(6)	111.68(11)	C(8)-C(7)-H(7A)	111.2
C(13)-C(1)-C(2)	110.03(11)	O(2)-C(7)-H(7B)	111.2
C(6)-C(1)-C(2)	106.63(11)	C(8)-C(7)-H(7B)	111.2
C(13)-C(1)-H(1)	111.2(12)	H(7A)-C(7)-H(7B)	109.1
C(6)-C(1)-H(1)	110.1(12)	O(2)-C(7)-H(7C)	109.8
C(2)-C(1)-H(1)	106.9(12)	C(8B)-C(7)-H(7C)	109.8
O(2)-C(2)-O(3)	106.92(11)	O(2)-C(7)-H(7D)	109.8
O(2)-C(2)-C(3)	110.84(11)	C(8B)-C(7)-H(7D)	109.8
O(3)-C(2)-C(3)	109.96(11)	H(7C)-C(7)-H(7D)	108.2
O(2)-C(2)-C(1)	110.84(11)	O(3)-C(8)-C(7)	103.11(14)
O(3)-C(2)-C(1)	108.36(11)	O(3)-C(8)-H(8A)	111.1
C(3)-C(2)-C(1)	109.84(12)	C(7)-C(8)-H(8A)	111.1
C(2)-O(2)-C(7)	108.27(12)	O(3)-C(8)-H(8B)	111.1
C(4)-C(3)-C(9)	120.12(14)	C(7)-C(8)-H(8B)	111.1
C(4)-C(3)-C(2)	120.78(12)	H(8A)-C(8)-H(8B)	109.1
C(9)-C(3)-C(2)	119.07(13)	O(3)-C(8B)-C(7)	101.1(6)
C(8)-O(3)-C(2)	106.71(12)	O(3)-C(8B)-H(8B1)	111.5
C(2)-O(3)-C(8B)	110.2(4)	C(7)-C(8B)-H(8B1)	111.5
C(3)-C(4)-C(12)	118.59(13)	O(3)-C(8B)-H(8B2)	111.5
C(3)-C(4)-C(5)	122.60(13)	C(7)-C(8B)-H(8B2)	111.5
C(12)-C(4)-C(5)	118.74(13)	H(8B1)-C(8B)-H(8B2)	109.4
C(23)-C(5)-C(4)	112.79(12)	C(10)-C(9)-C(3)	120.47(15)
C(23)-C(5)-C(6)	109.57(11)	C(10)-C(9)-H(9)	120.8(13)
C(4)-C(5)-C(6)	111.60(11)	C(3)-C(9)-H(9)	118.7(13)

C(11)-C(10)-C(9)	119.63(15)
C(11)-C(10)-H(10)	120.4(14)
C(9)-C(10)-H(10)	120.0(14)
C(10)-C(11)-C(12)	120.18(15)
C(10)-C(11)-H(11)	117.4(14)
C(12)-C(11)-H(11)	122.3(15)
C(11)-C(12)-C(4)	121.01(15)
C(11)-C(12)-H(12)	118.5(13)
C(4)-C(12)-H(12)	120.5(13)
O(13)-C(13)-N(13)	118.64(13)
O(13)-C(13)-C(1)	122.79(13)
N(13)-C(13)-C(1)	118.48(12)
C(13)-N(13)-C(14)	128.83(12)
C(13)-N(13)-C(16)	120.94(12)
C(14)-N(13)-C(16)	109.49(11)
O(14)-C(14)-O(15)	122.40(13)
O(14)-C(14)-N(13)	128.77(13)
O(15)-C(14)-N(13)	108.75(13)
O(15)-C(15)-C(16)	103.55(12)
O(15)-C(15)-H(15A)	107.2(14)
C(16)-C(15)-H(15A)	113.3(14)
O(15)-C(15)-H(15B)	107.2(13)
C(16)-C(15)-H(15B)	115.0(13)
H(15A)-C(15)-H(15B)	109.9(19)
C(14)-O(15)-C(15)	109.07(12)
N(13)-C(16)-C(17)	112.45(12)
N(13)-C(16)-C(15)	98.94(12)
C(17)-C(16)-C(15)	113.05(12)
N(13)-C(16)-H(16)	109.3(11)
C(17)-C(16)-H(16)	112.0(11)
C(15)-C(16)-H(16)	110.3(11)
C(22)-C(17)-C(18)	119.13(15)
C(22)-C(17)-C(16)	122.65(13)
C(18)-C(17)-C(16)	118.20(14)
C(19)-C(18)-C(17)	120.01(17)
C(19)-C(18)-H(18)	121.0(14)
C(17)-C(18)-H(18)	119.0(14)
C(20)-C(19)-C(18)	120.57(16)
C(20)-C(19)-H(19)	119.1(16)
C(18)-C(19)-H(19)	120.3(16)
C(19)-C(20)-C(21)	119.80(16)
C(19)-C(20)-H(20)	118.2(15)
C(21)-C(20)-H(20)	122.0(15)
C(20)-C(21)-C(22)	119.95(17)
C(20)-C(21)-H(21)	120.9(14)
C(22)-C(21)-H(21)	119.1(14)
C(17)-C(22)-C(21)	120.52(15)
C(17)-C(22)-H(22)	123.1(13)
C(21)-C(22)-H(22)	116.4(13)
C(28)-C(23)-C(24)	118.66(14)
C(28)-C(23)-C(5)	121.46(13)
C(24)-C(23)-C(5)	119.79(13)
C(25)-C(24)-C(23)	121.07(15)
C(25)-C(24)-H(24)	118.9(13)
C(23)-C(24)-H(24)	120.0(13)
C(26)-C(25)-C(24)	119.83(15)
C(26)-C(25)-H(25)	119.5(14)
C(24)-C(25)-H(25)	120.6(14)
C(27)-C(26)-C(25)	119.63(15)
C(27)-C(26)-H(26)	119.9(13)
C(25)-C(26)-H(26)	120.5(13)
C(26)-C(27)-C(28)	120.51(16)
C(26)-C(27)-H(27)	121.0(15)
C(28)-C(27)-H(27)	118.5(15)
C(23)-C(28)-C(27)	120.28(15)
C(23)-C(28)-H(28)	119.1(14)
C(27)-C(28)-H(28)	120.5(14)
O(29)-C(29)-O(30)	124.39(13)
O(29)-C(29)-C(6)	123.84(14)
O(30)-C(29)-C(6)	111.71(12)
O(30)-C(30)-C(31)	106.80(15)
O(30)-C(30)-H(30A)	105.7(16)

C(31)-C(30)-H(30A)	111.5(16)	C(30)-C(31)-H(31B)	110.2(19)
O(30)-C(30)-H(30B)	109.7(15)	H(31A)-C(31)-H(31B)	111(3)
C(31)-C(30)-H(30B)	115.2(15)	C(30)-C(31)-H(31C)	108.4(17)
H(30A)-C(30)-H(30B)	108(2)	H(31A)-C(31)-H(31C)	110(2)
C(29)-O(30)-C(30)	115.79(12)	H(31B)-C(31)-H(31C)	107(2)
C(30)-C(31)-H(31A)	110(2)		

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters (Å2x 103) for JF3084MOFMI. The anisotropic displacement factor exponent takes the form: -2p2[h2 a*2U11 + ... + 2 h k a* b* U12]

	U11	U22	U33	U23	U13
C(1)	11(1)	14(1)	18(1)	-2(1)	0(1)
C(2)	10(1)	17(1)	22(1)	-2(1)	-1(1)
O(2)	11(1)	25(1)	30(1)	-3(1)	-5(1)
C(3)	13(1)	18(1)	22(1)	-4(1)	2(1)
O(3)	16(1)	16(1)	25(1)	2(1)	-1(1)
C(4)	14(1)	19(1)	21(1)	-2(1)	3(1)
C(5)	12(1)	16(1)	19(1)	0(1)	-1(1)
C(6)	10(1)	14(1)	19(1)	-2(1)	-1(1)
C(7)	25(1)	31(1)	35(1)	2(1)	-12(1)
C(8)	26(1)	18(1)	30(1)	1(1)	-5(1)
C(8B)	32(3)	26(3)	31(3)	2(3)	-6(3)
C(9)	16(1)	21(1)	30(1)	-5(1)	4(1)
C(10)	20(1)	25(1)	34(1)	-8(1)	10(1)
C(11)	24(1)	33(1)	25(1)	-8(1)	8(1)
C(12)	20(1)	29(1)	21(1)	-2(1)	2(1)
C(13)	13(1)	14(1)	21(1)	-2(1)	-1(1)
N(13)	14(1)	16(1)	17(1)	-1(1)	-1(1)
O(13)	18(1)	22(1)	22(1)	-2(1)	3(1)
C(14)	10(1)	16(1)	24(1)	-3(1)	0(1)
O(14)	15(1)	22(1)	22(1)	-1(1)	2(1)
C(15)	18(1)	27(1)	24(1)	0(1)	-6(1)
O(15)	14(1)	26(1)	26(1)	-2(1)	-4(1)
C(16)	18(1)	19(1)	17(1)	1(1)	-4(1)
C(17)	15(1)	19(1)	18(1)	-2(1)	0(1)
C(18)	24(1)	37(1)	17(1)	-1(1)	-2(1)
C(19)	28(1)	46(1)	21(1)	-13(1)	5(1)
C(20)	22(1)	32(1)	36(1)	-15(1)	8(1)
C(21)	24(1)	22(1)	32(1)	-3(1)	4(1)
C(22)	21(1)	20(1)	20(1)	-1(1)	3(1)
C(23)	14(1)	22(1)	16(1)	0(1)	0(1)
C(24)	17(1)	21(1)	21(1)	-3(1)	-1(1)

C(25)	20(1)	28(1)	23(1)	-5(1)	1(1)
C(26)	16(1)	39(1)	25(1)	0(1)	-4(1)
C(27)	18(1)	35(1)	31(1)	7(1)	-5(1)
C(28)	18(1)	23(1)	28(1)	6(1)	-2(1)
C(29)	14(1)	19(1)	21(1)	-2(1)	0(1)
O(29)	22(1)	17(1)	46(1)	-6(1)	-1(1)
C(30)	17(1)	30(1)	39(1)	-4(1)	2(1)
O(30)	11(1)	23(1)	29(1)	-3(1)	1(1)
C(31)	14(1)	45(1)	57(1)	6(1)	4(1)

Table 5. Hydrogen coordinates (x 104) and isotropic displacement parameters (Å2x 10 3) for JF3084MOFMI.

	x	y	z	U(eq)
H(1)	7371(18)	3585(15)	3228(11)	16(4)
H(5)	6036(18)	3667(15)	2099(11)	18(5)
H(6)	5410(17)	2301(15)	3240(11)	19(5)
H(7A)	8742	1731	4707	31(6)
H(7B)	9753	1155	4220	38(7)
H(7C)	9227	1750	4682	31(6)
H(7D)	9519	942	4048	38(7)
H(8A)	8335	265	3580	25(6)
H(8B)	7671	368	4395	38(7)
H(8B1)	7756	303	4359	35
H(8B2)	7314	1288	4777	35
H(9)	9390(18)	1231(16)	2475(12)	26(5)
H(10)	9520(20)	965(17)	1151(13)	34(6)
H(11)	8110(20)	1595(18)	314(15)	39(6)
H(12)	6430(20)	2476(16)	805(12)	26(5)
H(15A)	9340(20)	4520(18)	6027(13)	34(6)
H(15B)	9733(19)	3539(17)	5645(12)	26(5)
H(16)	7684(17)	3183(14)	5743(11)	17(5)
H(18)	7220(20)	4194(19)	6932(14)	42(7)
H(19)	5920(20)	5460(20)	7411(15)	44(7)
H(20)	5020(20)	6573(19)	6609(14)	42(6)
H(21)	5300(20)	6442(18)	5260(13)	34(6)
H(22)	6503(18)	5234(14)	4796(12)	19(5)
H(24)	4791(19)	1244(15)	2060(11)	21(5)
H(25)	2890(20)	811(16)	1587(12)	26(5)
H(26)	1590(20)	1992(17)	1065(12)	32(6)
H(27)	2220(20)	3643(18)	1046(14)	37(6)
H(28)	4110(20)	4075(17)	1573(13)	31(6)
H(30A)	2900(20)	4559(19)	3131(15)	41(7)
H(30B)	2850(20)	4417(19)	4012(14)	39(6)

H(31A)	1430(30)	3070(30)	3856(19)	76(10)
H(31B)	1550(30)	3240(20)	2909(19)	65(9)
H(31C)	930(30)	4040(20)	3421(15)	48(7)

Table 6. Torsion angles [°] for JF3084MOFMI.

C(13)-C(1)-C(2)-O(2)	-56.22(15)	C(4)-C(5)-C(6)-C(29)	168.02(11)
C(6)-C(1)-C(2)-O(2)	-177.51(11)	C(23)-C(5)-C(6)-C(1)	172.06(11)
C(13)-C(1)-C(2)-O(3)	60.81(14)	C(4)-C(5)-C(6)-C(1)	46.40(15)
C(6)-C(1)-C(2)-O(3)	-60.47(14)	C(2)-O(2)-C(7)-C(8B)	-8.1(6)
C(13)-C(1)-C(2)-C(3)	-179.04(11)	C(2)-O(2)-C(7)-C(8)	24.06(17)
C(6)-C(1)-C(2)-C(3)	59.67(14)	C(2)-O(3)-C(8)-C(7)	32.03(18)
O(3)-C(2)-O(2)-C(7)	-4.95(15)	O(2)-C(7)-C(8)-O(3)	-34.20(19)
C(3)-C(2)-O(2)-C(7)	-124.80(14)	C(2)-O(3)-C(8B)-C(7)	-20.4(8)
C(1)-C(2)-O(2)-C(7)	112.97(14)	O(2)-C(7)-C(8B)-O(3)	17.1(8)
O(2)-C(2)-C(3)-C(4)	-150.42(13)	C(4)-C(3)-C(9)-C(10)	-0.3(2)
O(3)-C(2)-C(3)-C(4)	91.57(15)	C(2)-C(3)-C(9)-C(10)	177.65(14)
C(1)-C(2)-C(3)-C(4)	-27.60(18)	C(3)-C(9)-C(10)-C(11)	0.8(2)
O(2)-C(2)-C(3)-C(9)	31.68(18)	C(9)-C(10)-C(11)-C(12)	-0.4(3)
O(3)-C(2)-C(3)-C(9)	-86.33(15)	C(10)-C(11)-C(12)-C(4)	-0.5(3)
C(1)-C(2)-C(3)-C(9)	154.50(13)	C(3)-C(4)-C(12)-C(11)	1.0(2)
O(2)-C(2)-O(3)-C(8)	-17.70(16)	C(5)-C(4)-C(12)-C(11)	178.03(14)
C(3)-C(2)-O(3)-C(8)	102.71(14)	C(6)-C(1)-C(13)-O(13)	28.69(19)
C(1)-C(2)-O(3)-C(8)	-137.22(13)	C(2)-C(1)-C(13)-O(13)	-89.52(16)
O(2)-C(2)-O(3)-C(8B)	16.6(5)	C(6)-C(1)-C(13)-N(13)	-154.78(12)
C(3)-C(2)-O(3)-C(8B)	137.0(5)	C(2)-C(1)-C(13)-N(13)	87.00(15)
C(1)-C(2)-O(3)-C(8B)	-103.0(5)	O(13)-C(13)-N(13)-C(14)	-167.32(14)
C(9)-C(3)-C(4)-C(12)	-0.6(2)	C(1)-C(13)-N(13)-C(14)	16.0(2)
C(2)-C(3)-C(4)-C(12)	-178.51(14)	O(13)-C(13)-N(13)-C(16)	1.7(2)
C(9)-C(3)-C(4)-C(5)	-177.51(13)	C(1)-C(13)-N(13)-C(16)	-174.96(12)
C(2)-C(3)-C(4)-C(5)	4.6(2)	C(13)-N(13)-C(14)-O(14)	8.0(2)
C(3)-C(4)-C(5)-C(23)	-137.68(14)	C(16)-N(13)-C(14)-O(14)	-162.03(15)
C(12)-C(4)-C(5)-C(23)	45.44(18)	C(13)-N(13)-C(14)-O(15)	-175.39(13)
C(3)-C(4)-C(5)-C(6)	-13.83(18)	C(16)-N(13)-C(14)-O(15)	14.58(16)
C(12)-C(4)-C(5)-C(6)	169.30(13)	O(14)-C(14)-O(15)-C(15)	-176.04(14)
C(13)-C(1)-C(6)-C(29)	49.26(16)	N(13)-C(14)-O(15)-C(15)	7.09(16)
C(2)-C(1)-C(6)-C(29)	169.49(12)	C(16)-C(15)-O(15)-C(14)	-24.56(16)
C(13)-C(1)-C(6)-C(5)	169.16(11)	C(13)-N(13)-C(16)-C(17)	-79.32(16)
C(2)-C(1)-C(6)-C(5)	-70.62(14)	C(14)-N(13)-C(16)-C(17)	91.64(14)
C(23)-C(5)-C(6)-C(29)	-66.32(14)	C(13)-N(13)-C(16)-C(15)	161.09(12)

C(14)-N(13)-C(16)-C(15)	-27.96(15)
O(15)-C(15)-C(16)-N(13)	30.52(14)
O(15)-C(15)-C(16)-C(17)	-88.62(15)
N(13)-C(16)-C(17)-C(22)	-9.9(2)
C(15)-C(16)-C(17)-C(22)	101.15(17)
N(13)-C(16)-C(17)-C(18)	171.47(13)
C(15)-C(16)-C(17)-C(18)	-77.52(17)
C(22)-C(17)-C(18)-C(19)	-0.7(2)
C(16)-C(17)-C(18)-C(19)	178.05(15)
C(17)-C(18)-C(19)-C(20)	-0.2(3)
C(18)-C(19)-C(20)-C(21)	1.0(3)
C(19)-C(20)-C(21)-C(22)	-1.0(3)
C(18)-C(17)-C(22)-C(21)	0.7(2)
C(16)-C(17)-C(22)-C(21)	-177.92(14)
C(20)-C(21)-C(22)-C(17)	0.1(2)
C(4)-C(5)-C(23)-C(28)	-131.65(15)
C(6)-C(5)-C(23)-C(28)	103.38(16)
C(4)-C(5)-C(23)-C(24)	51.84(18)
C(6)-C(5)-C(23)-C(24)	-73.13(16)
C(28)-C(23)-C(24)-C(25)	-1.5(2)
C(5)-C(23)-C(24)-C(25)	175.15(14)
C(23)-C(24)-C(25)-C(26)	1.0(2)
C(24)-C(25)-C(26)-C(27)	0.0(3)
C(25)-C(26)-C(27)-C(28)	-0.6(3)
C(24)-C(23)-C(28)-C(27)	0.9(2)
C(5)-C(23)-C(28)-C(27)	-175.70(15)
C(26)-C(27)-C(28)-C(23)	0.2(3)
C(1)-C(6)-C(29)-O(29)	37.2(2)
C(5)-C(6)-C(29)-O(29)	-82.64(18)
C(1)-C(6)-C(29)-O(30)	-145.59(12)
C(5)-C(6)-C(29)-O(30)	94.54(14)
O(29)-C(29)-O(30)-C(30)	9.7(2)
C(6)-C(29)-O(30)-C(30)	-167.48(13)
C(31)-C(30)-O(30)-C(29)	167.68(16)

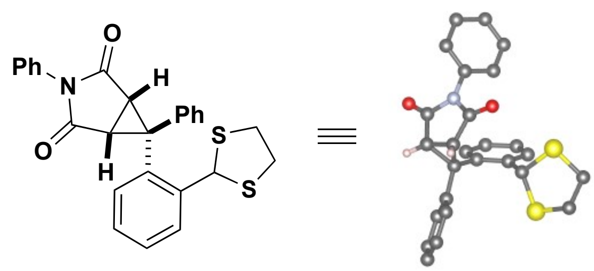
Symmetry transformations used to generate equivalent atoms:

Table 7. Hydrogen bonds for JF3084MOFMI [Å and °].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
C(1)-H(1)...O(14)	0.93(2)	2.28(2)	2.9571(17)	129.2(15)
C(8B^b)-H(8B2^b)...O(13)	0.99	2.57	3.190(12)	120.5
C(15)-H(15B)...O(13)#1	0.96(2)	2.52(2)	3.447(2)	162.4(17)
C(31)-H(31C)...O(14)#2	0.96(3)	2.52(3)	3.402(2)	153(2)

Symmetry transformations used to generate equivalent atoms:

#1 x+1/2,-y+1/2,-z+1   #2 x-1,y,z



CCDC 2087415

Table 1. Crystal data and structure refinement for $[C_{26}H_{21}NO_2S_2]_4[H_2O]$

Identification code	JF2975KFMI (MG-4-44-C)	
Empirical formula	C104 H86 N4 O9 S8	
Formula weight	1792.24	
Temperature	190(2) K	
Wavelength	1.54178 Å	
Crystal system	Triclinic	
Space group	P-1	
Unit cell dimensions	a = 8.6339(2) Å	〈= 83.1131(13)°.
	b = 15.2440(3) Å	®= 89.8510(13)°.
	c = 33.4220(6) Å	© = 83.6116(14)°.
Volume	4339.73(15) Å^3	
Z	2	
Density (calculated)	1.372 Mg/m^3	
Absorption coefficient	2.424 mm^{-1}	
F(000)	1876	

Crystal size	0.192 x 0.083 x 0.016 mm^3
Crystal color and habit	Colorless Plate
Diffractometer	Bruker Photon100 CMOS
Theta range for data collection	2.663 to 68.681°.
Index ranges	-10<=h<=9, -18<=k<=18, -40<=l<=40
Reflections collected	28242
Independent reflections	15752 [R(int) = 0.0406]
Observed reflections (I > 2sigma(I))	12023
Completeness to theta = 67.679°	98.5 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.8384 and 0.7250
Solution method	SHELXT (Sheldrick, 2014)
Refinement method	SHELXL-2017/1 (Sheldrick, 2017) Full-matrix least-squares on F^2
Data / restraints / parameters	15752 / 14 / 1175
Goodness-of-fit on F^2	1.101
Final R indices [I>2sigma(I)]	R1 = 0.0609, wR2 = 0.1288
R indices (all data)	R1 = 0.0823, wR2 = 0.1436
Extinction coefficient	0.00127(6)
Largest diff. peak and hole	0.411 and -0.457 e.$Å^{-3}$

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for JF2975KFMI. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
C(1)	839(4)	2467(2)	5410(1)	33(1)
C(2)	832(4)	1473(2)	5523(1)	35(1)
C(3)	1598(4)	1792(2)	5138(1)	36(1)
C(4)	3276(4)	1483(2)	5191(1)	36(1)
N(4)	3527(3)	1108(2)	5592(1)	35(1)
O(4)	4288(3)	1517(2)	4939(1)	44(1)
C(5)	2130(4)	1053(2)	5801(1)	36(1)
O(5)	2033(3)	720(2)	6146(1)	45(1)
C(6)	1827(4)	2960(2)	5660(1)	35(1)
C(7)	1394(4)	3103(2)	6054(1)	37(1)
C(8)	2354(5)	3551(2)	6275(1)	47(1)
C(9)	3693(5)	3855(2)	6117(1)	50(1)
C(10)	4122(4)	3712(2)	5728(1)	47(1)
C(11)	3183(4)	3278(2)	5501(1)	39(1)
C(12)	-113(4)	2823(2)	6236(1)	42(1)
S(12)	108(1)	2218(1)	6744(1)	50(1)
C(13)	-2505(15)	3400(30)	6697(3)	60(2)
C(13B)	-2440(100)	3400(200)	6673(18)	60(2)
S(13)	-1465(3)	3829(1)	6272(1)	65(1)
S(13B)	-1785(17)	3505(10)	6167(4)	63(3)
C(14)	-1283(5)	2941(4)	6993(1)	69(1)
C(15)	-644(4)	2984(2)	5229(1)	35(1)
C(16)	-854(4)	3910(2)	5205(1)	38(1)
C(17)	-2150(4)	4390(2)	5006(1)	43(1)
C(18)	-3260(4)	3961(2)	4836(1)	46(1)
C(19)	-3078(4)	3045(3)	4864(1)	49(1)
C(20)	-1787(4)	2558(2)	5060(1)	44(1)
C(21)	5035(4)	838(2)	5768(1)	38(1)
C(22)	6017(5)	198(3)	5607(1)	49(1)
C(23)	7501(5)	-45(3)	5774(1)	58(1)
C(24)	7967(5)	327(3)	6097(1)	61(1)

C(25)	6967(5)	961(3)	6260(1)	62(1)
C(26)	5493(5)	1229(3)	6093(1)	51(1)
C(31)	4976(4)	7531(2)	6322(1)	33(1)
C(32)	5051(4)	8441(2)	6465(1)	36(1)
C(33)	4107(4)	8377(2)	6091(1)	38(1)
C(34)	2460(4)	8609(2)	6202(1)	38(1)
N(34)	2416(3)	8691(2)	6613(1)	33(1)
O(34)	1315(3)	8716(2)	5984(1)	46(1)
C(35)	3912(4)	8652(2)	6780(1)	35(1)
C(36)	4106(4)	6844(2)	6558(1)	33(1)
O(36)	4175(3)	8770(2)	7122(1)	43(1)
C(37)	4677(4)	6405(2)	6930(1)	36(1)
C(38)	3870(4)	5739(2)	7125(1)	48(1)
C(39)	2561(5)	5485(3)	6954(1)	50(1)
C(40)	2011(4)	5902(2)	6582(1)	45(1)
C(41)	2789(4)	6568(2)	6387(1)	38(1)
C(42)	6186(4)	6626(2)	7101(1)	39(1)
S(42)	7860(1)	5869(1)	6980(1)	56(1)
C(43)	8077(7)	5240(4)	7456(2)	49(1)
C(43B)	8760(20)	5673(15)	7485(6)	55(5)
S(43)	6167(1)	6650(1)	7646(1)	45(1)
C(44)	7798(6)	5841(3)	7779(1)	65(1)
C(45)	6388(4)	7142(2)	6110(1)	36(1)
C(46)	6319(5)	6343(2)	5952(1)	48(1)
C(47)	7603(6)	5957(3)	5760(1)	62(1)
C(48)	8962(5)	6350(3)	5722(1)	61(1)
C(49)	9028(5)	7137(3)	5875(1)	55(1)
C(50)	7768(4)	7537(3)	6067(1)	45(1)
C(51)	1012(4)	8830(2)	6840(1)	33(1)
C(52)	499(4)	9673(2)	6922(1)	38(1)
C(53)	-845(4)	9807(2)	7145(1)	46(1)
C(54)	-1636(4)	9101(3)	7285(1)	46(1)
C(55)	-1100(5)	8254(3)	7204(1)	52(1)
C(56)	235(5)	8116(2)	6977(1)	48(1)
C(61)	697(3)	7216(2)	9599(1)	29(1)
C(62)	1142(4)	6232(2)	9578(1)	32(1)

C(63)	157(4)	6511(2)	9925(1)	33(1)
C(64)	-1388(4)	6209(2)	9869(1)	34(1)
N(64)	-1388(3)	5858(2)	9498(1)	32(1)
O(64)	-2484(3)	6246(2)	10095(1)	44(1)
C(65)	82(4)	5833(2)	9318(1)	33(1)
O(65)	397(3)	5541(2)	9004(1)	44(1)
C(66)	-449(3)	7730(2)	9293(1)	31(1)
C(67)	-106(4)	7865(2)	8882(1)	33(1)
C(68)	-1238(4)	8335(2)	8616(1)	41(1)
C(69)	-2678(4)	8670(3)	8750(1)	48(1)
C(70)	-3000(4)	8551(2)	9156(1)	46(1)
C(71)	-1889(4)	8091(2)	9424(1)	37(1)
C(72)	1480(4)	7565(2)	8721(1)	33(1)
S(72)	1436(1)	6995(1)	8267(1)	44(1)
C(73)	3499(5)	8193(3)	8158(1)	49(1)
S(73)	2531(1)	8542(1)	8599(1)	49(1)
C(74)	2309(5)	7806(3)	7925(1)	53(1)
C(75)	1906(4)	7730(2)	9756(1)	32(1)
C(76)	1411(4)	8530(2)	9902(1)	41(1)
C(77)	2483(5)	8999(3)	10074(1)	50(1)
C(78)	4028(5)	8678(3)	10100(1)	50(1)
C(79)	4528(4)	7892(3)	9957(1)	50(1)
C(80)	3478(4)	7413(2)	9784(1)	42(1)
C(81)	-2771(4)	5662(2)	9310(1)	33(1)
C(82)	-3206(4)	6084(2)	8932(1)	44(1)
C(83)	-4576(4)	5912(3)	8756(1)	49(1)
C(84)	-5521(4)	5341(2)	8959(1)	42(1)
C(85)	-5080(4)	4920(2)	9338(1)	39(1)
C(86)	-3696(4)	5077(2)	9513(1)	36(1)
C(91)	5581(4)	2182(2)	8762(1)	31(1)
C(92)	5208(4)	3155(2)	8588(1)	34(1)
C(93)	6106(4)	2936(2)	8982(1)	34(1)
C(94)	7682(4)	3202(2)	8902(1)	34(1)
N(94)	7794(3)	3444(2)	8484(1)	35(1)
O(94)	8713(3)	3228(2)	9141(1)	43(1)
C(95)	6372(4)	3458(2)	8285(1)	34(1)

O(95)	6141(3)	3680(2)	7927(1)	44(1)
C(96)	6761(4)	1600(2)	8549(1)	31(1)
C(97)	6429(4)	1353(2)	8169(1)	31(1)
C(98)	7564(4)	821(2)	7984(1)	36(1)
C(99)	8995(4)	528(2)	8165(1)	40(1)
C(100)	9306(4)	755(2)	8543(1)	40(1)
C(101)	8199(4)	1280(2)	8733(1)	37(1)
C(102)	4855(4)	1622(2)	7963(1)	35(1)
S(102)	3698(1)	679(1)	8028(1)	53(1)
C(103)	2974(5)	749(3)	7521(1)	53(1)
S(103)	4928(1)	2007(1)	7424(1)	47(1)
C(104)	4203(5)	1056(3)	7240(1)	57(1)
C(105)	4261(4)	1742(2)	8961(1)	33(1)
C(106)	2985(4)	2223(2)	9118(1)	41(1)
C(107)	1818(4)	1803(2)	9318(1)	44(1)
C(108)	1896(4)	884(2)	9362(1)	44(1)
C(109)	3149(4)	389(2)	9207(1)	39(1)
C(110)	4326(4)	812(2)	9008(1)	36(1)
C(111)	9241(4)	3574(2)	8284(1)	34(1)
C(112)	9792(4)	2993(2)	8012(1)	38(1)
C(113)	11181(4)	3123(2)	7818(1)	43(1)
C(114)	12013(4)	3811(2)	7895(1)	45(1)
C(115)	11454(4)	4372(2)	8169(1)	46(1)
C(116)	10066(4)	4255(2)	8367(1)	39(1)
O(121)	2059(14)	9525(7)	5178(3)	81(3)
O(122)	1059(16)	9654(8)	5185(4)	99(4)

Table 3. Bond lengths [Å] and angles [°] for JF2975KFMI.

C(1)-C(15)	1.513(4)
C(1)-C(6)	1.513(4)
C(1)-C(2)	1.518(4)
C(1)-C(3)	1.544(4)
C(2)-C(5)	1.494(5)
C(2)-C(3)	1.497(4)
C(2)-H(2)	1.0000
C(3)-C(4)	1.477(5)
C(3)-H(3)	1.0000
C(4)-O(4)	1.212(4)
C(4)-N(4)	1.401(4)
N(4)-C(5)	1.398(4)
N(4)-C(21)	1.427(4)
C(5)-O(5)	1.208(4)
C(6)-C(11)	1.397(5)
C(6)-C(7)	1.401(4)
C(7)-C(8)	1.397(5)
C(7)-C(12)	1.517(5)
C(8)-C(9)	1.374(5)
C(8)-H(8)	0.9500
C(9)-C(10)	1.387(5)
C(9)-H(9)	0.9500
C(10)-C(11)	1.383(5)
C(10)-H(10)	0.9500
C(11)-H(11)	0.9500
C(12)-S(13B)	1.681(15)
C(12)-S(12)	1.833(3)
C(12)-S(13)	1.837(4)
C(12)-H(12)	1.0000
C(12)-H(12E)	1.0000
S(12)-C(14)	1.808(4)
C(13)-C(14)	1.500(6)
C(13)-S(13)	1.779(16)
C(13)-H(13A)	0.9900

C(13)-H(13B)	0.9900
C(13B)-C(14)	1.500(11)
C(13B)-S(13B)	1.779(18)
C(13B)-H(13C)	0.9900
C(13B)-H(13D)	0.9900
C(14)-H(14A)	0.9900
C(14)-H(14B)	0.9900
C(15)-C(16)	1.394(5)
C(15)-C(20)	1.398(5)
C(16)-C(17)	1.390(5)
C(16)-H(16)	0.9500
C(17)-C(18)	1.379(5)
C(17)-H(17)	0.9500
C(18)-C(19)	1.379(5)
C(18)-H(18)	0.9500
C(19)-C(20)	1.388(5)
C(19)-H(19)	0.9500
C(20)-H(20)	0.9500
C(21)-C(22)	1.379(5)
C(21)-C(26)	1.379(5)
C(22)-C(23)	1.392(6)
C(22)-H(22)	0.9500
C(23)-C(24)	1.361(6)
C(23)-H(23)	0.9500
C(24)-C(25)	1.382(6)
C(24)-H(24)	0.9500
C(25)-C(26)	1.389(6)
C(25)-H(25)	0.9500
C(26)-H(26)	0.9500
C(31)-C(36)	1.503(4)
C(31)-C(45)	1.509(4)
C(31)-C(32)	1.529(4)
C(31)-C(33)	1.539(4)
C(32)-C(35)	1.478(4)
C(32)-C(33)	1.512(5)
C(32)-H(32)	1.0000

C(33)-C(34)	1.483(5)
C(33)-H(33)	1.0000
C(34)-O(34)	1.214(4)
C(34)-N(34)	1.395(4)
N(34)-C(35)	1.401(4)
N(34)-C(51)	1.437(4)
C(35)-O(36)	1.205(4)
C(36)-C(41)	1.401(5)
C(36)-C(37)	1.403(4)
C(37)-C(38)	1.392(5)
C(37)-C(42)	1.512(5)
C(38)-C(39)	1.380(5)
C(38)-H(38)	0.9500
C(39)-C(40)	1.388(5)
C(39)-H(39)	0.9500
C(40)-C(41)	1.377(5)
C(40)-H(40)	0.9500
C(41)-H(41)	0.9500
C(42)-S(42)	1.823(3)
C(42)-S(43)	1.826(3)
C(42)-H(42)	1.0000
S(42)-C(43)	1.756(5)
S(42)-C(43B)	1.836(19)
C(43)-C(44)	1.499(7)
C(43)-H(43A)	0.9900
C(43)-H(43B)	0.9900
C(43B)-C(44)	1.31(2)
C(43B)-H(43C)	0.9900
C(43B)-H(43D)	0.9900
S(43)-C(44)	1.785(4)
C(44)-H(44A)	0.9900
C(44)-H(44B)	0.9900
C(44)-H(44C)	0.9900
C(44)-H(44D)	0.9900
C(45)-C(46)	1.392(5)
C(45)-C(50)	1.393(5)

C(46)-C(47)	1.388(5)
C(46)-H(46)	0.9500
C(47)-C(48)	1.375(7)
C(47)-H(47)	0.9500
C(48)-C(49)	1.366(6)
C(48)-H(48)	0.9500
C(49)-C(50)	1.382(5)
C(49)-H(49)	0.9500
C(50)-H(50)	0.9500
C(51)-C(52)	1.370(4)
C(51)-C(56)	1.374(5)
C(52)-C(53)	1.388(5)
C(52)-H(52)	0.9500
C(53)-C(54)	1.373(5)
C(53)-H(53)	0.9500
C(54)-C(55)	1.381(5)
C(54)-H(54)	0.9500
C(55)-C(56)	1.389(5)
C(55)-H(55)	0.9500
C(56)-H(56)	0.9500
C(61)-C(75)	1.504(4)
C(61)-C(66)	1.509(4)
C(61)-C(62)	1.516(4)
C(61)-C(63)	1.544(4)
C(62)-C(65)	1.489(4)
C(62)-C(63)	1.510(4)
C(62)-H(62)	1.0000
C(63)-C(64)	1.478(5)
C(63)-H(63)	1.0000
C(64)-O(64)	1.211(4)
C(64)-N(64)	1.408(4)
N(64)-C(65)	1.401(4)
N(64)-C(81)	1.428(4)
C(65)-O(65)	1.207(4)
C(66)-C(71)	1.394(4)
C(66)-C(67)	1.401(4)

C(67)-C(68)	1.398(4)
C(67)-C(72)	1.513(4)
C(68)-C(69)	1.384(5)
C(68)-H(68)	0.9500
C(69)-C(70)	1.380(5)
C(69)-H(69)	0.9500
C(70)-C(71)	1.385(5)
C(70)-H(70)	0.9500
C(71)-H(71)	0.9500
C(72)-S(73)	1.833(3)
C(72)-S(72)	1.839(3)
C(72)-H(72)	1.0000
S(72)-C(74)	1.809(4)
C(73)-C(74)	1.503(5)
C(73)-S(73)	1.798(4)
C(73)-H(73A)	0.9900
C(73)-H(73B)	0.9900
C(74)-H(74A)	0.9900
C(74)-H(74B)	0.9900
C(75)-C(80)	1.388(5)
C(75)-C(76)	1.392(5)
C(76)-C(77)	1.395(5)
C(76)-H(76)	0.9500
C(77)-C(78)	1.368(6)
C(77)-H(77)	0.9500
C(78)-C(79)	1.367(6)
C(78)-H(78)	0.9500
C(79)-C(80)	1.393(5)
C(79)-H(79)	0.9500
C(80)-H(80)	0.9500
C(81)-C(86)	1.380(4)
C(81)-C(82)	1.381(4)
C(82)-C(83)	1.386(5)
C(82)-H(82)	0.9500
C(83)-C(84)	1.376(5)
C(83)-H(83)	0.9500

C(84)-C(85)	1.385(5)
C(84)-H(84)	0.9500
C(85)-C(86)	1.388(5)
C(85)-H(85)	0.9500
C(86)-H(86)	0.9500
C(91)-C(105)	1.501(4)
C(91)-C(96)	1.509(4)
C(91)-C(92)	1.527(4)
C(91)-C(93)	1.545(4)
C(92)-C(95)	1.495(4)
C(92)-C(93)	1.513(4)
C(92)-H(92)	1.0000
C(93)-C(94)	1.477(5)
C(93)-H(93)	1.0000
C(94)-O(94)	1.205(4)
C(94)-N(94)	1.410(4)
N(94)-C(95)	1.395(4)
N(94)-C(111)	1.437(4)
C(95)-O(95)	1.214(4)
C(96)-C(101)	1.398(4)
C(96)-C(97)	1.404(4)
C(97)-C(98)	1.393(4)
C(97)-C(102)	1.518(4)
C(98)-C(99)	1.381(5)
C(98)-H(98)	0.9500
C(99)-C(100)	1.383(5)
C(99)-H(99)	0.9500
C(100)-C(101)	1.382(5)
C(100)-H(100)	0.9500
C(101)-H(101)	0.9500
C(102)-S(103)	1.827(3)
C(102)-S(102)	1.833(3)
C(102)-H(102)	1.0000
S(102)-C(103)	1.794(4)
C(103)-C(104)	1.493(6)
C(103)-H(10A)	0.9900

C(103)-H(10B)	0.9900
S(103)-C(104)	1.816(4)
C(104)-H(10C)	0.9900
C(104)-H(10D)	0.9900
C(105)-C(106)	1.392(4)
C(105)-C(110)	1.402(4)
C(106)-C(107)	1.380(5)
C(106)-H(106)	0.9500
C(107)-C(108)	1.386(5)
C(107)-H(107)	0.9500
C(108)-C(109)	1.385(5)
C(108)-H(108)	0.9500
C(109)-C(110)	1.388(5)
C(109)-H(109)	0.9500
C(110)-H(110)	0.9500
C(111)-C(116)	1.378(4)
C(111)-C(112)	1.390(4)
C(112)-C(113)	1.383(5)
C(112)-H(112)	0.9500
C(113)-C(114)	1.384(5)
C(113)-H(113)	0.9500
C(114)-C(115)	1.378(5)
C(114)-H(114)	0.9500
C(115)-C(116)	1.386(5)
C(115)-H(115)	0.9500
C(116)-H(116)	0.9500
O(121)-H(12A)	0.842(5)
O(121)-H(12B)	0.842(5)
O(122)-H(12C)	0.842(5)
O(122)-H(12D)	0.842(5)

C(15)-C(1)-C(6)	116.4(3)
C(15)-C(1)-C(2)	117.4(3)
C(6)-C(1)-C(2)	118.3(3)
C(15)-C(1)-C(3)	112.9(3)
C(6)-C(1)-C(3)	121.0(3)

C(2)-C(1)-C(3)	58.5(2)
C(5)-C(2)-C(3)	105.6(3)
C(5)-C(2)-C(1)	114.2(3)
C(3)-C(2)-C(1)	61.6(2)
C(5)-C(2)-H(2)	120.3
C(3)-C(2)-H(2)	120.3
C(1)-C(2)-H(2)	120.3
C(4)-C(3)-C(2)	106.4(3)
C(4)-C(3)-C(1)	118.9(3)
C(2)-C(3)-C(1)	59.9(2)
C(4)-C(3)-H(3)	118.8
C(2)-C(3)-H(3)	118.8
C(1)-C(3)-H(3)	118.8
O(4)-C(4)-N(4)	124.2(3)
O(4)-C(4)-C(3)	128.0(3)
N(4)-C(4)-C(3)	107.8(3)
C(5)-N(4)-C(4)	112.0(3)
C(5)-N(4)-C(21)	124.2(3)
C(4)-N(4)-C(21)	123.8(3)
O(5)-C(5)-N(4)	124.6(3)
O(5)-C(5)-C(2)	127.7(3)
N(4)-C(5)-C(2)	107.8(3)
C(11)-C(6)-C(7)	119.3(3)
C(11)-C(6)-C(1)	120.2(3)
C(7)-C(6)-C(1)	120.6(3)
C(8)-C(7)-C(6)	118.5(3)
C(8)-C(7)-C(12)	119.7(3)
C(6)-C(7)-C(12)	121.8(3)
C(9)-C(8)-C(7)	121.9(3)
C(9)-C(8)-H(8)	119.1
C(7)-C(8)-H(8)	119.1
C(8)-C(9)-C(10)	119.6(3)
C(8)-C(9)-H(9)	120.2
C(10)-C(9)-H(9)	120.2
C(11)-C(10)-C(9)	119.7(4)
C(11)-C(10)-H(10)	120.2

C(9)-C(10)-H(10)	120.2
C(10)-C(11)-C(6)	121.1(3)
C(10)-C(11)-H(11)	119.5
C(6)-C(11)-H(11)	119.5
C(7)-C(12)-S(13B)	120.7(6)
C(7)-C(12)-S(12)	114.2(2)
S(13B)-C(12)-S(12)	113.3(5)
C(7)-C(12)-S(13)	108.3(2)
S(12)-C(12)-S(13)	107.00(18)
C(7)-C(12)-H(12)	109.1
S(12)-C(12)-H(12)	109.1
S(13)-C(12)-H(12)	109.1
C(7)-C(12)-H(12E)	101.5
S(13B)-C(12)-H(12E)	101.5
S(12)-C(12)-H(12E)	101.5
C(14)-S(12)-C(12)	97.69(19)
C(14)-C(13)-S(13)	105.5(8)
C(14)-C(13)-H(13A)	110.6
S(13)-C(13)-H(13A)	110.6
C(14)-C(13)-H(13B)	110.6
S(13)-C(13)-H(13B)	110.6
H(13A)-C(13)-H(13B)	108.8
C(14)-C(13B)-S(13B)	117.7(15)
C(14)-C(13B)-H(13C)	107.9
S(13B)-C(13B)-H(13C)	107.9
C(14)-C(13B)-H(13D)	107.9
S(13B)-C(13B)-H(13D)	107.9
H(13C)-C(13B)-H(13D)	107.2
C(13)-S(13)-C(12)	96.9(11)
C(12)-S(13B)-C(13B)	97(3)
C(13)-C(14)-S(12)	110.0(10)
C(13B)-C(14)-S(12)	106(7)
C(13)-C(14)-H(14A)	109.7
S(12)-C(14)-H(14A)	109.7
C(13)-C(14)-H(14B)	109.7
S(12)-C(14)-H(14B)	109.7

H(14A)-C(14)-H(14B)	108.2
C(16)-C(15)-C(20)	118.2(3)
C(16)-C(15)-C(1)	120.4(3)
C(20)-C(15)-C(1)	121.2(3)
C(17)-C(16)-C(15)	120.4(3)
C(17)-C(16)-H(16)	119.8
C(15)-C(16)-H(16)	119.8
C(18)-C(17)-C(16)	120.7(3)
C(18)-C(17)-H(17)	119.6
C(16)-C(17)-H(17)	119.6
C(19)-C(18)-C(17)	119.5(3)
C(19)-C(18)-H(18)	120.3
C(17)-C(18)-H(18)	120.3
C(18)-C(19)-C(20)	120.4(4)
C(18)-C(19)-H(19)	119.8
C(20)-C(19)-H(19)	119.8
C(19)-C(20)-C(15)	120.7(3)
C(19)-C(20)-H(20)	119.6
C(15)-C(20)-H(20)	119.6
C(22)-C(21)-C(26)	121.1(3)
C(22)-C(21)-N(4)	119.4(3)
C(26)-C(21)-N(4)	119.6(3)
C(21)-C(22)-C(23)	119.0(4)
C(21)-C(22)-H(22)	120.5
C(23)-C(22)-H(22)	120.5
C(24)-C(23)-C(22)	120.7(4)
C(24)-C(23)-H(23)	119.7
C(22)-C(23)-H(23)	119.7
C(23)-C(24)-C(25)	119.9(4)
C(23)-C(24)-H(24)	120.1
C(25)-C(24)-H(24)	120.1
C(24)-C(25)-C(26)	120.6(4)
C(24)-C(25)-H(25)	119.7
C(26)-C(25)-H(25)	119.7
C(21)-C(26)-C(25)	118.7(4)
C(21)-C(26)-H(26)	120.6

C(25)-C(26)-H(26)	120.6
C(36)-C(31)-C(45)	113.6(3)
C(36)-C(31)-C(32)	120.8(3)
C(45)-C(31)-C(32)	117.1(3)
C(36)-C(31)-C(33)	121.1(3)
C(45)-C(31)-C(33)	114.6(3)
C(32)-C(31)-C(33)	59.1(2)
C(35)-C(32)-C(33)	106.2(3)
C(35)-C(32)-C(31)	114.3(3)
C(33)-C(32)-C(31)	60.8(2)
C(35)-C(32)-H(32)	120.2
C(33)-C(32)-H(32)	120.2
C(31)-C(32)-H(32)	120.2
C(34)-C(33)-C(32)	105.3(3)
C(34)-C(33)-C(31)	116.9(3)
C(32)-C(33)-C(31)	60.1(2)
C(34)-C(33)-H(33)	119.6
C(32)-C(33)-H(33)	119.6
C(31)-C(33)-H(33)	119.6
O(34)-C(34)-N(34)	123.9(3)
O(34)-C(34)-C(33)	128.0(3)
N(34)-C(34)-C(33)	108.1(3)
C(34)-N(34)-C(35)	112.0(3)
C(34)-N(34)-C(51)	124.7(3)
C(35)-N(34)-C(51)	123.3(2)
O(36)-C(35)-N(34)	124.4(3)
O(36)-C(35)-C(32)	127.8(3)
N(34)-C(35)-C(32)	107.8(3)
C(41)-C(36)-C(37)	118.9(3)
C(41)-C(36)-C(31)	119.7(3)
C(37)-C(36)-C(31)	121.1(3)
C(38)-C(37)-C(36)	118.6(3)
C(38)-C(37)-C(42)	121.4(3)
C(36)-C(37)-C(42)	119.9(3)
C(39)-C(38)-C(37)	121.6(3)
C(39)-C(38)-H(38)	119.2

C(37)-C(38)-H(38)	119.2
C(38)-C(39)-C(40)	120.1(3)
C(38)-C(39)-H(39)	119.9
C(40)-C(39)-H(39)	119.9
C(41)-C(40)-C(39)	119.0(3)
C(41)-C(40)-H(40)	120.5
C(39)-C(40)-H(40)	120.5
C(40)-C(41)-C(36)	121.7(3)
C(40)-C(41)-H(41)	119.1
C(36)-C(41)-H(41)	119.1
C(37)-C(42)-S(42)	112.5(2)
C(37)-C(42)-S(43)	113.9(2)
S(42)-C(42)-S(43)	108.26(17)
C(37)-C(42)-H(42)	107.3
S(42)-C(42)-H(42)	107.3
S(43)-C(42)-H(42)	107.3
C(43)-S(42)-C(42)	96.9(2)
C(42)-S(42)-C(43B)	97.2(6)
C(44)-C(43)-S(42)	109.7(3)
C(44)-C(43)-H(43A)	109.7
S(42)-C(43)-H(43A)	109.7
C(44)-C(43)-H(43B)	109.7
S(42)-C(43)-H(43B)	109.7
H(43A)-C(43)-H(43B)	108.2
C(44)-C(43B)-S(42)	114.7(13)
C(44)-C(43B)-H(43C)	108.6
S(42)-C(43B)-H(43C)	108.6
C(44)-C(43B)-H(43D)	108.6
S(42)-C(43B)-H(43D)	108.6
H(43C)-C(43B)-H(43D)	107.6
C(44)-S(43)-C(42)	98.62(18)
C(43B)-C(44)-S(43)	115.8(9)
C(43)-C(44)-S(43)	110.1(3)
C(43)-C(44)-H(44A)	109.6
S(43)-C(44)-H(44A)	109.6
C(43)-C(44)-H(44B)	109.6

S(43)-C(44)-H(44B)	109.6
H(44A)-C(44)-H(44B)	108.2
C(43B)-C(44)-H(44C)	108.3
S(43)-C(44)-H(44C)	108.3
C(43B)-C(44)-H(44D)	108.3
S(43)-C(44)-H(44D)	108.3
H(44C)-C(44)-H(44D)	107.4
C(46)-C(45)-C(50)	118.1(3)
C(46)-C(45)-C(31)	118.6(3)
C(50)-C(45)-C(31)	123.4(3)
C(47)-C(46)-C(45)	120.2(4)
C(47)-C(46)-H(46)	119.9
C(45)-C(46)-H(46)	119.9
C(48)-C(47)-C(46)	121.1(4)
C(48)-C(47)-H(47)	119.4
C(46)-C(47)-H(47)	119.4
C(49)-C(48)-C(47)	118.8(4)
C(49)-C(48)-H(48)	120.6
C(47)-C(48)-H(48)	120.6
C(48)-C(49)-C(50)	121.4(4)
C(48)-C(49)-H(49)	119.3
C(50)-C(49)-H(49)	119.3
C(49)-C(50)-C(45)	120.4(4)
C(49)-C(50)-H(50)	119.8
C(45)-C(50)-H(50)	119.8
C(52)-C(51)-C(56)	121.7(3)
C(52)-C(51)-N(34)	119.0(3)
C(56)-C(51)-N(34)	119.3(3)
C(51)-C(52)-C(53)	119.0(3)
C(51)-C(52)-H(52)	120.5
C(53)-C(52)-H(52)	120.5
C(54)-C(53)-C(52)	120.2(3)
C(54)-C(53)-H(53)	119.9
C(52)-C(53)-H(53)	119.9
C(53)-C(54)-C(55)	120.2(3)
C(53)-C(54)-H(54)	119.9

C(55)-C(54)-H(54)	119.9
C(54)-C(55)-C(56)	119.9(3)
C(54)-C(55)-H(55)	120.0
C(56)-C(55)-H(55)	120.0
C(51)-C(56)-C(55)	119.0(3)
C(51)-C(56)-H(56)	120.5
C(55)-C(56)-H(56)	120.5
C(75)-C(61)-C(66)	116.1(3)
C(75)-C(61)-C(62)	117.5(3)
C(66)-C(61)-C(62)	119.0(2)
C(75)-C(61)-C(63)	112.5(2)
C(66)-C(61)-C(63)	120.5(3)
C(62)-C(61)-C(63)	59.1(2)
C(65)-C(62)-C(63)	105.5(3)
C(65)-C(62)-C(61)	113.8(3)
C(63)-C(62)-C(61)	61.4(2)
C(65)-C(62)-H(62)	120.4
C(63)-C(62)-H(62)	120.4
C(61)-C(62)-H(62)	120.4
C(64)-C(63)-C(62)	106.3(2)
C(64)-C(63)-C(61)	117.6(3)
C(62)-C(63)-C(61)	59.52(19)
C(64)-C(63)-H(63)	119.3
C(62)-C(63)-H(63)	119.3
C(61)-C(63)-H(63)	119.3
O(64)-C(64)-N(64)	124.5(3)
O(64)-C(64)-C(63)	127.5(3)
N(64)-C(64)-C(63)	108.0(3)
C(65)-N(64)-C(64)	111.7(3)
C(65)-N(64)-C(81)	124.7(3)
C(64)-N(64)-C(81)	123.2(3)
O(65)-C(65)-N(64)	124.7(3)
O(65)-C(65)-C(62)	127.1(3)
N(64)-C(65)-C(62)	108.2(3)
C(71)-C(66)-C(67)	118.8(3)
C(71)-C(66)-C(61)	119.1(3)

C(67)-C(66)-C(61)	122.1(3)
C(68)-C(67)-C(66)	118.8(3)
C(68)-C(67)-C(72)	119.1(3)
C(66)-C(67)-C(72)	122.0(3)
C(69)-C(68)-C(67)	121.6(3)
C(69)-C(68)-H(68)	119.2
C(67)-C(68)-H(68)	119.2
C(70)-C(69)-C(68)	119.4(3)
C(70)-C(69)-H(69)	120.3
C(68)-C(69)-H(69)	120.3
C(69)-C(70)-C(71)	119.7(3)
C(69)-C(70)-H(70)	120.1
C(71)-C(70)-H(70)	120.1
C(70)-C(71)-C(66)	121.6(3)
C(70)-C(71)-H(71)	119.2
C(66)-C(71)-H(71)	119.2
C(67)-C(72)-S(73)	108.7(2)
C(67)-C(72)-S(72)	114.7(2)
S(73)-C(72)-S(72)	107.84(16)
C(67)-C(72)-H(72)	108.5
S(73)-C(72)-H(72)	108.5
S(72)-C(72)-H(72)	108.5
C(74)-S(72)-C(72)	97.73(16)
C(74)-C(73)-S(73)	106.5(3)
C(74)-C(73)-H(73A)	110.4
S(73)-C(73)-H(73A)	110.4
C(74)-C(73)-H(73B)	110.4
S(73)-C(73)-H(73B)	110.4
H(73A)-C(73)-H(73B)	108.6
C(73)-S(73)-C(72)	97.21(16)
C(73)-C(74)-S(72)	107.9(2)
C(73)-C(74)-H(74A)	110.1
S(72)-C(74)-H(74A)	110.1
C(73)-C(74)-H(74B)	110.1
S(72)-C(74)-H(74B)	110.1
H(74A)-C(74)-H(74B)	108.4

C(80)-C(75)-C(76)	118.7(3)
C(80)-C(75)-C(61)	122.8(3)
C(76)-C(75)-C(61)	118.4(3)
C(75)-C(76)-C(77)	120.1(3)
C(75)-C(76)-H(76)	119.9
C(77)-C(76)-H(76)	119.9
C(78)-C(77)-C(76)	120.4(4)
C(78)-C(77)-H(77)	119.8
C(76)-C(77)-H(77)	119.8
C(79)-C(78)-C(77)	120.0(3)
C(79)-C(78)-H(78)	120.0
C(77)-C(78)-H(78)	120.0
C(78)-C(79)-C(80)	120.6(4)
C(78)-C(79)-H(79)	119.7
C(80)-C(79)-H(79)	119.7
C(75)-C(80)-C(79)	120.2(3)
C(75)-C(80)-H(80)	119.9
C(79)-C(80)-H(80)	119.9
C(86)-C(81)-C(82)	120.3(3)
C(86)-C(81)-N(64)	119.8(3)
C(82)-C(81)-N(64)	119.8(3)
C(81)-C(82)-C(83)	119.5(3)
C(81)-C(82)-H(82)	120.3
C(83)-C(82)-H(82)	120.3
C(84)-C(83)-C(82)	120.7(3)
C(84)-C(83)-H(83)	119.6
C(82)-C(83)-H(83)	119.6
C(83)-C(84)-C(85)	119.6(3)
C(83)-C(84)-H(84)	120.2
C(85)-C(84)-H(84)	120.2
C(84)-C(85)-C(86)	120.0(3)
C(84)-C(85)-H(85)	120.0
C(86)-C(85)-H(85)	120.0
C(81)-C(86)-C(85)	119.9(3)
C(81)-C(86)-H(86)	120.1
C(85)-C(86)-H(86)	120.1

C(105)-C(91)-C(96)	116.6(3)
C(105)-C(91)-C(92)	116.2(3)
C(96)-C(91)-C(92)	118.4(3)
C(105)-C(91)-C(93)	114.1(2)
C(96)-C(91)-C(93)	120.1(3)
C(92)-C(91)-C(93)	59.01(19)
C(95)-C(92)-C(93)	105.1(3)
C(95)-C(92)-C(91)	112.9(3)
C(93)-C(92)-C(91)	61.11(19)
C(95)-C(92)-H(92)	120.8
C(93)-C(92)-H(92)	120.8
C(91)-C(92)-H(92)	120.8
C(94)-C(93)-C(92)	106.5(3)
C(94)-C(93)-C(91)	118.4(3)
C(92)-C(93)-C(91)	59.89(19)
C(94)-C(93)-H(93)	118.9
C(92)-C(93)-H(93)	118.9
C(91)-C(93)-H(93)	118.9
O(94)-C(94)-N(94)	124.1(3)
O(94)-C(94)-C(93)	128.3(3)
N(94)-C(94)-C(93)	107.5(3)
C(95)-N(94)-C(94)	112.1(3)
C(95)-N(94)-C(111)	124.1(3)
C(94)-N(94)-C(111)	123.5(3)
O(95)-C(95)-N(94)	125.2(3)
O(95)-C(95)-C(92)	126.7(3)
N(94)-C(95)-C(92)	108.1(3)
C(101)-C(96)-C(97)	118.9(3)
C(101)-C(96)-C(91)	120.0(3)
C(97)-C(96)-C(91)	121.1(3)
C(98)-C(97)-C(96)	118.8(3)
C(98)-C(97)-C(102)	119.2(3)
C(96)-C(97)-C(102)	122.0(3)
C(99)-C(98)-C(97)	121.8(3)
C(99)-C(98)-H(98)	119.1
C(97)-C(98)-H(98)	119.1

C(98)-C(99)-C(100)	119.3(3)
C(98)-C(99)-H(99)	120.3
C(100)-C(99)-H(99)	120.3
C(101)-C(100)-C(99)	120.0(3)
C(101)-C(100)-H(100)	120.0
C(99)-C(100)-H(100)	120.0
C(100)-C(101)-C(96)	121.1(3)
C(100)-C(101)-H(101)	119.4
C(96)-C(101)-H(101)	119.4
C(97)-C(102)-S(103)	115.2(2)
C(97)-C(102)-S(102)	109.3(2)
S(103)-C(102)-S(102)	108.22(16)
C(97)-C(102)-H(102)	108.0
S(103)-C(102)-H(102)	108.0
S(102)-C(102)-H(102)	108.0
C(103)-S(102)-C(102)	98.51(17)
C(104)-C(103)-S(102)	108.5(3)
C(104)-C(103)-H(10A)	110.0
S(102)-C(103)-H(10A)	110.0
C(104)-C(103)-H(10B)	110.0
S(102)-C(103)-H(10B)	110.0
H(10A)-C(103)-H(10B)	108.4
C(104)-S(103)-C(102)	97.60(17)
C(103)-C(104)-S(103)	108.0(3)
C(103)-C(104)-H(10C)	110.1
S(103)-C(104)-H(10C)	110.1
C(103)-C(104)-H(10D)	110.1
S(103)-C(104)-H(10D)	110.1
H(10C)-C(104)-H(10D)	108.4
C(106)-C(105)-C(110)	118.0(3)
C(106)-C(105)-C(91)	122.3(3)
C(110)-C(105)-C(91)	119.6(3)
C(107)-C(106)-C(105)	121.4(3)
C(107)-C(106)-H(106)	119.3
C(105)-C(106)-H(106)	119.3
C(106)-C(107)-C(108)	120.0(3)

C(106)-C(107)-H(107)	120.0
C(108)-C(107)-H(107)	120.0
C(109)-C(108)-C(107)	119.8(3)
C(109)-C(108)-H(108)	120.1
C(107)-C(108)-H(108)	120.1
C(108)-C(109)-C(110)	120.2(3)
C(108)-C(109)-H(109)	119.9
C(110)-C(109)-H(109)	119.9
C(109)-C(110)-C(105)	120.6(3)
C(109)-C(110)-H(110)	119.7
C(105)-C(110)-H(110)	119.7
C(116)-C(111)-C(112)	121.2(3)
C(116)-C(111)-N(94)	120.1(3)
C(112)-C(111)-N(94)	118.7(3)
C(113)-C(112)-C(111)	118.6(3)
C(113)-C(112)-H(112)	120.7
C(111)-C(112)-H(112)	120.7
C(112)-C(113)-C(114)	120.9(3)
C(112)-C(113)-H(113)	119.6
C(114)-C(113)-H(113)	119.6
C(115)-C(114)-C(113)	119.6(3)
C(115)-C(114)-H(114)	120.2
C(113)-C(114)-H(114)	120.2
C(114)-C(115)-C(116)	120.6(3)
C(114)-C(115)-H(115)	119.7
C(116)-C(115)-H(115)	119.7
C(111)-C(116)-C(115)	119.2(3)
C(111)-C(116)-H(116)	120.4
C(115)-C(116)-H(116)	120.4
H(12A)-O(121)-H(12B)	106.5(9)
H(12C)-O(122)-H(12D)	106.6(9)

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($Å^2 x 10^3$) for JF2975KFMI. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2 a^{*2}U^{11} + ... + 2 h k a^* b^* U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
C(1)	39(2)	30(2)	29(2)	-3(1)	2(1)	-4(1)
C(2)	42(2)	31(2)	33(2)	-5(1)	3(1)	-7(1)
C(3)	45(2)	35(2)	29(2)	-5(1)	1(1)	-5(1)
C(4)	51(2)	30(2)	30(2)	-7(1)	6(1)	-9(1)
N(4)	38(2)	35(1)	30(1)	-2(1)	2(1)	-2(1)
O(4)	56(2)	43(1)	36(1)	-8(1)	11(1)	-8(1)
C(5)	46(2)	29(2)	34(2)	-3(1)	3(1)	-4(1)
O(5)	51(2)	47(1)	35(1)	6(1)	5(1)	-5(1)
C(6)	40(2)	27(2)	36(2)	-4(1)	-2(1)	-2(1)
C(7)	45(2)	34(2)	33(2)	-6(1)	-1(1)	-2(1)
C(8)	55(2)	48(2)	41(2)	-14(2)	-2(2)	-7(2)
C(9)	56(2)	46(2)	52(2)	-14(2)	-4(2)	-12(2)
C(10)	46(2)	38(2)	58(2)	-5(2)	-1(2)	-11(2)
C(11)	44(2)	33(2)	40(2)	-2(1)	4(2)	-5(1)
C(12)	44(2)	49(2)	31(2)	-4(1)	0(1)	0(2)
S(12)	59(1)	50(1)	37(1)	3(1)	-2(1)	-5(1)
C(13)	54(3)	76(5)	51(3)	-17(4)	13(2)	-1(3)
C(13B)	54(4)	76(6)	52(4)	-17(5)	13(3)	0(4)
S(13)	64(1)	58(1)	63(1)	9(1)	18(1)	17(1)
S(13B)	61(7)	79(9)	40(5)	3(5)	7(4)	15(6)
C(14)	55(3)	110(4)	40(2)	-15(2)	5(2)	0(3)
C(15)	41(2)	35(2)	30(2)	-2(1)	3(1)	-4(1)
C(16)	43(2)	39(2)	33(2)	-3(1)	1(1)	-6(2)
C(17)	50(2)	39(2)	37(2)	-5(1)	2(2)	3(2)
C(18)	45(2)	52(2)	38(2)	-4(2)	-2(2)	4(2)
C(19)	44(2)	55(2)	48(2)	-7(2)	-6(2)	-8(2)
C(20)	48(2)	35(2)	50(2)	-5(2)	-4(2)	-6(2)
C(21)	42(2)	36(2)	35(2)	-2(1)	3(1)	-6(1)
C(22)	51(2)	50(2)	47(2)	-15(2)	5(2)	1(2)
C(23)	50(2)	61(3)	60(2)	-1(2)	8(2)	9(2)
C(24)	44(2)	77(3)	58(2)	15(2)	-3(2)	-9(2)

C(25)	64(3)	70(3)	54(2)	-5(2)	-16(2)	-16(2)
C(26)	63(3)	46(2)	44(2)	-10(2)	-7(2)	-2(2)
C(31)	36(2)	33(2)	27(2)	-2(1)	1(1)	1(1)
C(32)	40(2)	36(2)	33(2)	-4(1)	5(1)	-3(1)
C(33)	46(2)	35(2)	28(2)	2(1)	5(1)	5(1)
C(34)	49(2)	29(2)	31(2)	-1(1)	5(2)	5(1)
N(34)	37(2)	32(1)	27(1)	-1(1)	2(1)	2(1)
O(34)	52(2)	52(1)	30(1)	-2(1)	-6(1)	10(1)
C(35)	43(2)	30(2)	33(2)	-4(1)	5(1)	-5(1)
C(36)	37(2)	32(2)	31(2)	-4(1)	5(1)	0(1)
O(36)	44(1)	50(1)	38(1)	-15(1)	3(1)	-6(1)
C(37)	36(2)	37(2)	34(2)	-2(1)	2(1)	0(1)
C(38)	50(2)	49(2)	42(2)	11(2)	-2(2)	-12(2)
C(39)	53(2)	47(2)	51(2)	4(2)	4(2)	-14(2)
C(40)	44(2)	41(2)	50(2)	-6(2)	-4(2)	-8(2)
C(41)	37(2)	39(2)	38(2)	-6(1)	-3(1)	4(1)
C(42)	36(2)	46(2)	31(2)	4(1)	0(1)	-1(1)
S(42)	44(1)	79(1)	41(1)	-2(1)	3(1)	13(1)
C(43)	58(3)	41(3)	43(3)	5(2)	3(2)	9(2)
C(43B)	55(12)	56(12)	50(11)	0(9)	-4(9)	1(10)
S(43)	44(1)	54(1)	34(1)	-2(1)	0(1)	3(1)
C(44)	79(3)	62(3)	48(2)	-6(2)	-17(2)	21(2)
C(45)	41(2)	39(2)	23(1)	0(1)	4(1)	6(1)
C(46)	61(2)	44(2)	39(2)	-11(2)	8(2)	3(2)
C(47)	84(3)	54(2)	42(2)	-11(2)	13(2)	18(2)
C(48)	62(3)	78(3)	34(2)	-2(2)	14(2)	28(2)
C(49)	39(2)	78(3)	42(2)	5(2)	7(2)	15(2)
C(50)	41(2)	54(2)	38(2)	-2(2)	2(2)	6(2)
C(51)	36(2)	33(2)	28(2)	-3(1)	1(1)	0(1)
C(52)	45(2)	36(2)	32(2)	-3(1)	6(1)	-1(1)
C(53)	53(2)	41(2)	43(2)	-8(2)	13(2)	4(2)
C(54)	39(2)	59(2)	40(2)	-8(2)	5(2)	-4(2)
C(55)	54(2)	56(2)	52(2)	-13(2)	15(2)	-24(2)
C(56)	55(2)	38(2)	55(2)	-13(2)	11(2)	-12(2)
C(61)	29(2)	32(2)	26(1)	-5(1)	1(1)	-2(1)
C(62)	29(2)	36(2)	29(2)	-5(1)	-4(1)	0(1)

C(63)	34(2)	40(2)	25(1)	-2(1)	-1(1)	-5(1)
C(64)	42(2)	34(2)	28(2)	-1(1)	2(1)	-6(1)
N(64)	29(1)	37(1)	29(1)	-3(1)	1(1)	-6(1)
O(64)	43(1)	57(2)	36(1)	-8(1)	12(1)	-18(1)
C(65)	32(2)	32(2)	35(2)	-3(1)	0(1)	0(1)
O(65)	44(1)	52(1)	42(1)	-19(1)	6(1)	-9(1)
C(66)	26(2)	34(2)	32(2)	-3(1)	2(1)	-5(1)
C(67)	32(2)	34(2)	32(2)	0(1)	0(1)	-4(1)
C(68)	40(2)	44(2)	36(2)	5(1)	1(1)	-3(2)
C(69)	34(2)	52(2)	52(2)	10(2)	-4(2)	4(2)
C(70)	33(2)	45(2)	54(2)	6(2)	6(2)	6(2)
C(71)	35(2)	37(2)	38(2)	0(1)	9(1)	1(1)
C(72)	32(2)	39(2)	27(1)	-4(1)	1(1)	-3(1)
S(72)	49(1)	48(1)	37(1)	-13(1)	3(1)	-9(1)
C(73)	48(2)	49(2)	48(2)	-4(2)	16(2)	-10(2)
S(73)	47(1)	51(1)	57(1)	-20(1)	17(1)	-19(1)
C(74)	58(2)	67(3)	32(2)	-2(2)	6(2)	-3(2)
C(75)	30(2)	42(2)	24(1)	-6(1)	2(1)	-7(1)
C(76)	42(2)	46(2)	36(2)	-9(1)	1(1)	-9(2)
C(77)	68(3)	49(2)	36(2)	-8(2)	1(2)	-20(2)
C(78)	58(2)	66(2)	30(2)	3(2)	-5(2)	-31(2)
C(79)	34(2)	73(3)	45(2)	-2(2)	1(2)	-20(2)
C(80)	34(2)	52(2)	41(2)	-7(2)	6(1)	-9(2)
C(81)	34(2)	32(2)	33(2)	-5(1)	1(1)	-5(1)
C(82)	46(2)	52(2)	34(2)	6(2)	-1(2)	-14(2)
C(83)	44(2)	61(2)	41(2)	1(2)	-9(2)	-9(2)
C(84)	34(2)	50(2)	45(2)	-11(2)	-1(1)	-6(2)
C(85)	34(2)	40(2)	46(2)	-10(2)	8(1)	-10(1)
C(86)	36(2)	35(2)	35(2)	-2(1)	1(1)	-6(1)
C(91)	34(2)	32(2)	24(1)	-4(1)	1(1)	0(1)
C(92)	37(2)	34(2)	28(2)	-1(1)	-2(1)	3(1)
C(93)	41(2)	29(2)	30(2)	-5(1)	-2(1)	1(1)
C(94)	43(2)	30(2)	29(2)	-10(1)	-4(1)	2(1)
N(94)	36(2)	36(1)	32(1)	-5(1)	-4(1)	-2(1)
O(94)	50(1)	45(1)	35(1)	-11(1)	-11(1)	0(1)
C(95)	36(2)	34(2)	32(2)	-2(1)	-7(1)	-3(1)

O(95)	44(1)	52(1)	34(1)	8(1)	-10(1)	-13(1)
C(96)	32(2)	31(2)	30(2)	-5(1)	2(1)	0(1)
C(97)	32(2)	32(2)	30(2)	-5(1)	5(1)	-3(1)
C(98)	36(2)	41(2)	34(2)	-12(1)	3(1)	-4(1)
C(99)	38(2)	40(2)	43(2)	-10(1)	6(2)	2(1)
C(100)	30(2)	43(2)	46(2)	-10(2)	-2(1)	5(1)
C(101)	41(2)	37(2)	35(2)	-10(1)	-5(1)	1(1)
C(102)	32(2)	44(2)	30(2)	-9(1)	2(1)	-5(1)
S(102)	57(1)	63(1)	42(1)	0(1)	-10(1)	-27(1)
C(103)	57(2)	53(2)	50(2)	-16(2)	-16(2)	-5(2)
S(103)	47(1)	62(1)	31(1)	2(1)	1(1)	-6(1)
C(104)	61(3)	72(3)	39(2)	-19(2)	-6(2)	1(2)
C(105)	34(2)	38(2)	26(1)	-5(1)	-1(1)	0(1)
C(106)	42(2)	38(2)	39(2)	-2(1)	2(2)	5(2)
C(107)	34(2)	56(2)	39(2)	-7(2)	3(1)	6(2)
C(108)	39(2)	54(2)	38(2)	-4(2)	1(2)	-7(2)
C(109)	45(2)	42(2)	29(2)	-4(1)	1(1)	-9(2)
C(110)	42(2)	38(2)	27(2)	-9(1)	1(1)	-2(1)
C(111)	34(2)	31(2)	34(2)	0(1)	-6(1)	-1(1)
C(112)	43(2)	33(2)	39(2)	-7(1)	-2(1)	-4(1)
C(113)	45(2)	43(2)	42(2)	-8(2)	1(2)	0(2)
C(114)	36(2)	47(2)	50(2)	5(2)	-8(2)	-4(2)
C(115)	45(2)	41(2)	53(2)	0(2)	-19(2)	-11(2)
C(116)	45(2)	32(2)	41(2)	-6(1)	-15(2)	-4(1)
O(121)	142(10)	61(5)	42(4)	-3(3)	5(6)	-21(6)
O(122)	147(11)	77(6)	80(6)	-23(4)	29(8)	-21(8)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for JF2975KFMI.

	x	y	z	U(eq)
H(2)	-163	1196	5516	42
H(3)	1078	1740	4877	43
H(8)	2073	3649	6543	57
H(9)	4322	4162	6274	60
H(10)	5056	3910	5618	57
H(11)	3465	3196	5232	47
H(12)	-580	2445	6054	50
H(12E)	-316	2339	6072	50
H(13A)	-3142	3883	6814	72
H(13B)	-3202	2970	6620	72
H(13C)	-2848	3958	6745	72
H(13D)	-3327	3003	6683	72
H(14A)	-1781	2589	7215	82
H(14B)	-739	3391	7110	82
H(16)	-107	4214	5324	46
H(17)	-2272	5021	4988	51
H(18)	-4142	4293	4701	55
H(19)	-3841	2746	4748	58
H(20)	-1680	1927	5079	53
H(22)	5687	-73	5385	59
H(23)	8195	-476	5661	70
H(24)	8977	152	6211	74
H(25)	7291	1215	6487	75
H(26)	4812	1672	6202	61
H(32)	6042	8726	6443	43
H(33)	4485	8614	5821	45
H(38)	4229	5451	7381	57
H(39)	2035	5025	7092	60
H(40)	1110	5731	6463	54
H(41)	2424	6847	6130	46

H(42)	6358	7235	6974	46
H(43A)	7324	4793	7483	59
H(43B)	9142	4922	7486	59
H(43C)	9211	5043	7535	66
H(43D)	9621	6047	7491	66
H(44A)	8737	6144	7814	78
H(44B)	7597	5486	8038	78
H(44C)	8396	6046	7996	78
H(44D)	7403	5279	7892	78
H(46)	5390	6061	5975	58
H(47)	7541	5412	5653	74
H(48)	9839	6078	5593	73
H(49)	9960	7416	5848	66
H(50)	7843	8085	6170	54
H(52)	1056	10159	6826	46
H(53)	-1219	10389	7201	55
H(54)	-2555	9196	7438	55
H(55)	-1643	7765	7304	63
H(56)	604	7536	6916	58
H(62)	2247	5963	9625	38
H(63)	630	6440	10201	40
H(68)	-1014	8426	8337	50
H(69)	-3436	8980	8563	58
H(70)	-3981	8783	9251	55
H(71)	-2114	8020	9704	45
H(72)	2074	7154	8938	39
H(73A)	3885	8706	7993	58
H(73B)	4395	7741	8236	58
H(74A)	2814	7519	7700	64
H(74B)	1501	8281	7810	64
H(76)	340	8758	9885	49
H(77)	2138	9544	10174	60
H(78)	4753	9002	10216	60
H(79)	5602	7670	9977	60
H(80)	3838	6869	9685	50
H(82)	-2572	6490	8793	53

H(83)	-4866	6191	8494	59
H(84)	-6469	5237	8839	50
H(85)	-5725	4523	9479	47
H(86)	-3385	4782	9772	43
H(92)	4113	3451	8579	40
H(93)	5575	3073	9237	40
H(98)	7347	655	7727	44
H(99)	9758	174	8031	49
H(100)	10280	549	8671	48
H(101)	8418	1427	8994	45
H(102)	4300	2114	8099	42
H(10A)	2715	159	7464	63
H(10B)	2016	1173	7485	63
H(10C)	3760	1225	6965	68
H(10D)	5063	572	7229	68
H(106)	2916	2854	9088	49
H(107)	961	2145	9424	52
H(108)	1093	594	9498	52
H(109)	3204	-242	9236	46
H(110)	5184	468	8903	43
H(112)	9227	2518	7960	46
H(113)	11568	2734	7630	52
H(114)	12962	3896	7759	54
H(115)	12025	4844	8223	55
H(116)	9689	4639	8558	47
H(12A)	2170(140)	9160(50)	5390(17)	122
H(12B)	2650(110)	9310(70)	5010(20)	122
H(12C)	830(180)	9580(70)	5430(12)	149
H(12D)	1000(200)	9160(40)	5100(30)	149

Table 6. Torsion angles [°] for JF2975KFMI.

C(15)-C(1)-C(2)-C(5)	-163.4(3)
C(6)-C(1)-C(2)-C(5)	-15.6(4)
C(3)-C(1)-C(2)-C(5)	95.3(3)
C(15)-C(1)-C(2)-C(3)	101.3(3)
C(6)-C(1)-C(2)-C(3)	-110.9(3)
C(5)-C(2)-C(3)-C(4)	4.8(3)
C(1)-C(2)-C(3)-C(4)	114.3(3)
C(5)-C(2)-C(3)-C(1)	-109.5(3)
C(15)-C(1)-C(3)-C(4)	157.8(3)
C(6)-C(1)-C(3)-C(4)	13.2(4)
C(2)-C(1)-C(3)-C(4)	-93.1(3)
C(15)-C(1)-C(3)-C(2)	-109.1(3)
C(6)-C(1)-C(3)-C(2)	106.3(3)
C(2)-C(3)-C(4)-O(4)	171.7(3)
C(1)-C(3)-C(4)-O(4)	-124.1(3)
C(2)-C(3)-C(4)-N(4)	-6.8(3)
C(1)-C(3)-C(4)-N(4)	57.4(4)
O(4)-C(4)-N(4)-C(5)	-172.1(3)
C(3)-C(4)-N(4)-C(5)	6.4(3)
O(4)-C(4)-N(4)-C(21)	9.6(5)
C(3)-C(4)-N(4)-C(21)	-171.8(3)
C(4)-N(4)-C(5)-O(5)	176.7(3)
C(21)-N(4)-C(5)-O(5)	-5.1(5)
C(4)-N(4)-C(5)-C(2)	-3.3(3)
C(21)-N(4)-C(5)-C(2)	174.9(3)
C(3)-C(2)-C(5)-O(5)	178.9(3)
C(1)-C(2)-C(5)-O(5)	113.5(4)
C(3)-C(2)-C(5)-N(4)	-1.2(3)
C(1)-C(2)-C(5)-N(4)	-66.6(3)
C(15)-C(1)-C(6)-C(11)	-103.2(3)
C(2)-C(1)-C(6)-C(11)	108.7(3)
C(3)-C(1)-C(6)-C(11)	40.3(4)
C(15)-C(1)-C(6)-C(7)	76.7(4)
C(2)-C(1)-C(6)-C(7)	-71.4(4)

C(3)-C(1)-C(6)-C(7)	-139.8(3)
C(11)-C(6)-C(7)-C(8)	-0.9(5)
C(1)-C(6)-C(7)-C(8)	179.2(3)
C(11)-C(6)-C(7)-C(12)	176.3(3)
C(1)-C(6)-C(7)-C(12)	-3.7(5)
C(6)-C(7)-C(8)-C(9)	0.3(5)
C(12)-C(7)-C(8)-C(9)	-176.9(3)
C(7)-C(8)-C(9)-C(10)	-0.4(6)
C(8)-C(9)-C(10)-C(11)	1.1(6)
C(9)-C(10)-C(11)-C(6)	-1.7(5)
C(7)-C(6)-C(11)-C(10)	1.6(5)
C(1)-C(6)-C(11)-C(10)	-178.5(3)
C(8)-C(7)-C(12)-S(13B)	90.2(6)
C(6)-C(7)-C(12)-S(13B)	-86.9(6)
C(8)-C(7)-C(12)-S(12)	-50.3(4)
C(6)-C(7)-C(12)-S(12)	132.6(3)
C(8)-C(7)-C(12)-S(13)	68.8(4)
C(6)-C(7)-C(12)-S(13)	-108.3(3)
C(7)-C(12)-S(12)-C(14)	123.8(3)
S(13B)-C(12)-S(12)-C(14)	-19.7(6)
S(13)-C(12)-S(12)-C(14)	3.9(3)
C(14)-C(13)-S(13)-C(12)	46(3)
C(7)-C(12)-S(13)-C(13)	-150.9(12)
S(12)-C(12)-S(13)-C(13)	-27.3(12)
C(7)-C(12)-S(13B)-C(13B)	-135(11)
S(12)-C(12)-S(13B)-C(13B)	6(11)
C(14)-C(13B)-S(13B)-C(12)	15(23)
S(13)-C(13)-C(14)-S(12)	-49(3)
S(13B)-C(13B)-C(14)-S(12)	-28(24)
C(12)-S(12)-C(14)-C(13)	27.2(18)
C(12)-S(12)-C(14)-C(13B)	27(12)
C(6)-C(1)-C(15)-C(16)	16.7(4)
C(2)-C(1)-C(15)-C(16)	165.1(3)
C(3)-C(1)-C(15)-C(16)	-129.7(3)
C(6)-C(1)-C(15)-C(20)	-167.6(3)
C(2)-C(1)-C(15)-C(20)	-19.1(4)

C(3)-C(1)-C(15)-C(20)	46.1(4)
C(20)-C(15)-C(16)-C(17)	-1.7(5)
C(1)-C(15)-C(16)-C(17)	174.1(3)
C(15)-C(16)-C(17)-C(18)	1.0(5)
C(16)-C(17)-C(18)-C(19)	0.0(5)
C(17)-C(18)-C(19)-C(20)	-0.2(6)
C(18)-C(19)-C(20)-C(15)	-0.6(6)
C(16)-C(15)-C(20)-C(19)	1.5(5)
C(1)-C(15)-C(20)-C(19)	-174.3(3)
C(5)-N(4)-C(21)-C(22)	122.0(4)
C(4)-N(4)-C(21)-C(22)	-60.0(4)
C(5)-N(4)-C(21)-C(26)	-58.7(5)
C(4)-N(4)-C(21)-C(26)	119.3(4)
C(26)-C(21)-C(22)-C(23)	-0.9(6)
N(4)-C(21)-C(22)-C(23)	178.4(3)
C(21)-C(22)-C(23)-C(24)	1.4(6)
C(22)-C(23)-C(24)-C(25)	-0.7(7)
C(23)-C(24)-C(25)-C(26)	-0.7(7)
C(22)-C(21)-C(26)-C(25)	-0.4(6)
N(4)-C(21)-C(26)-C(25)	-179.7(3)
C(24)-C(25)-C(26)-C(21)	1.2(6)
C(36)-C(31)-C(32)-C(35)	-14.5(4)
C(45)-C(31)-C(32)-C(35)	-160.6(3)
C(33)-C(31)-C(32)-C(35)	95.6(3)
C(36)-C(31)-C(32)-C(33)	-110.1(3)
C(45)-C(31)-C(32)-C(33)	103.8(3)
C(35)-C(32)-C(33)-C(34)	3.4(3)
C(31)-C(32)-C(33)-C(34)	112.6(3)
C(35)-C(32)-C(33)-C(31)	-109.2(3)
C(36)-C(31)-C(33)-C(34)	16.7(4)
C(45)-C(31)-C(33)-C(34)	159.0(3)
C(32)-C(31)-C(33)-C(34)	-92.9(3)
C(36)-C(31)-C(33)-C(32)	109.6(3)
C(45)-C(31)-C(33)-C(32)	-108.1(3)
C(32)-C(33)-C(34)-O(34)	173.2(3)
C(31)-C(33)-C(34)-O(34)	-122.9(4)

C(32)-C(33)-C(34)-N(34)	-6.8(3)
C(31)-C(33)-C(34)-N(34)	57.1(4)
O(34)-C(34)-N(34)-C(35)	-172.0(3)
C(33)-C(34)-N(34)-C(35)	8.0(3)
O(34)-C(34)-N(34)-C(51)	6.0(5)
C(33)-C(34)-N(34)-C(51)	-174.0(3)
C(34)-N(34)-C(35)-O(36)	174.5(3)
C(51)-N(34)-C(35)-O(36)	-3.5(5)
C(34)-N(34)-C(35)-C(32)	-5.8(3)
C(51)-N(34)-C(35)-C(32)	176.2(3)
C(33)-C(32)-C(35)-O(36)	-179.1(3)
C(31)-C(32)-C(35)-O(36)	116.2(4)
C(33)-C(32)-C(35)-N(34)	1.2(3)
C(31)-C(32)-C(35)-N(34)	-63.6(3)
C(45)-C(31)-C(36)-C(41)	-97.4(3)
C(32)-C(31)-C(36)-C(41)	115.4(3)
C(33)-C(31)-C(36)-C(41)	45.3(4)
C(45)-C(31)-C(36)-C(37)	76.0(4)
C(32)-C(31)-C(36)-C(37)	-71.2(4)
C(33)-C(31)-C(36)-C(37)	-141.4(3)
C(41)-C(36)-C(37)-C(38)	-2.9(5)
C(31)-C(36)-C(37)-C(38)	-176.3(3)
C(41)-C(36)-C(37)-C(42)	173.8(3)
C(31)-C(36)-C(37)-C(42)	0.4(5)
C(36)-C(37)-C(38)-C(39)	2.0(6)
C(42)-C(37)-C(38)-C(39)	-174.7(4)
C(37)-C(38)-C(39)-C(40)	-0.5(6)
C(38)-C(39)-C(40)-C(41)	0.0(6)
C(39)-C(40)-C(41)-C(36)	-1.0(5)
C(37)-C(36)-C(41)-C(40)	2.5(5)
C(31)-C(36)-C(41)-C(40)	176.0(3)
C(38)-C(37)-C(42)-S(42)	81.5(4)
C(36)-C(37)-C(42)-S(42)	-95.2(3)
C(38)-C(37)-C(42)-S(43)	-42.2(4)
C(36)-C(37)-C(42)-S(43)	141.1(3)
C(37)-C(42)-S(42)-C(43)	-103.8(3)

S(43)-C(42)-S(42)-C(43)	23.0(3)
C(37)-C(42)-S(42)-C(43B)	-134.3(8)
S(43)-C(42)-S(42)-C(43B)	-7.6(8)
C(42)-S(42)-C(43)-C(44)	-39.7(4)
C(42)-S(42)-C(43B)-C(44)	21.2(16)
C(37)-C(42)-S(43)-C(44)	122.8(3)
S(42)-C(42)-S(43)-C(44)	-3.2(3)
S(42)-C(43B)-C(44)-S(43)	-26.8(18)
S(42)-C(43)-C(44)-S(43)	42.0(5)
C(42)-S(43)-C(44)-C(43B)	18.7(12)
C(42)-S(43)-C(44)-C(43)	-22.7(4)
C(36)-C(31)-C(45)-C(46)	35.8(4)
C(32)-C(31)-C(45)-C(46)	-175.7(3)
C(33)-C(31)-C(45)-C(46)	-109.3(3)
C(36)-C(31)-C(45)-C(50)	-143.6(3)
C(32)-C(31)-C(45)-C(50)	4.9(4)
C(33)-C(31)-C(45)-C(50)	71.2(4)
C(50)-C(45)-C(46)-C(47)	0.5(5)
C(31)-C(45)-C(46)-C(47)	-179.0(3)
C(45)-C(46)-C(47)-C(48)	0.0(6)
C(46)-C(47)-C(48)-C(49)	-0.6(6)
C(47)-C(48)-C(49)-C(50)	0.6(6)
C(48)-C(49)-C(50)-C(45)	-0.1(6)
C(46)-C(45)-C(50)-C(49)	-0.5(5)
C(31)-C(45)-C(50)-C(49)	178.9(3)
C(34)-N(34)-C(51)-C(52)	-99.5(4)
C(35)-N(34)-C(51)-C(52)	78.2(4)
C(34)-N(34)-C(51)-C(56)	81.7(4)
C(35)-N(34)-C(51)-C(56)	-100.6(4)
C(56)-C(51)-C(52)-C(53)	-0.4(5)
N(34)-C(51)-C(52)-C(53)	-179.2(3)
C(51)-C(52)-C(53)-C(54)	0.6(5)
C(52)-C(53)-C(54)-C(55)	-0.1(6)
C(53)-C(54)-C(55)-C(56)	-0.7(6)
C(52)-C(51)-C(56)-C(55)	-0.3(6)
N(34)-C(51)-C(56)-C(55)	178.5(3)

C(54)-C(55)-C(56)-C(51)	0.9(6)
C(75)-C(61)-C(62)-C(65)	-163.7(3)
C(66)-C(61)-C(62)-C(65)	-14.9(4)
C(63)-C(61)-C(62)-C(65)	95.3(3)
C(75)-C(61)-C(62)-C(63)	101.0(3)
C(66)-C(61)-C(62)-C(63)	-110.2(3)
C(65)-C(62)-C(63)-C(64)	3.8(3)
C(61)-C(62)-C(63)-C(64)	112.8(3)
C(65)-C(62)-C(63)-C(61)	-109.0(3)
C(75)-C(61)-C(63)-C(64)	157.0(3)
C(66)-C(61)-C(63)-C(64)	14.2(4)
C(62)-C(61)-C(63)-C(64)	-93.4(3)
C(75)-C(61)-C(63)-C(62)	-109.5(3)
C(66)-C(61)-C(63)-C(62)	107.7(3)
C(62)-C(63)-C(64)-O(64)	174.5(3)
C(61)-C(63)-C(64)-O(64)	-121.8(4)
C(62)-C(63)-C(64)-N(64)	-5.5(3)
C(61)-C(63)-C(64)-N(64)	58.2(3)
O(64)-C(64)-N(64)-C(65)	-174.8(3)
C(63)-C(64)-N(64)-C(65)	5.1(3)
O(64)-C(64)-N(64)-C(81)	12.5(5)
C(63)-C(64)-N(64)-C(81)	-167.6(3)
C(64)-N(64)-C(65)-O(65)	178.1(3)
C(81)-N(64)-C(65)-O(65)	-9.3(5)
C(64)-N(64)-C(65)-C(62)	-2.6(3)
C(81)-N(64)-C(65)-C(62)	170.0(3)
C(63)-C(62)-C(65)-O(65)	178.4(3)
C(61)-C(62)-C(65)-O(65)	113.3(4)
C(63)-C(62)-C(65)-N(64)	-0.9(3)
C(61)-C(62)-C(65)-N(64)	-66.0(3)
C(75)-C(61)-C(66)-C(71)	-95.6(3)
C(62)-C(61)-C(66)-C(71)	115.2(3)
C(63)-C(61)-C(66)-C(71)	46.0(4)
C(75)-C(61)-C(66)-C(67)	83.8(4)
C(62)-C(61)-C(66)-C(67)	-65.4(4)
C(63)-C(61)-C(66)-C(67)	-134.6(3)

C(71)-C(66)-C(67)-C(68)	-1.8(5)
C(61)-C(66)-C(67)-C(68)	178.8(3)
C(71)-C(66)-C(67)-C(72)	174.5(3)
C(61)-C(66)-C(67)-C(72)	-4.9(5)
C(66)-C(67)-C(68)-C(69)	0.2(5)
C(72)-C(67)-C(68)-C(69)	-176.2(3)
C(67)-C(68)-C(69)-C(70)	0.9(6)
C(68)-C(69)-C(70)-C(71)	-0.5(6)
C(69)-C(70)-C(71)-C(66)	-1.0(6)
C(67)-C(66)-C(71)-C(70)	2.2(5)
C(61)-C(66)-C(71)-C(70)	-178.4(3)
C(68)-C(67)-C(72)-S(73)	71.9(3)
C(66)-C(67)-C(72)-S(73)	-104.3(3)
C(68)-C(67)-C(72)-S(72)	-48.8(4)
C(66)-C(67)-C(72)-S(72)	134.9(3)
C(67)-C(72)-S(72)-C(74)	115.4(3)
S(73)-C(72)-S(72)-C(74)	-5.8(2)
C(74)-C(73)-S(73)-C(72)	42.6(3)
C(67)-C(72)-S(73)-C(73)	-143.5(2)
S(72)-C(72)-S(73)-C(73)	-18.6(2)
S(73)-C(73)-C(74)-S(72)	-51.1(3)
C(72)-S(72)-C(74)-C(73)	34.7(3)
C(66)-C(61)-C(75)-C(80)	-133.2(3)
C(62)-C(61)-C(75)-C(80)	16.5(4)
C(63)-C(61)-C(75)-C(80)	82.2(4)
C(66)-C(61)-C(75)-C(76)	51.1(4)
C(62)-C(61)-C(75)-C(76)	-159.2(3)
C(63)-C(61)-C(75)-C(76)	-93.5(3)
C(80)-C(75)-C(76)-C(77)	-0.1(5)
C(61)-C(75)-C(76)-C(77)	175.8(3)
C(75)-C(76)-C(77)-C(78)	0.1(5)
C(76)-C(77)-C(78)-C(79)	-0.3(5)
C(77)-C(78)-C(79)-C(80)	0.3(5)
C(76)-C(75)-C(80)-C(79)	0.1(5)
C(61)-C(75)-C(80)-C(79)	-175.6(3)
C(78)-C(79)-C(80)-C(75)	-0.2(5)

C(65)-N(64)-C(81)-C(86)	130.5(3)
C(64)-N(64)-C(81)-C(86)	-57.7(4)
C(65)-N(64)-C(81)-C(82)	-51.9(4)
C(64)-N(64)-C(81)-C(82)	119.9(3)
C(86)-C(81)-C(82)-C(83)	-0.4(5)
N(64)-C(81)-C(82)-C(83)	-177.9(3)
C(81)-C(82)-C(83)-C(84)	1.5(6)
C(82)-C(83)-C(84)-C(85)	-1.4(6)
C(83)-C(84)-C(85)-C(86)	0.2(5)
C(82)-C(81)-C(86)-C(85)	-0.8(5)
N(64)-C(81)-C(86)-C(85)	176.8(3)
C(84)-C(85)-C(86)-C(81)	0.9(5)
C(105)-C(91)-C(92)-C(95)	-161.2(3)
C(96)-C(91)-C(92)-C(95)	-14.7(4)
C(93)-C(91)-C(92)-C(95)	95.2(3)
C(105)-C(91)-C(92)-C(93)	103.5(3)
C(96)-C(91)-C(92)-C(93)	-109.9(3)
C(95)-C(92)-C(93)-C(94)	5.5(3)
C(91)-C(92)-C(93)-C(94)	113.6(3)
C(95)-C(92)-C(93)-C(91)	-108.1(3)
C(105)-C(91)-C(93)-C(94)	159.3(3)
C(96)-C(91)-C(93)-C(94)	13.6(4)
C(92)-C(91)-C(93)-C(94)	-93.4(3)
C(105)-C(91)-C(93)-C(92)	-107.2(3)
C(96)-C(91)-C(93)-C(92)	107.0(3)
C(92)-C(93)-C(94)-O(94)	171.6(3)
C(91)-C(93)-C(94)-O(94)	-124.1(3)
C(92)-C(93)-C(94)-N(94)	-7.5(3)
C(91)-C(93)-C(94)-N(94)	56.8(3)
O(94)-C(94)-N(94)-C(95)	-172.4(3)
C(93)-C(94)-N(94)-C(95)	6.8(3)
O(94)-C(94)-N(94)-C(111)	13.4(5)
C(93)-C(94)-N(94)-C(111)	-167.4(3)
C(94)-N(94)-C(95)-O(95)	176.9(3)
C(111)-N(94)-C(95)-O(95)	-9.0(5)
C(94)-N(94)-C(95)-C(92)	-3.2(3)

C(111)-N(94)-C(95)-C(92)	171.0(3)
C(93)-C(92)-C(95)-O(95)	178.3(3)
C(91)-C(92)-C(95)-O(95)	113.7(4)
C(93)-C(92)-C(95)-N(94)	-1.6(3)
C(91)-C(92)-C(95)-N(94)	-66.2(3)
C(105)-C(91)-C(96)-C(101)	-101.6(3)
C(92)-C(91)-C(96)-C(101)	112.1(3)
C(93)-C(91)-C(96)-C(101)	43.4(4)
C(105)-C(91)-C(96)-C(97)	76.9(4)
C(92)-C(91)-C(96)-C(97)	-69.5(4)
C(93)-C(91)-C(96)-C(97)	-138.2(3)
C(101)-C(96)-C(97)-C(98)	-2.0(5)
C(91)-C(96)-C(97)-C(98)	179.5(3)
C(101)-C(96)-C(97)-C(102)	175.8(3)
C(91)-C(96)-C(97)-C(102)	-2.6(5)
C(96)-C(97)-C(98)-C(99)	0.4(5)
C(102)-C(97)-C(98)-C(99)	-177.5(3)
C(97)-C(98)-C(99)-C(100)	1.1(5)
C(98)-C(99)-C(100)-C(101)	-0.9(5)
C(99)-C(100)-C(101)-C(96)	-0.7(5)
C(97)-C(96)-C(101)-C(100)	2.2(5)
C(91)-C(96)-C(101)-C(100)	-179.3(3)
C(98)-C(97)-C(102)-S(103)	-45.4(4)
C(96)-C(97)-C(102)-S(103)	136.8(3)
C(98)-C(97)-C(102)-S(102)	76.7(3)
C(96)-C(97)-C(102)-S(102)	-101.2(3)
C(97)-C(102)-S(102)-C(103)	-135.1(2)
S(103)-C(102)-S(102)-C(103)	-8.9(2)
C(102)-S(102)-C(103)-C(104)	34.6(3)
C(97)-C(102)-S(103)-C(104)	109.1(3)
S(102)-C(102)-S(103)-C(104)	-13.5(2)
S(102)-C(103)-C(104)-S(103)	-47.5(3)
C(102)-S(103)-C(104)-C(103)	37.3(3)
C(96)-C(91)-C(105)-C(106)	-170.9(3)
C(92)-C(91)-C(105)-C(106)	-23.8(4)
C(93)-C(91)-C(105)-C(106)	42.1(4)

C(96)-C(91)-C(105)-C(110)	11.9(4)
C(92)-C(91)-C(105)-C(110)	159.0(3)
C(93)-C(91)-C(105)-C(110)	-135.1(3)
C(110)-C(105)-C(106)-C(107)	0.4(5)
C(91)-C(105)-C(106)-C(107)	-176.9(3)
C(105)-C(106)-C(107)-C(108)	-0.4(5)
C(106)-C(107)-C(108)-C(109)	0.2(5)
C(107)-C(108)-C(109)-C(110)	0.2(5)
C(108)-C(109)-C(110)-C(105)	-0.2(5)
C(106)-C(105)-C(110)-C(109)	-0.1(5)
C(91)-C(105)-C(110)-C(109)	177.3(3)
C(95)-N(94)-C(111)-C(116)	121.6(3)
C(94)-N(94)-C(111)-C(116)	-64.8(4)
C(95)-N(94)-C(111)-C(112)	-59.4(4)
C(94)-N(94)-C(111)-C(112)	114.2(3)
C(116)-C(111)-C(112)-C(113)	-1.4(5)
N(94)-C(111)-C(112)-C(113)	179.7(3)
C(111)-C(112)-C(113)-C(114)	0.5(5)
C(112)-C(113)-C(114)-C(115)	0.3(5)
C(113)-C(114)-C(115)-C(116)	-0.3(5)
C(112)-C(111)-C(116)-C(115)	1.4(5)
N(94)-C(111)-C(116)-C(115)	-179.6(3)
C(114)-C(115)-C(116)-C(111)	-0.6(5)

Symmetry transformations used to generate equivalent atoms:

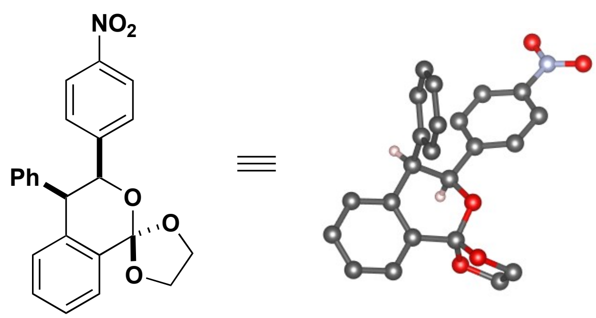
Table 7. Hydrogen bonds for JF2975KFMI [Å and °].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
C(22)-H(22)...O(4)#1	0.95	2.57	3.397(4)	146
C(43)-H(43A)...O(95)	0.99	2.43	3.300(6)	147
C(52)-H(52)...O(5)#2	0.95	2.51	3.239(4)	133
C(63)-H(63)...O(94)#3	1.00	2.40	3.355(4)	160
C(73)-H(73A)...S(102)#2	0.99	3.01	3.785(4)	136
C(116)-H(116)...O(65)#4	0.95	2.27	3.097(4)	144
O(121)-H(12A)...O(34)	0.842(5)	2.17(5)	2.925(10)	148(9)
O(122)-H(12C)...O(34)	0.842(5)	2.16(8)	2.872(13)	143(12)

Symmetry transformations used to generate equivalent atoms:

#1 -x+1,-y,-z+1 #2 x,y+1,z #3 -x+1,-y+1,-z+2

#4 x+1,y,z



CCDC 2087128

Table 1. Crystal data and structure refinement for $[C_{23}H_{19}NO_5]_{0.91:0.09}$.

Identification code	JF2983FMI (MG-4-62-2) (Whole Molecule Disorder, 0.91:0.09)	
Empirical formula	C23 H19 N O5	
Formula weight	389.39	
Temperature	90(2) K	
Wavelength	1.54178 Å	
Crystal system	Orthorhombic	
Space group	$Pca2_1$	
Unit cell dimensions	a = 19.1967(9) Å	α= 90°.
	b = 13.7962(6) Å	β= 90°.
	c = 13.8480(6) Å	γ = 90°.
Volume	3667.5(3) $Å^3$	

Z, Z’	8, 2
Density (calculated)	1.410 Mg/m^3
Absorption coefficient	0.823 mm^{-1}
F(000)	1632
Crystal size	0.549 x 0.333 x 0.178 mm^3
Crystal color and habit	colourless Block
Diffractometer	Bruker APEX-II CCD
Theta range for data collection	3.203 to 69.545°.
Index ranges	-21<=h<=23, -16<=k<=16, -16<=l<=16
Reflections collected	17934
Independent reflections	6717 [R(int) = 0.0207]
Observed reflections (I > 2sigma(I))	6644
Completeness to theta = 67.679°	99.9 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.8116 and 0.7343
Solution method	SHELXT (Sheldrick, 2014)
Refinement method	SHELXL-2017/1 (Sheldrick, 2017) Full-matrix least-squares on F^2
Data / restraints / parameters	6717 / 432 / 683
Goodness-of-fit on F^2	1.045
Final R indices [I>2sigma(I)]	R1 = 0.0341, wR2 = 0.0903
R indices (all data)	R1 = 0.0343, wR2 = 0.0906
Absolute structure parameters	Flack = 0.02(4); Hooft = 0.02(3); Parson’s = 0.06(3)
Largest diff. peak and hole	0.156 and -0.400 e.Å^{-3}

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for JF2983FMI. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
C(1)	3110(1)	5068(2)	4560(2)	14(1)
O(1)	2590(1)	4502(2)	4128(2)	15(1)
C(2)	1969(1)	5055(1)	3946(2)	13(1)
O(2)	3409(1)	5700(1)	3877(1)	16(1)
C(3)	1608(1)	5256(2)	4925(1)	13(1)
O(3)	3639(1)	4422(1)	4822(1)	17(1)
C(4)	2130(1)	5772(2)	5569(2)	16(1)
C(5)	2845(1)	5651(2)	5399(2)	15(1)
C(6)	3328(1)	6119(2)	5990(2)	16(1)
C(7)	3100(1)	6705(2)	6751(2)	18(1)
C(8)	2390(2)	6827(2)	6908(2)	17(1)
C(9)	1911(1)	6366(2)	6324(2)	16(1)
C(10)	3892(1)	5128(2)	3321(2)	25(1)
C(11)	4016(1)	4232(2)	3943(2)	21(1)
C(12)	1535(1)	4519(1)	3214(2)	14(1)
C(13)	930(1)	4950(2)	2853(2)	15(1)
C(14)	539(1)	4502(1)	2143(2)	15(1)
C(15)	760(1)	3605(1)	1810(1)	14(1)
N(15)	353(1)	3135(2)	1051(2)	17(1)
O(15)	-167(1)	3553(1)	745(1)	23(1)
C(16)	1352(1)	3157(2)	2150(2)	17(1)
O(16)	554(1)	2346(1)	738(1)	24(1)
C(17)	1740(1)	3617(2)	2859(2)	18(1)
C(18)	1321(1)	4340(2)	5400(2)	16(1)
C(19)	1739(1)	3753(2)	5970(2)	18(1)
C(20)	1480(1)	2902(2)	6366(2)	27(1)
C(21)	804(2)	2634(2)	6205(3)	36(1)
C(22)	372(1)	3214(2)	5623(2)	30(1)
C(23)	635(1)	4063(2)	5238(2)	23(1)
C(31)	1883(1)	9928(2)	6883(2)	18(1)
O(31)	2424(1)	9364(1)	6485(1)	16(1)

C(32)	3038(1)	9933(1)	6306(2)	14(1)
O(32)	1587(1)	10524(1)	6167(1)	20(1)
C(33)	3376(1)	10158(2)	7292(2)	15(1)
O(33)	1364(1)	9276(1)	7154(1)	20(1)
C(34)	2833(1)	10677(2)	7904(2)	17(1)
C(35)	2124(1)	10546(2)	7712(2)	18(1)
C(36)	1629(1)	11015(2)	8283(2)	20(1)
C(37)	1833(1)	11597(2)	9046(2)	24(1)
C(38)	2540(1)	11722(2)	9244(2)	23(1)
C(39)	3032(1)	11265(2)	8673(2)	20(1)
C(40)	1098(1)	9932(2)	5645(2)	27(1)
C(41)	1006(1)	9035(2)	6271(2)	26(1)
C(42)	3488(1)	9412(2)	5580(2)	16(1)
C(43)	4096(1)	9856(2)	5241(2)	16(1)
C(44)	4484(1)	9442(2)	4511(2)	18(1)
C(45)	4263(1)	8570(2)	4125(2)	17(1)
N(45)	4659(1)	8151(2)	3319(2)	20(1)
O(45)	5189(1)	8569(1)	3051(1)	27(1)
C(46)	3674(1)	8098(2)	4449(2)	19(1)
O(46)	4438(1)	7405(1)	2934(1)	28(1)
C(47)	3285(1)	8527(2)	5176(2)	18(1)
C(48)	3656(2)	9266(2)	7821(3)	17(1)
C(49)	3222(1)	8711(2)	8405(2)	17(1)
C(50)	3485(1)	7929(2)	8921(2)	19(1)
C(51)	4186(1)	7698(2)	8864(2)	21(1)
C(52)	4618(1)	8241(2)	8270(2)	24(1)
C(53)	4354(1)	9022(2)	7749(2)	21(1)
C(101)	1865(9)	5036(14)	4659(14)	21(2)
O(101)	2413(11)	4446(18)	4210(20)	20(4)
C(102)	3029(11)	4989(18)	4039(16)	34(3)
O(102)	1602(10)	5570(14)	3884(15)	42(3)
C(103)	3367(11)	5170(17)	5013(15)	28(3)
O(103)	1389(11)	4339(15)	5038(18)	26(3)
C(104)	2912(10)	5749(19)	5610(15)	16(3)
C(105)	2197(11)	5661(19)	5477(16)	15(2)
C(106)	1741(8)	6139(17)	6093(17)	27(4)

C(107)	1999(12)	6706(13)	6842(14)	30(4)
C(108)	2714(13)	6794(12)	6974(12)	21(3)
C(109)	3170(9)	6316(16)	6358(15)	20(4)
C(110)	1140(13)	4917(16)	3368(17)	30(3)
C(111)	1005(13)	4077(17)	4048(19)	33(3)
C(112)	3487(8)	4442(12)	3361(11)	35(3)
C(113)	4072(9)	4903(10)	2988(13)	36(3)
C(114)	4453(7)	4469(11)	2252(12)	36(3)
C(115)	4249(7)	3573(10)	1890(9)	36(3)
C(116)	3664(8)	3112(9)	2263(12)	36(3)
C(117)	3283(7)	3546(12)	2998(12)	36(4)
N(115)	4663(9)	3156(13)	1121(12)	33(3)
O(115)	4338(12)	2454(16)	1041(19)	38(3)
O(116)	5154(9)	3552(13)	822(14)	41(3)
C(118)	3674(8)	4323(10)	5592(13)	28(3)
C(119)	4363(8)	4044(13)	5457(14)	28(3)
C(120)	4613(7)	3206(14)	5893(17)	21(4)
C(121)	4173(8)	2646(11)	6464(15)	30(3)
C(122)	3484(8)	2925(11)	6598(13)	28(3)
C(123)	3235(6)	3764(12)	6162(14)	29(3)
C(131)	3096(9)	10078(13)	7210(14)	14(4)
O(131)	2590(8)	9484(13)	6805(14)	20(3)
O(132)	3607(12)	9423(17)	7567(18)	16(7)
C(132)	1946(12)	10020(30)	6638(16)	16(4)
O(133)	3400(8)	10659(11)	6514(12)	22(3)
C(133)	1621(9)	10241(13)	7604(12)	17(3)
C(134)	2133(8)	10783(13)	8216(13)	20(3)
C(135)	2843(9)	10651(15)	8072(13)	16(4)
C(136)	3321(7)	11107(15)	8674(14)	22(4)
C(137)	3088(8)	11696(12)	9422(12)	25(3)
C(138)	2377(9)	11829(14)	9567(13)	27(3)
C(139)	1900(7)	11372(15)	8964(15)	25(4)
C(140)	4001(12)	9201(16)	6622(18)	27(5)
C(141)	3893(14)	10061(19)	5980(20)	41(7)
C(142)	1518(8)	9488(12)	5911(11)	27(3)
C(143)	918(9)	9929(10)	5558(13)	26(3)

C(144)	534(7)	9484(11)	4832(13)	24(2)
C(145)	749(7)	8598(10)	4459(11)	26(3)
C(146)	1348(8)	8157(9)	4811(12)	27(3)
C(147)	1733(7)	8602(11)	5538(11)	24(2)
N(145)	346(11)	8147(15)	3712(18)	28(3)
O(145)	-172(8)	8562(12)	3417(13)	28(2)
O(146)	579(9)	7396(12)	3419(15)	29(2)
C(148)	1321(7)	9328(9)	8115(11)	17(3)
C(149)	1752(6)	8760(10)	8690(12)	17(4)
C(150)	1490(8)	7931(10)	9130(12)	17(6)
C(151)	797(9)	7671(11)	8995(16)	33(6)
C(152)	367(7)	8239(13)	8420(17)	22(4)
C(153)	628(7)	9068(11)	7980(13)	18(4)

Table 3. Bond lengths [Å] and angles [°] for JF2983FMI.

C(1)-O(3)	1.399(2)
C(1)-O(1)	1.400(3)
C(1)-O(2)	1.408(3)
C(1)-C(5)	1.503(3)
O(1)-C(2)	1.437(3)
C(2)-C(12)	1.507(3)
C(2)-C(3)	1.548(3)
C(2)-H(2)	1.0000
O(2)-C(10)	1.441(3)
C(3)-C(4)	1.518(3)
C(3)-C(18)	1.526(3)
C(3)-H(3)	1.0000
O(3)-C(11)	1.440(3)
C(4)-C(9)	1.393(3)
C(4)-C(5)	1.403(3)
C(5)-C(6)	1.395(3)
C(6)-C(7)	1.397(3)
C(6)-H(6)	0.9500
C(7)-C(8)	1.392(3)
C(7)-H(7)	0.9500
C(8)-C(9)	1.379(3)
C(8)-H(8)	0.9500
C(9)-H(9)	0.9500
C(10)-C(11)	1.526(3)
C(10)-H(10A)	0.9900
C(10)-H(10B)	0.9900
C(11)-H(11A)	0.9900
C(11)-H(11B)	0.9900
C(12)-C(17)	1.396(3)
C(12)-C(13)	1.396(3)
C(13)-C(14)	1.384(3)
C(13)-H(13)	0.9500
C(14)-C(15)	1.387(3)
C(14)-H(14)	0.9500

C(15)-C(16)	1.377(3)
C(15)-N(15)	1.461(3)
N(15)-O(15)	1.228(3)
N(15)-O(16)	1.233(3)
C(16)-C(17)	1.386(3)
C(16)-H(16)	0.9500
C(17)-H(17)	0.9500
C(18)-C(19)	1.387(3)
C(18)-C(23)	1.391(3)
C(19)-C(20)	1.389(3)
C(19)-H(19)	0.9500
C(20)-C(21)	1.367(4)
C(20)-H(20)	0.9500
C(21)-C(22)	1.407(4)
C(21)-H(21)	0.9500
C(22)-C(23)	1.383(4)
C(22)-H(22)	0.9500
C(23)-H(23)	0.9500
C(31)-O(33)	1.394(3)
C(31)-O(32)	1.408(3)
C(31)-O(31)	1.410(3)
C(31)-C(35)	1.505(4)
O(31)-C(32)	1.437(2)
C(32)-C(42)	1.508(3)
C(32)-C(33)	1.544(3)
C(32)-H(32)	1.0000
O(32)-C(40)	1.440(3)
C(33)-C(34)	1.522(3)
C(33)-C(48)	1.530(4)
C(33)-H(33)	1.0000
O(33)-C(41)	1.441(3)
C(34)-C(39)	1.392(3)
C(34)-C(35)	1.398(3)
C(35)-C(36)	1.396(3)
C(36)-C(37)	1.383(4)
C(36)-H(36)	0.9500

C(37)-C(38)	1.397(4)
C(37)-H(37)	0.9500
C(38)-C(39)	1.384(3)
C(38)-H(38)	0.9500
C(39)-H(39)	0.9500
C(40)-C(41)	1.522(4)
C(40)-H(40A)	0.9900
C(40)-H(40B)	0.9900
C(41)-H(41A)	0.9900
C(41)-H(41B)	0.9900
C(42)-C(43)	1.399(3)
C(42)-C(47)	1.399(3)
C(43)-C(44)	1.381(3)
C(43)-H(43)	0.9500
C(44)-C(45)	1.382(3)
C(44)-H(44)	0.9500
C(45)-C(46)	1.380(3)
C(45)-N(45)	1.469(3)
N(45)-O(45)	1.227(3)
N(45)-O(46)	1.233(3)
C(46)-C(47)	1.386(3)
C(46)-H(46)	0.9500
C(47)-H(47)	0.9500
C(48)-C(53)	1.385(4)
C(48)-C(49)	1.391(4)
C(49)-C(50)	1.389(3)
C(49)-H(49)	0.9500
C(50)-C(51)	1.385(3)
C(50)-H(50)	0.9500
C(51)-C(52)	1.389(4)
C(51)-H(51)	0.9500
C(52)-C(53)	1.393(3)
C(52)-H(52)	0.9500
C(53)-H(53)	0.9500
C(101)-O(102)	1.40(2)
C(101)-O(103)	1.43(2)

C(101)-O(101)	1.47(2)
C(101)-C(105)	1.560(19)
O(101)-C(102)	1.420(14)
C(102)-C(112)	1.492(18)
C(102)-C(103)	1.52(2)
C(102)-H(10C)	1.0000
O(102)-C(110)	1.452(14)
C(103)-C(104)	1.44(2)
C(103)-C(118)	1.53(3)
C(103)-H(103)	1.0000
O(103)-C(111)	1.60(3)
C(104)-C(105)	1.3900
C(104)-C(109)	1.3900
C(105)-C(106)	1.3900
C(106)-C(107)	1.3900
C(106)-H(106)	0.9500
C(107)-C(108)	1.3900
C(107)-H(107)	0.9500
C(108)-C(109)	1.3900
C(108)-H(108)	0.9500
C(109)-H(109)	0.9500
C(110)-C(111)	1.52(2)
C(110)-H(11C)	0.9900
C(110)-H(11D)	0.9900
C(111)-H(11E)	0.9900
C(111)-H(11F)	0.9900
C(112)-C(113)	1.3900
C(112)-C(117)	1.3900
C(113)-C(114)	1.3900
C(113)-H(113)	0.9500
C(114)-C(115)	1.3900
C(114)-H(114)	0.9500
C(115)-C(116)	1.3900
C(115)-N(115)	1.448(16)
C(116)-C(117)	1.3900
C(116)-H(116)	0.9500

C(117)-H(117)	0.9500
N(115)-O(115)	1.16(2)
N(115)-O(116)	1.165(19)
C(118)-C(119)	1.3900
C(118)-C(123)	1.3900
C(119)-C(120)	1.3900
C(119)-H(119)	0.9500
C(120)-C(121)	1.3900
C(120)-H(120)	0.9500
C(121)-C(122)	1.3900
C(121)-H(121)	0.9500
C(122)-C(123)	1.3900
C(122)-H(122)	0.9500
C(123)-H(123)	0.9500
C(131)-O(133)	1.38(2)
C(131)-O(131)	1.39(2)
C(131)-O(132)	1.42(2)
C(131)-C(135)	1.511(18)
O(131)-C(132)	1.46(3)
O(132)-C(140)	1.54(3)
C(132)-C(142)	1.493(18)
C(132)-C(133)	1.51(2)
C(132)-H(132)	1.0000
O(133)-C(141)	1.46(3)
C(133)-C(134)	1.498(18)
C(133)-C(148)	1.555(18)
C(133)-H(133)	1.0000
C(134)-C(135)	1.3900
C(134)-C(139)	1.3900
C(135)-C(136)	1.3900
C(136)-C(137)	1.3900
C(136)-H(136)	0.9500
C(137)-C(138)	1.3900
C(137)-H(137)	0.9500
C(138)-C(139)	1.3900
C(138)-H(138)	0.9500

C(139)-H(139)	0.9500
C(140)-C(141)	1.50(2)
C(140)-H(14A)	0.9900
C(140)-H(14B)	0.9900
C(141)-H(14C)	0.9900
C(141)-H(14D)	0.9900
C(142)-C(143)	1.3900
C(142)-C(147)	1.3900
C(143)-C(144)	1.3900
C(143)-H(143)	0.9500
C(144)-C(145)	1.3900
C(144)-H(144)	0.9500
C(145)-C(146)	1.3900
C(145)-N(145)	1.43(2)
C(146)-C(147)	1.3900
C(146)-H(146)	0.9500
C(147)-H(147)	0.9500
N(145)-O(146)	1.20(2)
N(145)-O(145)	1.22(2)
C(148)-C(149)	1.3900
C(148)-C(153)	1.3900
C(149)-C(150)	1.3900
C(149)-H(149)	0.9500
C(150)-C(151)	1.3900
C(150)-H(150)	0.9500
C(151)-C(152)	1.3900
C(151)-H(151)	0.9500
C(152)-C(153)	1.3900
C(152)-H(152)	0.9500
C(153)-H(153)	0.9500
O(3)-C(1)-O(1)	105.88(17)
O(3)-C(1)-O(2)	105.81(16)
O(1)-C(1)-O(2)	110.37(19)
O(3)-C(1)-C(5)	112.73(19)
O(1)-C(1)-C(5)	112.80(18)

O(2)-C(1)-C(5)	109.01(18)
C(1)-O(1)-C(2)	111.72(17)
O(1)-C(2)-C(12)	108.46(17)
O(1)-C(2)-C(3)	108.30(17)
C(12)-C(2)-C(3)	115.40(16)
O(1)-C(2)-H(2)	108.2
C(12)-C(2)-H(2)	108.2
C(3)-C(2)-H(2)	108.2
C(1)-O(2)-C(10)	106.40(16)
C(4)-C(3)-C(18)	111.9(2)
C(4)-C(3)-C(2)	107.57(17)
C(18)-C(3)-C(2)	112.96(17)
C(4)-C(3)-H(3)	108.1
C(18)-C(3)-H(3)	108.1
C(2)-C(3)-H(3)	108.1
C(1)-O(3)-C(11)	105.17(16)
C(9)-C(4)-C(5)	119.4(2)
C(9)-C(4)-C(3)	121.2(2)
C(5)-C(4)-C(3)	119.5(2)
C(6)-C(5)-C(4)	119.8(2)
C(6)-C(5)-C(1)	118.4(2)
C(4)-C(5)-C(1)	121.7(2)
C(5)-C(6)-C(7)	120.1(2)
C(5)-C(6)-H(6)	119.9
C(7)-C(6)-H(6)	119.9
C(8)-C(7)-C(6)	119.7(2)
C(8)-C(7)-H(7)	120.2
C(6)-C(7)-H(7)	120.2
C(9)-C(8)-C(7)	120.3(2)
C(9)-C(8)-H(8)	119.9
C(7)-C(8)-H(8)	119.9
C(8)-C(9)-C(4)	120.7(2)
C(8)-C(9)-H(9)	119.6
C(4)-C(9)-H(9)	119.6
O(2)-C(10)-C(11)	104.02(19)
O(2)-C(10)-H(10A)	111.0

C(11)-C(10)-H(10A)	111.0
O(2)-C(10)-H(10B)	111.0
C(11)-C(10)-H(10B)	111.0
H(10A)-C(10)-H(10B)	109.0
O(3)-C(11)-C(10)	104.53(17)
O(3)-C(11)-H(11A)	110.8
C(10)-C(11)-H(11A)	110.8
O(3)-C(11)-H(11B)	110.8
C(10)-C(11)-H(11B)	110.8
H(11A)-C(11)-H(11B)	108.9
C(17)-C(12)-C(13)	119.25(19)
C(17)-C(12)-C(2)	121.21(19)
C(13)-C(12)-C(2)	119.48(18)
C(14)-C(13)-C(12)	121.02(19)
C(14)-C(13)-H(13)	119.5
C(12)-C(13)-H(13)	119.5
C(13)-C(14)-C(15)	117.96(18)
C(13)-C(14)-H(14)	121.0
C(15)-C(14)-H(14)	121.0
C(16)-C(15)-C(14)	122.68(19)
C(16)-C(15)-N(15)	119.22(19)
C(14)-C(15)-N(15)	118.09(19)
O(15)-N(15)-O(16)	123.2(2)
O(15)-N(15)-C(15)	118.3(2)
O(16)-N(15)-C(15)	118.47(19)
C(15)-C(16)-C(17)	118.72(19)
C(15)-C(16)-H(16)	120.6
C(17)-C(16)-H(16)	120.6
C(16)-C(17)-C(12)	120.38(19)
C(16)-C(17)-H(17)	119.8
C(12)-C(17)-H(17)	119.8
C(19)-C(18)-C(23)	118.7(2)
C(19)-C(18)-C(3)	121.4(2)
C(23)-C(18)-C(3)	119.9(2)
C(18)-C(19)-C(20)	120.7(2)
C(18)-C(19)-H(19)	119.6

C(20)-C(19)-H(19)	119.6
C(21)-C(20)-C(19)	120.3(2)
C(21)-C(20)-H(20)	119.9
C(19)-C(20)-H(20)	119.9
C(20)-C(21)-C(22)	120.0(2)
C(20)-C(21)-H(21)	120.0
C(22)-C(21)-H(21)	120.0
C(23)-C(22)-C(21)	119.2(2)
C(23)-C(22)-H(22)	120.4
C(21)-C(22)-H(22)	120.4
C(22)-C(23)-C(18)	121.1(2)
C(22)-C(23)-H(23)	119.5
C(18)-C(23)-H(23)	119.5
O(33)-C(31)-O(32)	106.14(19)
O(33)-C(31)-O(31)	106.1(2)
O(32)-C(31)-O(31)	110.2(2)
O(33)-C(31)-C(35)	112.3(2)
O(32)-C(31)-C(35)	109.3(2)
O(31)-C(31)-C(35)	112.6(2)
C(31)-O(31)-C(32)	111.70(16)
O(31)-C(32)-C(42)	108.90(16)
O(31)-C(32)-C(33)	107.61(17)
C(42)-C(32)-C(33)	116.42(17)
O(31)-C(32)-H(32)	107.9
C(42)-C(32)-H(32)	107.9
C(33)-C(32)-H(32)	107.9
C(31)-O(32)-C(40)	106.57(17)
C(34)-C(33)-C(48)	110.6(2)
C(34)-C(33)-C(32)	107.37(19)
C(48)-C(33)-C(32)	114.12(19)
C(34)-C(33)-H(33)	108.2
C(48)-C(33)-H(33)	108.2
C(32)-C(33)-H(33)	108.2
C(31)-O(33)-C(41)	105.10(18)
C(39)-C(34)-C(35)	119.2(2)
C(39)-C(34)-C(33)	120.7(2)

C(35)-C(34)-C(33)	120.0(2)
C(36)-C(35)-C(34)	119.8(2)
C(36)-C(35)-C(31)	119.1(2)
C(34)-C(35)-C(31)	121.2(2)
C(37)-C(36)-C(35)	120.6(2)
C(37)-C(36)-H(36)	119.7
C(35)-C(36)-H(36)	119.7
C(36)-C(37)-C(38)	119.8(2)
C(36)-C(37)-H(37)	120.1
C(38)-C(37)-H(37)	120.1
C(39)-C(38)-C(37)	119.7(2)
C(39)-C(38)-H(38)	120.2
C(37)-C(38)-H(38)	120.2
C(38)-C(39)-C(34)	121.0(2)
C(38)-C(39)-H(39)	119.5
C(34)-C(39)-H(39)	119.5
O(32)-C(40)-C(41)	104.5(2)
O(32)-C(40)-H(40A)	110.9
C(41)-C(40)-H(40A)	110.9
O(32)-C(40)-H(40B)	110.9
C(41)-C(40)-H(40B)	110.9
H(40A)-C(40)-H(40B)	108.9
O(33)-C(41)-C(40)	103.95(18)
O(33)-C(41)-H(41A)	111.0
C(40)-C(41)-H(41A)	111.0
O(33)-C(41)-H(41B)	111.0
C(40)-C(41)-H(41B)	111.0
H(41A)-C(41)-H(41B)	109.0
C(43)-C(42)-C(47)	118.7(2)
C(43)-C(42)-C(32)	119.53(19)
C(47)-C(42)-C(32)	121.53(19)
C(44)-C(43)-C(42)	121.0(2)
C(44)-C(43)-H(43)	119.5
C(42)-C(43)-H(43)	119.5
C(43)-C(44)-C(45)	118.5(2)
C(43)-C(44)-H(44)	120.7

C(45)-C(44)-H(44)	120.7
C(46)-C(45)-C(44)	122.5(2)
C(46)-C(45)-N(45)	119.0(2)
C(44)-C(45)-N(45)	118.5(2)
O(45)-N(45)-O(46)	123.1(2)
O(45)-N(45)-C(45)	118.2(2)
O(46)-N(45)-C(45)	118.7(2)
C(45)-C(46)-C(47)	118.5(2)
C(45)-C(46)-H(46)	120.8
C(47)-C(46)-H(46)	120.8
C(46)-C(47)-C(42)	120.8(2)
C(46)-C(47)-H(47)	119.6
C(42)-C(47)-H(47)	119.6
C(53)-C(48)-C(49)	119.2(3)
C(53)-C(48)-C(33)	120.0(3)
C(49)-C(48)-C(33)	120.7(2)
C(50)-C(49)-C(48)	120.5(2)
C(50)-C(49)-H(49)	119.7
C(48)-C(49)-H(49)	119.7
C(51)-C(50)-C(49)	120.3(2)
C(51)-C(50)-H(50)	119.9
C(49)-C(50)-H(50)	119.9
C(50)-C(51)-C(52)	119.3(2)
C(50)-C(51)-H(51)	120.4
C(52)-C(51)-H(51)	120.4
C(51)-C(52)-C(53)	120.5(2)
C(51)-C(52)-H(52)	119.8
C(53)-C(52)-H(52)	119.8
C(48)-C(53)-C(52)	120.2(2)
C(48)-C(53)-H(53)	119.9
C(52)-C(53)-H(53)	119.9
O(102)-C(101)-O(103)	114.1(16)
O(102)-C(101)-O(101)	103(2)
O(103)-C(101)-O(101)	103.9(18)
O(102)-C(101)-C(105)	114.4(18)
O(103)-C(101)-C(105)	111.5(19)

O(101)-C(101)-C(105)	108.5(16)
C(102)-O(101)-C(101)	112.1(17)
O(101)-C(102)-C(112)	109.3(18)
O(101)-C(102)-C(103)	107.0(17)
C(112)-C(102)-C(103)	113.0(17)
O(101)-C(102)-H(10C)	109.2
C(112)-C(102)-H(10C)	109.2
C(103)-C(102)-H(10C)	109.2
C(101)-O(102)-C(110)	105.7(16)
C(104)-C(103)-C(102)	109.9(17)
C(104)-C(103)-C(118)	110.7(18)
C(102)-C(103)-C(118)	120.2(18)
C(104)-C(103)-H(103)	104.9
C(102)-C(103)-H(103)	104.9
C(118)-C(103)-H(103)	104.9
C(101)-O(103)-C(111)	97.6(16)
C(105)-C(104)-C(109)	120.0
C(105)-C(104)-C(103)	118.2(17)
C(109)-C(104)-C(103)	121.5(17)
C(106)-C(105)-C(104)	120.0
C(106)-C(105)-C(101)	116.7(16)
C(104)-C(105)-C(101)	123.3(16)
C(105)-C(106)-C(107)	120.0
C(105)-C(106)-H(106)	120.0
C(107)-C(106)-H(106)	120.0
C(108)-C(107)-C(106)	120.0
C(108)-C(107)-H(107)	120.0
C(106)-C(107)-H(107)	120.0
C(107)-C(108)-C(109)	120.0
C(107)-C(108)-H(108)	120.0
C(109)-C(108)-H(108)	120.0
C(108)-C(109)-C(104)	120.0
C(108)-C(109)-H(109)	120.0
C(104)-C(109)-H(109)	120.0
O(102)-C(110)-C(111)	105.9(17)
O(102)-C(110)-H(11C)	110.6

C(111)-C(110)-H(11C)	110.6
O(102)-C(110)-H(11D)	110.6
C(111)-C(110)-H(11D)	110.6
H(11C)-C(110)-H(11D)	108.7
C(110)-C(111)-O(103)	106.3(15)
C(110)-C(111)-H(11E)	110.5
O(103)-C(111)-H(11E)	110.5
C(110)-C(111)-H(11F)	110.5
O(103)-C(111)-H(11F)	110.5
H(11E)-C(111)-H(11F)	108.7
C(113)-C(112)-C(117)	120.0
C(113)-C(112)-C(102)	118.6(13)
C(117)-C(112)-C(102)	120.8(13)
C(114)-C(113)-C(112)	120.0
C(114)-C(113)-H(113)	120.0
C(112)-C(113)-H(113)	120.0
C(115)-C(114)-C(113)	120.0
C(115)-C(114)-H(114)	120.0
C(113)-C(114)-H(114)	120.0
C(114)-C(115)-C(116)	120.0
C(114)-C(115)-N(115)	117.6(10)
C(116)-C(115)-N(115)	122.4(10)
C(115)-C(116)-C(117)	120.0
C(115)-C(116)-H(116)	120.0
C(117)-C(116)-H(116)	120.0
C(116)-C(117)-C(112)	120.0
C(116)-C(117)-H(117)	120.0
C(112)-C(117)-H(117)	120.0
O(115)-N(115)-O(116)	143(2)
O(115)-N(115)-C(115)	96.1(19)
O(116)-N(115)-C(115)	121.3(18)
C(119)-C(118)-C(123)	120.0
C(119)-C(118)-C(103)	120.4(13)
C(123)-C(118)-C(103)	119.1(13)
C(118)-C(119)-C(120)	120.0
C(118)-C(119)-H(119)	120.0

C(120)-C(119)-H(119)	120.0
C(121)-C(120)-C(119)	120.0
C(121)-C(120)-H(120)	120.0
C(119)-C(120)-H(120)	120.0
C(120)-C(121)-C(122)	120.0
C(120)-C(121)-H(121)	120.0
C(122)-C(121)-H(121)	120.0
C(123)-C(122)-C(121)	120.0
C(123)-C(122)-H(122)	120.0
C(121)-C(122)-H(122)	120.0
C(122)-C(123)-C(118)	120.0
C(122)-C(123)-H(123)	120.0
C(118)-C(123)-H(123)	120.0
O(133)-C(131)-O(131)	110.9(16)
O(133)-C(131)-O(132)	108.6(16)
O(131)-C(131)-O(132)	104.4(17)
O(133)-C(131)-C(135)	112.5(16)
O(131)-C(131)-C(135)	113.8(15)
O(132)-C(131)-C(135)	106.2(18)
C(131)-O(131)-C(132)	110.9(17)
C(131)-O(132)-C(140)	99.7(17)
O(131)-C(132)-C(142)	109(2)
O(131)-C(132)-C(133)	108.2(18)
C(142)-C(132)-C(133)	118.0(18)
O(131)-C(132)-H(132)	107.0
C(142)-C(132)-H(132)	107.0
C(133)-C(132)-H(132)	107.0
C(131)-O(133)-C(141)	107.4(14)
C(134)-C(133)-C(132)	109.4(14)
C(134)-C(133)-C(148)	113.0(14)
C(132)-C(133)-C(148)	113.1(18)
C(134)-C(133)-H(133)	107.0
C(132)-C(133)-H(133)	107.0
C(148)-C(133)-H(133)	107.0
C(135)-C(134)-C(139)	120.0
C(135)-C(134)-C(133)	119.8(13)

C(139)-C(134)-C(133)	120.1(13)
C(136)-C(135)-C(134)	120.0
C(136)-C(135)-C(131)	120.0(12)
C(134)-C(135)-C(131)	119.8(12)
C(135)-C(136)-C(137)	120.0
C(135)-C(136)-H(136)	120.0
C(137)-C(136)-H(136)	120.0
C(138)-C(137)-C(136)	120.0
C(138)-C(137)-H(137)	120.0
C(136)-C(137)-H(137)	120.0
C(139)-C(138)-C(137)	120.0
C(139)-C(138)-H(138)	120.0
C(137)-C(138)-H(138)	120.0
C(138)-C(139)-C(134)	120.0
C(138)-C(139)-H(139)	120.0
C(134)-C(139)-H(139)	120.0
C(141)-C(140)-O(132)	106.1(16)
C(141)-C(140)-H(14A)	110.5
O(132)-C(140)-H(14A)	110.5
C(141)-C(140)-H(14B)	110.5
O(132)-C(140)-H(14B)	110.5
H(14A)-C(140)-H(14B)	108.7
O(133)-C(141)-C(140)	103.9(16)
O(133)-C(141)-H(14C)	111.0
C(140)-C(141)-H(14C)	111.0
O(133)-C(141)-H(14D)	111.0
C(140)-C(141)-H(14D)	111.0
H(14C)-C(141)-H(14D)	109.0
C(143)-C(142)-C(147)	120.0
C(143)-C(142)-C(132)	118.6(16)
C(147)-C(142)-C(132)	121.3(16)
C(142)-C(143)-C(144)	120.0
C(142)-C(143)-H(143)	120.0
C(144)-C(143)-H(143)	120.0
C(143)-C(144)-C(145)	120.0
C(143)-C(144)-H(144)	120.0

C(145)-C(144)-H(144)	120.0
C(146)-C(145)-C(144)	120.0
C(146)-C(145)-N(145)	120.7(12)
C(144)-C(145)-N(145)	119.3(12)
C(147)-C(146)-C(145)	120.0
C(147)-C(146)-H(146)	120.0
C(145)-C(146)-H(146)	120.0
C(146)-C(147)-C(142)	120.0
C(146)-C(147)-H(147)	120.0
C(142)-C(147)-H(147)	120.0
O(146)-N(145)-O(145)	127(2)
O(146)-N(145)-C(145)	114.6(18)
O(145)-N(145)-C(145)	118.6(18)
C(149)-C(148)-C(153)	120.0
C(149)-C(148)-C(133)	119.8(11)
C(153)-C(148)-C(133)	120.2(11)
C(148)-C(149)-C(150)	120.0
C(148)-C(149)-H(149)	120.0
C(150)-C(149)-H(149)	120.0
C(151)-C(150)-C(149)	120.0
C(151)-C(150)-H(150)	120.0
C(149)-C(150)-H(150)	120.0
C(152)-C(151)-C(150)	120.0
C(152)-C(151)-H(151)	120.0
C(150)-C(151)-H(151)	120.0
C(151)-C(152)-C(153)	120.0
C(151)-C(152)-H(152)	120.0
C(153)-C(152)-H(152)	120.0
C(152)-C(153)-C(148)	120.0
C(152)-C(153)-H(153)	120.0
C(148)-C(153)-H(153)	120.0

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($Å^2$x 10^3) for JF2983FMI. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2 a^{*2}U^{11} + ... + 2 h k a^* b^* U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
C(1)	14(1)	17(1)	11(1)	0(1)	-3(1)	-2(1)
O(1)	12(1)	17(1)	16(1)	-1(1)	-1(1)	1(1)
C(2)	13(1)	13(1)	13(1)	-1(1)	-1(1)	1(1)
O(2)	16(1)	17(1)	15(1)	0(1)	3(1)	-1(1)
C(3)	14(1)	14(1)	10(1)	-1(1)	2(1)	2(1)
O(3)	16(1)	21(1)	15(1)	-1(1)	-1(1)	4(1)
C(4)	19(1)	14(1)	13(1)	1(1)	1(1)	-1(1)
C(5)	20(1)	13(1)	12(1)	2(1)	-3(1)	-1(1)
C(6)	19(1)	16(1)	14(1)	-2(1)	1(1)	0(1)
C(7)	22(1)	18(1)	12(1)	-2(1)	-1(1)	-3(1)
C(8)	20(1)	16(1)	14(1)	-1(1)	1(1)	-3(1)
C(9)	21(1)	13(1)	13(1)	-3(1)	-1(1)	-2(1)
C(10)	26(1)	27(1)	21(1)	-3(1)	7(1)	3(1)
C(11)	20(1)	26(1)	17(1)	-2(1)	2(1)	5(1)
C(12)	18(1)	14(1)	11(1)	0(1)	2(1)	-3(1)
C(13)	15(1)	16(1)	14(1)	-3(1)	1(1)	1(1)
C(14)	12(1)	19(1)	14(1)	1(1)	0(1)	0(1)
C(15)	16(1)	16(1)	10(1)	-1(1)	2(1)	-5(1)
N(15)	18(1)	22(1)	13(1)	-2(1)	1(1)	-4(1)
O(15)	19(1)	29(1)	21(1)	-5(1)	-6(1)	2(1)
C(16)	21(1)	14(1)	17(1)	-2(1)	-1(1)	0(1)
O(16)	24(1)	22(1)	24(1)	-9(1)	-3(1)	-1(1)
C(17)	18(1)	16(1)	18(1)	2(1)	-3(1)	2(1)
C(18)	21(1)	16(1)	11(1)	-6(1)	6(1)	0(1)
C(19)	21(1)	14(1)	18(1)	0(1)	2(1)	1(1)
C(20)	34(1)	16(1)	31(1)	5(1)	9(1)	2(1)
C(21)	38(2)	18(1)	51(2)	2(1)	15(1)	-7(1)
C(22)	22(1)	26(1)	42(2)	-3(1)	8(1)	-6(1)
C(23)	19(1)	21(1)	29(1)	-3(1)	2(1)	1(1)
C(31)	14(1)	18(1)	20(1)	5(1)	2(1)	3(1)
O(31)	14(1)	15(1)	19(1)	2(1)	1(1)	-1(1)

C(32)	13(1)	14(1)	16(1)	3(1)	0(1)	-1(1)
O(32)	19(1)	21(1)	21(1)	6(1)	-3(1)	3(1)
C(33)	14(1)	15(1)	15(1)	2(1)	0(1)	-1(1)
O(33)	16(1)	24(1)	18(1)	2(1)	1(1)	-4(1)
C(34)	21(1)	13(1)	16(1)	5(1)	3(1)	1(1)
C(35)	20(1)	13(1)	20(1)	4(1)	2(1)	1(1)
C(36)	20(1)	18(1)	22(1)	4(1)	3(1)	2(1)
C(37)	31(1)	17(1)	23(1)	3(1)	11(1)	5(1)
C(38)	32(1)	15(1)	22(1)	0(1)	4(1)	-1(1)
C(39)	24(1)	14(1)	21(1)	2(1)	2(1)	-2(1)
C(40)	26(1)	30(1)	24(1)	-1(1)	-6(1)	2(1)
C(41)	20(1)	36(1)	23(1)	-1(1)	-2(1)	-9(1)
C(42)	16(1)	16(1)	15(1)	5(1)	-3(1)	3(1)
C(43)	15(1)	16(1)	17(1)	2(1)	-2(1)	0(1)
C(44)	13(1)	22(1)	19(1)	5(1)	-2(1)	-2(1)
C(45)	17(1)	18(1)	17(1)	1(1)	-1(1)	4(1)
N(45)	19(1)	21(1)	21(1)	-1(1)	1(1)	4(1)
O(45)	18(1)	31(1)	30(1)	-4(1)	8(1)	-3(1)
C(46)	18(1)	16(1)	22(1)	0(1)	-2(1)	-2(1)
O(46)	31(1)	22(1)	32(1)	-7(1)	7(1)	-1(1)
C(47)	16(1)	16(1)	22(1)	4(1)	-1(1)	-1(1)
C(48)	20(1)	14(1)	16(2)	-1(1)	-3(1)	1(1)
C(49)	20(1)	15(1)	17(1)	-1(1)	0(1)	0(1)
C(50)	28(1)	15(1)	15(1)	0(1)	-2(1)	-2(1)
C(51)	29(1)	16(1)	17(1)	1(1)	-8(1)	1(1)
C(52)	19(1)	22(1)	32(1)	0(1)	-5(1)	2(1)
C(53)	18(1)	20(1)	24(1)	3(1)	-1(1)	-2(1)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for JF2983FMI.

	x	y	z	U(eq)
H(2)	2109	5691	3659	16
H(3)	1209	5707	4806	15
H(6)	3812	6038	5876	19
H(7)	3429	7018	7157	21
H(8)	2234	7230	7421	20
H(9)	1427	6455	6438	19
H(10A)	4332	5486	3213	30
H(10B)	3690	4948	2688	30
H(11A)	3835	3643	3620	25
H(11B)	4518	4143	4075	25
H(13)	786	5561	3099	18
H(14)	131	4798	1891	18
H(16)	1491	2544	1904	21
H(17)	2149	3316	3104	21
H(19)	2209	3935	6091	21
H(20)	1773	2503	6750	32
H(21)	626	2057	6487	43
H(22)	-95	3025	5496	36
H(23)	341	4464	4856	28
H(32)	2887	10561	6012	17
H(33)	3773	10614	7182	18
H(36)	1147	10934	8147	24
H(37)	1492	11910	9435	28
H(38)	2683	12119	9768	27
H(39)	3513	11354	8807	24
H(40A)	1283	9757	5001	32
H(40B)	649	10275	5560	32
H(41A)	507	8903	6393	32
H(41B)	1218	8459	5961	32
H(43)	4243	10452	5518	19

H(44)	4894	9748	4279	22
H(46)	3538	7494	4179	23
H(47)	2875	8215	5403	21
H(49)	2741	8867	8451	21
H(50)	3184	7552	9315	23
H(51)	4369	7172	9228	25
H(52)	5098	8079	8218	29
H(53)	4653	9389	7342	25
H(10C)	2901	5625	3741	40
H(103)	3774	5601	4870	33
H(106)	1252	6078	6002	32
H(107)	1686	7032	7263	36
H(108)	2890	7182	7486	25
H(109)	3659	6377	6449	24
H(11C)	1362	4686	2766	36
H(11D)	699	5248	3201	36
H(11E)	1194	3468	3776	40
H(11F)	499	3995	4156	40
H(113)	4211	5515	3236	43
H(114)	4852	4784	1997	44
H(116)	3525	2500	2015	43
H(117)	2883	3231	3253	43
H(119)	4664	4427	5067	34
H(120)	5083	3015	5801	25
H(121)	4343	2073	6762	36
H(122)	3184	2543	6988	33
H(123)	2764	3955	6254	34
H(132)	2079	10654	6340	19
H(133)	1221	10689	7482	21
H(136)	3806	11016	8575	26
H(137)	3414	12008	9834	30
H(138)	2218	12231	10078	32
H(139)	1415	11463	9063	29
H(14A)	4504	9104	6752	32
H(14B)	3814	8608	6314	32
H(14C)	4336	10412	5874	49

H(14D)	3698	9864	5350	49
H(143)	771	10535	5813	31
H(144)	125	9785	4591	28
H(146)	1495	7551	4556	32
H(147)	2142	8301	5779	29
H(149)	2225	8939	8783	20
H(150)	1784	7543	9523	21
H(151)	618	7104	9296	40
H(152)	-107	8060	8327	26
H(153)	334	9456	7587	22

Table 6. Torsion angles [°] for JF2983FMI.

O(3)-C(1)-O(1)-C(2)	171.70(17)
O(2)-C(1)-O(1)-C(2)	-74.2(2)
C(5)-C(1)-O(1)-C(2)	48.0(3)
C(1)-O(1)-C(2)-C(12)	161.94(18)
C(1)-O(1)-C(2)-C(3)	-72.1(2)
O(3)-C(1)-O(2)-C(10)	35.2(2)
O(1)-C(1)-O(2)-C(10)	-79.0(2)
C(5)-C(1)-O(2)-C(10)	156.63(19)
O(1)-C(2)-C(3)-C(4)	56.8(2)
C(12)-C(2)-C(3)-C(4)	178.52(18)
O(1)-C(2)-C(3)-C(18)	-67.2(2)
C(12)-C(2)-C(3)-C(18)	54.5(2)
O(1)-C(1)-O(3)-C(11)	79.0(2)
O(2)-C(1)-O(3)-C(11)	-38.2(2)
C(5)-C(1)-O(3)-C(11)	-157.21(18)
C(18)-C(3)-C(4)-C(9)	-80.0(3)
C(2)-C(3)-C(4)-C(9)	155.3(2)
C(18)-C(3)-C(4)-C(5)	100.2(2)
C(2)-C(3)-C(4)-C(5)	-24.5(3)
C(9)-C(4)-C(5)-C(6)	0.6(3)
C(3)-C(4)-C(5)-C(6)	-179.6(3)
C(9)-C(4)-C(5)-C(1)	-176.3(3)
C(3)-C(4)-C(5)-C(1)	3.5(3)
O(3)-C(1)-C(5)-C(6)	49.7(3)
O(1)-C(1)-C(5)-C(6)	169.5(2)
O(2)-C(1)-C(5)-C(6)	-67.5(3)
O(3)-C(1)-C(5)-C(4)	-133.5(2)
O(1)-C(1)-C(5)-C(4)	-13.6(3)
O(2)-C(1)-C(5)-C(4)	109.4(2)
C(4)-C(5)-C(6)-C(7)	0.1(3)
C(1)-C(5)-C(6)-C(7)	177.0(2)
C(5)-C(6)-C(7)-C(8)	-0.6(3)
C(6)-C(7)-C(8)-C(9)	0.6(3)
C(7)-C(8)-C(9)-C(4)	0.0(3)

C(5)-C(4)-C(9)-C(8)	-0.6(3)
C(3)-C(4)-C(9)-C(8)	179.6(2)
C(1)-O(2)-C(10)-C(11)	-17.8(2)
C(1)-O(3)-C(11)-C(10)	25.8(2)
O(2)-C(10)-C(11)-O(3)	-4.8(2)
O(1)-C(2)-C(12)-C(17)	2.8(3)
C(3)-C(2)-C(12)-C(17)	-118.9(2)
O(1)-C(2)-C(12)-C(13)	-174.48(18)
C(3)-C(2)-C(12)-C(13)	63.9(2)
C(17)-C(12)-C(13)-C(14)	-0.8(3)
C(2)-C(12)-C(13)-C(14)	176.57(18)
C(12)-C(13)-C(14)-C(15)	0.8(3)
C(13)-C(14)-C(15)-C(16)	-0.6(3)
C(13)-C(14)-C(15)-N(15)	-179.21(19)
C(16)-C(15)-N(15)-O(15)	-178.9(2)
C(14)-C(15)-N(15)-O(15)	-0.2(3)
C(16)-C(15)-N(15)-O(16)	0.0(3)
C(14)-C(15)-N(15)-O(16)	178.71(19)
C(14)-C(15)-C(16)-C(17)	0.4(3)
N(15)-C(15)-C(16)-C(17)	178.96(19)
C(15)-C(16)-C(17)-C(12)	-0.3(3)
C(13)-C(12)-C(17)-C(16)	0.5(3)
C(2)-C(12)-C(17)-C(16)	-176.78(19)
C(4)-C(3)-C(18)-C(19)	-36.6(3)
C(2)-C(3)-C(18)-C(19)	85.0(3)
C(4)-C(3)-C(18)-C(23)	145.5(2)
C(2)-C(3)-C(18)-C(23)	-92.9(2)
C(23)-C(18)-C(19)-C(20)	0.4(3)
C(3)-C(18)-C(19)-C(20)	-177.4(2)
C(18)-C(19)-C(20)-C(21)	-0.6(4)
C(19)-C(20)-C(21)-C(22)	1.1(4)
C(20)-C(21)-C(22)-C(23)	-1.5(4)
C(21)-C(22)-C(23)-C(18)	1.4(4)
C(19)-C(18)-C(23)-C(22)	-0.9(4)
C(3)-C(18)-C(23)-C(22)	177.0(2)
O(33)-C(31)-O(31)-C(32)	-171.34(17)

O(32)-C(31)-O(31)-C(32)	74.2(2)
C(35)-C(31)-O(31)-C(32)	-48.1(3)
C(31)-O(31)-C(32)-C(42)	-159.93(18)
C(31)-O(31)-C(32)-C(33)	73.0(2)
O(33)-C(31)-O(32)-C(40)	-32.5(3)
O(31)-C(31)-O(32)-C(40)	81.9(2)
C(35)-C(31)-O(32)-C(40)	-153.85(19)
O(31)-C(32)-C(33)-C(34)	-57.3(2)
C(42)-C(32)-C(33)-C(34)	-179.84(17)
O(31)-C(32)-C(33)-C(48)	65.7(2)
C(42)-C(32)-C(33)-C(48)	-56.8(3)
O(32)-C(31)-O(33)-C(41)	38.4(2)
O(31)-C(31)-O(33)-C(41)	-78.8(2)
C(35)-C(31)-O(33)-C(41)	157.8(2)
C(48)-C(33)-C(34)-C(39)	77.6(3)
C(32)-C(33)-C(34)-C(39)	-157.3(2)
C(48)-C(33)-C(34)-C(35)	-100.8(3)
C(32)-C(33)-C(34)-C(35)	24.3(3)
C(39)-C(34)-C(35)-C(36)	0.9(3)
C(33)-C(34)-C(35)-C(36)	179.2(2)
C(39)-C(34)-C(35)-C(31)	179.3(2)
C(33)-C(34)-C(35)-C(31)	-2.3(3)
O(33)-C(31)-C(35)-C(36)	-49.4(3)
O(32)-C(31)-C(35)-C(36)	68.1(3)
O(31)-C(31)-C(35)-C(36)	-169.09(19)
O(33)-C(31)-C(35)-C(34)	132.2(2)
O(32)-C(31)-C(35)-C(34)	-110.3(2)
O(31)-C(31)-C(35)-C(34)	12.5(3)
C(34)-C(35)-C(36)-C(37)	-1.0(3)
C(31)-C(35)-C(36)-C(37)	-179.4(2)
C(35)-C(36)-C(37)-C(38)	0.4(3)
C(36)-C(37)-C(38)-C(39)	0.2(3)
C(37)-C(38)-C(39)-C(34)	-0.3(3)
C(35)-C(34)-C(39)-C(38)	-0.2(3)
C(33)-C(34)-C(39)-C(38)	-178.6(2)
C(31)-O(32)-C(40)-C(41)	13.7(3)

C(31)-O(33)-C(41)-C(40)	-28.5(2)
O(32)-C(40)-C(41)-O(33)	8.9(2)
O(31)-C(32)-C(42)-C(43)	175.84(18)
C(33)-C(32)-C(42)-C(43)	-62.3(3)
O(31)-C(32)-C(42)-C(47)	1.0(3)
C(33)-C(32)-C(42)-C(47)	122.8(2)
C(47)-C(42)-C(43)-C(44)	1.1(3)
C(32)-C(42)-C(43)-C(44)	-173.87(19)
C(42)-C(43)-C(44)-C(45)	-0.6(3)
C(43)-C(44)-C(45)-C(46)	-0.6(3)
C(43)-C(44)-C(45)-N(45)	177.31(19)
C(46)-C(45)-N(45)-O(45)	-178.7(2)
C(44)-C(45)-N(45)-O(45)	3.3(3)
C(46)-C(45)-N(45)-O(46)	2.5(3)
C(44)-C(45)-N(45)-O(46)	-175.5(2)
C(44)-C(45)-C(46)-C(47)	1.1(3)
N(45)-C(45)-C(46)-C(47)	-176.7(2)
C(45)-C(46)-C(47)-C(42)	-0.6(3)
C(43)-C(42)-C(47)-C(46)	-0.5(3)
C(32)-C(42)-C(47)-C(46)	174.4(2)
C(34)-C(33)-C(48)-C(53)	-142.3(3)
C(32)-C(33)-C(48)-C(53)	96.5(3)
C(34)-C(33)-C(48)-C(49)	35.4(3)
C(32)-C(33)-C(48)-C(49)	-85.8(3)
C(53)-C(48)-C(49)-C(50)	0.9(4)
C(33)-C(48)-C(49)-C(50)	-176.8(2)
C(48)-C(49)-C(50)-C(51)	0.4(3)
C(49)-C(50)-C(51)-C(52)	-1.4(3)
C(50)-C(51)-C(52)-C(53)	1.1(4)
C(49)-C(48)-C(53)-C(52)	-1.2(4)
C(33)-C(48)-C(53)-C(52)	176.5(2)
C(51)-C(52)-C(53)-C(48)	0.2(4)
O(102)-C(101)-O(101)-C(102)	77(2)
O(103)-C(101)-O(101)-C(102)	-163(2)
C(105)-C(101)-O(101)-C(102)	-44(3)
C(101)-O(101)-C(102)-C(112)	-165(2)

C(101)-O(101)-C(102)-C(103)	72(3)
O(103)-C(101)-O(102)-C(110)	-33(3)
O(101)-C(101)-O(102)-C(110)	79(2)
C(105)-C(101)-O(102)-C(110)	-163.0(19)
O(101)-C(102)-C(103)-C(104)	-63(3)
C(112)-C(102)-C(103)-C(104)	177(2)
O(101)-C(102)-C(103)-C(118)	67(2)
C(112)-C(102)-C(103)-C(118)	-53(2)
O(102)-C(101)-O(103)-C(111)	33(2)
O(101)-C(101)-O(103)-C(111)	-79(2)
C(105)-C(101)-O(103)-C(111)	164.4(18)
C(102)-C(103)-C(104)-C(105)	30(2)
C(118)-C(103)-C(104)-C(105)	-105.0(17)
C(102)-C(103)-C(104)-C(109)	-155.6(17)
C(118)-C(103)-C(104)-C(109)	69(2)
C(109)-C(104)-C(105)-C(106)	0.0
C(103)-C(104)-C(105)-C(106)	174(2)
C(109)-C(104)-C(105)-C(101)	-180(2)
C(103)-C(104)-C(105)-C(101)	-5(2)
O(102)-C(101)-C(105)-C(106)	76(2)
O(103)-C(101)-C(105)-C(106)	-55(2)
O(101)-C(101)-C(105)-C(106)	-169.0(17)
O(102)-C(101)-C(105)-C(104)	-104(2)
O(103)-C(101)-C(105)-C(104)	124.6(18)
O(101)-C(101)-C(105)-C(104)	11(3)
C(104)-C(105)-C(106)-C(107)	0.0
C(101)-C(105)-C(106)-C(107)	180(2)
C(105)-C(106)-C(107)-C(108)	0.0
C(106)-C(107)-C(108)-C(109)	0.0
C(107)-C(108)-C(109)-C(104)	0.0
C(105)-C(104)-C(109)-C(108)	0.0
C(103)-C(104)-C(109)-C(108)	-174(2)
C(101)-O(102)-C(110)-C(111)	15(3)
O(102)-C(110)-C(111)-O(103)	4(3)
C(101)-O(103)-C(111)-C(110)	-21(2)
O(101)-C(102)-C(112)-C(113)	171.1(16)

C(103)-C(102)-C(112)-C(113)	-70(2)
O(101)-C(102)-C(112)-C(117)	0(3)
C(103)-C(102)-C(112)-C(117)	119.4(17)
C(117)-C(112)-C(113)-C(114)	0.0
C(102)-C(112)-C(113)-C(114)	-170.8(15)
C(112)-C(113)-C(114)-C(115)	0.0
C(113)-C(114)-C(115)-C(116)	0.0
C(113)-C(114)-C(115)-N(115)	179.7(4)
C(114)-C(115)-C(116)-C(117)	0.0
N(115)-C(115)-C(116)-C(117)	-179.7(4)
C(115)-C(116)-C(117)-C(112)	0.0
C(113)-C(112)-C(117)-C(116)	0.0
C(102)-C(112)-C(117)-C(116)	170.6(16)
C(114)-C(115)-N(115)-O(115)	179.6(5)
C(116)-C(115)-N(115)-O(115)	-0.7(8)
C(114)-C(115)-N(115)-O(116)	0.7(10)
C(116)-C(115)-N(115)-O(116)	-179.6(7)
C(104)-C(103)-C(118)-C(119)	-141.0(17)
C(102)-C(103)-C(118)-C(119)	89(2)
C(104)-C(103)-C(118)-C(123)	47(2)
C(102)-C(103)-C(118)-C(123)	-83.0(19)
C(123)-C(118)-C(119)-C(120)	0.0
C(103)-C(118)-C(119)-C(120)	-172.1(17)
C(118)-C(119)-C(120)-C(121)	0.0
C(119)-C(120)-C(121)-C(122)	0.0
C(120)-C(121)-C(122)-C(123)	0.0
C(121)-C(122)-C(123)-C(118)	0.0
C(119)-C(118)-C(123)-C(122)	0.0
C(103)-C(118)-C(123)-C(122)	172.2(17)
O(133)-C(131)-O(131)-C(132)	-78(2)
O(132)-C(131)-O(131)-C(132)	164.7(19)
C(135)-C(131)-O(131)-C(132)	49(2)
O(133)-C(131)-O(132)-C(140)	-38(2)
O(131)-C(131)-O(132)-C(140)	80(2)
C(135)-C(131)-O(132)-C(140)	-159.0(17)
C(131)-O(131)-C(132)-C(142)	160.3(19)

C(131)-O(131)-C(132)-C(133)	-70(2)
O(131)-C(131)-O(133)-C(141)	-78(2)
O(132)-C(131)-O(133)-C(141)	36(2)
C(135)-C(131)-O(133)-C(141)	153.7(18)
O(131)-C(132)-C(133)-C(134)	56(3)
C(142)-C(132)-C(133)-C(134)	-179(2)
O(131)-C(132)-C(133)-C(148)	-71(2)
C(142)-C(132)-C(133)-C(148)	54(3)
C(132)-C(133)-C(134)-C(135)	-28(2)
C(148)-C(133)-C(134)-C(135)	99.3(16)
C(132)-C(133)-C(134)-C(139)	156.1(19)
C(148)-C(133)-C(134)-C(139)	-76.9(18)
C(139)-C(134)-C(135)-C(136)	0.0
C(133)-C(134)-C(135)-C(136)	-176.2(17)
C(139)-C(134)-C(135)-C(131)	-175(2)
C(133)-C(134)-C(135)-C(131)	9(2)
O(133)-C(131)-C(135)-C(136)	-66.9(19)
O(131)-C(131)-C(135)-C(136)	166.0(14)
O(132)-C(131)-C(135)-C(136)	52(2)
O(133)-C(131)-C(135)-C(134)	108.0(17)
O(131)-C(131)-C(135)-C(134)	-19(2)
O(132)-C(131)-C(135)-C(134)	-133.3(17)
C(134)-C(135)-C(136)-C(137)	0.0
C(131)-C(135)-C(136)-C(137)	175(2)
C(135)-C(136)-C(137)-C(138)	0.0
C(136)-C(137)-C(138)-C(139)	0.0
C(137)-C(138)-C(139)-C(134)	0.0
C(135)-C(134)-C(139)-C(138)	0.0
C(133)-C(134)-C(139)-C(138)	176.2(17)
C(131)-O(132)-C(140)-C(141)	26(3)
C(131)-O(133)-C(141)-C(140)	-17(3)
O(132)-C(140)-C(141)-O(133)	-6(3)
O(131)-C(132)-C(142)-C(143)	-172.5(15)
C(133)-C(132)-C(142)-C(143)	64(3)
O(131)-C(132)-C(142)-C(147)	3(3)
C(133)-C(132)-C(142)-C(147)	-121(2)

C(147)-C(142)-C(143)-C(144)	0.0
C(132)-C(142)-C(143)-C(144)	175.5(19)
C(142)-C(143)-C(144)-C(145)	0.0
C(143)-C(144)-C(145)-C(146)	0.0
C(143)-C(144)-C(145)-N(145)	179.8(18)
C(144)-C(145)-C(146)-C(147)	0.0
N(145)-C(145)-C(146)-C(147)	-179.8(19)
C(145)-C(146)-C(147)-C(142)	0.0
C(143)-C(142)-C(147)-C(146)	0.0
C(132)-C(142)-C(147)-C(146)	-175(2)
C(146)-C(145)-N(145)-O(146)	-2(3)
C(144)-C(145)-N(145)-O(146)	178.4(18)
C(146)-C(145)-N(145)-O(145)	-179.3(19)
C(144)-C(145)-N(145)-O(145)	1(3)
C(134)-C(133)-C(148)-C(149)	-38.3(18)
C(132)-C(133)-C(148)-C(149)	86.6(17)
C(134)-C(133)-C(148)-C(153)	143.2(14)
C(132)-C(133)-C(148)-C(153)	-91.9(17)
C(153)-C(148)-C(149)-C(150)	0.0
C(133)-C(148)-C(149)-C(150)	-178.5(15)
C(148)-C(149)-C(150)-C(151)	0.0
C(149)-C(150)-C(151)-C(152)	0.0
C(150)-C(151)-C(152)-C(153)	0.0
C(151)-C(152)-C(153)-C(148)	0.0
C(149)-C(148)-C(153)-C(152)	0.0
C(133)-C(148)-C(153)-C(152)	178.5(15)

Symmetry transformations used to generate equivalent atoms:

Table 7. Hydrogen bonds for JF2983FMI [Å and °].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
C(3^a)-H(3^a)...O(15^a)#1	1.00	2.60	3.412(3)	138.8
C(33^a)-H(33^a)...O(45^a)#2	1.00	2.59	3.432(3)	142.2
C(46^a)-H(46^a)...O(2^a)	0.95	2.52	3.441(3)	162.4
C(133^b)-H(133^b)...O(145^b)#3	1.00	2.61	3.42(2)	138.9

Symmetry transformations used to generate equivalent atoms:
#1 -x,-y+1,z+1/2 #2 -x+1,-y+2,z+1/2 #3 -x,-y+2,z+1/2

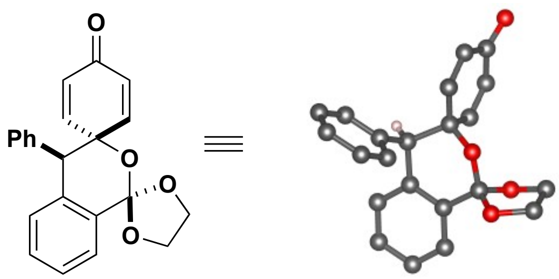


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Table 1. Crystal data and structure refinement for [$C_{22}H_{18}O_4$].

Identification code	JF2998FMI (MG-4-175)	
Empirical formula	C22 H18 O4	
Formula weight	346.36	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Orthorhombic	
Space group	Pbca	
Unit cell dimensions	a = 9.7117(6) Å	〈= 90°.
	b = 17.1656(11) Å	®= 90°.
	c = 19.8546(13) Å	© = 90°.
Volume	3309.9(4) $Å^3$	
Z	8	
Density (calculated)	1.390 Mg/m^3	
Absorption coefficient	0.095 mm^{-1}	
F(000)	1456	
Crystal size	0.395 x 0.170 x 0.150 mm^3	

Crystal color and habit	Yellow Block
Diffractometer	Bruker Photon100 CMOS
Theta range for data collection	2.051 to 27.496°.
Index ranges	-12<=h<=12, -22<=k<=22, -25<=l<=25
Reflections collected	28507
Independent reflections	3807 [R(int) = 0.0282]
Observed reflections (I > 2sigma(I))	3347
Completeness to theta = 25.242°	100.0 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.9873 and 0.9155
Solution method	SHELXT (Sheldrick, 2014)
Refinement method	SHELXL-2017/1 (Sheldrick, 2017) Full-matrix least-squares on F^2
Data / restraints / parameters	3807 / 0 / 308
Goodness-of-fit on F^2	1.041
Final R indices [I>2sigma(I)]	R1 = 0.0417, wR2 = 0.1076
R indices (all data)	R1 = 0.0476, wR2 = 0.1131
Extinction coefficient	0.0115(9)
Largest diff. peak and hole	0.383 and -0.324 e.Å^{-3}

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for JF2998FMI. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
C(1)	2203(1)	5023(1)	5957(1)	19(1)
O(1)	3628(1)	5102(1)	5816(1)	19(1)
C(2)	4572(1)	4861(1)	6343(1)	19(1)
O(2)	1559(1)	5088(1)	5329(1)	21(1)
C(3)	4387(1)	3972(1)	6477(1)	19(1)
O(3)	1715(1)	5642(1)	6351(1)	21(1)
C(4)	2867(1)	3778(1)	6555(1)	18(1)
C(5)	1848(1)	4266(1)	6303(1)	18(1)
C(6)	1256(2)	5904(1)	5225(1)	27(1)
C(7)	1557(2)	6290(1)	5899(1)	26(1)
C(8)	4310(1)	5302(1)	6990(1)	21(1)
C(9)	5180(2)	5816(1)	7249(1)	23(1)
C(10)	6485(2)	6012(1)	6912(1)	25(1)
O(10)	7226(1)	6546(1)	7110(1)	36(1)
C(11)	6843(1)	5548(1)	6311(1)	24(1)
C(12)	5961(1)	5041(1)	6043(1)	22(1)
C(13)	5033(1)	3446(1)	5948(1)	18(1)
C(14)	6084(1)	2935(1)	6131(1)	21(1)
C(15)	6666(1)	2436(1)	5658(1)	24(1)
C(16)	6213(1)	2441(1)	4997(1)	24(1)
C(17)	5171(1)	2952(1)	4810(1)	24(1)
C(18)	4575(1)	3447(1)	5281(1)	22(1)
C(19)	2482(1)	3080(1)	6870(1)	22(1)
C(20)	1107(2)	2879(1)	6929(1)	25(1)
C(21)	89(1)	3376(1)	6683(1)	25(1)
C(22)	458(1)	4070(1)	6375(1)	22(1)

Table 3. Bond lengths [Å] and angles [°] for JF2998FMI.

C(1)-O(2)	1.3983(15)
C(1)-O(3)	1.4016(15)
C(1)-O(1)	1.4178(15)
C(1)-C(5)	1.5106(17)
O(1)-C(2)	1.4509(15)
C(2)-C(12)	1.5065(18)
C(2)-C(8)	1.5123(17)
C(2)-C(3)	1.5602(17)
O(2)-C(6)	1.4475(16)
C(3)-C(13)	1.5209(17)
C(3)-C(4)	1.5209(17)
C(3)-H(3)	0.971(16)
O(3)-C(7)	1.4371(16)
C(4)-C(5)	1.3898(18)
C(4)-C(19)	1.4023(18)
C(5)-C(22)	1.3981(18)
C(6)-C(7)	1.521(2)
C(6)-H(6A)	0.968(19)
C(6)-H(6B)	1.00(2)
C(7)-H(7A)	0.987(19)
C(7)-H(7B)	0.96(2)
C(8)-C(9)	1.3265(19)
C(8)-H(8)	0.967(18)
C(9)-C(10)	1.472(2)
C(9)-H(9)	0.962(18)
C(10)-O(10)	1.2293(17)
C(10)-C(11)	1.475(2)
C(11)-C(12)	1.3327(19)
C(11)-H(11)	0.967(17)
C(12)-H(12)	0.960(18)
C(13)-C(14)	1.3928(17)
C(13)-C(18)	1.3977(18)
C(14)-C(15)	1.3910(19)
C(14)-H(14)	0.959(17)

C(15)-C(16)	1.385(2)
C(15)-H(15)	0.969(19)
C(16)-C(17)	1.3895(19)
C(16)-H(16)	0.941(16)
C(17)-C(18)	1.3890(19)
C(17)-H(17)	0.957(17)
C(18)-H(18)	0.967(18)
C(19)-C(20)	1.384(2)
C(19)-H(19)	0.966(17)
C(20)-C(21)	1.394(2)
C(20)-H(20)	0.968(17)
C(21)-C(22)	1.3858(19)
C(21)-H(21)	0.95(2)
C(22)-H(22)	0.970(17)

O(2)-C(1)-O(3)	106.65(10)
O(2)-C(1)-O(1)	104.72(10)
O(3)-C(1)-O(1)	111.53(10)
O(2)-C(1)-C(5)	111.78(10)
O(3)-C(1)-C(5)	108.70(10)
O(1)-C(1)-C(5)	113.24(10)
C(1)-O(1)-C(2)	116.63(9)
O(1)-C(2)-C(12)	102.82(10)
O(1)-C(2)-C(8)	111.31(10)
C(12)-C(2)-C(8)	112.67(11)
O(1)-C(2)-C(3)	109.16(10)
C(12)-C(2)-C(3)	111.78(10)
C(8)-C(2)-C(3)	108.96(10)
C(1)-O(2)-C(6)	107.16(10)
C(13)-C(3)-C(4)	109.97(10)
C(13)-C(3)-C(2)	114.61(10)
C(4)-C(3)-C(2)	110.09(10)
C(13)-C(3)-H(3)	108.5(9)
C(4)-C(3)-H(3)	107.8(9)
C(2)-C(3)-H(3)	105.6(9)
C(1)-O(3)-C(7)	105.86(10)

C(5)-C(4)-C(19)	119.05(12)
C(5)-C(4)-C(3)	121.50(11)
C(19)-C(4)-C(3)	119.42(11)
C(4)-C(5)-C(22)	120.34(12)
C(4)-C(5)-C(1)	121.31(11)
C(22)-C(5)-C(1)	118.34(11)
O(2)-C(6)-C(7)	104.82(11)
O(2)-C(6)-H(6A)	107.2(11)
C(7)-C(6)-H(6A)	112.3(11)
O(2)-C(6)-H(6B)	108.3(11)
C(7)-C(6)-H(6B)	110.6(11)
H(6A)-C(6)-H(6B)	113.1(15)
O(3)-C(7)-C(6)	103.51(11)
O(3)-C(7)-H(7A)	107.5(10)
C(6)-C(7)-H(7A)	113.6(10)
O(3)-C(7)-H(7B)	108.7(12)
C(6)-C(7)-H(7B)	114.4(12)
H(7A)-C(7)-H(7B)	108.8(15)
C(9)-C(8)-C(2)	123.63(13)
C(9)-C(8)-H(8)	119.5(10)
C(2)-C(8)-H(8)	116.9(10)
C(8)-C(9)-C(10)	121.66(13)
C(8)-C(9)-H(9)	122.9(10)
C(10)-C(9)-H(9)	115.4(10)
O(10)-C(10)-C(9)	121.88(14)
O(10)-C(10)-C(11)	121.50(14)
C(9)-C(10)-C(11)	116.59(12)
C(12)-C(11)-C(10)	121.60(13)
C(12)-C(11)-H(11)	122.6(10)
C(10)-C(11)-H(11)	115.8(10)
C(11)-C(12)-C(2)	123.43(13)
C(11)-C(12)-H(12)	120.5(11)
C(2)-C(12)-H(12)	116.0(11)
C(14)-C(13)-C(18)	118.76(12)
C(14)-C(13)-C(3)	119.78(11)
C(18)-C(13)-C(3)	121.45(11)

C(15)-C(14)-C(13)	120.65(12)
C(15)-C(14)-H(14)	120.6(10)
C(13)-C(14)-H(14)	118.7(10)
C(16)-C(15)-C(14)	120.43(12)
C(16)-C(15)-H(15)	120.7(10)
C(14)-C(15)-H(15)	118.9(10)
C(15)-C(16)-C(17)	119.22(12)
C(15)-C(16)-H(16)	121.6(10)
C(17)-C(16)-H(16)	119.2(10)
C(18)-C(17)-C(16)	120.69(13)
C(18)-C(17)-H(17)	118.8(10)
C(16)-C(17)-H(17)	120.5(10)
C(17)-C(18)-C(13)	120.25(12)
C(17)-C(18)-H(18)	119.5(10)
C(13)-C(18)-H(18)	120.2(10)
C(20)-C(19)-C(4)	120.53(12)
C(20)-C(19)-H(19)	119.2(10)
C(4)-C(19)-H(19)	120.2(10)
C(19)-C(20)-C(21)	120.12(12)
C(19)-C(20)-H(20)	118.5(10)
C(21)-C(20)-H(20)	121.3(10)
C(22)-C(21)-C(20)	119.81(13)
C(22)-C(21)-H(21)	119.8(11)
C(20)-C(21)-H(21)	120.4(11)
C(21)-C(22)-C(5)	120.12(13)
C(21)-C(22)-H(22)	120.9(10)
C(5)-C(22)-H(22)	119.0(10)

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($Å^2$x 10^3) for JF2998FMI. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2 a^{*2}U^{11} + ... + 2 h k a^* b^* U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
C(1)	18(1)	20(1)	18(1)	-2(1)	0(1)	0(1)
O(1)	19(1)	20(1)	18(1)	1(1)	0(1)	0(1)
C(2)	18(1)	19(1)	20(1)	-1(1)	-1(1)	0(1)
O(2)	25(1)	20(1)	19(1)	0(1)	-4(1)	2(1)
C(3)	20(1)	19(1)	17(1)	0(1)	-2(1)	0(1)
O(3)	24(1)	18(1)	20(1)	-2(1)	2(1)	3(1)
C(4)	22(1)	18(1)	15(1)	-3(1)	1(1)	0(1)
C(5)	21(1)	19(1)	16(1)	-2(1)	1(1)	0(1)
C(6)	33(1)	21(1)	27(1)	3(1)	-5(1)	2(1)
C(7)	31(1)	20(1)	28(1)	0(1)	-1(1)	4(1)
C(8)	23(1)	20(1)	20(1)	0(1)	-2(1)	3(1)
C(9)	30(1)	19(1)	21(1)	-1(1)	-6(1)	2(1)
C(10)	29(1)	20(1)	27(1)	5(1)	-11(1)	-2(1)
O(10)	44(1)	28(1)	36(1)	2(1)	-11(1)	-14(1)
C(11)	21(1)	20(1)	33(1)	5(1)	-3(1)	0(1)
C(12)	21(1)	19(1)	25(1)	2(1)	1(1)	2(1)
C(13)	18(1)	16(1)	21(1)	-1(1)	0(1)	-2(1)
C(14)	20(1)	21(1)	22(1)	2(1)	-1(1)	0(1)
C(15)	22(1)	20(1)	31(1)	4(1)	4(1)	3(1)
C(16)	23(1)	19(1)	29(1)	-4(1)	6(1)	-2(1)
C(17)	24(1)	27(1)	21(1)	-4(1)	0(1)	-1(1)
C(18)	21(1)	23(1)	23(1)	-2(1)	-2(1)	2(1)
C(19)	29(1)	20(1)	17(1)	-1(1)	0(1)	0(1)
C(20)	33(1)	22(1)	19(1)	-1(1)	4(1)	-7(1)
C(21)	24(1)	29(1)	21(1)	-3(1)	3(1)	-7(1)
C(22)	22(1)	26(1)	19(1)	-3(1)	1(1)	-1(1)

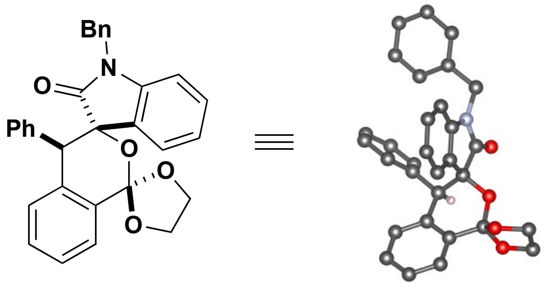
Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for JF2998FMI.

	x	y	z	U(eq)
H(3)	4833(16)	3873(9)	6906(8)	18(4)
H(6A)	290(20)	5942(11)	5101(9)	35(5)
H(6B)	1890(20)	6107(11)	4870(10)	41(5)
H(7A)	2428(19)	6586(10)	5905(9)	30(4)
H(7B)	830(20)	6619(11)	6064(10)	38(5)
H(8)	3470(18)	5179(9)	7230(9)	24(4)
H(9)	4997(17)	6097(10)	7658(9)	28(4)
H(11)	7741(17)	5649(9)	6119(8)	22(4)
H(12)	6175(18)	4780(10)	5628(9)	28(4)
H(14)	6396(17)	2933(10)	6589(9)	26(4)
H(15)	7383(19)	2080(11)	5801(9)	32(4)
H(16)	6591(16)	2105(9)	4671(8)	21(4)
H(17)	4845(17)	2966(10)	4356(9)	27(4)
H(18)	3838(18)	3791(10)	5144(8)	27(4)
H(19)	3175(17)	2736(9)	7052(8)	21(4)
H(20)	876(17)	2388(10)	7141(8)	26(4)
H(21)	-850(20)	3244(11)	6729(9)	36(5)
H(22)	-238(17)	4426(10)	6208(9)	25(4)

Table 6. Torsion angles [°] for JF2998FMI.

O(2)-C(1)-O(1)-C(2)	-164.55(9)
O(3)-C(1)-O(1)-C(2)	80.47(12)
C(5)-C(1)-O(1)-C(2)	-42.52(14)
C(1)-O(1)-C(2)-C(12)	-178.44(10)
C(1)-O(1)-C(2)-C(8)	-57.58(14)
C(1)-O(1)-C(2)-C(3)	62.74(13)
O(3)-C(1)-O(2)-C(6)	28.17(13)
O(1)-C(1)-O(2)-C(6)	-90.17(11)
C(5)-C(1)-O(2)-C(6)	146.85(11)
O(1)-C(2)-C(3)-C(13)	76.28(13)
C(12)-C(2)-C(3)-C(13)	-36.79(15)
C(8)-C(2)-C(3)-C(13)	-161.97(10)
O(1)-C(2)-C(3)-C(4)	-48.31(13)
C(12)-C(2)-C(3)-C(4)	-161.37(10)
C(8)-C(2)-C(3)-C(4)	73.44(12)
O(2)-C(1)-O(3)-C(7)	-36.21(13)
O(1)-C(1)-O(3)-C(7)	77.57(12)
C(5)-C(1)-O(3)-C(7)	-156.89(10)
C(13)-C(3)-C(4)-C(5)	-106.29(13)
C(2)-C(3)-C(4)-C(5)	20.92(16)
C(13)-C(3)-C(4)-C(19)	71.67(14)
C(2)-C(3)-C(4)-C(19)	-161.12(11)
C(19)-C(4)-C(5)-C(22)	1.31(18)
C(3)-C(4)-C(5)-C(22)	179.27(11)
C(19)-C(4)-C(5)-C(1)	-179.79(11)
C(3)-C(4)-C(5)-C(1)	-1.83(18)
O(2)-C(1)-C(5)-C(4)	128.56(12)
O(3)-C(1)-C(5)-C(4)	-113.98(12)
O(1)-C(1)-C(5)-C(4)	10.56(16)
O(2)-C(1)-C(5)-C(22)	-52.51(15)
O(3)-C(1)-C(5)-C(22)	64.95(14)
O(1)-C(1)-C(5)-C(22)	-170.51(11)
C(1)-O(2)-C(6)-C(7)	-9.49(14)
C(1)-O(3)-C(7)-C(6)	28.81(14)

O(2)-C(6)-C(7)-O(3)	-11.73(14)
O(1)-C(2)-C(8)-C(9)	-112.00(14)
C(12)-C(2)-C(8)-C(9)	2.90(18)
C(3)-C(2)-C(8)-C(9)	127.56(13)
C(2)-C(8)-C(9)-C(10)	1.0(2)
C(8)-C(9)-C(10)-O(10)	172.12(13)
C(8)-C(9)-C(10)-C(11)	-6.15(19)
O(10)-C(10)-C(11)-C(12)	-170.83(13)
C(9)-C(10)-C(11)-C(12)	7.44(19)
C(10)-C(11)-C(12)-C(2)	-3.6(2)
O(1)-C(2)-C(12)-C(11)	118.36(13)
C(8)-C(2)-C(12)-C(11)	-1.57(18)
C(3)-C(2)-C(12)-C(11)	-124.68(13)
C(4)-C(3)-C(13)-C(14)	-117.53(12)
C(2)-C(3)-C(13)-C(14)	117.82(13)
C(4)-C(3)-C(13)-C(18)	60.93(15)
C(2)-C(3)-C(13)-C(18)	-63.72(16)
C(18)-C(13)-C(14)-C(15)	-0.10(19)
C(3)-C(13)-C(14)-C(15)	178.41(12)
C(13)-C(14)-C(15)-C(16)	0.4(2)
C(14)-C(15)-C(16)-C(17)	0.0(2)
C(15)-C(16)-C(17)-C(18)	-0.7(2)
C(16)-C(17)-C(18)-C(13)	1.0(2)
C(14)-C(13)-C(18)-C(17)	-0.55(19)
C(3)-C(13)-C(18)-C(17)	-179.03(12)
C(5)-C(4)-C(19)-C(20)	0.00(18)
C(3)-C(4)-C(19)-C(20)	-178.00(11)
C(4)-C(19)-C(20)-C(21)	-0.88(19)
C(19)-C(20)-C(21)-C(22)	0.5(2)
C(20)-C(21)-C(22)-C(5)	0.85(19)
C(4)-C(5)-C(22)-C(21)	-1.74(19)
C(1)-C(5)-C(22)-C(21)	179.32(11)



CCDC 2087130

Table 1. Crystal data and structure refinement for [$C_{31}H_{25}NO_4$].

Identification code	JF2999FMI (MG-4-165)	
Empirical formula	C31 H25 N O4	
Formula weight	475.52	
Temperature	90(2) K	
Wavelength	1.54178 Å	
Crystal system	Triclinic	
Space group	P-1	
Unit cell dimensions	a = 10.2681(8) Å	〈= 75.214(3)°.
	b = 13.4445(10) Å	®= 78.879(3)°.
	c = 18.5225(14) Å	© = 68.820(2)°.
Volume	2290.9(3) $Å^3$	
Z, Z'	4, 2	
Density (calculated)	1.379 Mg/m^3	
Absorption coefficient	0.732 mm^{-1}	
F(000)	1000	
Crystal size	0.271 x 0.184 x 0.056 mm^3	
Crystal color and habit	Pale Yellow Block	
Diffractometer	Bruker Duo APEXII CCD	
Theta range for data collection	2.483 to 67.903°.	
Index ranges	-12<=h<=12, -16<=k<=16, -22<=l<=22	
Reflections collected	14547	
Independent reflections	7860 [R(int) = 0.0144]	
Observed reflections (I > 2sigma(I))	7357	
Completeness to theta = 67.679°	94.3 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.9126 and 0.8432	
Solution method	SHELXT (Sheldrick, 2014)	

Refinement method	SHELXL-2017/1 (Sheldrick, 2017) Full-matrix least-squares on F^2
Data / restraints / parameters	7860 / 0 / 850
Goodness-of-fit on F^2	1.045
Final R indices [I>2sigma(I)]	R1 = 0.0328, wR2 = 0.0875
R indices (all data)	R1 = 0.0347, wR2 = 0.0893
Extinction coefficient	0.00103(12)
Largest diff. peak and hole	0.228 and -0.248 e.Å^{-3}

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for JF2999FMI. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
C(1)	3219(1)	8214(1)	3208(1)	18(1)
O(1)	2960(1)	8386(1)	2447(1)	21(1)
C(2)	1630(1)	9102(1)	2240(1)	19(1)
O(2)	1759(1)	10110(1)	1843(1)	23(1)
C(3)	484(1)	9278(1)	2888(1)	20(1)
O(3)	1291(1)	8658(1)	1721(1)	23(1)
C(4)	684(1)	8627(1)	3605(1)	19(1)
C(5)	2098(1)	7740(1)	3713(1)	18(1)
C(6)	4707(1)	7354(1)	3265(1)	19(1)
N(6)	5461(1)	7734(1)	3596(1)	19(1)
O(6)	5113(1)	6489(1)	3062(1)	24(1)
C(7)	4707(1)	8806(1)	3692(1)	19(1)
C(8)	3379(1)	9158(1)	3449(1)	19(1)
C(9)	2390(2)	9935(1)	1105(1)	31(1)
C(10)	1755(2)	9146(1)	981(1)	36(1)
C(11)	-771(1)	10127(1)	2762(1)	23(1)
C(12)	-1834(1)	10335(1)	3348(1)	25(1)
C(13)	-1636(1)	9695(1)	4062(1)	24(1)
C(14)	-395(1)	8841(1)	4189(1)	22(1)
C(15)	2432(1)	7242(1)	4515(1)	19(1)
C(16)	2266(1)	7862(1)	5050(1)	21(1)
C(17)	2617(1)	7353(1)	5772(1)	24(1)
C(18)	3164(1)	6225(1)	5968(1)	24(1)
C(19)	3341(1)	5607(1)	5442(1)	24(1)
C(20)	2965(1)	6112(1)	4724(1)	22(1)
C(21)	2486(1)	10205(1)	3492(1)	21(1)
C(22)	2941(1)	10877(1)	3774(1)	25(1)
C(23)	4262(1)	10504(1)	4018(1)	25(1)
C(24)	5166(1)	9451(1)	3985(1)	23(1)
C(25)	6949(1)	7198(1)	3690(1)	21(1)
C(26)	7278(1)	6884(1)	4499(1)	20(1)

C(27)	6240(1)	6895(1)	5105(1)	22(1)
C(28)	6595(1)	6572(1)	5838(1)	23(1)
C(29)	7987(1)	6232(1)	5969(1)	23(1)
C(30)	9029(1)	6217(1)	5366(1)	24(1)
C(31)	8678(1)	6544(1)	4635(1)	22(1)
C(41)	-592(1)	6880(1)	1602(1)	18(1)
O(41)	-1566(1)	7908(1)	1725(1)	22(1)
C(42)	-2719(1)	8416(1)	1295(1)	19(1)
O(42)	-2486(1)	9308(1)	762(1)	24(1)
C(43)	-3035(1)	7681(1)	908(1)	19(1)
O(43)	-3879(1)	8861(1)	1791(1)	24(1)
C(44)	-2432(1)	6549(1)	1105(1)	18(1)
C(45)	-1454(1)	6099(1)	1715(1)	18(1)
C(46)	398(1)	6469(1)	2230(1)	18(1)
N(46)	1749(1)	6154(1)	1893(1)	17(1)
O(46)	33(1)	6407(1)	2896(1)	25(1)
C(47)	1795(1)	6432(1)	1107(1)	17(1)
C(48)	432(1)	6901(1)	895(1)	18(1)
C(49)	-2737(2)	10118(1)	1195(1)	30(1)
C(50)	-3923(2)	9940(1)	1785(1)	36(1)
C(51)	-3938(1)	8148(1)	349(1)	21(1)
C(52)	-4234(1)	7495(1)	-23(1)	22(1)
C(53)	-3633(1)	6370(1)	167(1)	22(1)
C(54)	-2750(1)	5902(1)	730(1)	20(1)
C(55)	-582(1)	4903(1)	1804(1)	18(1)
C(56)	-629(1)	4237(1)	2513(1)	22(1)
C(57)	113(1)	3126(1)	2626(1)	25(1)
C(58)	919(1)	2668(1)	2028(1)	24(1)
C(59)	1000(1)	3328(1)	1321(1)	22(1)
C(60)	259(1)	4440(1)	1205(1)	19(1)
C(61)	2980(1)	6294(1)	592(1)	21(1)
C(62)	2780(1)	6659(1)	-167(1)	22(1)
C(63)	1438(1)	7149(1)	-391(1)	22(1)
C(64)	256(1)	7273(1)	141(1)	21(1)
C(65)	2981(1)	5792(1)	2294(1)	19(1)
C(66)	3994(1)	4684(1)	2187(1)	18(1)

C(67)	5426(1)	4448(1)	2210(1)	19(1)
C(68)	6361(1)	3411(1)	2164(1)	22(1)
C(69)	5875(1)	2610(1)	2088(1)	23(1)
C(70)	4450(1)	2843(1)	2058(1)	22(1)
C(71)	3516(1)	3877(1)	2105(1)	20(1)

Table 3. Bond lengths [Å] and angles [°] for JF2999FMI.

C(1)-O(1)	1.4305(14)
C(1)-C(8)	1.5184(16)
C(1)-C(6)	1.5512(16)
C(1)-C(5)	1.5543(16)
O(1)-C(2)	1.4147(14)
C(2)-O(3)	1.4060(14)
C(2)-O(2)	1.4069(14)
C(2)-C(3)	1.5102(17)
O(2)-C(9)	1.4343(17)
C(3)-C(11)	1.3910(17)
C(3)-C(4)	1.3970(17)
O(3)-C(10)	1.4317(18)
C(4)-C(14)	1.3954(17)
C(4)-C(5)	1.5188(16)
C(5)-C(15)	1.5145(17)
C(5)-H(5)	0.982(14)
C(6)-O(6)	1.2174(14)
C(6)-N(6)	1.3646(16)
N(6)-C(7)	1.4076(15)
N(6)-C(25)	1.4582(15)
C(7)-C(24)	1.3798(17)
C(7)-C(8)	1.3954(16)
C(8)-C(21)	1.3880(16)
C(9)-C(10)	1.512(2)
C(9)-H(9A)	1.047(18)
C(9)-H(9B)	0.997(17)
C(10)-H(10A)	1.05(2)
C(10)-H(10B)	0.96(2)
C(11)-C(12)	1.3870(18)
C(11)-H(11)	1.001(16)
C(12)-C(13)	1.3896(19)
C(12)-H(12)	0.978(15)
C(13)-C(14)	1.3849(18)
C(13)-H(13)	0.985(15)

C(14)-H(14)	1.003(15)
C(15)-C(20)	1.3929(17)
C(15)-C(16)	1.3987(17)
C(16)-C(17)	1.3895(18)
C(16)-H(16)	0.969(15)
C(17)-C(18)	1.3889(18)
C(17)-H(17)	0.975(15)
C(18)-C(19)	1.3828(19)
C(18)-H(18)	0.978(16)
C(19)-C(20)	1.3875(18)
C(19)-H(19)	0.976(16)
C(20)-H(20)	1.000(15)
C(21)-C(22)	1.3953(18)
C(21)-H(21)	0.992(15)
C(22)-C(23)	1.3871(18)
C(22)-H(22)	0.958(16)
C(23)-C(24)	1.3936(18)
C(23)-H(23)	0.965(16)
C(24)-H(24)	0.967(15)
C(25)-C(26)	1.5183(17)
C(25)-H(25A)	0.968(16)
C(25)-H(25B)	0.979(15)
C(26)-C(27)	1.3898(17)
C(26)-C(31)	1.3953(17)
C(27)-C(28)	1.3926(18)
C(27)-H(27)	0.990(15)
C(28)-C(29)	1.3851(18)
C(28)-H(28)	0.978(16)
C(29)-C(30)	1.3885(19)
C(29)-H(29)	0.955(16)
C(30)-C(31)	1.3872(18)
C(30)-H(30)	0.985(16)
C(31)-H(31)	0.982(15)
C(41)-O(41)	1.4271(13)
C(41)-C(48)	1.5140(16)
C(41)-C(46)	1.5529(15)

C(41)-C(45)	1.5558(16)
O(41)-C(42)	1.4163(14)
C(42)-O(43)	1.4014(14)
C(42)-O(42)	1.4078(14)
C(42)-C(43)	1.5105(17)
O(42)-C(49)	1.4341(15)
C(43)-C(51)	1.3935(17)
C(43)-C(44)	1.3977(16)
O(43)-C(50)	1.4315(16)
C(44)-C(54)	1.3950(17)
C(44)-C(45)	1.5168(16)
C(45)-C(55)	1.5153(15)
C(45)-H(45)	0.979(15)
C(46)-O(46)	1.2092(15)
C(46)-N(46)	1.3680(15)
N(46)-C(47)	1.4022(15)
N(46)-C(65)	1.4572(14)
C(47)-C(61)	1.3804(17)
C(47)-C(48)	1.3988(16)
C(48)-C(64)	1.3825(17)
C(49)-C(50)	1.516(2)
C(49)-H(49A)	0.995(16)
C(49)-H(49B)	1.014(17)
C(50)-H(50A)	0.98(2)
C(50)-H(50B)	1.05(2)
C(51)-C(52)	1.3858(18)
C(51)-H(51)	0.988(14)
C(52)-C(53)	1.3887(18)
C(52)-H(52)	0.986(15)
C(53)-C(54)	1.3872(17)
C(53)-H(53)	0.981(16)
C(54)-H(54)	0.969(15)
C(55)-C(56)	1.3916(18)
C(55)-C(60)	1.3988(17)
C(56)-C(57)	1.3914(17)
C(56)-H(56)	0.980(15)

C(57)-C(58)	1.3837(19)
C(57)-H(57)	0.966(17)
C(58)-C(59)	1.3887(19)
C(58)-H(58)	0.949(16)
C(59)-C(60)	1.3916(17)
C(59)-H(59)	0.991(16)
C(60)-H(60)	0.978(15)
C(61)-C(62)	1.3954(18)
C(61)-H(61)	0.981(15)
C(62)-C(63)	1.3886(18)
C(62)-H(62)	0.967(15)
C(63)-C(64)	1.3964(18)
C(63)-H(63)	0.960(16)
C(64)-H(64)	0.974(16)
C(65)-C(66)	1.5146(15)
C(65)-H(65A)	0.995(15)
C(65)-H(65B)	0.965(15)
C(66)-C(71)	1.3920(17)
C(66)-C(67)	1.3943(17)
C(67)-C(68)	1.3909(17)
C(67)-H(67)	0.976(15)
C(68)-C(69)	1.3859(18)
C(68)-H(68)	0.968(15)
C(69)-C(70)	1.3901(18)
C(69)-H(69)	0.977(15)
C(70)-C(71)	1.3873(17)
C(70)-H(70)	0.993(15)
C(71)-H(71)	0.956(15)

O(1)-C(1)-C(8)	116.97(9)
O(1)-C(1)-C(6)	105.24(9)
C(8)-C(1)-C(6)	102.22(9)
O(1)-C(1)-C(5)	106.89(9)
C(8)-C(1)-C(5)	114.67(9)
C(6)-C(1)-C(5)	110.29(9)
C(2)-O(1)-C(1)	117.70(9)

O(3)-C(2)-O(2)	105.90(9)
O(3)-C(2)-O(1)	105.85(9)
O(2)-C(2)-O(1)	109.16(9)
O(3)-C(2)-C(3)	111.16(9)
O(2)-C(2)-C(3)	109.66(9)
O(1)-C(2)-C(3)	114.70(10)
C(2)-O(2)-C(9)	105.01(9)
C(11)-C(3)-C(4)	120.40(11)
C(11)-C(3)-C(2)	118.45(11)
C(4)-C(3)-C(2)	121.13(10)
C(2)-O(3)-C(10)	108.19(10)
C(14)-C(4)-C(3)	118.88(11)
C(14)-C(4)-C(5)	123.20(11)
C(3)-C(4)-C(5)	117.88(11)
C(15)-C(5)-C(4)	116.84(10)
C(15)-C(5)-C(1)	113.81(9)
C(4)-C(5)-C(1)	106.30(9)
C(15)-C(5)-H(5)	107.0(8)
C(4)-C(5)-H(5)	107.1(8)
C(1)-C(5)-H(5)	105.0(8)
O(6)-C(6)-N(6)	126.48(11)
O(6)-C(6)-C(1)	125.73(10)
N(6)-C(6)-C(1)	107.78(9)
C(6)-N(6)-C(7)	111.03(9)
C(6)-N(6)-C(25)	124.25(10)
C(7)-N(6)-C(25)	123.54(10)
C(24)-C(7)-C(8)	122.72(11)
C(24)-C(7)-N(6)	126.66(11)
C(8)-C(7)-N(6)	110.61(10)
C(21)-C(8)-C(7)	118.96(11)
C(21)-C(8)-C(1)	133.25(11)
C(7)-C(8)-C(1)	107.73(10)
O(2)-C(9)-C(10)	102.70(11)
O(2)-C(9)-H(9A)	109.6(9)
C(10)-C(9)-H(9A)	111.9(9)
O(2)-C(9)-H(9B)	109.0(10)

C(10)-C(9)-H(9B)	115.1(10)
H(9A)-C(9)-H(9B)	108.3(13)
O(3)-C(10)-C(9)	104.56(11)
O(3)-C(10)-H(10A)	109.0(11)
C(9)-C(10)-H(10A)	112.2(11)
O(3)-C(10)-H(10B)	110.5(12)
C(9)-C(10)-H(10B)	112.2(12)
H(10A)-C(10)-H(10B)	108.4(16)
C(12)-C(11)-C(3)	120.20(12)
C(12)-C(11)-H(11)	122.1(9)
C(3)-C(11)-H(11)	117.7(9)
C(11)-C(12)-C(13)	119.65(12)
C(11)-C(12)-H(12)	120.2(9)
C(13)-C(12)-H(12)	120.1(9)
C(14)-C(13)-C(12)	120.32(12)
C(14)-C(13)-H(13)	119.0(9)
C(12)-C(13)-H(13)	120.7(9)
C(13)-C(14)-C(4)	120.54(12)
C(13)-C(14)-H(14)	119.5(8)
C(4)-C(14)-H(14)	120.0(8)
C(20)-C(15)-C(16)	118.41(11)
C(20)-C(15)-C(5)	118.31(11)
C(16)-C(15)-C(5)	123.26(10)
C(17)-C(16)-C(15)	120.37(11)
C(17)-C(16)-H(16)	119.5(9)
C(15)-C(16)-H(16)	120.2(9)
C(18)-C(17)-C(16)	120.46(12)
C(18)-C(17)-H(17)	119.8(9)
C(16)-C(17)-H(17)	119.7(9)
C(19)-C(18)-C(17)	119.53(12)
C(19)-C(18)-H(18)	121.3(9)
C(17)-C(18)-H(18)	119.2(9)
C(18)-C(19)-C(20)	120.14(12)
C(18)-C(19)-H(19)	119.6(9)
C(20)-C(19)-H(19)	120.3(9)
C(19)-C(20)-C(15)	121.08(12)

C(19)-C(20)-H(20)	121.2(8)
C(15)-C(20)-H(20)	117.7(8)
C(8)-C(21)-C(22)	119.14(11)
C(8)-C(21)-H(21)	121.3(8)
C(22)-C(21)-H(21)	119.6(8)
C(23)-C(22)-C(21)	120.77(11)
C(23)-C(22)-H(22)	119.0(9)
C(21)-C(22)-H(22)	120.2(9)
C(22)-C(23)-C(24)	120.77(11)
C(22)-C(23)-H(23)	119.7(9)
C(24)-C(23)-H(23)	119.5(9)
C(7)-C(24)-C(23)	117.61(11)
C(7)-C(24)-H(24)	119.6(9)
C(23)-C(24)-H(24)	122.8(9)
N(6)-C(25)-C(26)	114.55(10)
N(6)-C(25)-H(25A)	107.5(9)
C(26)-C(25)-H(25A)	110.5(9)
N(6)-C(25)-H(25B)	105.8(8)
C(26)-C(25)-H(25B)	110.4(8)
H(25A)-C(25)-H(25B)	107.8(12)
C(27)-C(26)-C(31)	119.11(11)
C(27)-C(26)-C(25)	122.35(11)
C(31)-C(26)-C(25)	118.51(11)
C(26)-C(27)-C(28)	120.36(11)
C(26)-C(27)-H(27)	118.4(9)
C(28)-C(27)-H(27)	121.2(9)
C(29)-C(28)-C(27)	120.23(12)
C(29)-C(28)-H(28)	120.0(9)
C(27)-C(28)-H(28)	119.8(9)
C(28)-C(29)-C(30)	119.66(12)
C(28)-C(29)-H(29)	120.6(9)
C(30)-C(29)-H(29)	119.7(9)
C(31)-C(30)-C(29)	120.24(12)
C(31)-C(30)-H(30)	119.1(9)
C(29)-C(30)-H(30)	120.7(9)
C(30)-C(31)-C(26)	120.39(12)

C(30)-C(31)-H(31)	121.5(9)
C(26)-C(31)-H(31)	118.1(9)
O(41)-C(41)-C(48)	116.34(9)
O(41)-C(41)-C(46)	105.94(9)
C(48)-C(41)-C(46)	102.19(9)
O(41)-C(41)-C(45)	106.97(9)
C(48)-C(41)-C(45)	115.74(9)
C(46)-C(41)-C(45)	108.95(9)
C(42)-O(41)-C(41)	118.62(9)
O(43)-C(42)-O(42)	105.90(9)
O(43)-C(42)-O(41)	106.02(9)
O(42)-C(42)-O(41)	108.74(9)
O(43)-C(42)-C(43)	110.57(9)
O(42)-C(42)-C(43)	109.87(10)
O(41)-C(42)-C(43)	115.29(9)
C(42)-O(42)-C(49)	104.11(9)
C(51)-C(43)-C(44)	120.38(11)
C(51)-C(43)-C(42)	118.95(10)
C(44)-C(43)-C(42)	120.66(11)
C(42)-O(43)-C(50)	107.67(10)
C(54)-C(44)-C(43)	118.72(11)
C(54)-C(44)-C(45)	123.81(10)
C(43)-C(44)-C(45)	117.47(10)
C(55)-C(45)-C(44)	116.31(10)
C(55)-C(45)-C(41)	114.62(9)
C(44)-C(45)-C(41)	107.08(9)
C(55)-C(45)-H(45)	106.4(8)
C(44)-C(45)-H(45)	107.9(8)
C(41)-C(45)-H(45)	103.6(8)
O(46)-C(46)-N(46)	126.52(11)
O(46)-C(46)-C(41)	125.99(11)
N(46)-C(46)-C(41)	107.44(10)
C(46)-N(46)-C(47)	111.32(9)
C(46)-N(46)-C(65)	123.58(10)
C(47)-N(46)-C(65)	123.89(10)
C(61)-C(47)-C(48)	122.68(11)

C(61)-C(47)-N(46)	127.00(11)
C(48)-C(47)-N(46)	110.32(10)
C(64)-C(48)-C(47)	119.09(11)
C(64)-C(48)-C(41)	132.94(11)
C(47)-C(48)-C(41)	107.97(10)
O(42)-C(49)-C(50)	102.89(10)
O(42)-C(49)-H(49A)	107.6(9)
C(50)-C(49)-H(49A)	114.7(9)
O(42)-C(49)-H(49B)	109.3(9)
C(50)-C(49)-H(49B)	111.4(10)
H(49A)-C(49)-H(49B)	110.5(13)
O(43)-C(50)-C(49)	104.45(11)
O(43)-C(50)-H(50A)	110.1(12)
C(49)-C(50)-H(50A)	111.4(12)
O(43)-C(50)-H(50B)	106.2(11)
C(49)-C(50)-H(50B)	111.8(11)
H(50A)-C(50)-H(50B)	112.5(16)
C(52)-C(51)-C(43)	120.26(11)
C(52)-C(51)-H(51)	121.6(8)
C(43)-C(51)-H(51)	118.1(8)
C(51)-C(52)-C(53)	119.68(11)
C(51)-C(52)-H(52)	121.0(8)
C(53)-C(52)-H(52)	119.3(8)
C(54)-C(53)-C(52)	120.21(11)
C(54)-C(53)-H(53)	120.2(9)
C(52)-C(53)-H(53)	119.5(9)
C(53)-C(54)-C(44)	120.73(11)
C(53)-C(54)-H(54)	119.6(9)
C(44)-C(54)-H(54)	119.7(9)
C(56)-C(55)-C(60)	118.71(11)
C(56)-C(55)-C(45)	118.31(11)
C(60)-C(55)-C(45)	122.98(11)
C(57)-C(56)-C(55)	121.03(12)
C(57)-C(56)-H(56)	120.8(9)
C(55)-C(56)-H(56)	118.2(9)
C(58)-C(57)-C(56)	119.94(12)

C(58)-C(57)-H(57)	120.6(9)
C(56)-C(57)-H(57)	119.5(9)
C(57)-C(58)-C(59)	119.61(11)
C(57)-C(58)-H(58)	119.5(9)
C(59)-C(58)-H(58)	120.8(9)
C(58)-C(59)-C(60)	120.62(12)
C(58)-C(59)-H(59)	119.3(9)
C(60)-C(59)-H(59)	120.0(9)
C(59)-C(60)-C(55)	120.06(11)
C(59)-C(60)-H(60)	119.1(8)
C(55)-C(60)-H(60)	120.8(8)
C(47)-C(61)-C(62)	117.39(11)
C(47)-C(61)-H(61)	121.2(9)
C(62)-C(61)-H(61)	121.4(9)
C(63)-C(62)-C(61)	120.98(11)
C(63)-C(62)-H(62)	120.3(8)
C(61)-C(62)-H(62)	118.7(8)
C(62)-C(63)-C(64)	120.56(12)
C(62)-C(63)-H(63)	119.5(9)
C(64)-C(63)-H(63)	120.0(9)
C(48)-C(64)-C(63)	119.27(11)
C(48)-C(64)-H(64)	121.4(9)
C(63)-C(64)-H(64)	119.4(9)
N(46)-C(65)-C(66)	113.25(9)
N(46)-C(65)-H(65A)	105.4(8)
C(66)-C(65)-H(65A)	110.1(8)
N(46)-C(65)-H(65B)	109.2(8)
C(66)-C(65)-H(65B)	110.0(8)
H(65A)-C(65)-H(65B)	108.8(12)
C(71)-C(66)-C(67)	119.34(11)
C(71)-C(66)-C(65)	121.24(10)
C(67)-C(66)-C(65)	119.32(10)
C(68)-C(67)-C(66)	120.19(11)
C(68)-C(67)-H(67)	121.4(8)
C(66)-C(67)-H(67)	118.4(8)
C(69)-C(68)-C(67)	120.08(11)

C(69)-C(68)-H(68)	121.3(9)
C(67)-C(68)-H(68)	118.6(9)
C(68)-C(69)-C(70)	119.98(11)
C(68)-C(69)-H(69)	119.8(9)
C(70)-C(69)-H(69)	120.2(9)
C(71)-C(70)-C(69)	119.98(11)
C(71)-C(70)-H(70)	119.9(8)
C(69)-C(70)-H(70)	120.2(8)
C(70)-C(71)-C(66)	120.42(11)
C(70)-C(71)-H(71)	120.3(9)
C(66)-C(71)-H(71)	119.3(9)

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($Å^2$x 10^3) for JF2999FMI. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2 a^{*2}U^{11} + ... + 2 h k a^* b^* U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
C(1)	22(1)	18(1)	15(1)	-3(1)	-5(1)	-5(1)
O(1)	21(1)	23(1)	16(1)	-4(1)	-5(1)	-3(1)
C(2)	23(1)	16(1)	19(1)	-2(1)	-7(1)	-7(1)
O(2)	30(1)	17(1)	21(1)	-2(1)	-2(1)	-8(1)
C(3)	22(1)	19(1)	21(1)	-6(1)	-5(1)	-9(1)
O(3)	29(1)	25(1)	18(1)	-5(1)	-6(1)	-11(1)
C(4)	21(1)	18(1)	22(1)	-5(1)	-5(1)	-9(1)
C(5)	22(1)	16(1)	18(1)	-5(1)	-3(1)	-7(1)
C(6)	22(1)	20(1)	13(1)	-1(1)	-3(1)	-6(1)
N(6)	18(1)	19(1)	17(1)	-4(1)	-2(1)	-4(1)
O(6)	27(1)	20(1)	24(1)	-8(1)	-6(1)	-3(1)
C(7)	22(1)	19(1)	14(1)	-1(1)	-1(1)	-7(1)
C(8)	22(1)	19(1)	14(1)	-1(1)	-2(1)	-8(1)
C(9)	39(1)	26(1)	22(1)	0(1)	1(1)	-9(1)
C(10)	52(1)	40(1)	19(1)	-7(1)	-1(1)	-20(1)
C(11)	25(1)	22(1)	23(1)	-4(1)	-8(1)	-7(1)
C(12)	21(1)	25(1)	30(1)	-8(1)	-7(1)	-5(1)
C(13)	21(1)	28(1)	26(1)	-10(1)	-2(1)	-9(1)
C(14)	24(1)	24(1)	22(1)	-5(1)	-4(1)	-11(1)
C(15)	19(1)	20(1)	19(1)	-3(1)	-2(1)	-7(1)
C(16)	22(1)	20(1)	21(1)	-4(1)	-2(1)	-6(1)
C(17)	25(1)	30(1)	19(1)	-7(1)	-1(1)	-10(1)
C(18)	24(1)	30(1)	18(1)	1(1)	-3(1)	-11(1)
C(19)	25(1)	20(1)	24(1)	1(1)	-3(1)	-8(1)
C(20)	24(1)	20(1)	21(1)	-4(1)	-2(1)	-8(1)
C(21)	23(1)	18(1)	22(1)	-1(1)	-5(1)	-6(1)
C(22)	30(1)	18(1)	25(1)	-3(1)	-5(1)	-7(1)
C(23)	34(1)	24(1)	24(1)	-4(1)	-6(1)	-14(1)
C(24)	24(1)	25(1)	21(1)	-2(1)	-4(1)	-11(1)
C(25)	18(1)	25(1)	19(1)	-4(1)	-3(1)	-4(1)
C(26)	23(1)	16(1)	19(1)	-4(1)	-4(1)	-6(1)

C(27)	21(1)	21(1)	22(1)	-4(1)	-3(1)	-6(1)
C(28)	27(1)	22(1)	20(1)	-4(1)	-1(1)	-9(1)
C(29)	30(1)	21(1)	19(1)	-2(1)	-7(1)	-8(1)
C(30)	23(1)	24(1)	25(1)	-5(1)	-7(1)	-6(1)
C(31)	21(1)	22(1)	21(1)	-5(1)	-2(1)	-6(1)
C(41)	18(1)	16(1)	19(1)	-5(1)	-3(1)	-2(1)
O(41)	21(1)	18(1)	26(1)	-9(1)	-8(1)	0(1)
C(42)	18(1)	17(1)	20(1)	-2(1)	-3(1)	-2(1)
O(42)	32(1)	20(1)	22(1)	-2(1)	-5(1)	-11(1)
C(43)	16(1)	20(1)	19(1)	-5(1)	1(1)	-5(1)
O(43)	21(1)	21(1)	28(1)	-9(1)	1(1)	-3(1)
C(44)	15(1)	20(1)	17(1)	-3(1)	2(1)	-6(1)
C(45)	17(1)	19(1)	16(1)	-4(1)	0(1)	-4(1)
C(46)	20(1)	16(1)	17(1)	-5(1)	-2(1)	-4(1)
N(46)	18(1)	17(1)	16(1)	-3(1)	-4(1)	-4(1)
O(46)	23(1)	32(1)	18(1)	-7(1)	-2(1)	-3(1)
C(47)	22(1)	14(1)	17(1)	-3(1)	-4(1)	-7(1)
C(48)	20(1)	14(1)	20(1)	-4(1)	-3(1)	-6(1)
C(49)	43(1)	19(1)	30(1)	-4(1)	-12(1)	-10(1)
C(50)	49(1)	23(1)	36(1)	-13(1)	1(1)	-9(1)
C(51)	18(1)	20(1)	23(1)	-2(1)	-2(1)	-4(1)
C(52)	18(1)	27(1)	22(1)	-3(1)	-4(1)	-6(1)
C(53)	19(1)	25(1)	23(1)	-7(1)	-2(1)	-9(1)
C(54)	17(1)	19(1)	22(1)	-4(1)	1(1)	-6(1)
C(55)	16(1)	18(1)	21(1)	-3(1)	-4(1)	-6(1)
C(56)	20(1)	24(1)	21(1)	-3(1)	-3(1)	-8(1)
C(57)	24(1)	22(1)	27(1)	3(1)	-7(1)	-10(1)
C(58)	22(1)	16(1)	35(1)	-2(1)	-9(1)	-6(1)
C(59)	19(1)	22(1)	28(1)	-9(1)	-4(1)	-6(1)
C(60)	19(1)	20(1)	20(1)	-4(1)	-4(1)	-7(1)
C(61)	19(1)	21(1)	22(1)	-4(1)	-4(1)	-7(1)
C(62)	24(1)	25(1)	20(1)	-5(1)	0(1)	-11(1)
C(63)	27(1)	24(1)	17(1)	-1(1)	-4(1)	-10(1)
C(64)	22(1)	20(1)	21(1)	-2(1)	-6(1)	-7(1)
C(65)	20(1)	19(1)	19(1)	-5(1)	-7(1)	-5(1)
C(66)	21(1)	19(1)	11(1)	-1(1)	-2(1)	-5(1)

C(67)	22(1)	22(1)	14(1)	-3(1)	-3(1)	-8(1)
C(68)	19(1)	28(1)	16(1)	-5(1)	-3(1)	-4(1)
C(69)	26(1)	20(1)	18(1)	-5(1)	-3(1)	-1(1)
C(70)	27(1)	20(1)	20(1)	-4(1)	-4(1)	-7(1)
C(71)	20(1)	22(1)	18(1)	-4(1)	-3(1)	-6(1)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for JF2999FMI.

	x	y	z	U(eq)
H(5)	2118(14)	7147(11)	3488(8)	17(3)
H(9A)	3483(19)	9595(14)	1101(9)	41(4)
H(9B)	2171(17)	10649(14)	744(10)	38(4)
H(10A)	890(20)	9542(16)	673(12)	61(6)
H(10B)	2430(20)	8599(17)	726(12)	58(6)
H(11)	-857(15)	10588(12)	2244(9)	28(4)
H(12)	-2723(16)	10923(12)	3257(8)	28(4)
H(13)	-2373(15)	9840(12)	4487(9)	26(4)
H(14)	-266(15)	8386(12)	4708(9)	25(4)
H(16)	1907(15)	8650(12)	4918(8)	24(4)
H(17)	2477(15)	7792(12)	6144(9)	27(4)
H(18)	3438(16)	5885(12)	6474(9)	29(4)
H(19)	3743(16)	4816(13)	5576(9)	32(4)
H(20)	3085(15)	5677(12)	4336(8)	24(4)
H(21)	1528(16)	10480(11)	3334(8)	23(3)
H(22)	2336(16)	11601(13)	3809(8)	28(4)
H(23)	4559(16)	10978(13)	4214(9)	30(4)
H(24)	6088(16)	9164(12)	4158(8)	27(4)
H(25A)	7445(15)	7682(12)	3390(9)	26(4)
H(25B)	7246(15)	6551(12)	3471(8)	23(3)
H(27)	5253(16)	7115(12)	5002(8)	28(4)
H(28)	5856(16)	6588(12)	6261(9)	29(4)
H(29)	8239(15)	6000(12)	6470(9)	26(4)
H(30)	10024(17)	5980(12)	5450(9)	32(4)
H(31)	9400(16)	6537(12)	4201(9)	26(4)
H(45)	-2029(14)	6189(11)	2196(8)	19(3)
H(49A)	-2980(16)	10841(13)	847(9)	31(4)
H(49B)	-1858(18)	9974(13)	1431(9)	39(4)
H(50A)	-3770(20)	9986(16)	2281(12)	58(6)
H(50B)	-4910(20)	10464(16)	1625(11)	58(5)

H(51)	-4334(14)	8951(12)	220(8)	21(3)
H(52)	-4853(15)	7817(11)	-427(8)	23(3)
H(53)	-3827(16)	5910(12)	-104(9)	28(4)
H(54)	-2345(15)	5116(12)	863(8)	23(4)
H(56)	-1213(15)	4570(12)	2930(9)	25(4)
H(57)	43(16)	2677(13)	3121(9)	31(4)
H(58)	1412(16)	1908(13)	2108(9)	30(4)
H(59)	1599(16)	3000(12)	898(9)	29(4)
H(60)	327(14)	4887(11)	701(8)	21(3)
H(61)	3925(16)	5957(12)	755(8)	27(4)
H(62)	3596(15)	6554(11)	-538(8)	21(3)
H(63)	1327(15)	7391(12)	-917(9)	26(4)
H(64)	-677(17)	7620(12)	-27(9)	30(4)
H(65A)	2607(15)	5767(11)	2834(9)	23(4)
H(65B)	3456(15)	6327(11)	2135(8)	21(3)
H(67)	5747(15)	5024(12)	2263(8)	25(4)
H(68)	7349(16)	3266(12)	2188(8)	26(4)
H(69)	6539(16)	1888(13)	2044(8)	27(4)
H(70)	4097(15)	2269(12)	2010(8)	27(4)
H(71)	2533(16)	4036(11)	2096(8)	24(4)

Table 6. Torsion angles [°] for JF2999FMI.

C(8)-C(1)-O(1)-C(2)	-70.52(13)
C(6)-C(1)-O(1)-C(2)	176.85(9)
C(5)-C(1)-O(1)-C(2)	59.57(12)
C(1)-O(1)-C(2)-O(3)	-144.02(9)
C(1)-O(1)-C(2)-O(2)	102.39(11)
C(1)-O(1)-C(2)-C(3)	-21.10(14)
O(3)-C(2)-O(2)-C(9)	-36.67(12)
O(1)-C(2)-O(2)-C(9)	76.88(11)
C(3)-C(2)-O(2)-C(9)	-156.69(10)
O(3)-C(2)-C(3)-C(11)	-72.88(13)
O(2)-C(2)-C(3)-C(11)	43.88(14)
O(1)-C(2)-C(3)-C(11)	167.10(10)
O(3)-C(2)-C(3)-C(4)	108.89(12)
O(2)-C(2)-C(3)-C(4)	-134.35(11)
O(1)-C(2)-C(3)-C(4)	-11.13(15)
O(2)-C(2)-O(3)-C(10)	22.72(13)
O(1)-C(2)-O(3)-C(10)	-93.10(11)
C(3)-C(2)-O(3)-C(10)	141.76(11)
C(11)-C(3)-C(4)-C(14)	0.16(17)
C(2)-C(3)-C(4)-C(14)	178.36(10)
C(11)-C(3)-C(4)-C(5)	-177.69(10)
C(2)-C(3)-C(4)-C(5)	0.51(16)
C(14)-C(4)-C(5)-C(15)	-12.99(16)
C(3)-C(4)-C(5)-C(15)	164.76(10)
C(14)-C(4)-C(5)-C(1)	-141.26(11)
C(3)-C(4)-C(5)-C(1)	36.49(13)
O(1)-C(1)-C(5)-C(15)	165.21(9)
C(8)-C(1)-C(5)-C(15)	-63.41(13)
C(6)-C(1)-C(5)-C(15)	51.30(12)
O(1)-C(1)-C(5)-C(4)	-64.76(11)
C(8)-C(1)-C(5)-C(4)	66.62(12)
C(6)-C(1)-C(5)-C(4)	-178.67(9)
O(1)-C(1)-C(6)-O(6)	-50.55(15)
C(8)-C(1)-C(6)-O(6)	-173.23(12)

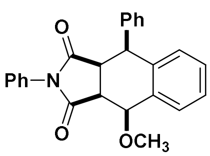
C(5)-C(1)-C(6)-O(6)	64.41(15)
O(1)-C(1)-C(6)-N(6)	130.62(10)
C(8)-C(1)-C(6)-N(6)	7.94(12)
C(5)-C(1)-C(6)-N(6)	-114.42(10)
O(6)-C(6)-N(6)-C(7)	174.53(12)
C(1)-C(6)-N(6)-C(7)	-6.65(13)
O(6)-C(6)-N(6)-C(25)	6.61(19)
C(1)-C(6)-N(6)-C(25)	-174.58(10)
C(6)-N(6)-C(7)-C(24)	-177.81(12)
C(25)-N(6)-C(7)-C(24)	-9.78(18)
C(6)-N(6)-C(7)-C(8)	2.41(13)
C(25)-N(6)-C(7)-C(8)	170.43(10)
C(24)-C(7)-C(8)-C(21)	0.95(18)
N(6)-C(7)-C(8)-C(21)	-179.26(10)
C(24)-C(7)-C(8)-C(1)	-176.75(11)
N(6)-C(7)-C(8)-C(1)	3.04(13)
O(1)-C(1)-C(8)-C(21)	61.93(17)
C(6)-C(1)-C(8)-C(21)	176.27(13)
C(5)-C(1)-C(8)-C(21)	-64.40(17)
O(1)-C(1)-C(8)-C(7)	-120.83(11)
C(6)-C(1)-C(8)-C(7)	-6.49(12)
C(5)-C(1)-C(8)-C(7)	112.84(11)
C(2)-O(2)-C(9)-C(10)	35.10(13)
C(2)-O(3)-C(10)-C(9)	-0.59(14)
O(2)-C(9)-C(10)-O(3)	-20.98(14)
C(4)-C(3)-C(11)-C(12)	0.04(18)
C(2)-C(3)-C(11)-C(12)	-178.20(11)
C(3)-C(11)-C(12)-C(13)	0.48(18)
C(11)-C(12)-C(13)-C(14)	-1.22(19)
C(12)-C(13)-C(14)-C(4)	1.43(18)
C(3)-C(4)-C(14)-C(13)	-0.90(17)
C(5)-C(4)-C(14)-C(13)	176.84(11)
C(4)-C(5)-C(15)-C(20)	132.92(11)
C(1)-C(5)-C(15)-C(20)	-102.54(12)
C(4)-C(5)-C(15)-C(16)	-48.76(16)
C(1)-C(5)-C(15)-C(16)	75.78(14)

C(20)-C(15)-C(16)-C(17)	-0.50(18)
C(5)-C(15)-C(16)-C(17)	-178.82(11)
C(15)-C(16)-C(17)-C(18)	1.36(19)
C(16)-C(17)-C(18)-C(19)	-0.90(19)
C(17)-C(18)-C(19)-C(20)	-0.41(19)
C(18)-C(19)-C(20)-C(15)	1.28(19)
C(16)-C(15)-C(20)-C(19)	-0.82(18)
C(5)-C(15)-C(20)-C(19)	177.59(11)
C(7)-C(8)-C(21)-C(22)	0.21(17)
C(1)-C(8)-C(21)-C(22)	177.20(12)
C(8)-C(21)-C(22)-C(23)	-0.77(19)
C(21)-C(22)-C(23)-C(24)	0.2(2)
C(8)-C(7)-C(24)-C(23)	-1.49(18)
N(6)-C(7)-C(24)-C(23)	178.75(11)
C(22)-C(23)-C(24)-C(7)	0.89(19)
C(6)-N(6)-C(25)-C(26)	-121.54(12)
C(7)-N(6)-C(25)-C(26)	72.01(14)
N(6)-C(25)-C(26)-C(27)	12.83(16)
N(6)-C(25)-C(26)-C(31)	-168.96(10)
C(31)-C(26)-C(27)-C(28)	0.08(17)
C(25)-C(26)-C(27)-C(28)	178.29(11)
C(26)-C(27)-C(28)-C(29)	-0.34(18)
C(27)-C(28)-C(29)-C(30)	0.22(18)
C(28)-C(29)-C(30)-C(31)	0.16(18)
C(29)-C(30)-C(31)-C(26)	-0.42(18)
C(27)-C(26)-C(31)-C(30)	0.29(17)
C(25)-C(26)-C(31)-C(30)	-177.98(11)
C(48)-C(41)-O(41)-C(42)	75.45(13)
C(46)-C(41)-O(41)-C(42)	-171.82(9)
C(45)-C(41)-O(41)-C(42)	-55.69(13)
C(41)-O(41)-C(42)-O(43)	139.41(10)
C(41)-O(41)-C(42)-O(42)	-107.12(11)
C(41)-O(41)-C(42)-C(43)	16.74(15)
O(43)-C(42)-O(42)-C(49)	39.18(12)
O(41)-C(42)-O(42)-C(49)	-74.37(11)
C(43)-C(42)-O(42)-C(49)	158.61(10)

O(43)-C(42)-C(43)-C(51)	73.55(14)
O(42)-C(42)-C(43)-C(51)	-42.97(14)
O(41)-C(42)-C(43)-C(51)	-166.23(11)
O(43)-C(42)-C(43)-C(44)	-106.45(12)
O(42)-C(42)-C(43)-C(44)	137.02(11)
O(41)-C(42)-C(43)-C(44)	13.76(16)
O(42)-C(42)-O(43)-C(50)	-26.51(13)
O(41)-C(42)-O(43)-C(50)	88.91(12)
C(43)-C(42)-O(43)-C(50)	-145.47(11)
C(51)-C(43)-C(44)-C(54)	0.19(17)
C(42)-C(43)-C(44)-C(54)	-179.80(10)
C(51)-C(43)-C(44)-C(45)	179.70(10)
C(42)-C(43)-C(44)-C(45)	-0.29(16)
C(54)-C(44)-C(45)-C(55)	11.99(16)
C(43)-C(44)-C(45)-C(55)	-167.50(10)
C(54)-C(44)-C(45)-C(41)	141.65(11)
C(43)-C(44)-C(45)-C(41)	-37.84(14)
O(41)-C(41)-C(45)-C(55)	-165.10(9)
C(48)-C(41)-C(45)-C(55)	63.43(13)
C(46)-C(41)-C(45)-C(55)	-51.00(13)
O(41)-C(41)-C(45)-C(44)	64.28(11)
C(48)-C(41)-C(45)-C(44)	-67.18(12)
C(46)-C(41)-C(45)-C(44)	178.39(9)
O(41)-C(41)-C(46)-O(46)	51.37(15)
C(48)-C(41)-C(46)-O(46)	173.63(11)
C(45)-C(41)-C(46)-O(46)	-63.41(14)
O(41)-C(41)-C(46)-N(46)	-130.92(9)
C(48)-C(41)-C(46)-N(46)	-8.65(11)
C(45)-C(41)-C(46)-N(46)	114.30(10)
O(46)-C(46)-N(46)-C(47)	-174.70(11)
C(41)-C(46)-N(46)-C(47)	7.60(12)
O(46)-C(46)-N(46)-C(65)	-6.80(18)
C(41)-C(46)-N(46)-C(65)	175.50(9)
C(46)-N(46)-C(47)-C(61)	176.11(11)
C(65)-N(46)-C(47)-C(61)	8.25(17)
C(46)-N(46)-C(47)-C(48)	-3.22(13)

C(65)-N(46)-C(47)-C(48)	-171.07(10)
C(61)-C(47)-C(48)-C(64)	-2.02(17)
N(46)-C(47)-C(48)-C(64)	177.34(10)
C(61)-C(47)-C(48)-C(41)	177.86(10)
N(46)-C(47)-C(48)-C(41)	-2.78(12)
O(41)-C(41)-C(48)-C(64)	-58.50(17)
C(46)-C(41)-C(48)-C(64)	-173.37(12)
C(45)-C(41)-C(48)-C(64)	68.40(16)
O(41)-C(41)-C(48)-C(47)	121.65(10)
C(46)-C(41)-C(48)-C(47)	6.78(11)
C(45)-C(41)-C(48)-C(47)	-111.45(11)
C(42)-O(42)-C(49)-C(50)	-35.35(12)
C(42)-O(43)-C(50)-C(49)	3.90(14)
O(42)-C(49)-C(50)-O(43)	19.30(14)
C(44)-C(43)-C(51)-C(52)	-0.74(18)
C(42)-C(43)-C(51)-C(52)	179.25(11)
C(43)-C(51)-C(52)-C(53)	0.38(19)
C(51)-C(52)-C(53)-C(54)	0.54(19)
C(52)-C(53)-C(54)-C(44)	-1.10(18)
C(43)-C(44)-C(54)-C(53)	0.73(17)
C(45)-C(44)-C(54)-C(53)	-178.75(11)
C(44)-C(45)-C(55)-C(56)	-126.99(11)
C(41)-C(45)-C(55)-C(56)	107.07(12)
C(44)-C(45)-C(55)-C(60)	52.54(15)
C(41)-C(45)-C(55)-C(60)	-73.41(14)
C(60)-C(55)-C(56)-C(57)	-1.65(17)
C(45)-C(55)-C(56)-C(57)	177.90(11)
C(55)-C(56)-C(57)-C(58)	0.33(18)
C(56)-C(57)-C(58)-C(59)	1.10(18)
C(57)-C(58)-C(59)-C(60)	-1.19(18)
C(58)-C(59)-C(60)-C(55)	-0.14(18)
C(56)-C(55)-C(60)-C(59)	1.55(17)
C(45)-C(55)-C(60)-C(59)	-177.98(10)
C(48)-C(47)-C(61)-C(62)	1.02(17)
N(46)-C(47)-C(61)-C(62)	-178.23(11)
C(47)-C(61)-C(62)-C(63)	0.46(18)

C(61)-C(62)-C(63)-C(64)	-0.92(18)
C(47)-C(48)-C(64)-C(63)	1.50(17)
C(41)-C(48)-C(64)-C(63)	-178.34(11)
C(62)-C(63)-C(64)-C(48)	-0.09(18)
C(46)-N(46)-C(65)-C(66)	125.52(11)
C(47)-N(46)-C(65)-C(66)	-68.09(14)
N(46)-C(65)-C(66)-C(71)	-33.79(16)
N(46)-C(65)-C(66)-C(67)	149.68(11)
C(71)-C(66)-C(67)-C(68)	-1.01(17)
C(65)-C(66)-C(67)-C(68)	175.59(11)
C(66)-C(67)-C(68)-C(69)	0.57(18)
C(67)-C(68)-C(69)-C(70)	-0.02(18)
C(68)-C(69)-C(70)-C(71)	-0.08(18)
C(69)-C(70)-C(71)-C(66)	-0.37(18)
C(67)-C(66)-C(71)-C(70)	0.91(17)
C(65)-C(66)-C(71)-C(70)	-175.62(11)



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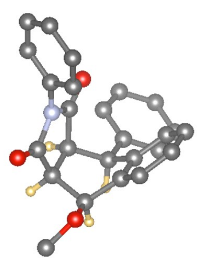

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CCDC 2240749

Table 1. Crystal data and structure refinement for [$C_{28}H_{26}N_2O_3$].

Identification code	JF3055FMI (JMR-II-175)	
Empirical formula	C28 H26 N2 O3	
Formula weight	438.51	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	$P2_1/n$	
Unit cell dimensions	a = 7.9089(3) Å	α= 90°.
	b = 21.0205(9) Å	β= 96.0784(16)°.
	c = 13.3410(6) Å	γ = 90°.
Volume	2205.46(16) $Å^3$	

Z	4
Density (calculated)	1.321 Mg/m^3
Absorption coefficient	0.086 mm^{-1}
F(000)	928
Crystal size	0.401 x 0.302 x 0.150 mm^3
Crystal color and habit	Colorless Block
Diffractometer	Bruker Photon2 CMOS
Theta range for data collection	2.472 to 29.999°.
Index ranges	-11<=h<=11, -29<=k<=29, -18<=l<=18
Reflections collected	24830
Independent reflections	6426 [R(int) = 0.0166]
Observed reflections (I > 2sigma(I))	5835
Completeness to theta = 25.242°	99.8 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.9749 and 0.9261
Solution method	SHELXT (Sheldrick, 2014)
Refinement method	SHELXL-2018/3 (Sheldrick, 2018) Full-matrix least-squares on F^2
Data / restraints / parameters	6426 / 0 / 402
Goodness-of-fit on F^2	1.039
Final R indices [I>2sigma(I)]	R1 = 0.0373, wR2 = 0.0945
R indices (all data)	R1 = 0.0413, wR2 = 0.0978
Largest diff. peak and hole	0.393 and -0.191 e.Å^{-3}

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for JF3055FMI. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
C(1)	5436(1)	3419(1)	2173(1)	13(1)
C(2)	5230(1)	3274(1)	3277(1)	15(1)
C(3)	6171(1)	2807(1)	2683(1)	15(1)
C(4)	7988(1)	2824(1)	3126(1)	16(1)
N(4)	8130(1)	3296(1)	3869(1)	16(1)
O(4)	9144(1)	2496(1)	2900(1)	20(1)
C(5)	6556(1)	3568(1)	4019(1)	16(1)
O(5)	6353(1)	3968(1)	4645(1)	23(1)
C(6)	6581(1)	3959(1)	1942(1)	13(1)
C(7)	8075(1)	3839(1)	1503(1)	16(1)
C(8)	9139(1)	4334(1)	1276(1)	19(1)
C(9)	8713(1)	4955(1)	1498(1)	21(1)
C(10)	7231(1)	5079(1)	1940(1)	19(1)
C(11)	6131(1)	4589(1)	2152(1)	15(1)
C(12)	4492(1)	4734(1)	2601(1)	16(1)
N(12)	3961(1)	5397(1)	2478(1)	15(1)
C(13)	2585(1)	5524(1)	3106(1)	18(1)
C(14)	2028(2)	6211(1)	2992(1)	24(1)
O(14)	1475(1)	6367(1)	1963(1)	23(1)
C(15)	2820(1)	6242(1)	1352(1)	21(1)
C(16)	3362(1)	5549(1)	1428(1)	16(1)
C(17)	3909(1)	3304(1)	1418(1)	14(1)
C(18)	2642(1)	2870(1)	1609(1)	17(1)
C(19)	1302(1)	2739(1)	874(1)	20(1)
C(20)	1191(1)	3040(1)	-56(1)	20(1)
C(21)	2435(1)	3476(1)	-251(1)	20(1)
C(22)	3784(1)	3608(1)	481(1)	17(1)
C(23)	9689(1)	3477(1)	4441(1)	17(1)
C(24)	10231(1)	4105(1)	4424(1)	24(1)
C(25)	11699(2)	4283(1)	5030(1)	29(1)
C(26)	12617(1)	3837(1)	5632(1)	27(1)

C(27)	12070(1)	3212(1)	5627(1)	24(1)
C(28)	10600(1)	3025(1)	5032(1)	20(1)

Table 3. Bond lengths [Å] and angles [°] for JF3055FMI.

C(1)-C(6)	1.5038(12)	C(14)-H(14A)	0.981(15)
C(1)-C(17)	1.5082(12)	C(14)-H(14B)	1.014(16)
C(1)-C(2)	1.5299(12)	O(14)-C(15)	1.4316(12)
C(1)-C(3)	1.5401(12)	C(15)-C(16)	1.5186(14)
C(2)-C(5)	1.4973(13)	C(15)-H(15A)	0.996(15)
C(2)-C(3)	1.5058(13)	C(15)-H(15B)	0.970(14)
C(2)-H(2)	0.956(14)	C(16)-H(16A)	1.015(14)
C(3)-C(4)	1.4953(13)	C(16)-H(16B)	0.996(13)
C(3)-H(3)	0.960(14)	C(17)-C(18)	1.3980(12)
C(4)-O(4)	1.2088(12)	C(17)-C(22)	1.3983(12)
C(4)-N(4)	1.3985(12)	C(18)-C(19)	1.3925(13)
N(4)-C(5)	1.4030(12)	C(18)-H(18)	0.956(15)
N(4)-C(23)	1.4312(12)	C(19)-C(20)	1.3881(14)
C(5)-O(5)	1.2068(12)	C(19)-H(19)	0.975(16)
C(6)-C(7)	1.3962(12)	C(20)-C(21)	1.3892(15)
C(6)-C(11)	1.4067(12)	C(20)-H(20)	0.960(15)
C(7)-C(8)	1.3910(13)	C(21)-C(22)	1.3959(13)
C(7)-H(7)	0.982(14)	C(21)-H(21)	0.958(16)
C(8)-C(9)	1.3884(14)	C(22)-H(22)	0.965(14)
C(8)-H(8)	0.971(14)	C(23)-C(28)	1.3870(13)
C(9)-C(10)	1.3915(14)	C(23)-C(24)	1.3884(14)
C(9)-H(9)	0.967(15)	C(24)-C(25)	1.3939(15)
C(10)-C(11)	1.3961(12)	C(24)-H(24)	1.005(16)
C(10)-H(10)	0.970(15)	C(25)-C(26)	1.3883(17)
C(11)-C(12)	1.5154(12)	C(25)-H(25)	0.956(19)
C(12)-N(12)	1.4609(11)	C(26)-C(27)	1.3842(17)
C(12)-H(12A)	1.001(14)	C(26)-H(26)	0.967(16)
C(12)-H(12B)	0.987(14)	C(27)-C(28)	1.3924(14)
N(12)-C(16)	1.4657(12)	C(27)-H(27)	0.969(16)
N(12)-C(13)	1.4659(12)	C(28)-H(28)	0.976(15)
C(13)-C(14)	1.5132(14)		
C(13)-H(13A)	0.963(14)	C(6)-C(1)-C(17)	116.23(7)
C(13)-H(13B)	1.008(15)	C(6)-C(1)-C(2)	118.38(7)
C(14)-O(14)	1.4342(12)	C(17)-C(1)-C(2)	116.84(7)

C(6)-C(1)-C(3)	120.89(7)	C(9)-C(10)-C(11)	121.29(9)
C(17)-C(1)-C(3)	113.51(7)	C(9)-C(10)-H(10)	120.8(9)
C(2)-C(1)-C(3)	58.74(6)	C(11)-C(10)-H(10)	117.9(9)
C(5)-C(2)-C(3)	105.47(7)	C(10)-C(11)-C(6)	118.53(8)
C(5)-C(2)-C(1)	114.57(7)	C(10)-C(11)-C(12)	120.63(8)
C(3)-C(2)-C(1)	60.97(6)	C(6)-C(11)-C(12)	120.84(8)
C(5)-C(2)-H(2)	119.3(8)	N(12)-C(12)-C(11)	113.26(7)
C(3)-C(2)-H(2)	123.8(8)	N(12)-C(12)-H(12A)	110.8(8)
C(1)-C(2)-H(2)	119.2(8)	C(11)-C(12)-H(12A)	108.6(8)
C(4)-C(3)-C(2)	106.49(7)	N(12)-C(12)-H(12B)	107.2(8)
C(4)-C(3)-C(1)	117.14(7)	C(11)-C(12)-H(12B)	109.9(8)
C(2)-C(3)-C(1)	60.29(6)	H(12A)-C(12)-H(12B)	106.9(11)
C(4)-C(3)-H(3)	118.7(8)	C(12)-N(12)-C(16)	112.01(7)
C(2)-C(3)-H(3)	123.1(8)	C(12)-N(12)-C(13)	109.32(7)
C(1)-C(3)-H(3)	117.8(8)	C(16)-N(12)-C(13)	108.80(7)
O(4)-C(4)-N(4)	125.14(9)	N(12)-C(13)-C(14)	109.99(8)
O(4)-C(4)-C(3)	127.46(9)	N(12)-C(13)-H(13A)	109.3(8)
N(4)-C(4)-C(3)	107.40(8)	C(14)-C(13)-H(13A)	108.2(8)
C(4)-N(4)-C(5)	112.57(8)	N(12)-C(13)-H(13B)	112.0(8)
C(4)-N(4)-C(23)	124.48(8)	C(14)-C(13)-H(13B)	108.8(8)
C(5)-N(4)-C(23)	122.92(8)	H(13A)-C(13)-H(13B)	108.5(12)
O(5)-C(5)-N(4)	124.52(9)	O(14)-C(14)-C(13)	111.77(8)
O(5)-C(5)-C(2)	127.58(9)	O(14)-C(14)-H(14A)	106.7(9)
N(4)-C(5)-C(2)	107.89(8)	C(13)-C(14)-H(14A)	110.0(9)
C(7)-C(6)-C(11)	119.74(8)	O(14)-C(14)-H(14B)	109.1(9)
C(7)-C(6)-C(1)	120.31(8)	C(13)-C(14)-H(14B)	108.5(9)
C(11)-C(6)-C(1)	119.94(8)	H(14A)-C(14)-H(14B)	110.7(13)
C(8)-C(7)-C(6)	121.03(9)	C(15)-O(14)-C(14)	109.44(8)
C(8)-C(7)-H(7)	119.7(8)	O(14)-C(15)-C(16)	111.14(8)
C(6)-C(7)-H(7)	119.2(8)	O(14)-C(15)-H(15A)	109.6(8)
C(9)-C(8)-C(7)	119.37(9)	C(16)-C(15)-H(15A)	109.8(8)
C(9)-C(8)-H(8)	120.2(8)	O(14)-C(15)-H(15B)	105.7(8)
C(7)-C(8)-H(8)	120.4(8)	C(16)-C(15)-H(15B)	111.4(9)
C(8)-C(9)-C(10)	120.00(9)	H(15A)-C(15)-H(15B)	109.1(12)
C(8)-C(9)-H(9)	120.7(9)	N(12)-C(16)-C(15)	109.42(8)
C(10)-C(9)-H(9)	119.3(9)	N(12)-C(16)-H(16A)	111.5(8)

C(15)-C(16)-H(16A)	110.8(8)	C(21)-C(22)-H(22)	119.0(8)
N(12)-C(16)-H(16B)	108.8(8)	C(17)-C(22)-H(22)	120.3(8)
C(15)-C(16)-H(16B)	110.8(8)	C(28)-C(23)-C(24)	121.19(9)
H(16A)-C(16)-H(16B)	105.6(11)	C(28)-C(23)-N(4)	119.16(9)
C(18)-C(17)-C(22)	118.52(8)	C(24)-C(23)-N(4)	119.61(8)
C(18)-C(17)-C(1)	121.46(8)	C(23)-C(24)-C(25)	119.04(10)
C(22)-C(17)-C(1)	119.93(8)	C(23)-C(24)-H(24)	119.7(9)
C(19)-C(18)-C(17)	120.49(9)	C(25)-C(24)-H(24)	121.3(9)
C(19)-C(18)-H(18)	119.1(9)	C(26)-C(25)-C(24)	120.44(11)
C(17)-C(18)-H(18)	120.4(9)	C(26)-C(25)-H(25)	118.9(11)
C(20)-C(19)-C(18)	120.68(9)	C(24)-C(25)-H(25)	120.7(11)
C(20)-C(19)-H(19)	120.2(9)	C(27)-C(26)-C(25)	119.64(10)
C(18)-C(19)-H(19)	119.1(9)	C(27)-C(26)-H(26)	121.5(10)
C(19)-C(20)-C(21)	119.35(9)	C(25)-C(26)-H(26)	118.9(10)
C(19)-C(20)-H(20)	119.6(9)	C(26)-C(27)-C(28)	120.79(10)
C(21)-C(20)-H(20)	121.0(9)	C(26)-C(27)-H(27)	120.0(9)
C(20)-C(21)-C(22)	120.23(9)	C(28)-C(27)-H(27)	119.2(9)
C(20)-C(21)-H(21)	120.2(9)	C(23)-C(28)-C(27)	118.90(10)
C(22)-C(21)-H(21)	119.6(9)	C(23)-C(28)-H(28)	119.2(9)
C(21)-C(22)-C(17)	120.74(9)	C(27)-C(28)-H(28)	122.0(9)

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($Å^2$x 10^3) for JF3055FMI. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2 a^{*2}U^{11} + ... + 2 h k a^* b^* U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
C(1)	14(1)	11(1)	13(1)	1(1)	2(1)	0(1)
C(2)	16(1)	15(1)	13(1)	1(1)	2(1)	0(1)
C(3)	17(1)	12(1)	16(1)	1(1)	1(1)	1(1)
C(4)	20(1)	13(1)	15(1)	3(1)	1(1)	1(1)
N(4)	16(1)	16(1)	16(1)	0(1)	-1(1)	2(1)
O(4)	21(1)	19(1)	21(1)	1(1)	2(1)	6(1)
C(5)	17(1)	18(1)	14(1)	2(1)	1(1)	1(1)
O(5)	23(1)	27(1)	17(1)	-6(1)	0(1)	4(1)
C(6)	14(1)	12(1)	14(1)	1(1)	1(1)	-1(1)
C(7)	16(1)	15(1)	18(1)	0(1)	3(1)	1(1)
C(8)	14(1)	20(1)	25(1)	2(1)	5(1)	0(1)
C(9)	15(1)	18(1)	30(1)	4(1)	2(1)	-2(1)
C(10)	16(1)	13(1)	27(1)	1(1)	2(1)	-1(1)
C(11)	13(1)	13(1)	18(1)	0(1)	2(1)	0(1)
C(12)	16(1)	12(1)	22(1)	0(1)	5(1)	1(1)
N(12)	16(1)	12(1)	16(1)	-1(1)	1(1)	2(1)
C(13)	22(1)	17(1)	15(1)	-1(1)	4(1)	4(1)
C(14)	33(1)	20(1)	19(1)	-2(1)	2(1)	11(1)
O(14)	24(1)	24(1)	21(1)	2(1)	2(1)	10(1)
C(15)	21(1)	20(1)	21(1)	4(1)	1(1)	4(1)
C(16)	16(1)	18(1)	15(1)	0(1)	2(1)	1(1)
C(17)	15(1)	11(1)	14(1)	-1(1)	2(1)	1(1)
C(18)	17(1)	15(1)	19(1)	1(1)	2(1)	-2(1)
C(19)	16(1)	17(1)	26(1)	-3(1)	1(1)	-1(1)
C(20)	18(1)	18(1)	22(1)	-6(1)	-3(1)	4(1)
C(21)	23(1)	18(1)	16(1)	0(1)	-1(1)	4(1)
C(22)	20(1)	15(1)	16(1)	1(1)	2(1)	0(1)
C(23)	16(1)	20(1)	15(1)	2(1)	1(1)	0(1)
C(24)	27(1)	21(1)	24(1)	5(1)	-3(1)	-3(1)
C(25)	28(1)	28(1)	30(1)	2(1)	-2(1)	-10(1)
C(26)	16(1)	41(1)	22(1)	0(1)	0(1)	-5(1)

C(27)	16(1)	35(1)	23(1)	8(1)	1(1)	4(1)
C(28)	17(1)	21(1)	21(1)	6(1)	2(1)	2(1)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for JF3055FMI.

	x	y	z	U(eq)
H(2)	4117(17)	3199(6)	3471(10)	19(3)
H(3)	5695(17)	2408(7)	2443(10)	22(3)
H(7)	8375(17)	3399(7)	1353(10)	21(3)
H(8)	10175(18)	4246(7)	969(10)	22(3)
H(9)	9439(19)	5306(7)	1348(11)	26(3)
H(10)	6928(19)	5510(7)	2109(11)	28(4)
H(12A)	3584(18)	4441(7)	2289(10)	20(3)
H(12B)	4631(17)	4643(7)	3331(11)	21(3)
H(13A)	2992(17)	5451(7)	3803(11)	22(3)
H(13B)	1569(19)	5241(7)	2921(11)	25(3)
H(14A)	1060(19)	6289(7)	3378(12)	29(4)
H(14B)	3030(20)	6493(8)	3241(12)	34(4)
H(15A)	3809(18)	6521(7)	1567(11)	24(3)
H(15B)	2371(18)	6352(7)	669(11)	24(3)
H(16A)	2394(18)	5259(7)	1156(11)	23(3)
H(16B)	4299(17)	5464(6)	1002(10)	17(3)
H(18)	2692(18)	2655(7)	2243(11)	26(3)
H(19)	440(20)	2432(8)	1023(12)	34(4)
H(20)	248(19)	2950(7)	-549(11)	27(4)
H(21)	2390(20)	3681(7)	-895(12)	32(4)
H(22)	4638(17)	3911(6)	329(10)	19(3)
H(24)	9540(20)	4424(8)	3992(12)	33(4)
H(25)	12100(20)	4713(9)	5034(13)	45(5)
H(26)	13620(20)	3974(8)	6052(12)	34(4)
H(27)	12700(20)	2899(7)	6049(12)	31(4)
H(28)	10189(19)	2587(7)	5023(11)	27(3)

Table 6. Torsion angles [°] for JF3055FMI.

C(6)-C(1)-C(2)-C(5)	-16.09(11)	C(3)-C(1)-C(6)-C(11)	-135.86(9)
C(17)-C(1)-C(2)-C(5)	-162.86(8)	C(11)-C(6)-C(7)-C(8)	0.65(14)
C(3)-C(1)-C(2)-C(5)	94.68(8)	C(1)-C(6)-C(7)-C(8)	179.39(8)
C(6)-C(1)-C(2)-C(3)	-110.77(9)	C(6)-C(7)-C(8)-C(9)	0.45(15)
C(17)-C(1)-C(2)-C(3)	102.46(8)	C(7)-C(8)-C(9)-C(10)	-0.18(15)
C(5)-C(2)-C(3)-C(4)	2.40(9)	C(8)-C(9)-C(10)-C(11)	-1.21(16)
C(1)-C(2)-C(3)-C(4)	112.26(8)	C(9)-C(10)-C(11)-C(6)	2.28(14)
C(5)-C(2)-C(3)-C(1)	-109.86(8)	C(9)-C(10)-C(11)-C(12)	-177.93(9)
C(6)-C(1)-C(3)-C(4)	12.27(12)	C(7)-C(6)-C(11)-C(10)	-1.98(13)
C(17)-C(1)-C(3)-C(4)	157.54(8)	C(1)-C(6)-C(11)-C(10)	179.27(8)
C(2)-C(1)-C(3)-C(4)	-94.28(9)	C(7)-C(6)-C(11)-C(12)	178.23(8)
C(6)-C(1)-C(3)-C(2)	106.55(9)	C(1)-C(6)-C(11)-C(12)	-0.52(13)
C(17)-C(1)-C(3)-C(2)	-108.18(8)	C(10)-C(11)-C(12)-N(12)	18.33(12)
C(2)-C(3)-C(4)-O(4)	175.81(9)	C(6)-C(11)-C(12)-N(12)	-161.88(8)
C(1)-C(3)-C(4)-O(4)	-119.60(10)	C(11)-C(12)-N(12)-C(16)	70.90(10)
C(2)-C(3)-C(4)-N(4)	-4.02(9)	C(11)-C(12)-N(12)-C(13)	-168.43(8)
C(1)-C(3)-C(4)-N(4)	60.57(10)	C(12)-N(12)-C(13)-C(14)	179.65(8)
O(4)-C(4)-N(4)-C(5)	-175.56(9)	C(16)-N(12)-C(13)-C(14)	-57.75(10)
C(3)-C(4)-N(4)-C(5)	4.27(10)	N(12)-C(13)-C(14)-O(14)	58.01(12)
O(4)-C(4)-N(4)-C(23)	2.86(15)	C(13)-C(14)-O(14)-C(15)	-57.65(12)
C(3)-C(4)-N(4)-C(23)	-177.31(8)	C(14)-O(14)-C(15)-C(16)	58.55(11)
C(4)-N(4)-C(5)-O(5)	177.22(9)	C(12)-N(12)-C(16)-C(15)	179.62(7)
C(23)-N(4)-C(5)-O(5)	-1.23(15)	C(13)-N(12)-C(16)-C(15)	58.65(10)
C(4)-N(4)-C(5)-C(2)	-2.72(10)	O(14)-C(15)-C(16)-N(12)	-60.03(10)
C(23)-N(4)-C(5)-C(2)	178.83(8)	C(6)-C(1)-C(17)-C(18)	-171.94(8)
C(3)-C(2)-C(5)-O(5)	-179.91(9)	C(2)-C(1)-C(17)-C(18)	-24.46(12)
C(1)-C(2)-C(5)-O(5)	115.38(11)	C(3)-C(1)-C(17)-C(18)	41.08(11)
C(3)-C(2)-C(5)-N(4)	0.03(10)	C(6)-C(1)-C(17)-C(22)	11.56(12)
C(1)-C(2)-C(5)-N(4)	-64.68(10)	C(2)-C(1)-C(17)-C(22)	159.04(8)
C(17)-C(1)-C(6)-C(7)	-98.98(10)	C(3)-C(1)-C(17)-C(22)	-135.42(9)
C(2)-C(1)-C(6)-C(7)	114.05(10)	C(22)-C(17)-C(18)-C(19)	0.90(14)
C(3)-C(1)-C(6)-C(7)	45.40(12)	C(1)-C(17)-C(18)-C(19)	-175.65(8)
C(17)-C(1)-C(6)-C(11)	79.76(10)	C(17)-C(18)-C(19)-C(20)	-0.61(14)
C(2)-C(1)-C(6)-C(11)	-67.21(11)	C(18)-C(19)-C(20)-C(21)	0.10(14)

C(19)-C(20)-C(21)-C(22)	0.10(14)
C(20)-C(21)-C(22)-C(17)	0.21(14)
C(18)-C(17)-C(22)-C(21)	-0.70(14)
C(1)-C(17)-C(22)-C(21)	175.90(8)
C(4)-N(4)-C(23)-C(28)	-59.92(13)
C(5)-N(4)-C(23)-C(28)	118.35(10)
C(4)-N(4)-C(23)-C(24)	122.43(11)
C(5)-N(4)-C(23)-C(24)	-59.30(13)
C(28)-C(23)-C(24)-C(25)	-1.38(16)
N(4)-C(23)-C(24)-C(25)	176.22(10)
C(23)-C(24)-C(25)-C(26)	0.85(18)
C(24)-C(25)-C(26)-C(27)	0.13(18)
C(25)-C(26)-C(27)-C(28)	-0.61(17)
C(24)-C(23)-C(28)-C(27)	0.91(15)
N(4)-C(23)-C(28)-C(27)	-176.71(9)
C(26)-C(27)-C(28)-C(23)	0.10(16)

Symmetry transformations used to generate equivalent atoms:

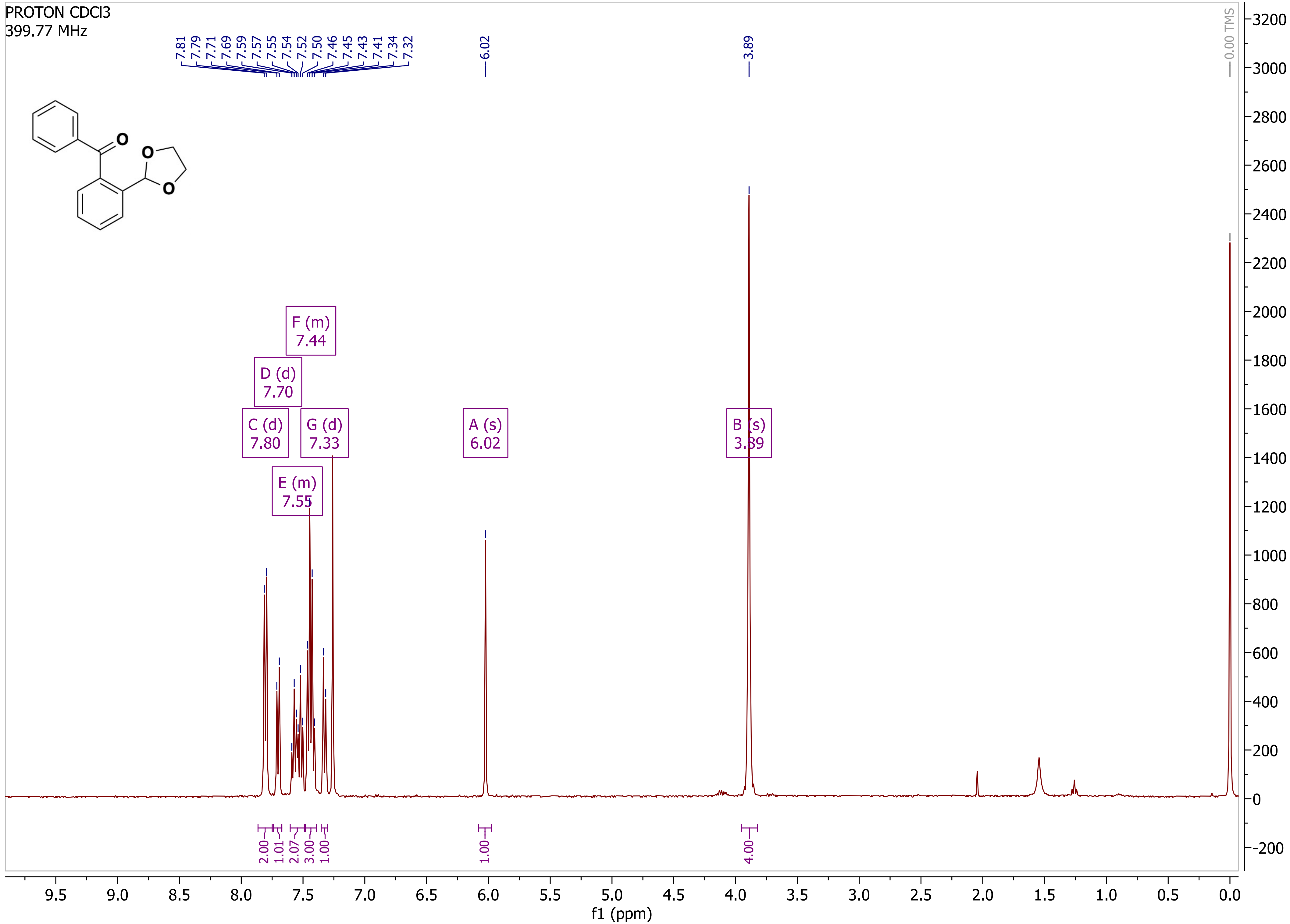
Table 7. Hydrogen bonds for JF3055FMI [Å and °].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
C(12)-H(12B)...O(5)	0.987(14)	2.537(14)	3.3684(12)	141.8(11)
C(13)-H(13A)...O(5)#1	0.963(14)	2.414(14)	3.2131(12)	140.1(11)

Symmetry transformations used to generate equivalent atoms:

#1 -x+1,-y+1,-z+1

Copy of NMR Spectra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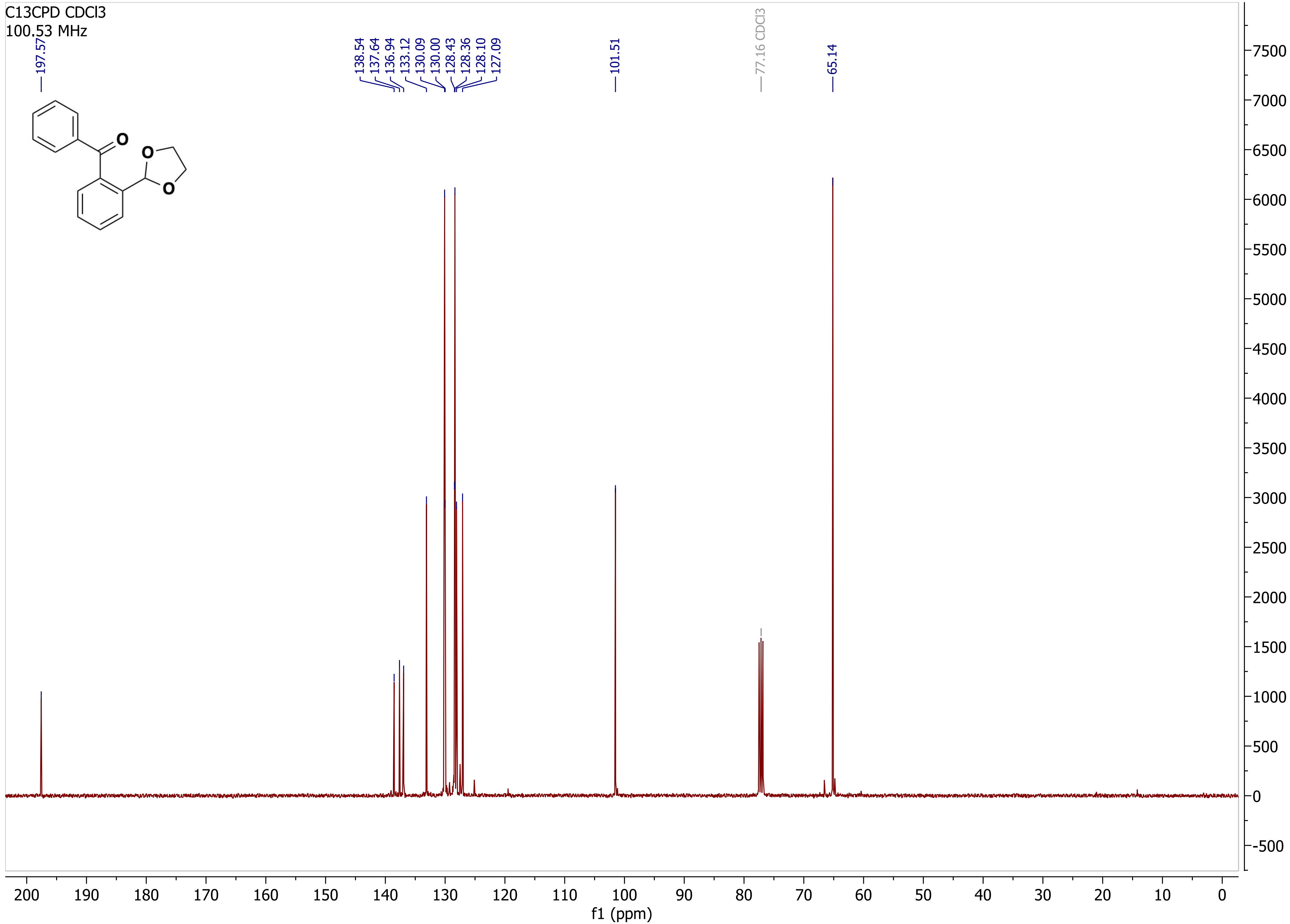
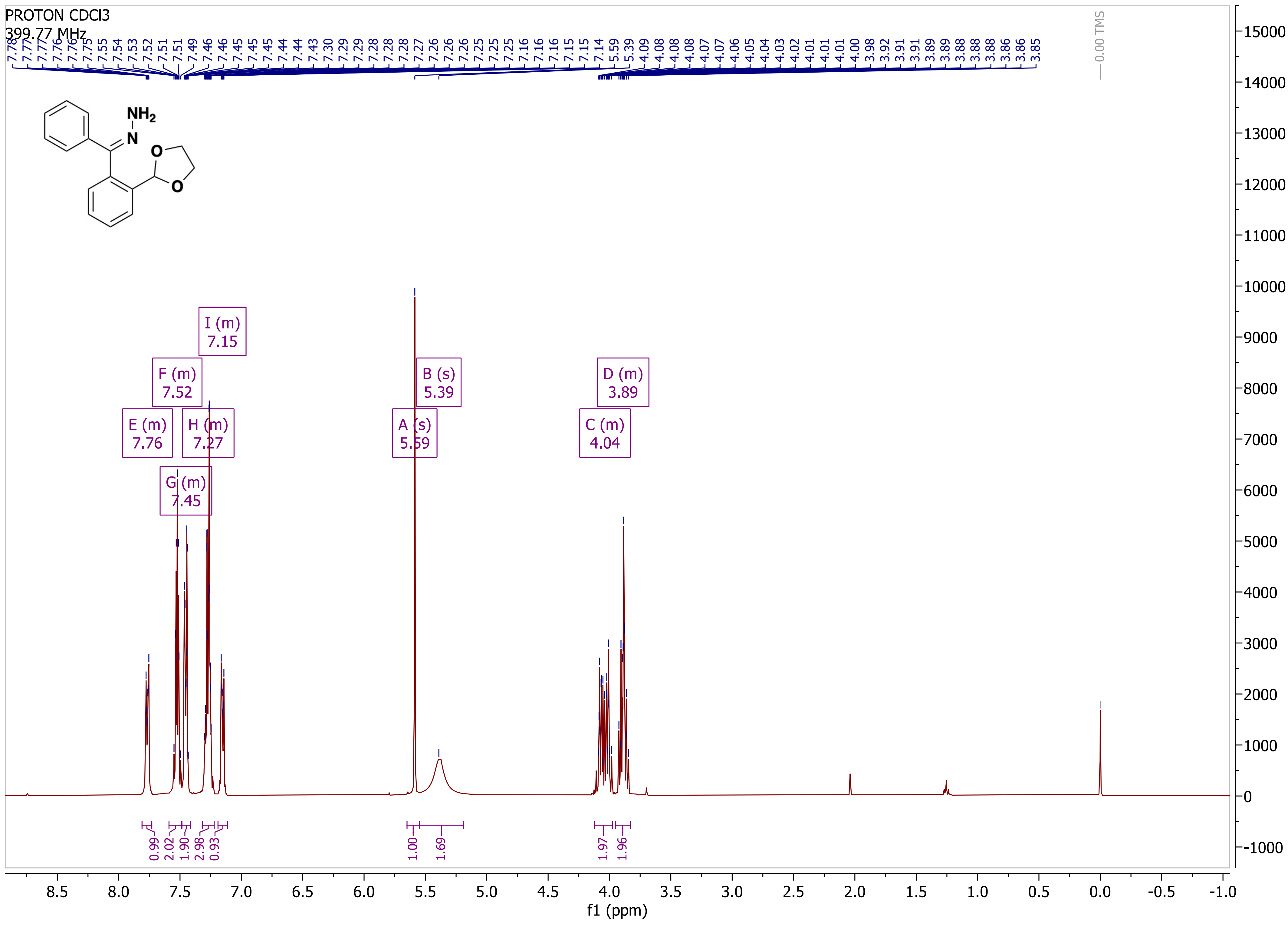
399.77 MHz
7.81
7.79
7.71
7.69
7.59
7.57
7.55
7.54
7.52
7.50
7.46
7.45
7.43
7.41
7.34
7.32
6.02
3.89
0.00 TMS
F (m)
7.44
D (d)
7.70
C (d)
7.80
G (d)
7.33
A (s)
6.02
B (s)
3.89
E (m)
7.55
2.00
1.01
2.07
3.00
1.00
1.00
4.00
f1 (ppm)


C13CPD CDCl3
100.53 MHz
197.57
138.54
137.64
136.94
133.12
130.09
130.00
128.43
128.36
128.10
127.09
101.51
77.16 CDCl3
65.14
O
O
O
f1 (ppm)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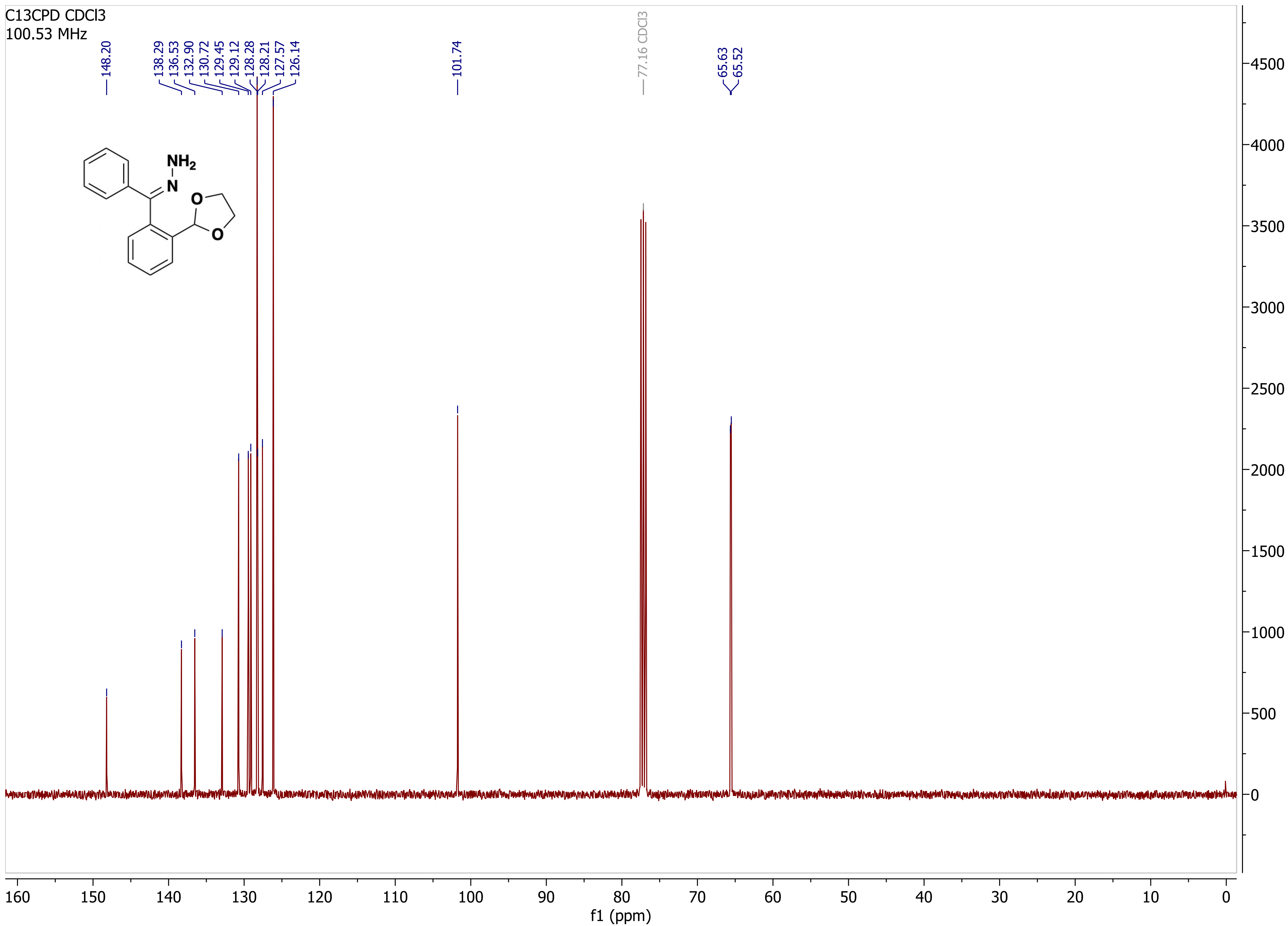
399.77 MHz
7.78 7.77 7.77 7.76 7.76 7.75 7.55 7.54 7.53 7.52 7.51 7.51 7.49 7.46 7.46 7.45 7.45 7.45 7.44 7.44 7.43 7.30 7.29 7.29 7.28 7.28 7.28 7.27 7.26 7.26 7.26 7.25 7.25 7.25 7.16 7.16 7.16 7.15 7.15 7.14 5.59 5.39 4.09 4.08 4.08 4.08 4.07 4.07 4.06 4.05 4.04 4.03 4.02 4.01 4.01 4.01 4.00 3.98 3.92 3.91 3.91 3.89 3.89 3.88 3.88 3.86 3.86 3.85
0.00 TMS
NH2
N
O
O
I (m) 7.15
F (m) 7.52
B (s) 5.39
D (m) 3.89
E (m) 7.76
H (m) 7.27
A (s) 5.59
C (m) 4.04
G (m) 7.45
0.99 2.02 1.90 2.98 0.93
1.00 1.69
1.97 1.96
f1 (ppm)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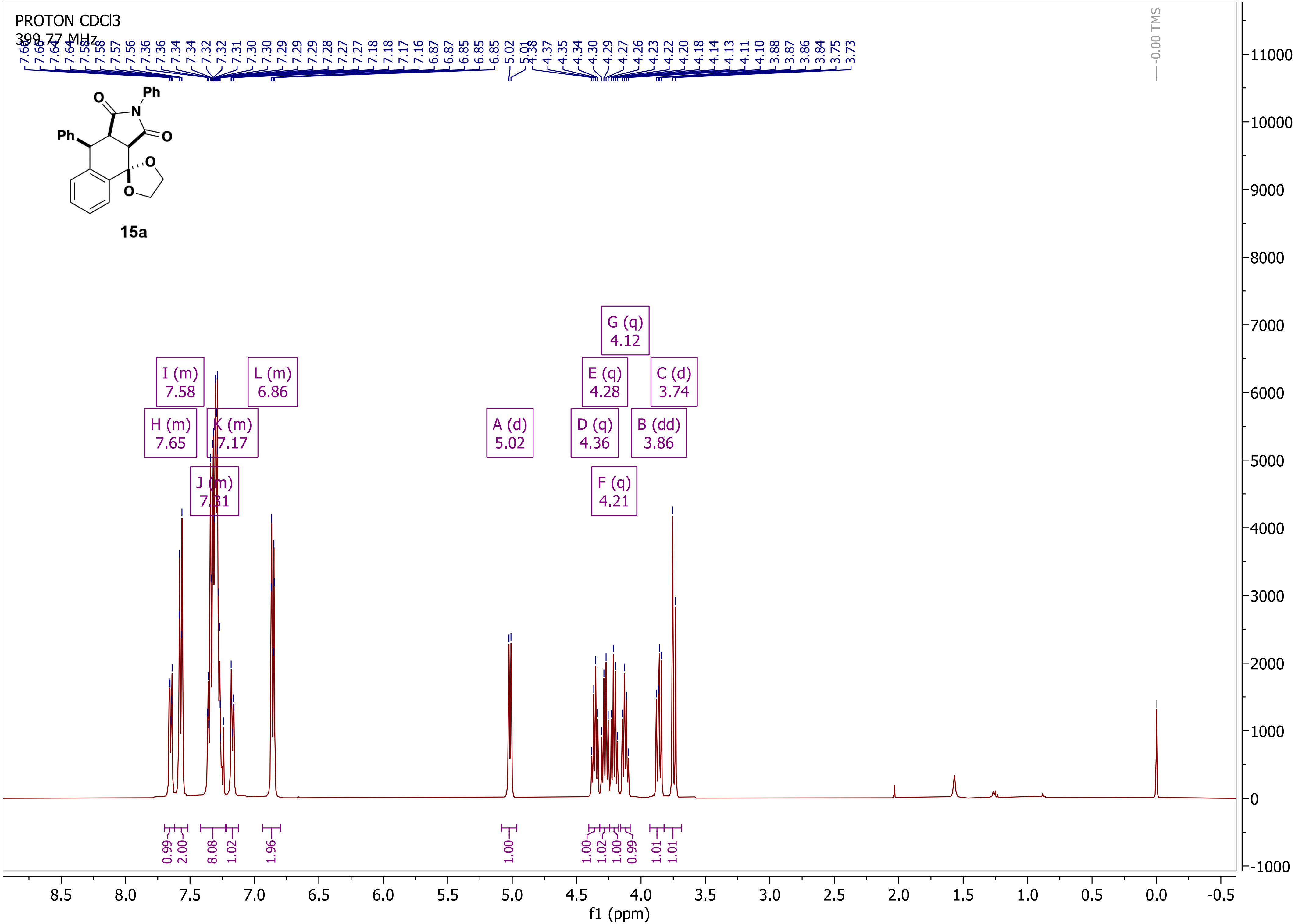
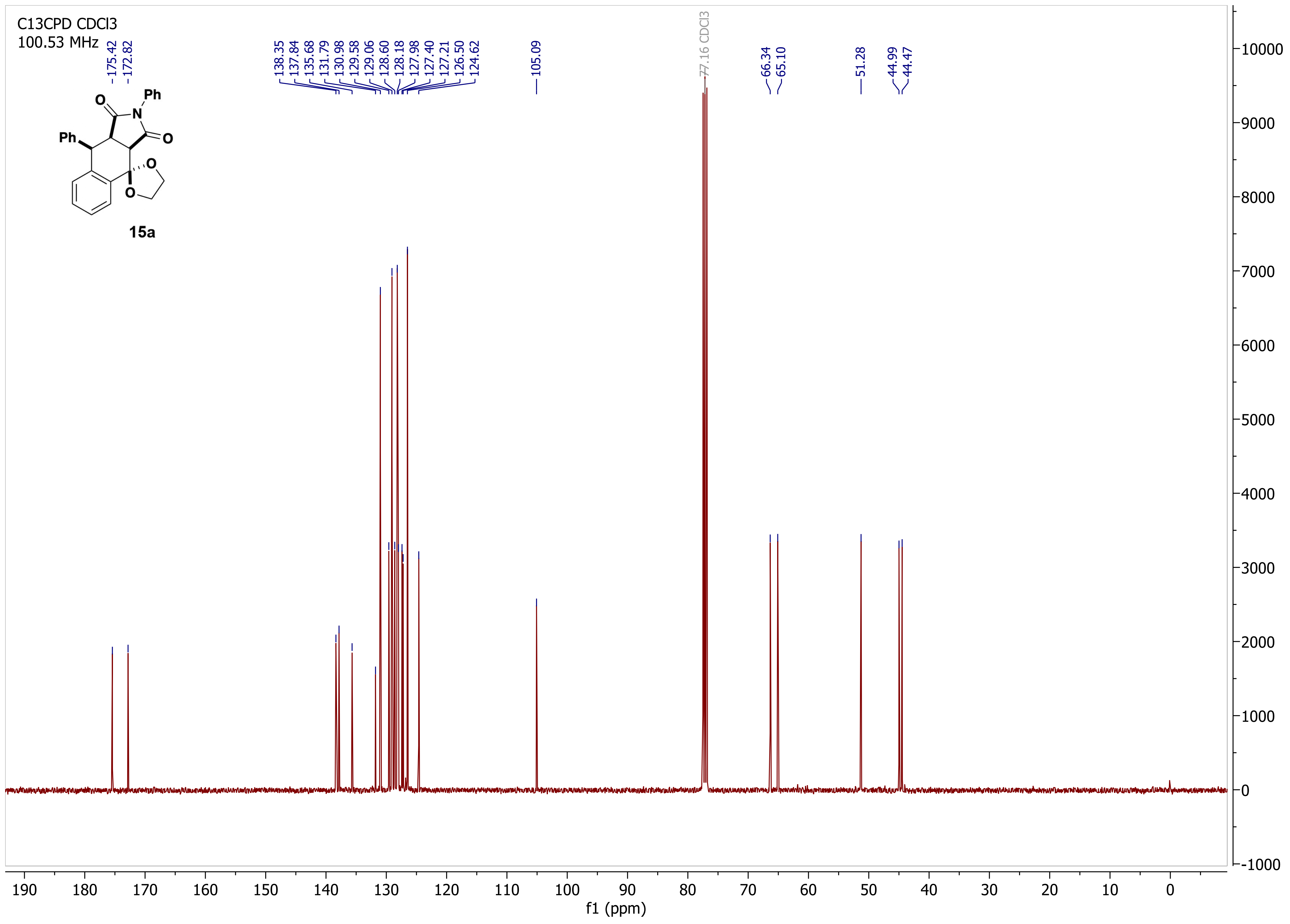
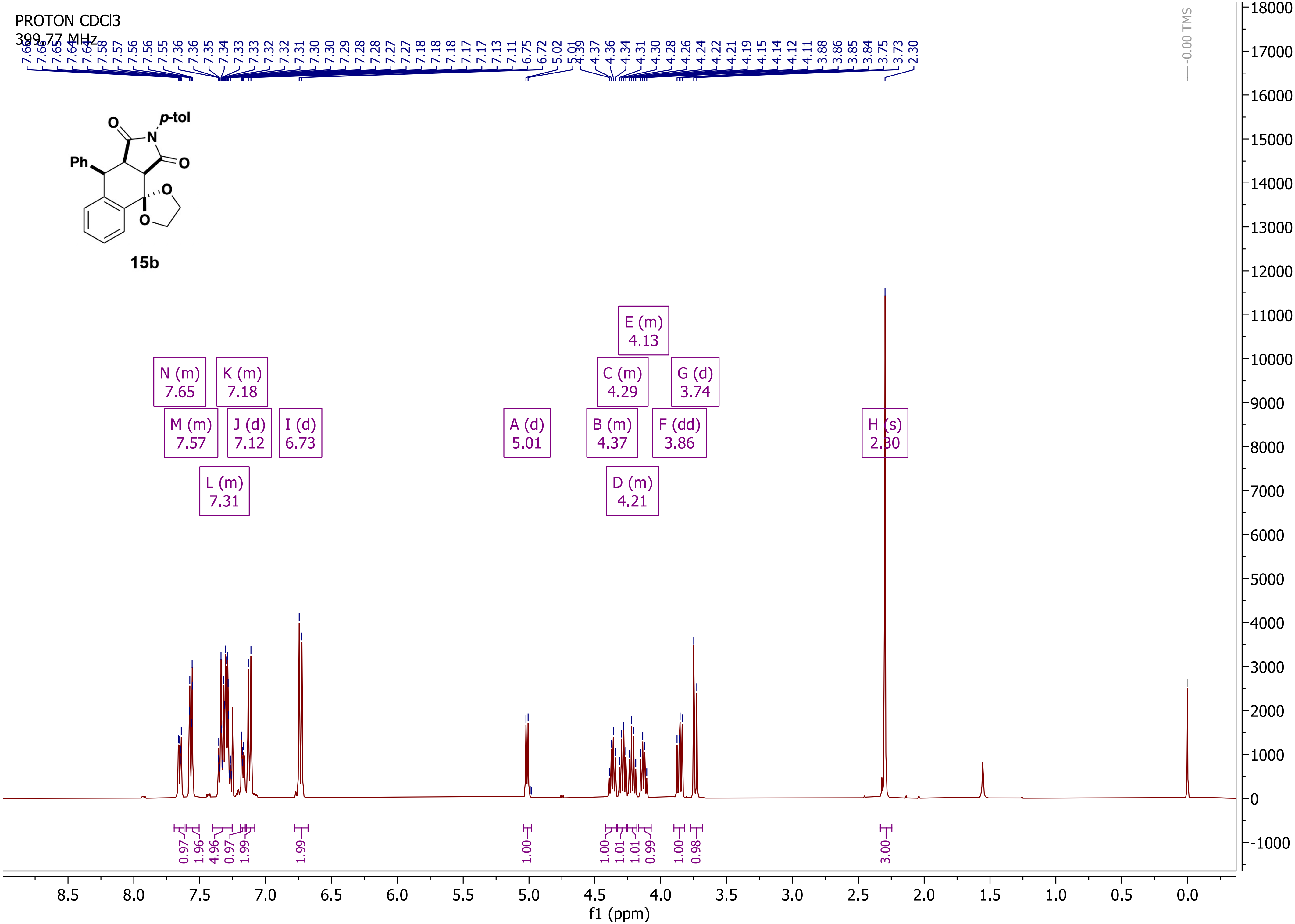
100.53 MHz
148.20
138.29
136.53
132.90
130.72
129.45
129.12
128.28
128.21
127.57
126.14
101.74
77.16 CDCl3
65.63
65.52
NH2
N
O
O
4500
4000
3500
3000
2500
2000
1500
1000
500
0
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

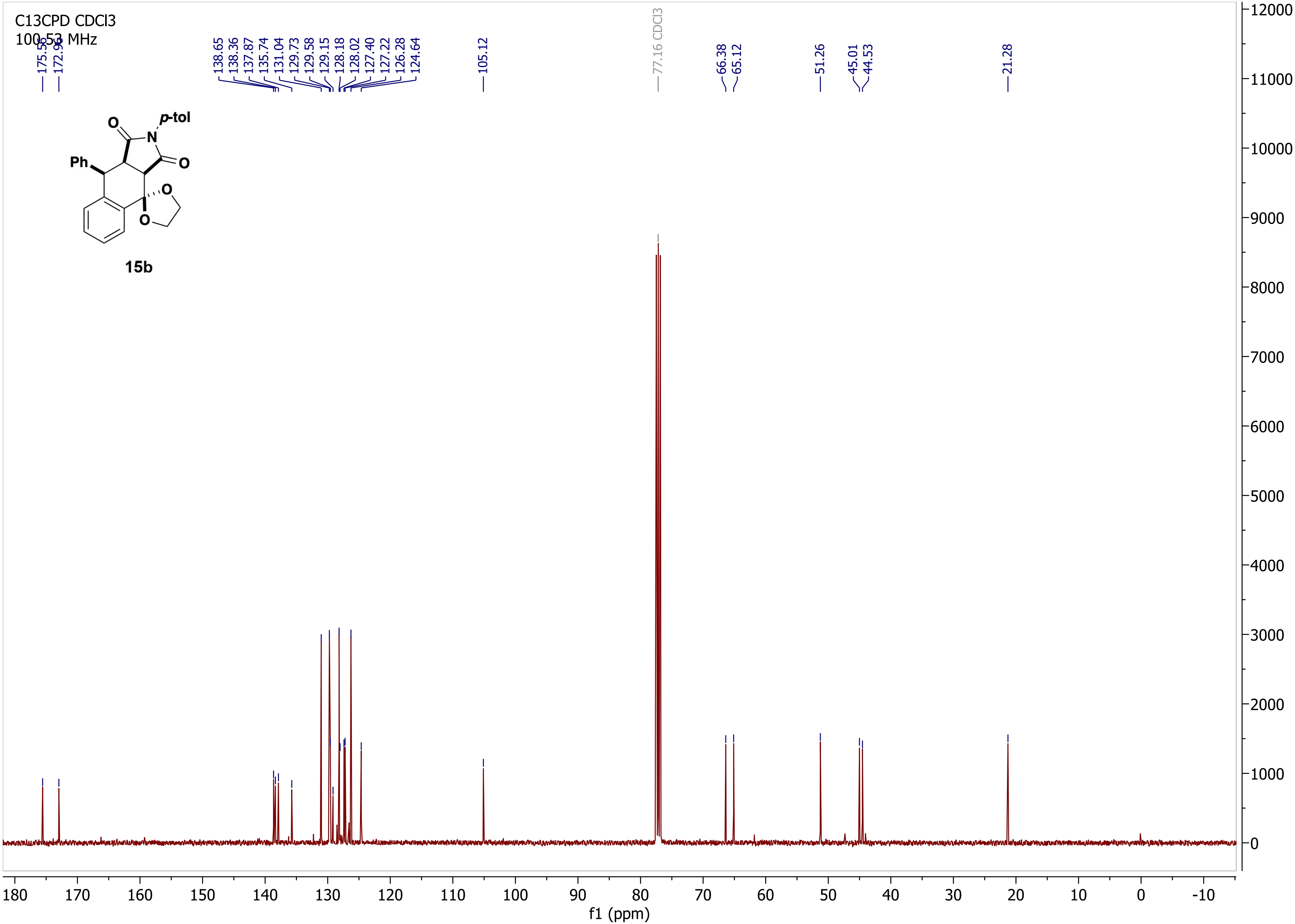


PROTON CDCl3
399.77 MHz
7.66 7.65 7.64 7.64 7.58 7.58 7.57 7.56 7.36 7.36 7.34 7.34 7.32 7.32 7.31 7.30 7.30 7.29 7.29 7.29 7.28 7.27 7.27 7.18 7.18 7.17 7.16 6.87 6.87 6.85 6.85 6.85
5.02 5.01 4.38 4.37 4.35 4.34 4.30 4.29 4.27 4.26 4.23 4.22 4.20 4.18 4.14 4.13 4.11 4.10 3.88 3.87 3.86 3.84 3.75 3.73
0.00 TMS
Ph
O
N
Ph
O
O
O
15a
I (m) 7.58
H (m) 7.65
K (m) 7.17
J (m) 7.31
L (m) 6.86
A (d) 5.02
G (q) 4.12
E (q) 4.28
D (q) 4.36
F (q) 4.21
C (d) 3.74
B (dd) 3.86
0.99 2.00 8.08 1.02 1.96 1.00 1.00 1.02 1.00 0.99 1.01 1.01
f1 (ppm)

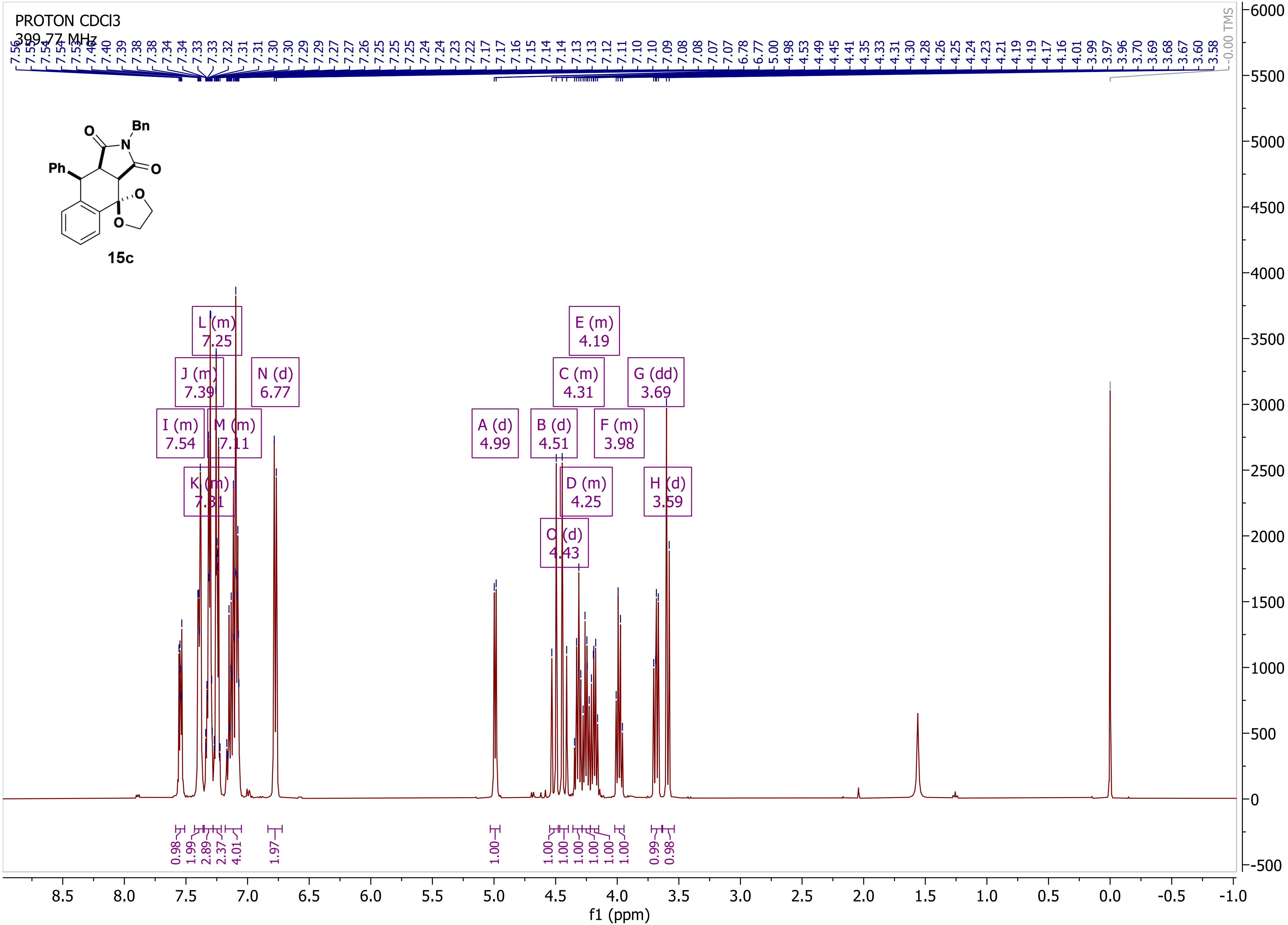


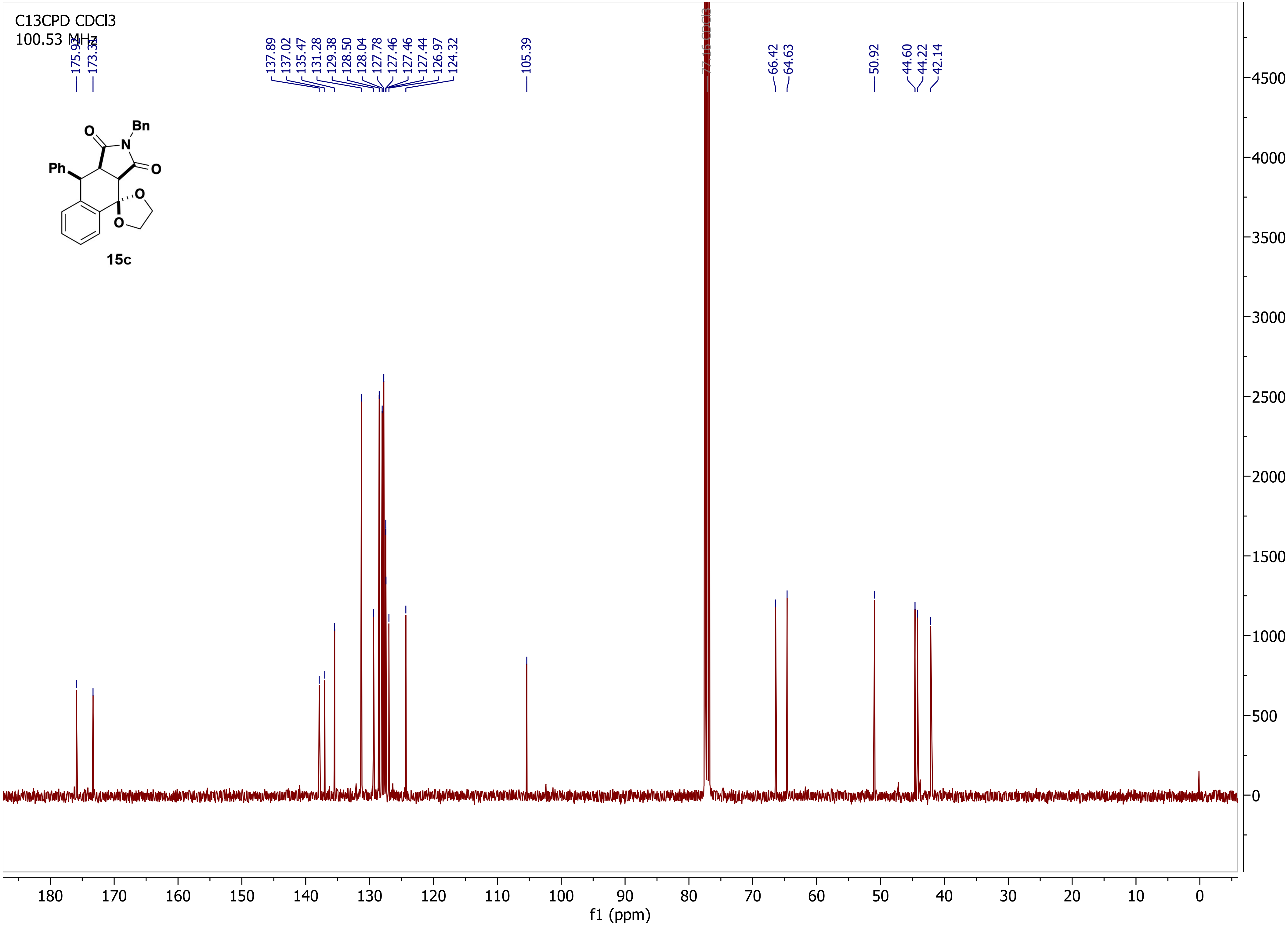
C13CPD CDCl3
100.53 MHz
175.42
172.82
138.35
137.84
135.68
131.79
130.98
129.58
129.06
128.60
128.18
127.98
127.40
127.21
126.50
124.62
105.09
77.16 CDCl3
66.34
65.10
51.28
44.99
44.47
Ph
O
N
O
Ph
O
O
15a
f1 (ppm)

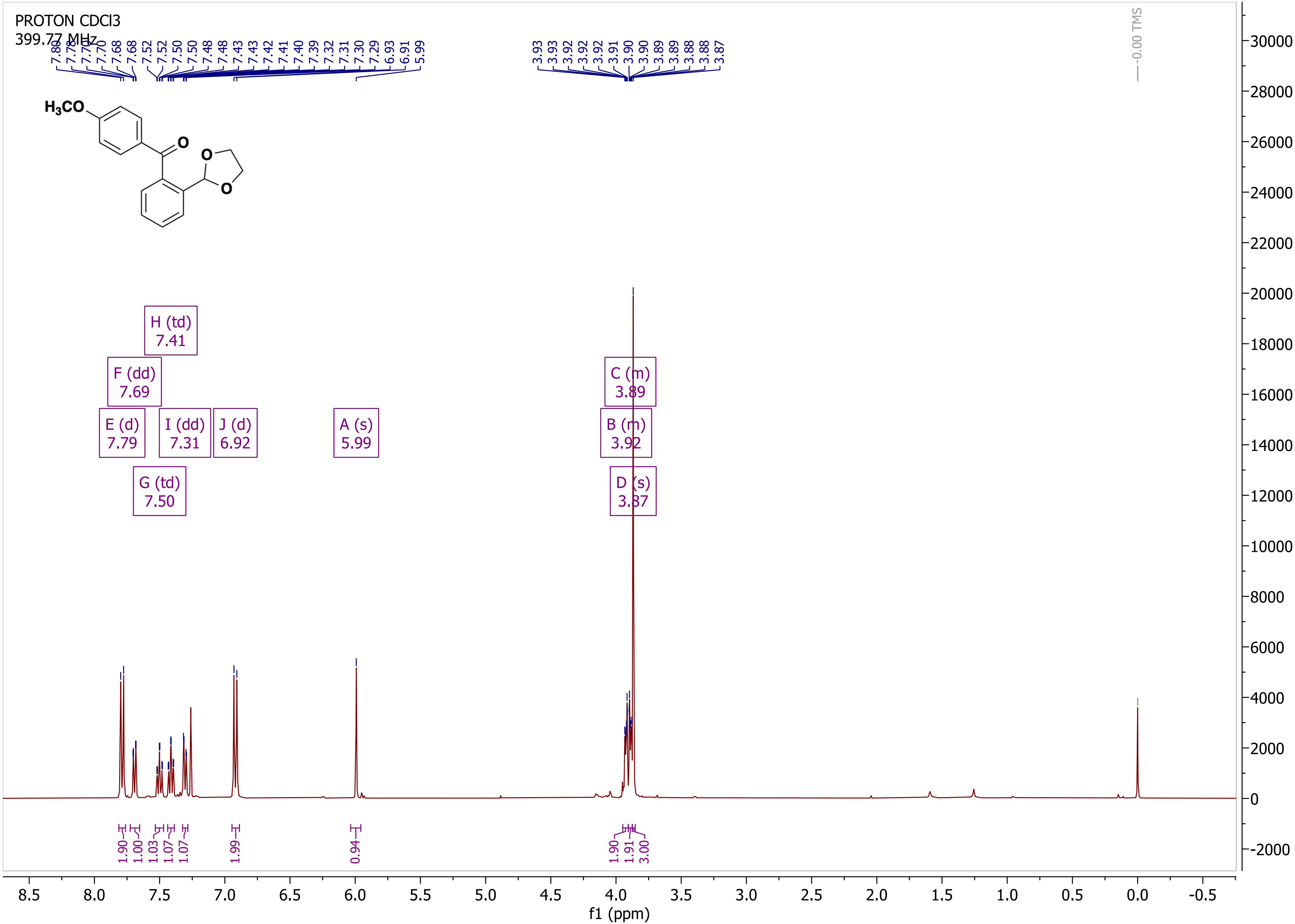

PROTON CDCl3
399.77 MHz
p-tol
O
N
O
Ph
O
O
15b
N (m) 7.65
M (m) 7.57
K (m) 7.18
L (m) 7.31
J (d) 7.12
I (d) 6.73
A (d) 5.01
B (m) 4.37
C (m) 4.29
D (m) 4.21
E (m) 4.13
F (dd) 3.86
G (d) 3.74
H (s) 2.30
0.00 TMS
0.97
1.96
4.96
0.97
1.99
1.99
1.00
1.00
1.01
1.01
0.99
1.00
0.98
3.00
f1 (ppm)



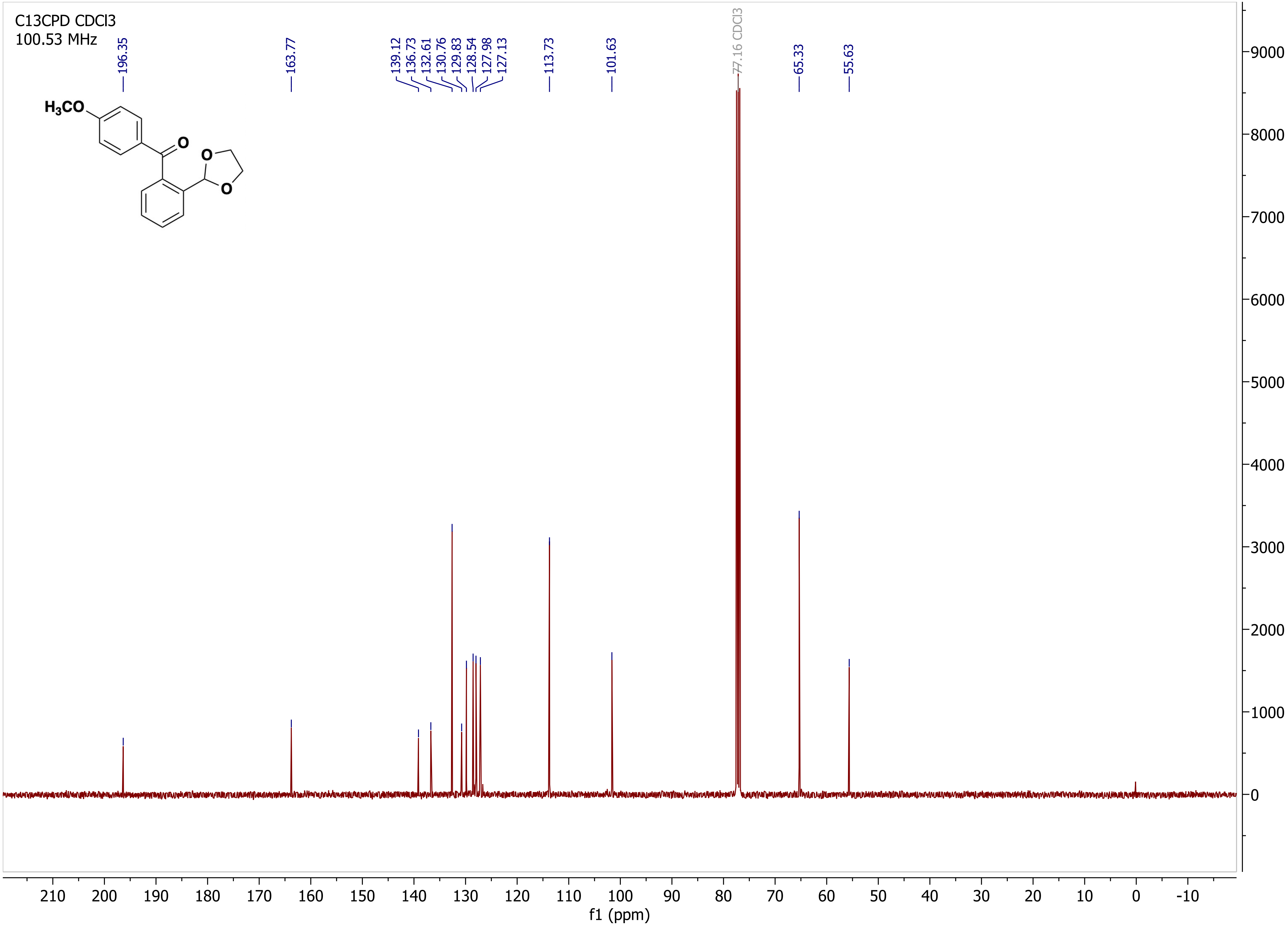
C13CPD CDCl3
100.53 MHz
175.5
172.9
138.65
138.36
137.87
135.74
131.04
129.73
129.58
129.15
128.18
128.02
127.40
127.22
126.28
124.64
105.12
77.16 CDCl3
66.38
65.12
51.26
45.01
44.53
21.28
p-tol
N
O
O
Ph
O
O
15b
12000
11000
10000
9000
8000
7000
6000
5000
4000
3000
2000
1000
0
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)


PROTON CDCl3
399.77 MHz
Bn
Ph
15c
I (m) 7.54
J (m) 7.39
K (m) 7.31
L (m) 7.25
M (m) 7.11
N (d) 6.77
A (d) 4.99
B (d) 4.51
O (d) 4.43
C (m) 4.31
D (m) 4.25
E (m) 4.19
F (m) 3.98
G (dd) 3.69
H (d) 3.59
-0.00 TMS
f1 (ppm)

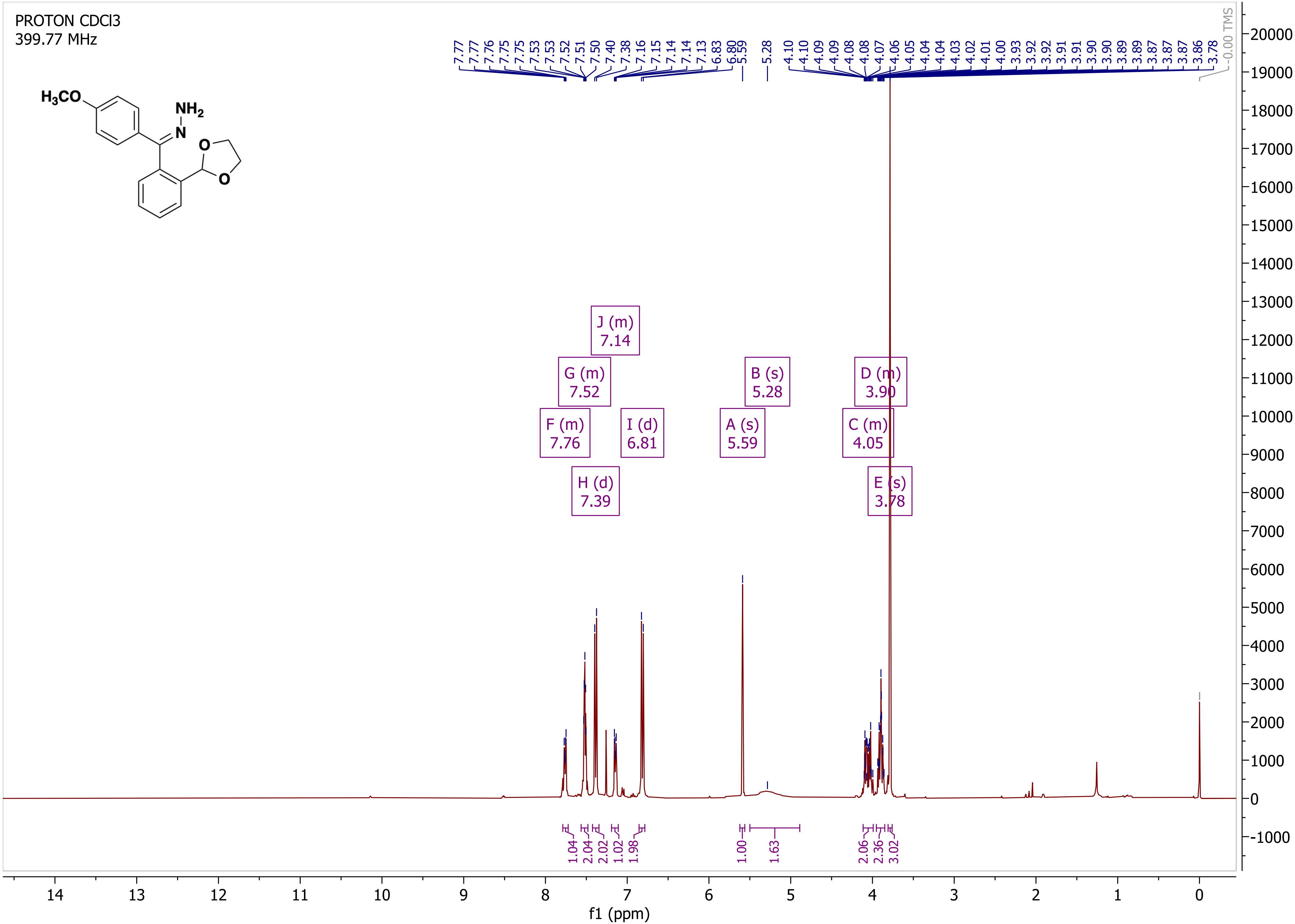

C13CPD CDCl3
100.53 MHz
175.93
173.36
137.89
137.02
135.47
131.28
129.38
128.50
128.04
127.78
127.46
127.46
127.44
126.97
124.32
105.39
77.16 CDCl3
66.42
64.63
50.92
44.60
44.22
42.14
Bn
O
N
O
Ph
O
O
15c
4500
4000
3500
3000
2500
2000
1500
1000
500
0
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

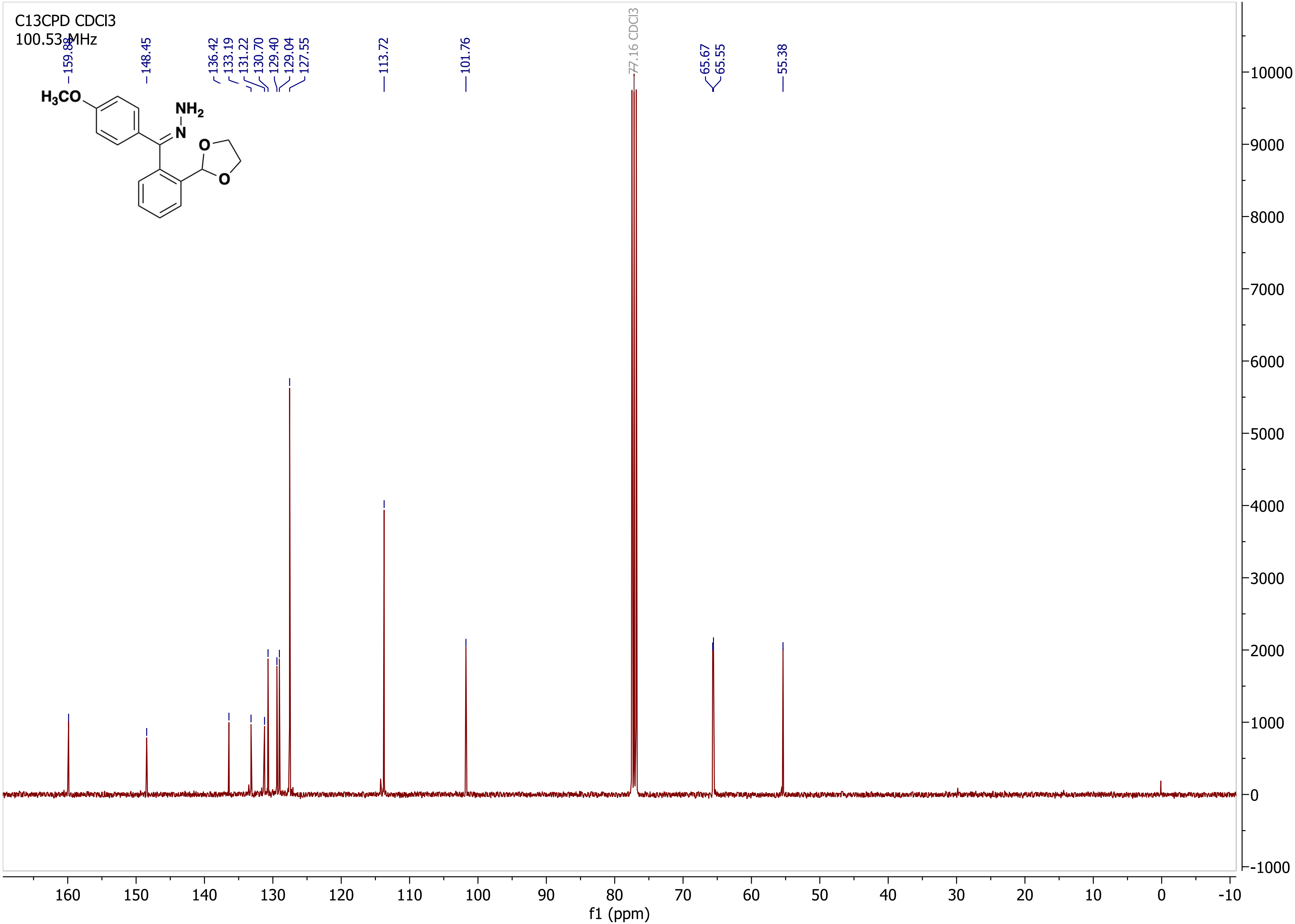


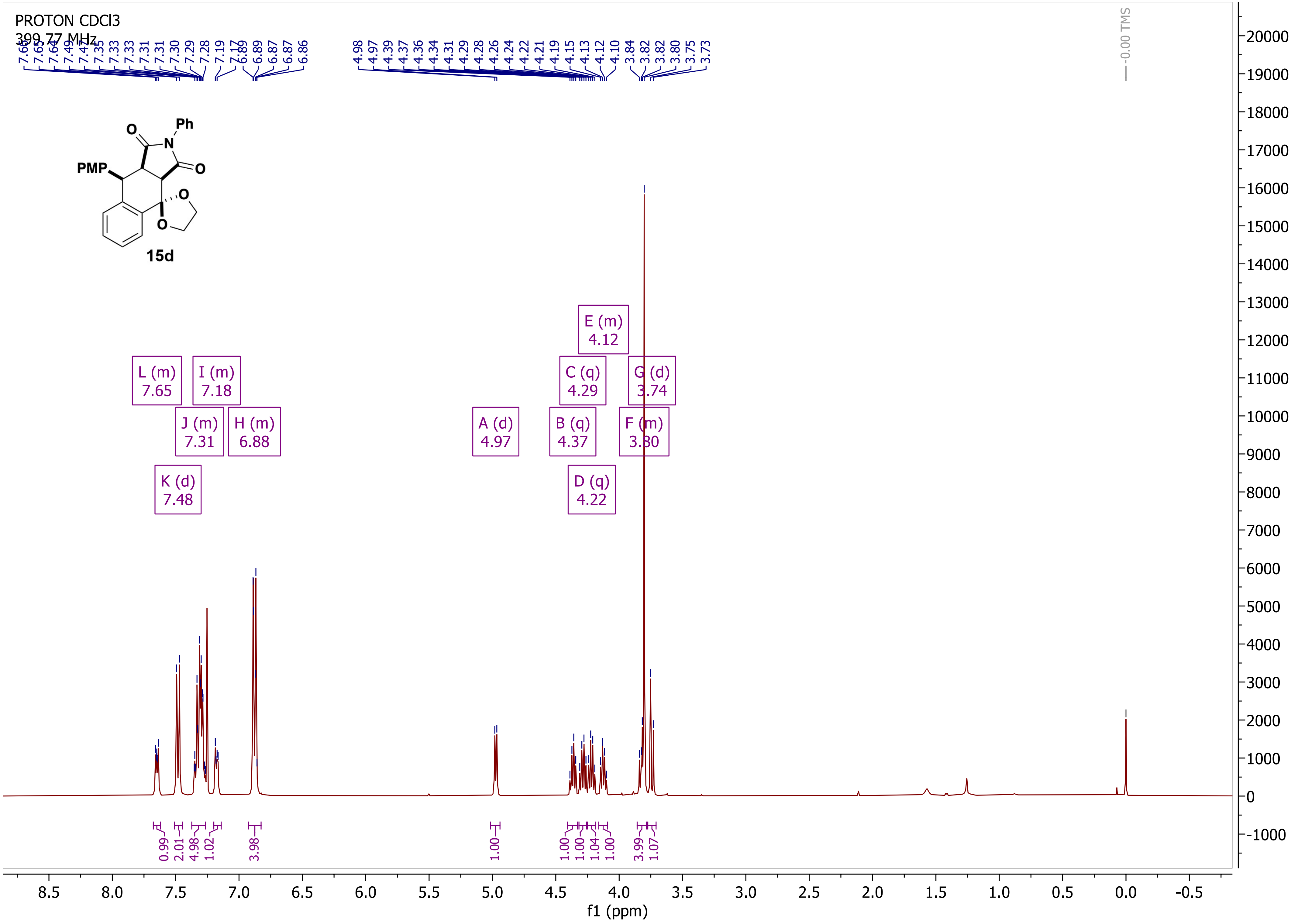
PROTON CDCl3
399.77 MHz
H3CO
O
O
O
H (td)
7.41
F (dd)
7.69
E (d)
7.79
I (dd)
7.31
J (d)
6.92
A (s)
5.99
C (m)
3.89
B (m)
3.92
G (td)
7.50
D (s)
3.87
0.00 TMS
1.90
1.00
1.03
1.07
1.07
1.99
0.94
1.90
1.91
3.00
f1 (ppm)

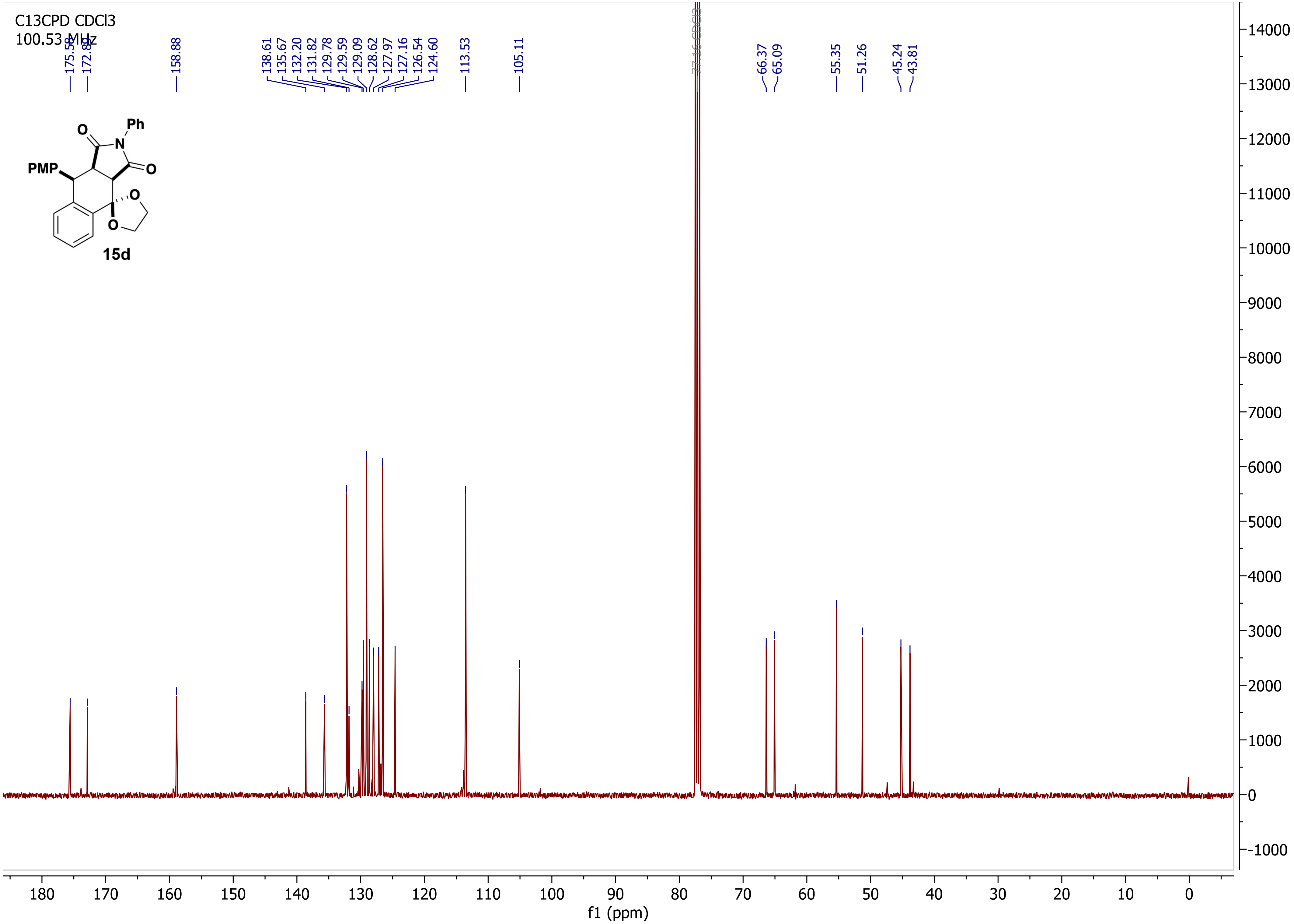


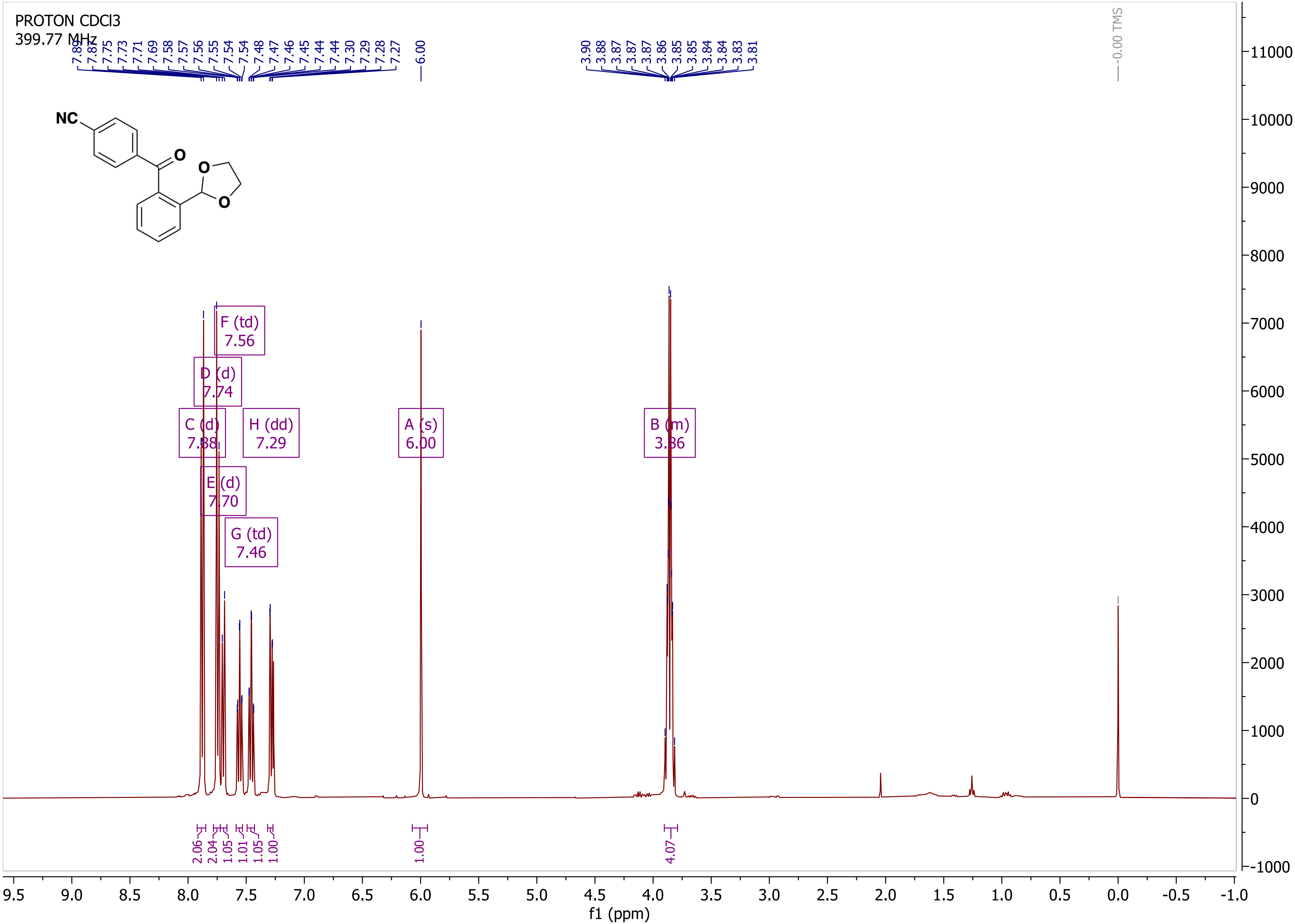
C13CPD CDCl3
100.53 MHz
196.35
163.77
139.12
136.73
132.61
130.76
129.83
128.54
127.98
127.13
113.73
101.63
77.16 CDCl3
65.33
55.63
H3CO
O
O
O
f1 (ppm)
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
9000
8000
7000
6000
5000
4000
3000
2000
1000
0


PROTON CDCl3
399.77 MHz
H3CO
NH2
N
O
O
7.77 7.77 7.76 7.75 7.75 7.53 7.53 7.52 7.51 7.50 7.40 7.38 7.16 7.15 7.14 7.14 7.13 6.83 6.80 5.59 5.28 4.10 4.10 4.09 4.09 4.08 4.08 4.07 4.06 4.05 4.04 4.04 4.03 4.02 4.01 4.00 3.93 3.92 3.92 3.91 3.91 3.90 3.90 3.89 3.89 3.87 3.87 3.87 3.86 3.78
-0.00 TMS
J (m) 7.14
G (m) 7.52
F (m) 7.76
I (d) 6.81
H (d) 7.39
A (s) 5.59
B (s) 5.28
D (m) 3.90
C (m) 4.05
E (s) 3.78
1.04 2.04 2.02 1.02 1.98 1.00 1.63 2.06 2.36 3.02
f1 (ppm)

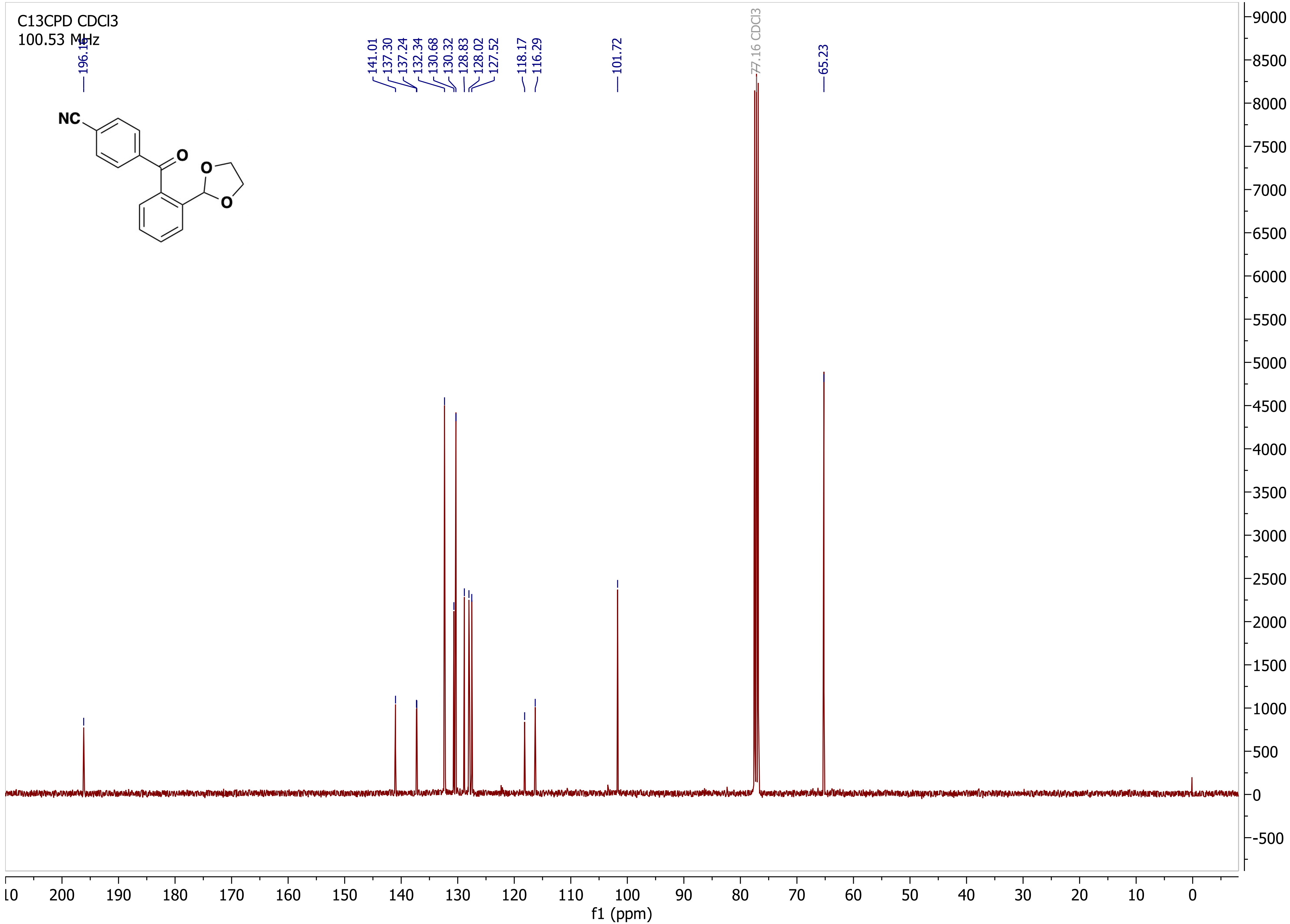

C13CPD CDCl3
100.53 MHz
159.88
148.45
136.42
133.19
131.22
130.70
129.40
129.04
127.55
113.72
101.76
77.16 CDCl3
65.67
65.55
55.38
H3CO
NH2
N
O
O
f1 (ppm)

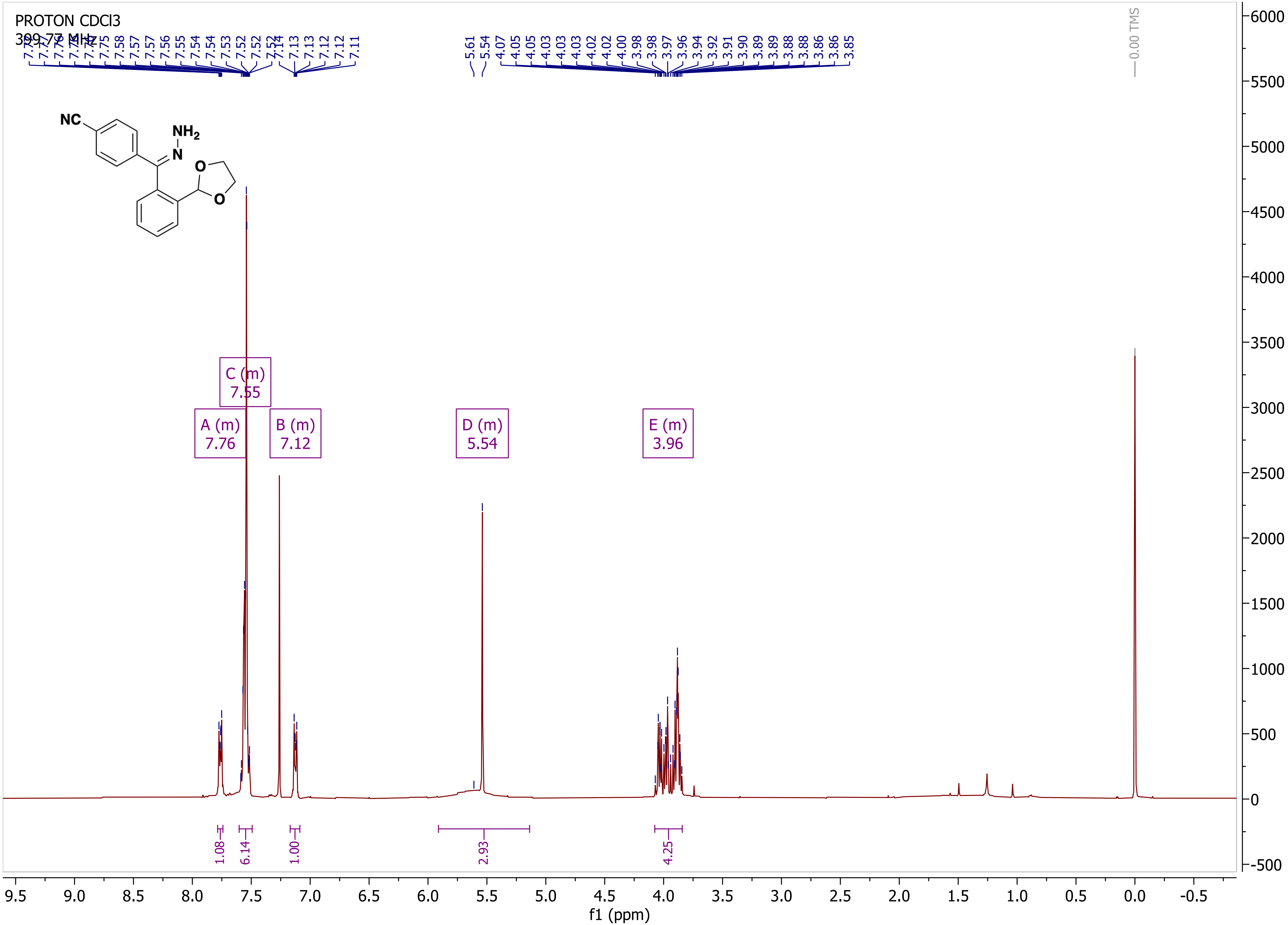

PROTON CDCl3
399.77 MHz
7.66 7.65 7.64 7.49 7.47 7.35 7.33 7.33 7.31 7.31 7.30 7.29 7.28 7.19 7.17 6.89 6.89 6.87 6.87 6.86
4.98 4.97 4.39 4.37 4.36 4.34 4.31 4.29 4.28 4.26 4.24 4.22 4.21 4.19 4.15 4.13 4.12 4.10 3.84 3.82 3.82 3.80 3.75 3.73
-0.00 TMS
Ph
N
O
O
PMP
O
O
15d
L (m) 7.65
I (m) 7.18
J (m) 7.31
H (m) 6.88
K (d) 7.48
A (d) 4.97
B (q) 4.37
C (q) 4.29
D (q) 4.22
E (m) 4.12
F (m) 3.80
G (d) 3.74
0.99 2.01 4.98 1.02 3.98 1.00 1.00 1.00 1.04 1.00 3.99 1.07
f1 (ppm)


C13CPD CDCl3
100.53 MHz
175.58
172.82
158.88
138.61
135.67
132.20
131.82
129.78
129.59
129.09
128.62
127.97
127.16
126.54
124.60
113.53
105.11
77.16 CDCl3
66.37
65.09
55.35
51.26
45.24
43.81
PMP
Ph
15d
f1 (ppm)

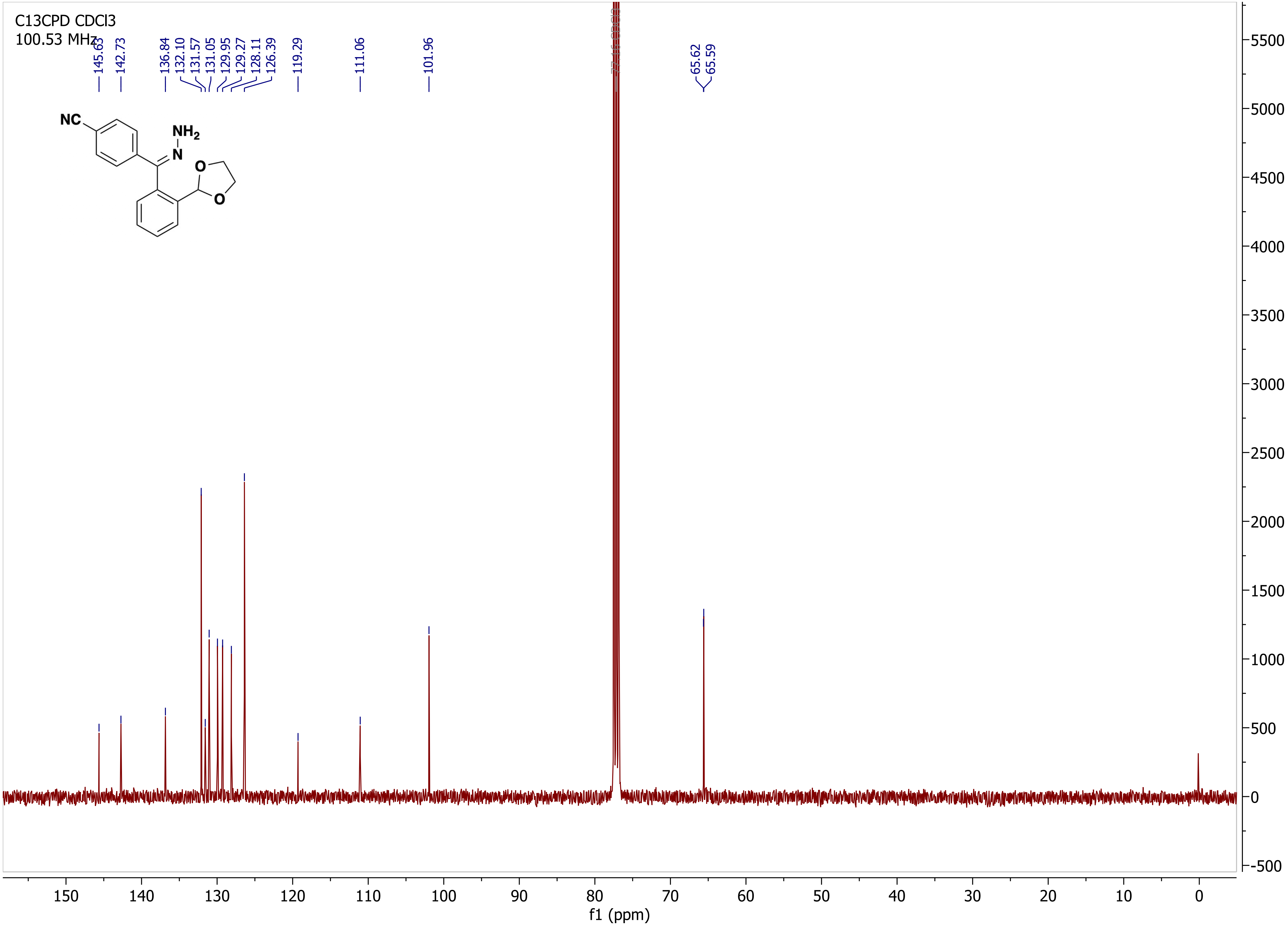


PROTON CDCl3
399.77 MHz
7.89
7.87
7.75
7.73
7.71
7.69
7.58
7.57
7.56
7.55
7.54
7.54
7.48
7.47
7.46
7.45
7.44
7.44
7.30
7.29
7.28
7.27
6.00
3.90
3.88
3.87
3.87
3.87
3.86
3.85
3.85
3.84
3.84
3.83
3.81
-0.00 TMS
NC
O
O
O
F (td) 7.56
D (d) 7.74
C (d) 7.88
H (dd) 7.29
A (s) 6.00
B (m) 3.86
E (d) 7.70
G (td) 7.46
2.06
2.04
1.05
1.01
1.05
1.00
1.00
4.07
f1 (ppm)

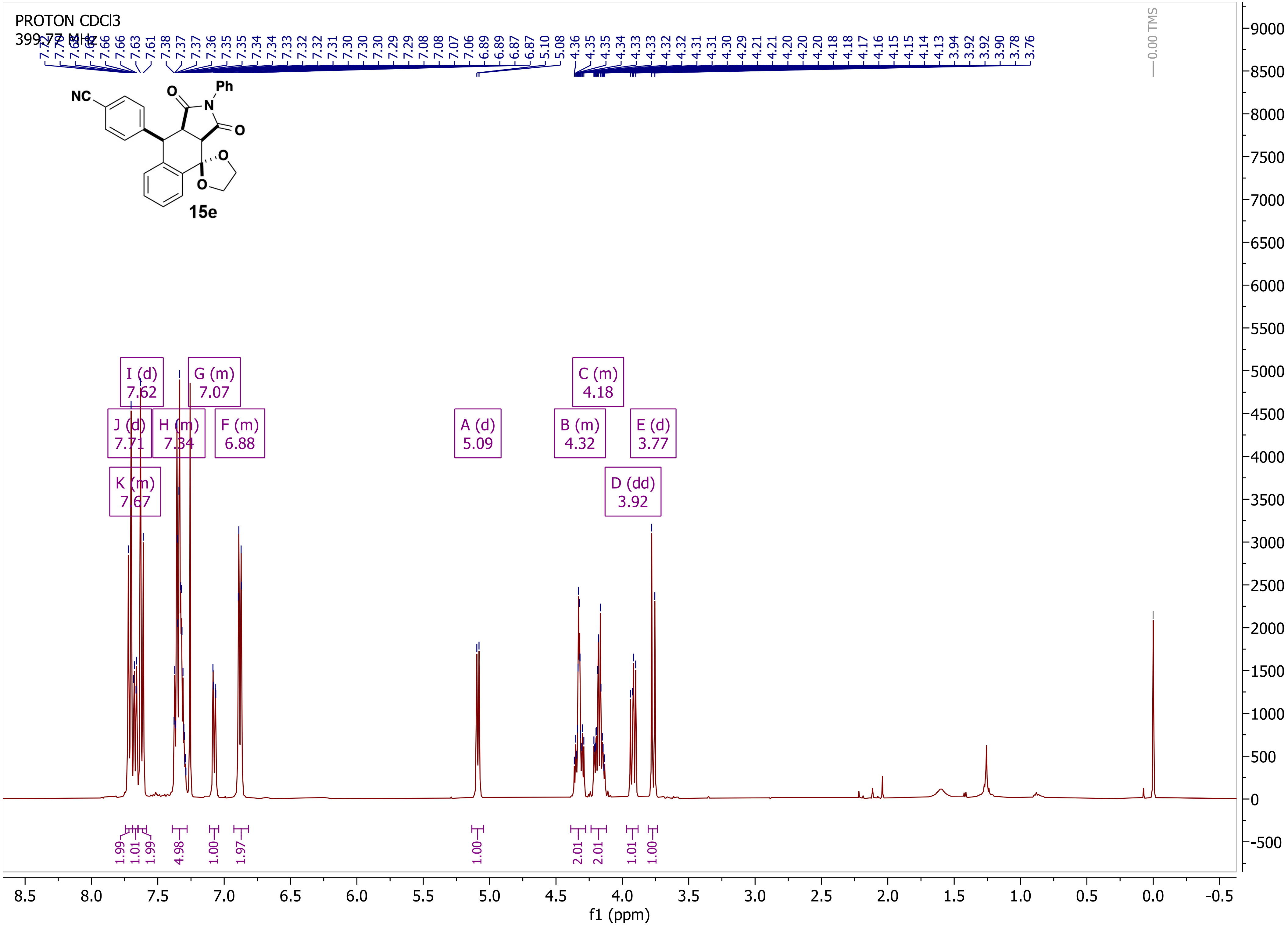

C13CPD CDCl3
100.53 MHz
196.15
141.01
137.30
137.24
132.34
130.68
130.32
128.83
128.02
127.52
118.17
116.29
101.72
77.16 CDCl3
65.23
NC
O
O
O
f1 (ppm)



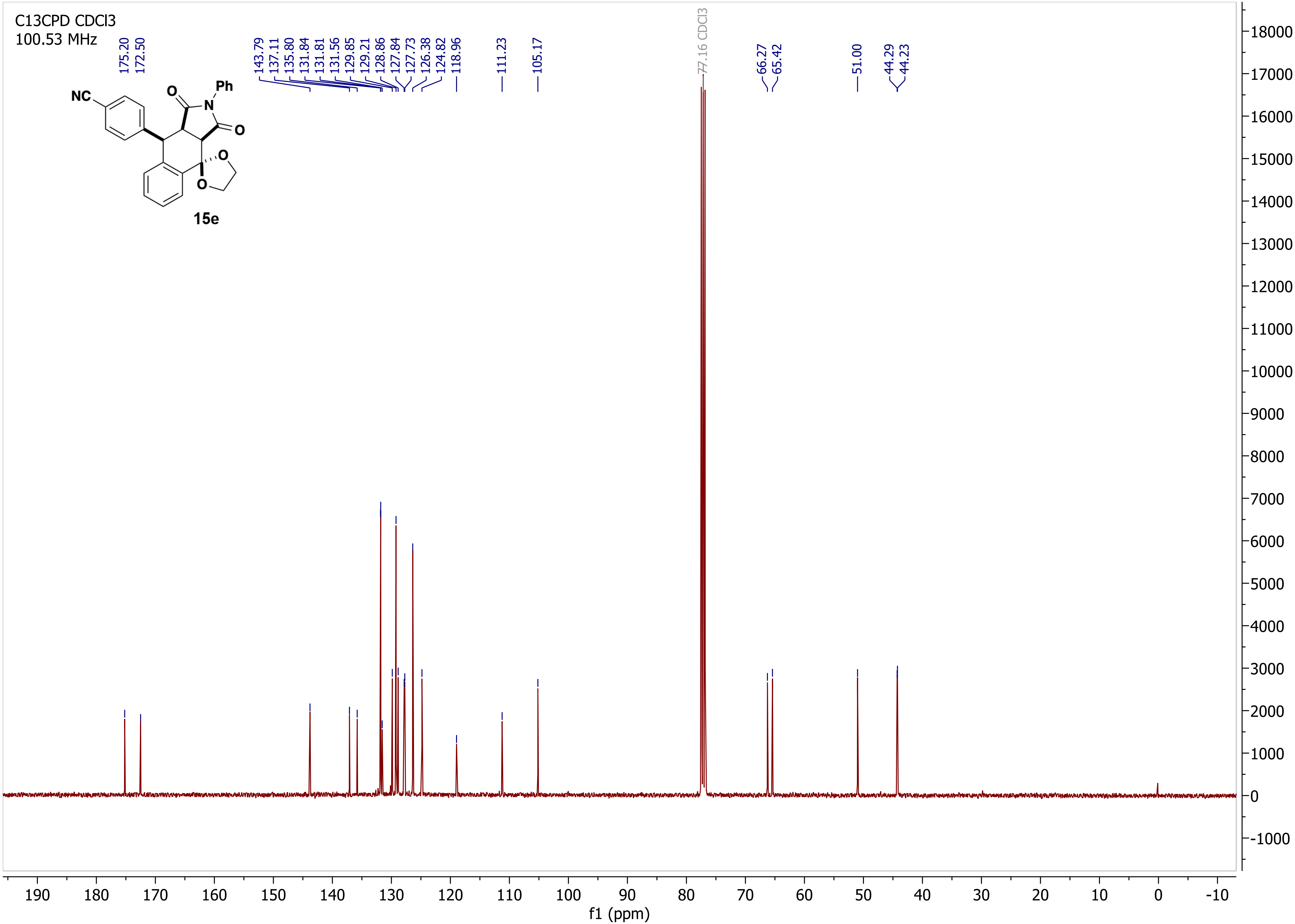
PROTON CDCl3
399.73 MHz
NC
NH2
N
O
O
A (m) 7.76
B (m) 7.12
C (m) 7.55
D (m) 5.54
E (m) 3.96
1.08
6.14
1.00
2.93
4.25
0.00 TMS
f1 (ppm)

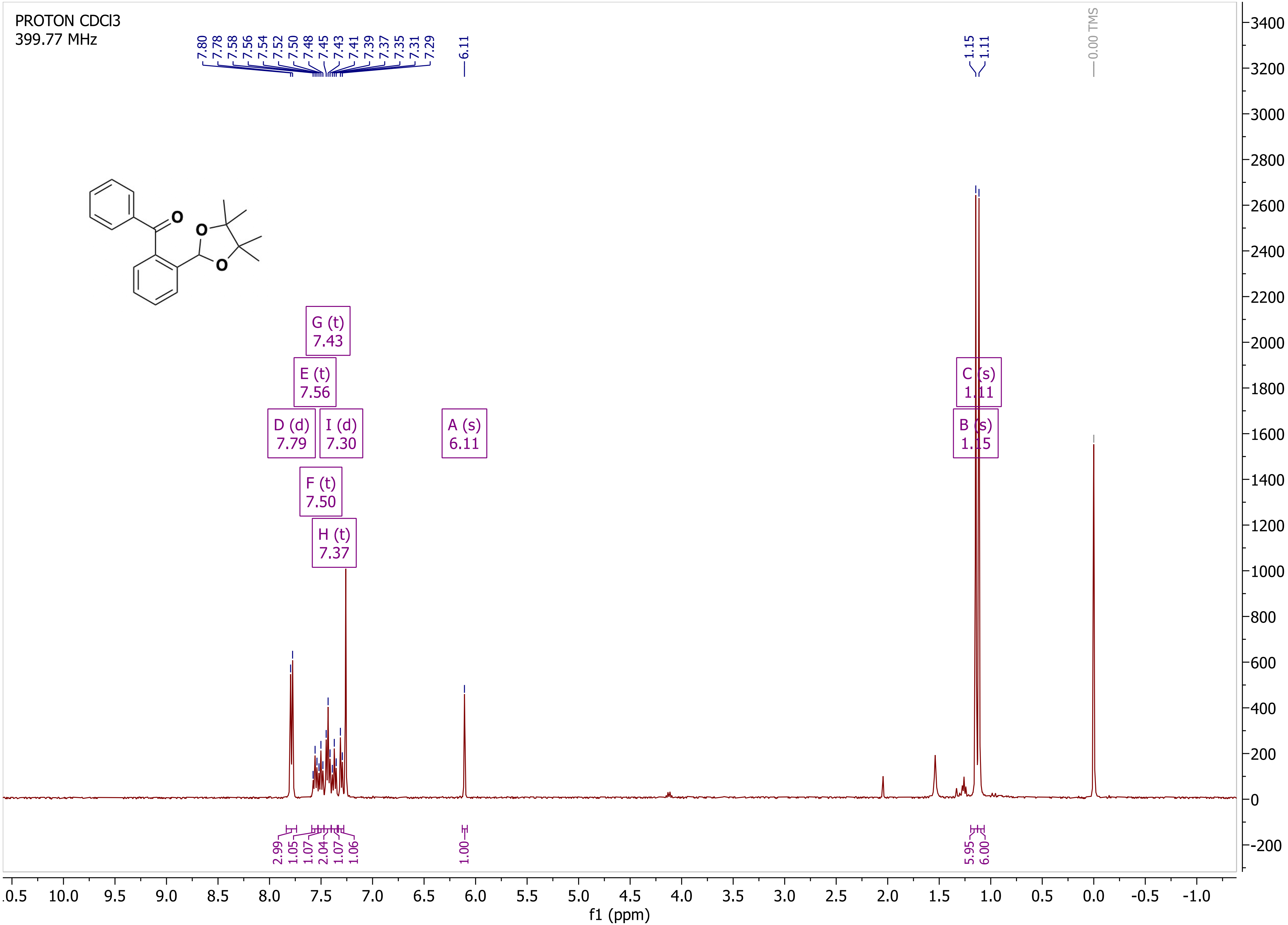


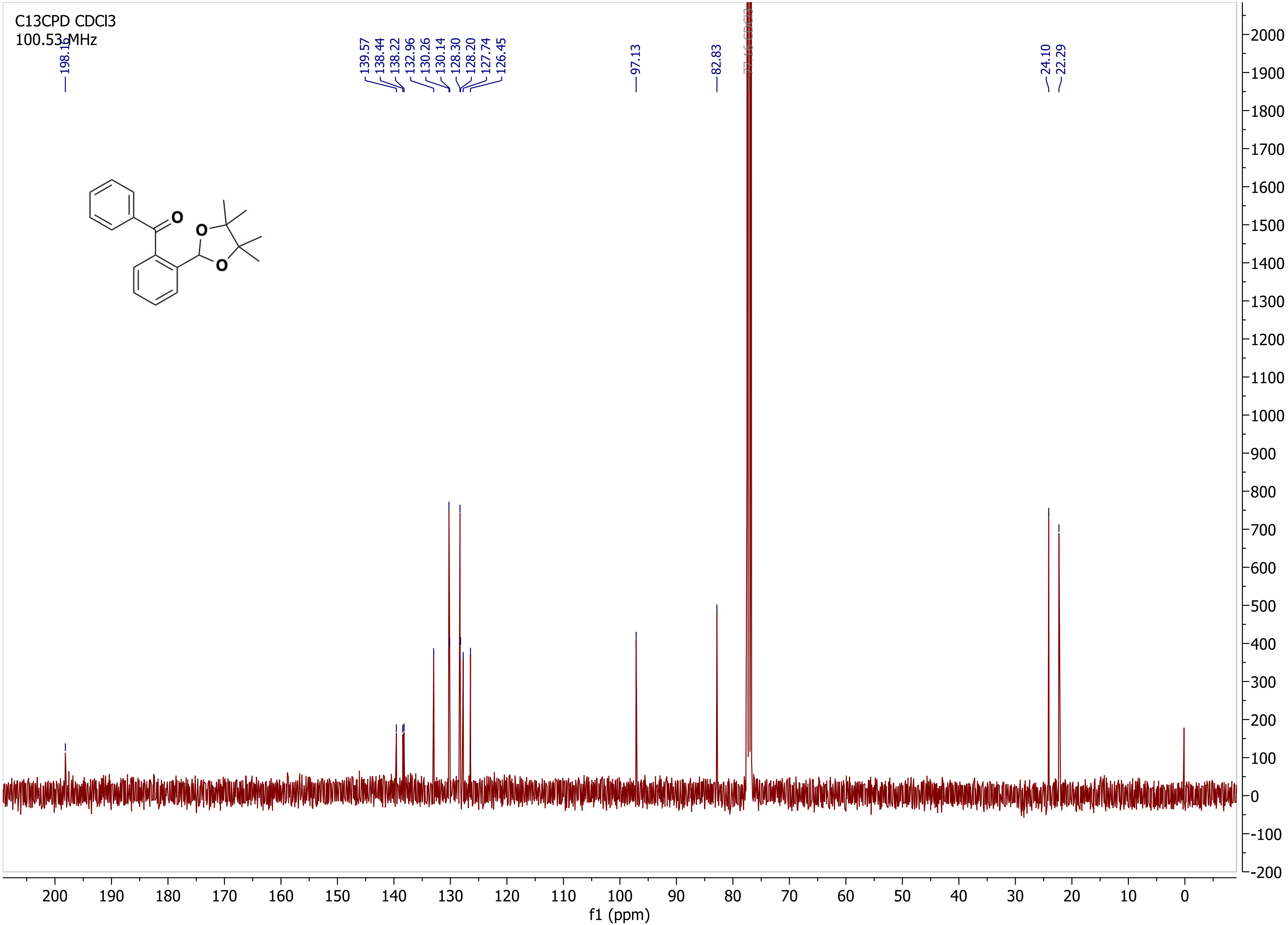
C13CPD CDCl3
100.53 MHz
145.63
142.73
136.84
132.10
131.57
131.05
129.95
129.27
128.11
126.39
119.29
111.06
101.96
65.62
65.59
NC
NH2
N
O
O
f1 (ppm)



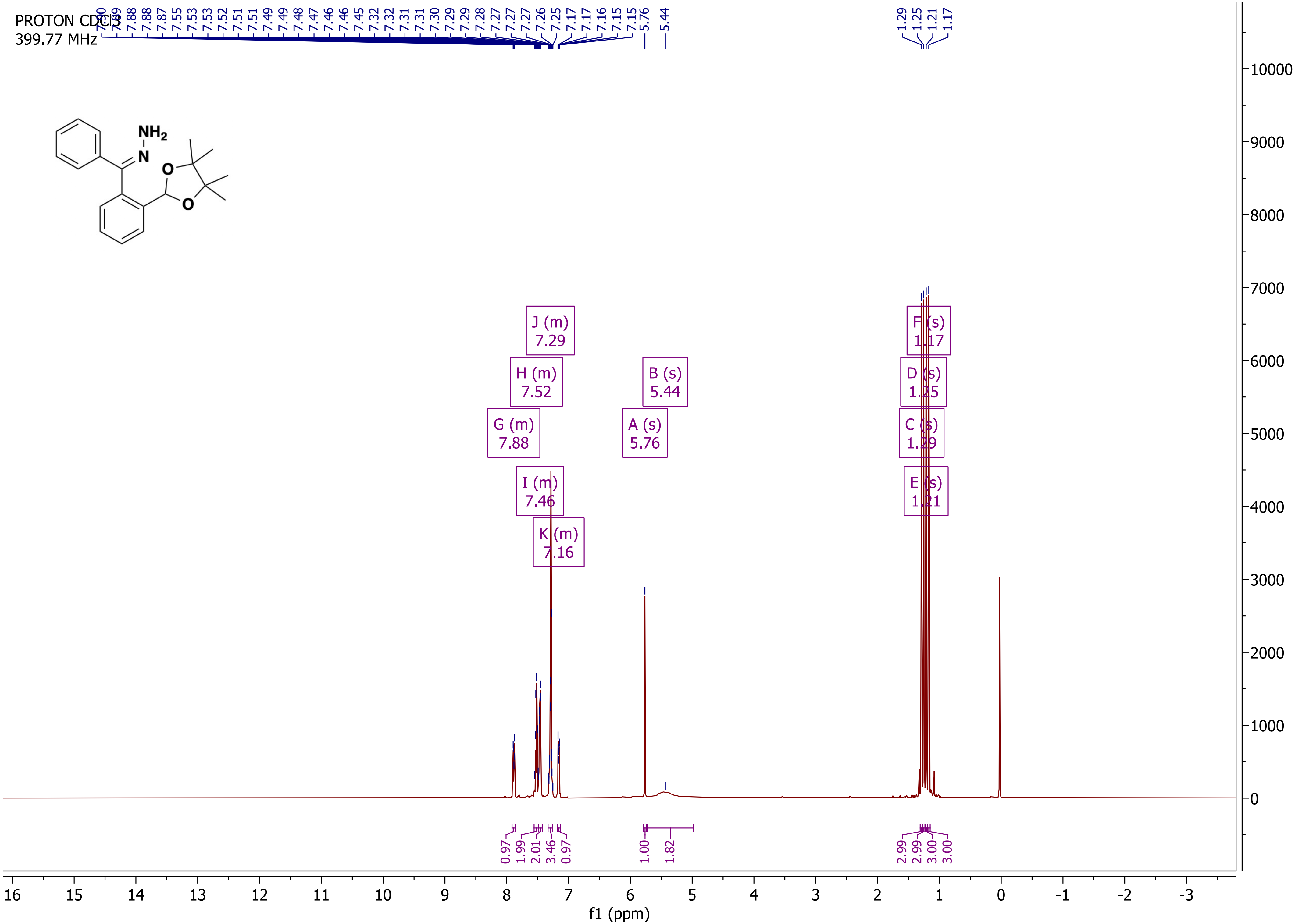
PROTON CDCl3
399.77 MHz
7.66
7.66
7.63
7.61
7.38
7.37
7.37
7.36
7.35
7.35
7.34
7.34
7.33
7.32
7.32
7.31
7.30
7.30
7.29
7.29
7.08
7.08
7.07
7.06
6.89
6.89
6.87
6.87
5.10
5.08
4.36
4.35
4.35
4.34
4.33
4.33
4.32
4.32
4.31
4.31
4.30
4.29
4.21
4.21
4.20
4.20
4.20
4.18
4.18
4.17
4.16
4.15
4.15
4.14
4.13
3.94
3.92
3.92
3.90
3.78
3.76
0.00 TMS
NC
O
N
Ph
O
O
O
15e
I (d) 7.62
G (m) 7.07
C (m) 4.18
J (d) 7.71
H (m) 7.34
F (m) 6.88
A (d) 5.09
B (m) 4.32
E (d) 3.77
K (m) 7.67
D (dd) 3.92
1.99
1.01
1.99
4.98
1.00
1.97
1.00
2.01
2.01
1.01
1.00
f1 (ppm)

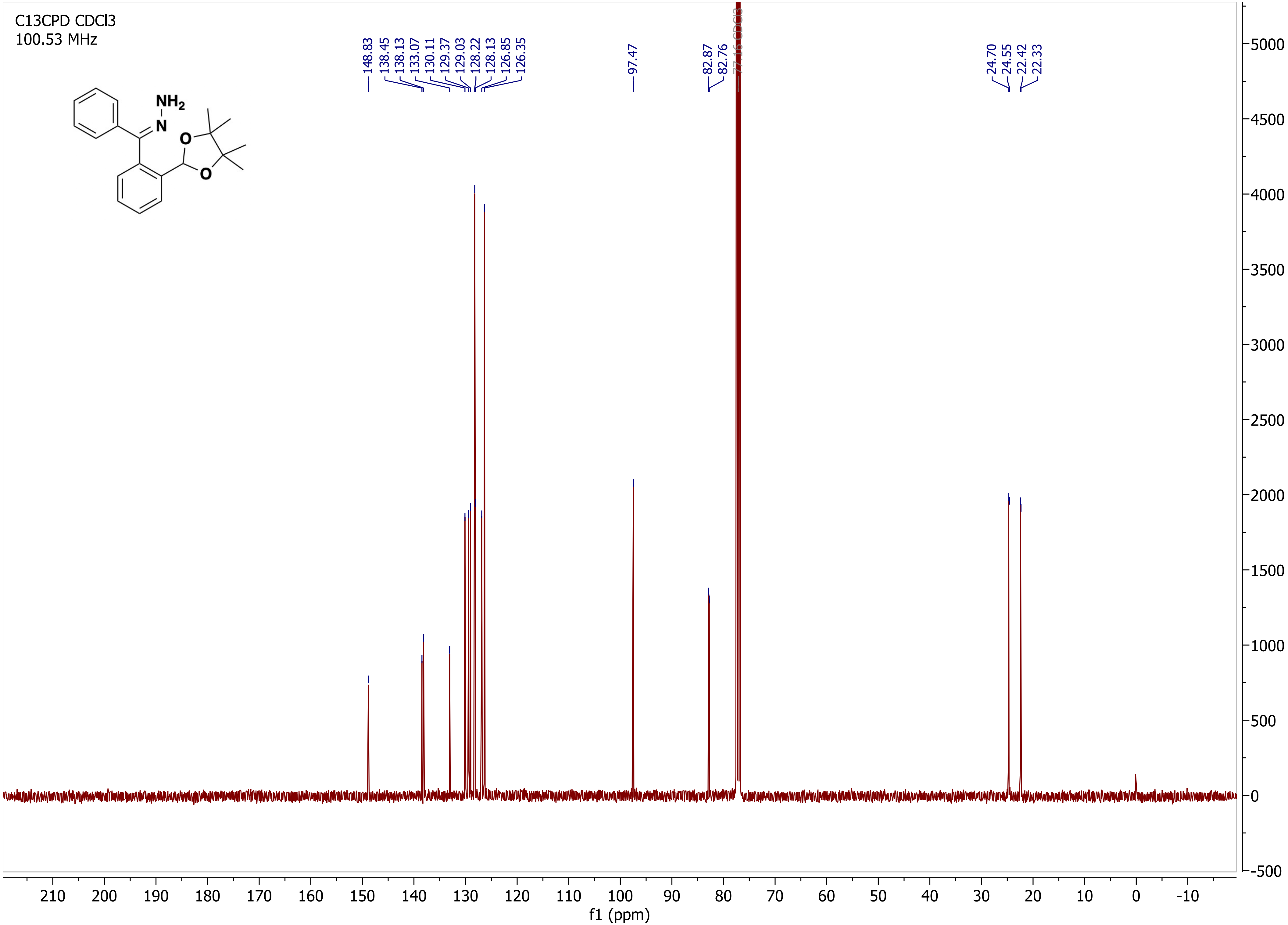

C13CPD CDCl3
100.53 MHz
175.20
172.50
143.79
137.11
135.80
131.84
131.81
131.56
129.85
129.21
128.86
127.84
127.73
126.38
124.82
118.96
111.23
105.17
77.16 CDCl3
66.27
65.42
51.00
44.29
44.23
NC
O
N
Ph
O
O
O
15e
f1 (ppm)

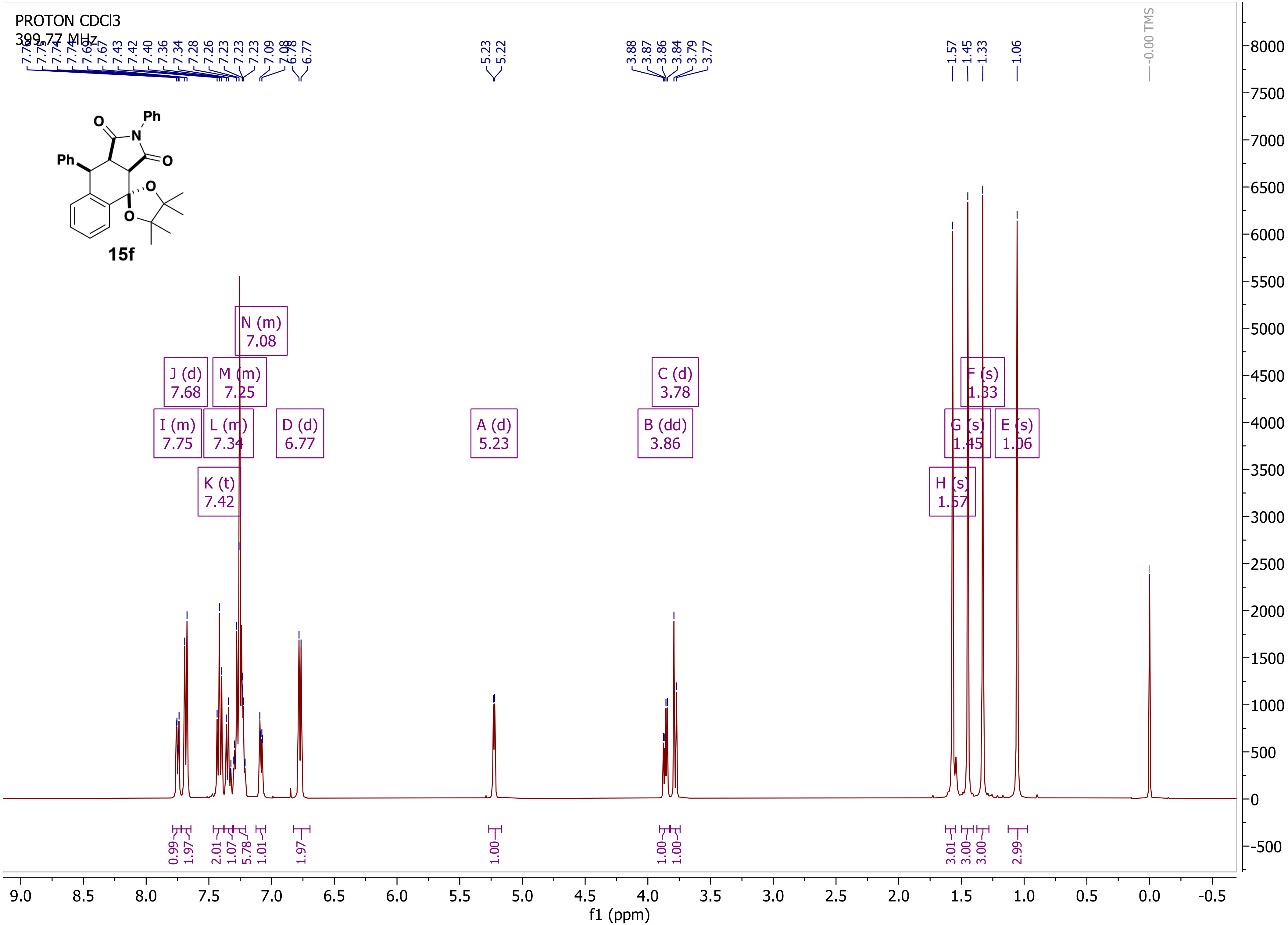

PROTON CDCl3
399.77 MHz
7.80
7.78
7.58
7.56
7.54
7.52
7.50
7.48
7.45
7.43
7.41
7.39
7.37
7.35
7.31
7.29
6.11
1.15
1.11
0.00 TMS
O
O
O
G (t)
7.43
E (t)
7.56
D (d)
7.79
I (d)
7.30
A (s)
6.11
F (t)
7.50
H (t)
7.37
C (s)
1.11
B (s)
1.15
2.99
1.05
1.07
2.04
1.07
1.06
1.00
5.95
6.00
f1 (ppm)

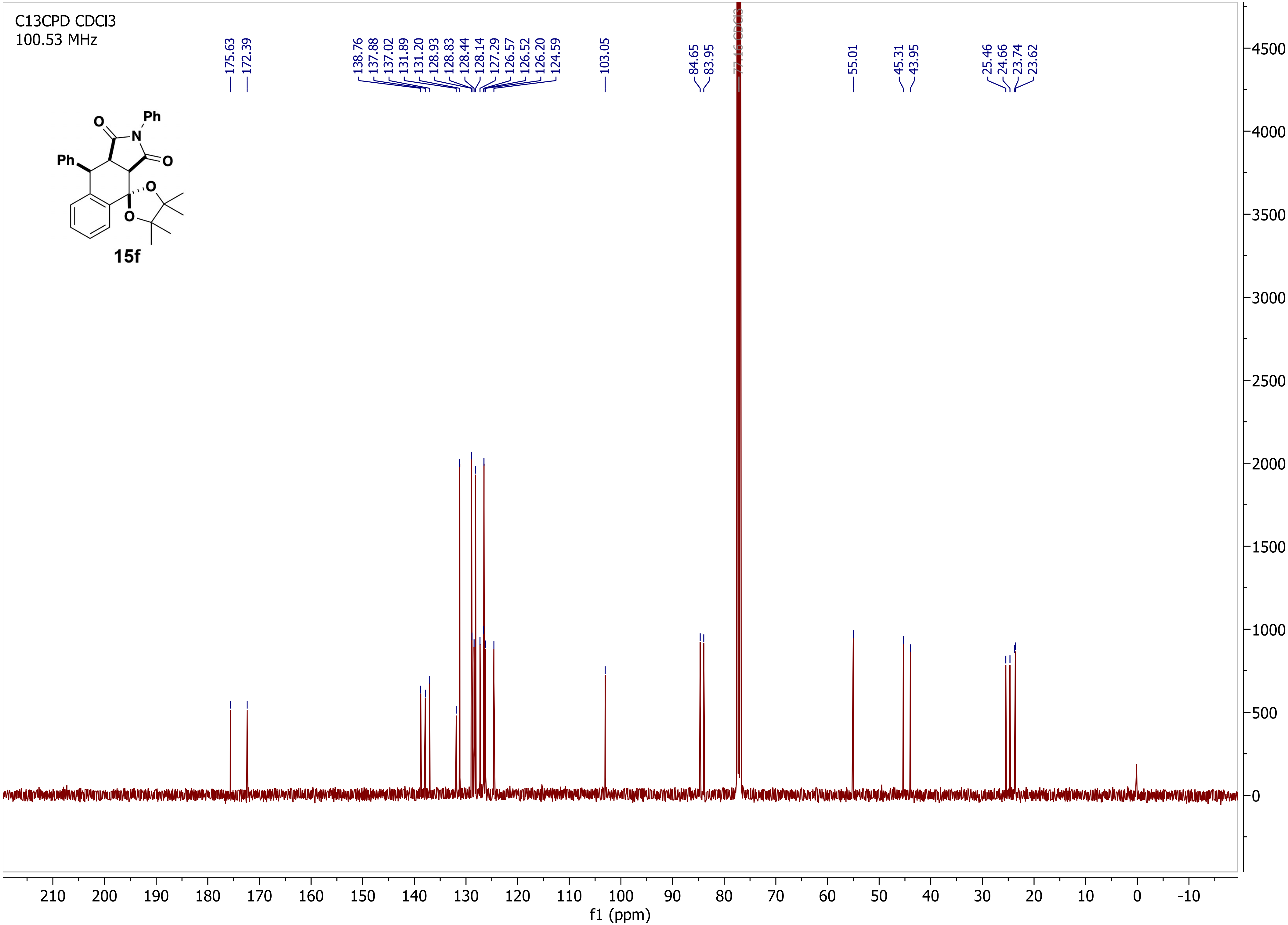


C13CPD CDCl3
100.53 MHz
198.16
139.57
138.44
138.22
132.96
130.26
130.14
128.30
128.20
127.74
126.45
97.13
82.83
77.16 CDCl3
24.10
22.29
O
O
O
f1 (ppm)

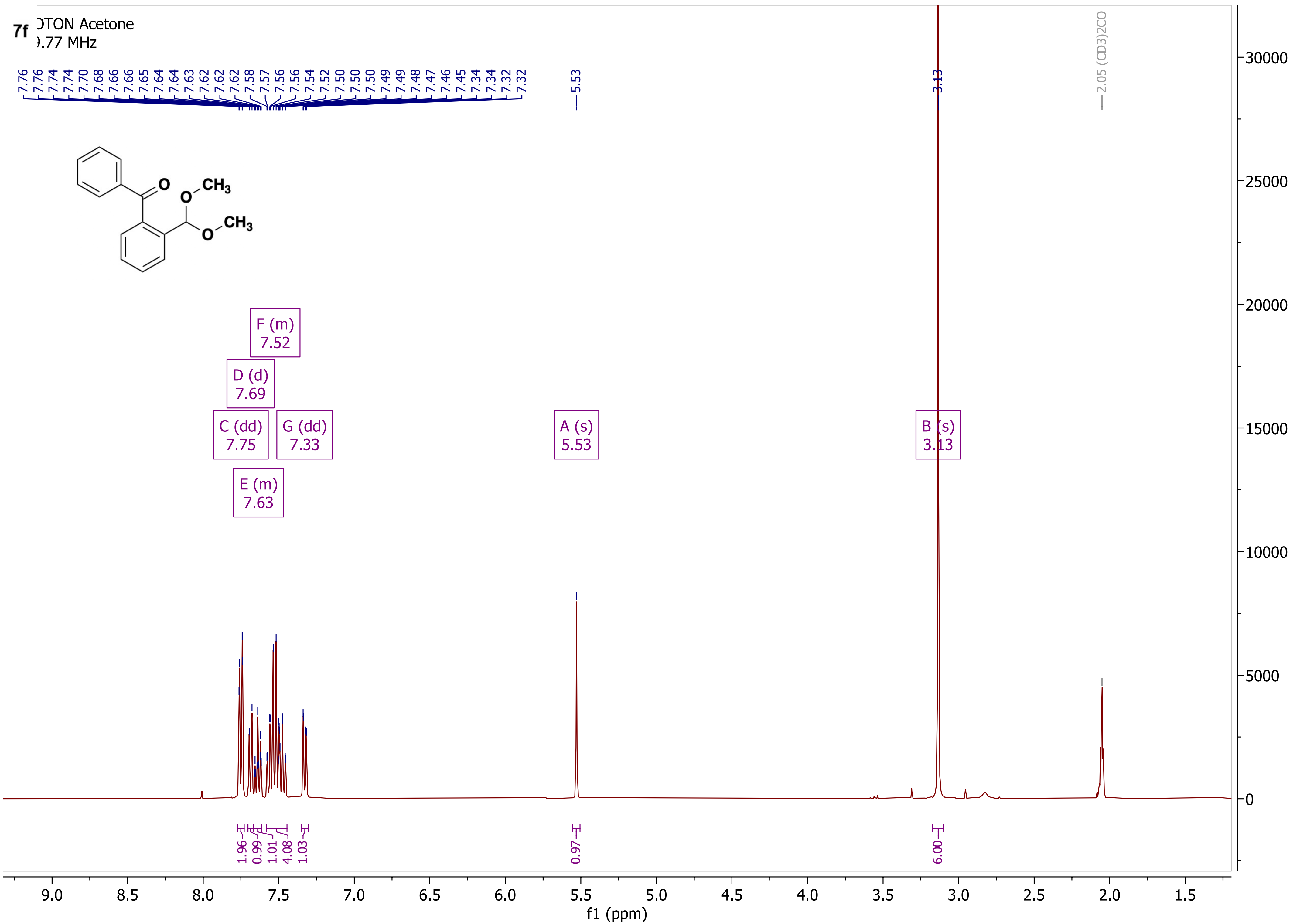

PROTON CDCl3
399.77 MHz
NH2
N
O
O
J (m) 7.29
H (m) 7.52
G (m) 7.88
I (m) 7.46
K (m) 7.16
B (s) 5.44
A (s) 5.76
F (s) 1.17
D (s) 1.25
C (s) 1.29
E (s) 1.21
0.97
1.99
2.01
3.46
0.97
1.00
1.82
2.99
2.99
3.00
3.00
f1 (ppm)


C13CPD CDCl3
100.53 MHz
NH2
N
O
O
148.83
138.45
138.13
133.07
130.11
129.37
129.03
128.22
128.13
126.85
126.35
97.47
82.87
82.76
77.16 CDCl3
24.70
24.55
22.42
22.33
f1 (ppm)

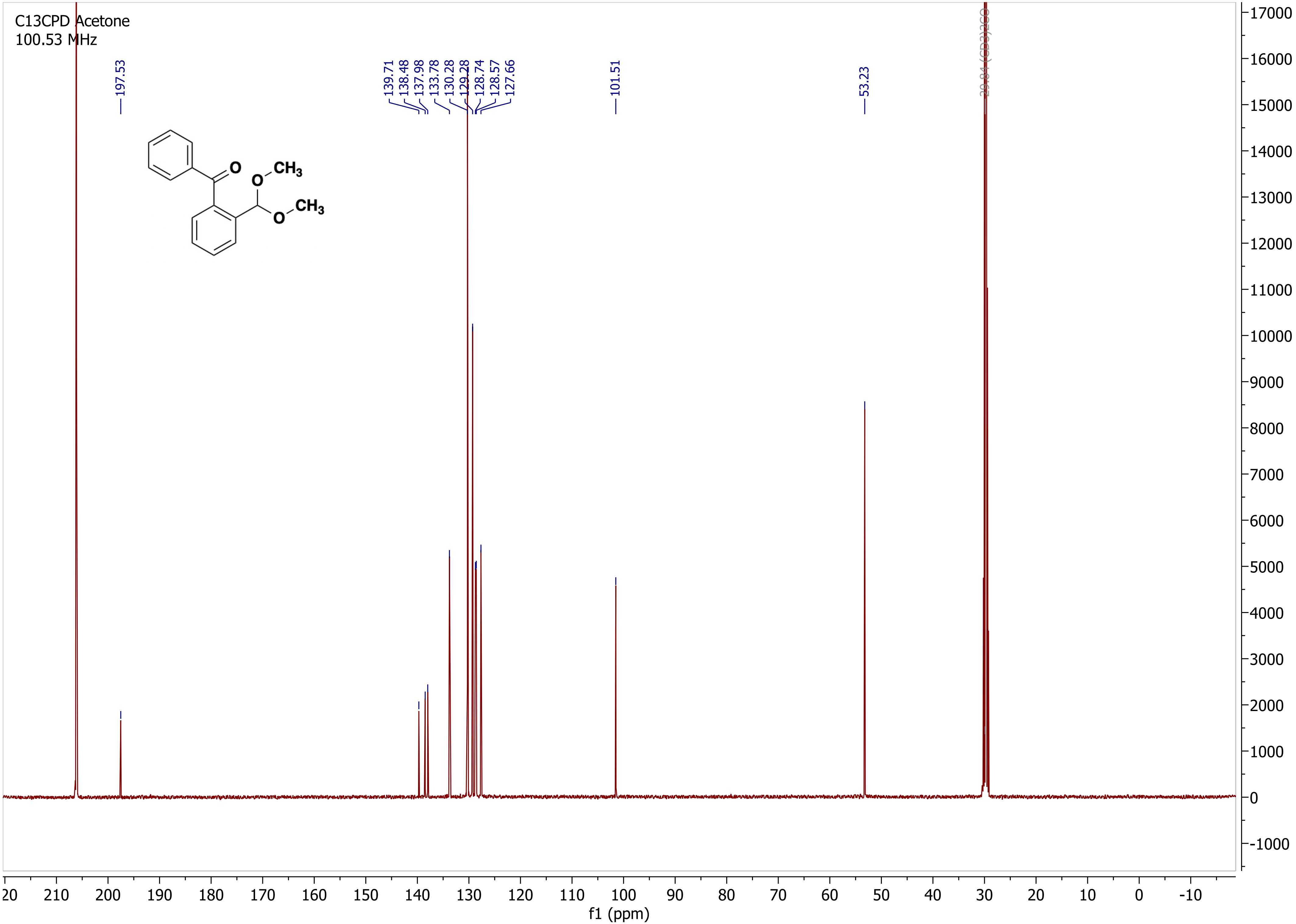

PROTON CDCl3
399.77 MHz
7.76 7.75 7.74 7.74 7.69 7.67 7.43 7.42 7.40 7.36 7.34 7.28 7.26 7.23 7.23 7.23 7.09 7.08 6.78 6.77
5.23 5.22
3.88 3.87 3.86 3.84 3.79 3.77
1.57 1.45 1.33 1.06
-0.00 TMS
O
N
Ph
Ph
O
O
O
15f
N (m) 7.08
J (d) 7.68
M (m) 7.25
I (m) 7.75
L (m) 7.34
D (d) 6.77
K (t) 7.42
A (d) 5.23
C (d) 3.78
B (dd) 3.86
F (s) 1.33
G (s) 1.45
E (s) 1.06
H (s) 1.57
0.99 1.97 2.01 1.07 5.78 1.01 1.97 1.00 1.00 1.00 3.01 3.00 3.00 2.99
f1 (ppm)

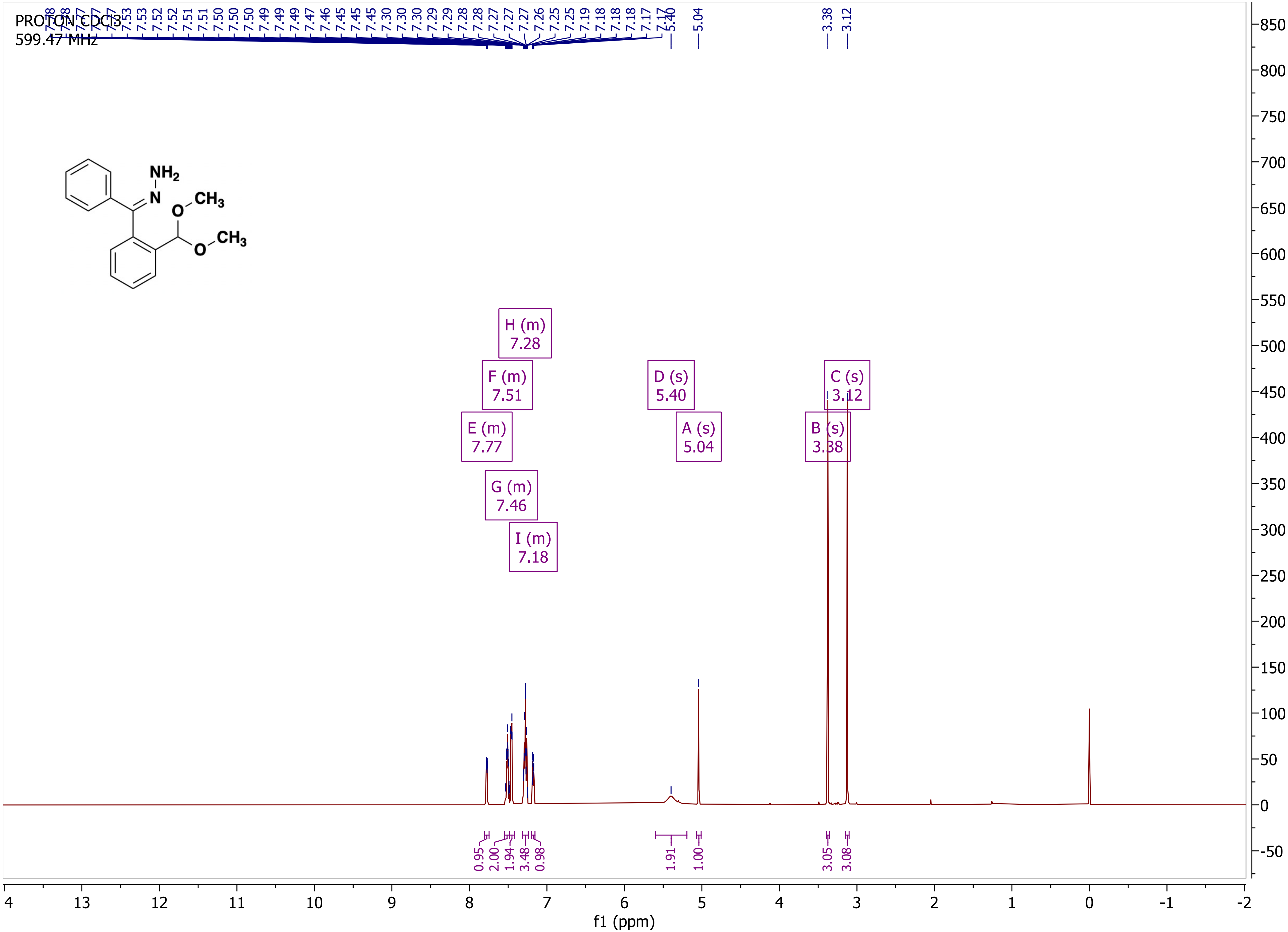

C13CPD CDCl3
100.53 MHz
175.63
172.39
138.76
137.88
137.02
131.89
131.20
128.93
128.83
128.44
128.14
127.29
126.57
126.52
126.20
124.59
103.05
84.65
83.95
77.16 CDCl3
55.01
45.31
43.95
25.46
24.66
23.74
23.62
O
N
Ph
O
Ph
O
O
15f
4500
4000
3500
3000
2500
2000
1500
1000
500
0
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

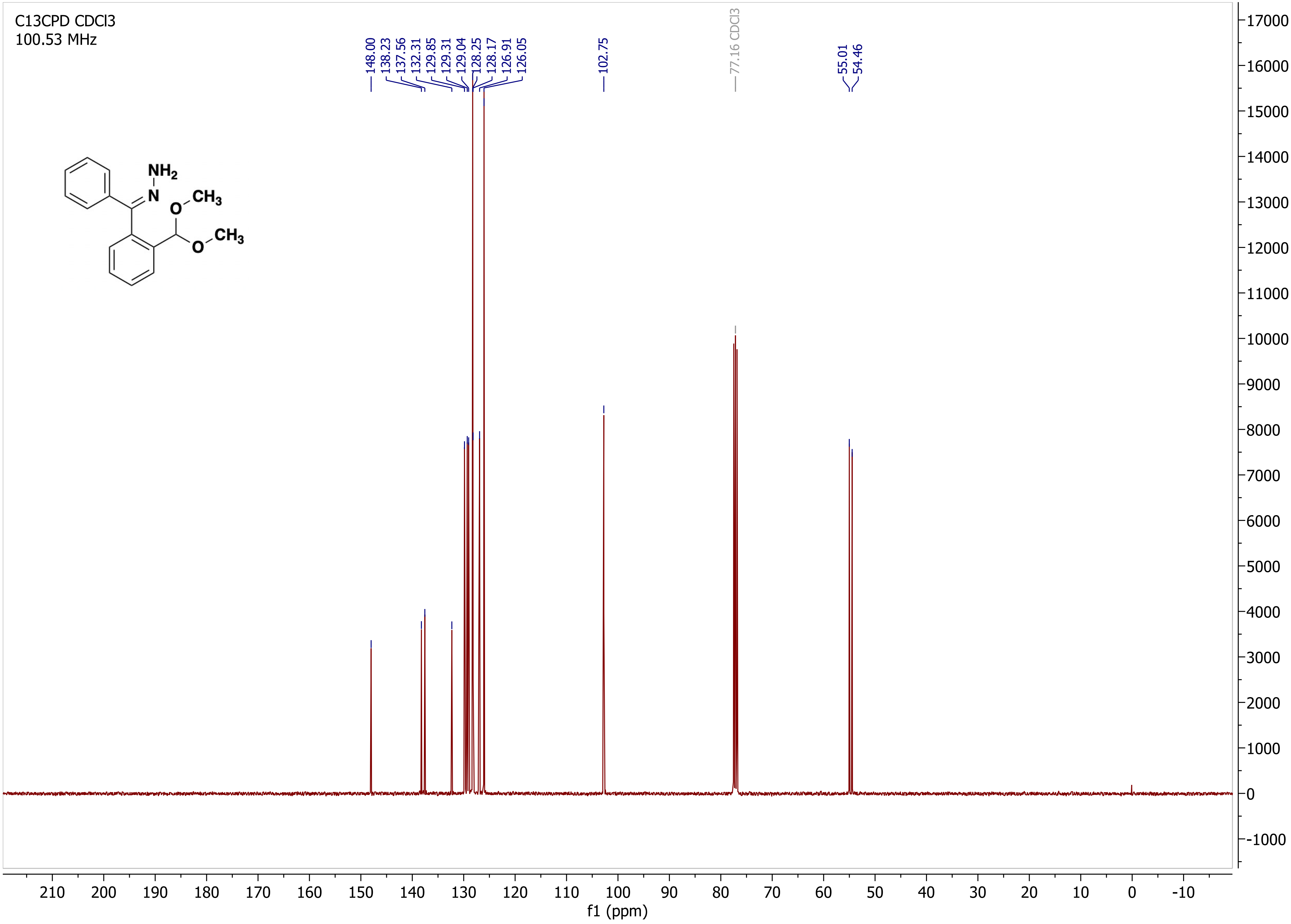
7f



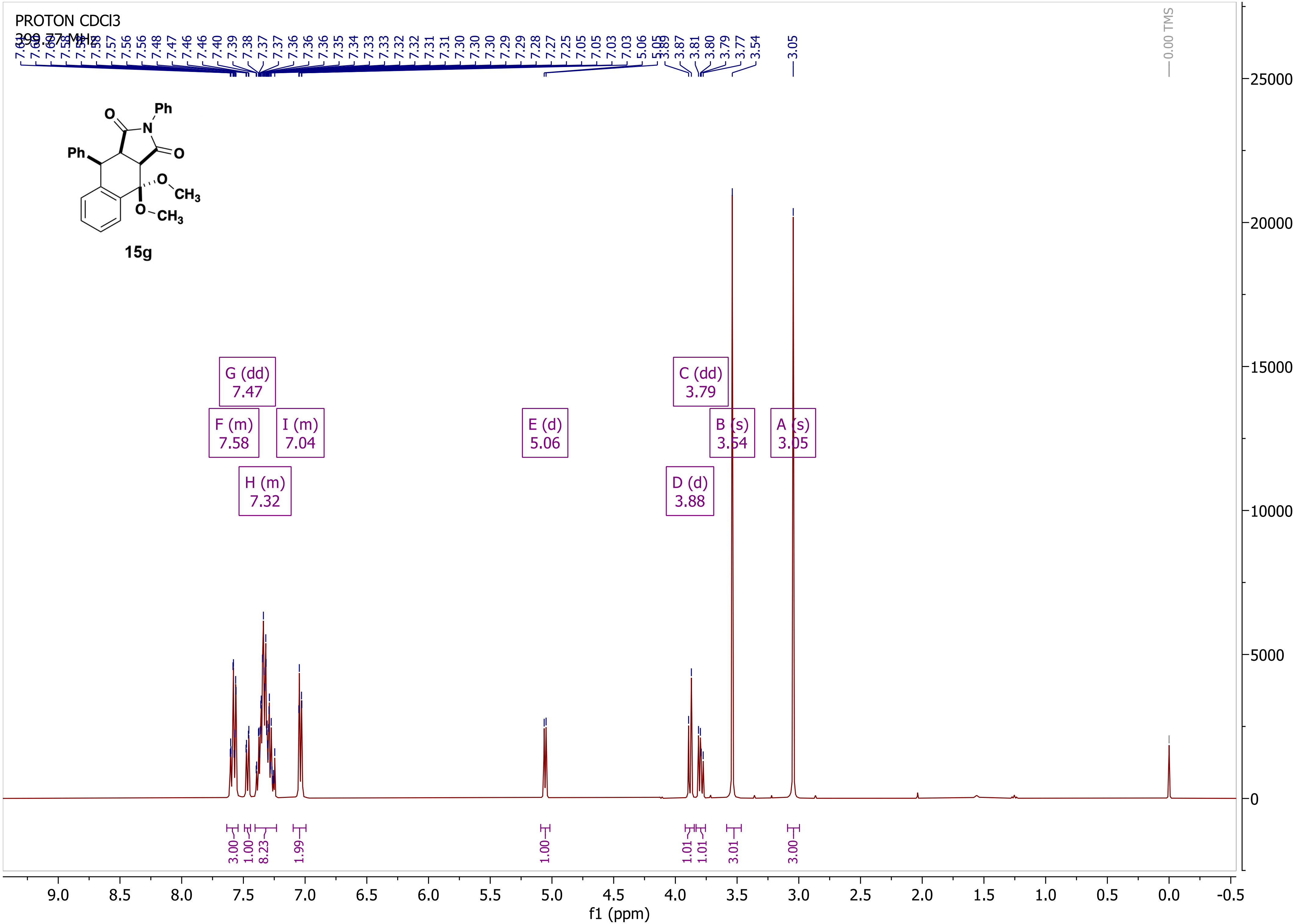
PROTON Acetone
.77 MHz
7.76 7.76 7.74 7.74 7.70 7.68 7.66 7.66 7.65 7.64 7.64 7.63 7.62 7.62 7.62 7.58 7.57 7.56 7.56 7.54 7.52 7.50 7.50 7.50 7.49 7.49 7.48 7.47 7.46 7.45 7.34 7.34 7.32 7.32
5.53
3.13
2.05 (CD3)2CO
O
O
CH3
O
CH3
F (m) 7.52
D (d) 7.69
C (dd) 7.75
G (dd) 7.33
E (m) 7.63
A (s) 5.53
B (s) 3.13
1.96
0.99
1.01
4.08
1.03
0.97
6.00
f1 (ppm)


C13CPD Acetone
100.53 MHz
197.53
139.71
138.48
137.98
133.78
130.28
129.28
128.74
128.57
127.66
101.51
53.23
29.84 (CD3)2CO
O
O
CH3
O
CH3
f1 (ppm)

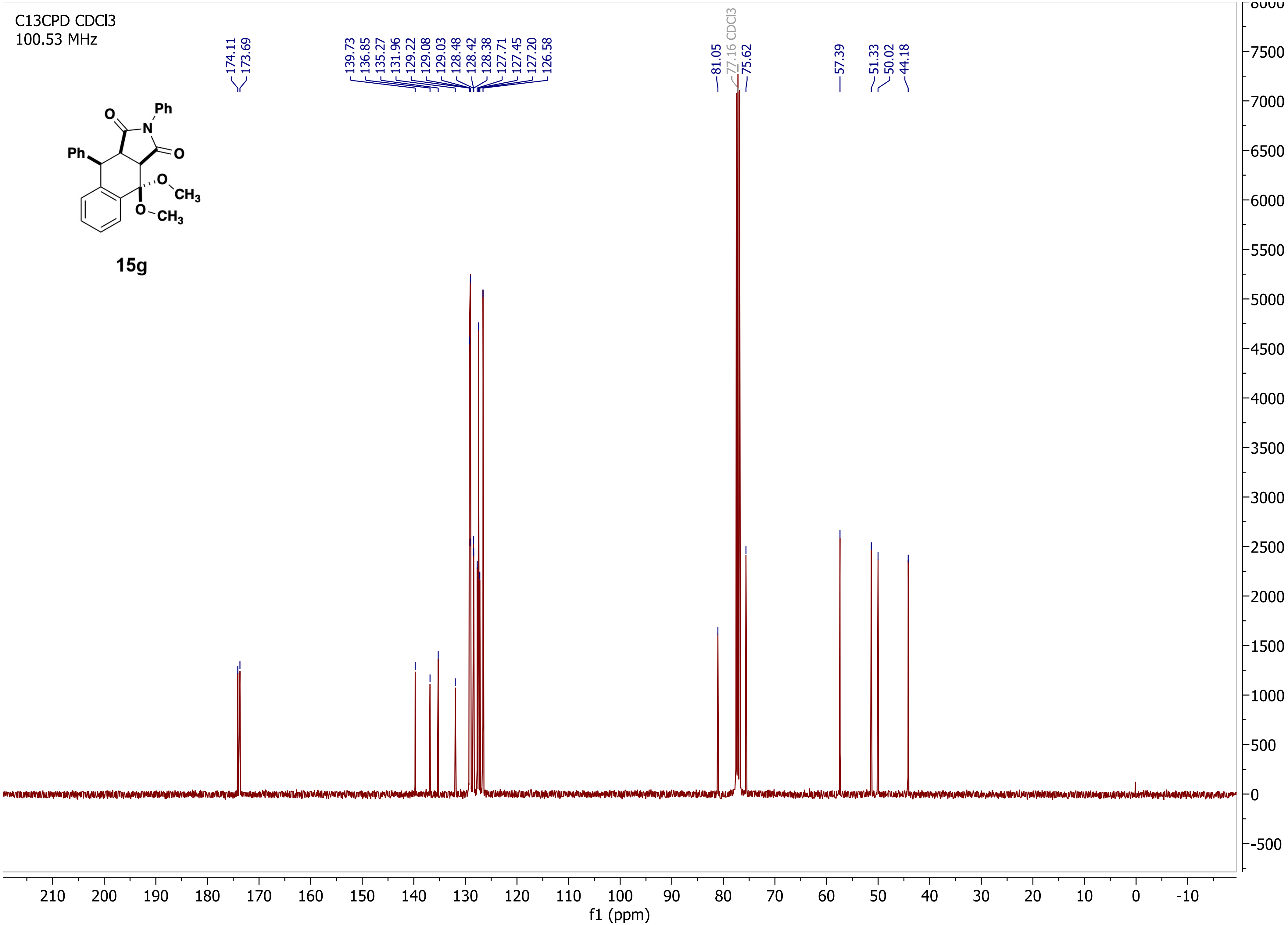

PROTON CDCl3
599.47 MHz
7.78
7.78
7.77
7.77
7.77
7.53
7.52
7.52
7.51
7.51
7.50
7.50
7.50
7.49
7.49
7.49
7.47
7.46
7.45
7.45
7.45
7.30
7.30
7.30
7.29
7.29
7.28
7.28
7.27
7.27
7.27
7.26
7.25
7.25
7.19
7.18
7.18
7.17
7.17
5.40
5.04
3.38
3.12
NH2
N
O
CH3
O
CH3
H (m)
7.28
F (m)
7.51
E (m)
7.77
G (m)
7.46
I (m)
7.18
D (s)
5.40
A (s)
5.04
C (s)
3.12
B (s)
3.38
0.95
2.00
1.94
3.48
0.98
1.91
1.00
3.05
3.08
f1 (ppm)



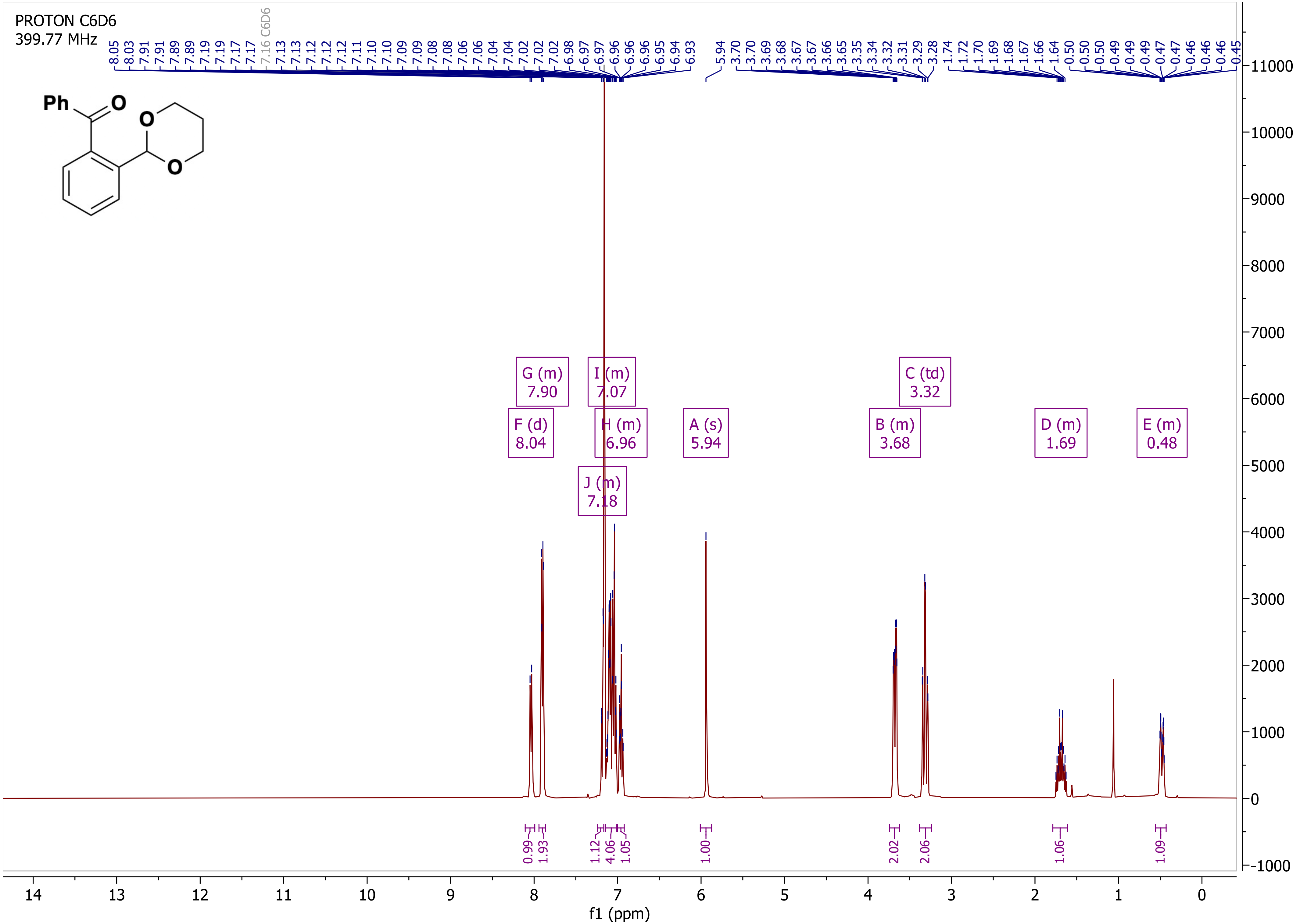
C13CPD CDCl3
100.53 MHz
148.00
138.23
137.56
132.31
129.85
129.31
129.04
128.25
128.17
126.91
126.05
102.75
77.16 CDCl3
55.01
54.46
NH2
N
O
CH3
O
CH3
f1 (ppm)


PROTON CDCl3
399.77 MHz
7.57 7.56 7.56 7.48 7.47 7.46 7.46 7.40 7.39 7.38 7.37 7.37 7.36 7.36 7.35 7.34 7.33 7.33 7.32 7.32 7.31 7.31 7.30 7.30 7.30 7.29 7.29 7.28 7.27 7.25 7.05 7.05 7.03 7.03 5.06
3.87 3.81 3.80 3.79 3.77 3.54 3.05
0.00 TMS
Ph
O
N
O
Ph
O
CH3
O
CH3
15g
G (dd) 7.47
F (m) 7.58
I (m) 7.04
H (m) 7.32
E (d) 5.06
C (dd) 3.79
B (s) 3.54
A (s) 3.05
D (d) 3.88
3.00
1.00
8.23
1.99
1.00
1.01
1.01
3.01
3.00
25000
20000
15000
10000
5000
0
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)

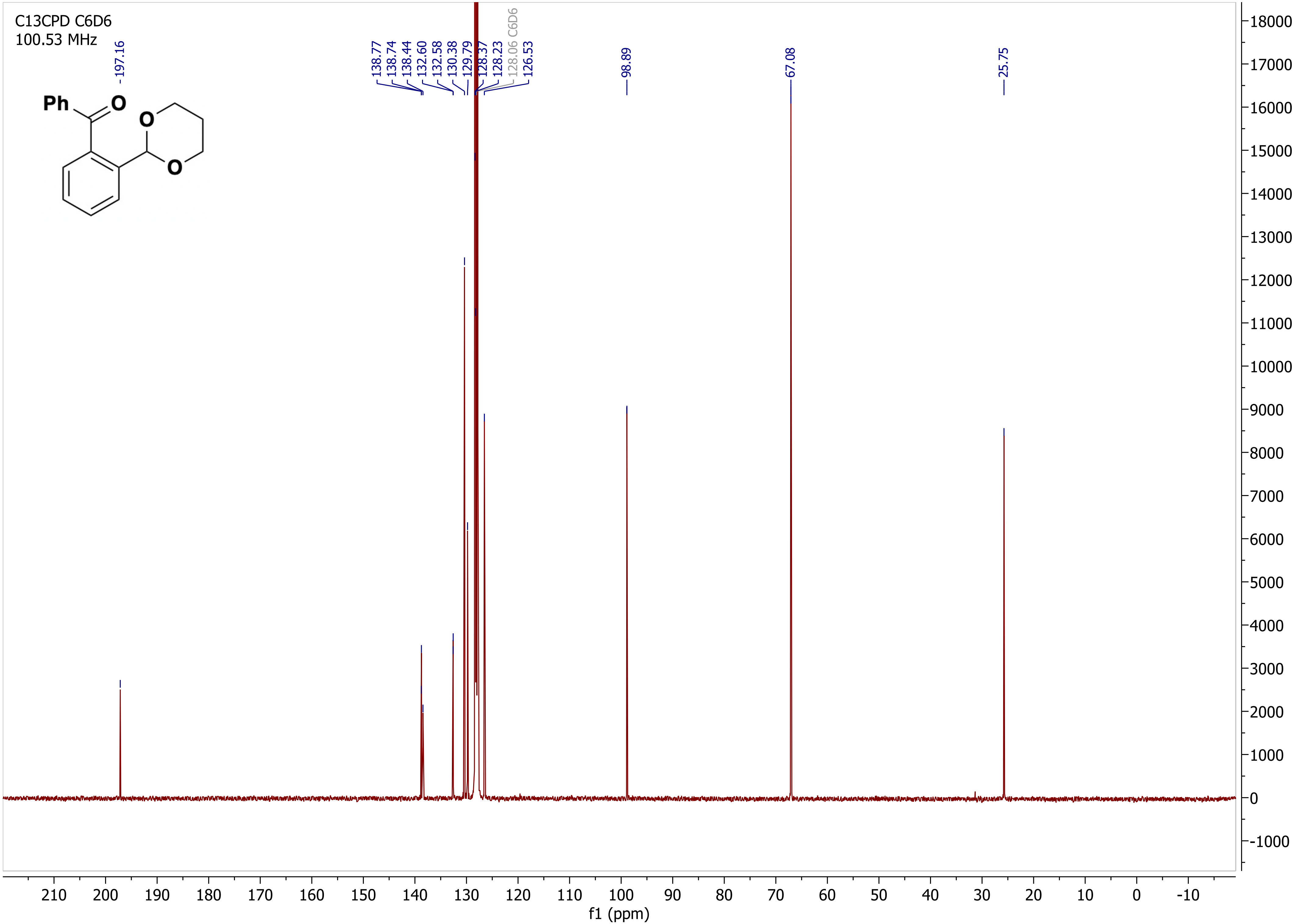
C13CPD CDCl3
100.53 MHz

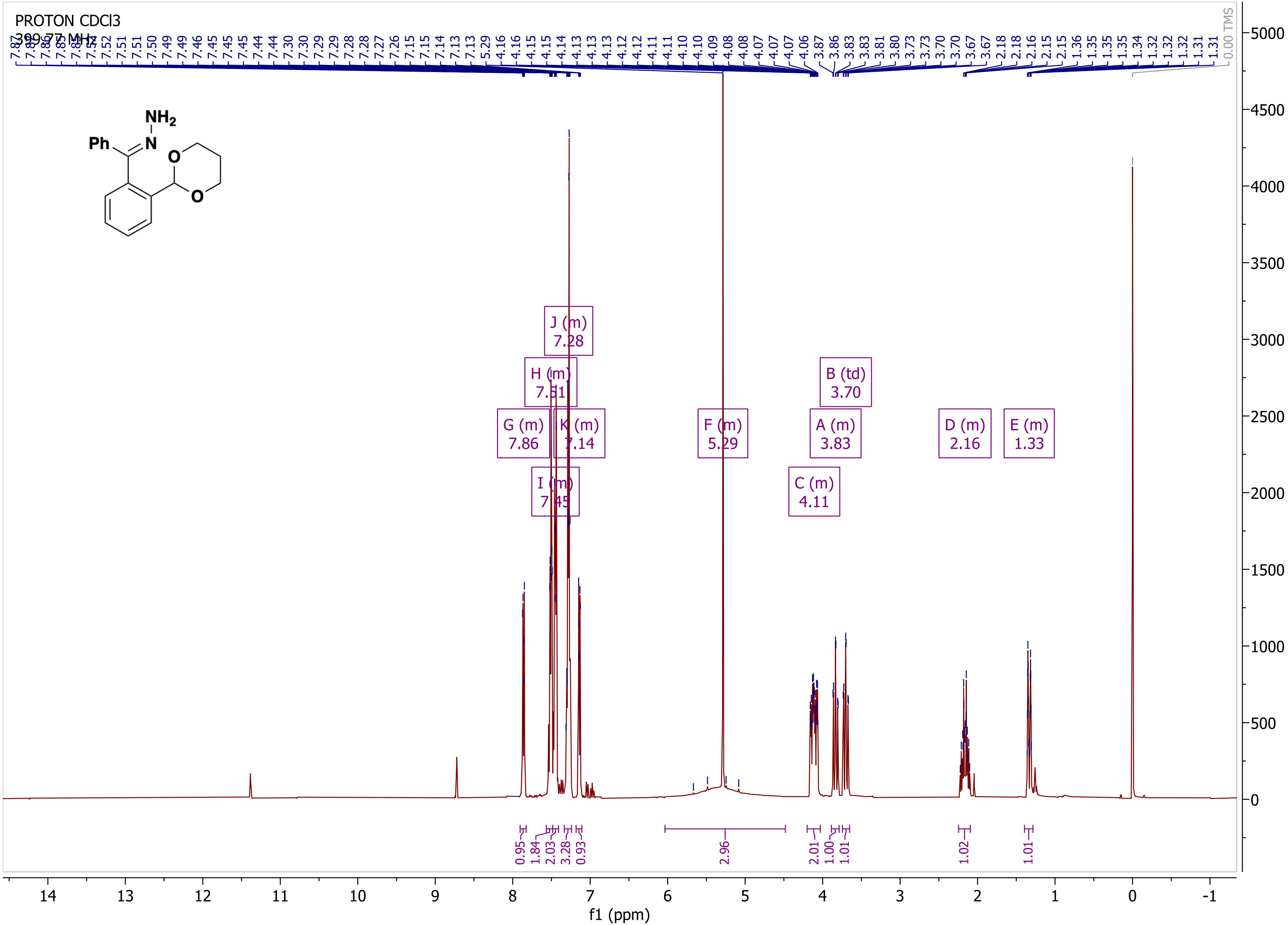


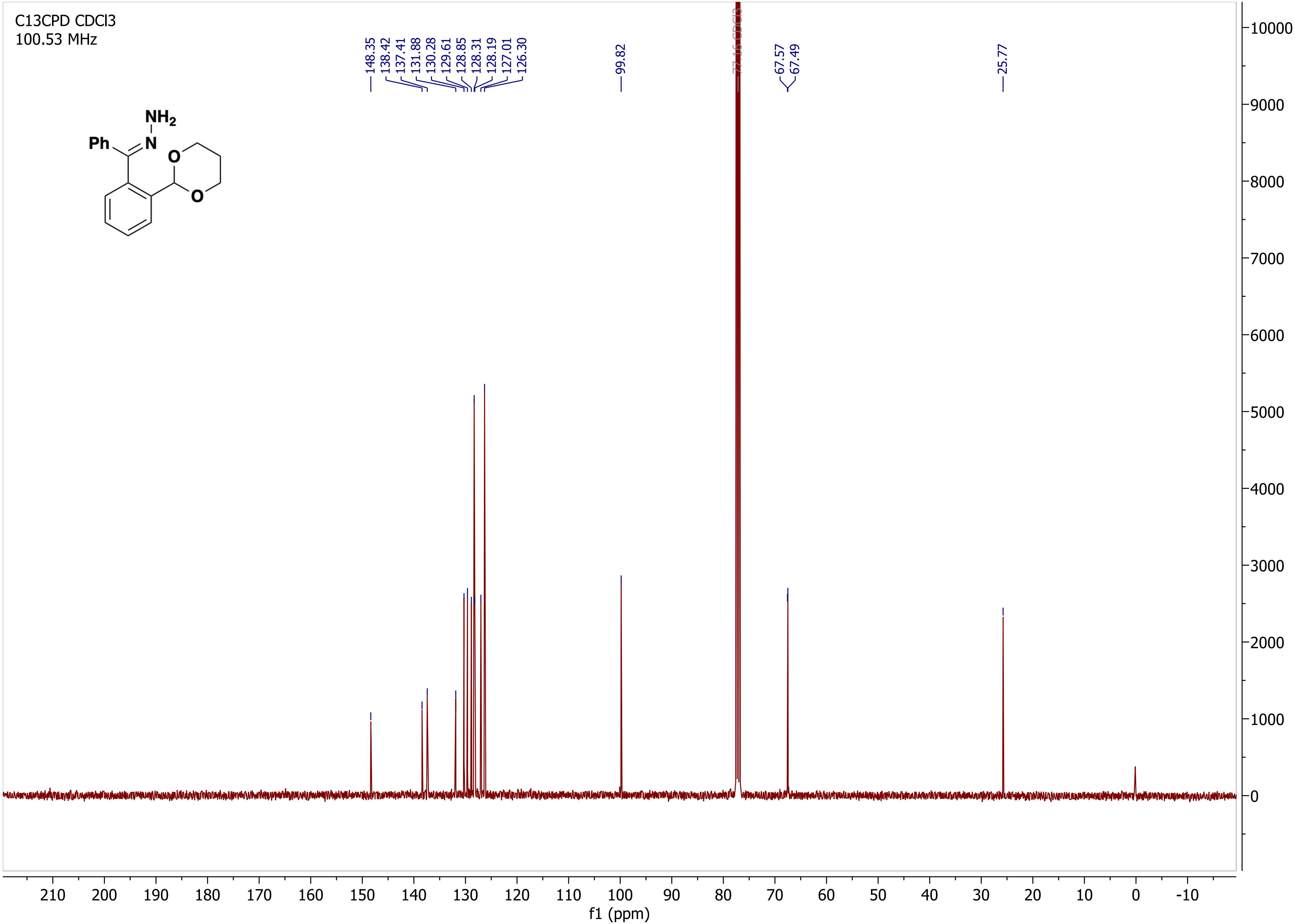
15g

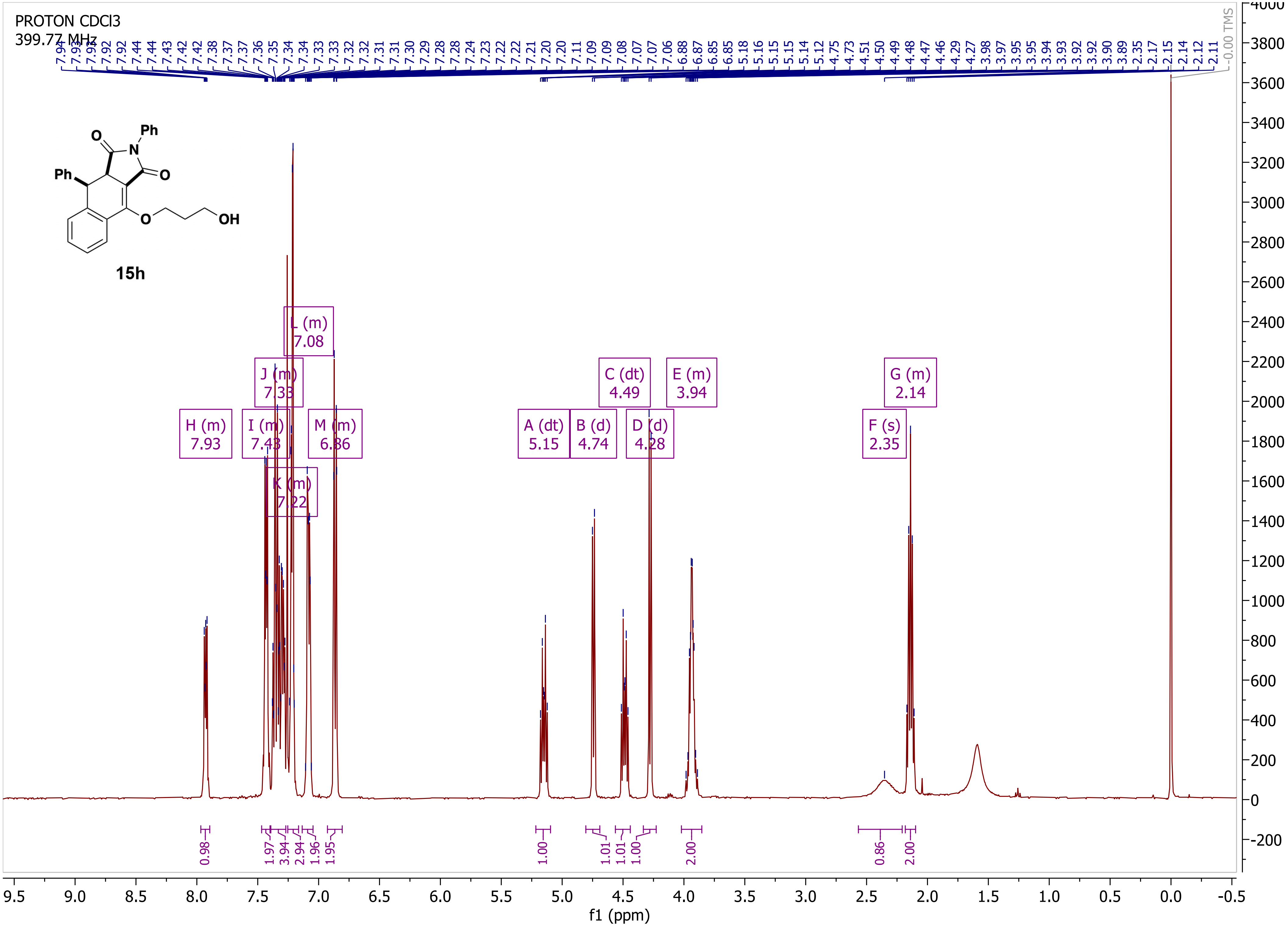


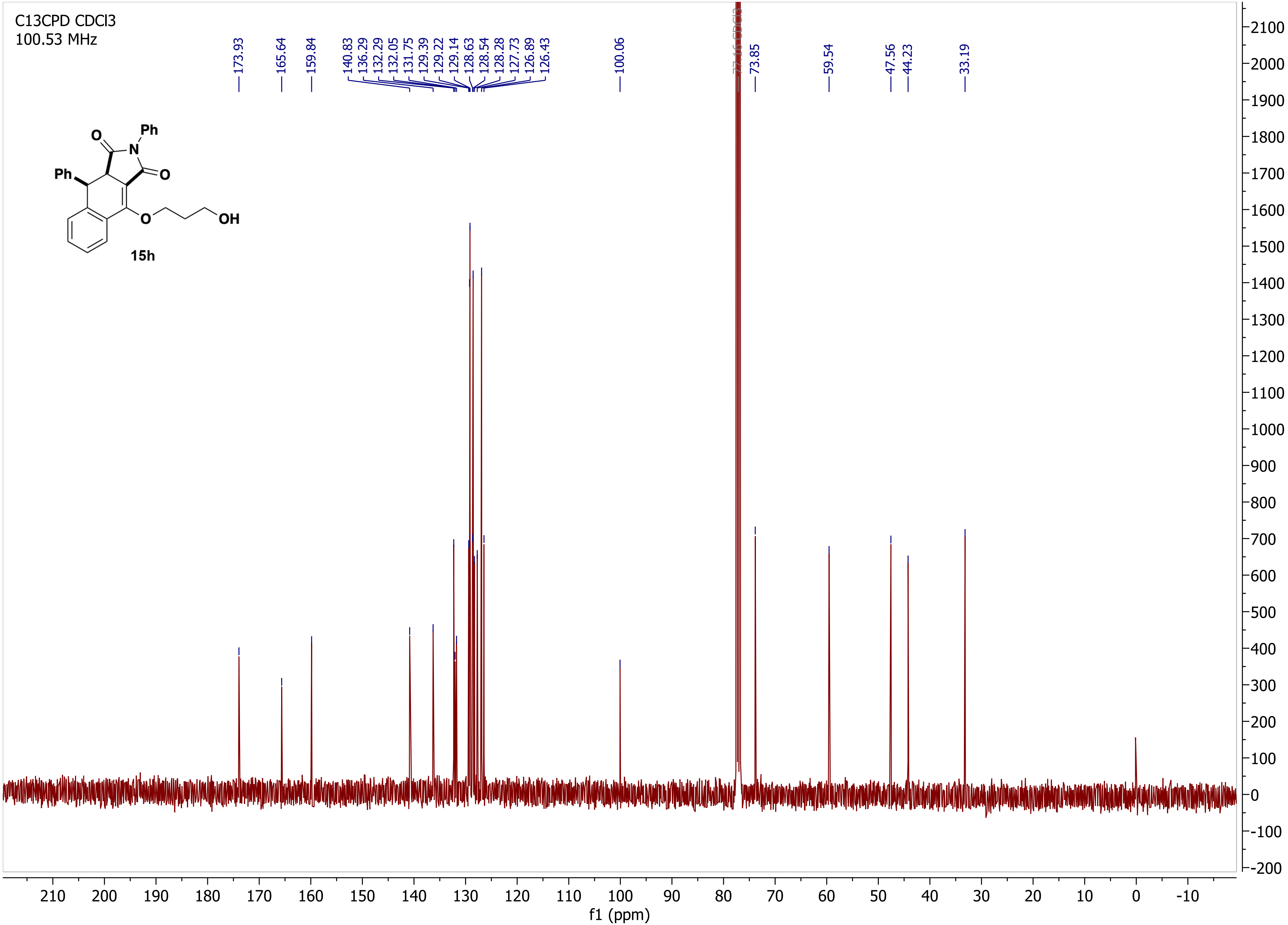
PROTON C6D6
399.77 MHz
Ph
O
O
O
G (m)
7.90
I (m)
7.07
C (td)
3.32
F (d)
8.04
H (m)
6.96
A (s)
5.94
B (m)
3.68
D (m)
1.69
E (m)
0.48
J (m)
7.18
f1 (ppm)


C13CPD C6D6
100.53 MHz
197.16
138.77
138.74
138.44
132.60
132.58
130.38
129.79
128.37
128.23
128.06 C6D6
126.53
98.89
67.08
25.75
Ph
O
O
O
f1 (ppm)

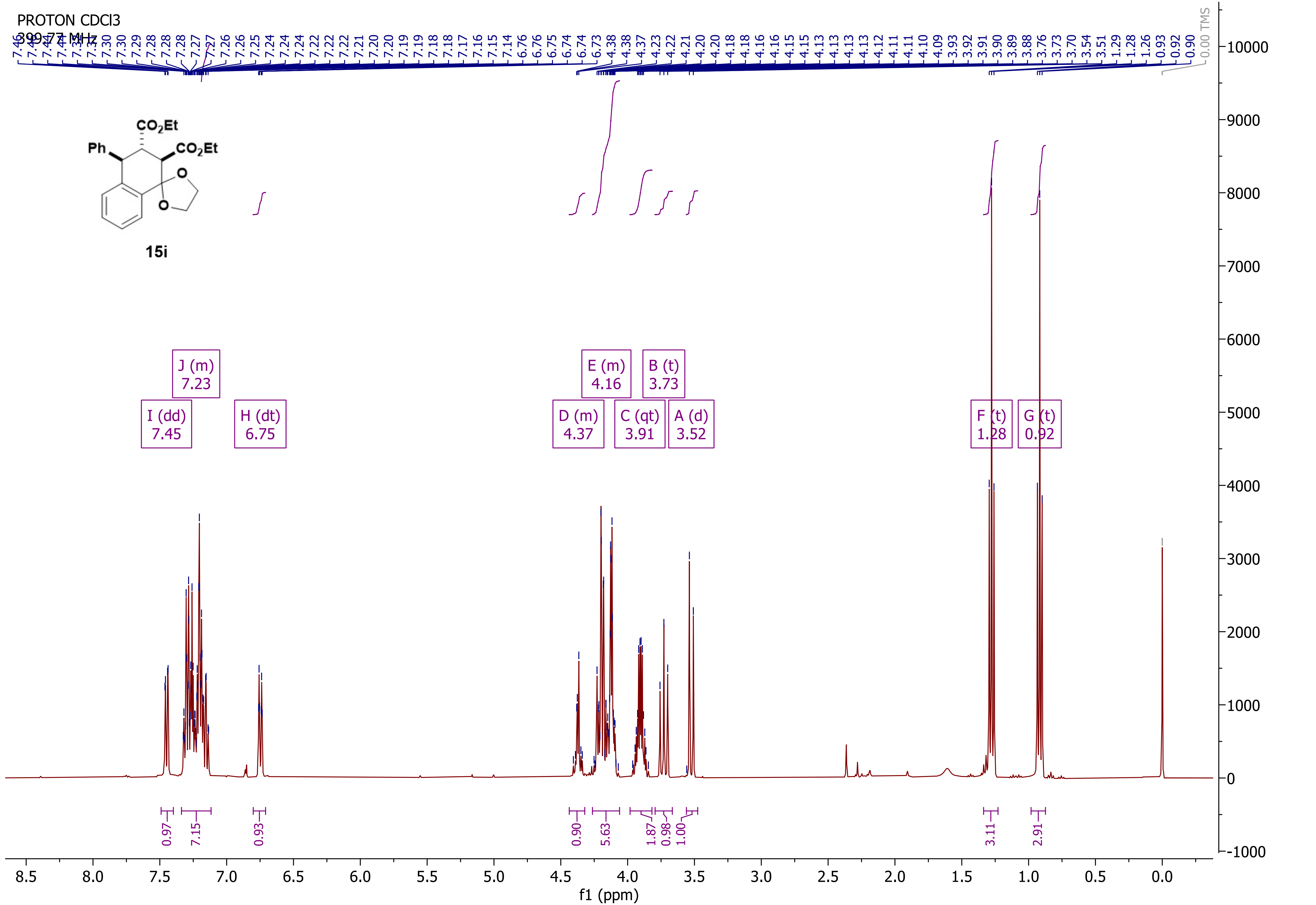

PROTON CDCl3
399.77 MHz
NH2
Ph
N
O
O
J (m)
7.28
H (m)
7.51
G (m)
7.86
K (m)
7.14
I (m)
7.45
F (m)
5.29
B (td)
3.70
A (m)
3.83
C (m)
4.11
D (m)
2.16
E (m)
1.33
0.95
1.84
2.03
3.28
0.93
2.96
2.01
1.00
1.01
1.02
1.01
0.00 TMS
f1 (ppm)

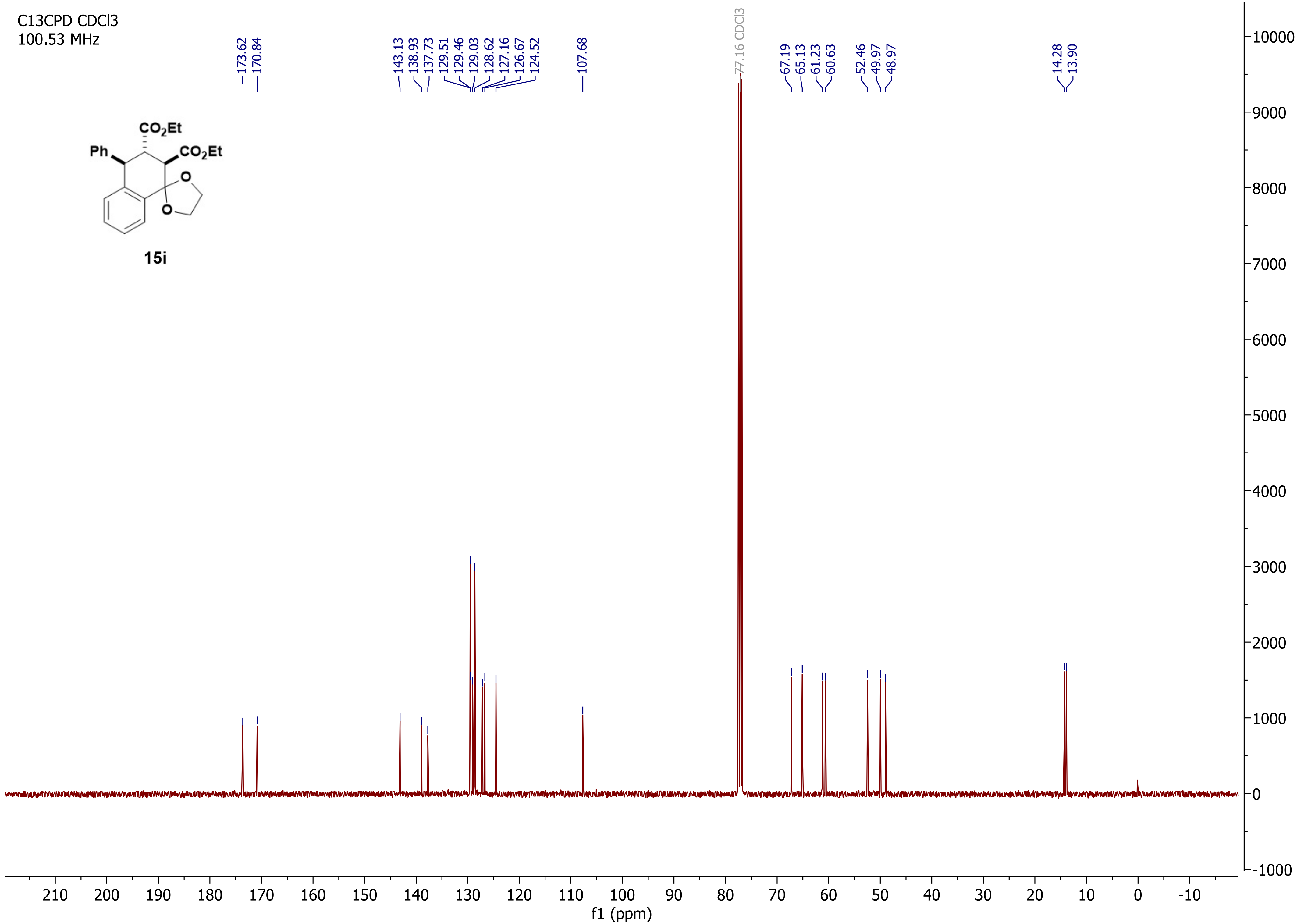

C13CPD CDCl3
100.53 MHz
148.35
138.42
137.41
131.88
130.28
129.61
128.85
128.31
128.19
127.01
126.30
99.82
77.16 CDCl3
67.57
67.49
25.77
NH2
Ph
N
O
O
f1 (ppm)

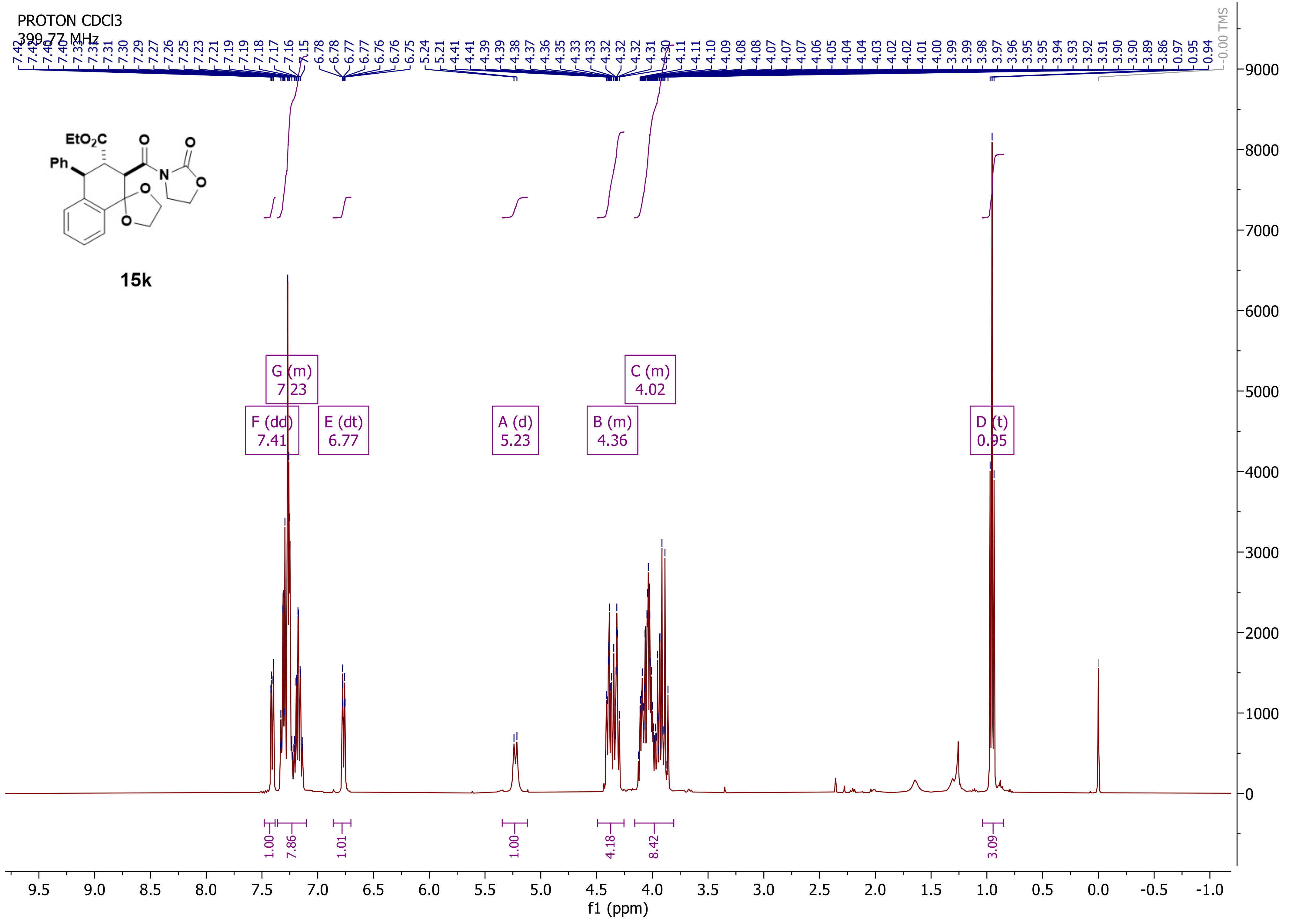

PROTON CDCl3
399.77 MHz
Ph
O
N
O
Ph
O
OH
15h
H (m) 7.93
I (m) 7.43
J (m) 7.33
K (m) 7.22
L (m) 7.08
M (m) 6.86
A (dt) 5.15
B (d) 4.74
C (dt) 4.49
D (d) 4.28
E (m) 3.94
F (s) 2.35
G (m) 2.14
-0.00 TMS
0.98
1.97
3.94
2.94
1.96
1.95
1.00
1.01
1.01
1.00
2.00
0.86
2.00
f1 (ppm)



C13CPD CDCl3
100.53 MHz
173.93
165.64
159.84
140.83
136.29
132.29
132.05
131.75
129.39
129.22
129.14
128.63
128.54
128.28
127.73
126.89
126.43
100.06
77.16 CDCl3
73.85
59.54
47.56
44.23
33.19
Ph
O
N
O
Ph
O
OH
15h
f1 (ppm)

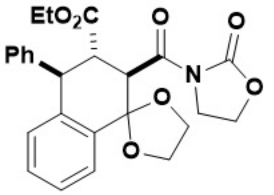

PROTON CDCl3
399.77 MHz
CO2Et
Ph
CO2Et
O
O
15i
I (dd) 7.45
J (m) 7.23
H (dt) 6.75
D (m) 4.37
E (m) 4.16
C (qt) 3.91
B (t) 3.73
A (d) 3.52
F (t) 1.28
G (t) 0.92
0.97
7.15
0.93
0.90
5.63
1.87
0.98
1.00
3.11
2.91
0.00 TMS
f1 (ppm)


C13CPD CDCl3
100.53 MHz
173.62
170.84
143.13
138.93
137.73
129.51
129.46
129.03
128.62
127.16
126.67
124.52
107.68
77.16 CDCl3
67.19
65.13
61.23
60.63
52.46
49.97
48.97
14.28
13.90
CO2Et
Ph
CO2Et
O
O
15i
f1 (ppm)

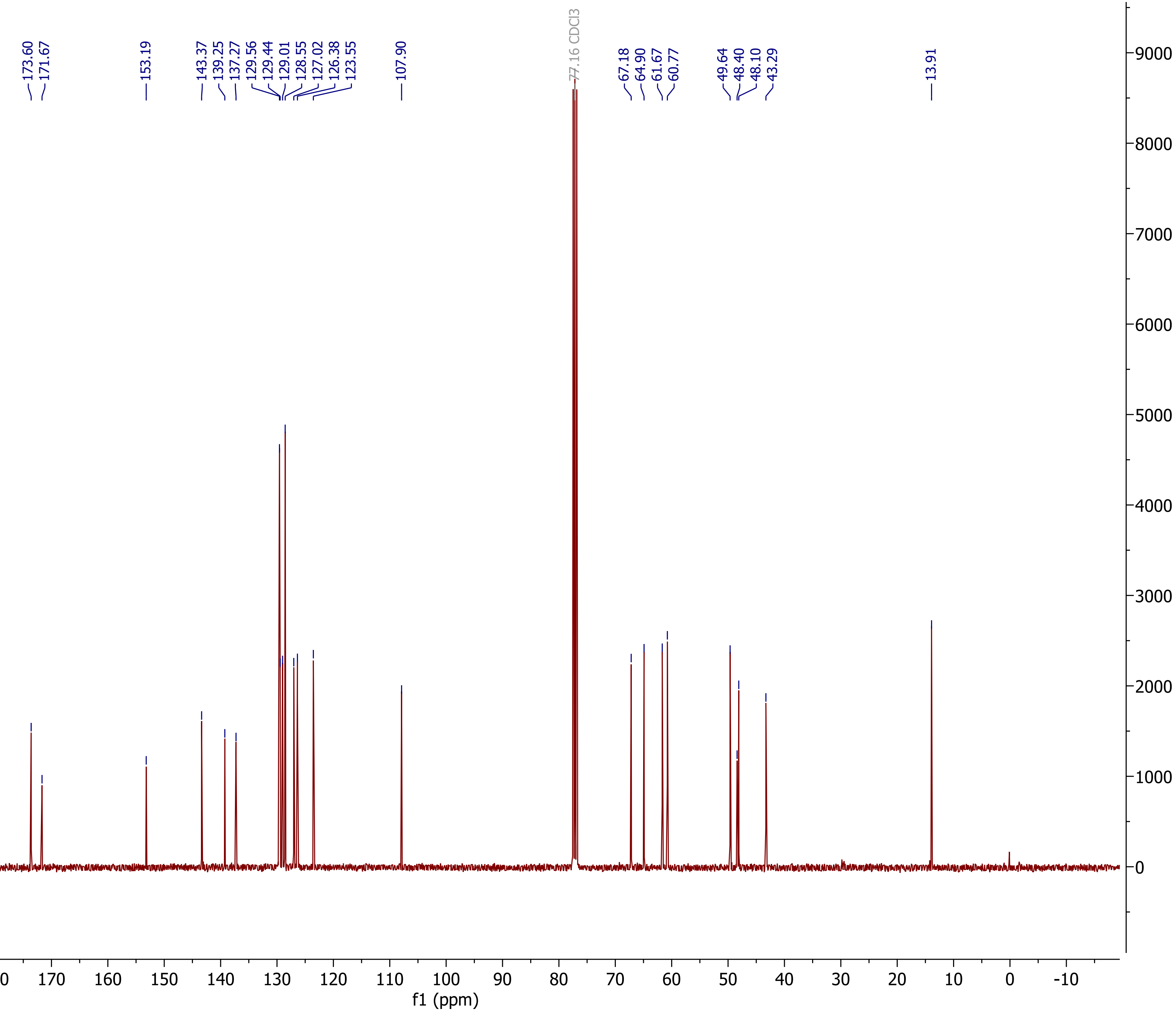


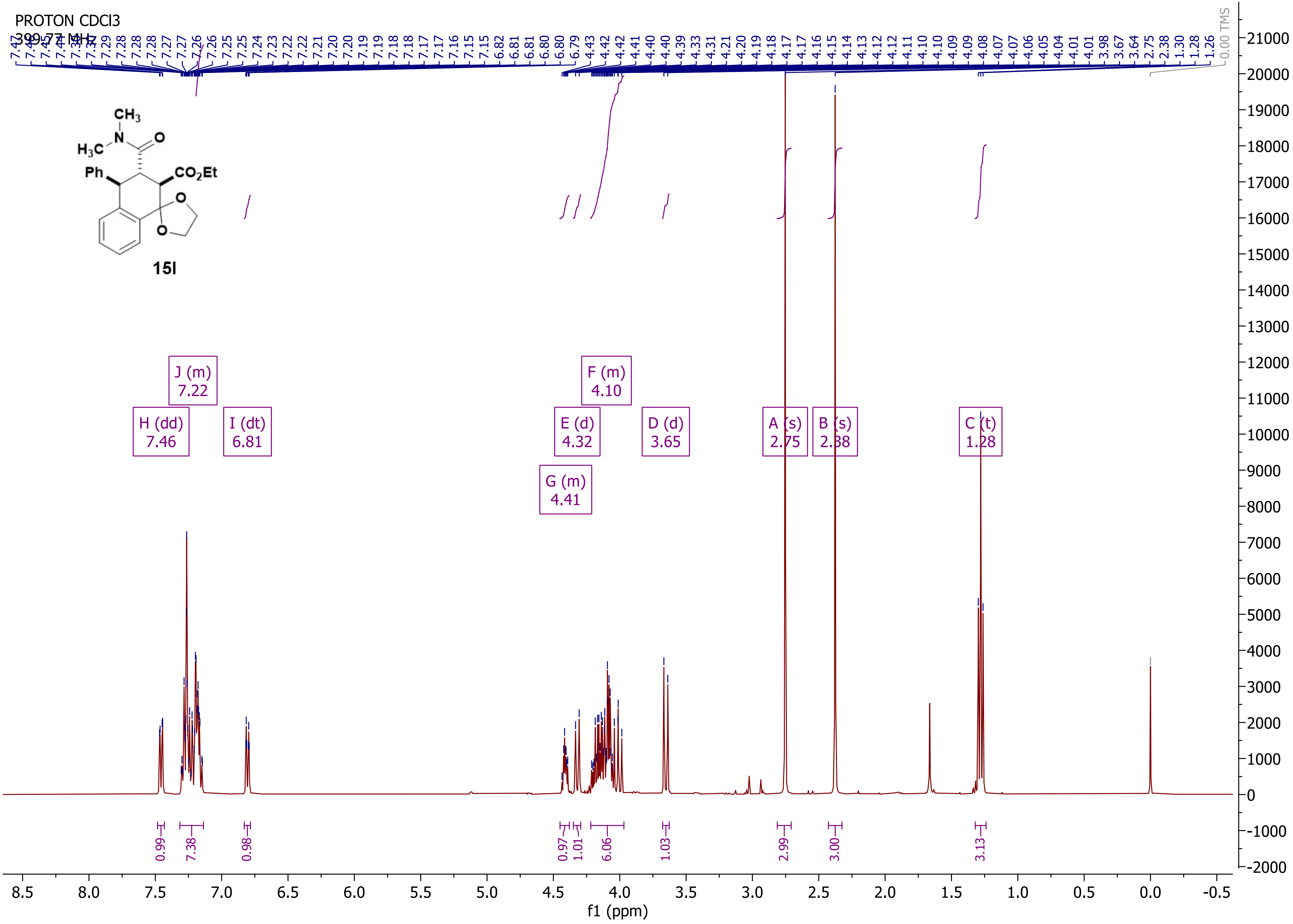
PROTON CDCl3
399.77 MHz
7.42 7.40 7.40 7.40 7.33 7.31 7.31 7.30 7.29 7.27 7.26 7.25 7.23 7.21 7.19 7.19 7.18 7.17 7.16 7.15 6.78 6.78 6.77 6.77 6.76 6.76 6.75 5.24 5.21 4.41 4.41 4.39 4.39 4.38 4.37 4.36 4.35 4.33 4.32 4.32 4.32 4.31 4.30 4.11 4.11 4.10 4.09 4.08 4.08 4.07 4.07 4.07 4.06 4.05 4.04 4.04 4.03 4.02 4.02 4.01 4.00 3.99 3.99 3.98 3.97 3.96 3.95 3.95 3.94 3.93 3.92 3.91 3.90 3.90 3.89 3.86 0.97 0.95 0.94
-0.00 TMS
EtO2C
O
O
Ph
N
O
O
O
15k
G (m) 7.23
C (m) 4.02
F (dd) 7.41
E (dt) 6.77
A (d) 5.23
B (m) 4.36
D (t) 0.95
1.00
7.86
1.01
1.00
4.18
8.42
3.09
f1 (ppm)

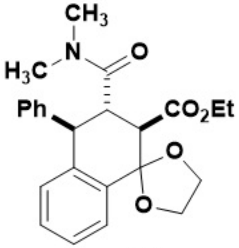
C13CPD CDCl3
100.53 MHz



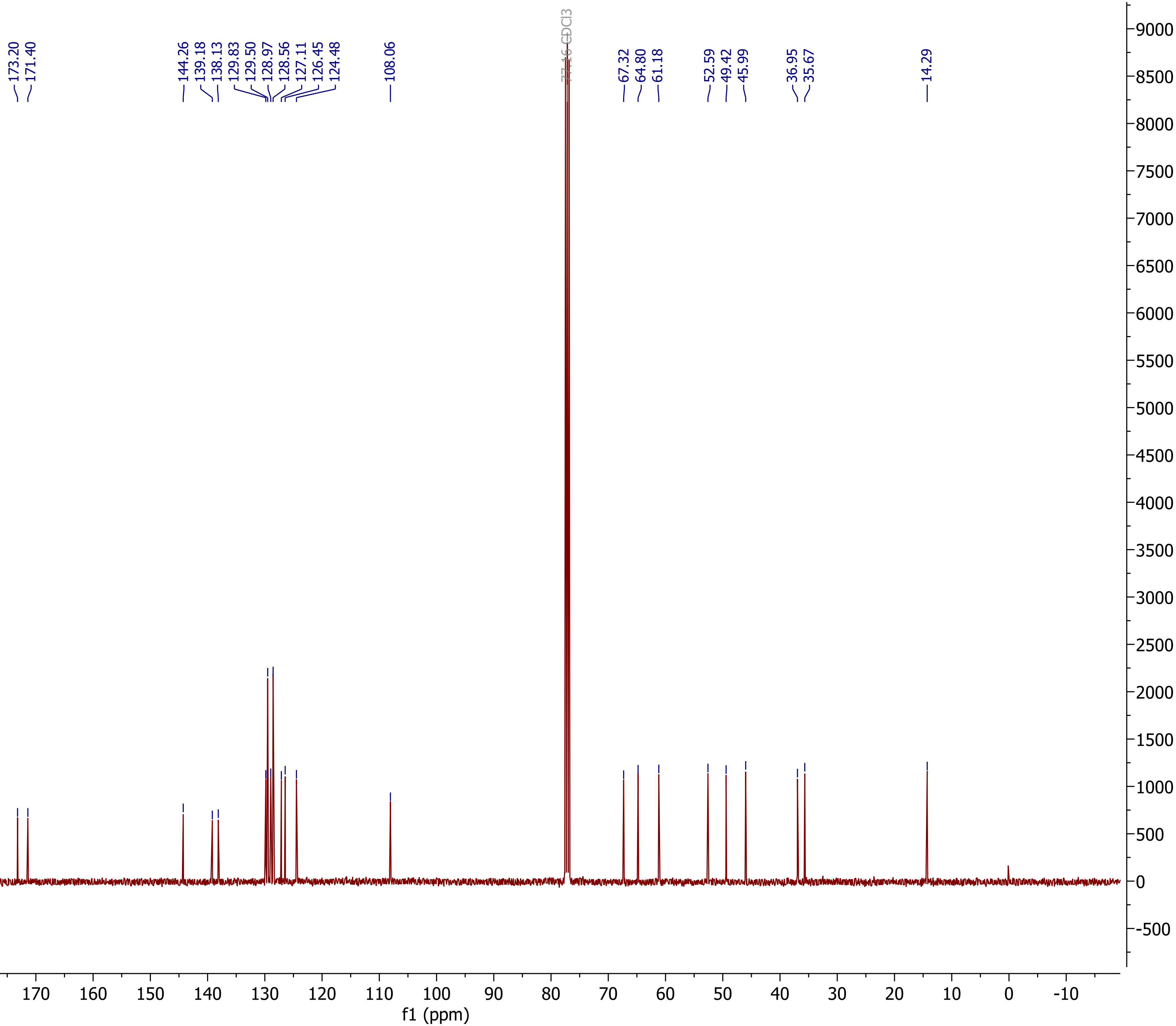
15k

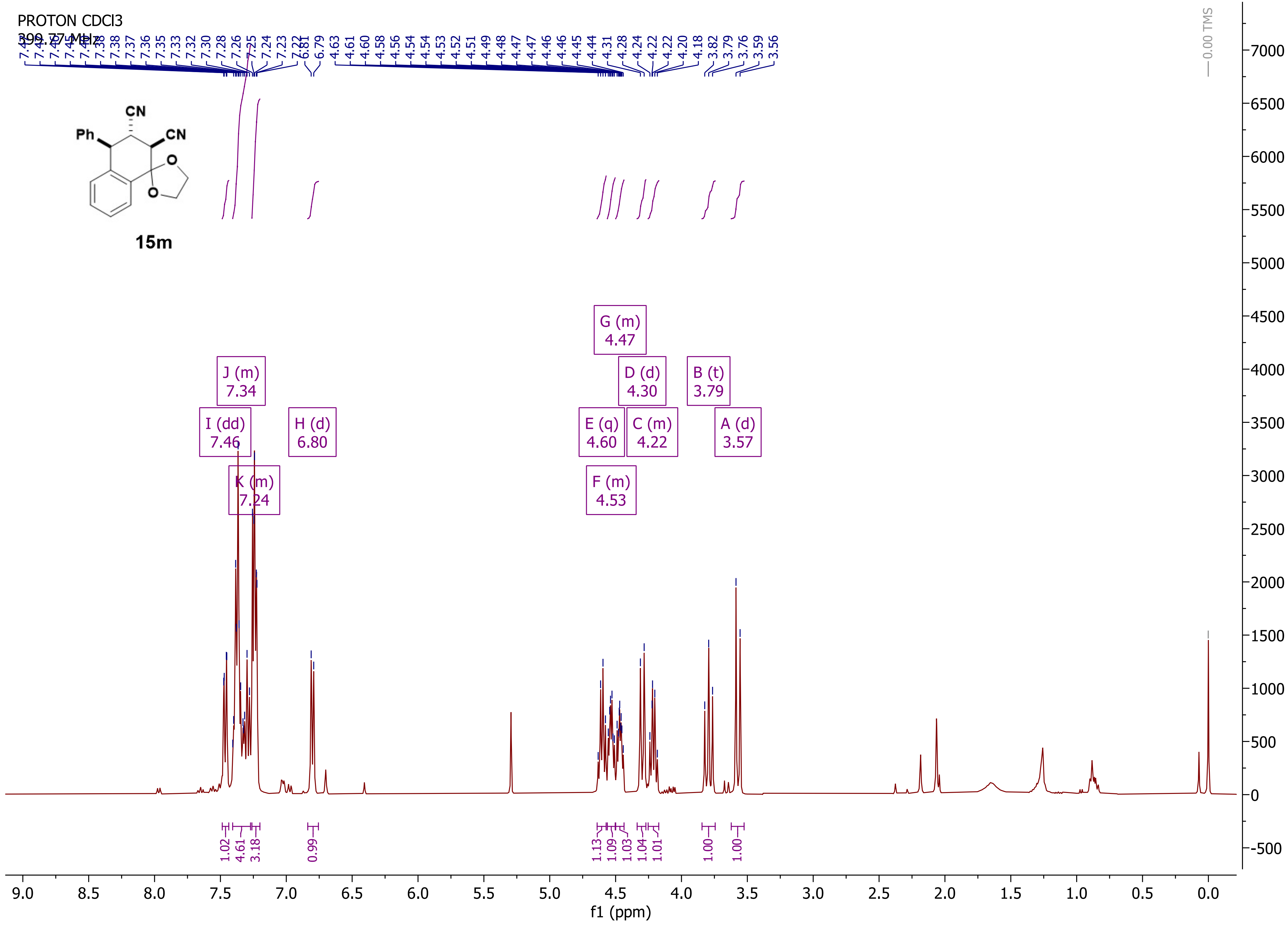


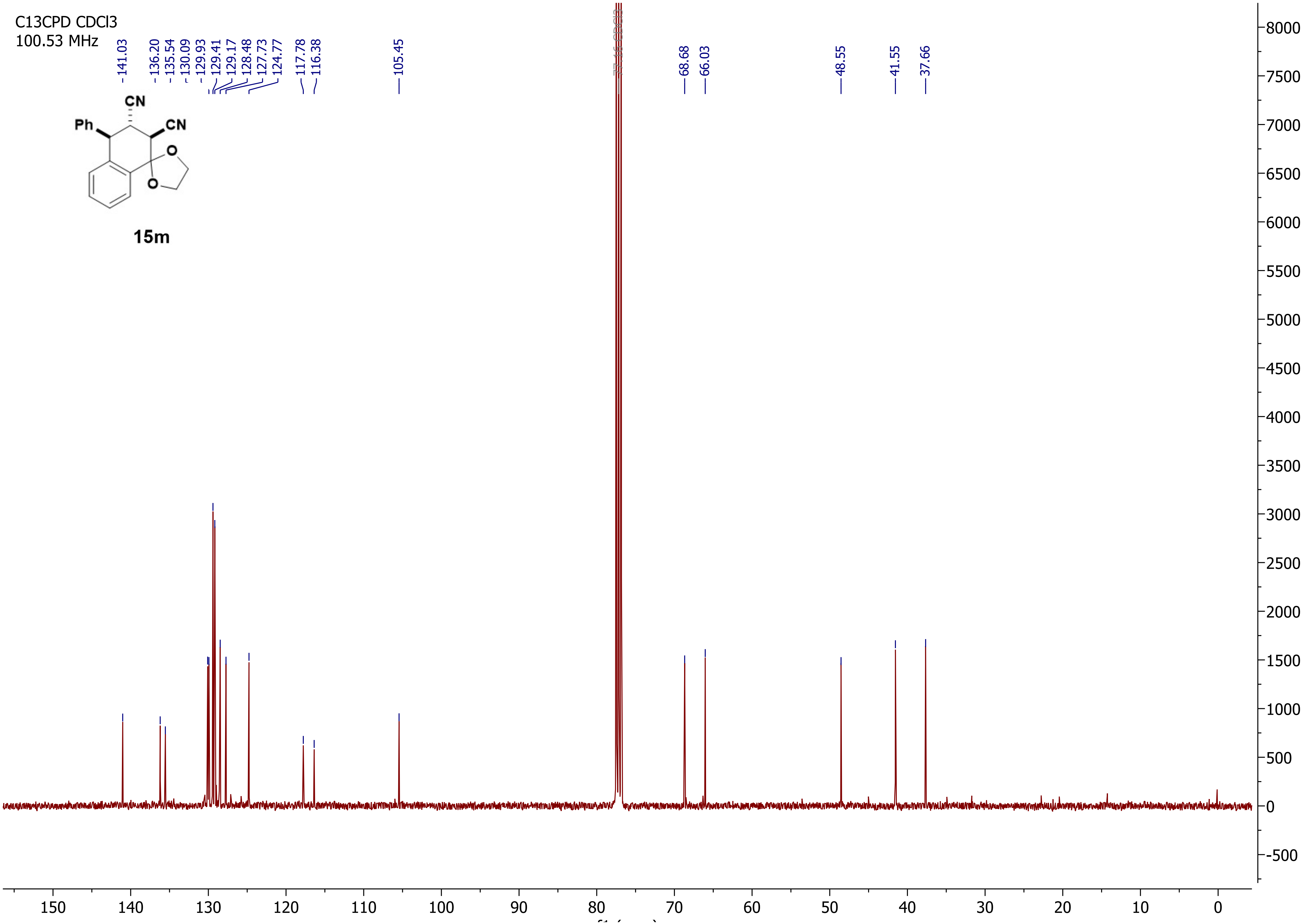

PROTON CDCl3
399.77 MHz
15l
J (m) 7.22
H (dd) 7.46
I (dt) 6.81
F (m) 4.10
E (d) 4.32
G (m) 4.41
D (d) 3.65
A (s) 2.75
B (s) 2.38
C (t) 1.28
0.99
7.38
0.98
0.97
1.01
6.06
1.03
2.99
3.00
3.13
f1 (ppm)

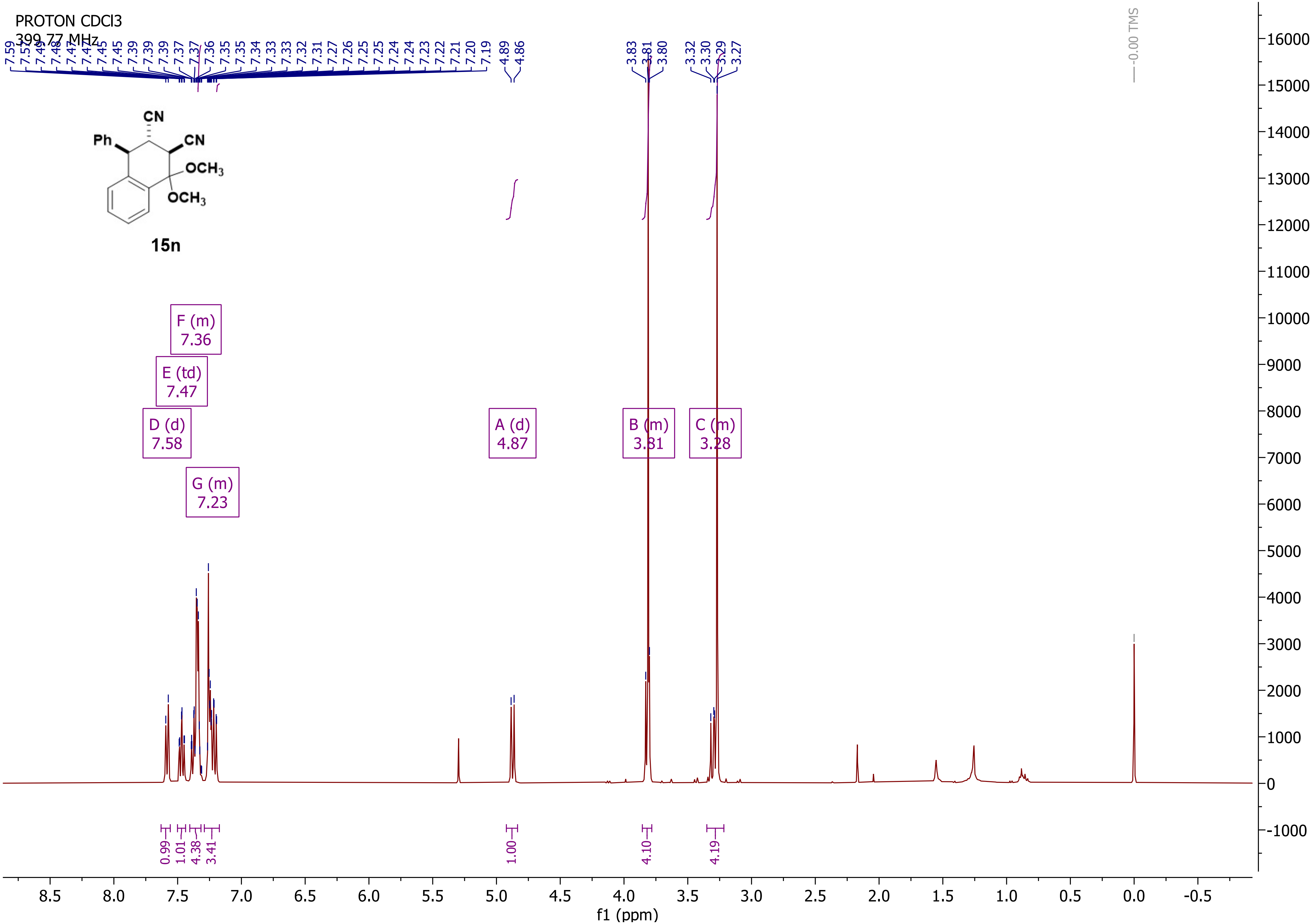

CH3
H3C
N
O
Ph
CO2Et
O
O

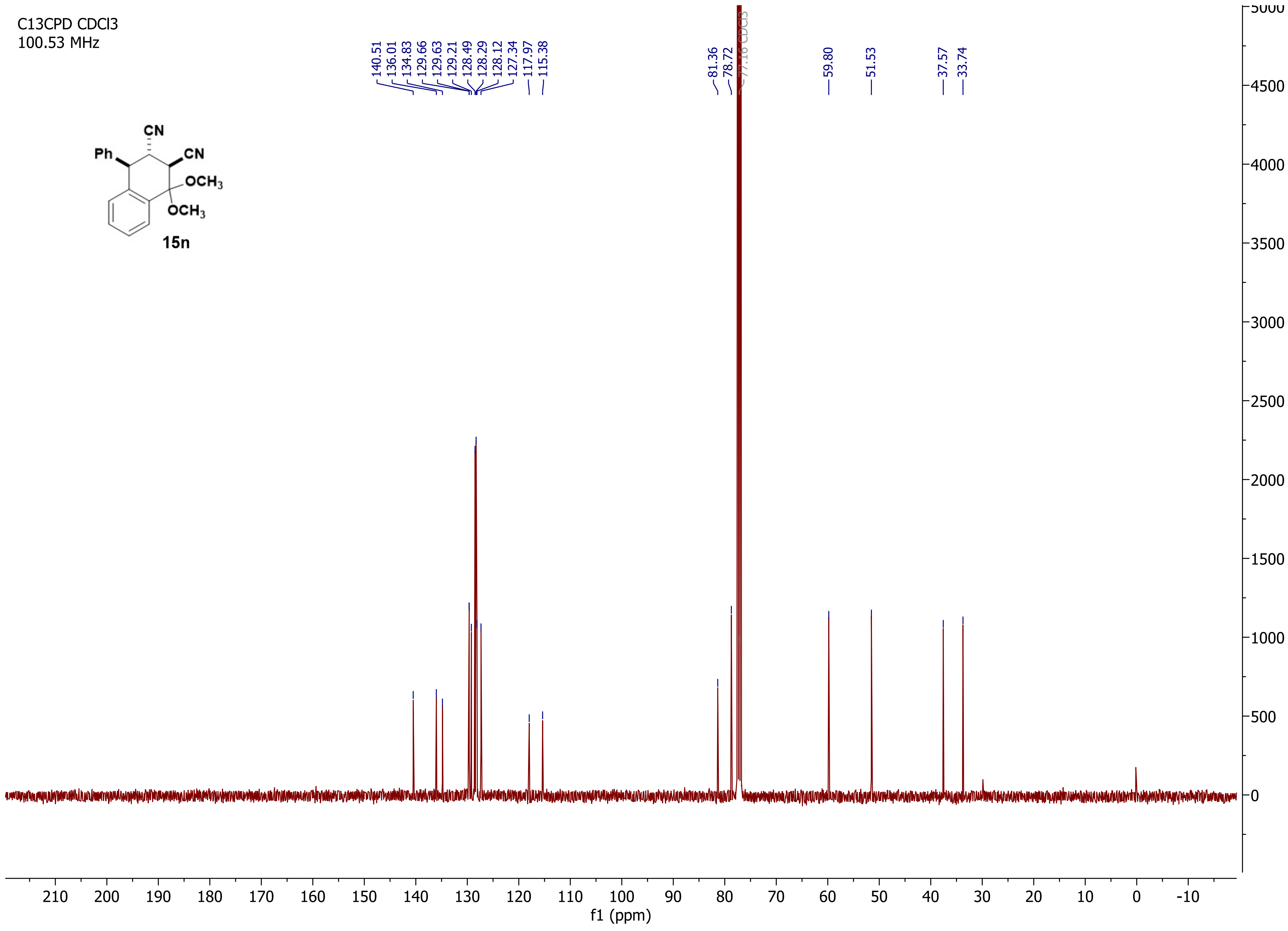
15l

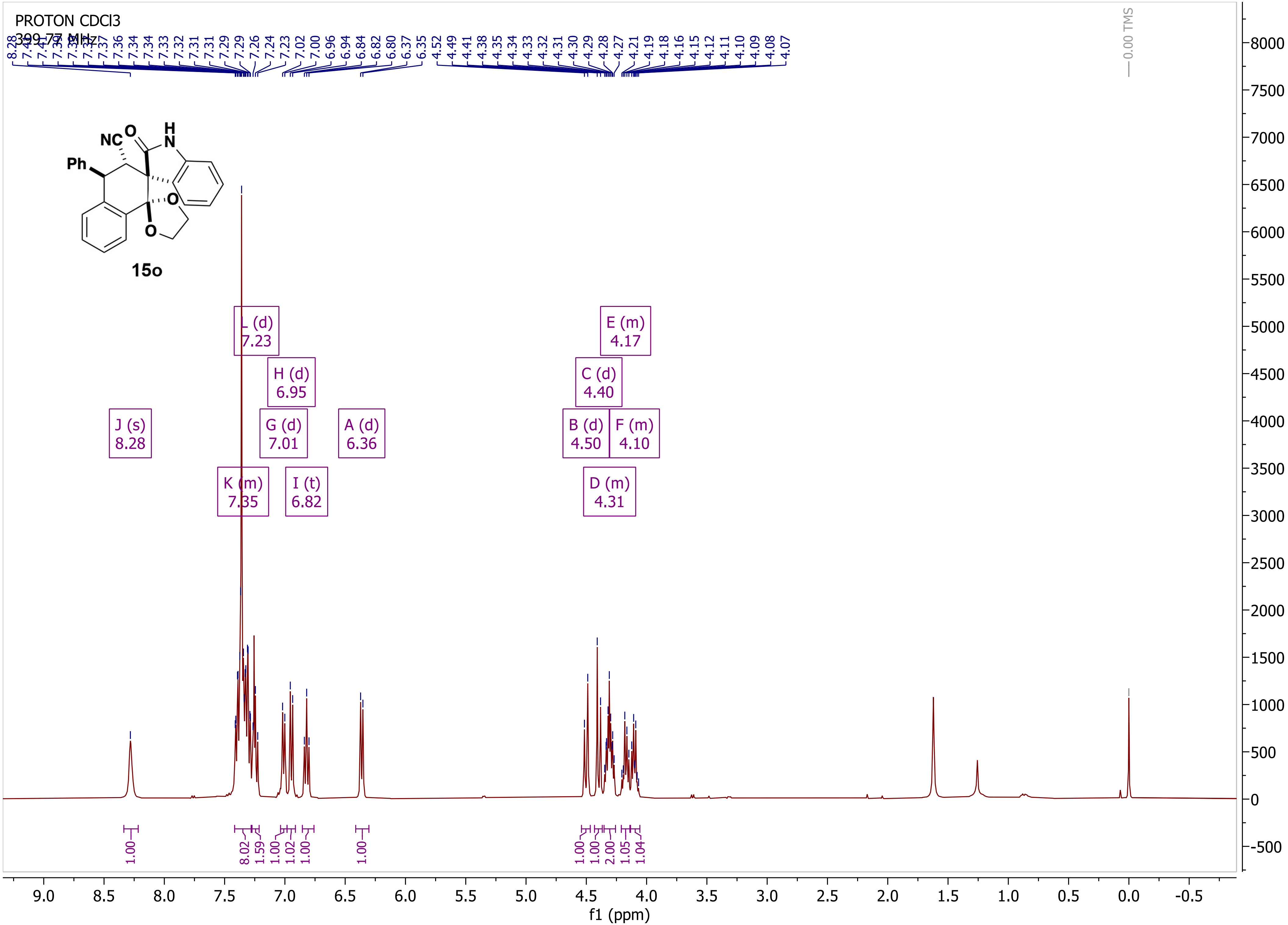

C13CPD CDCl3
100.53 MHz
173.20
171.40
144.26
139.18
138.13
129.83
129.50
128.97
128.56
127.11
126.45
124.48
108.06
77.16 CDCl3
67.32
64.80
61.18
52.59
49.42
45.99
36.95
35.67
14.29
f1 (ppm)


PROTON CDCl3
399.77 MHz
15m
J (m) 7.34
I (dd) 7.46
K (m) 7.24
H (d) 6.80
G (m) 4.47
D (d) 4.30
E (q) 4.60
C (m) 4.22
F (m) 4.53
B (t) 3.79
A (d) 3.57
0.00 TMS
f1 (ppm)

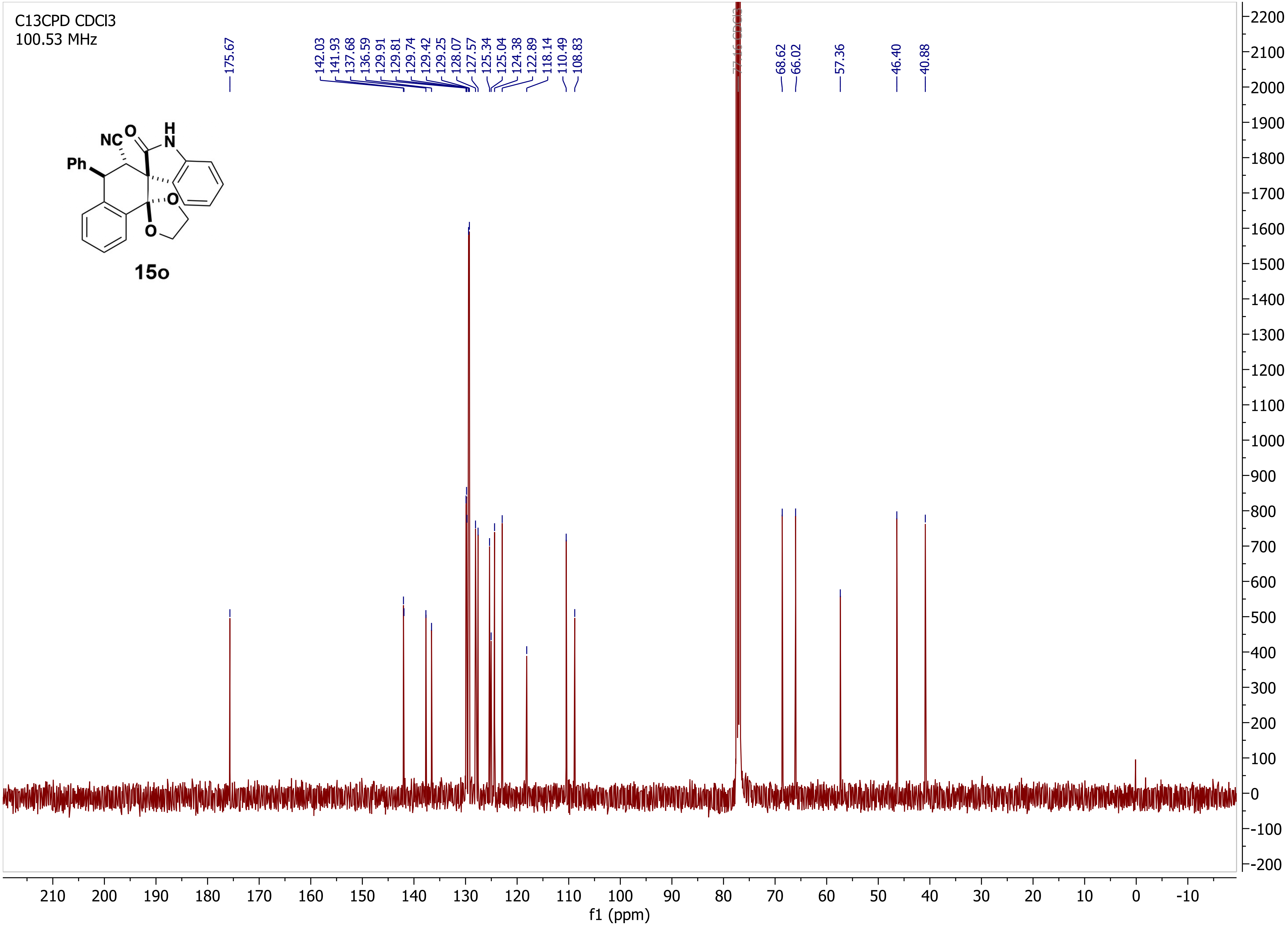

C13CPD CDCl3
100.53 MHz
141.03
136.20
135.54
130.09
129.93
129.41
129.17
128.48
127.73
124.77
117.78
116.38
105.45
68.68
66.03
48.55
41.55
37.66
Ph
CN
CN
O
O
15m
8000
7500
7000
6500
6000
5500
5000
4500
4000
3500
3000
2500
2000
1500
1000
500
0
-500
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0

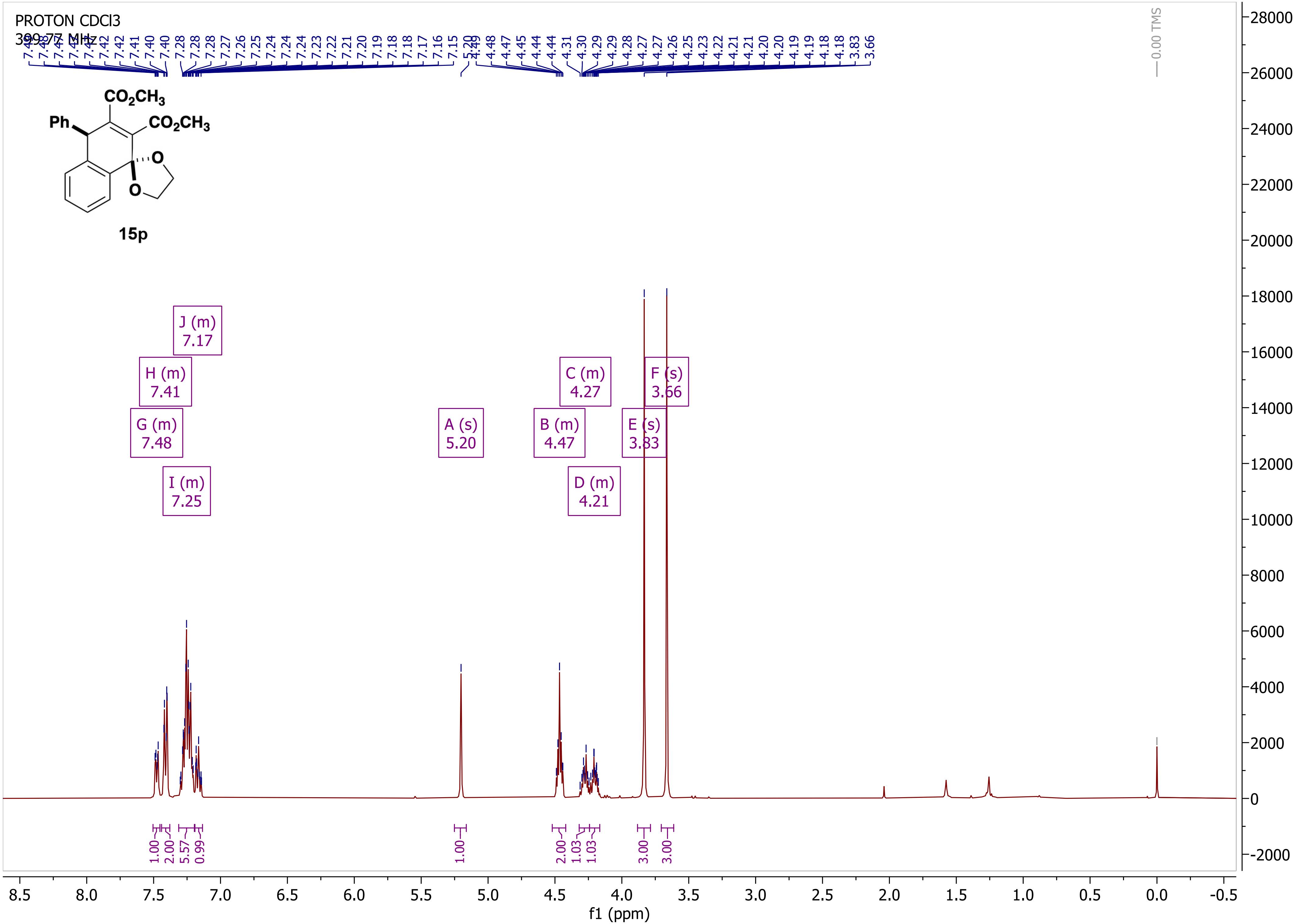

PROTON CDCl3
399.77 MHz
7.59 7.57 7.49 7.48 7.47 7.47 7.45 7.45 7.39 7.39 7.39 7.37 7.37 7.36 7.35 7.35 7.34 7.33 7.33 7.32 7.31 7.27 7.26 7.25 7.25 7.24 7.24 7.23 7.22 7.21 7.20 7.19 4.89 4.86
3.83 3.81 3.80 3.32 3.30 3.29 3.27
-0.00 TMS
CN
Ph
CN
OCH3
OCH3
15n
F (m) 7.36
E (td) 7.47
D (d) 7.58
G (m) 7.23
A (d) 4.87
B (m) 3.81
C (m) 3.28
0.99 1.01 4.38 3.41 1.00 4.10 4.19
f1 (ppm)

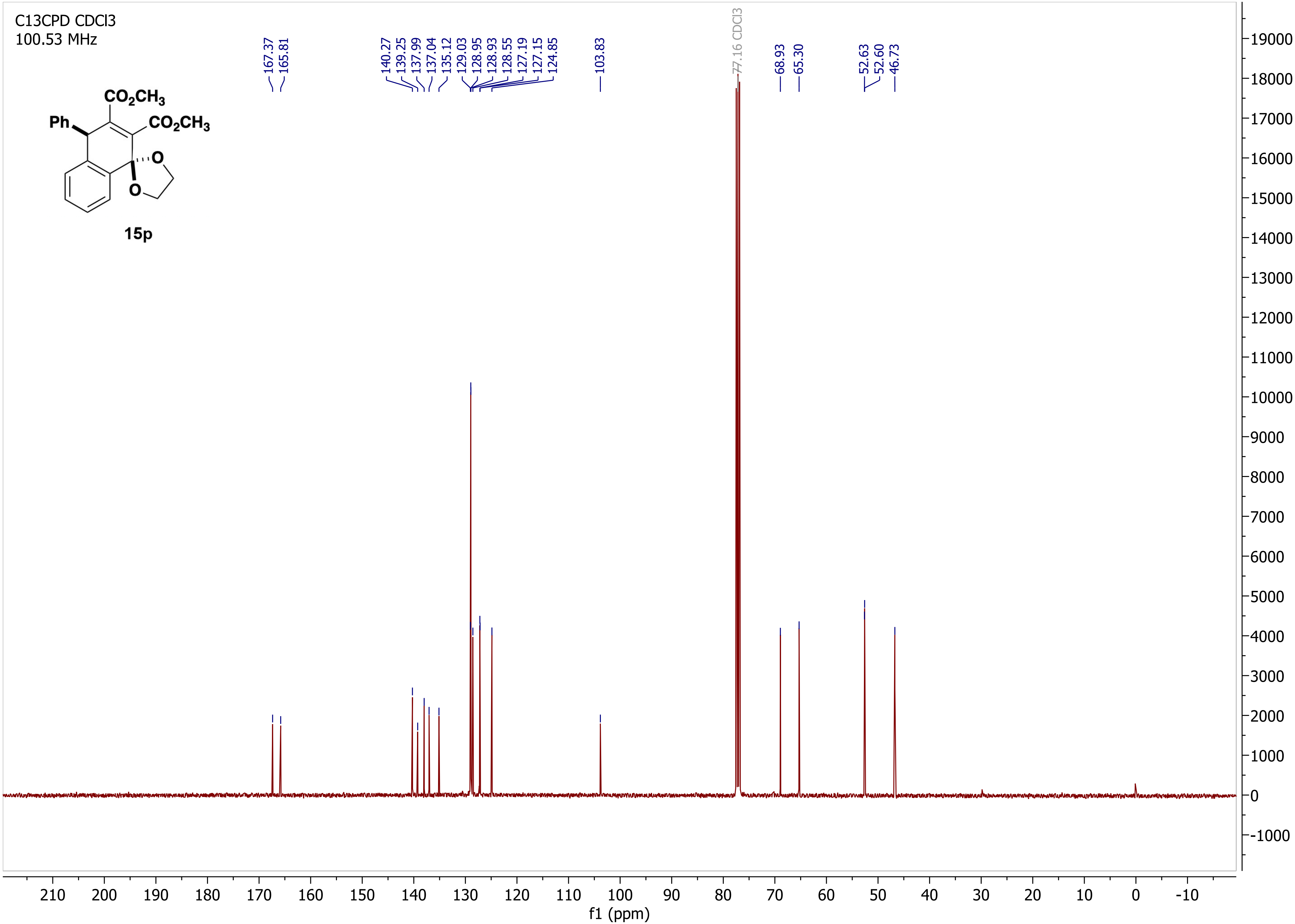

C13CPD CDCl3
100.53 MHz
140.51
136.01
134.83
129.66
129.63
129.21
128.49
128.29
128.12
127.34
117.97
115.38
81.36
78.72
77.16 CDCl3
59.80
51.53
37.57
33.74
Ph
CN
CN
OCH3
OCH3
15n
f1 (ppm)



15o
PROTON CDCl3
399.77 MHz
J (s) 8.28
K (m) 7.35
L (d) 7.23
G (d) 7.01
H (d) 6.95
I (t) 6.82
A (d) 6.36
B (d) 4.50
C (d) 4.40
D (m) 4.31
E (m) 4.17
F (m) 4.10
0.00 TMS
f1 (ppm)

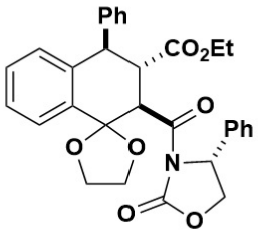

C13CPD CDCl3
100.53 MHz
175.67
142.03
141.93
137.68
136.59
129.91
129.81
129.74
129.42
129.25
128.07
127.57
125.34
125.04
124.38
122.89
118.14
110.49
108.83
77.16 CDCl3
68.62
66.02
57.36
46.40
40.88
NC
O
H
N
Ph
O
O
15o
f1 (ppm)


PROTON CDCl3
399.77 MHz
15p
J (m) 7.17
H (m) 7.41
G (m) 7.48
I (m) 7.25
A (s) 5.20
B (m) 4.47
C (m) 4.27
D (m) 4.21
E (s) 3.83
F (s) 3.66
0.00 TMS
f1 (ppm)

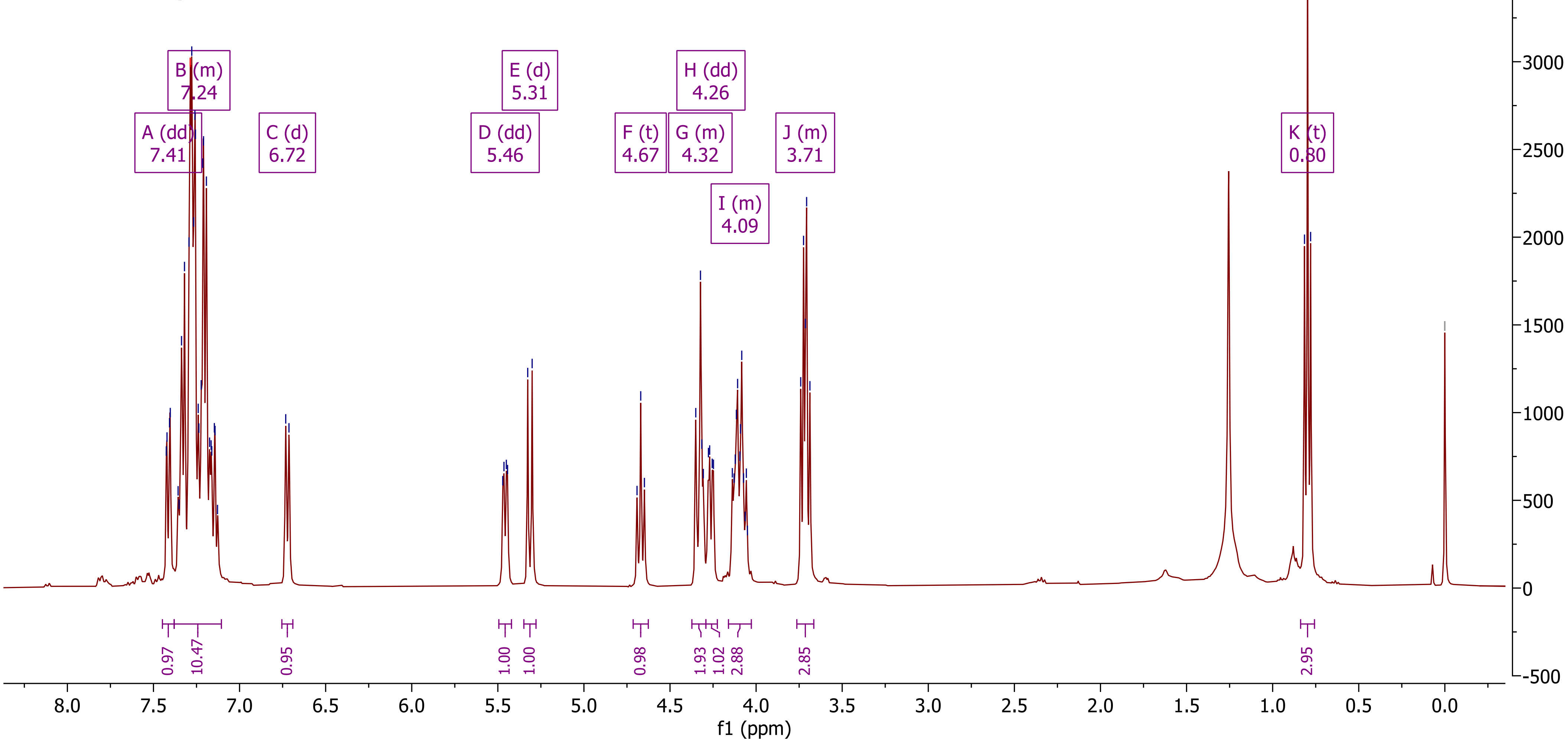

C13CPD CDCl3
100.53 MHz
CO2CH3
Ph
CO2CH3
O
O
167.37
165.81
140.27
139.25
137.99
137.04
135.12
129.03
128.95
128.93
128.55
127.19
127.15
124.85
103.83
77.16 CDCl3
68.93
65.30
52.63
52.60
46.73
f1 (ppm)

15p

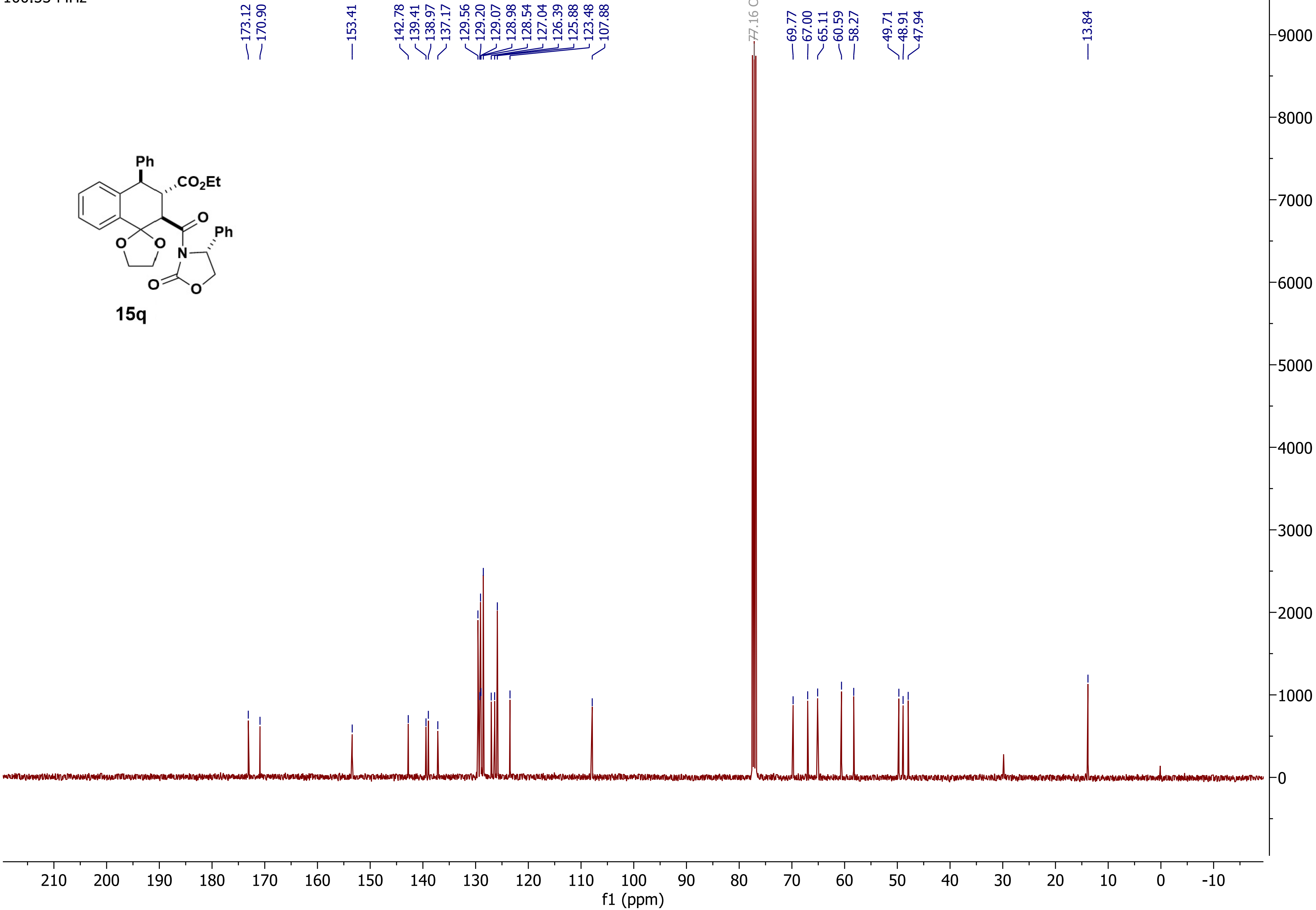
PROTON CDCl3 /home/nmrdata/Shaw amines19 6
399.77 MHz



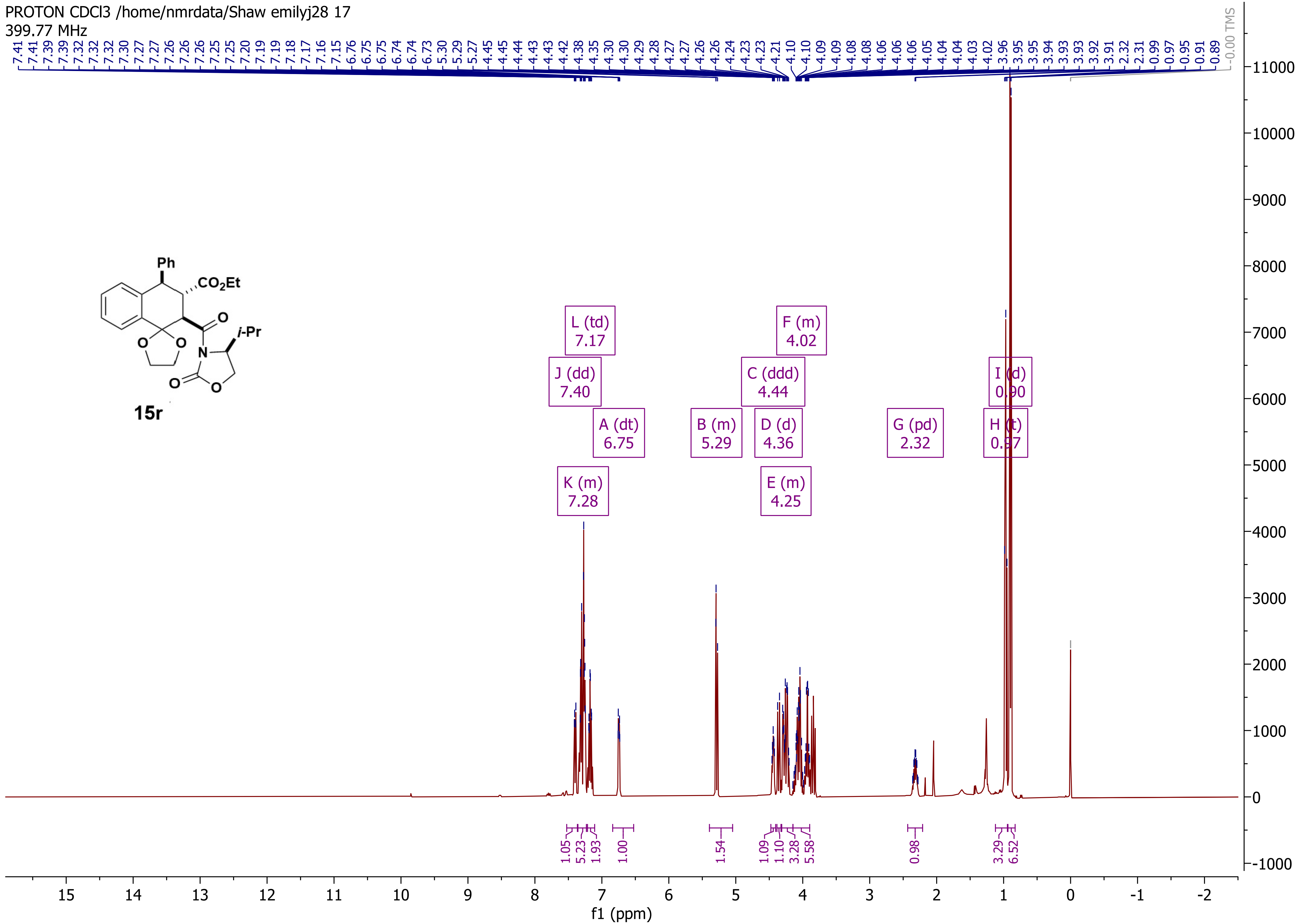
15q



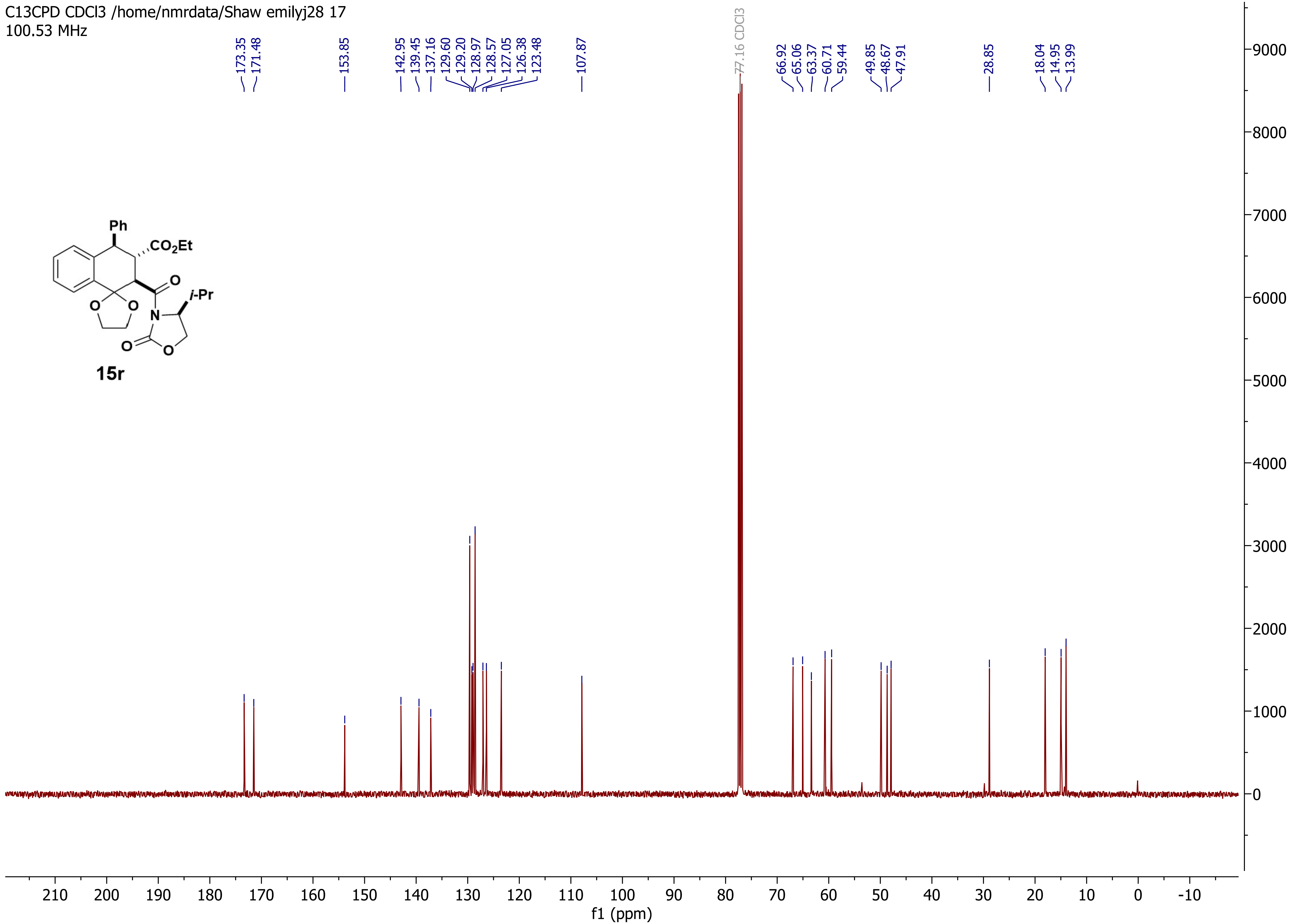
C13CPD CDCl3 /home/nmrdata/Shaw amines19 6
100.53 MHz

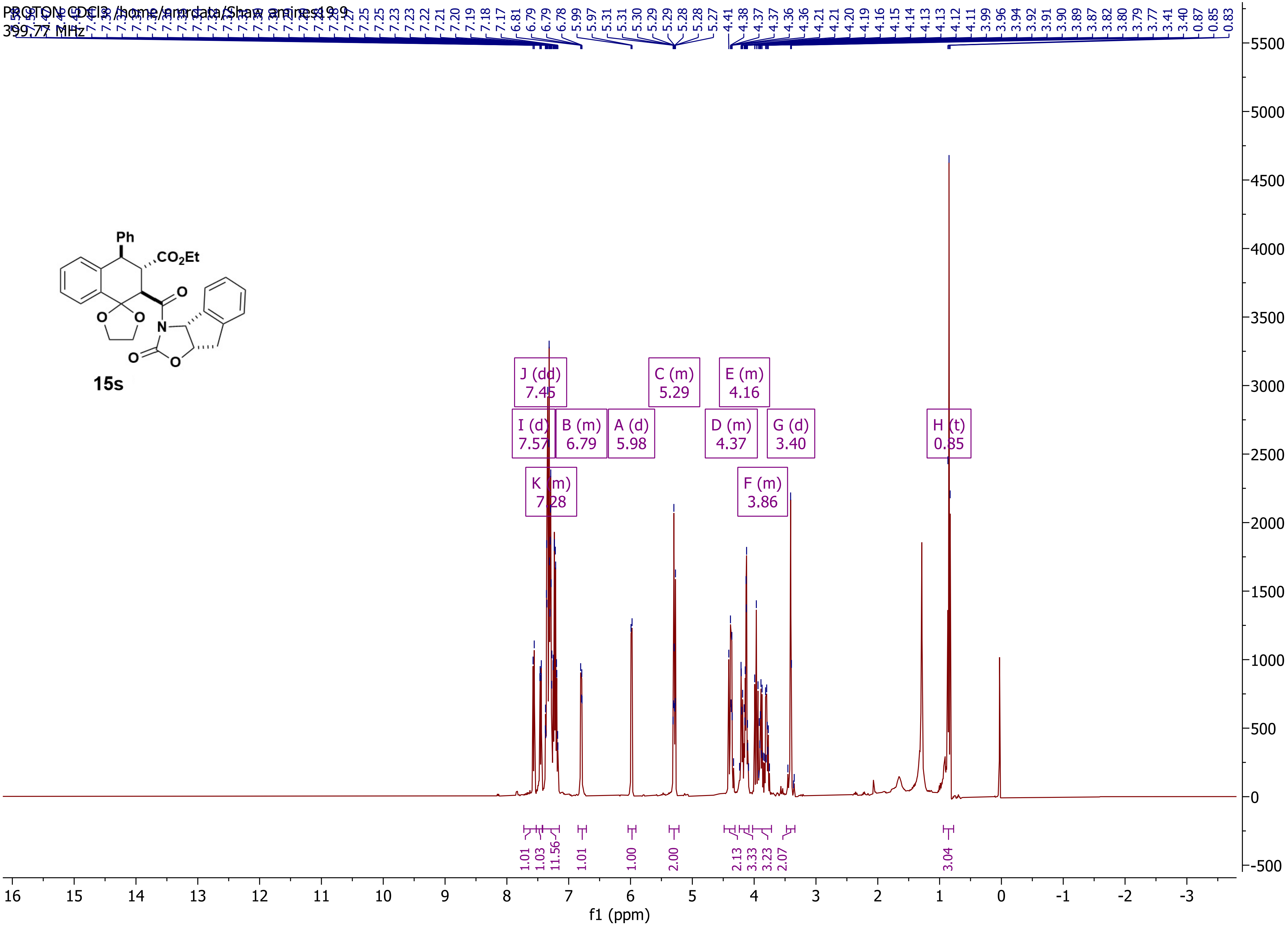


15q

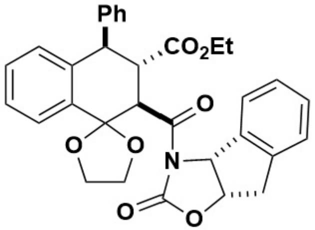


PROTON CDCl3 /home/nmrdata/Shaw emilyj28 17
399.77 MHz
7.41 7.41 7.39 7.39 7.32 7.32 7.32 7.30 7.27 7.27 7.26 7.26 7.26 7.25 7.25 7.20 7.19 7.19 7.18 7.17 7.16 7.15 6.76 6.75 6.75 6.74 6.74 6.73 5.30 5.29 5.27 4.45 4.45 4.44 4.43 4.43 4.42 4.38 4.35 4.30 4.30 4.29 4.28 4.27 4.27 4.26 4.26 4.24 4.23 4.23 4.21 4.10 4.10 4.09 4.09 4.08 4.08 4.06 4.06 4.06 4.05 4.04 4.04 4.03 4.02 3.96 3.95 3.95 3.94 3.93 3.93 3.92 3.91 2.32 2.31 0.99 0.97 0.95 0.91 0.89
-0.00 TMS
Ph
CO2Et
O
i-Pr
O
O
N
O
O
15r
L (td) 7.17
J (dd) 7.40
A (dt) 6.75
K (m) 7.28
B (m) 5.29
F (m) 4.02
C (ddd) 4.44
D (d) 4.36
E (m) 4.25
G (pd) 2.32
I (d) 0.90
H (t) 0.97
1.05 5.23 1.93 1.00 1.54 1.09 1.10 3.28 5.58 0.98 3.29 6.52
11000 10000 9000 8000 7000 6000 5000 4000 3000 2000 1000 0 -1000
15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1 -2
f1 (ppm)

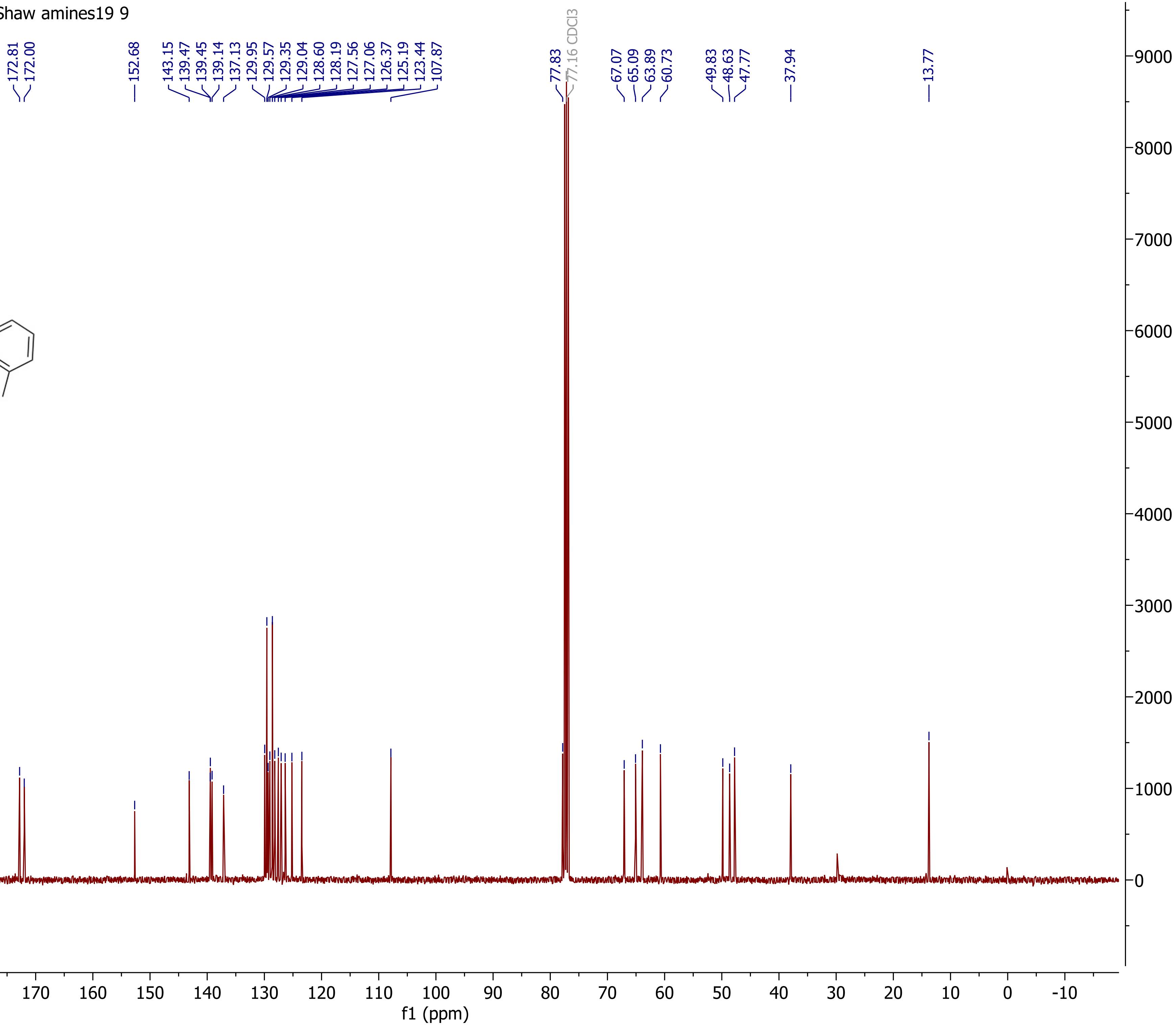

C13CPD CDCl3 /home/nmrdata/Shaw emilyj28 17
100.53 MHz
173.35
171.48
153.85
142.95
139.45
137.16
129.60
129.20
128.97
128.57
127.05
126.38
123.48
107.87
77.16 CDCl3
66.92
65.06
63.37
60.71
59.44
49.85
48.67
47.91
28.85
18.04
14.95
13.99
Ph
CO2Et
O
i-Pr
O
O
N
O
O
15r
f1 (ppm)

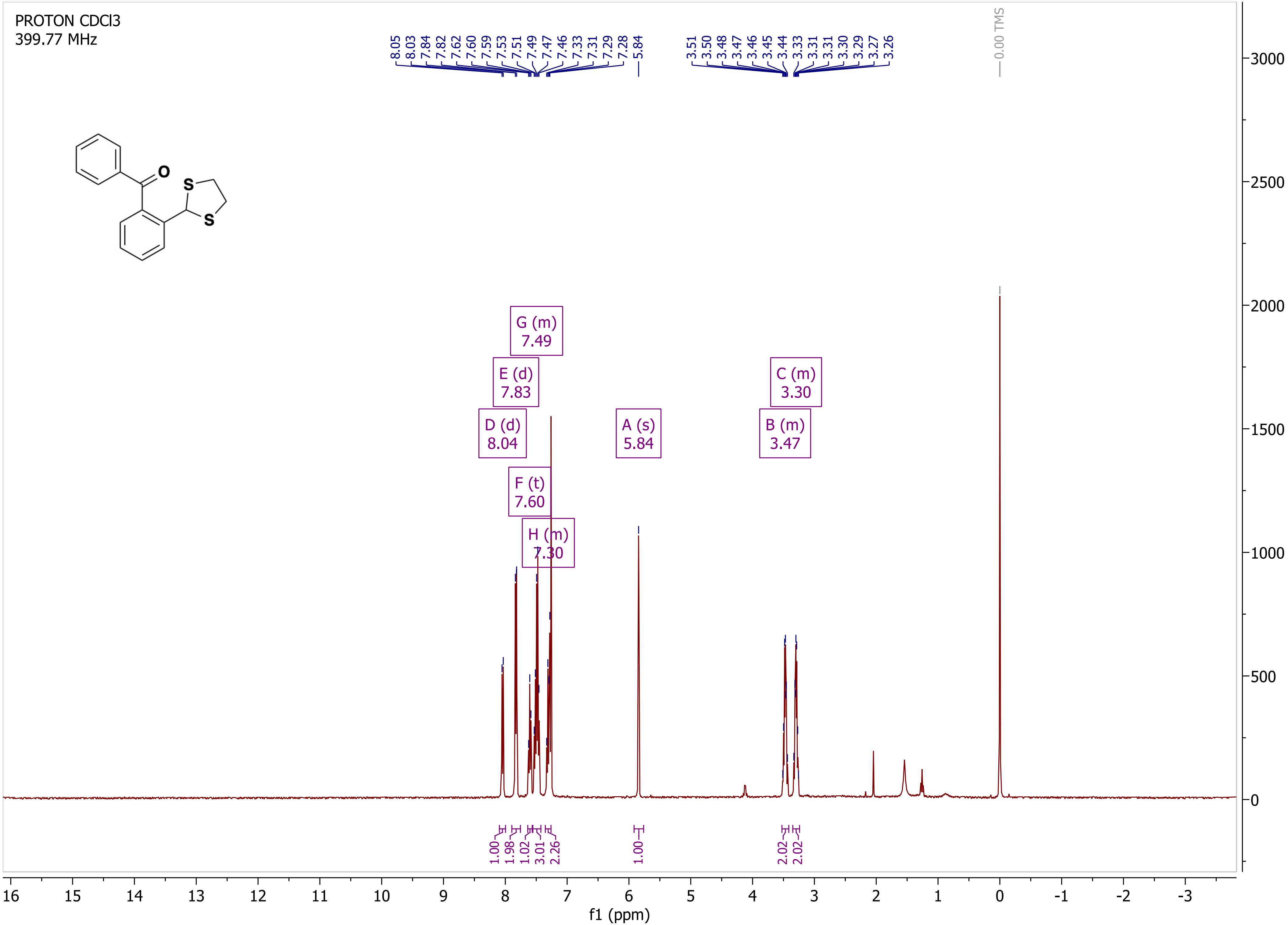

PROTON CDCl3 /home/nmrdata/Shaw amines19.9
399.77 MHz
7.25 7.25 7.23 7.23 7.22 7.21 7.20 7.19 7.18 7.17 6.81 6.79 6.79 6.78 5.99 5.97 5.31 5.31 5.30 5.29 5.29 5.28 5.28 5.27 4.41 4.38 4.37 4.37 4.36 4.36 4.21 4.21 4.20 4.19 4.16 4.15 4.14 4.13 4.13 4.12 4.11 3.99 3.96 3.94 3.92 3.91 3.90 3.89 3.87 3.82 3.80 3.79 3.77 3.41 3.40 0.87 0.85 0.83
Ph
CO2Et
O
N
O
O
O
O
15s
J (dd) 7.45
I (d) 7.57
B (m) 6.79
A (d) 5.98
K (m) 7.28
C (m) 5.29
E (m) 4.16
D (m) 4.37
G (d) 3.40
F (m) 3.86
H (t) 0.85
1.01
1.03
11.56
1.01
1.00
2.00
2.13
3.33
3.23
2.07
3.04
f1 (ppm)

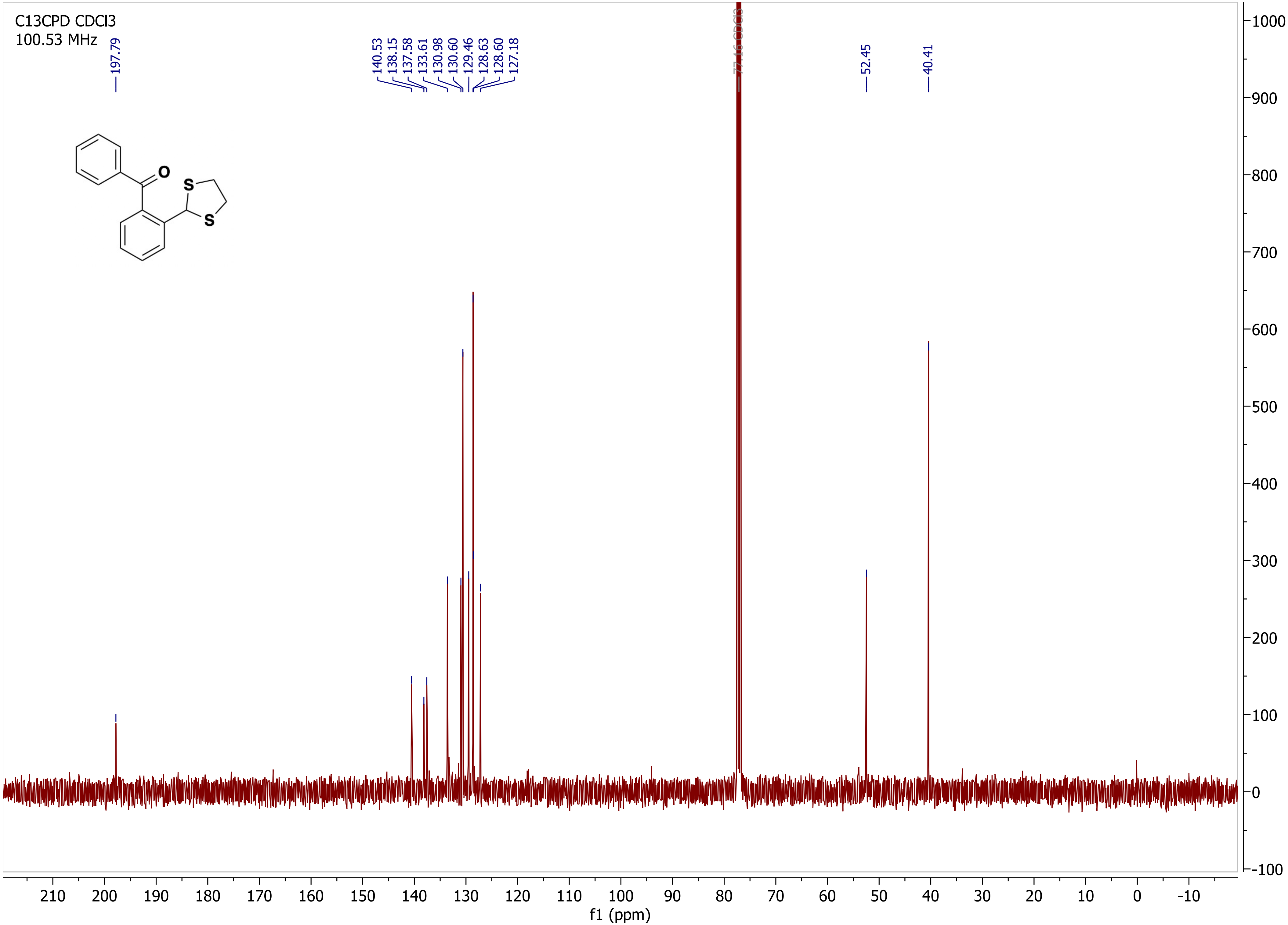
C13CPD CDCl3 /home/nmrdata/Shaw amines19 9
100.53 MHz

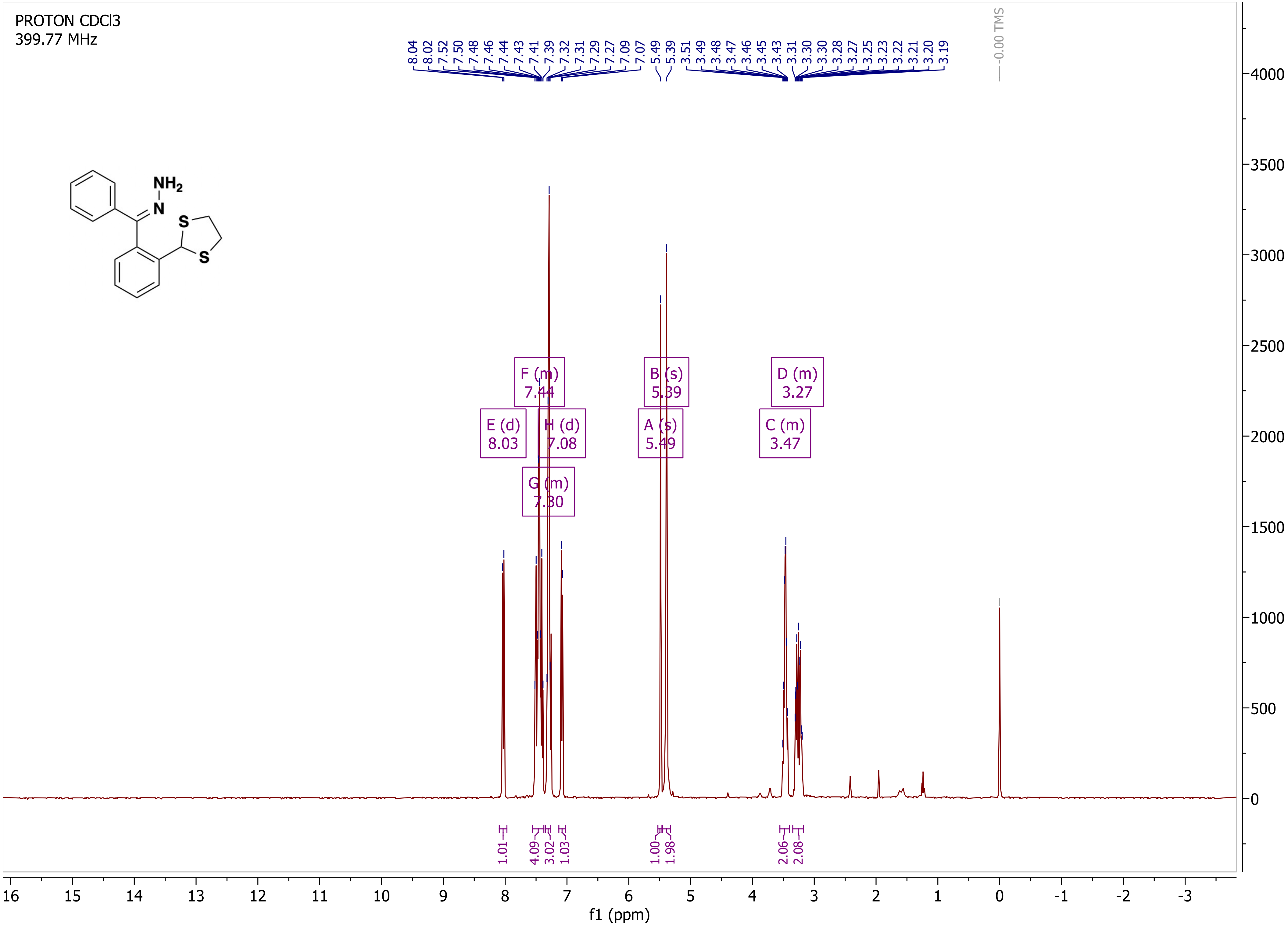


15s

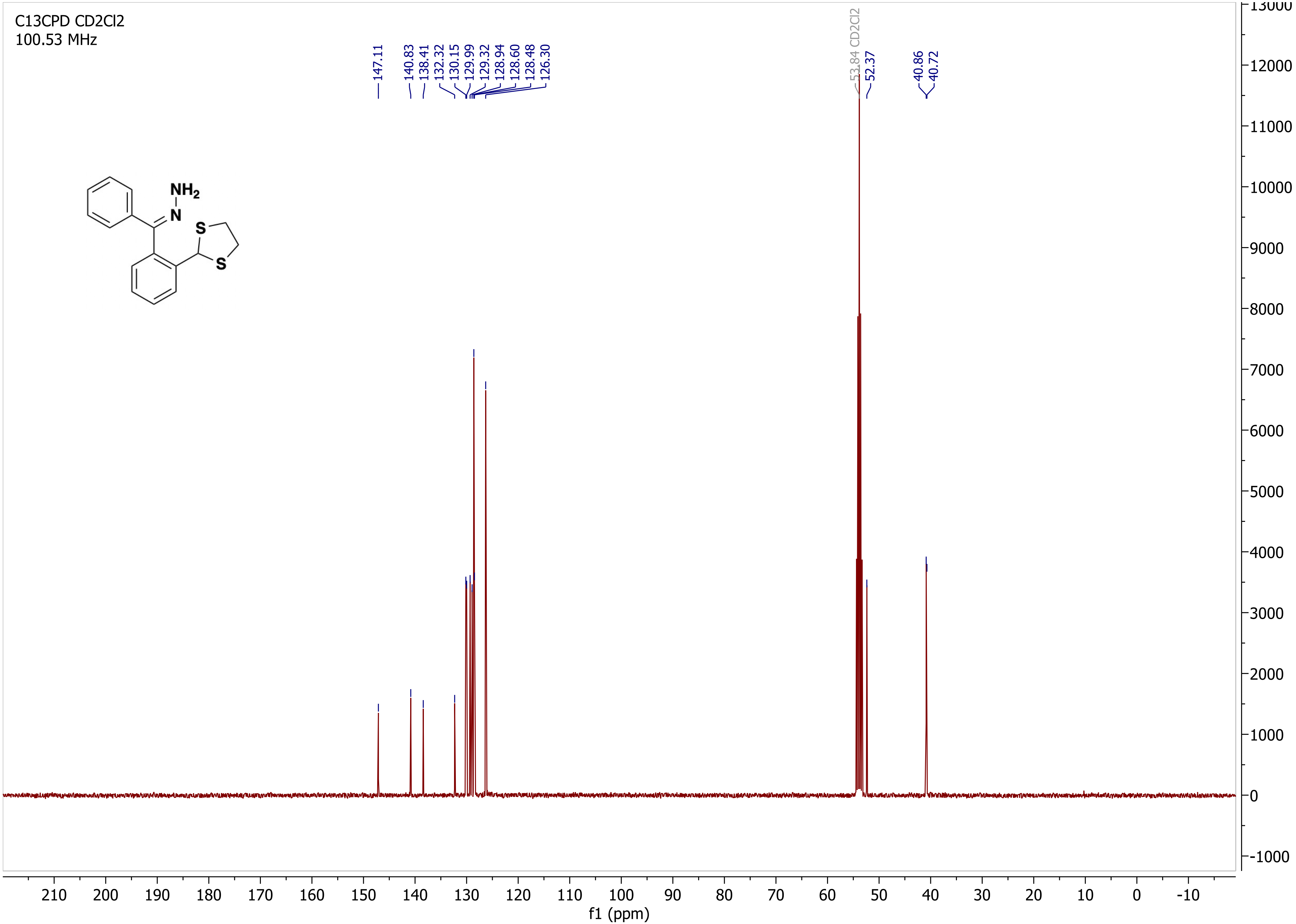



PROTON CDCl3
399.77 MHz
8.05
8.03
7.84
7.82
7.62
7.60
7.59
7.53
7.51
7.49
7.47
7.46
7.33
7.31
7.29
7.28
5.84
3.51
3.50
3.48
3.47
3.46
3.45
3.44
3.33
3.31
3.31
3.30
3.29
3.27
3.26
0.00 TMS
G (m) 7.49
E (d) 7.83
D (d) 8.04
F (t) 7.60
H (m) 7.30
A (s) 5.84
C (m) 3.30
B (m) 3.47
1.00
1.98
1.02
3.01
2.26
1.00
2.02
2.02
f1 (ppm)

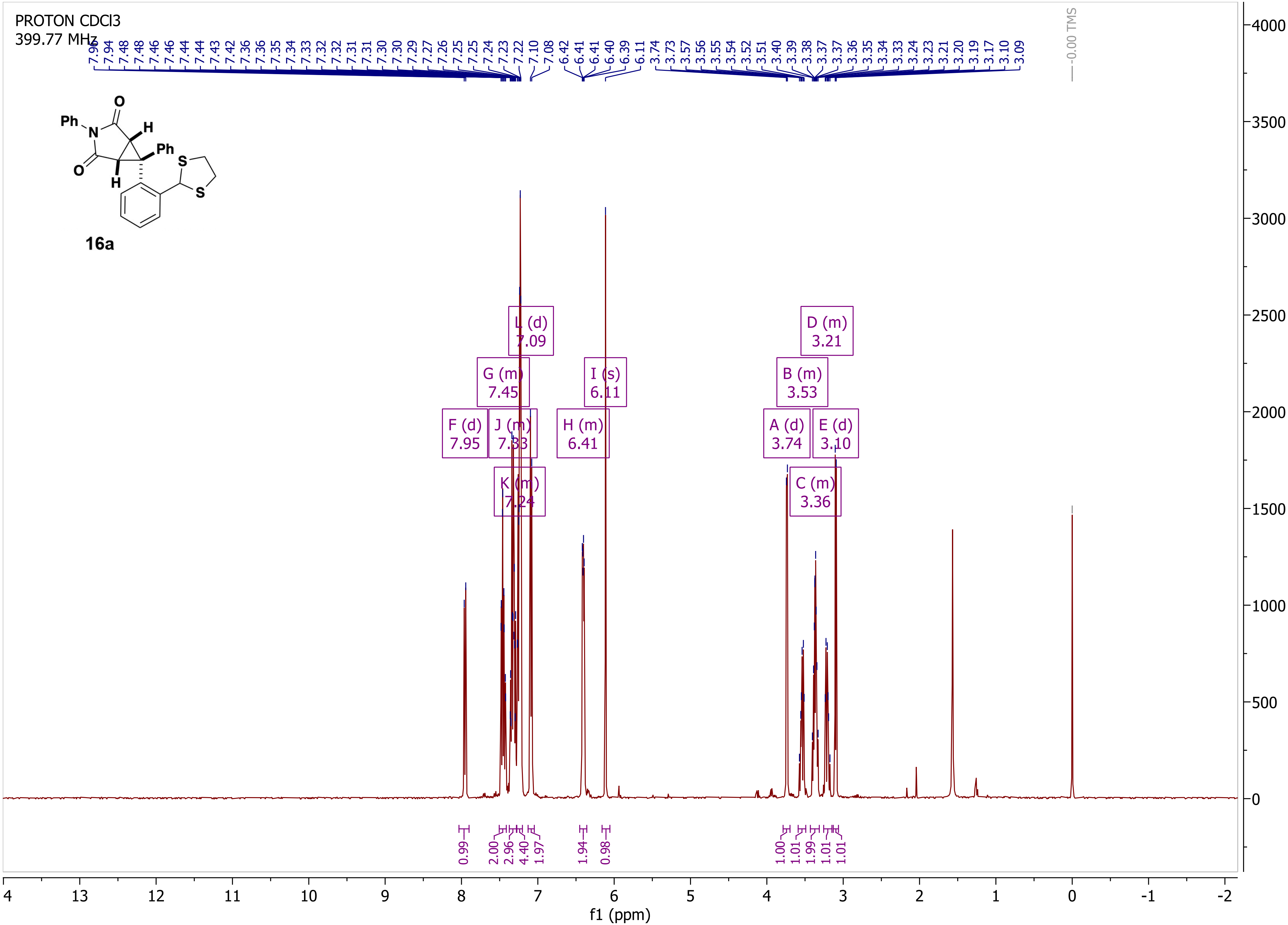

C13CPD CDCl3
100.53 MHz
197.79
140.53
138.15
137.58
133.61
130.98
130.60
129.46
128.63
128.60
127.18
77.16 CDCl3
52.45
40.41
O
S
S
f1 (ppm)



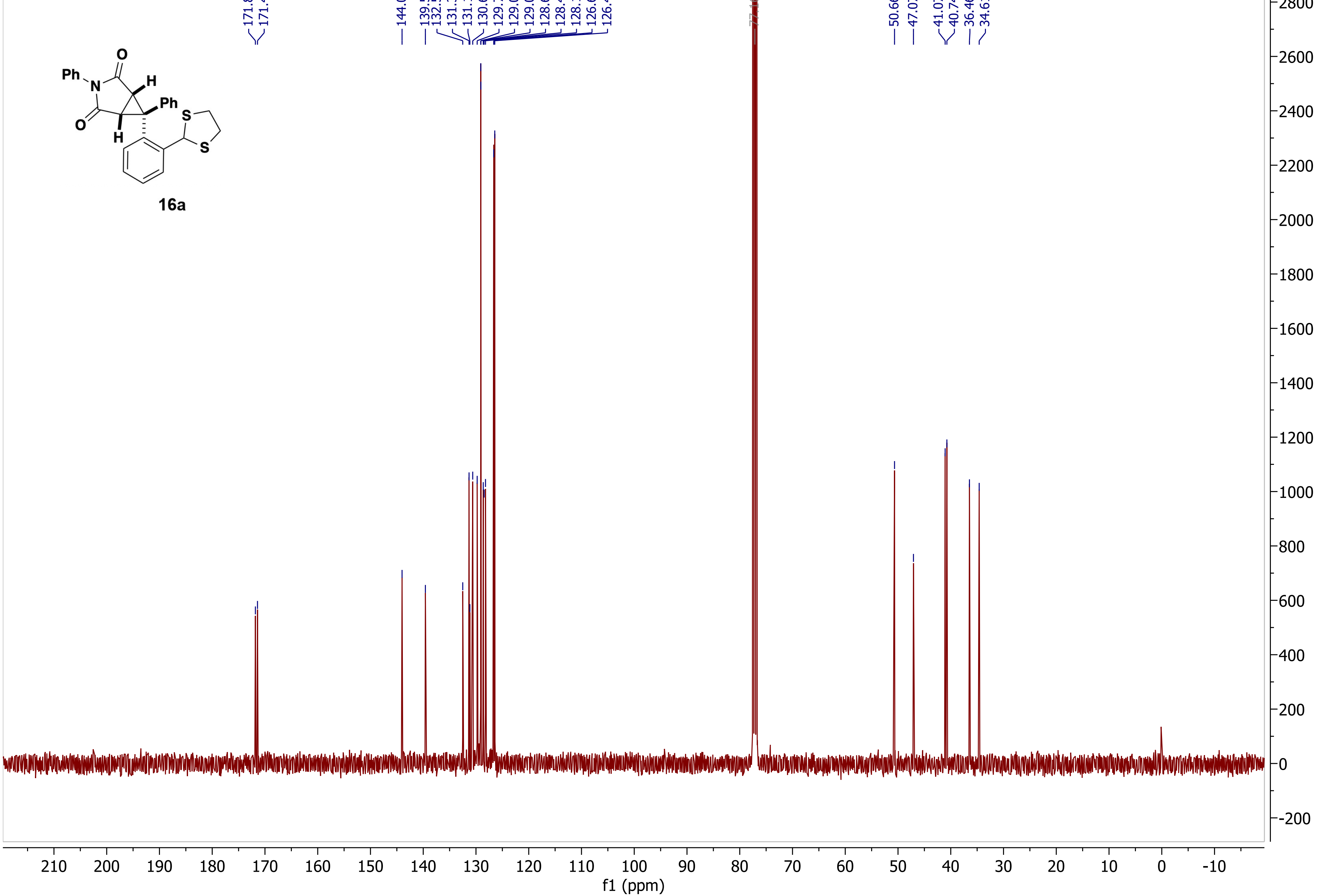
PROTON CDCl3
399.77 MHz
NH2
N
S
S
8.04
8.02
7.52
7.50
7.48
7.46
7.44
7.43
7.41
7.39
7.32
7.31
7.29
7.27
7.09
7.07
5.49
5.39
3.51
3.49
3.48
3.47
3.46
3.45
3.43
3.31
3.30
3.30
3.28
3.27
3.25
3.23
3.22
3.21
3.20
3.19
-0.00 TMS
F (m) 7.44
E (d) 8.03
H (d) 7.08
G (m) 7.30
B (s) 5.39
A (s) 5.49
D (m) 3.27
C (m) 3.47
1.01
4.09
3.02
1.03
1.00
1.98
2.06
2.08
f1 (ppm)

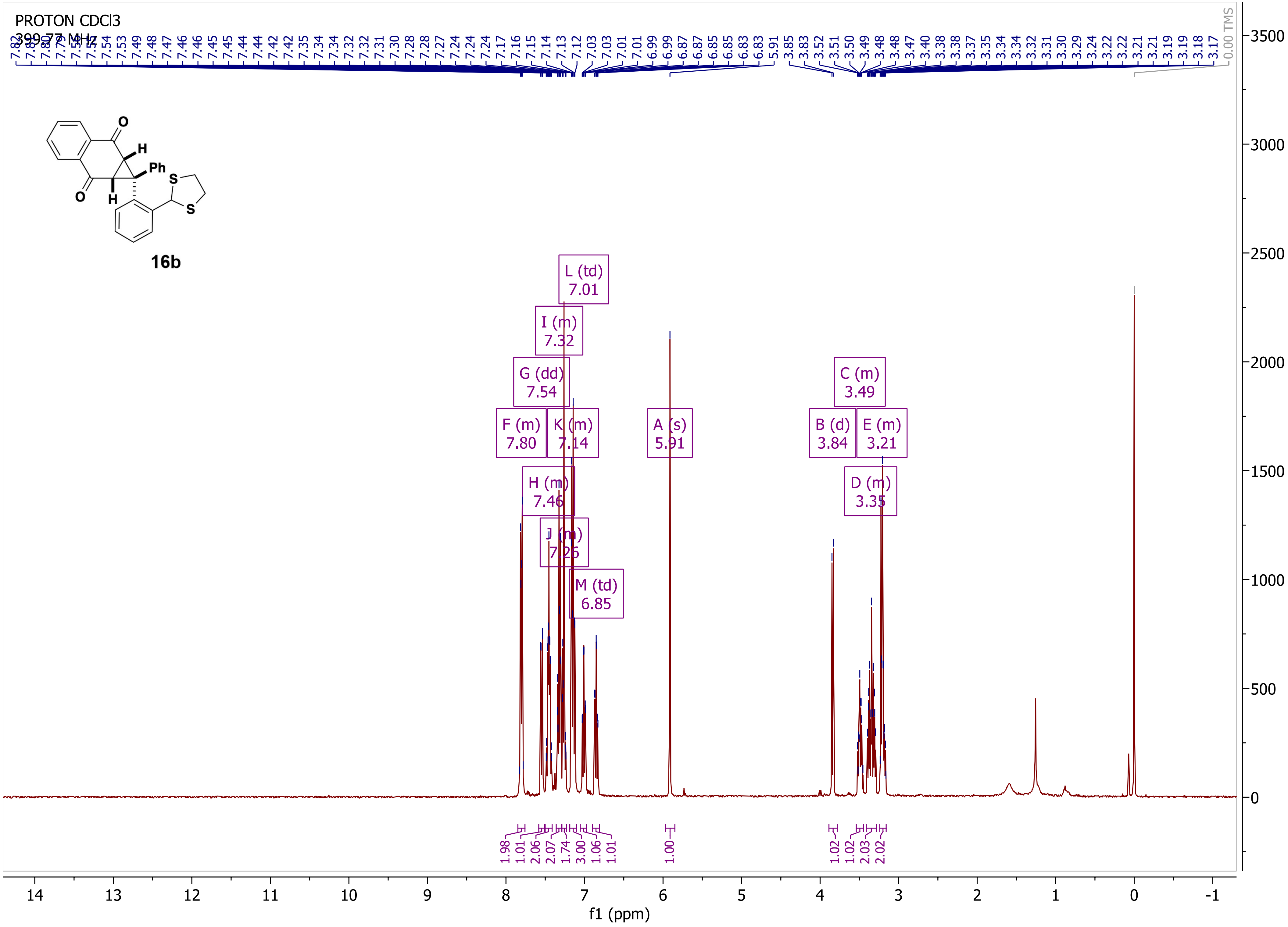


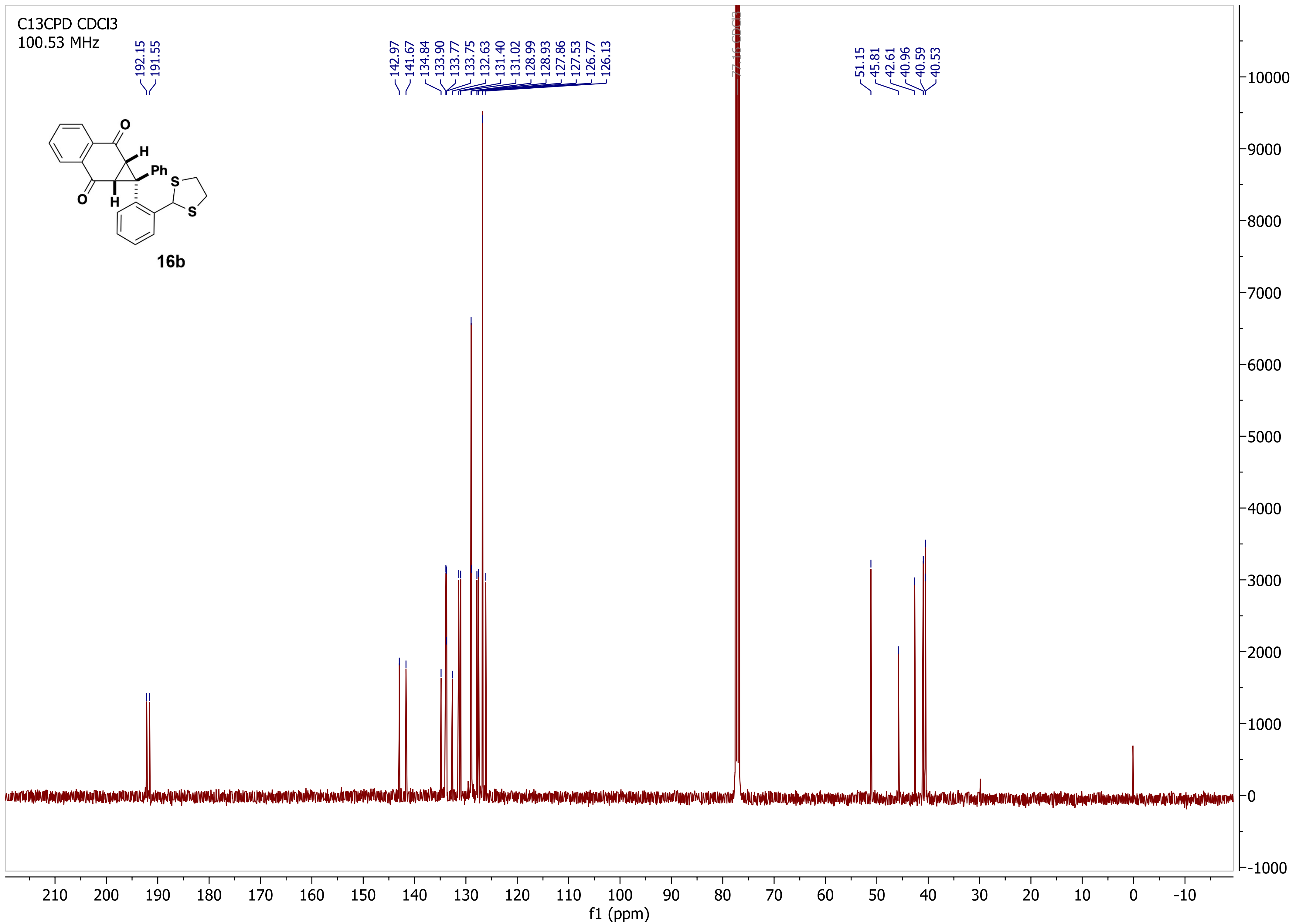
C13CPD CD2Cl2
100.53 MHz
147.11
140.83
138.41
132.32
130.15
129.99
129.32
128.94
128.60
128.48
126.30
53.84 CD2Cl2
52.37
40.86
40.72
NH2
N
S
S
f1 (ppm)

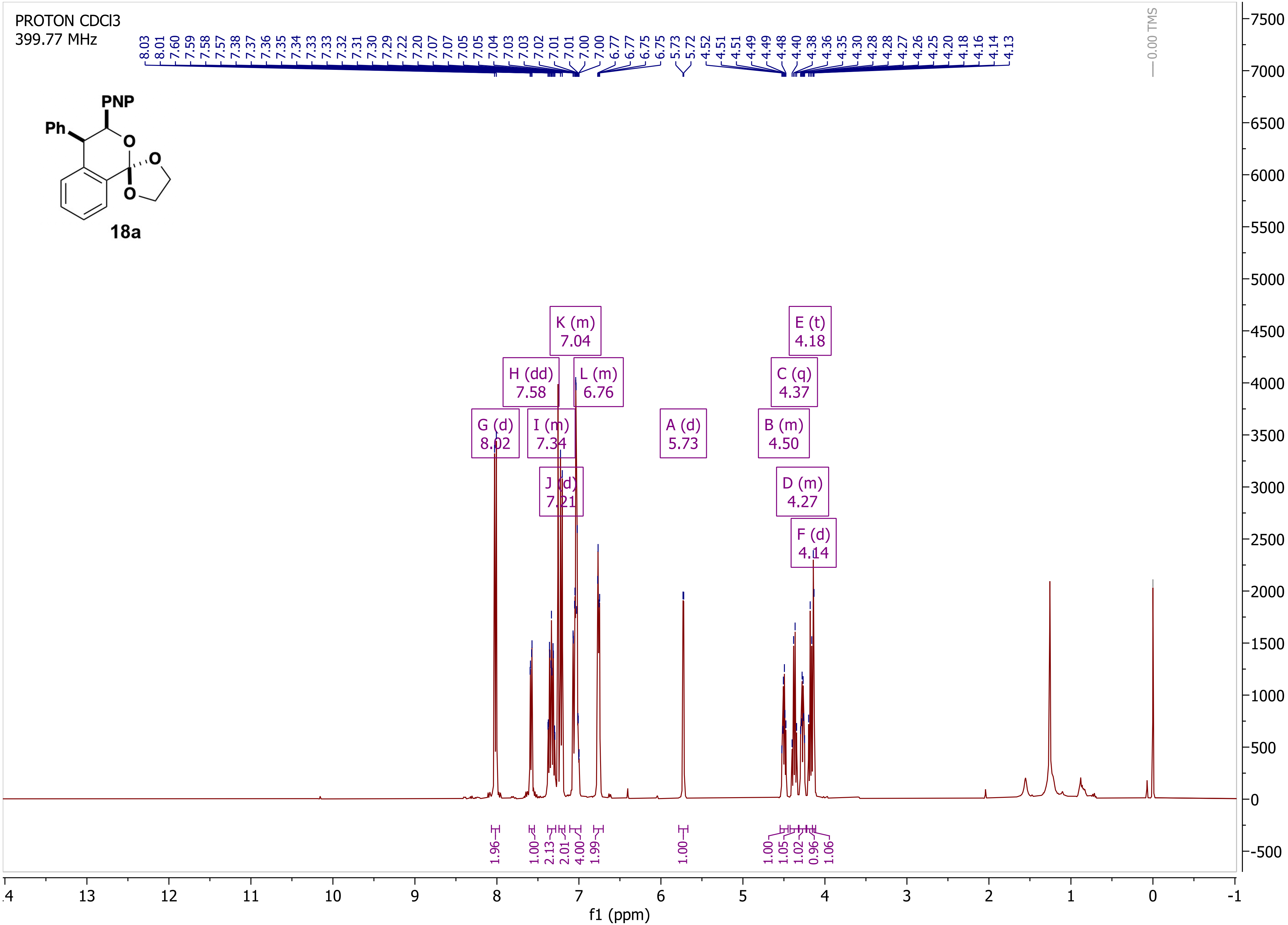

PROTON CDCl3
399.77 MHz
7.96 7.94 7.48 7.48 7.46 7.46 7.44 7.44 7.43 7.42 7.36 7.36 7.35 7.34 7.33 7.32 7.32 7.31 7.31 7.30 7.30 7.29 7.27 7.26 7.25 7.25 7.24 7.23 7.22 7.10 7.08 6.42 6.41 6.41 6.40 6.39 6.11 3.74 3.73 3.57 3.56 3.55 3.54 3.52 3.51 3.40 3.39 3.38 3.37 3.37 3.36 3.35 3.34 3.33 3.24 3.23 3.21 3.20 3.19 3.17 3.10 3.09
0.00 TMS
16a
L (d) 7.09
G (m) 7.45
I (s) 6.11
F (d) 7.95
J (m) 7.33
H (m) 6.41
K (m) 7.24
D (m) 3.21
B (m) 3.53
A (d) 3.74
E (d) 3.10
C (m) 3.36
0.99 2.00 2.96 4.40 1.97 1.94 0.98 1.00 1.01 1.99 1.01 1.01
f1 (ppm)

C13CPD CDCl3
100.53 MHz



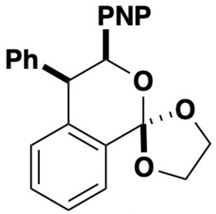

PROTON CDCl3
399.77 MHz
16b
A (s) 5.91
B (d) 3.84
C (m) 3.49
D (m) 3.35
E (m) 3.21
F (m) 7.80
G (dd) 7.54
H (m) 7.46
I (m) 7.32
J (m) 7.26
K (m) 7.14
L (td) 7.01
M (td) 6.85
0.00 TMS
1.98
1.01
2.06
2.07
1.74
3.00
1.06
1.01
1.00
1.02
1.02
2.03
2.02
f1 (ppm)

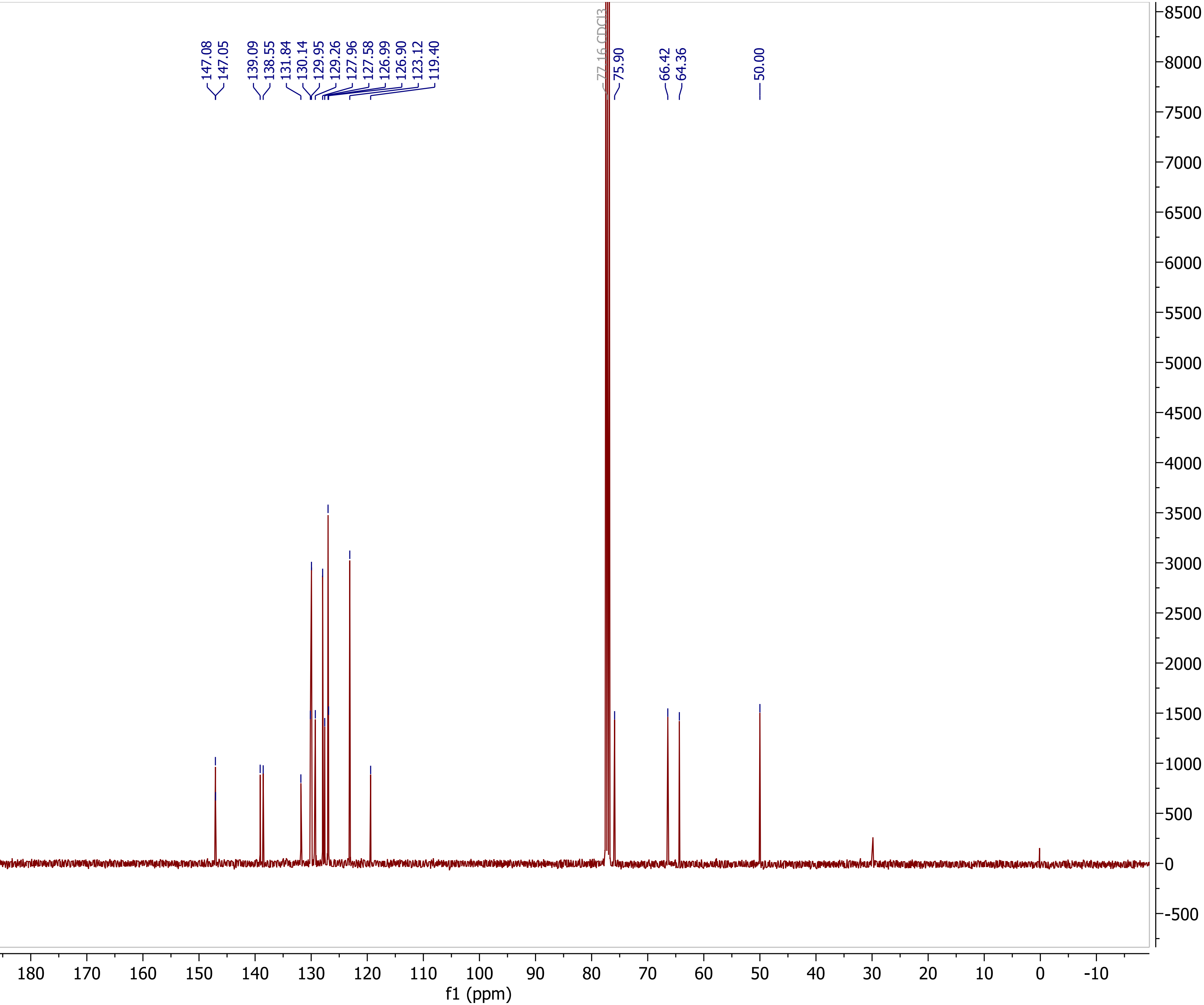

C13CPD CDCl3
100.53 MHz
192.15
191.55
142.97
141.67
134.84
133.90
133.77
133.75
132.63
131.40
131.02
128.99
128.93
127.86
127.53
126.77
126.13
77.16 CDCl3
51.15
45.81
42.61
40.96
40.59
40.53
16b
f1 (ppm)

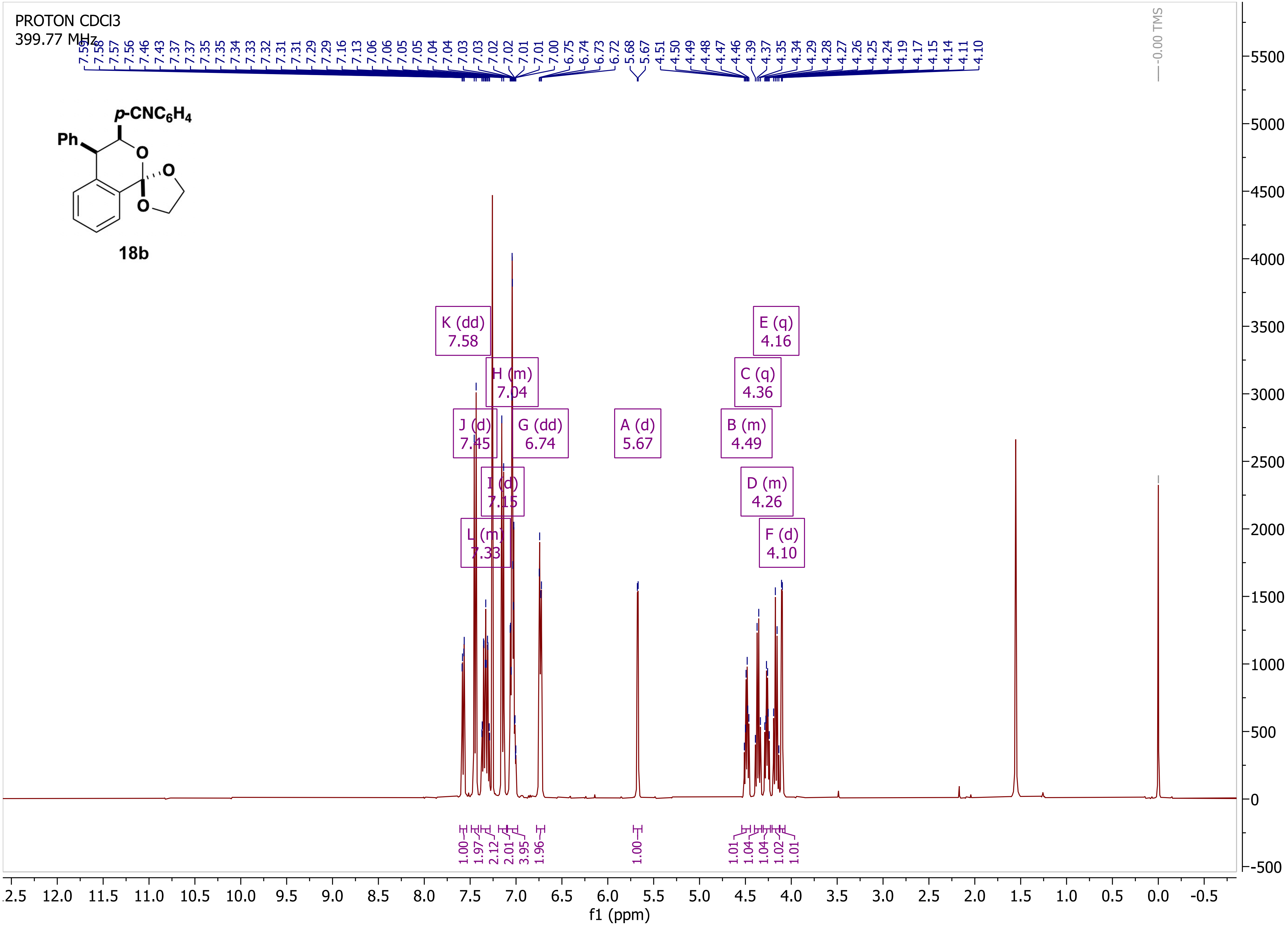


PROTON CDCl3
399.77 MHz
PNP
Ph
O
O
O
18a
8.03 8.01 7.60 7.59 7.58 7.57 7.38 7.37 7.36 7.35 7.34 7.33 7.33 7.32 7.31 7.30 7.29 7.22 7.20 7.07 7.07 7.05 7.05 7.04 7.03 7.03 7.02 7.01 7.01 7.00 7.00 6.77 6.77 6.75 6.75 5.73 5.72 4.52 4.51 4.51 4.49 4.49 4.48 4.40 4.38 4.36 4.35 4.30 4.28 4.28 4.27 4.26 4.25 4.20 4.18 4.16 4.14 4.13
0.00 TMS
G (d) 8.02
H (dd) 7.58
I (m) 7.34
J (d) 7.21
K (m) 7.04
L (m) 6.76
A (d) 5.73
B (m) 4.50
C (q) 4.37
D (m) 4.27
E (t) 4.18
F (d) 4.14
1.96 1.00 2.13 2.01 4.00 1.99 1.00 1.00 1.05 1.02 0.96 1.06
f1 (ppm)

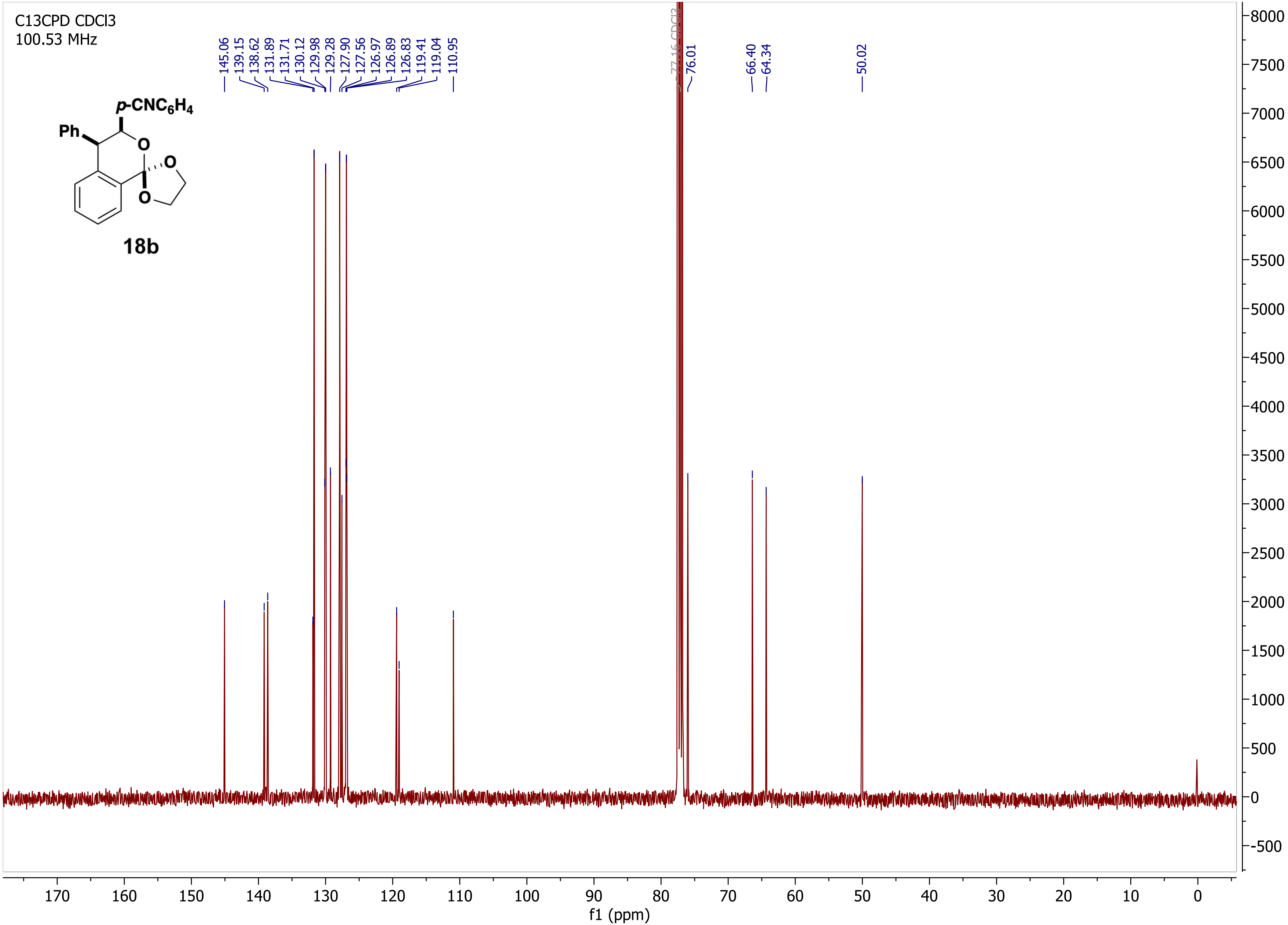
C13CPD CDCl3
100.53 MHz

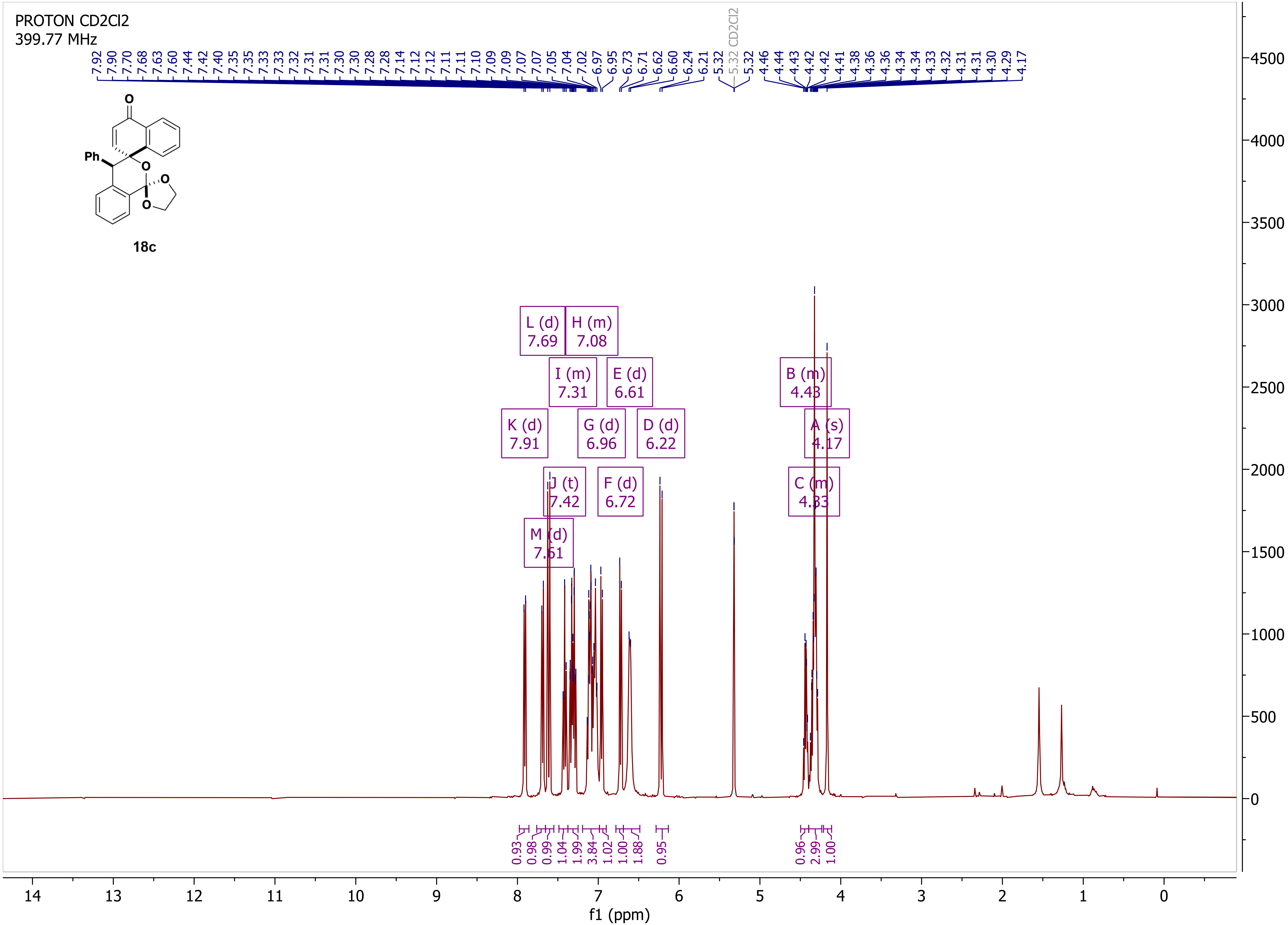

18a



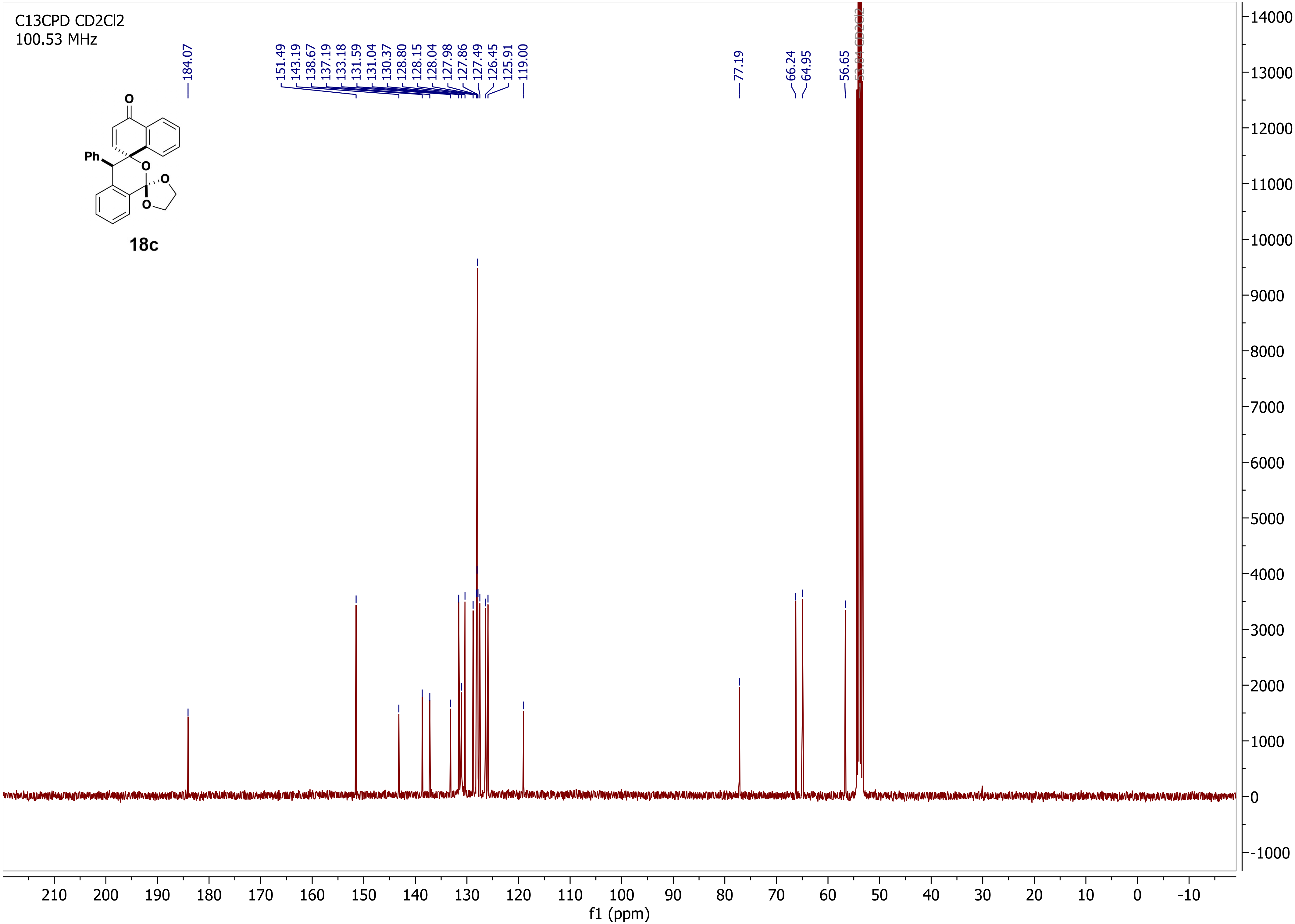


PROTON CDCl3
399.77 MHz
7.59 7.58 7.57 7.56 7.46 7.43 7.37 7.37 7.35 7.35 7.34 7.33 7.32 7.31 7.31 7.29 7.29 7.16 7.13 7.06 7.06 7.05 7.05 7.04 7.04 7.03 7.03 7.02 7.02 7.01 7.01 7.00 6.75 6.74 6.73 6.72 5.68 5.67 4.51 4.50 4.49 4.48 4.47 4.46 4.39 4.37 4.35 4.34 4.29 4.28 4.27 4.26 4.25 4.24 4.19 4.17 4.15 4.14 4.11 4.10
0.00 TMS
p-CNC6H4
Ph
O
O
O
18b
K (dd) 7.58
H (m) 7.04
J (d) 7.45
G (dd) 6.74
I (d) 7.15
L (m) 7.33
A (d) 5.67
E (q) 4.16
C (q) 4.36
B (m) 4.49
D (m) 4.26
F (d) 4.10
1.00 1.97 2.12 2.01 3.95 1.96 1.00 1.01 1.04 1.04 1.02 1.01
f1 (ppm)

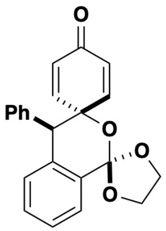

C13CPD CDCl3
100.53 MHz
145.06
139.15
138.62
131.89
131.71
130.12
129.98
129.28
127.90
127.56
126.97
126.89
126.83
119.41
119.04
110.95
77.16 CDCl3
76.01
66.40
64.34
50.02
p-CNC6H4
Ph
O
O
O
18b
f1 (ppm)



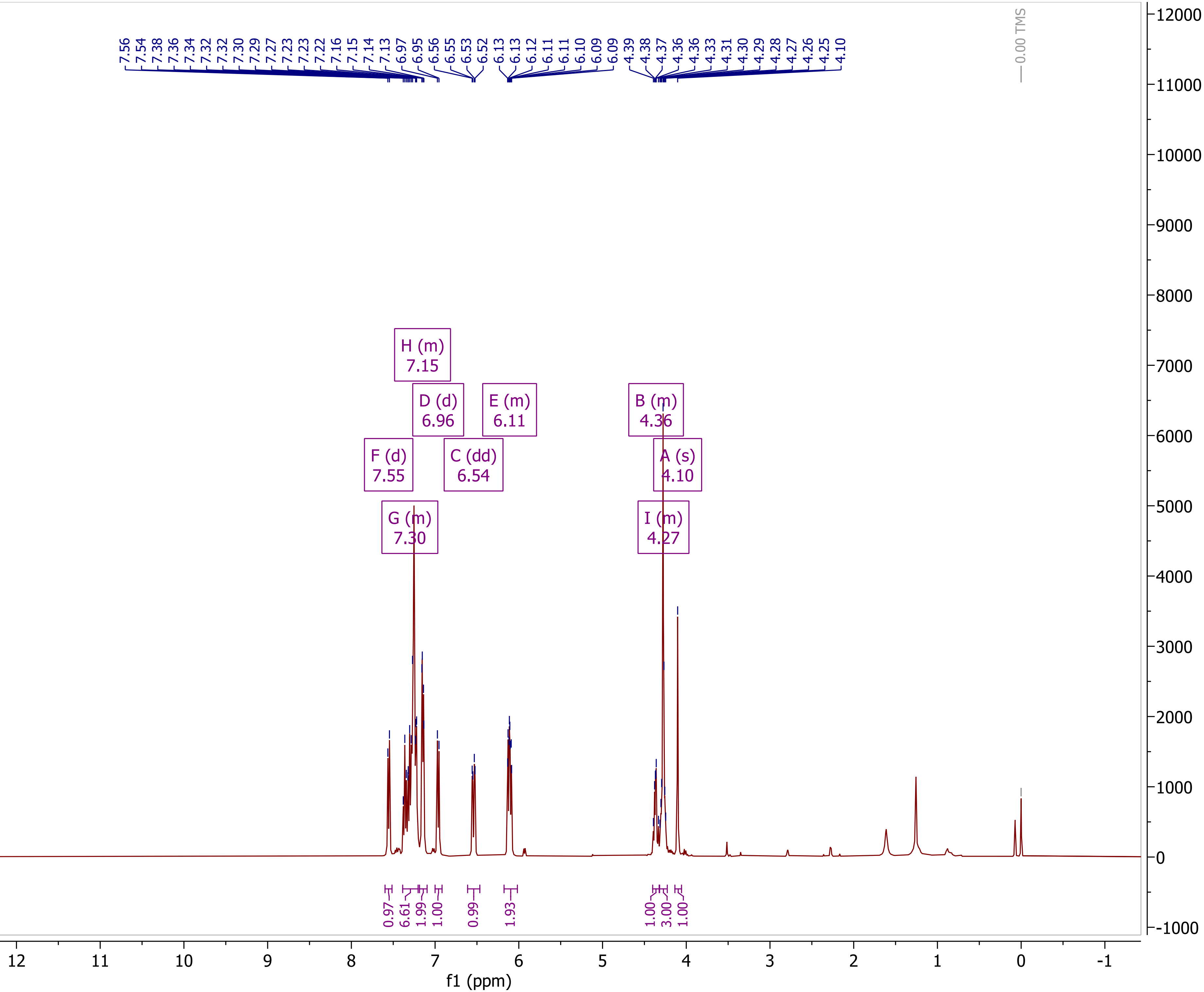
PROTON CD2Cl2
399.77 MHz
18c
L (d) 7.69
H (m) 7.08
I (m) 7.31
E (d) 6.61
K (d) 7.91
G (d) 6.96
D (d) 6.22
J (t) 7.42
F (d) 6.72
M (d) 7.61
B (m) 4.43
A (s) 4.17
C (m) 4.33
f1 (ppm)

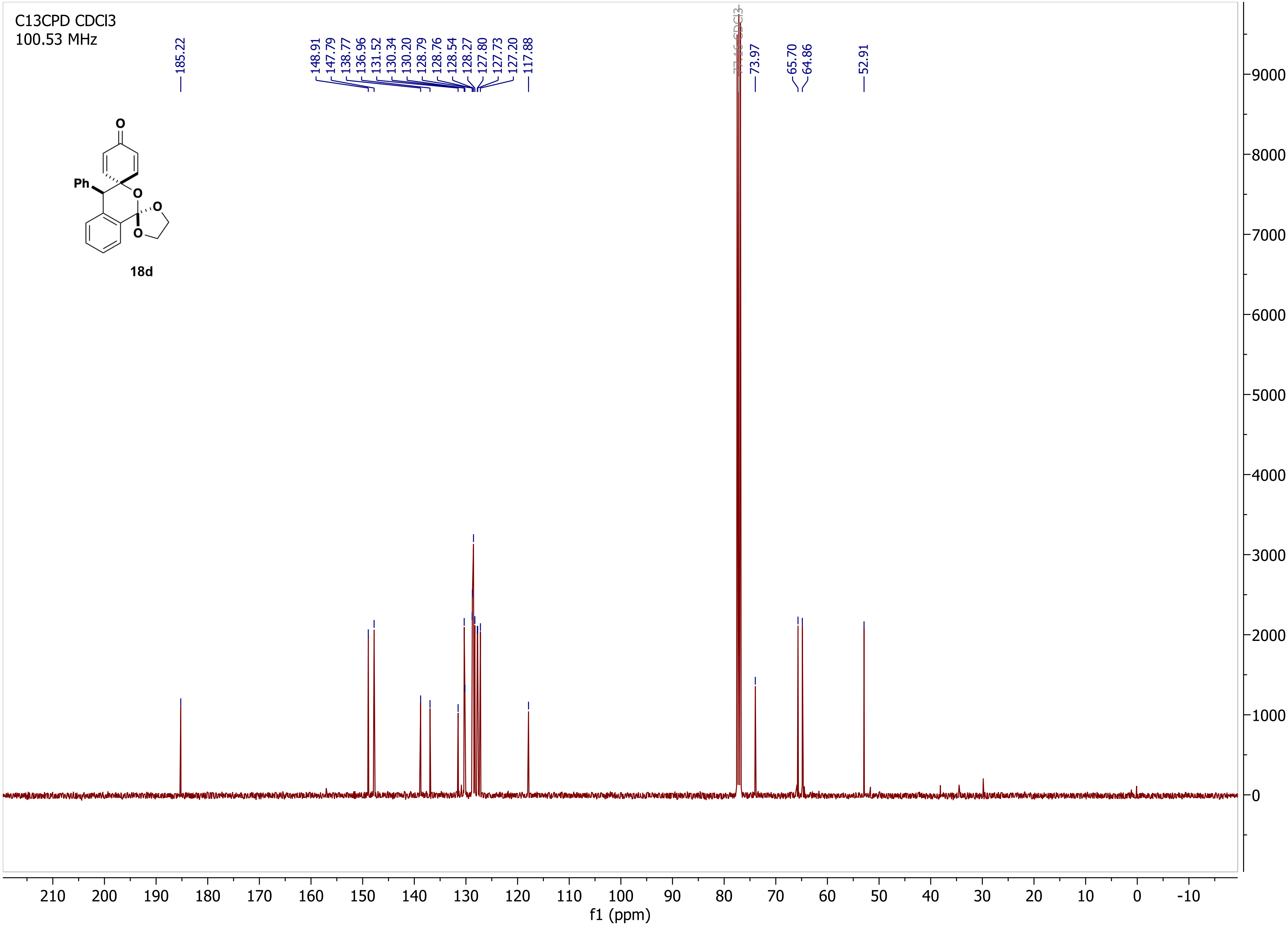

C13CPD CD2Cl2
100.53 MHz
184.07
151.49
143.19
138.67
137.19
133.18
131.59
131.04
130.37
128.80
128.15
128.04
127.98
127.86
127.49
126.45
125.91
119.00
77.19
66.24
64.95
56.65
Ph
O
O
O
O
18c
14000
13000
12000
11000
10000
9000
8000
7000
6000
5000
4000
3000
2000
1000
0
-1000
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

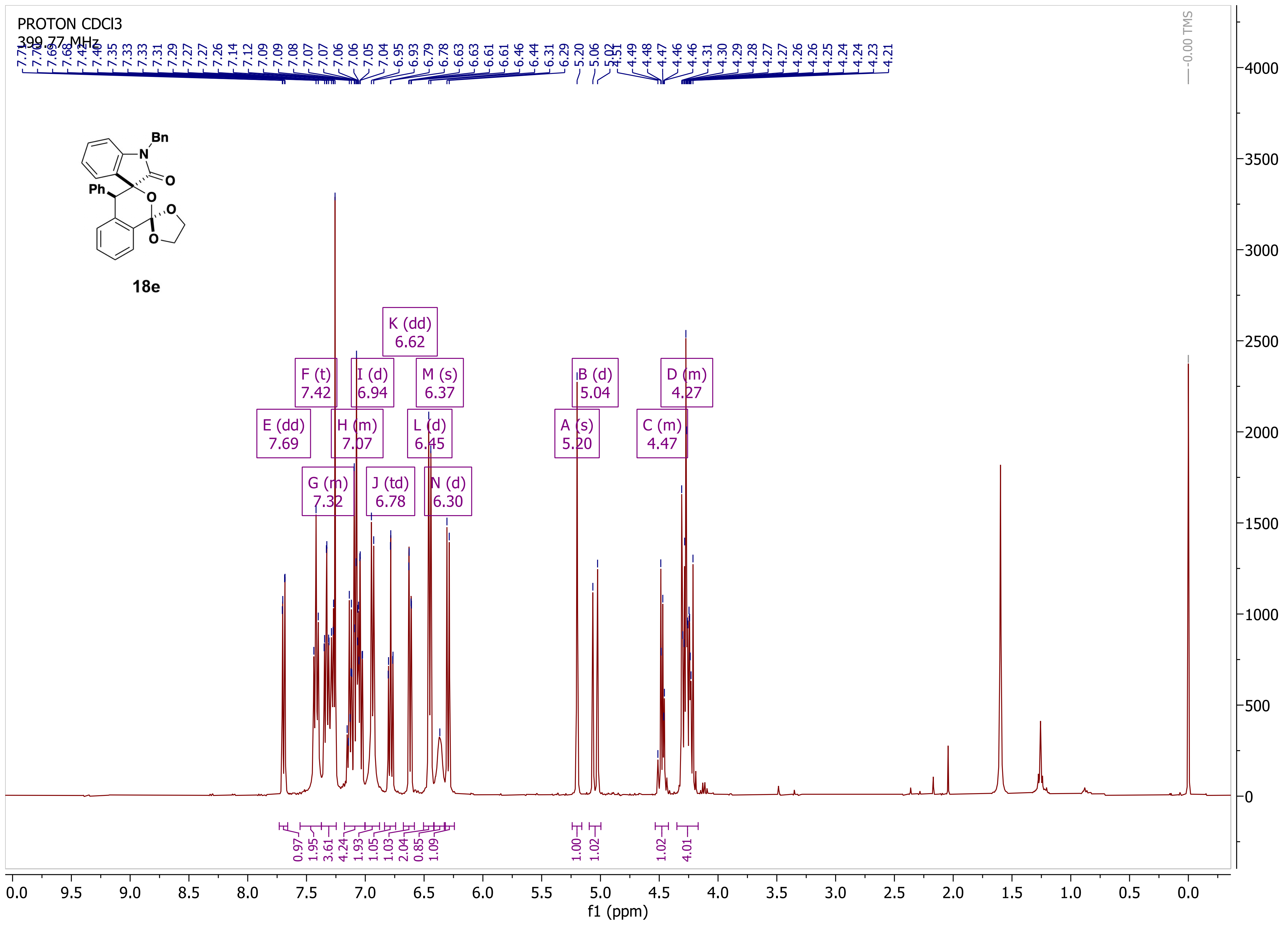
PROTON CDCl3
399.77 MHz



18d

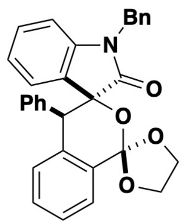



C13CPD CDCl3
100.53 MHz
185.22
148.91
147.79
138.77
136.96
131.52
130.34
130.20
128.79
128.76
128.54
128.27
127.80
127.73
127.20
117.88
77.16 CDCl3
73.97
65.70
64.86
52.91
O
Ph
O
O
O
18d
9000
8000
7000
6000
5000
4000
3000
2000
1000
0
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

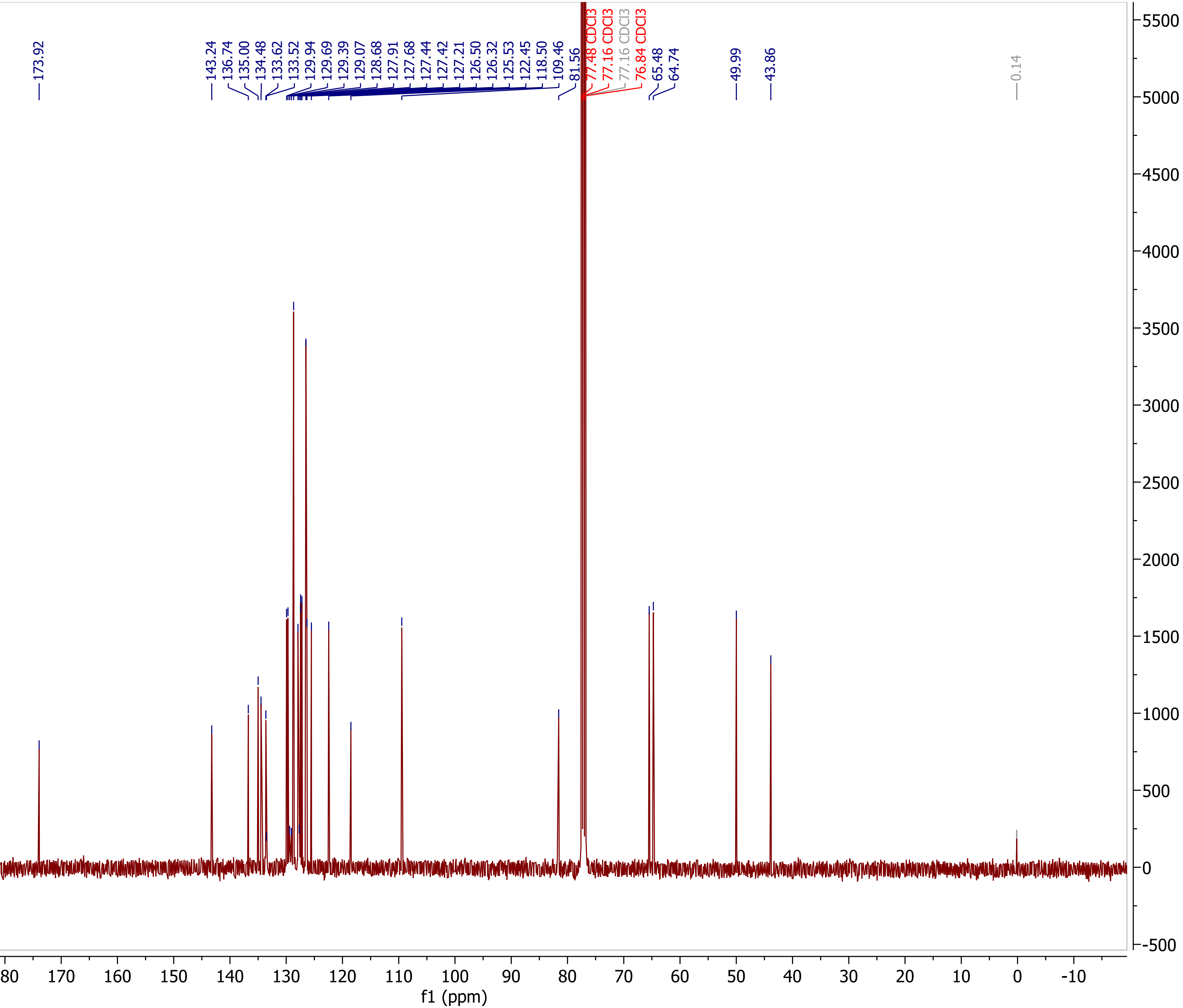


PROTON CDCl3
399.77 MHz
Bn
N
O
Ph
O
O
O
18e
E (dd) 7.69
F (t) 7.42
G (m) 7.32
H (m) 7.07
I (d) 6.94
J (td) 6.78
K (dd) 6.62
L (d) 6.45
M (s) 6.37
N (d) 6.30
A (s) 5.20
B (d) 5.04
C (m) 4.47
D (m) 4.27
0.97
1.95
3.61
4.24
1.93
1.05
1.03
2.04
0.85
1.09
1.00
1.02
1.02
4.01
-0.00 TMS
f1 (ppm)

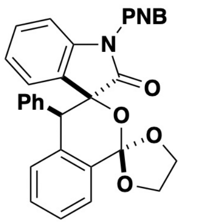
C13CPD CDCl3
100.53 MHz



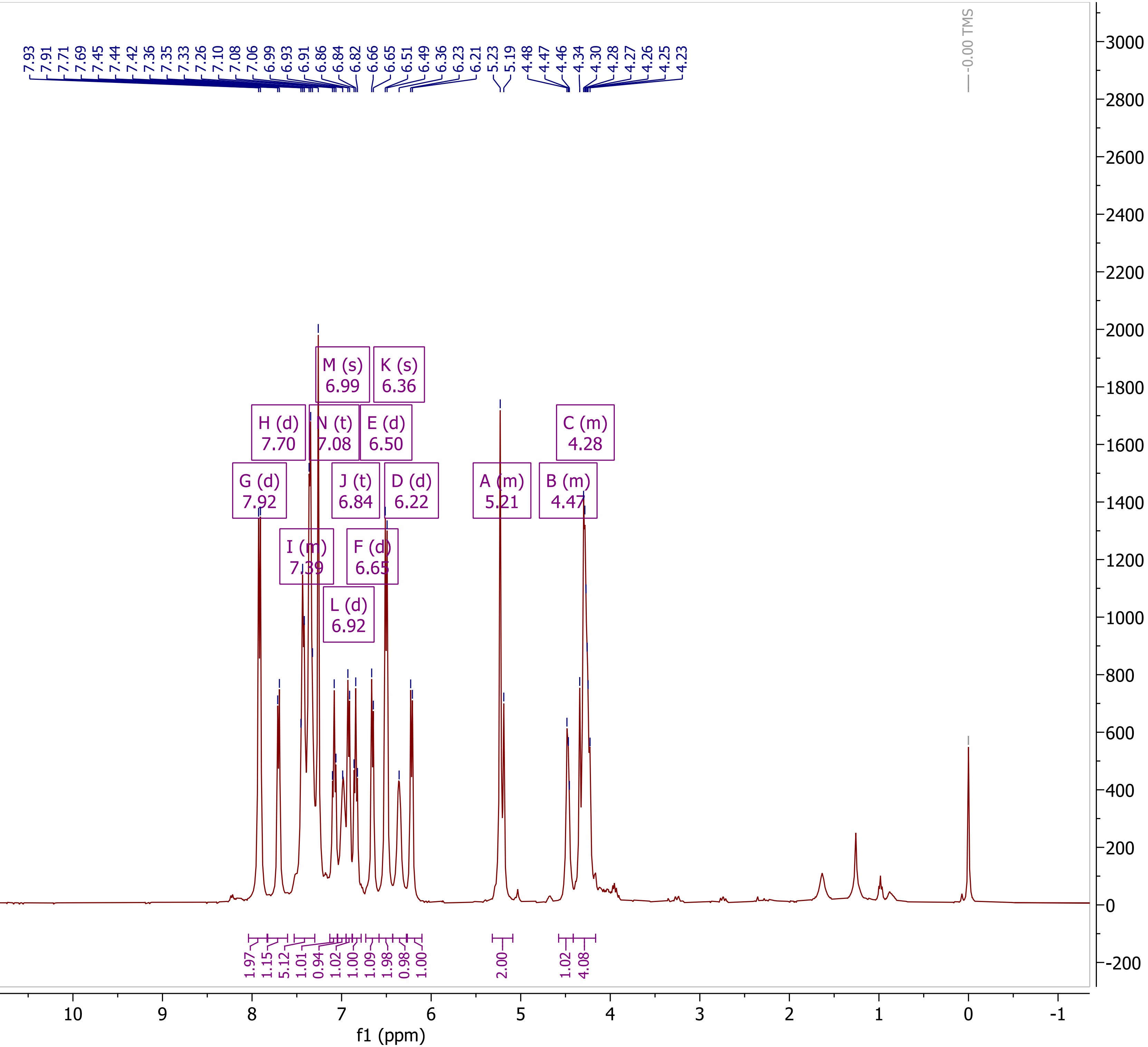
18e



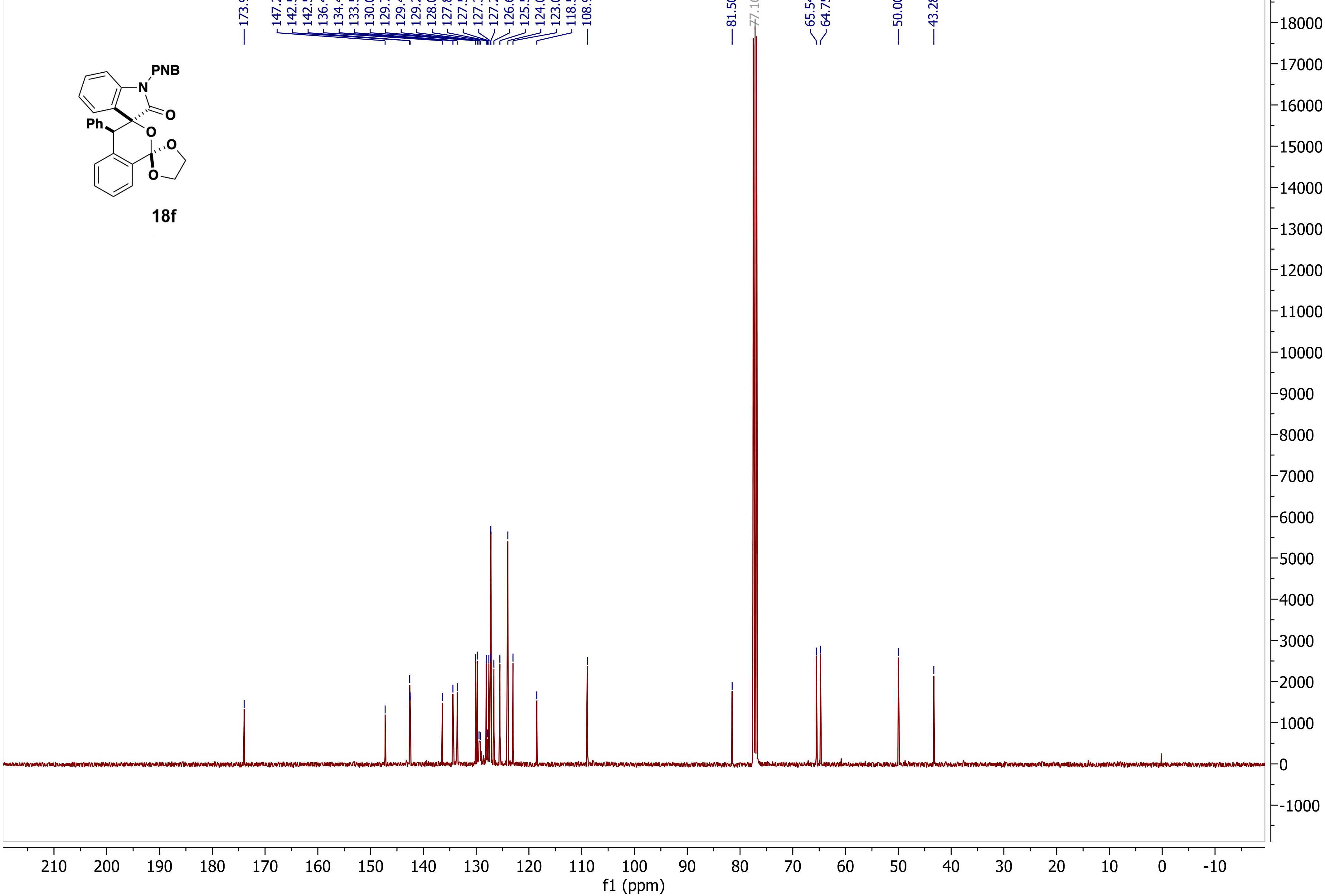
PROTON CDCl3
399.77 MHz

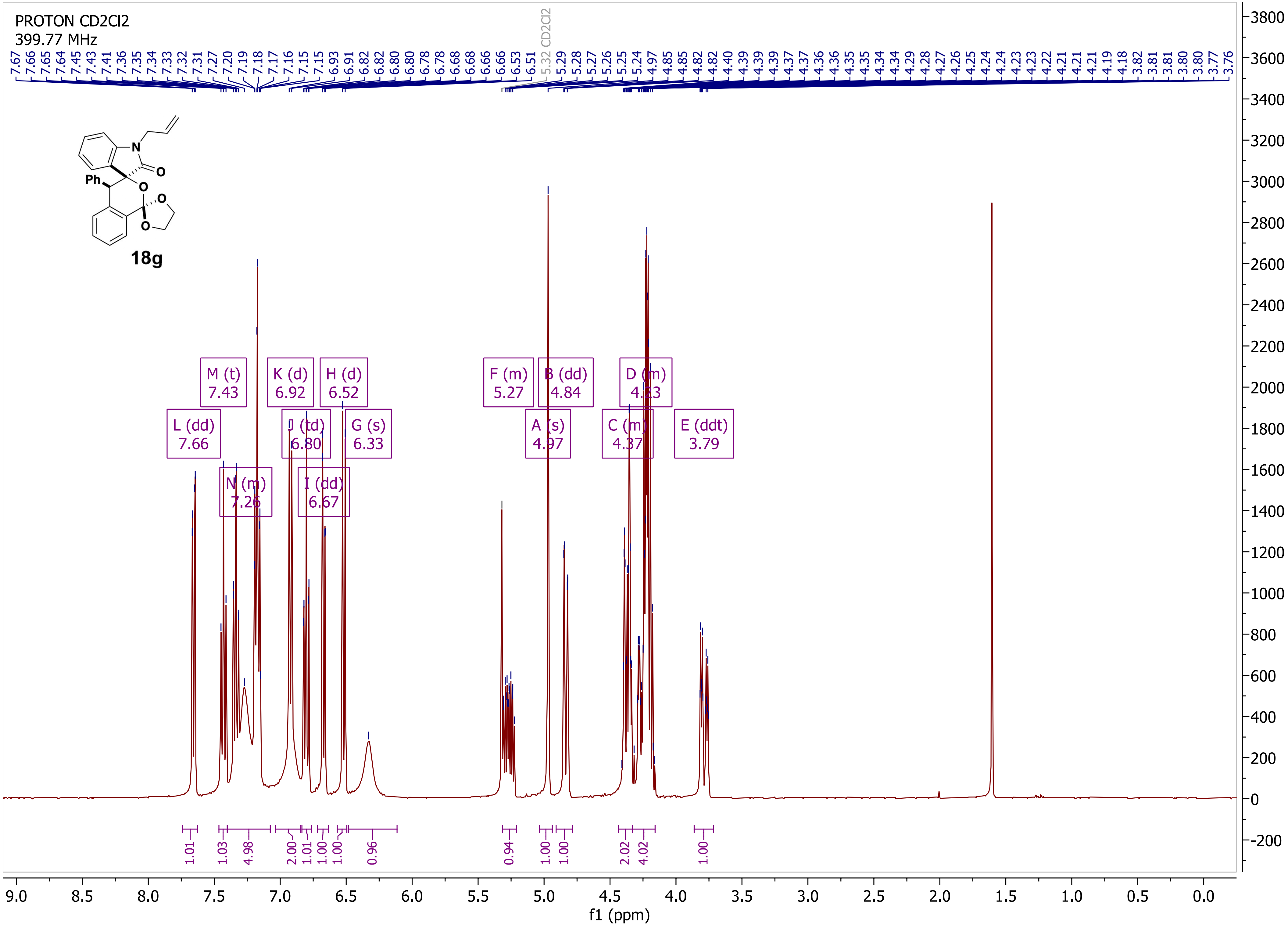


18f

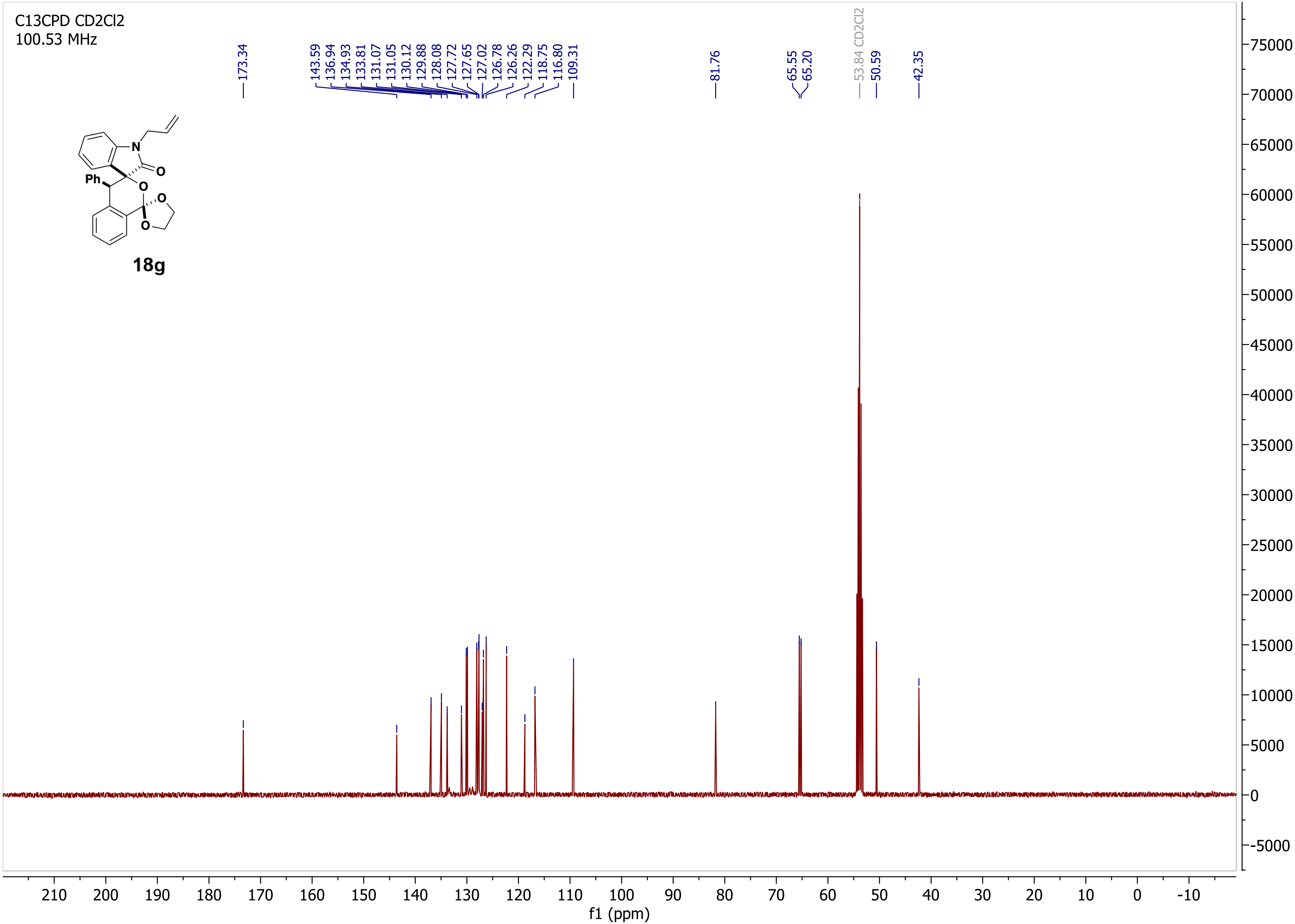


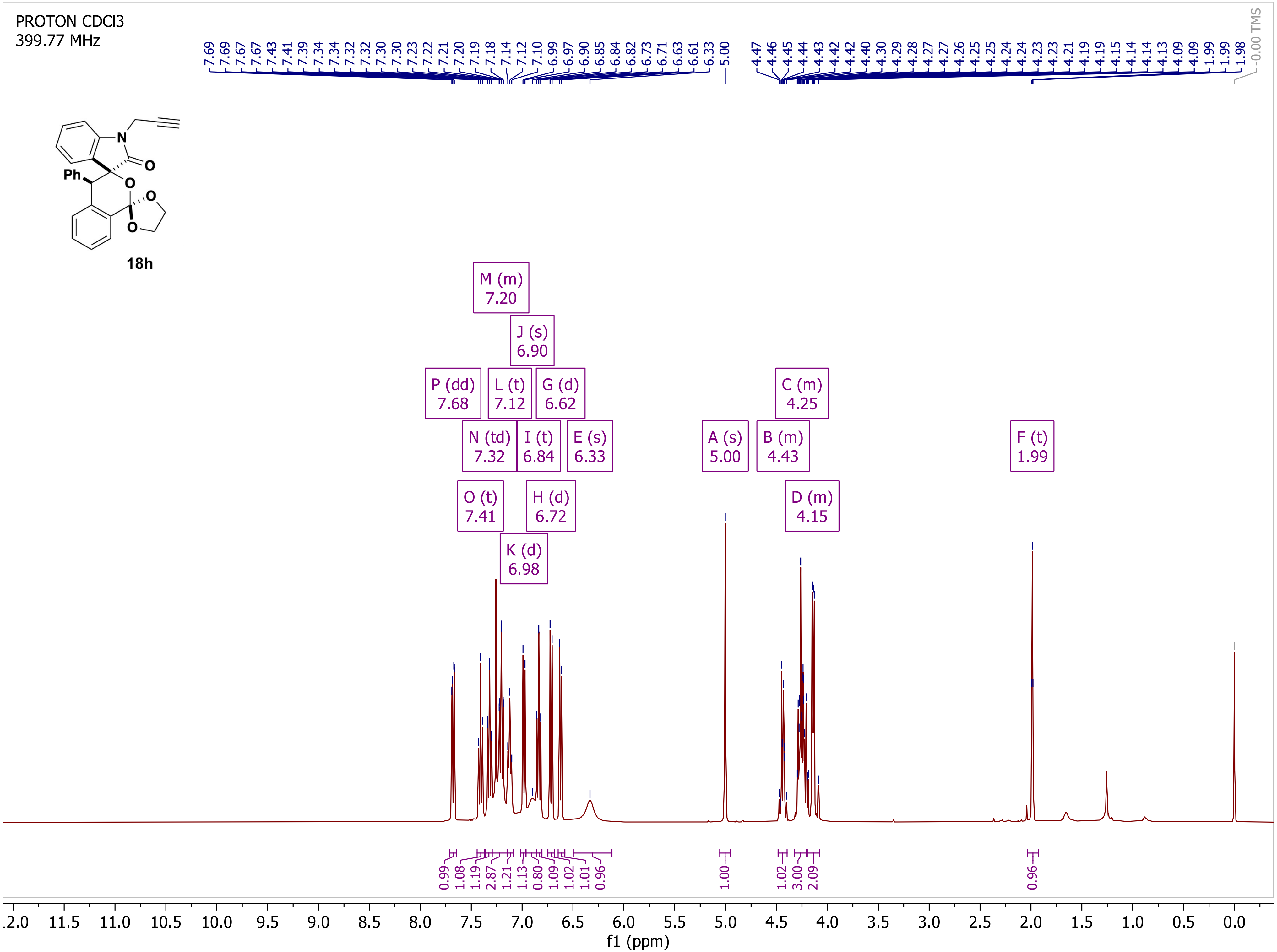
C13CPD CDCl3
100.53 MHz



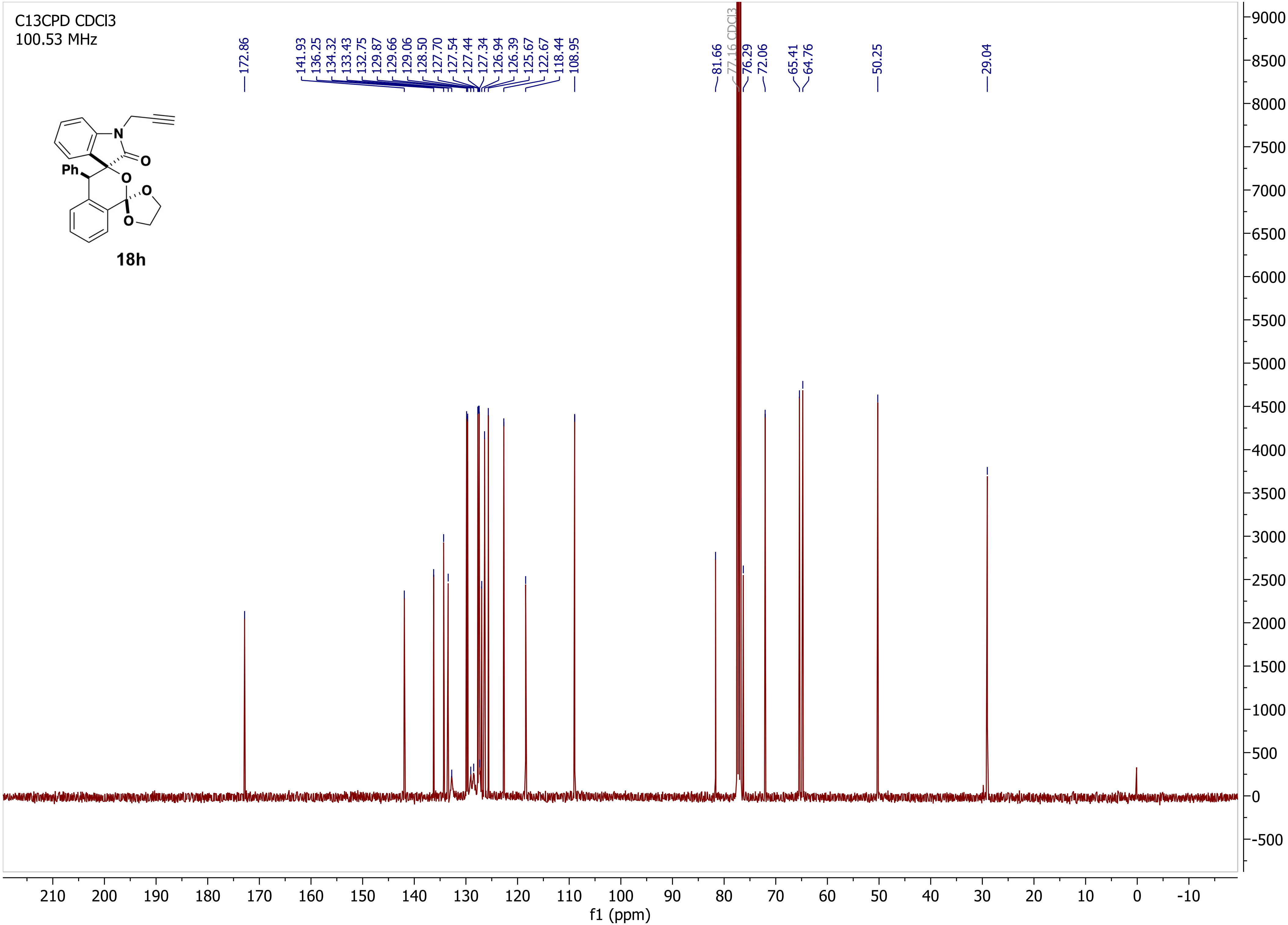


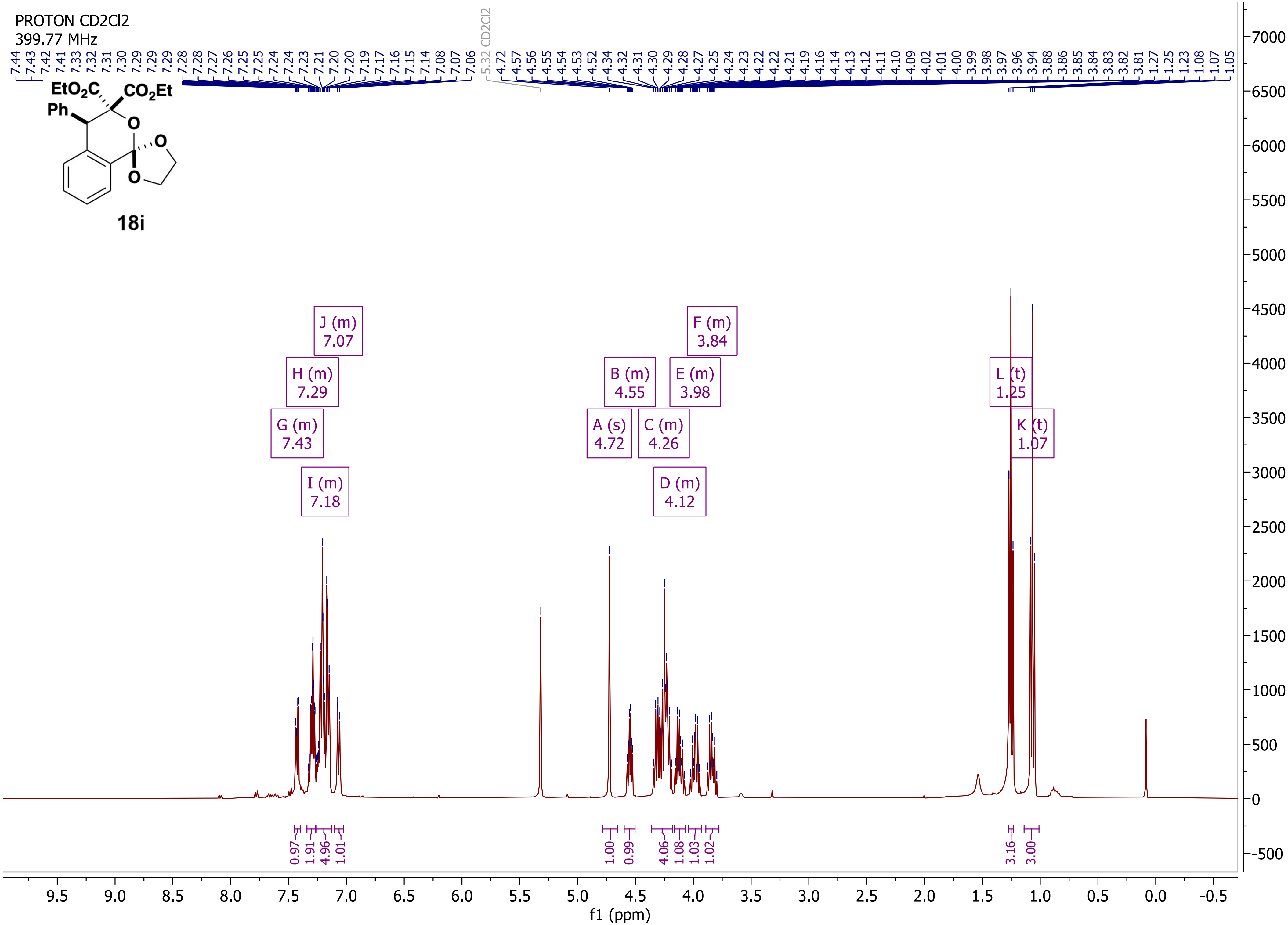
PROTON CD2Cl2
399.77 MHz
7.67 7.66 7.65 7.64 7.45 7.43 7.41 7.36 7.35 7.34 7.33 7.32 7.31 7.27 7.20 7.19 7.18 7.17 7.16 7.15 7.15 6.93 6.91 6.82 6.82 6.80 6.80 6.78 6.78 6.68 6.68 6.66 6.66 6.53 6.51 5.32 CD2Cl2 5.29 5.28 5.27 5.26 5.25 5.24 4.97 4.85 4.85 4.82 4.82 4.40 4.39 4.39 4.39 4.37 4.37 4.36 4.36 4.35 4.35 4.34 4.34 4.29 4.28 4.27 4.26 4.25 4.24 4.24 4.23 4.23 4.22 4.21 4.21 4.21 4.19 4.18 3.82 3.81 3.81 3.80 3.80 3.77 3.76
Ph
N
O
O
O
O
O
18g
M (t) 7.43
L (dd) 7.66
N (m) 7.26
K (d) 6.92
J (td) 6.80
I (dd) 6.67
H (d) 6.52
G (s) 6.33
F (m) 5.27
B (dd) 4.84
A (s) 4.97
D (m) 4.23
C (m) 4.37
E (ddt) 3.79
1.01 1.03 4.98 2.00 1.01 1.00 1.00 0.96 0.94 1.00 1.00 2.02 4.02 1.00
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)
3800 3600 3400 3200 3000 2800 2600 2400 2200 2000 1800 1600 1400 1200 1000 800 600 400 200 0 -200


C13CPD CD2Cl2
100.53 MHz
173.34
143.59
136.94
134.93
133.81
131.07
131.05
130.12
129.88
128.08
127.72
127.65
127.02
126.78
126.26
122.29
118.75
116.80
109.31
81.76
65.55
65.20
53.84 CD2Cl2
50.59
42.35
N
O
Ph
O
O
O
18g
f1 (ppm)



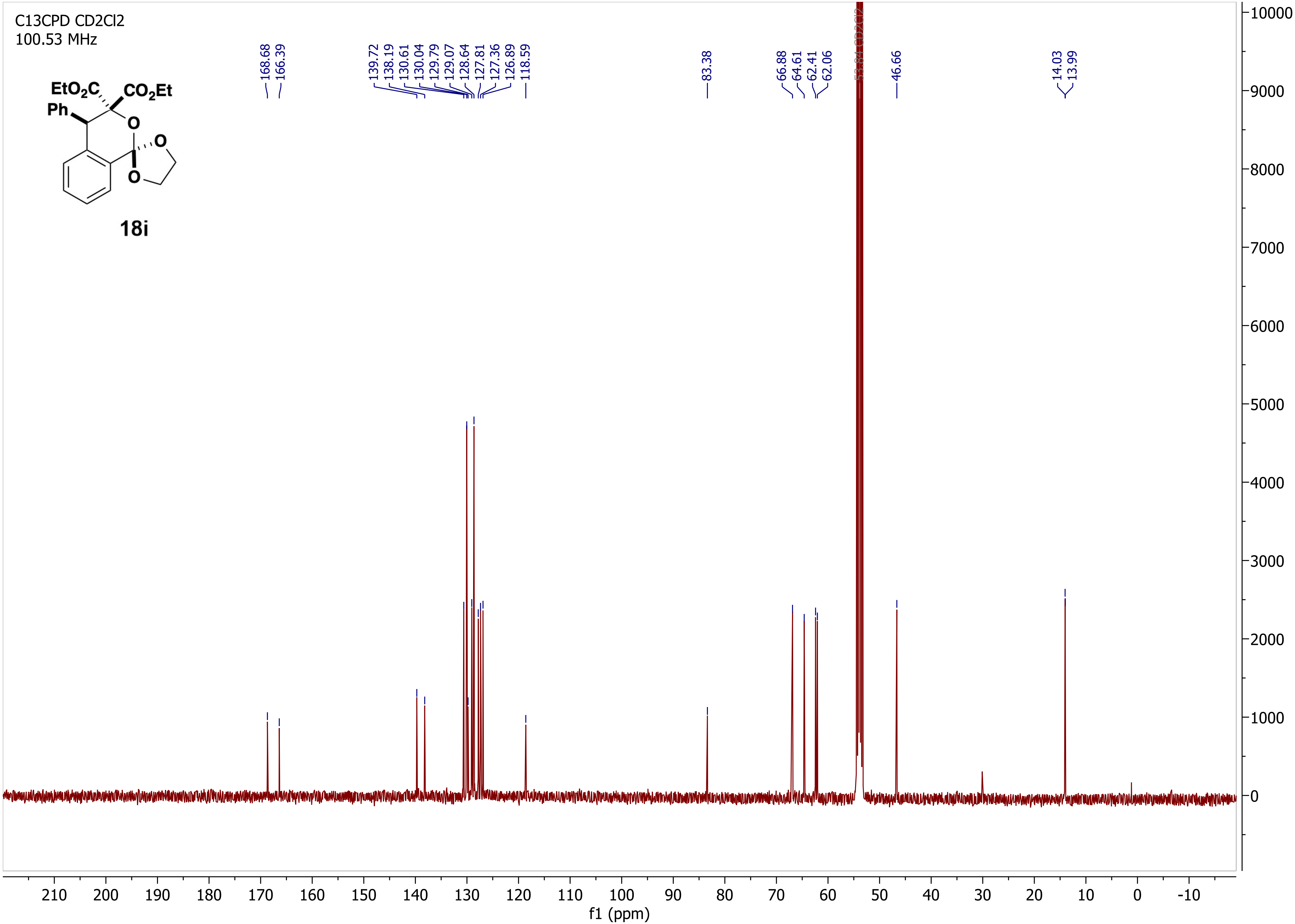
PROTON CDCl3
399.77 MHz
7.69 7.69 7.67 7.67 7.43 7.41 7.39 7.34 7.34 7.32 7.32 7.30 7.30 7.23 7.22 7.21 7.20 7.19 7.18 7.14 7.12 7.10 6.99 6.97 6.90 6.85 6.84 6.82 6.73 6.71 6.63 6.61 6.33 5.00 4.47 4.46 4.45 4.44 4.43 4.42 4.42 4.40 4.30 4.29 4.28 4.27 4.27 4.26 4.25 4.25 4.24 4.24 4.23 4.23 4.21 4.19 4.19 4.15 4.14 4.14 4.13 4.09 4.09 1.99 1.99 1.98
-0.00 TMS
N
O
Ph
O
O
O
18h
M (m) 7.20
J (s) 6.90
P (dd) 7.68
L (t) 7.12
G (d) 6.62
C (m) 4.25
N (td) 7.32
I (t) 6.84
E (s) 6.33
A (s) 5.00
B (m) 4.43
F (t) 1.99
O (t) 7.41
H (d) 6.72
D (m) 4.15
K (d) 6.98
0.99 1.08 1.19 2.87 1.21 1.13 0.80 1.09 1.02 1.01 0.96 1.00 1.02 3.00 2.09 0.96
f1 (ppm)

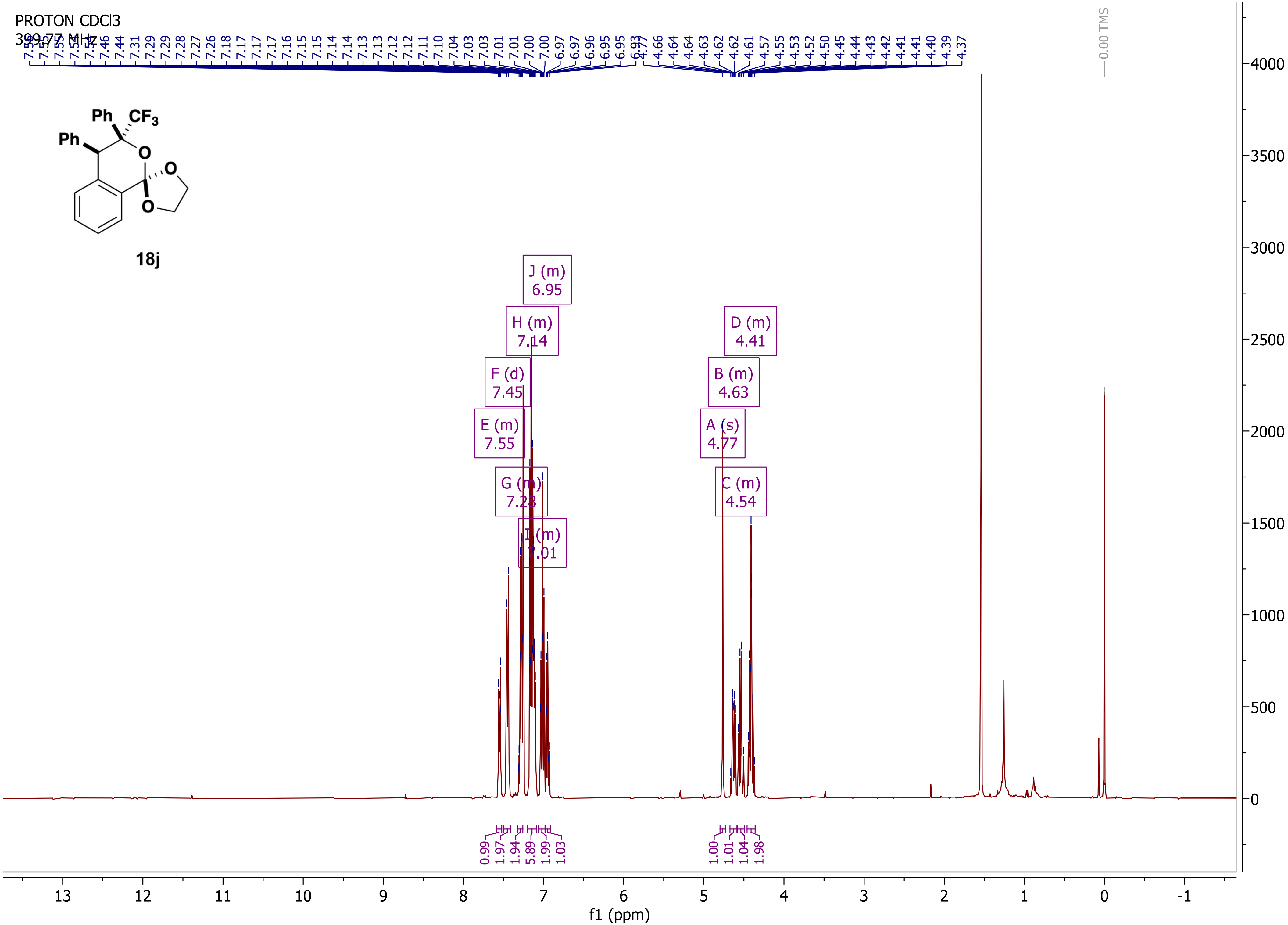

C13CPD CDCl3
100.53 MHz
172.86
141.93
136.25
134.32
133.43
132.75
129.87
129.66
129.06
128.50
127.70
127.54
127.44
127.34
126.94
126.39
125.67
122.67
118.44
108.95
81.66
77.16 CDCl3
76.29
72.06
65.41
64.76
50.25
29.04
Ph
N
O
18h
f1 (ppm)



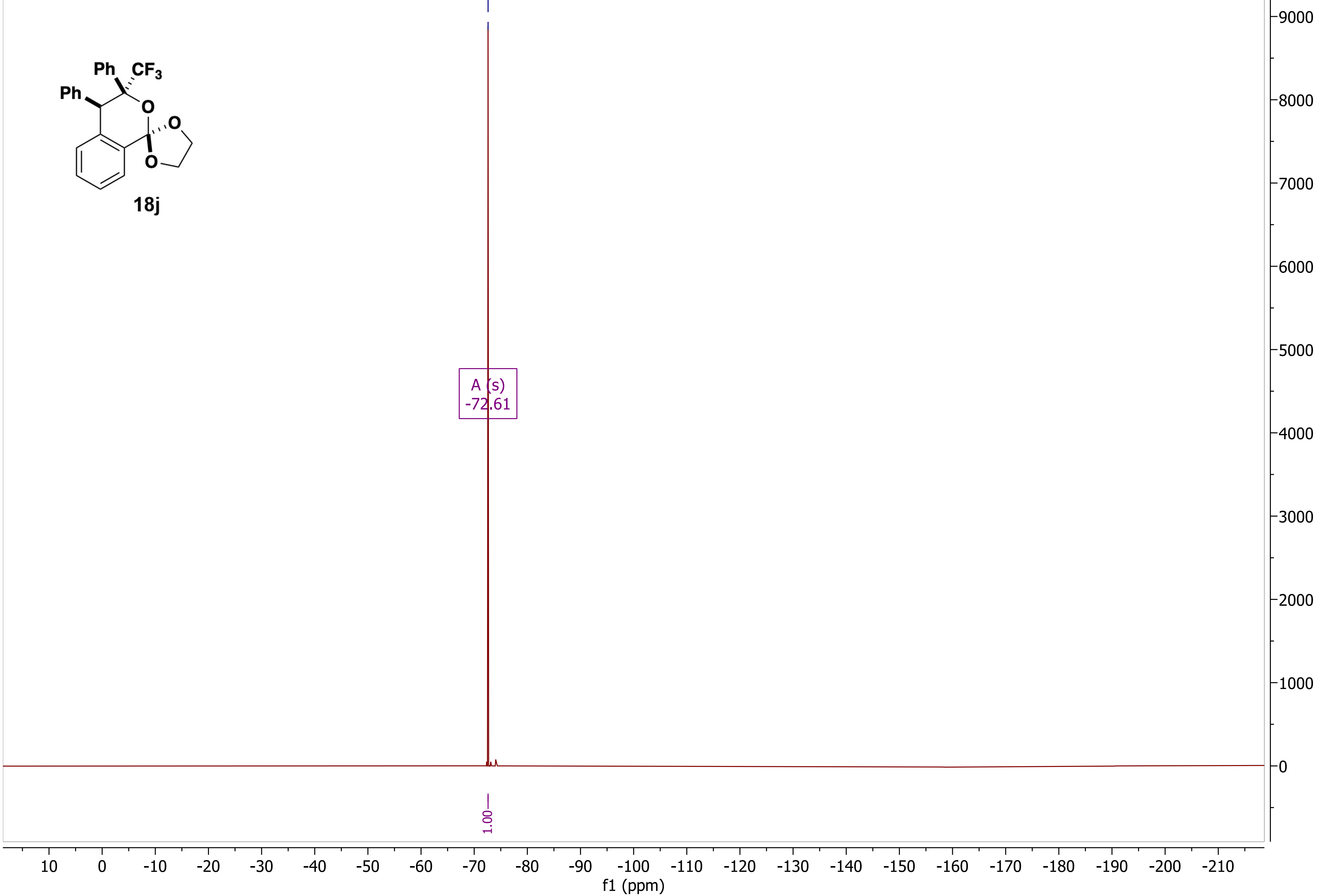
PROTON CD2Cl2
399.77 MHz
7.44 7.43 7.42 7.41 7.33 7.32 7.31 7.30 7.29 7.29 7.29 7.28 7.28 7.27 7.26 7.25 7.25 7.24 7.24 7.23 7.21 7.20 7.20 7.19 7.17 7.16 7.15 7.14 7.08 7.07 7.06
5.32 CD2Cl2
4.72 4.57 4.56 4.55 4.54 4.53 4.52 4.34 4.32 4.31 4.30 4.29 4.28 4.27 4.25 4.24 4.23 4.22 4.22 4.21 4.19 4.16 4.14 4.13 4.12 4.11 4.10 4.09 4.02 4.01 4.00 3.99 3.98 3.97 3.96 3.94 3.88 3.86 3.85 3.84 3.83 3.82 3.81 1.27 1.25 1.23 1.08 1.07 1.05
EtO2C
CO2Et
Ph
O
O
O
18i
J (m) 7.07
H (m) 7.29
G (m) 7.43
I (m) 7.18
A (s) 4.72
B (m) 4.55
C (m) 4.26
D (m) 4.12
E (m) 3.98
F (m) 3.84
L (t) 1.25
K (t) 1.07
0.97 1.91 4.96 1.01
1.00 0.99 4.06 1.08 1.03 1.02
3.16 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
f1 (ppm)
7000 6500 6000 5500 5000 4500 4000 3500 3000 2500 2000 1500 1000 500 0 -500

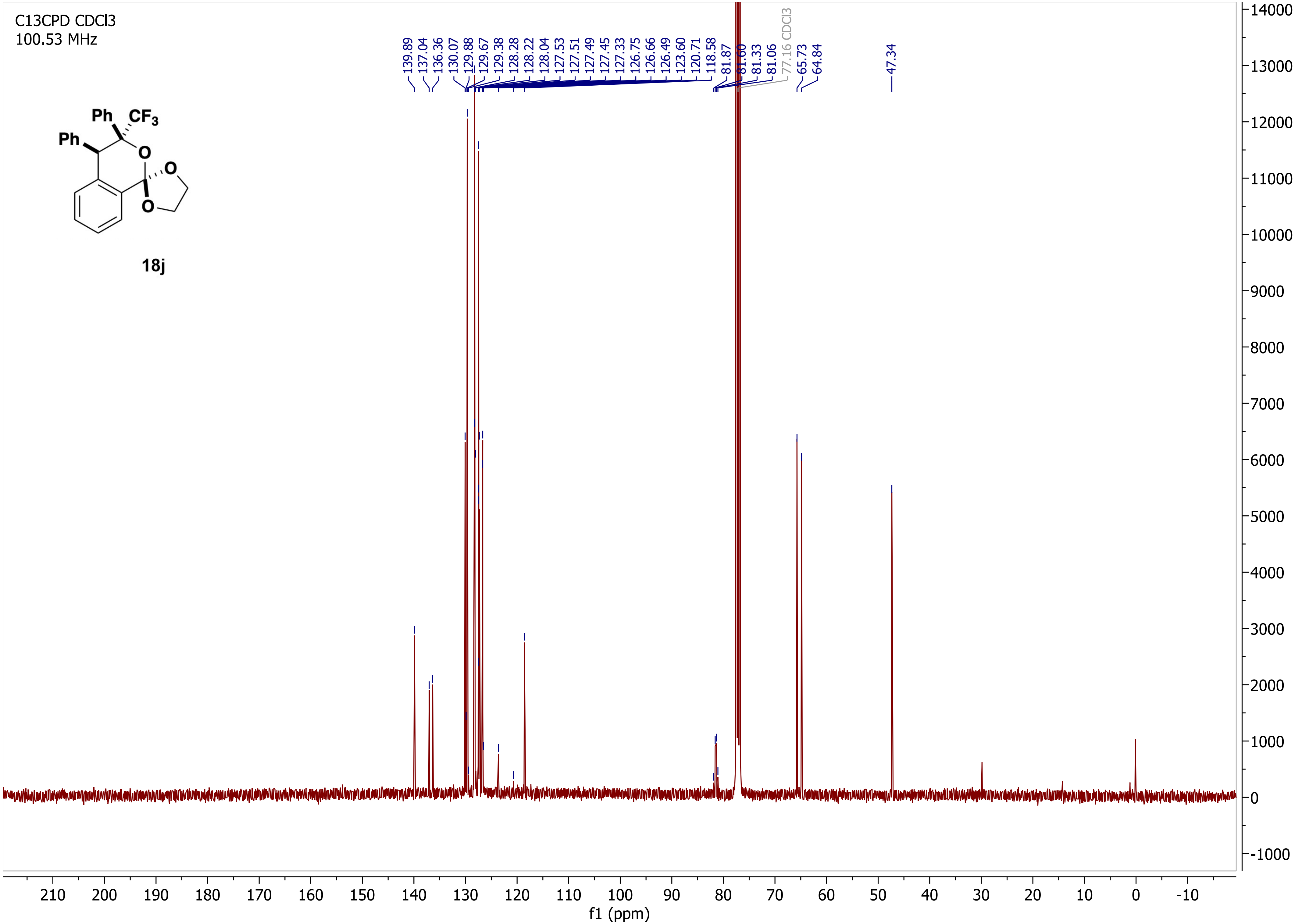
C13CPD CD2Cl2
100.53 MHz



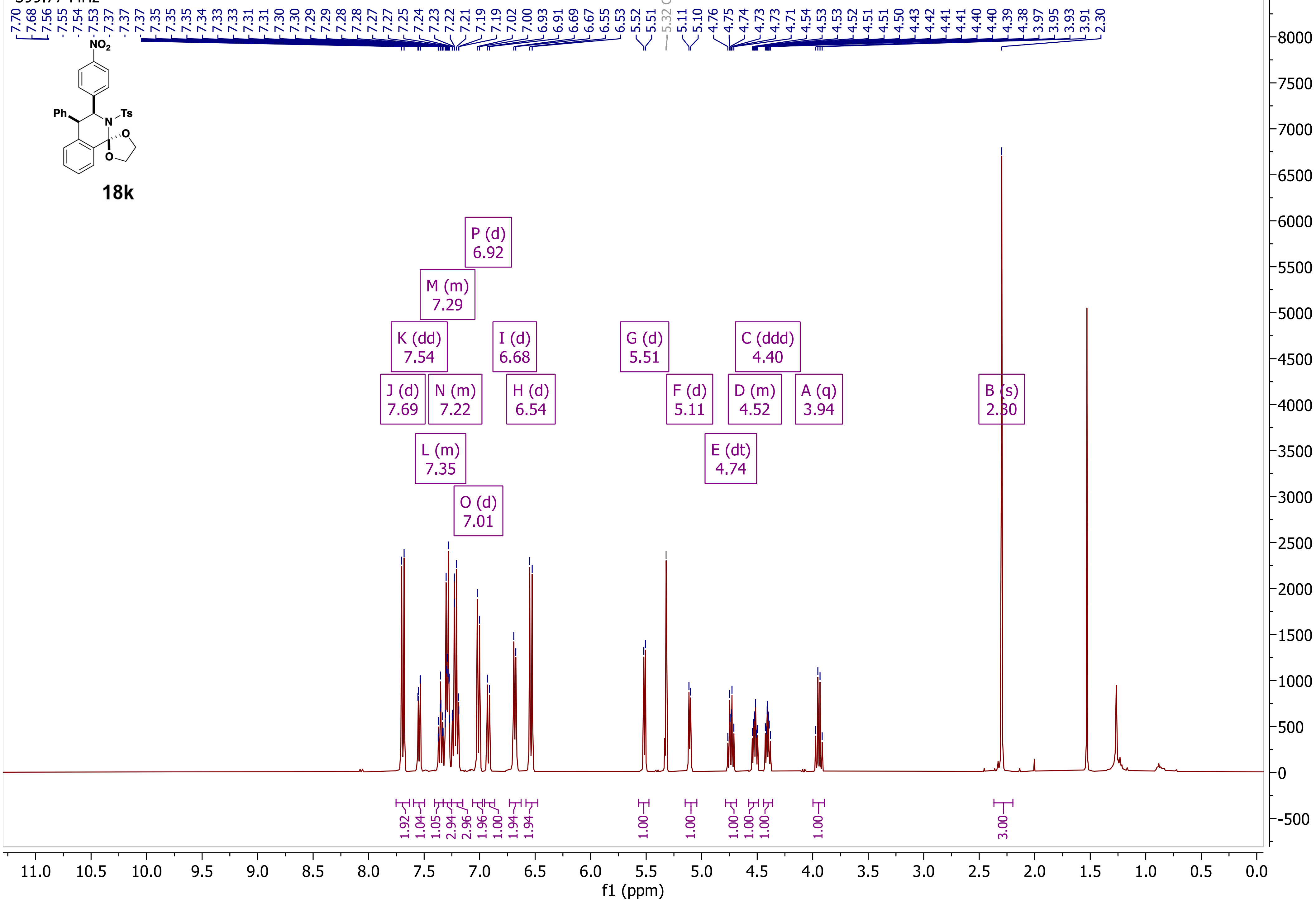

PROTON CDCl3
399.77 MHz
18j
J (m)
6.95
H (m)
7.14
F (d)
7.45
E (m)
7.55
G (m)
7.28
I (m)
7.01
D (m)
4.41
B (m)
4.63
A (s)
4.77
C (m)
4.54
0.00 TMS
f1 (ppm)

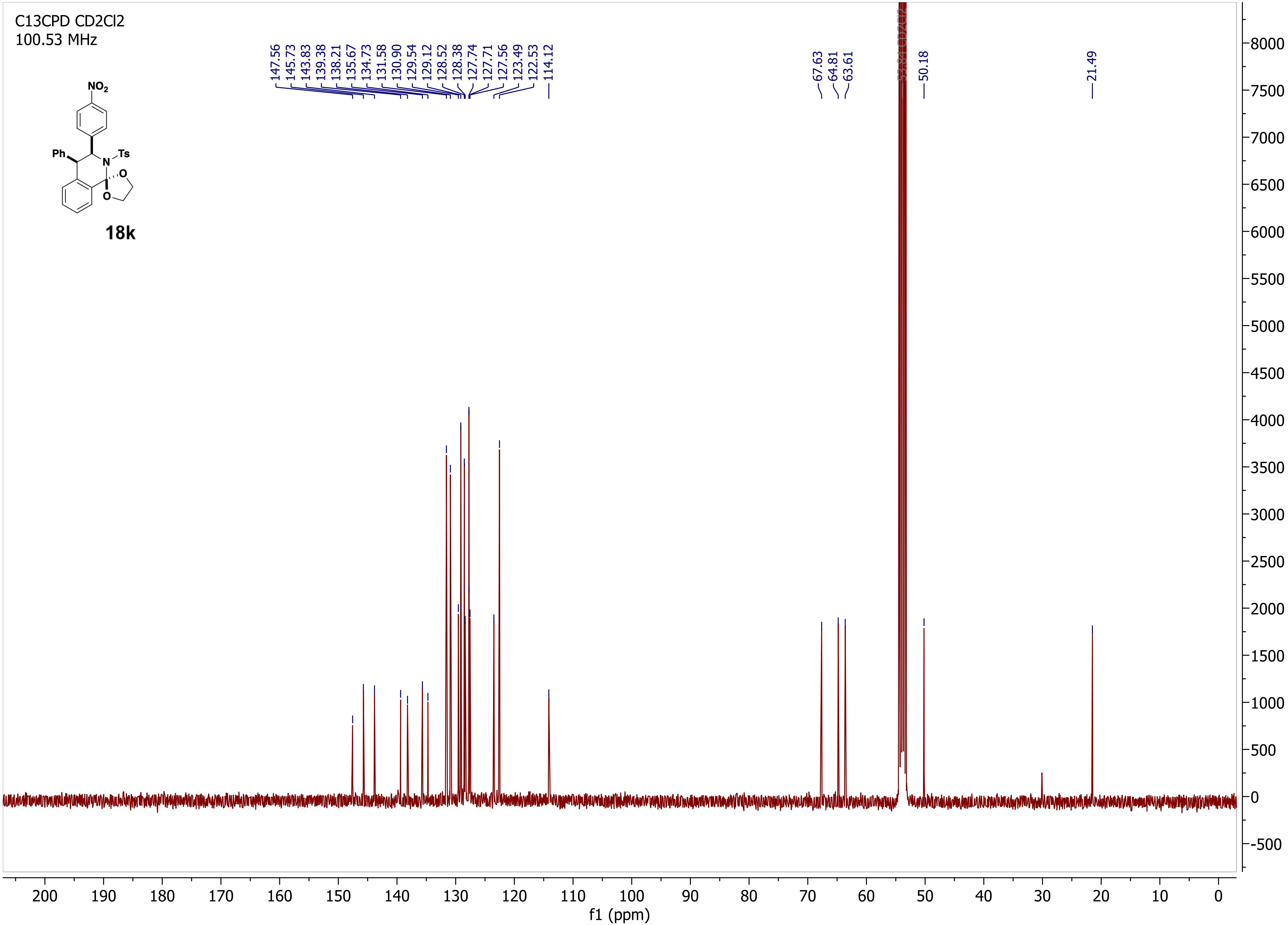
F19CPD CDCl3
376.12 MHz

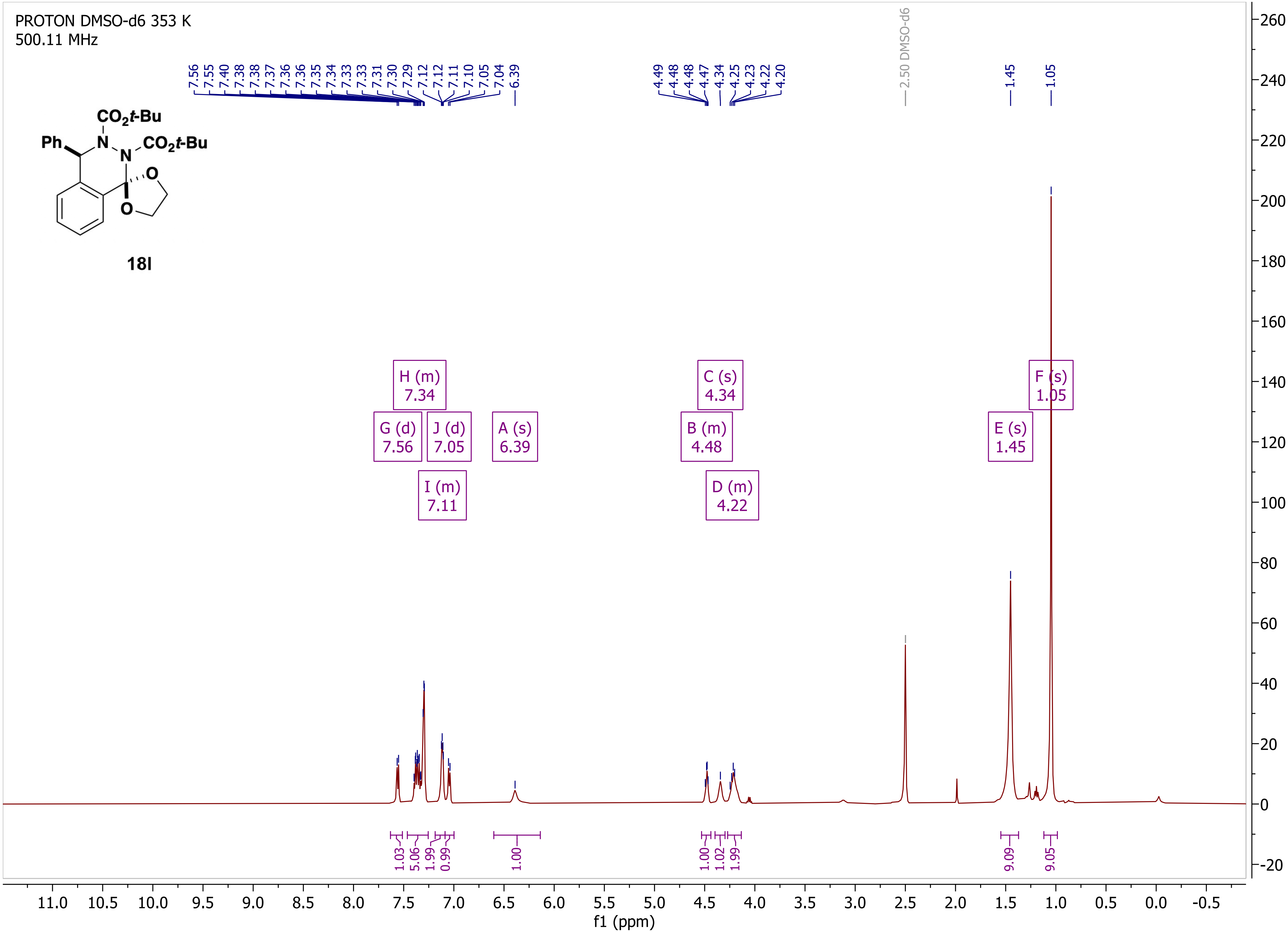



C13CPD CDCl3
100.53 MHz
18j
Ph
Ph
CF3
O
O
O
139.89
137.04
136.36
130.07
129.88
129.67
129.38
128.28
128.22
128.04
127.53
127.51
127.49
127.45
127.33
126.75
126.66
126.49
123.60
120.71
118.58
81.87
81.60
81.33
81.06
77.16 CDCl3
65.73
64.84
47.34
f1 (ppm)

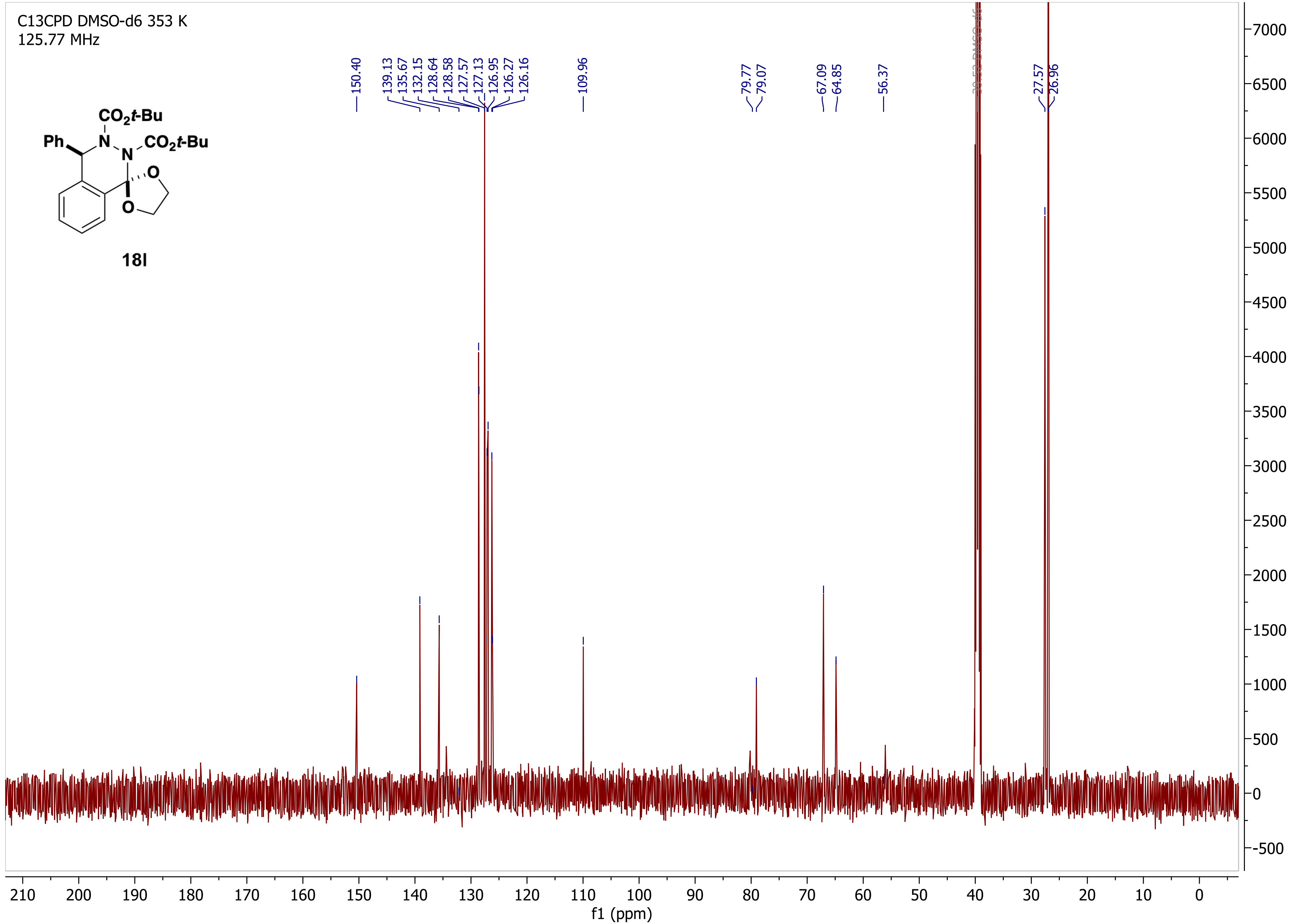
PROTON CD2Cl2
399.77 MHz



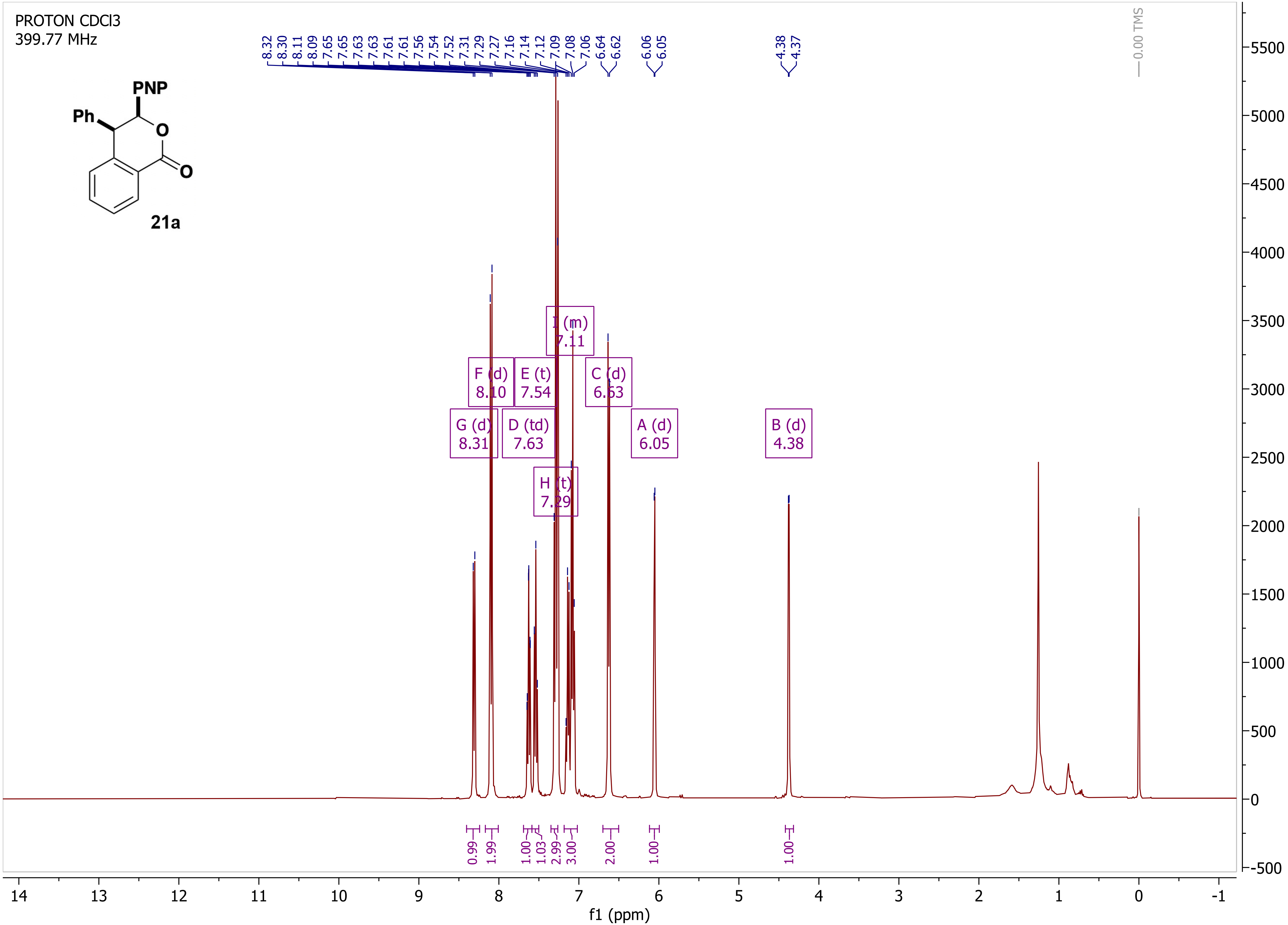

C13CPD CD2Cl2
100.53 MHz
NO2
Ph
N
Ts
O
O
18k
147.56
145.73
143.83
139.38
138.21
135.67
134.73
131.58
130.90
129.54
129.12
128.52
128.38
127.74
127.71
127.56
123.49
122.53
114.12
67.63
64.81
63.61
53.84 CD2Cl2
50.18
21.49
f1 (ppm)



PROTON DMSO-d6 353 K
500.11 MHz
18l
CO2t-Bu
Ph
N
N
CO2t-Bu
O
O
7.56
7.55
7.40
7.38
7.38
7.37
7.36
7.36
7.35
7.34
7.33
7.33
7.31
7.30
7.29
7.12
7.12
7.11
7.10
7.05
7.04
6.39
4.49
4.48
4.48
4.47
4.34
4.25
4.23
4.22
4.20
2.50 DMSO-d6
1.45
1.05
H (m) 7.34
G (d) 7.56
J (d) 7.05
I (m) 7.11
A (s) 6.39
C (s) 4.34
B (m) 4.48
D (m) 4.22
E (s) 1.45
F (s) 1.05
1.03
5.06
1.99
0.99
1.00
1.00
1.02
1.99
9.09
9.05
f1 (ppm)

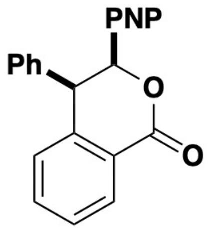


C13CPD DMSO-d6 353 K
125.77 MHz
150.40
139.13
135.67
132.15
128.64
128.58
127.57
127.13
126.95
126.27
126.16
109.96
79.77
79.07
67.09
64.85
56.37
27.57
26.96
Ph
N
N
CO2t-Bu
CO2t-Bu
O
O
18l
f1 (ppm)

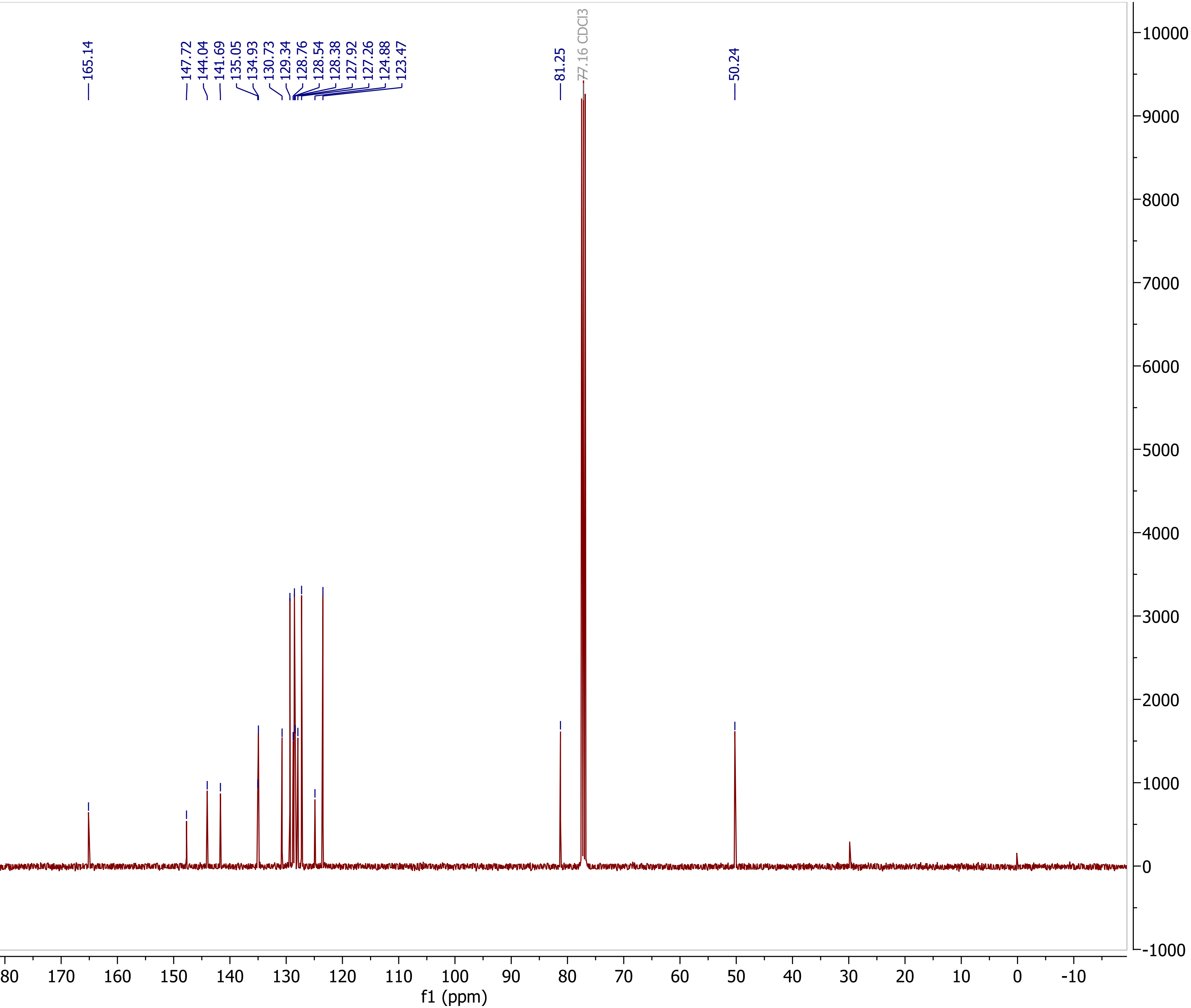


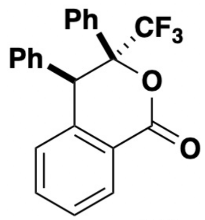
PROTON CDCl3
399.77 MHz
PNP
Ph
O
O
21a
8.32 8.30 8.11 8.09 7.65 7.65 7.63 7.63 7.61 7.61 7.56 7.54 7.52 7.31 7.29 7.27 7.16 7.14 7.12 7.09 7.08 7.06 6.64 6.62 6.06 6.05 4.38 4.37
0.00 TMS
G (d) 8.31
F (d) 8.10
D (td) 7.63
E (t) 7.54
H (t) 7.29
I (m) 7.11
C (d) 6.63
A (d) 6.05
B (d) 4.38
0.99 1.99 1.00 1.03 2.99 3.00 2.00 1.00 1.00
f1 (ppm)

C13CPD CDCl3
100.53 MHz

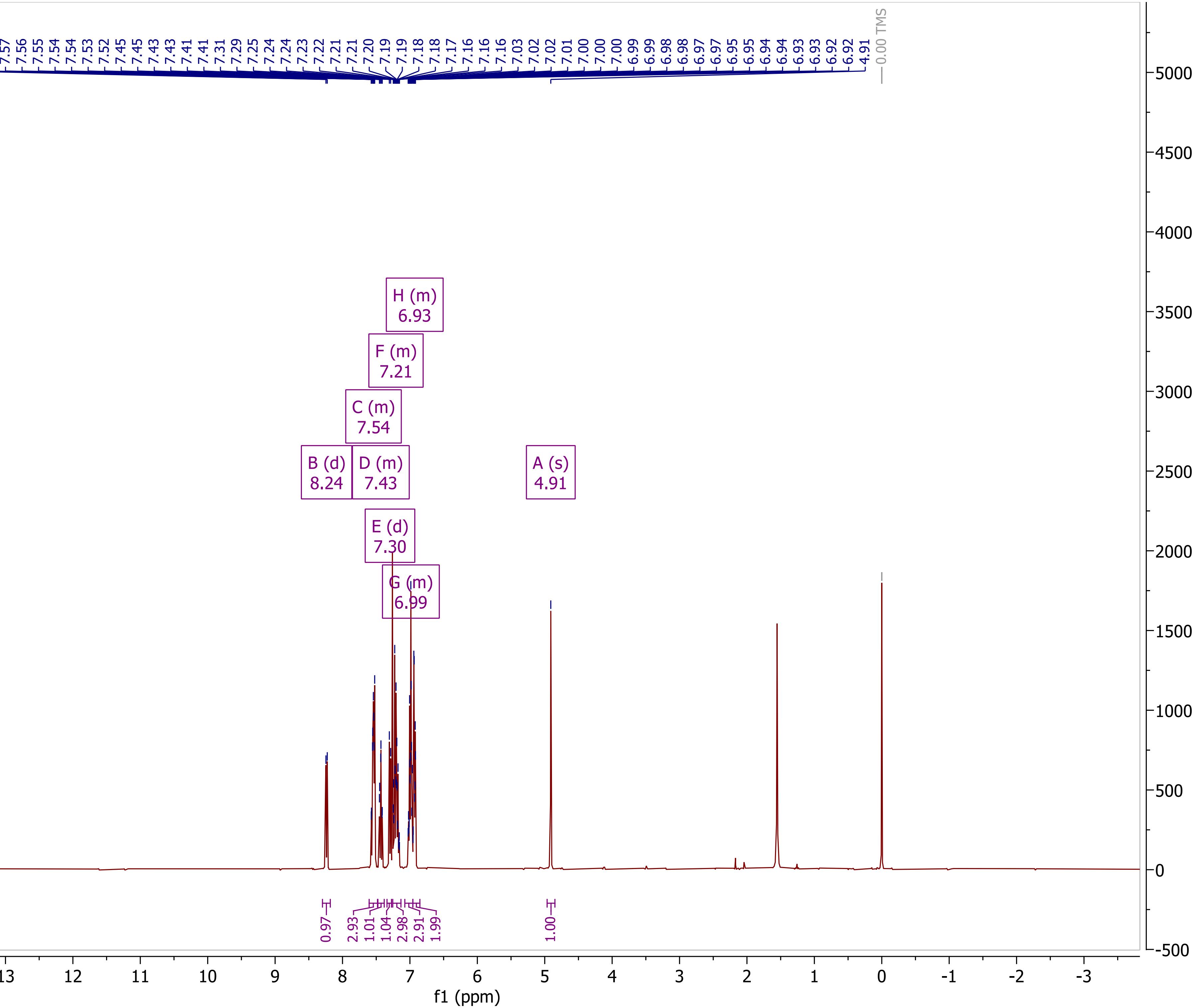


21a



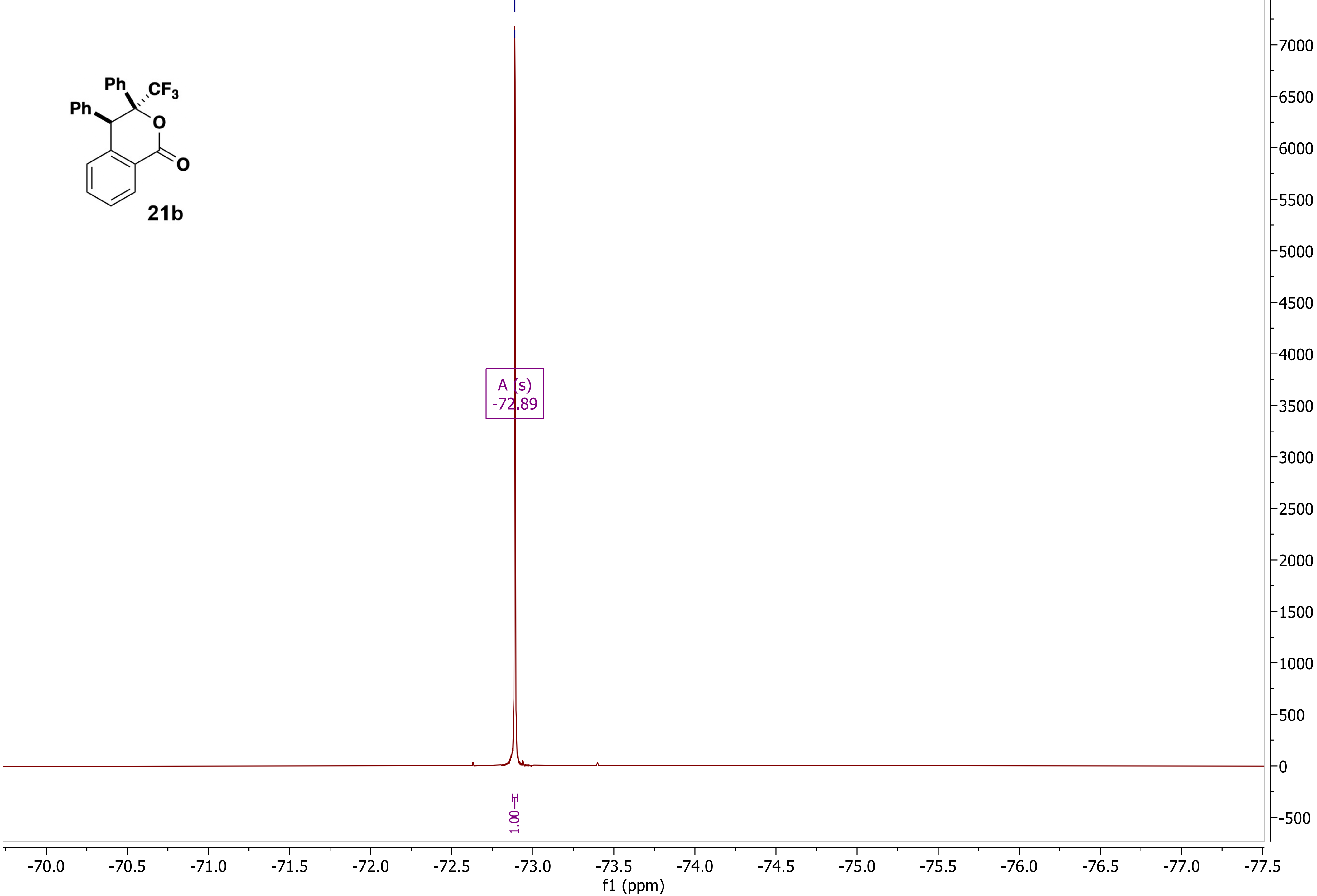


21b

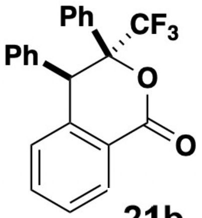


PROTON CDCl3
399.77 MHz
8.25 8.23 7.57 7.56 7.55 7.54 7.54 7.53 7.52 7.45 7.45 7.43 7.43 7.41 7.41 7.31 7.29 7.25 7.24 7.24 7.23 7.22 7.21 7.21 7.20 7.19 7.19 7.18 7.18 7.17 7.16 7.16 7.16 7.03 7.02 7.02 7.01 7.00 7.00 7.00 6.99 6.99 6.98 6.98 6.97 6.97 6.95 6.95 6.94 6.94 6.93 6.93 6.92 6.92 4.91
0.00 TMS
H (m) 6.93
F (m) 7.21
C (m) 7.54
B (d) 8.24
D (m) 7.43
A (s) 4.91
E (d) 7.30
G (m) 6.99
0.97
2.93
1.01
1.04
2.98
2.91
1.99
1.00
f1 (ppm)

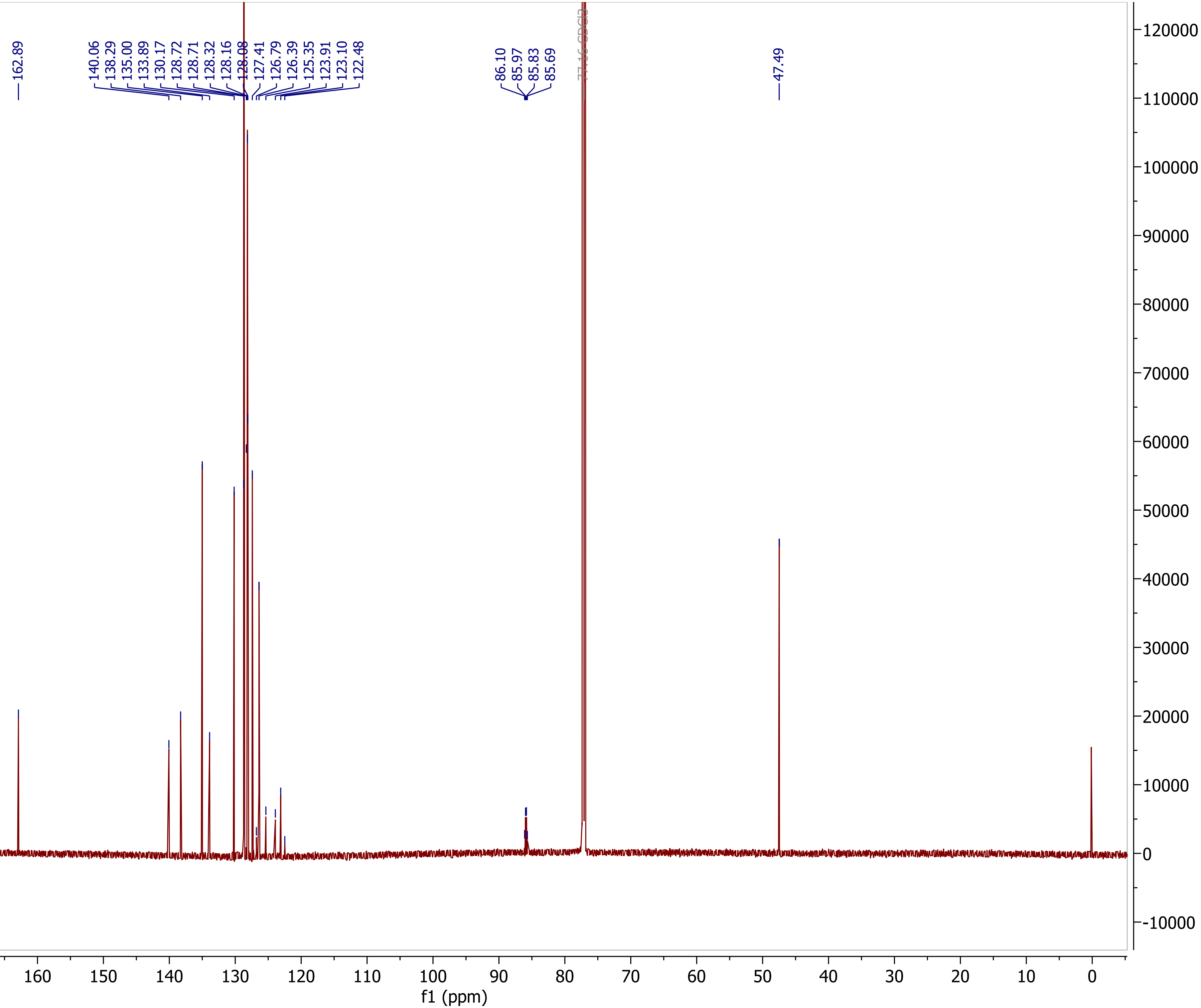
F19CPD CDCl3
376.12 MHz

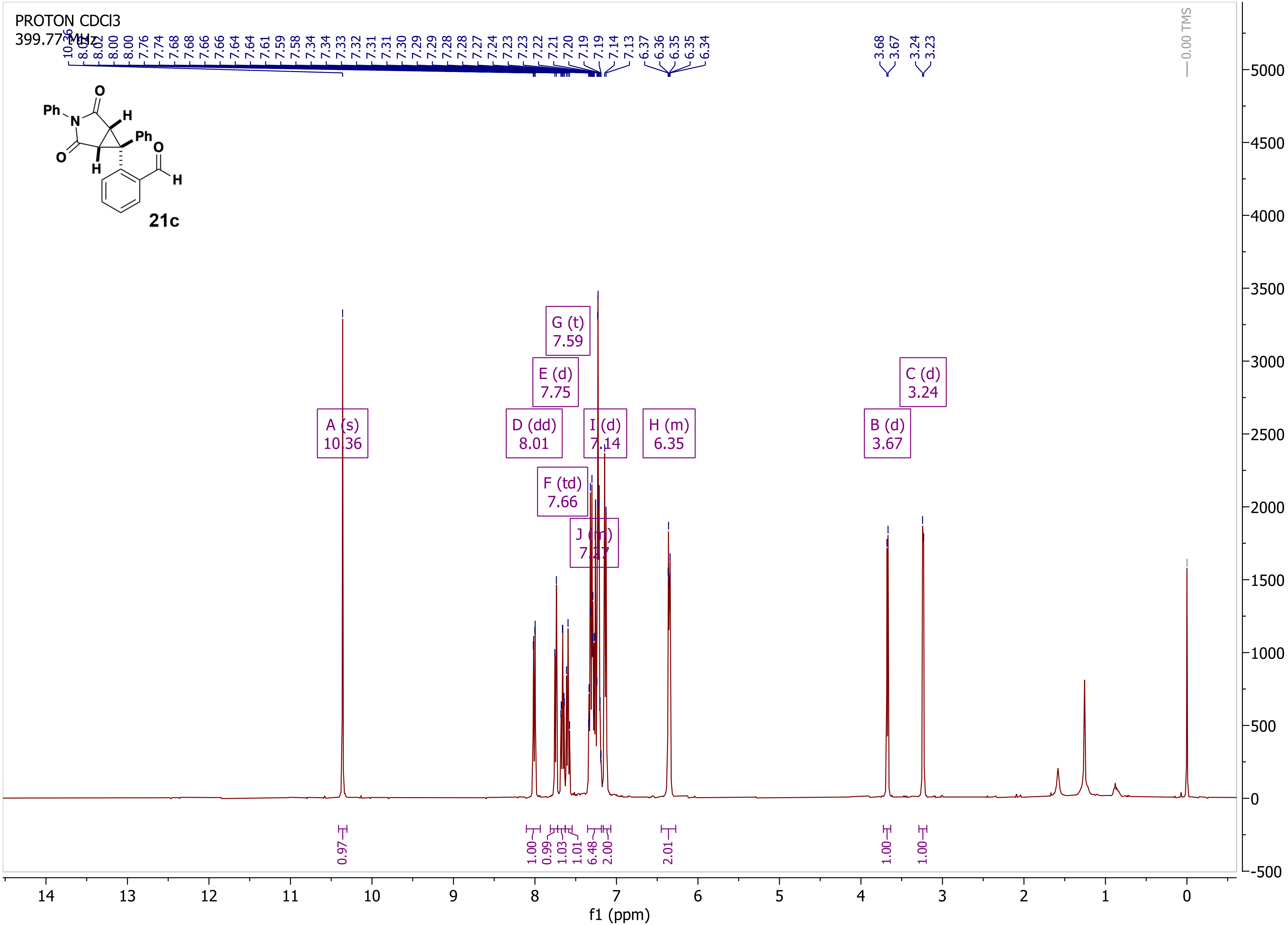


13C NMR, 800 MHz
201.22 MHz

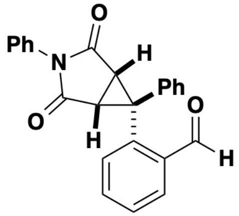


21b

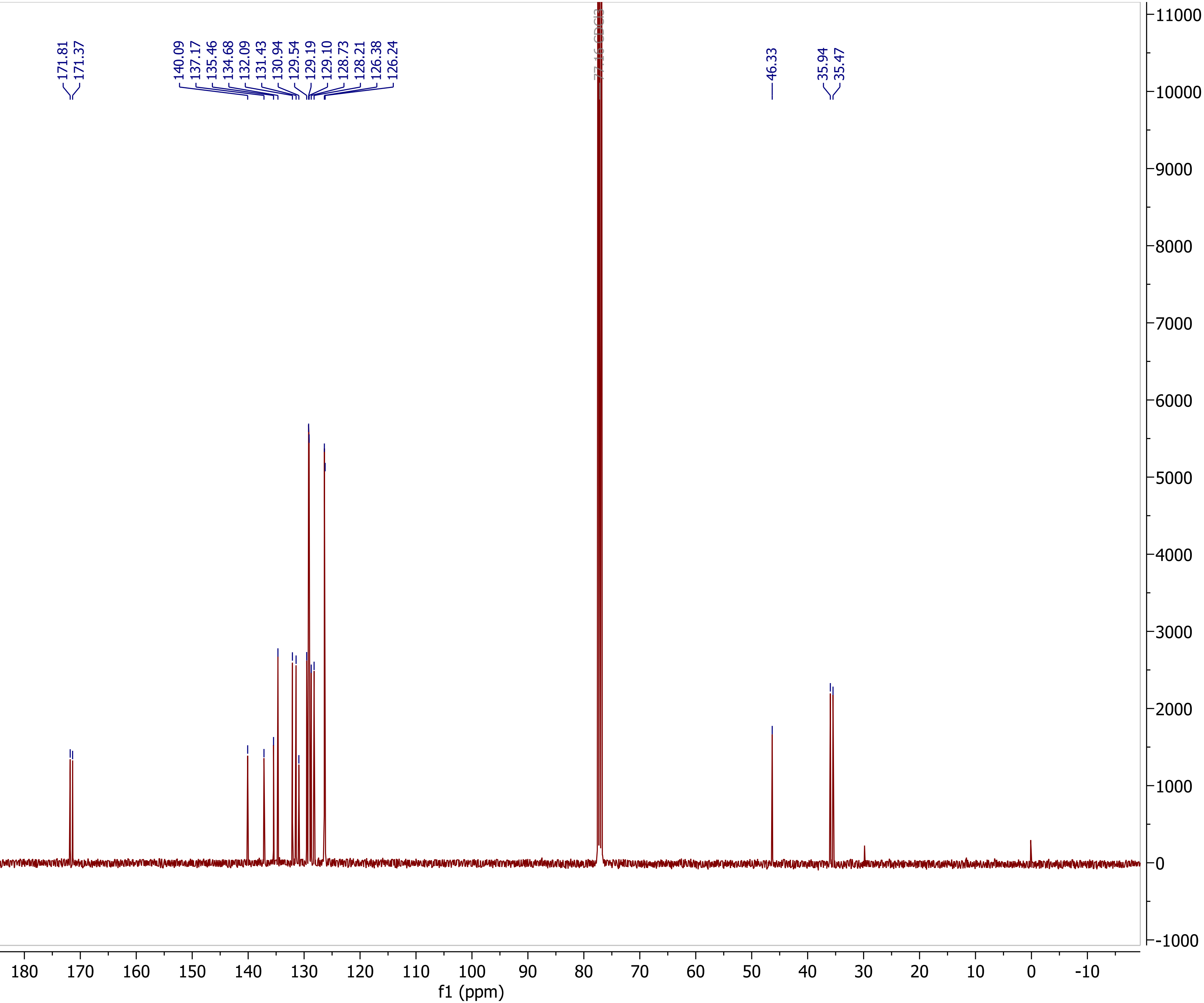


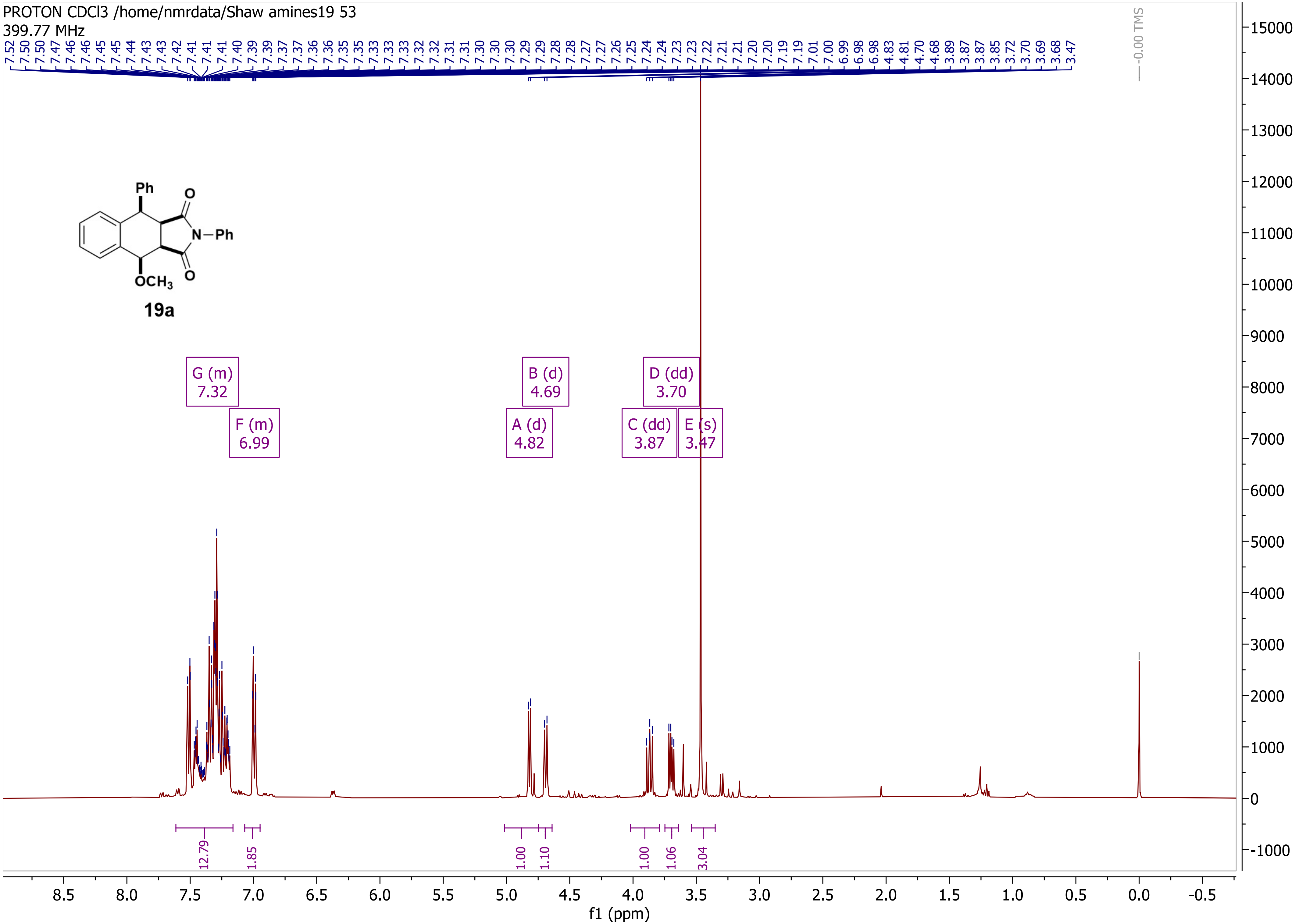

PROTON CDCl3
399.77 MHz
10.36 8.02 8.02 8.00 8.00 7.76 7.74 7.68 7.68 7.66 7.66 7.64 7.64 7.61 7.59 7.58 7.34 7.34 7.33 7.32 7.31 7.31 7.30 7.29 7.29 7.28 7.28 7.27 7.24 7.23 7.23 7.22 7.21 7.20 7.19 7.19 7.14 7.13 6.37 6.36 6.35 6.35 6.34
3.68 3.67 3.24 3.23
0.00 TMS
Ph
N
O
O
H
H
Ph
O
H
21c
A (s) 10.36
D (dd) 8.01
E (d) 7.75
G (t) 7.59
F (td) 7.66
I (d) 7.14
J (m) 7.27
H (m) 6.35
B (d) 3.67
C (d) 3.24
0.97
1.00
0.99
1.03
1.01
6.48
2.00
2.01
1.00
1.00
f1 (ppm)

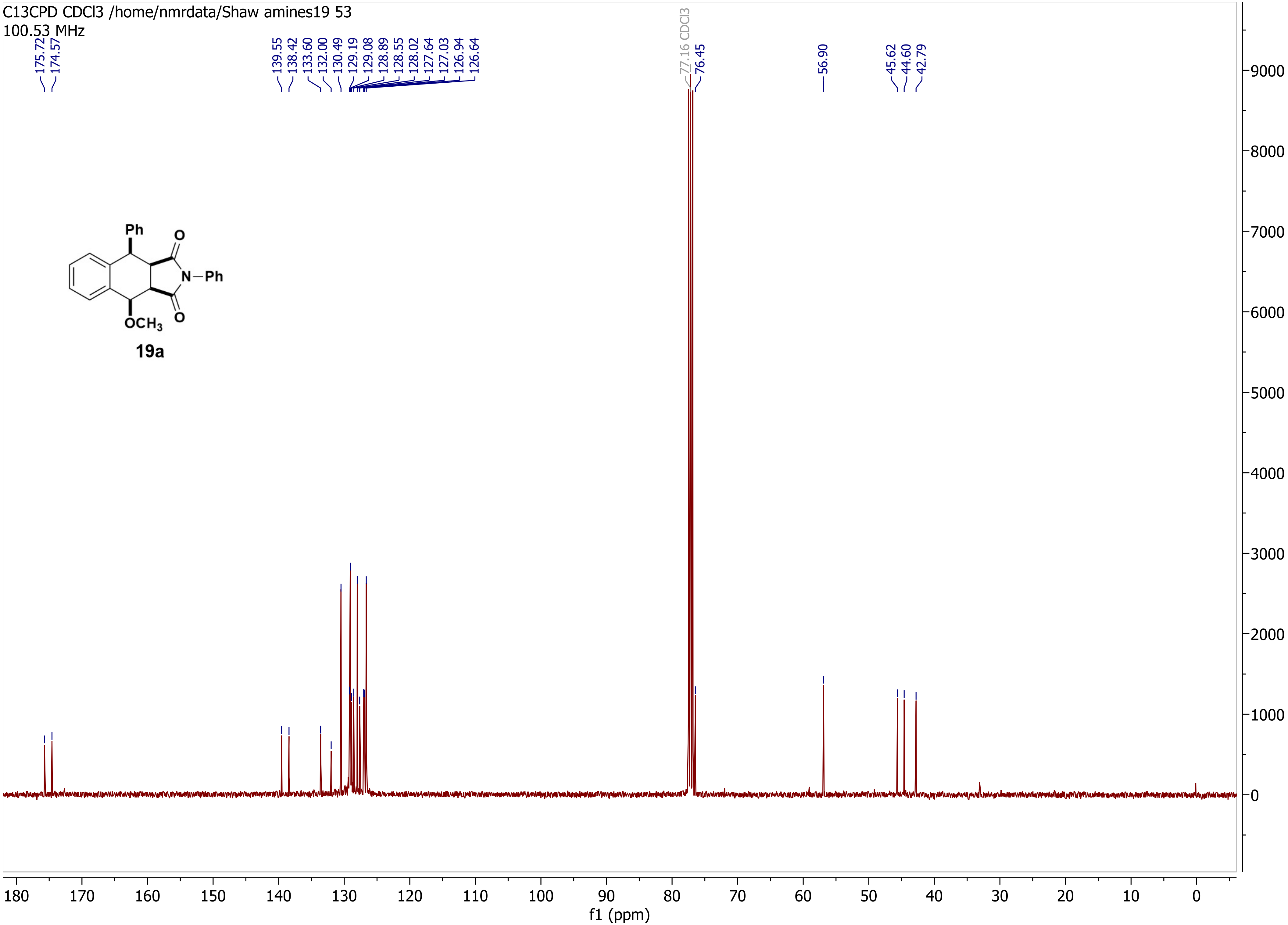
C13CPD CDCl3
100.53 MHz



21c

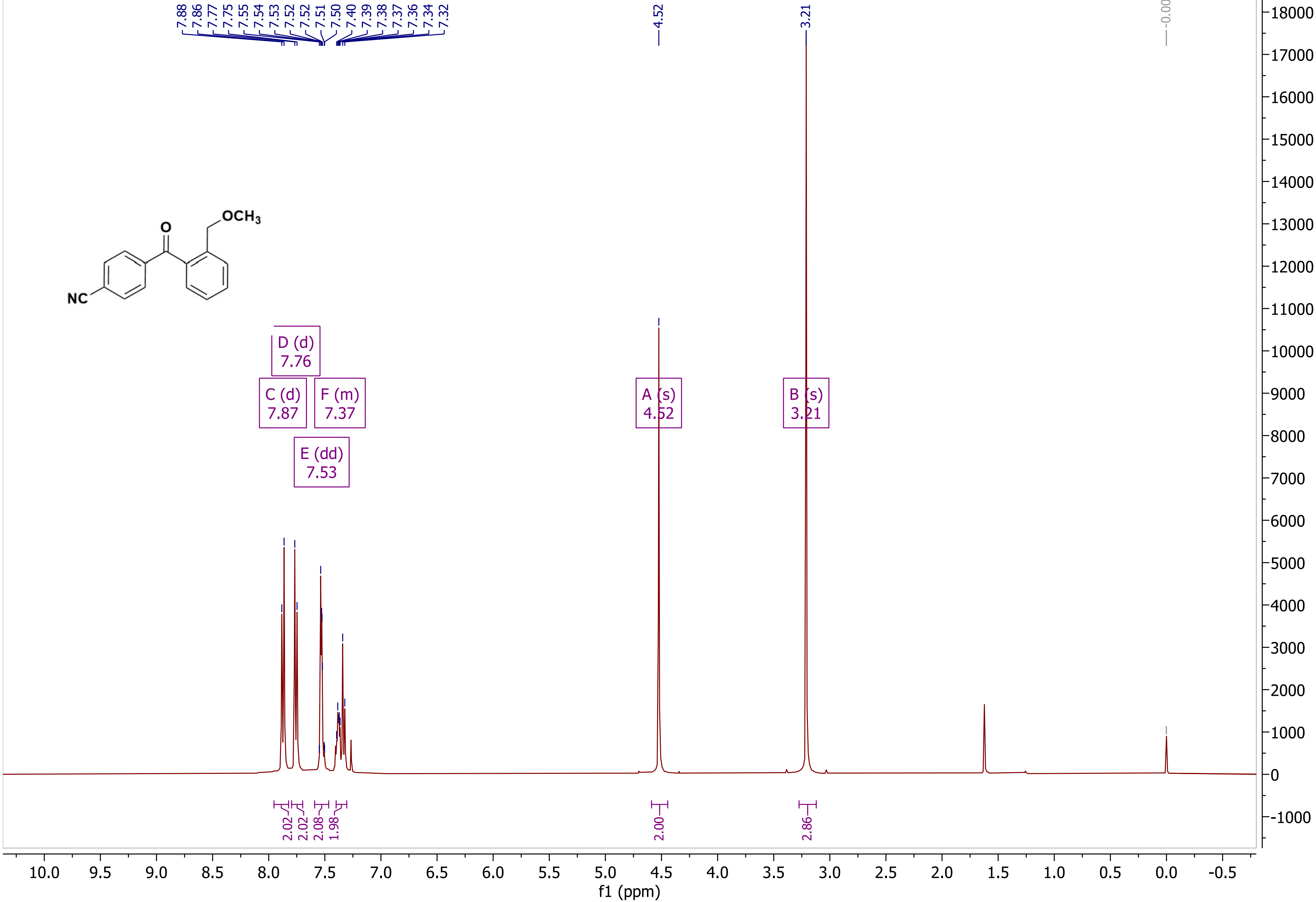


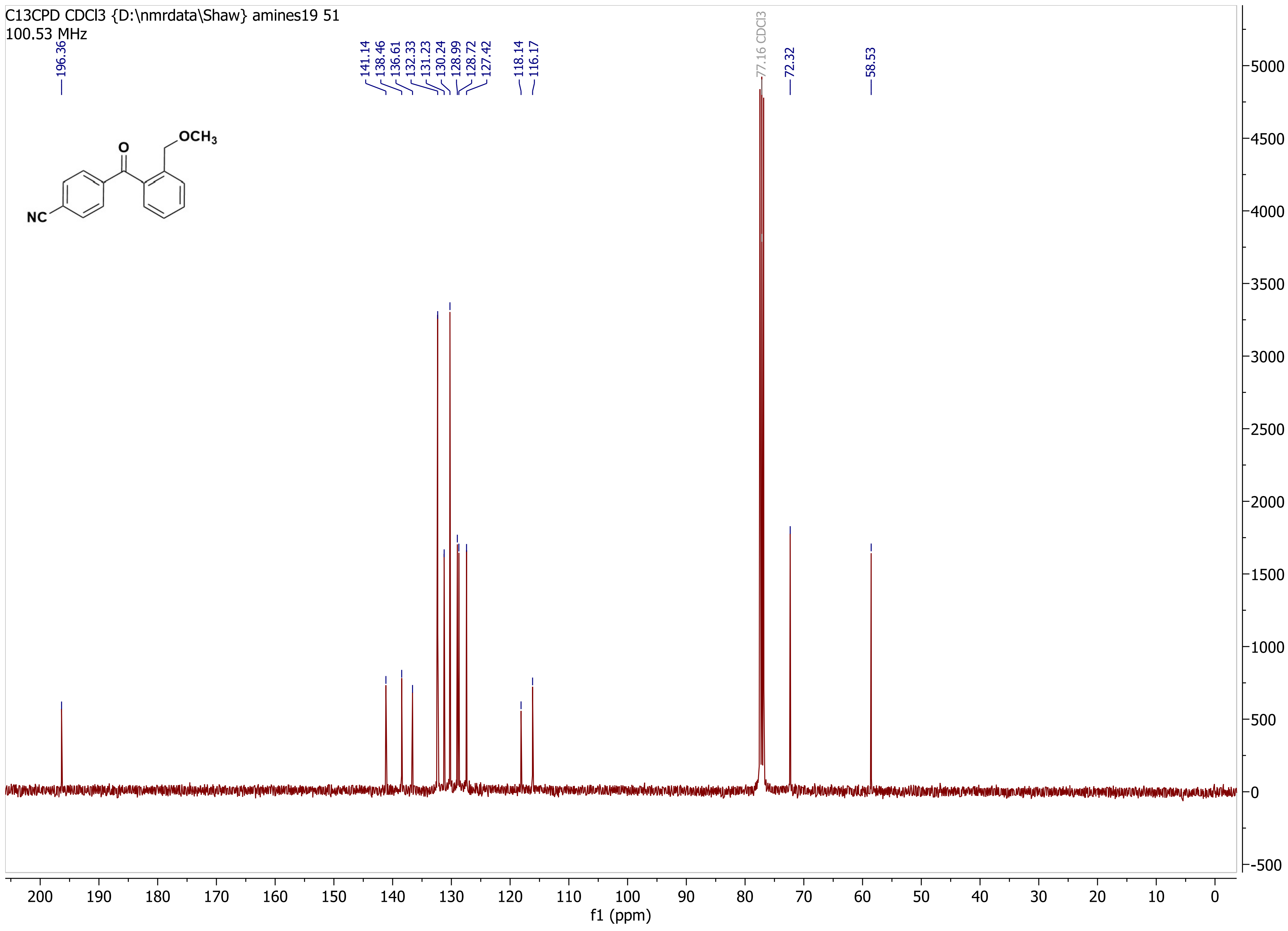

PROTON CDCl3 /home/nmrdata/Shaw amines19 53
399.77 MHz
7.52 7.50 7.50 7.47 7.46 7.46 7.45 7.45 7.44 7.43 7.43 7.42 7.41 7.41 7.41 7.41 7.40 7.39 7.39 7.37 7.37 7.36 7.36 7.35 7.35 7.33 7.33 7.33 7.32 7.32 7.31 7.31 7.30 7.30 7.30 7.29 7.29 7.28 7.28 7.27 7.26 7.25 7.24 7.24 7.23 7.23 7.22 7.21 7.21 7.20 7.20 7.19 7.19 7.01 7.00 6.99 6.98 6.98 4.83 4.81 4.70 4.68 3.89 3.87 3.85 3.72 3.70 3.69 3.68 3.47
0.00 TMS
Ph
O
N—Ph
O
OCH3
19a
G (m)
7.32
F (m)
6.99
B (d)
4.69
A (d)
4.82
D (dd)
3.70
C (dd)
3.87
E (s)
3.47
12.79
1.85
1.00
1.10
1.00
1.06
3.04
f1 (ppm)

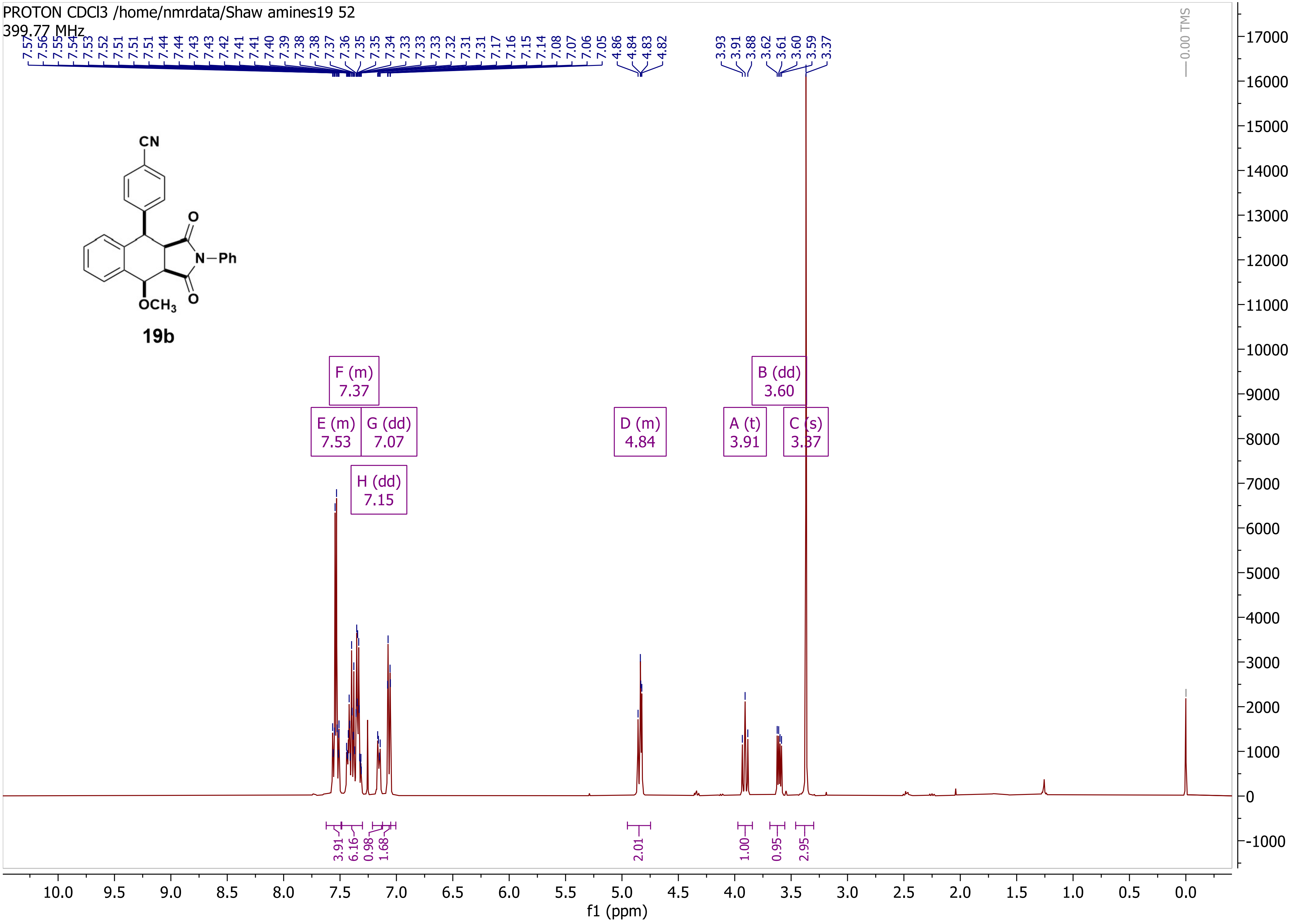


C13CPD CDCl3 /home/nmrdata/Shaw amines19 53
100.53 MHz
175.72
174.57
139.55
138.42
133.60
132.00
130.49
129.19
129.08
128.89
128.55
128.02
127.64
127.03
126.94
126.64
77.16 CDCl3
76.45
56.90
45.62
44.60
42.79
Ph
O
N—Ph
OCH3
O
19a
9000
8000
7000
6000
5000
4000
3000
2000
1000
0
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

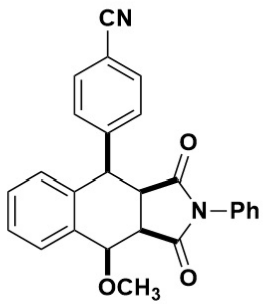
PROTON CDCl3 {D:\nmrdata\Shaw} amines19 51
399.77 MHz



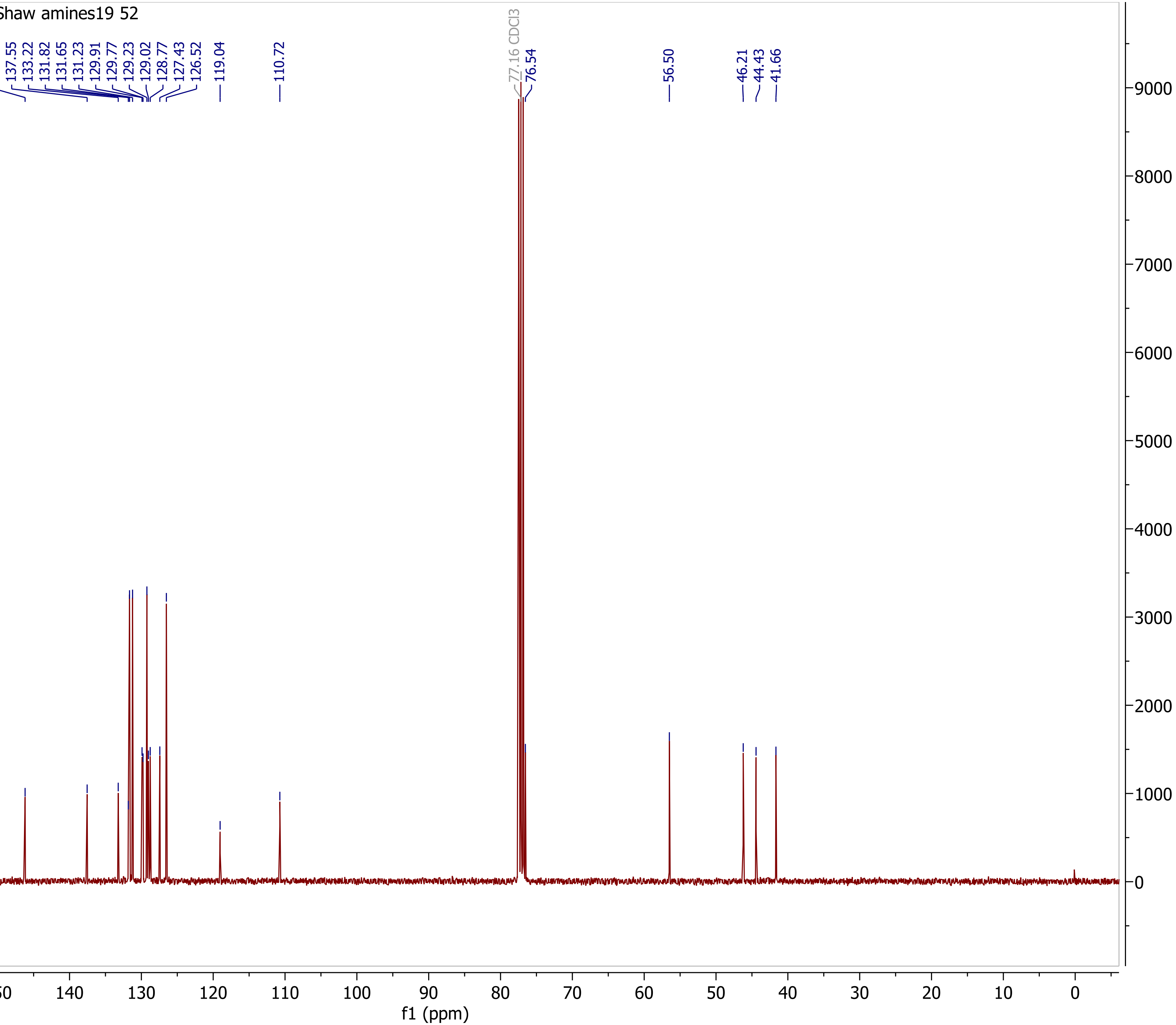

C13CPD CDCl3 {D:\nmrdata\Shaw} amines19 51
100.53 MHz
196.36
141.14
138.46
136.61
132.33
131.23
130.24
128.99
128.72
127.42
118.14
116.17
77.16 CDCl3
72.32
58.53
OCH3
O
NC
f1 (ppm)

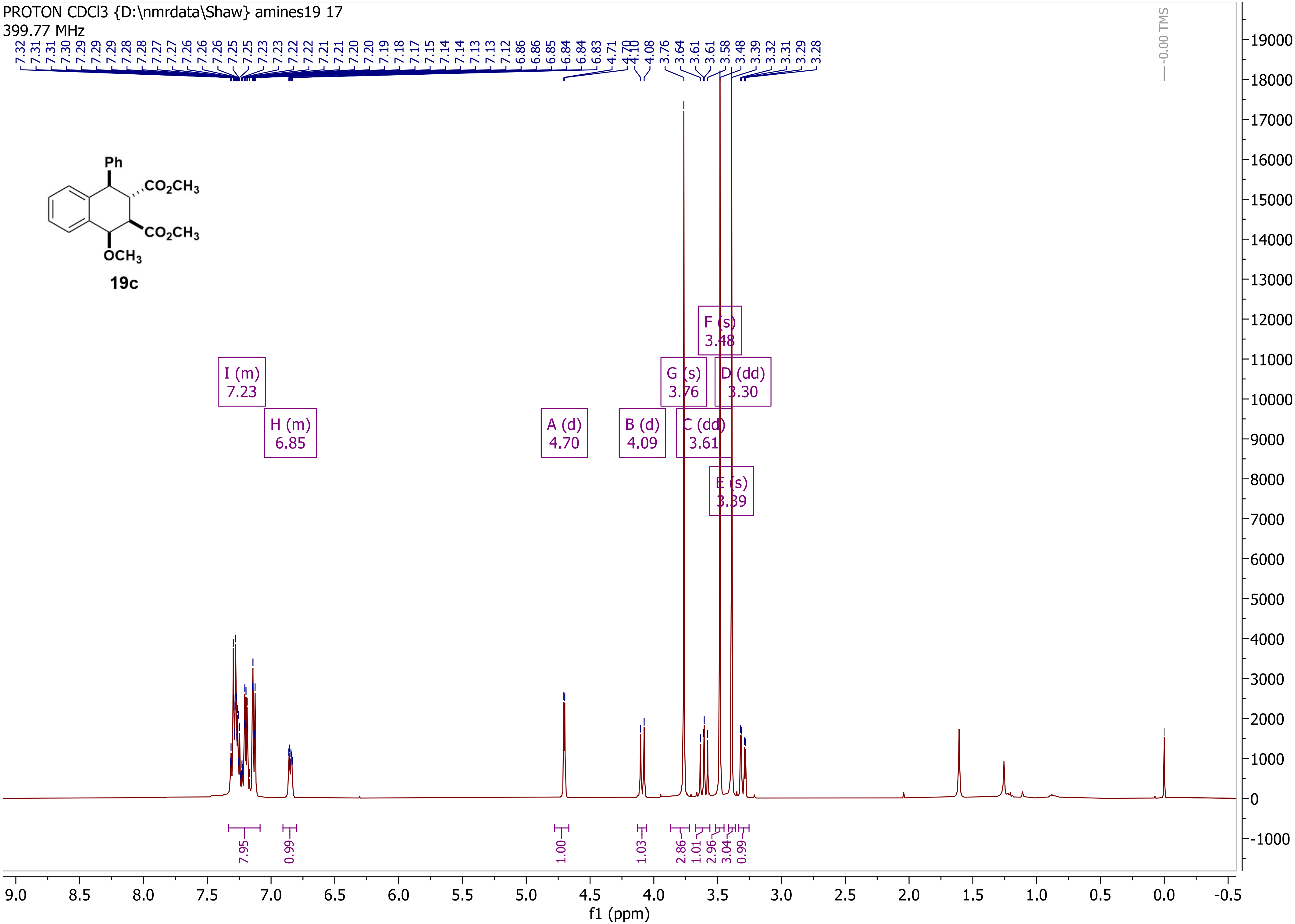

PROTON CDCl3 /home/nmrdata/Shaw amines19 52
399.77 MHz
7.57 7.56 7.55 7.54 7.53 7.52 7.51 7.51 7.51 7.44 7.44 7.43 7.43 7.42 7.41 7.41 7.40 7.39 7.38 7.38 7.37 7.36 7.35 7.35 7.34 7.33 7.33 7.33 7.32 7.31 7.31 7.17 7.16 7.15 7.14 7.08 7.07 7.06 7.05 4.86 4.84 4.83 4.82
3.93 3.91 3.88 3.62 3.61 3.60 3.59 3.37
0.00 TMS
CN
O
N—Ph
OCH3
O
19b
F (m)
7.37
E (m)
7.53
G (dd)
7.07
H (dd)
7.15
D (m)
4.84
B (dd)
3.60
A (t)
3.91
C (s)
3.37
3.91
6.16
0.98
1.68
2.01
1.00
0.95
2.95
f1 (ppm)

C13CPD CDCl3 /home/nmrdata/Shaw amines19 52
100.53 MHz



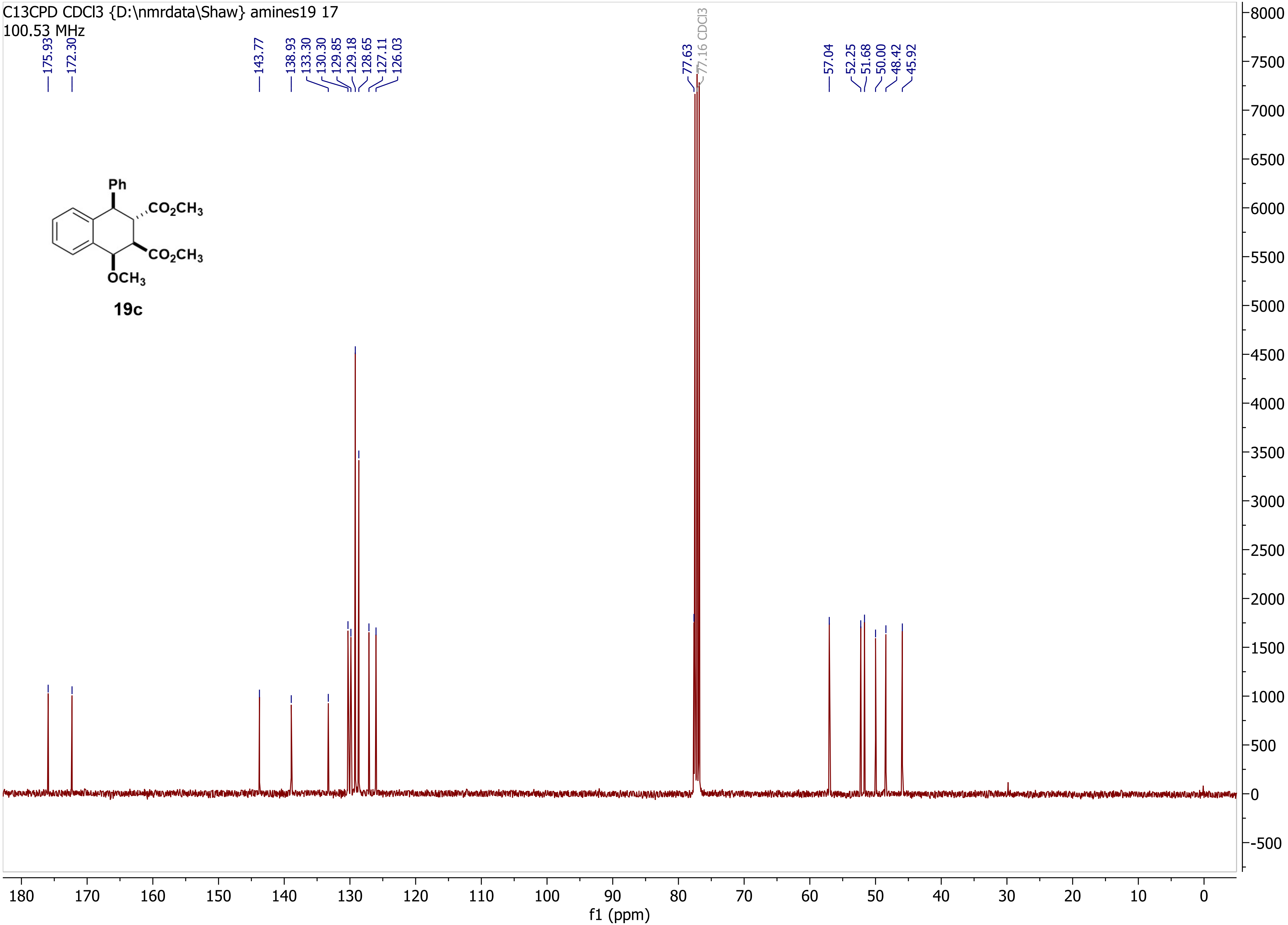
19b

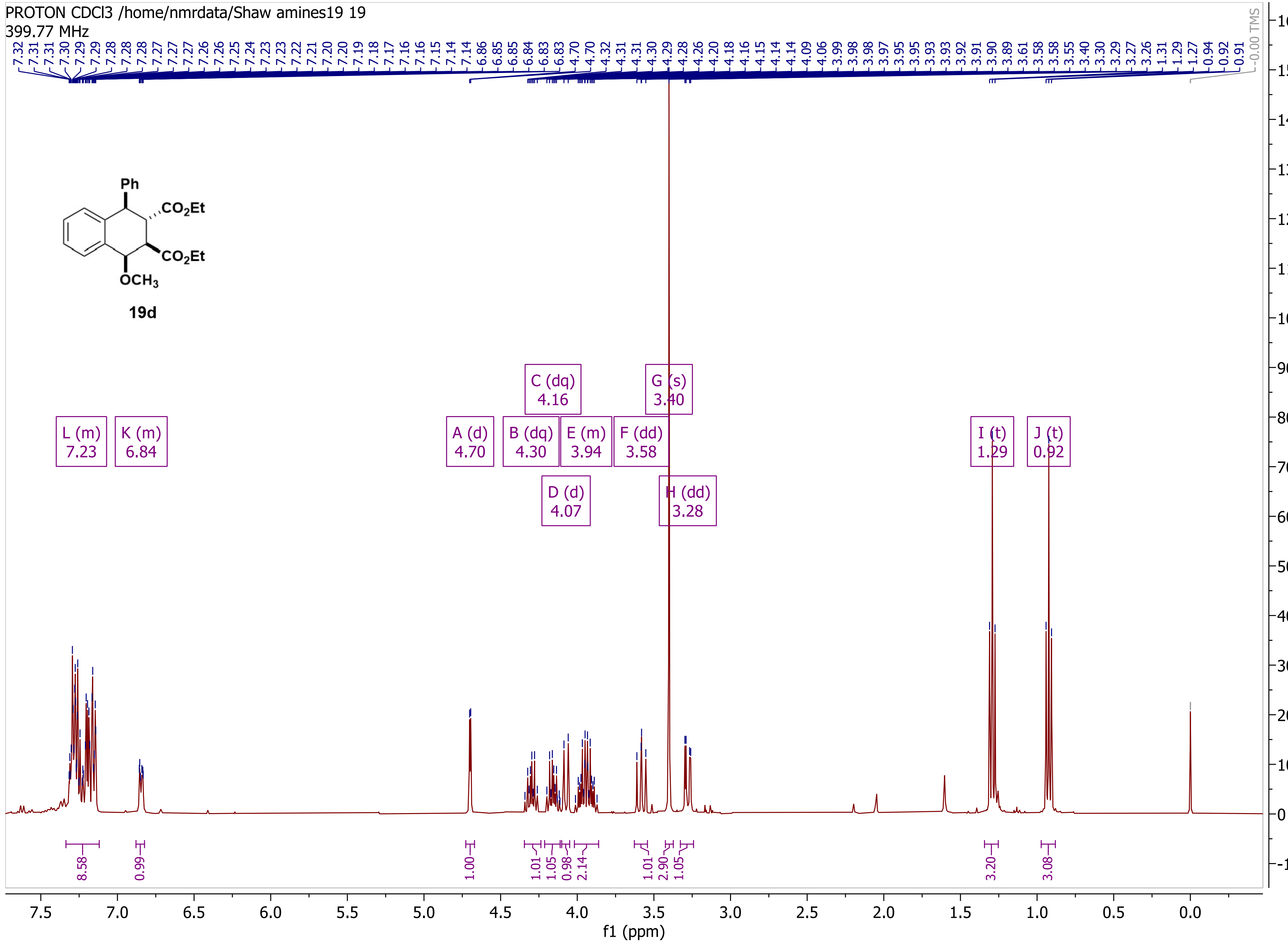


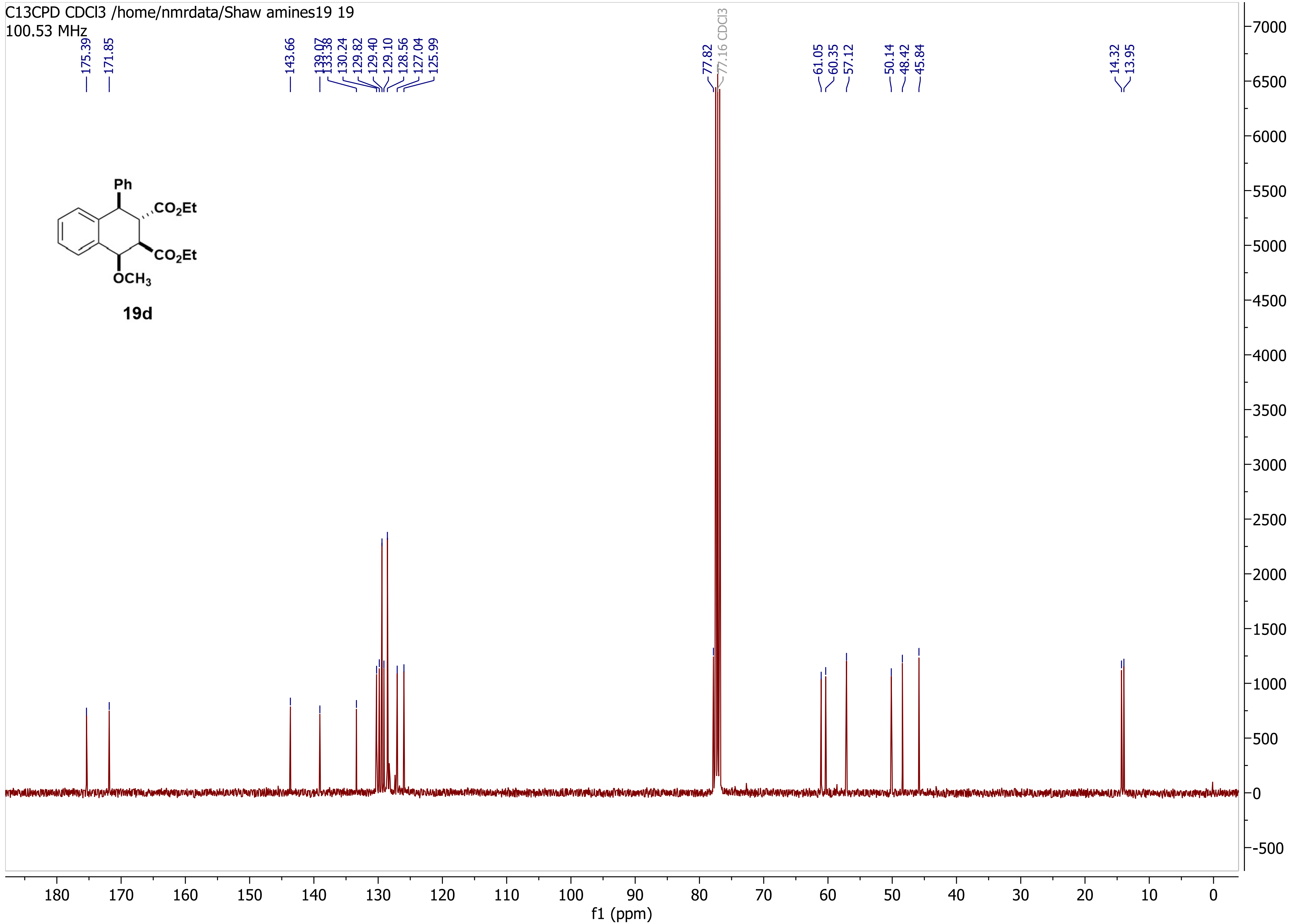


PROTON CDCl3 {D:\nmrdata\Shaw} amines19 17
399.77 MHz
7.32 7.31 7.31 7.30 7.29 7.29 7.29 7.28 7.28 7.27 7.27 7.26 7.26 7.26 7.25 7.25 7.23 7.23 7.22 7.22 7.21 7.21 7.20 7.20 7.19 7.18 7.17 7.15 7.14 7.14 7.13 7.13 7.12 6.86 6.86 6.85 6.84 6.84 6.83 4.71 4.70 4.10 4.08 3.76 3.64 3.61 3.61 3.58 3.48 3.39 3.32 3.31 3.29 3.28
0.00 TMS
Ph
CO2CH3
CO2CH3
OCH3
19c
I (m) 7.23
H (m) 6.85
A (d) 4.70
B (d) 4.09
G (s) 3.76
C (dd) 3.61
F (s) 3.48
E (s) 3.39
D (dd) 3.30
7.95
0.99
1.00
1.03
2.86
1.01
2.96
3.04
0.99
f1 (ppm)

C13CPD CDCl3 {D:\nmrdata\Shaw} amines19 17
100.53 MHz

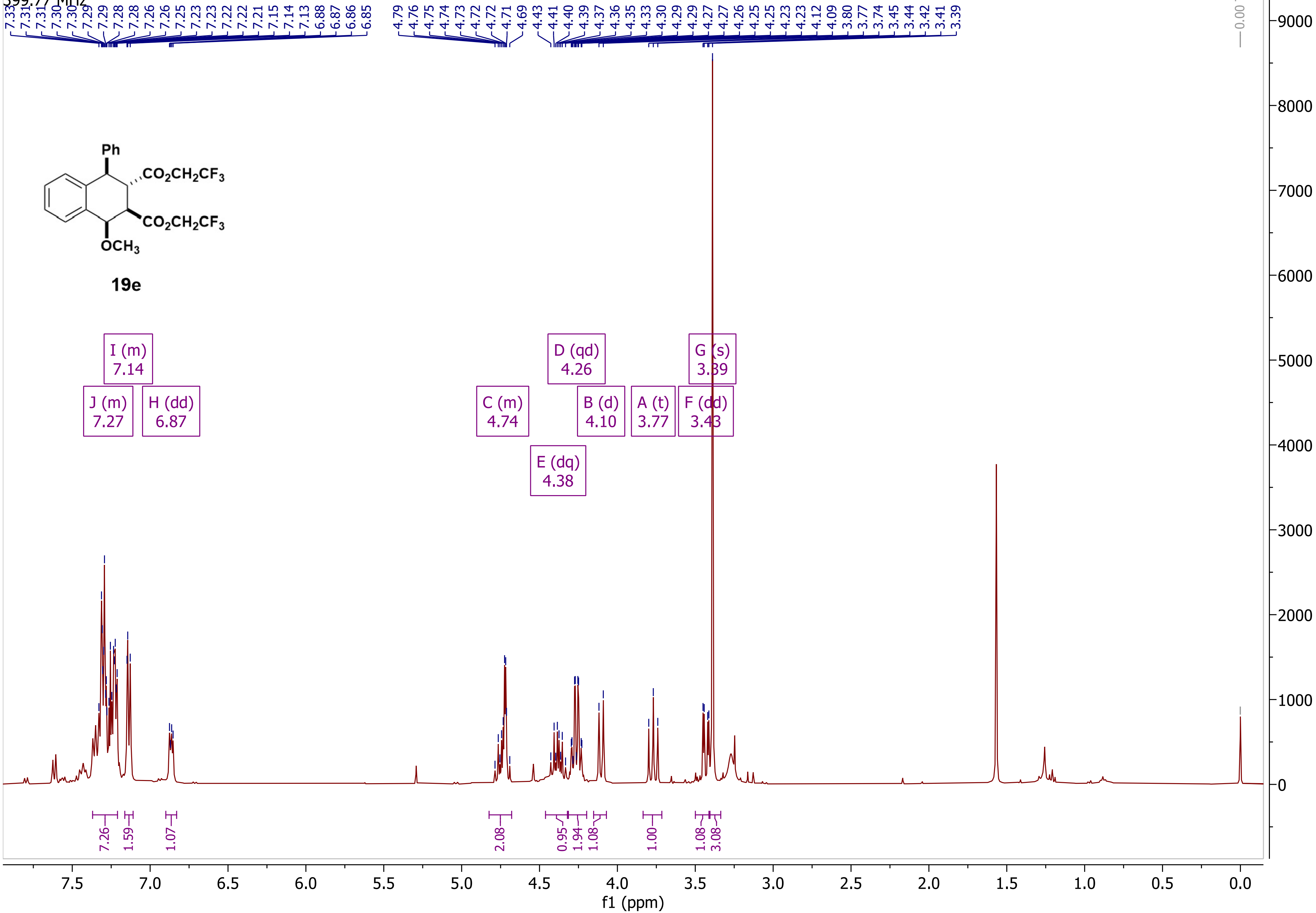



PROTON CDCl3 /home/nmrdata/Shaw amines19 19
399.77 MHz
Ph
CO2Et
CO2Et
OCH3
19d
L (m) 7.23
K (m) 6.84
A (d) 4.70
B (dq) 4.30
C (dq) 4.16
D (d) 4.07
E (m) 3.94
F (dd) 3.58
G (s) 3.40
H (dd) 3.28
I (t) 1.29
J (t) 0.92
8.58
0.99
1.00
1.01
1.05
0.98
2.14
1.01
2.90
1.05
3.20
3.08
-0.00 TMS
f1 (ppm)



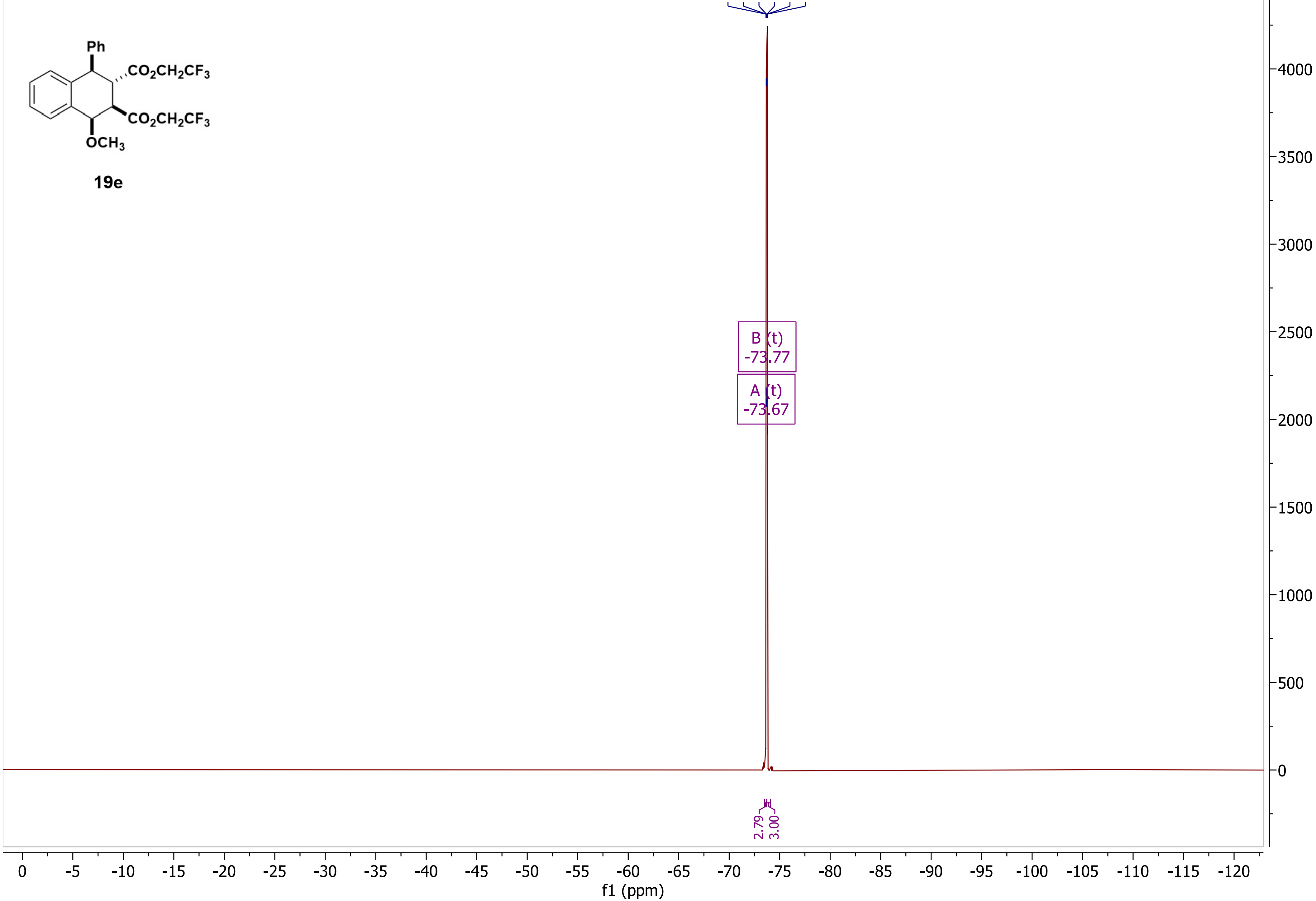
C13CPD CDCl3 /home/nmrdata/Shaw amines19 19
100.53 MHz
175.39
171.85
143.66
139.07
133.38
130.24
129.82
129.40
129.10
128.56
127.04
125.99
77.82
77.16 CDCl3
61.05
60.35
57.12
50.14
48.42
45.84
14.32
13.95
Ph
CO2Et
CO2Et
OCH3
19d
f1 (ppm)

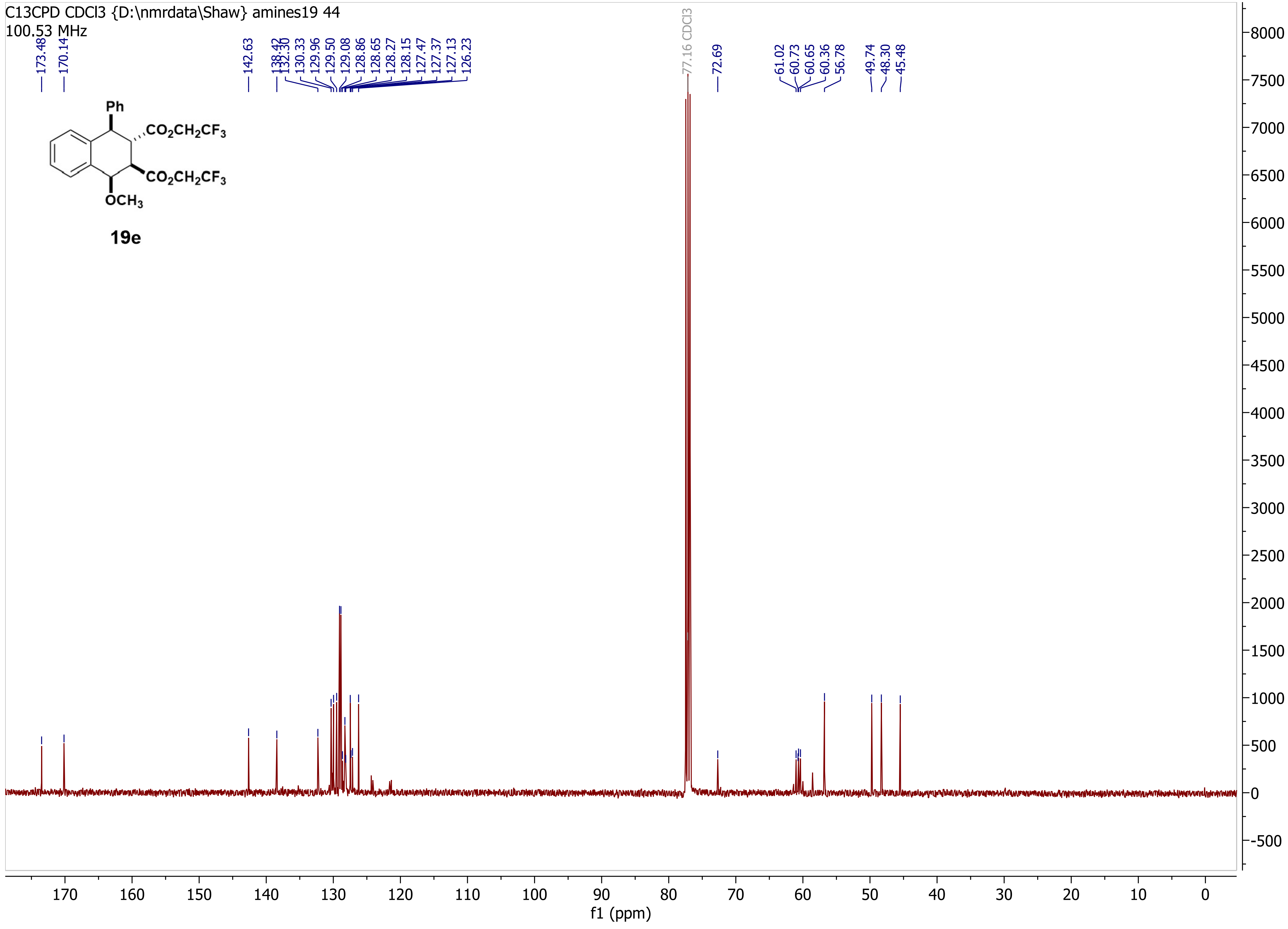
PROTON CDCl3 {D:\nmrdata\Shaw} amines19 44
399.77 MHz



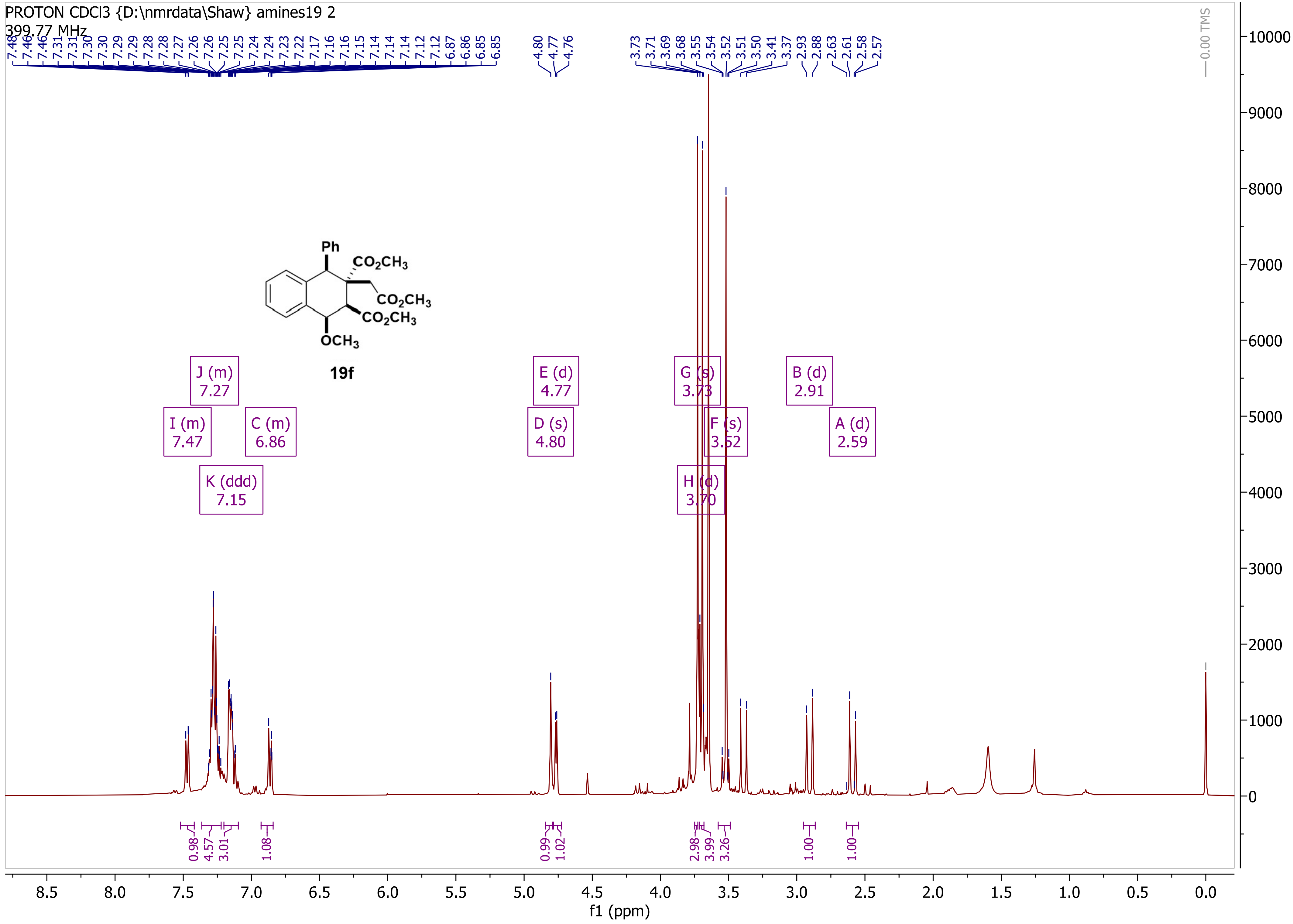
19e

F19 CDCl3 {D:\nmrdata\Shaw} amines19 44
376.12 MHz

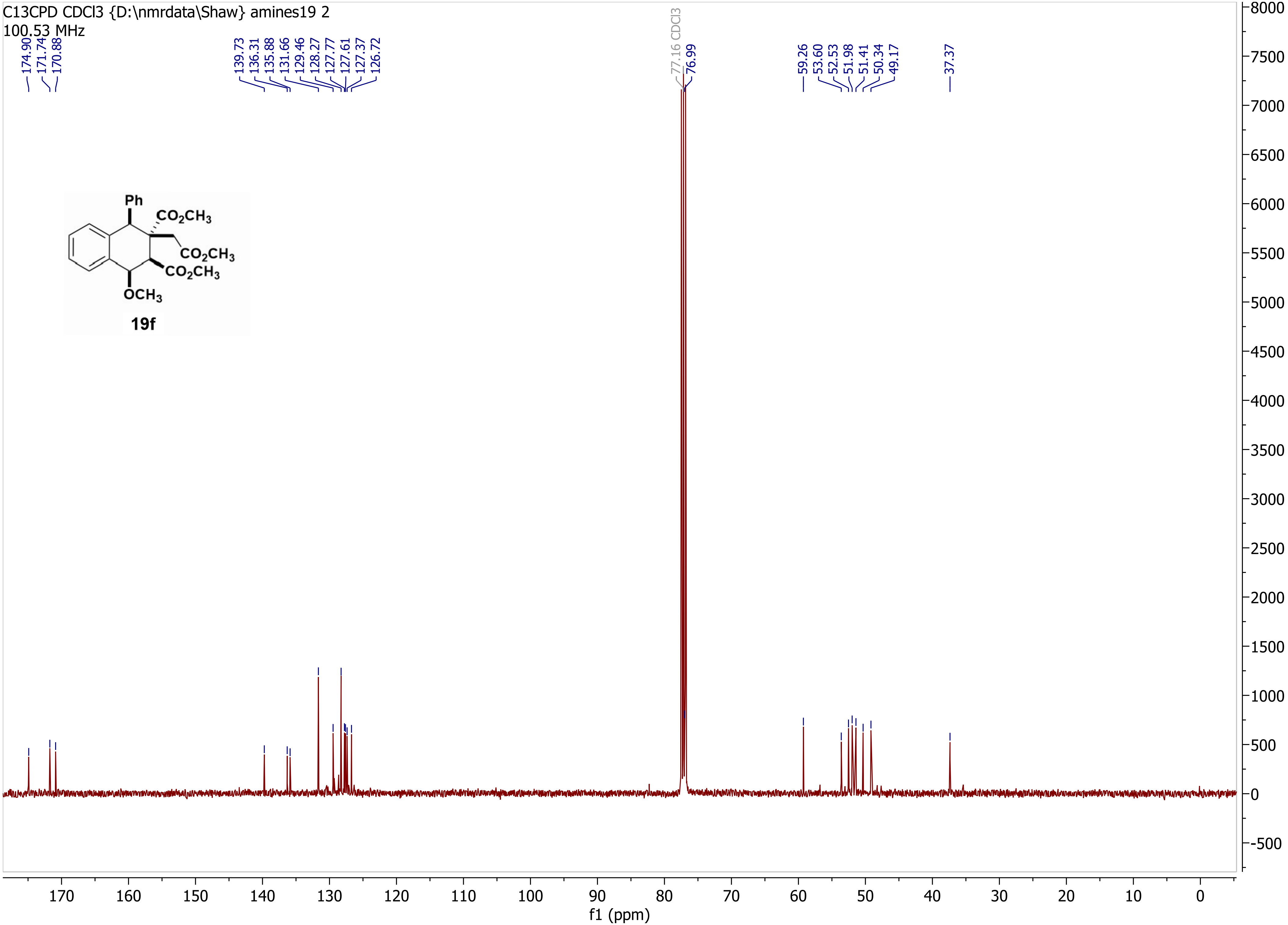


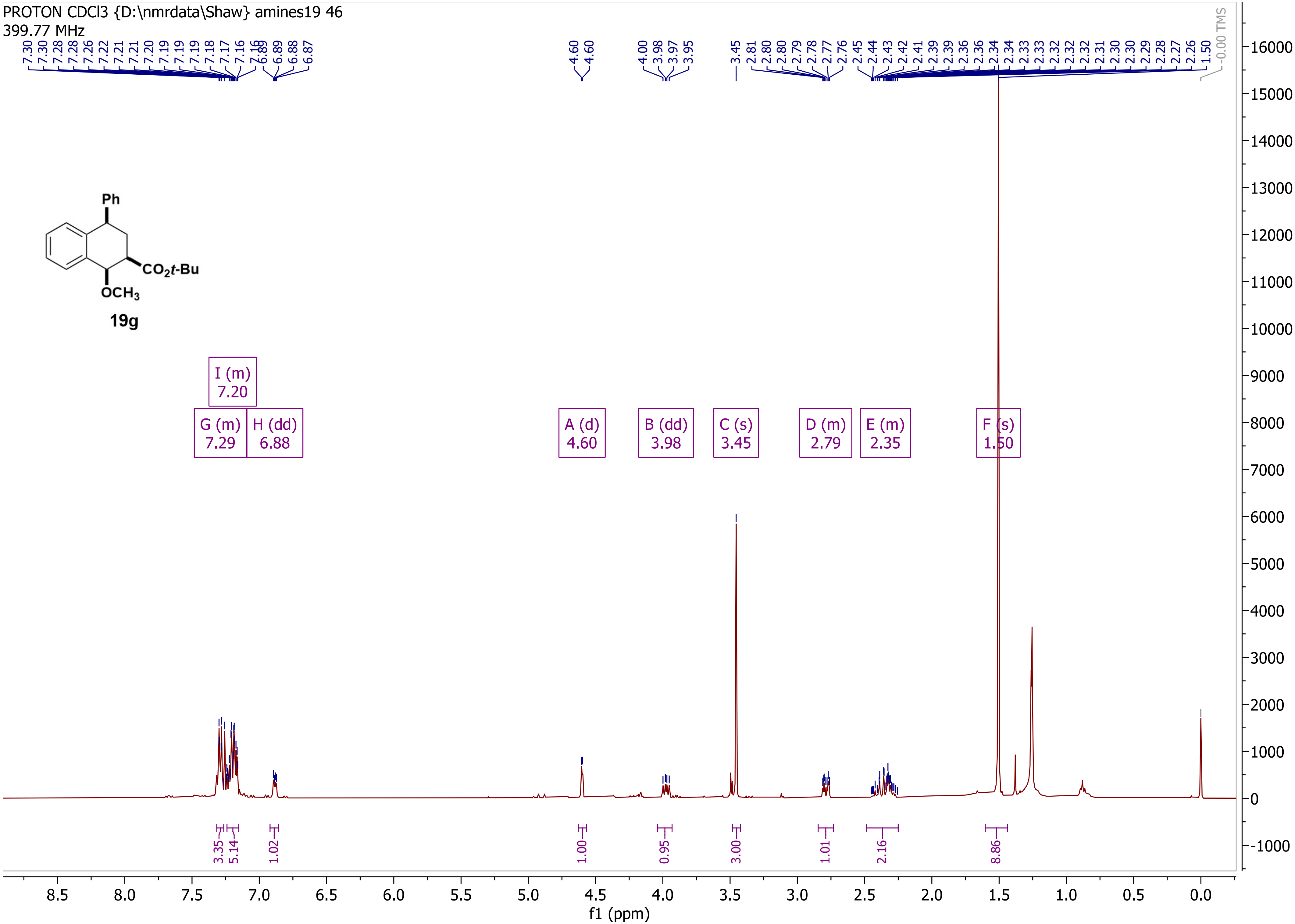


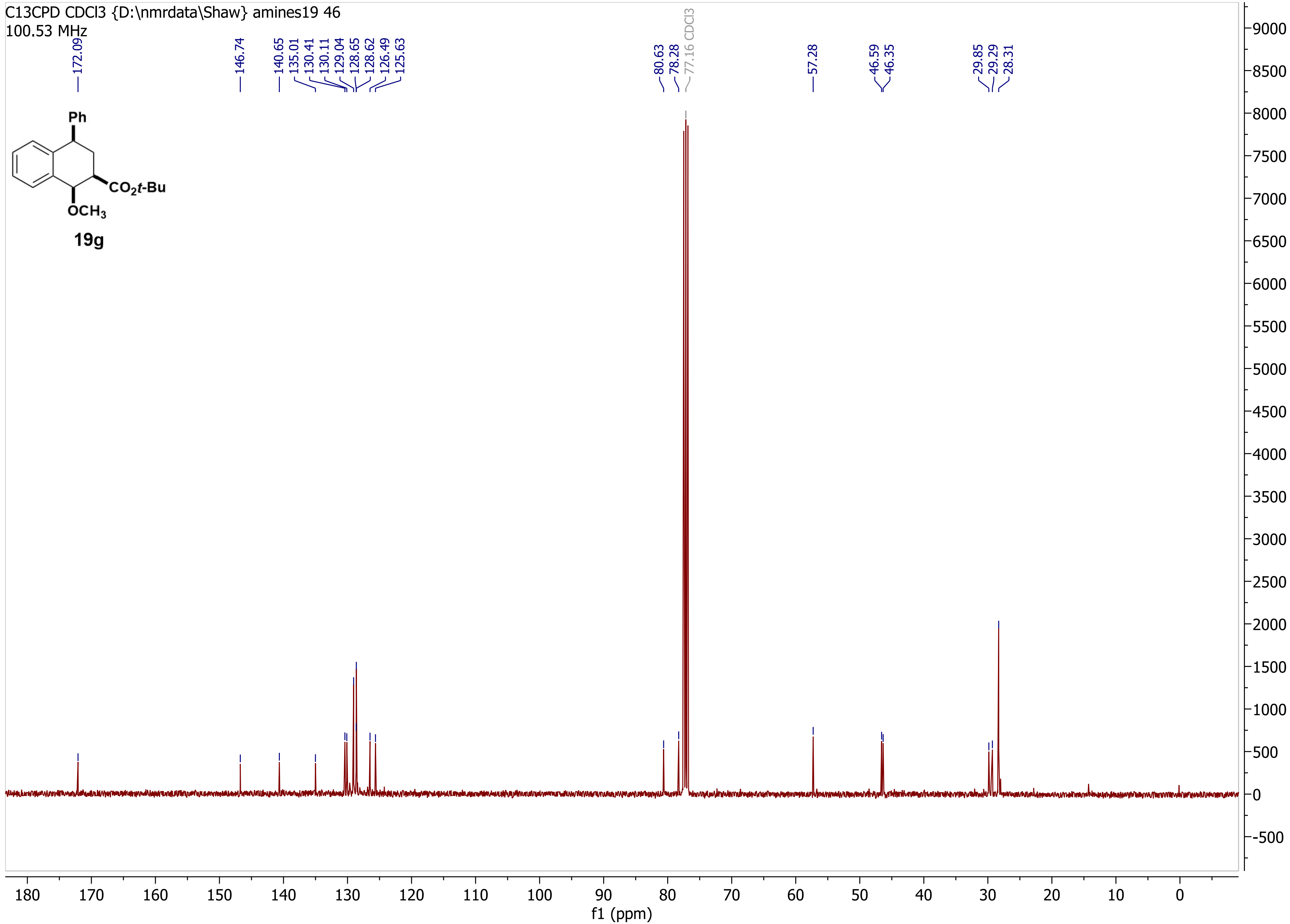
C13CPD CDCl3 {D:\nmrdata\Shaw} amines19 44
100.53 MHz
173.48
170.14
142.63
138.42
132.30
130.33
129.96
129.50
129.08
128.86
128.65
128.27
128.15
127.47
127.37
127.13
126.23
77.16 CDCl3
72.69
61.02
60.73
60.65
60.36
56.78
49.74
48.30
45.48
Ph
$CO_2CH_2CF_3$
$CO_2CH_2CF_3$
OCH_3
19e
f1 (ppm)


PROTON CDCl3 {D:\nmrdata\Shaw} amines19 2
399.77 MHz
7.48
7.46
7.46
7.31
7.31
7.30
7.30
7.29
7.29
7.28
7.28
7.27
7.26
7.26
7.25
7.25
7.24
7.24
7.23
7.22
7.17
7.16
7.16
7.15
7.14
7.14
7.14
7.12
7.12
6.87
6.86
6.85
6.85
4.80
4.77
4.76
3.73
3.71
3.69
3.68
3.55
3.54
3.52
3.51
3.50
3.41
3.37
2.93
2.88
2.63
2.61
2.58
2.57
0.00 TMS
Ph
CO2CH3
CO2CH3
CO2CH3
OCH3
19f
J (m) 7.27
I (m) 7.47
C (m) 6.86
K (ddd) 7.15
E (d) 4.77
D (s) 4.80
G (s) 3.73
F (s) 3.52
H (d) 3.70
B (d) 2.91
A (d) 2.59
0.98
4.57
3.01
1.08
0.99
1.02
2.98
3.99
3.26
1.00
1.00
f1 (ppm)

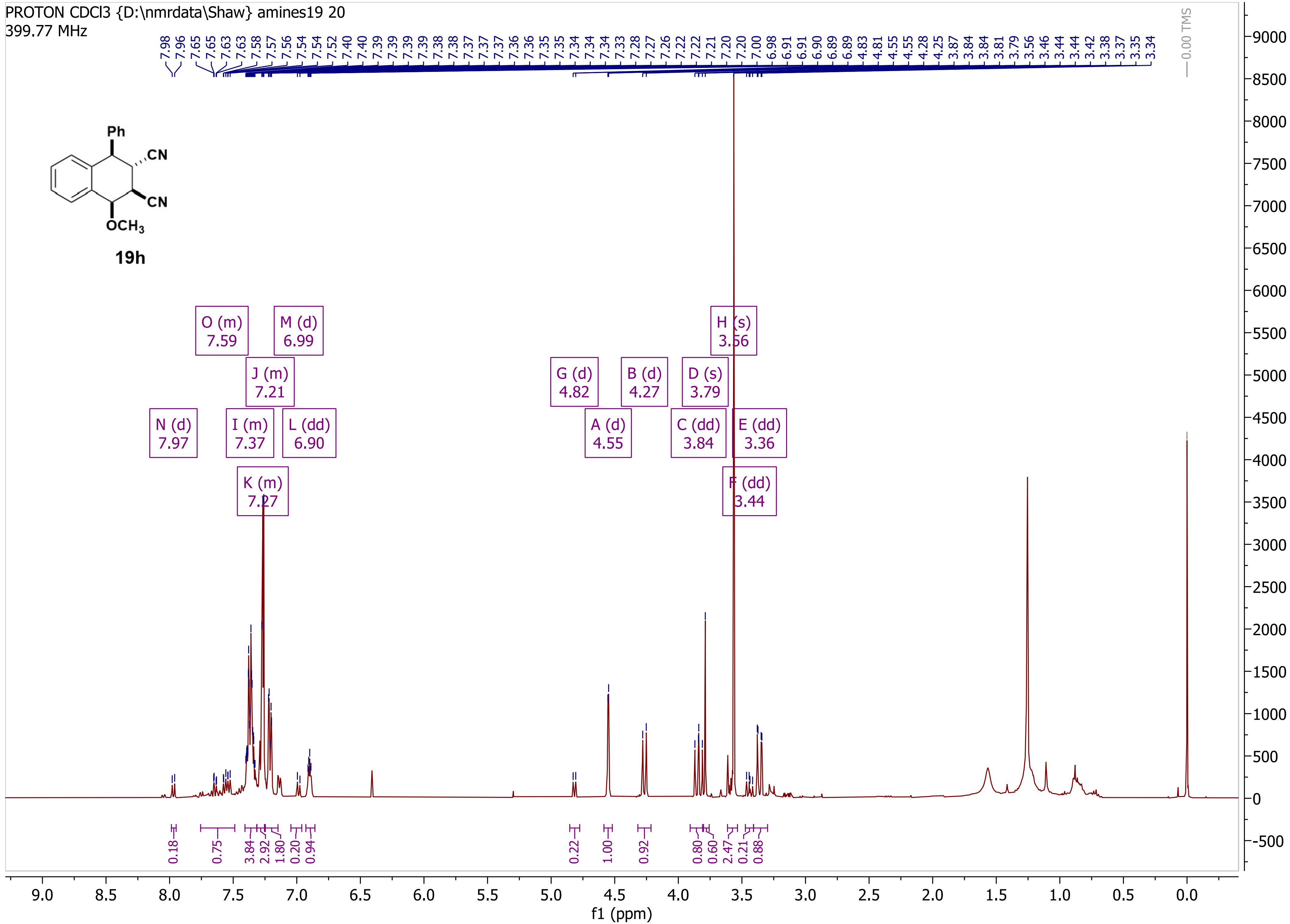
C13CPD CDCl3 {D:\nmrdata\Shaw} amines19 2
100.53 MHz



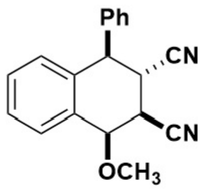

PROTON CDCl3 {D:\nmrdata\Shaw} amines19 46
399.77 MHz
Ph
CO2t-Bu
OCH3
19g
I (m) 7.20
G (m) 7.29
H (dd) 6.88
A (d) 4.60
B (dd) 3.98
C (s) 3.45
D (m) 2.79
E (m) 2.35
F (s) 1.50
3.35
5.14
1.02
1.00
0.95
3.00
1.01
2.16
8.86
-0.00 TMS
f1 (ppm)



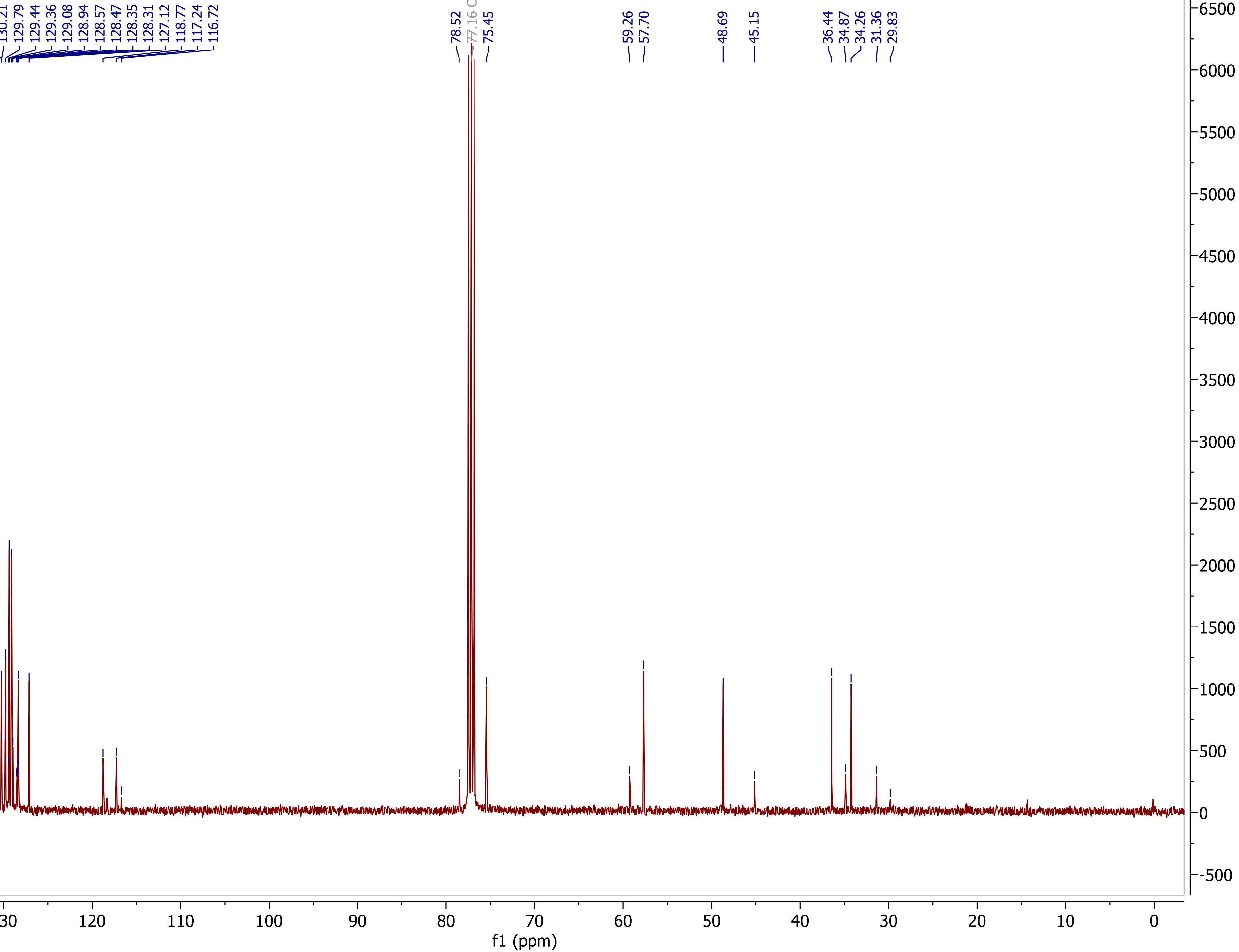
C13CPD CDCl3 {D:\nmrdata\Shaw} amines19 46
100.53 MHz
172.09
146.74
140.65
135.01
130.41
130.11
129.04
128.65
128.62
126.49
125.63
80.63
78.28
77.16 CDCl3
57.28
46.59
46.35
29.85
29.29
28.31
Ph
CO2t-Bu
OCH3
19g
9000
8500
8000
7500
7000
6500
6000
5500
5000
4500
4000
3500
3000
2500
2000
1500
1000
500
0
-500
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

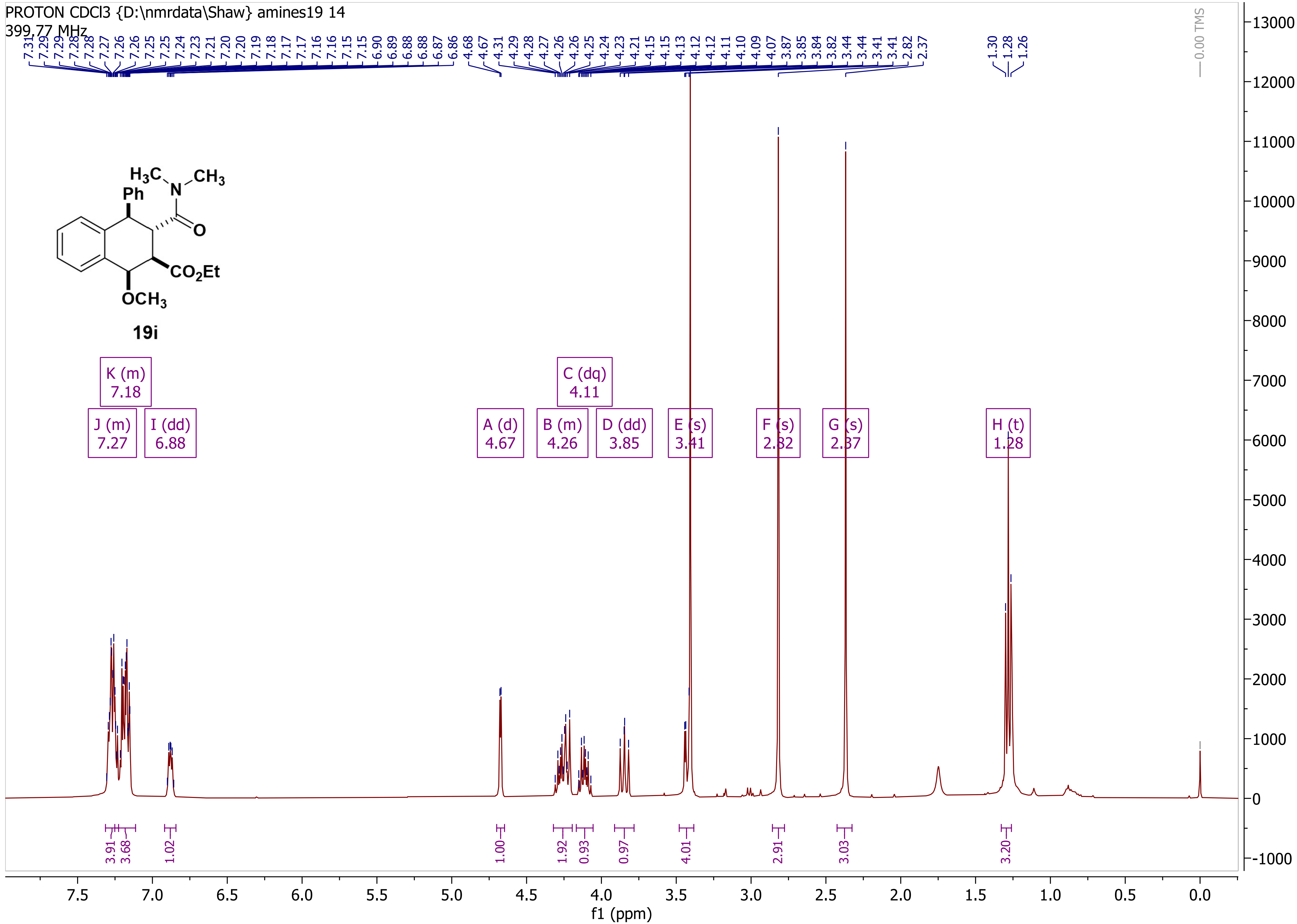

PROTON CDCl3 {D:\nmrdata\Shaw} amines19 20
399.77 MHz
7.98 7.96 7.65 7.63 7.63 7.58 7.57 7.56 7.54 7.54 7.52 7.40 7.40 7.39 7.39 7.39 7.39 7.38 7.38 7.37 7.37 7.37 7.36 7.36 7.35 7.35 7.34 7.34 7.34 7.33 7.28 7.27 7.26 7.22 7.22 7.21 7.20 7.20 7.00 6.98 6.91 6.91 6.90 6.89 6.89 4.83 4.81 4.55 4.55 4.28 4.25 3.87 3.84 3.84 3.81 3.79 3.56 3.46 3.44 3.44 3.42 3.38 3.37 3.35 3.34
0.00 TMS
Ph
CN
CN
OCH3
19h
O (m) 7.59
M (d) 6.99
H (s) 3.56
J (m) 7.21
G (d) 4.82
B (d) 4.27
D (s) 3.79
N (d) 7.97
I (m) 7.37
L (dd) 6.90
A (d) 4.55
C (dd) 3.84
E (dd) 3.36
K (m) 7.27
F (dd) 3.44
0.18 0.75 3.84 2.92 1.80 0.20 0.94 0.22 1.00 0.92 0.80 0.60 2.47 0.21 0.88
f1 (ppm)

C13CPD CDCl3 {D:\nmrdata\Shaw} amines19 44
100.53 MHz

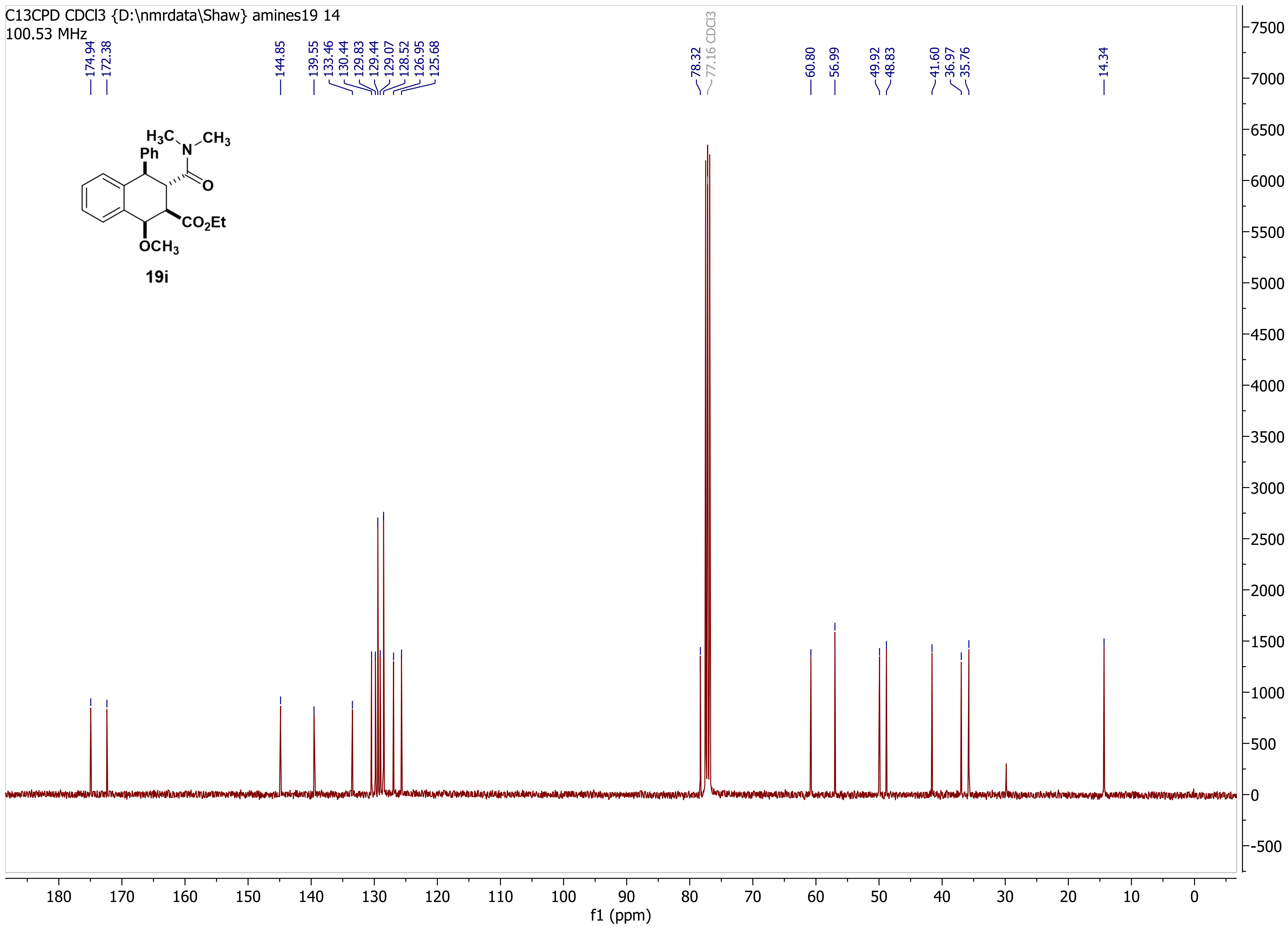


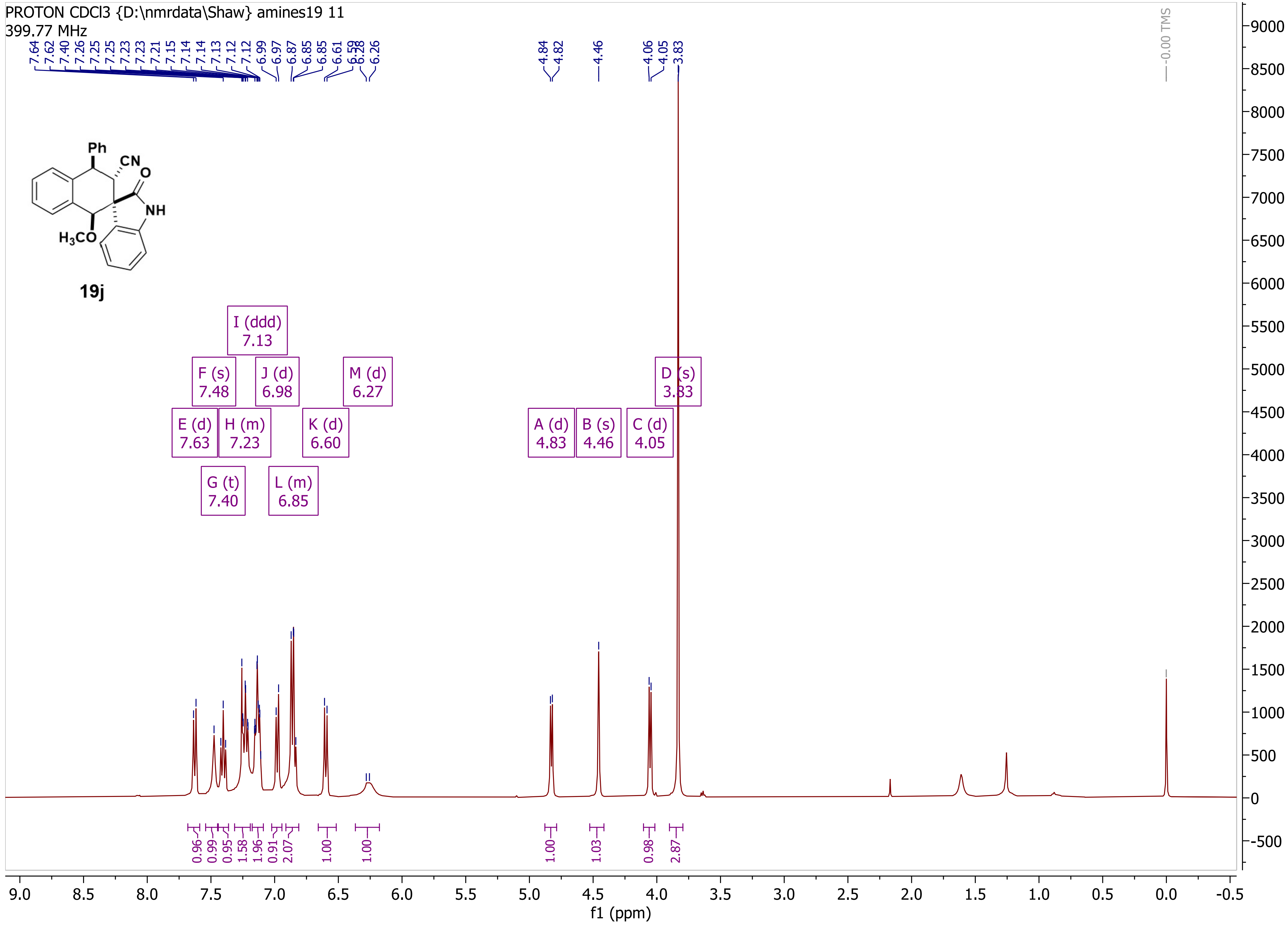
19h

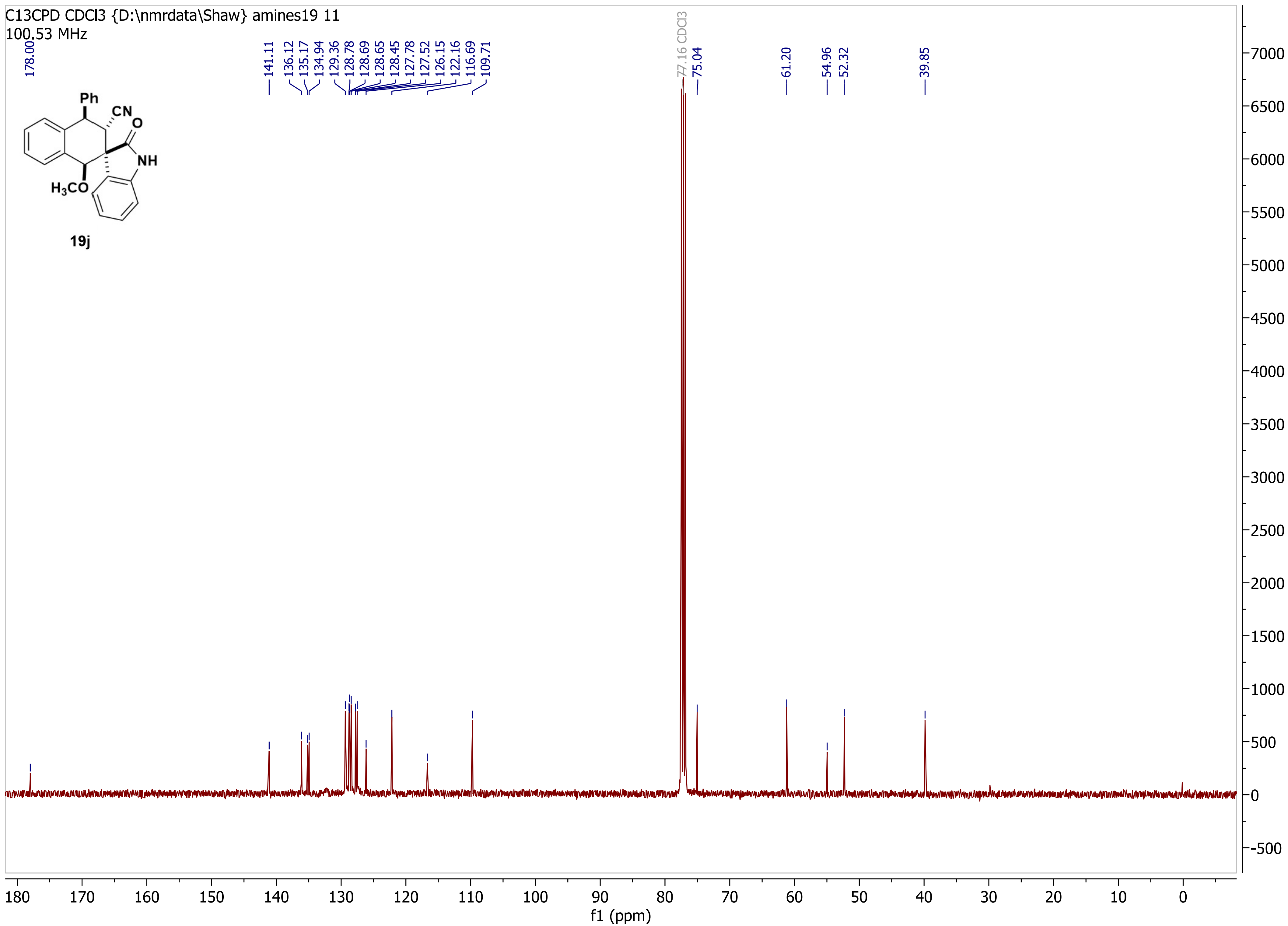




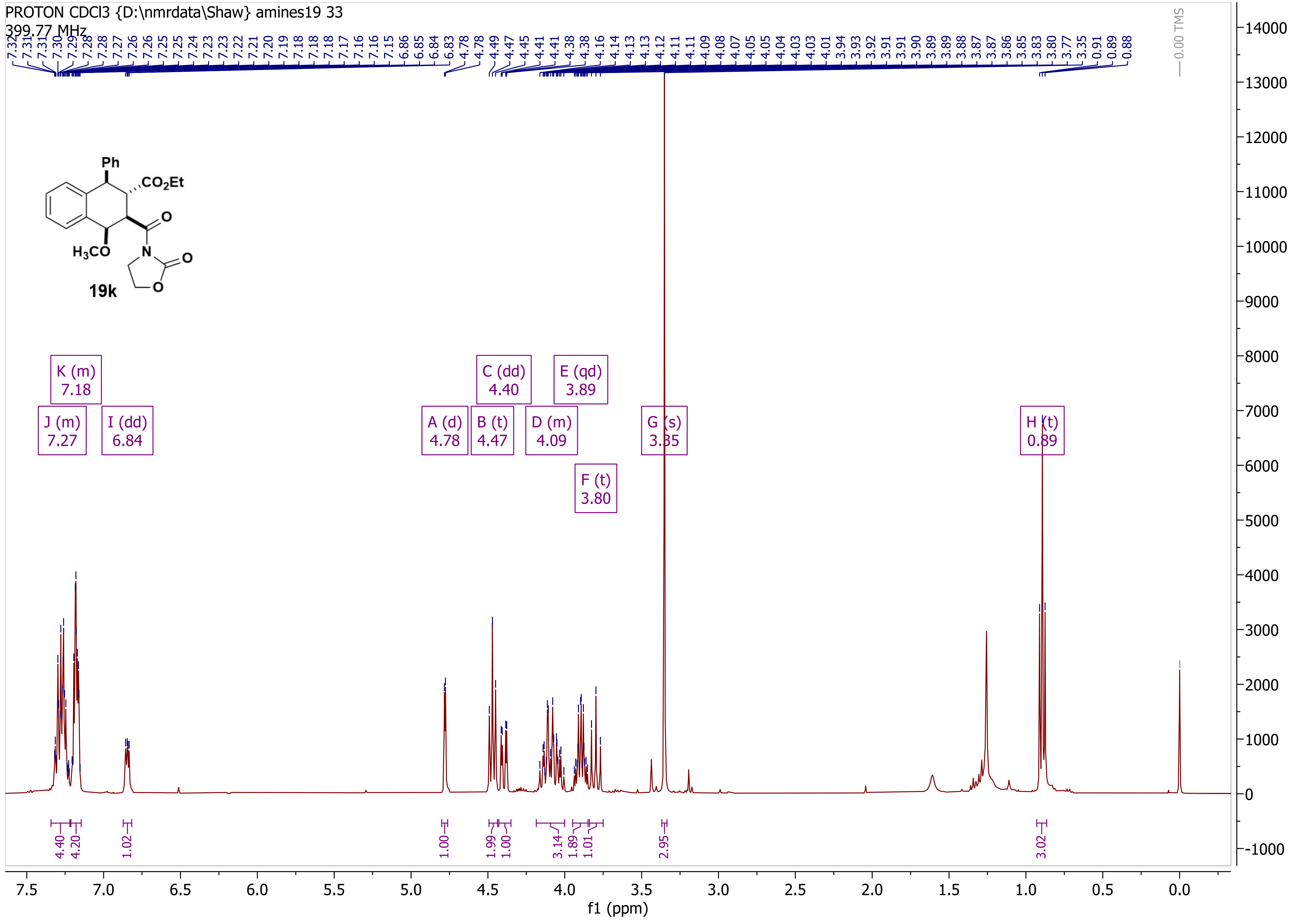
PROTON CDCl3 {D:\nmrdata\Shaw} amines19 14
399.77 MHz
7.31 7.29 7.29 7.28 7.28 7.27 7.26 7.26 7.25 7.25 7.24 7.23 7.21 7.20 7.20 7.19 7.18 7.17 7.17 7.16 7.16 7.15 7.15 6.90 6.89 6.88 6.88 6.87 6.86 4.68 4.67 4.31 4.29 4.28 4.27 4.26 4.26 4.25 4.24 4.23 4.21 4.15 4.15 4.13 4.12 4.12 4.11 4.10 4.09 4.07 3.87 3.85 3.84 3.82 3.44 3.44 3.41 3.41 2.82 2.37
1.30 1.28 1.26
0.00 TMS
H3C N CH3 Ph O CO2Et OCH3
19i
K (m) 7.18
C (dq) 4.11
J (m) 7.27
I (dd) 6.88
A (d) 4.67
B (m) 4.26
D (dd) 3.85
E (s) 3.41
F (s) 2.82
G (s) 2.37
H (t) 1.28
3.91 3.68 1.02 1.00 1.92 0.93 0.97 4.01 2.91 3.03 3.20
13000 12000 11000 10000 9000 8000 7000 6000 5000 4000 3000 2000 1000 0 -1000
7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

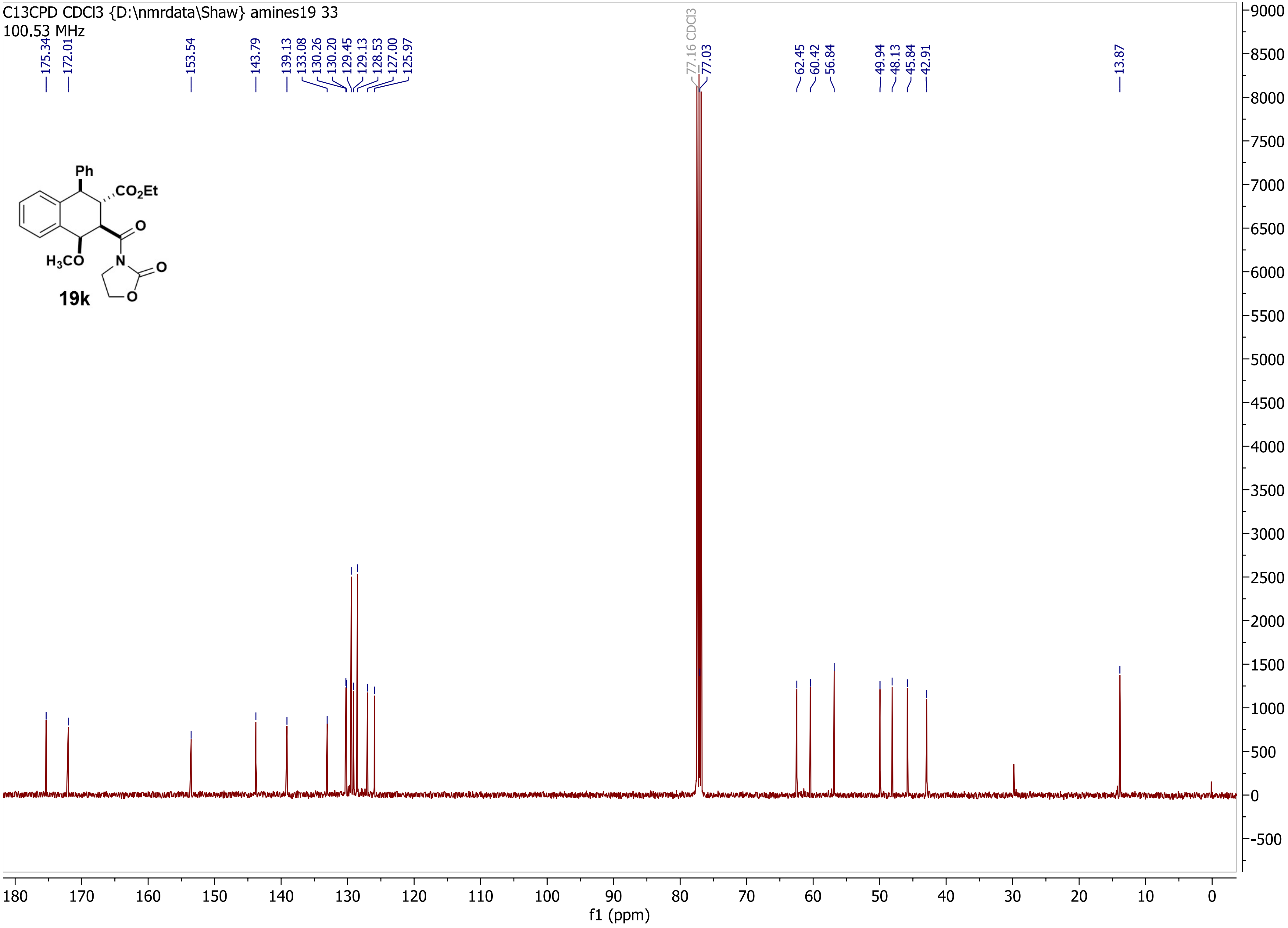

C13CPD CDCl3 {D:\nmrdata\Shaw} amines19 14
100.53 MHz
174.94
172.38
144.85
139.55
133.46
130.44
129.83
129.44
129.07
128.52
126.95
125.68
78.32
77.16 CDCl3
60.80
56.99
49.92
48.83
41.60
36.97
35.76
14.34
Ph
H_3C
N
CH_3
O
CO_2Et
OCH_3
19i
f1 (ppm)


PROTON CDCl3 {D:\nmrdata\Shaw} amines19 11
399.77 MHz
7.64 7.62 7.40 7.26 7.25 7.25 7.23 7.23 7.21 7.15 7.14 7.14 7.13 7.12 7.12 6.99 6.97 6.87 6.85 6.85 6.61 6.59 6.28 6.26
4.84 4.82
4.46
4.06 4.05 3.83
-0.00 TMS
Ph
CN
O
NH
H3CO
19j
I (ddd) 7.13
F (s) 7.48
J (d) 6.98
M (d) 6.27
D (s) 3.83
E (d) 7.63
H (m) 7.23
K (d) 6.60
A (d) 4.83
B (s) 4.46
C (d) 4.05
G (t) 7.40
L (m) 6.85
0.96 0.99 0.95 1.58 1.96 0.91 2.07 1.00 1.00 1.00 1.03 0.98 2.87
f1 (ppm)

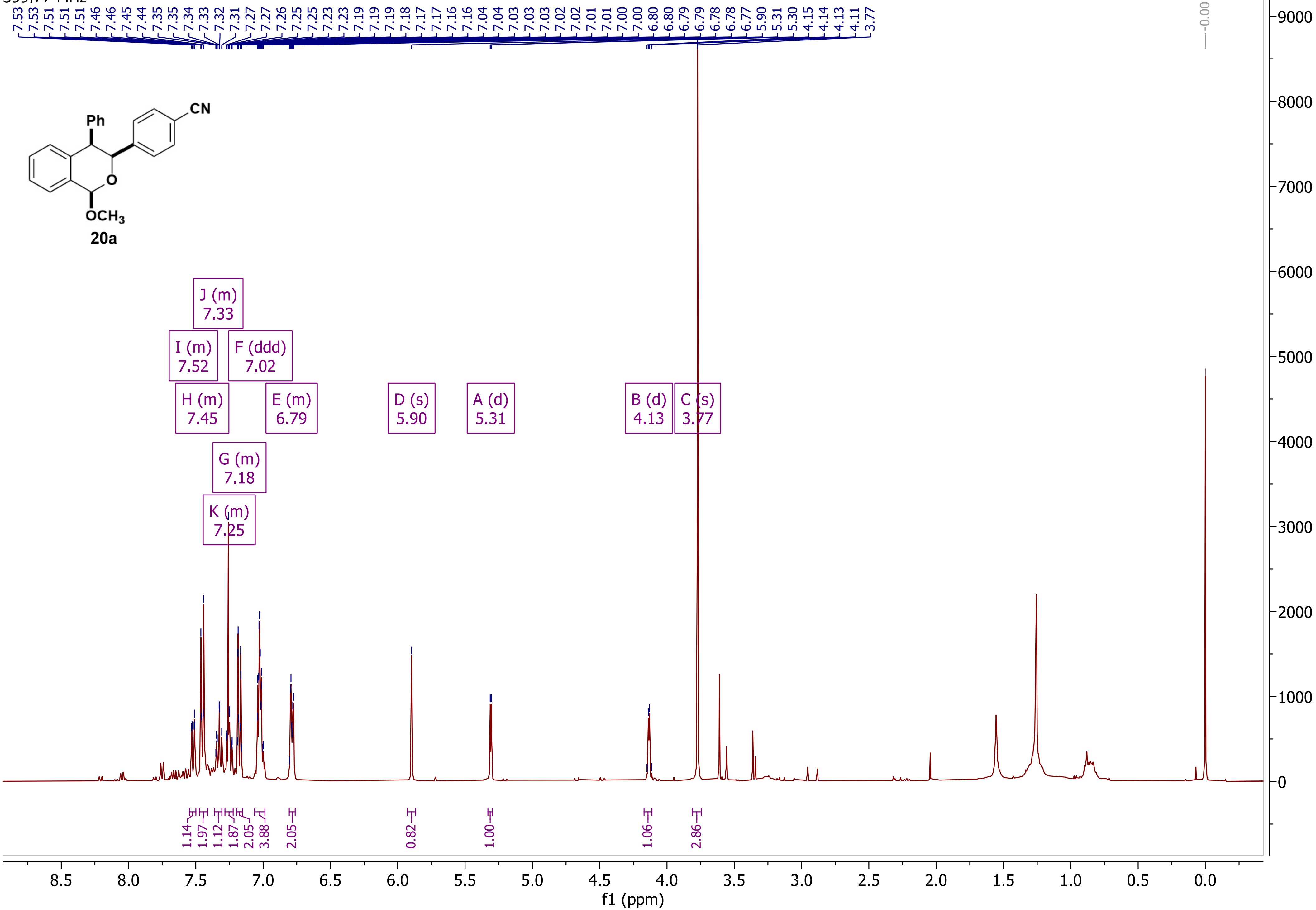


C13CPD CDCl3 {D:\nmrdata\Shaw} amines19 11
100.53 MHz
178.00
141.11
136.12
135.17
134.94
129.36
128.78
128.69
128.65
128.45
127.78
127.52
126.15
122.16
116.69
109.71
77.16 CDCl3
75.04
61.20
54.96
52.32
39.85
Ph
CN
O
NH
H_3CO
19j
f1 (ppm)

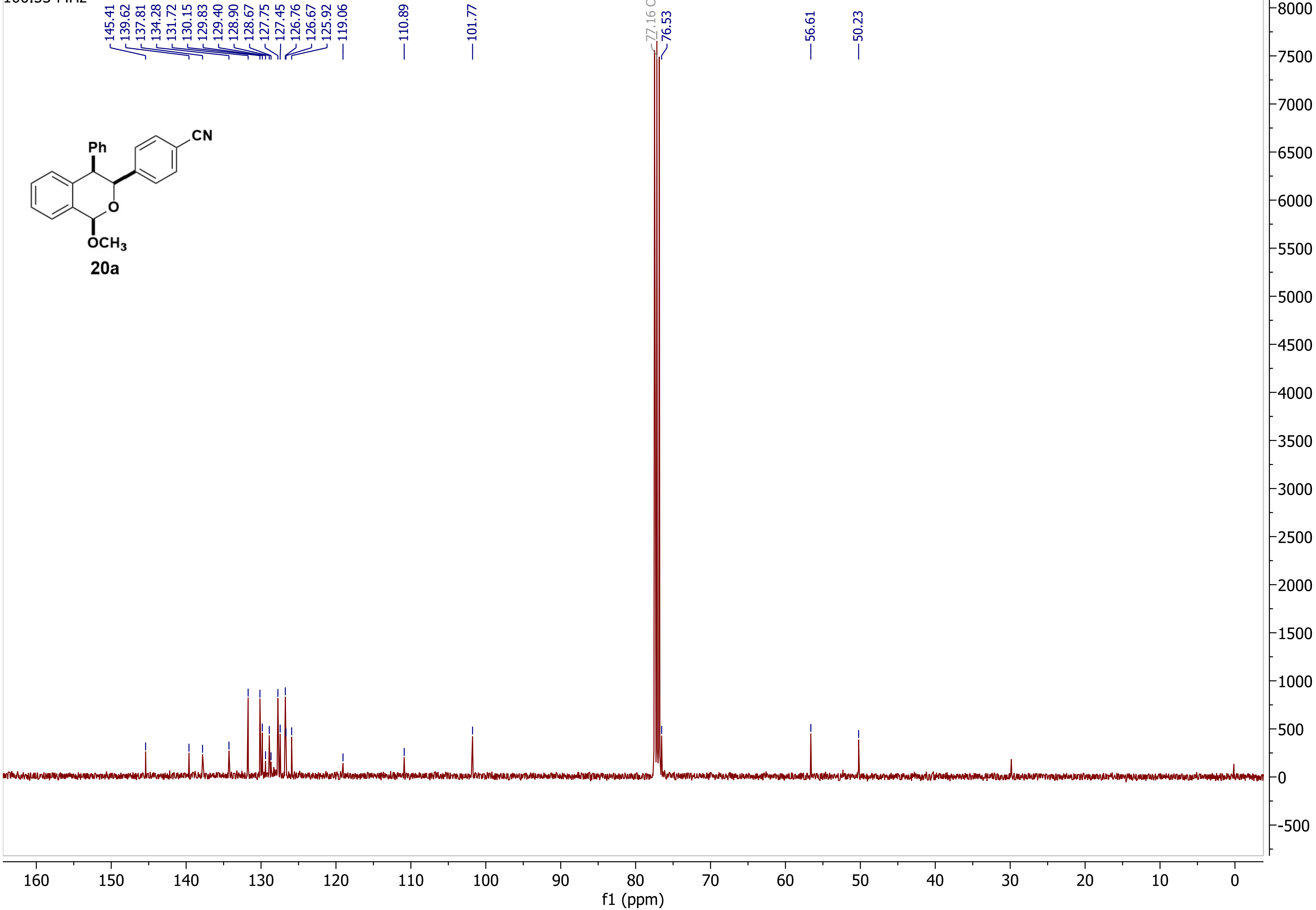

PROTON CDCl3 {D:\nmrdata\Shaw} amines19 33
399.77 MHz
7.32 7.31 7.31 7.30 7.29 7.28 7.28 7.27 7.26 7.26 7.25 7.25 7.24 7.23 7.23 7.22 7.21 7.20 7.19 7.18 7.18 7.18 7.17 7.16 7.16 7.15 6.86 6.85 6.84 6.83 4.78 4.78 4.49 4.47 4.45 4.41 4.41 4.38 4.38 4.16 4.14 4.13 4.13 4.12 4.11 4.11 4.09 4.08 4.07 4.05 4.05 4.04 4.03 4.03 4.01 3.94 3.93 3.92 3.91 3.91 3.90 3.89 3.89 3.88 3.87 3.87 3.86 3.85 3.83 3.80 3.77 3.35 0.91 0.89 0.88
0.00 TMS
Ph
CO2Et
O
H3CO
N
O
O
19k
K (m) 7.18
C (dd) 4.40
E (qd) 3.89
J (m) 7.27
I (dd) 6.84
A (d) 4.78
B (t) 4.47
D (m) 4.09
G (s) 3.35
H (t) 0.89
F (t) 3.80
4.40 4.20 1.02 1.00 1.99 1.00 3.14 1.89 1.01 2.95 3.02
14000 13000 12000 11000 10000 9000 8000 7000 6000 5000 4000 3000 2000 1000 0 -1000
7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)


C13CPD CDCl3 {D:\nmrdata\Shaw} amines19 33
100.53 MHz
175.34
172.01
153.54
143.79
139.13
133.08
130.26
130.20
129.45
129.13
128.53
127.00
125.97
77.16 CDCl3
77.03
62.45
60.42
56.84
49.94
48.13
45.84
42.91
13.87
Ph
CO2Et
O
N
O
O
H3CO
19k
f1 (ppm)

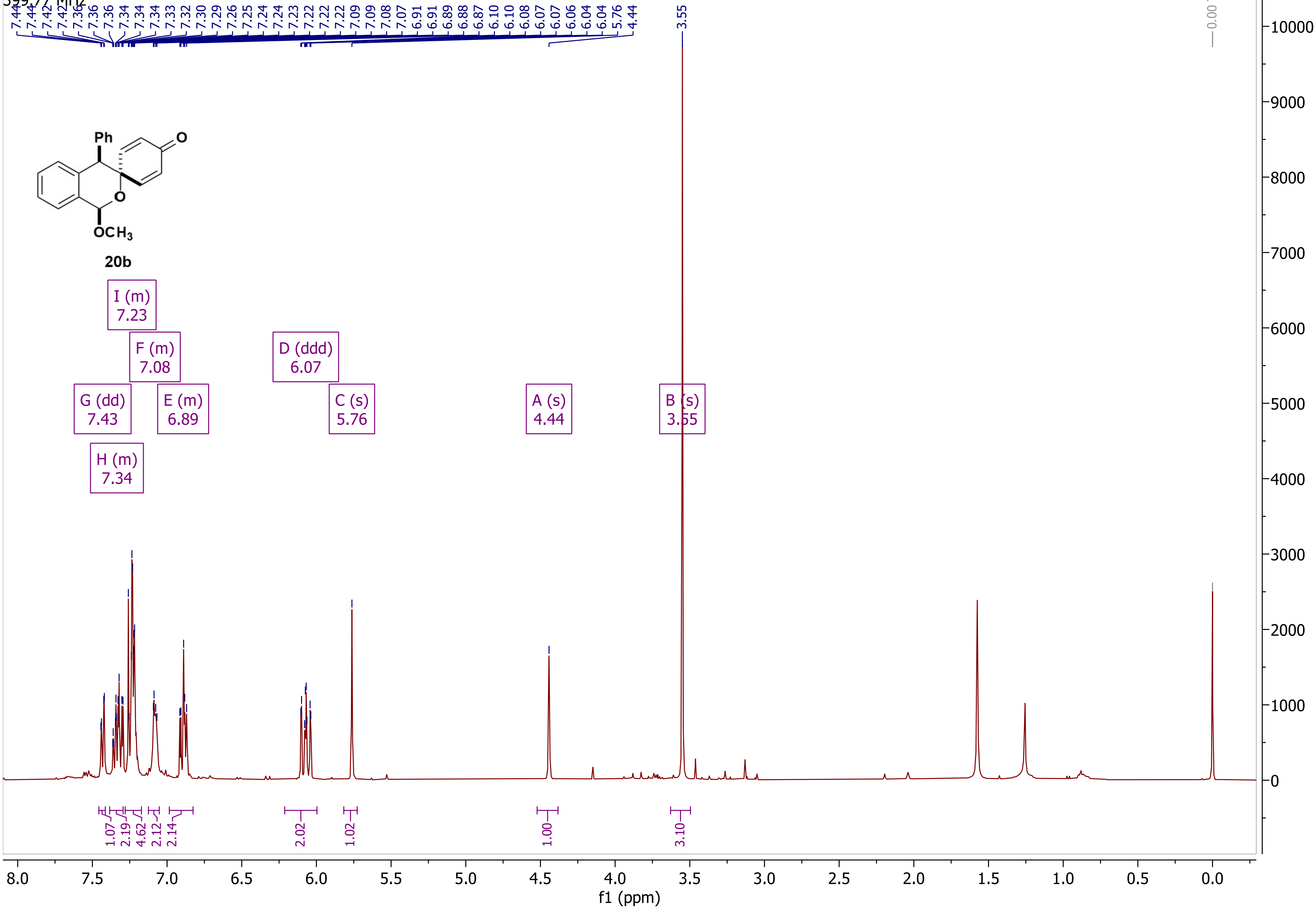
PROTON CDCl3 {D:\nmrdata\Shaw} amines19 36
399.77 MHz



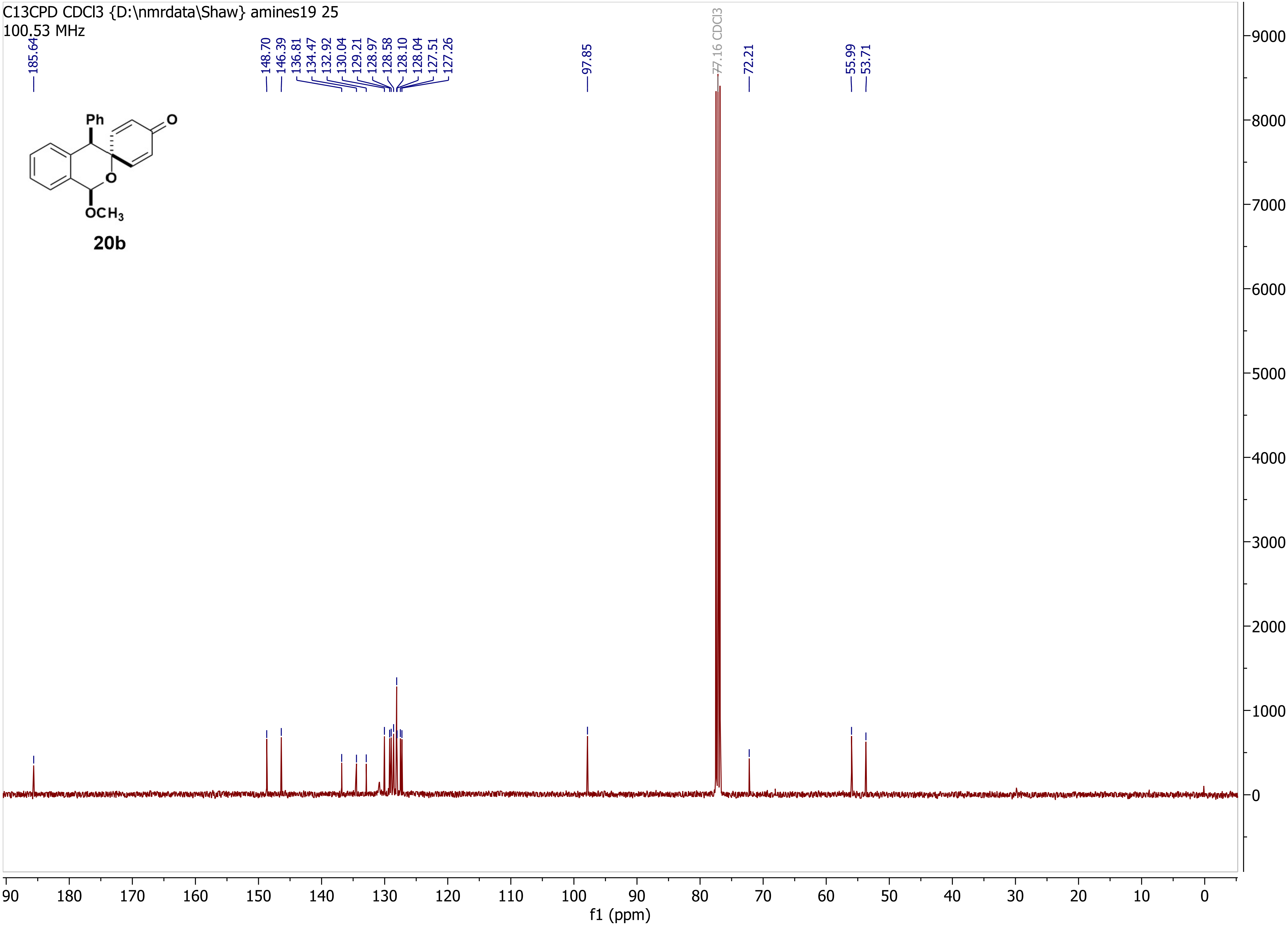
C13CPD CDCl3 {D:\nmrdata\Shaw} amines19 36
100.53 MHz

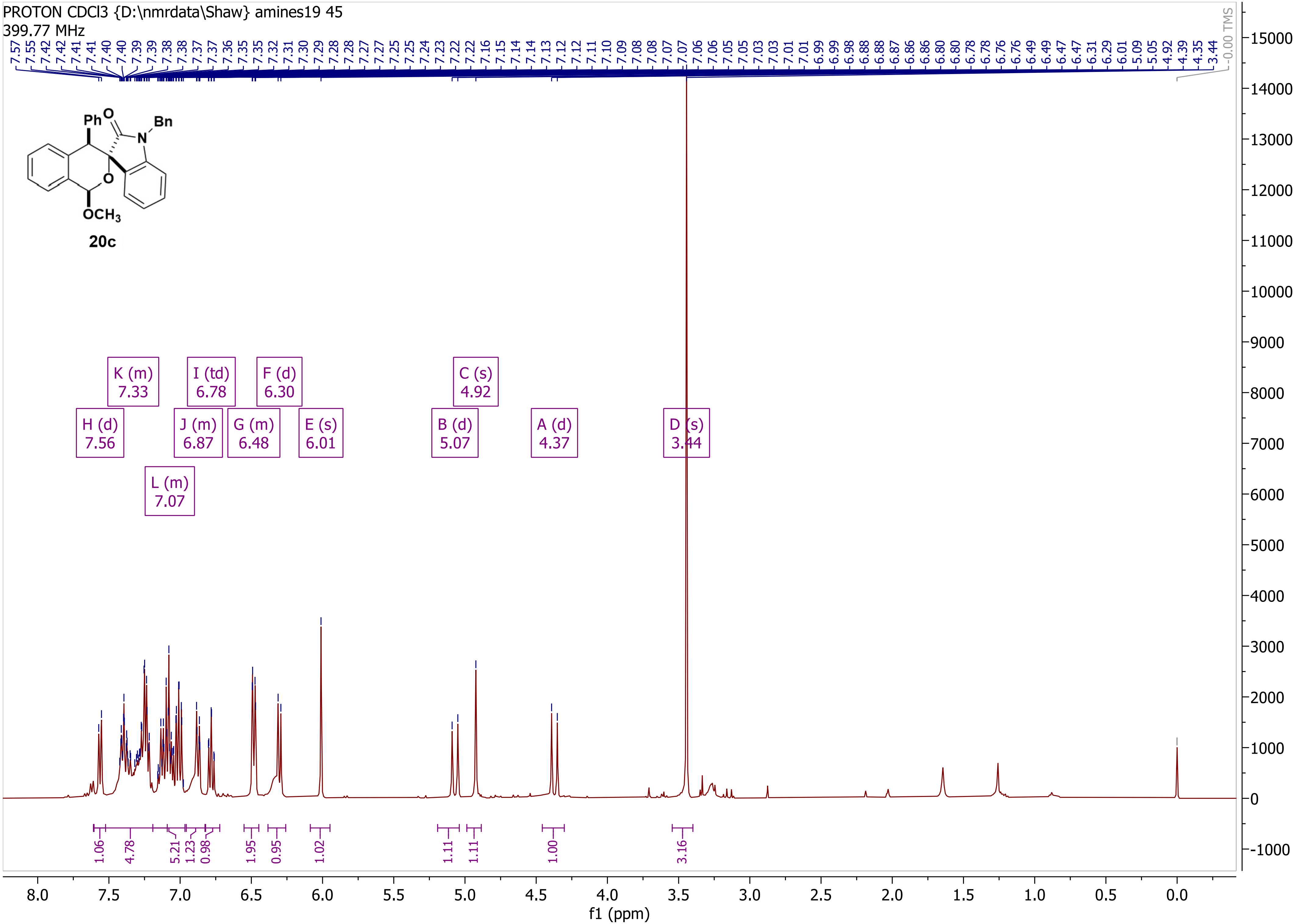


PROTON CDCl3 {D:\nmrdata\Shaw} amines19 25
399.77 MHz



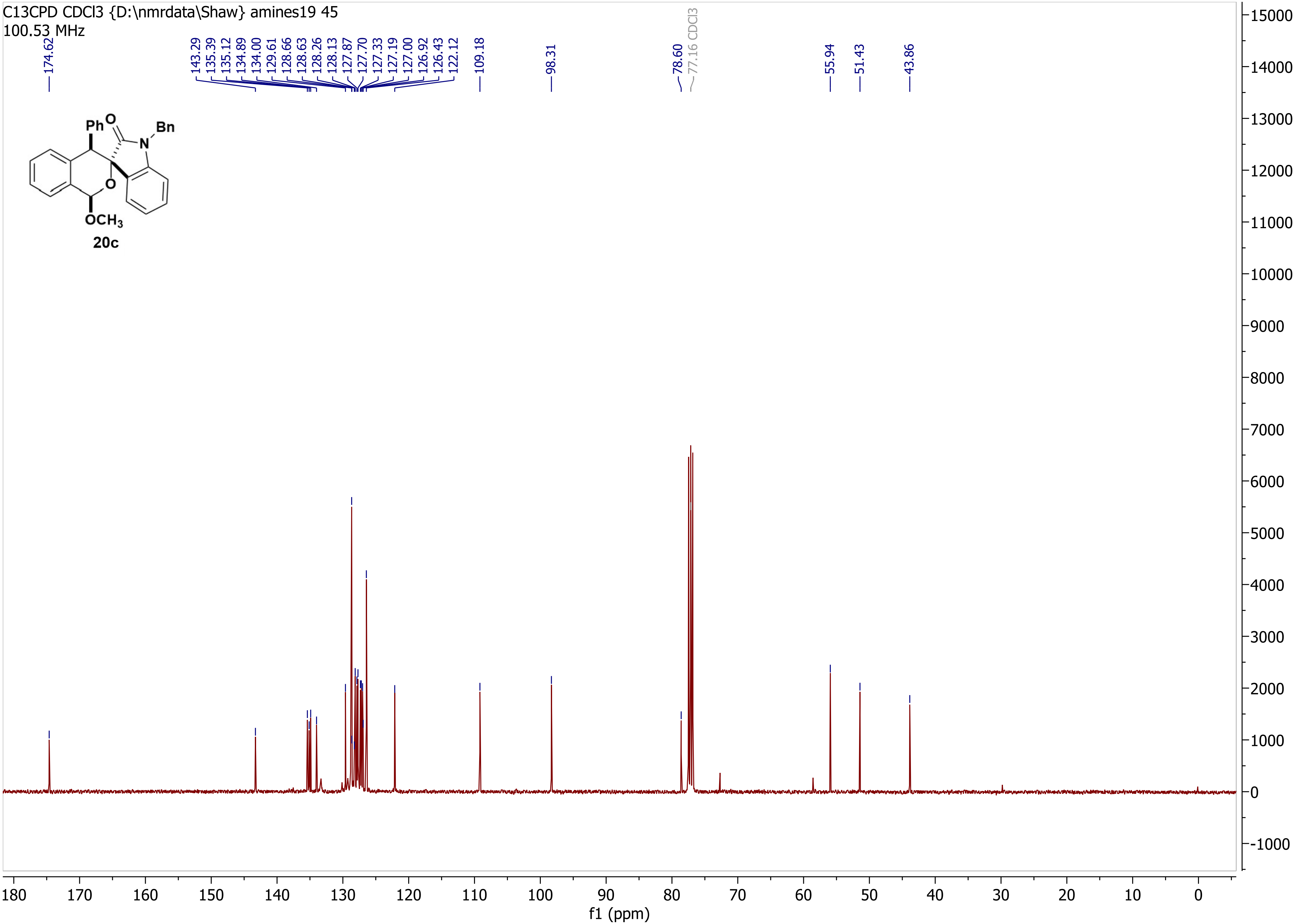
C13CPD CDCl3 {D:\nmrdata\Shaw} amines19 25
100.53 MHz

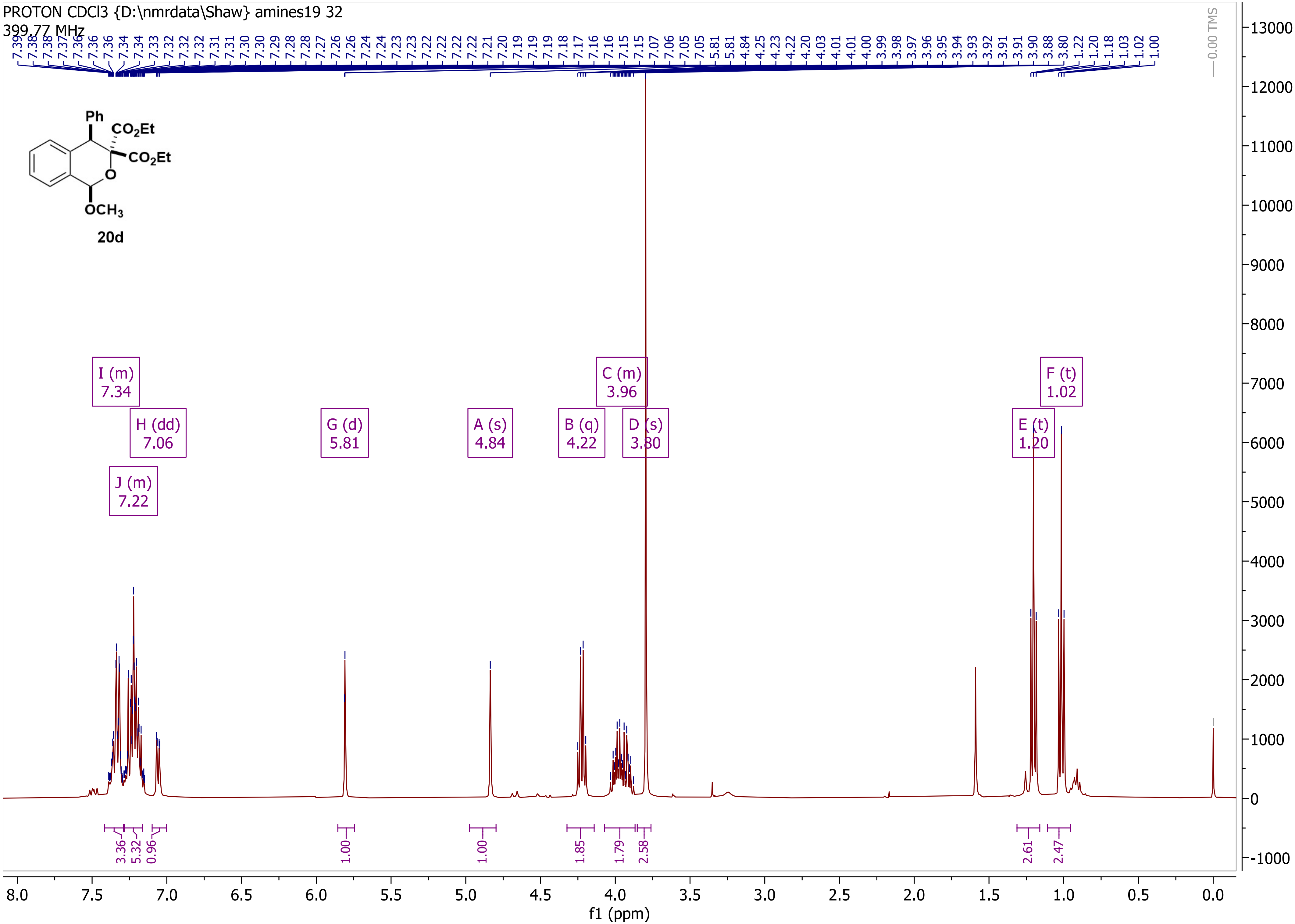


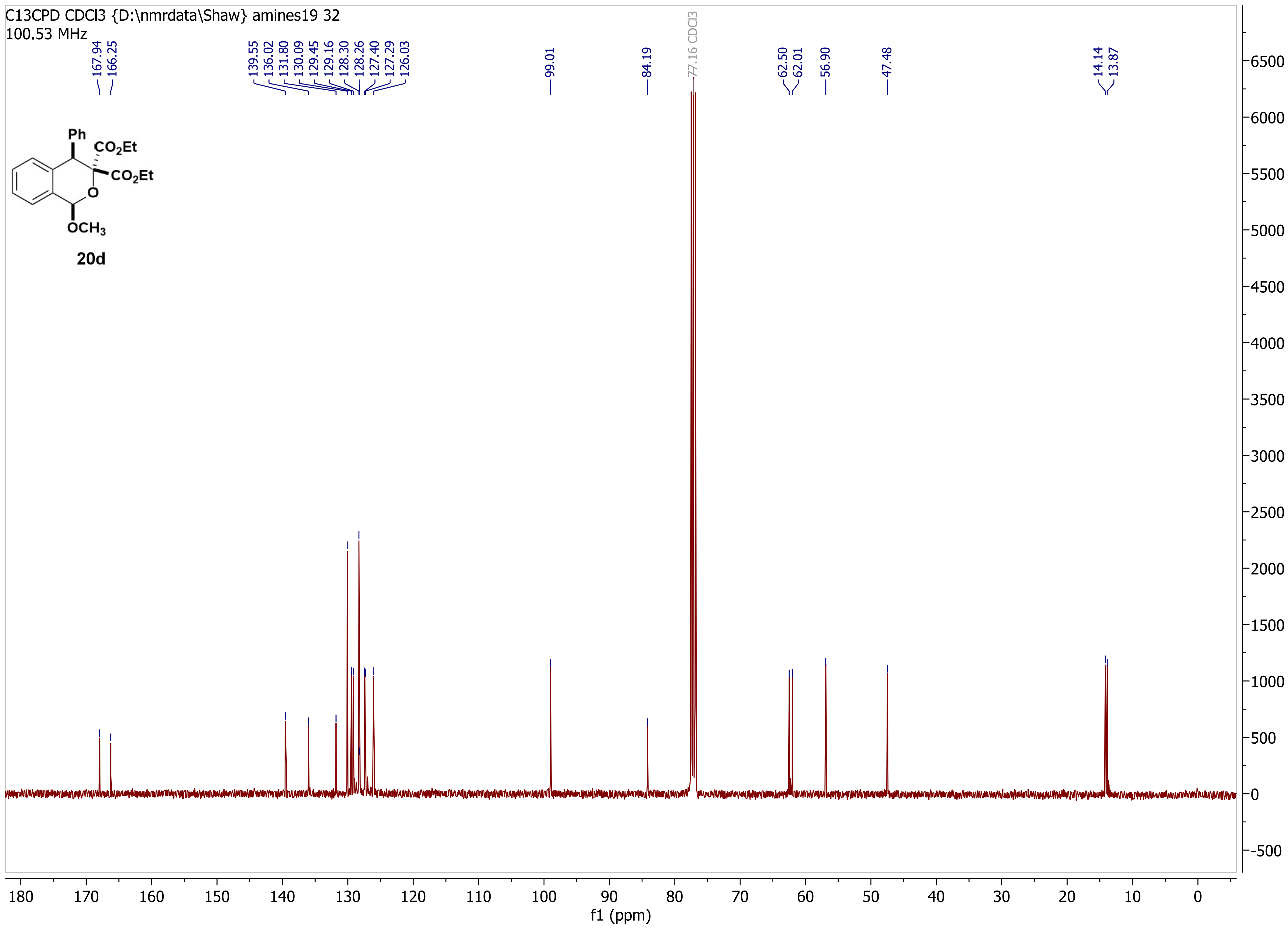


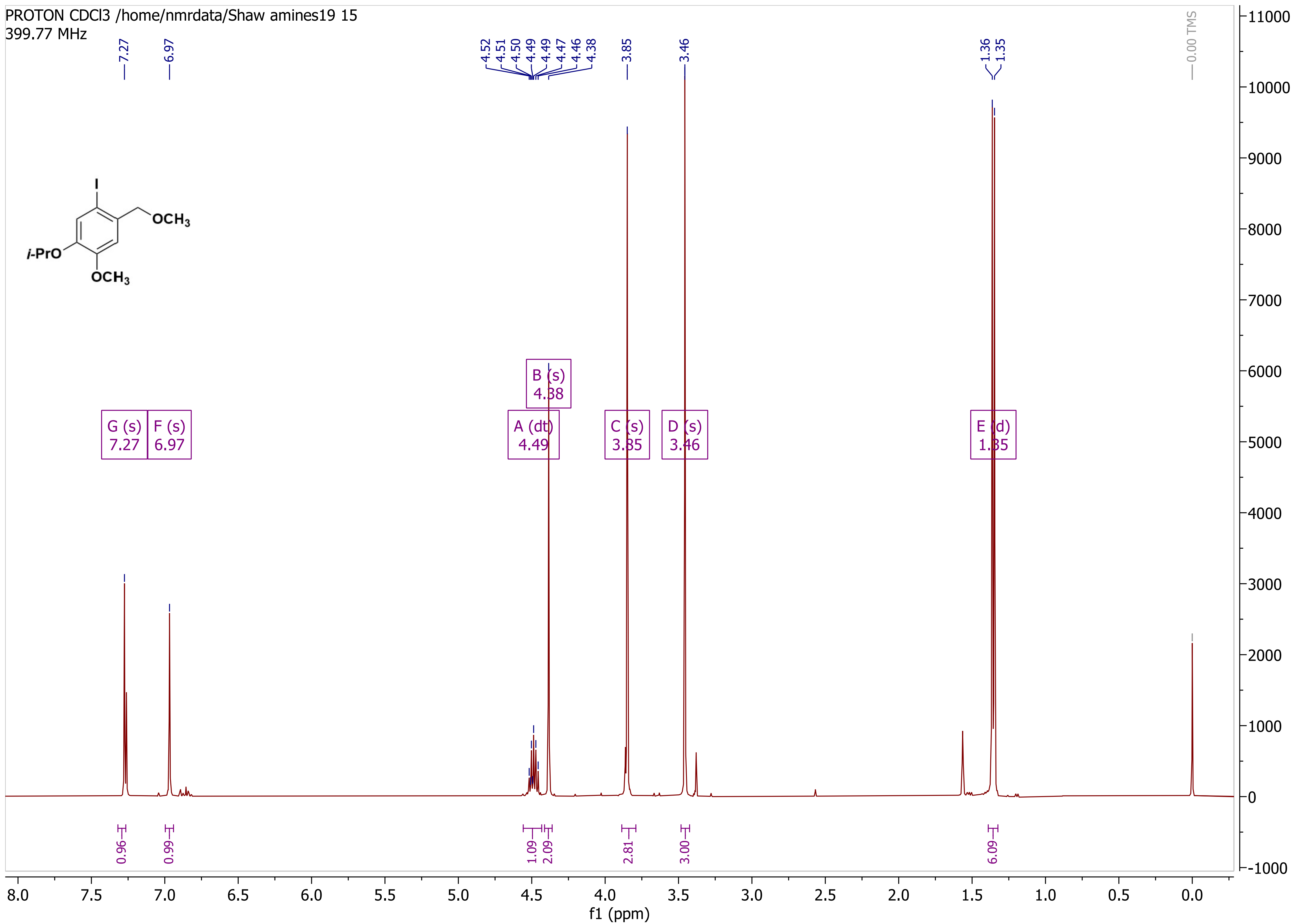
PROTON CDCl3 {D:\nmrdata\Shaw} amines19 45
399.77 MHz
7.57 7.55 7.42 7.42 7.41 7.41 7.40 7.40 7.39 7.39 7.38 7.38 7.37 7.37 7.36 7.35 7.35 7.32 7.31 7.30 7.29 7.28 7.28 7.27 7.27 7.25 7.25 7.24 7.23 7.22 7.22 7.16 7.15 7.14 7.14 7.13 7.12 7.12 7.11 7.10 7.09 7.08 7.08 7.07 7.07 7.06 7.06 7.05 7.05 7.03 7.03 7.01 7.01 6.99 6.99 6.98 6.88 6.88 6.87 6.86 6.86 6.80 6.80 6.78 6.78 6.76 6.76 6.49 6.49 6.47 6.47 6.31 6.29 6.01 5.09 5.05 4.92 4.39 4.35 3.44
0.00 TMS
Ph
O
N
Bn
O
OCH3
20c
K (m) 7.33
I (td) 6.78
F (d) 6.30
C (s) 4.92
H (d) 7.56
J (m) 6.87
G (m) 6.48
E (s) 6.01
B (d) 5.07
A (d) 4.37
D (s) 3.44
L (m) 7.07
1.06
4.78
5.21
1.23
0.98
1.95
0.95
1.02
1.11
1.11
1.00
3.16
8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)
15000 14000 13000 12000 11000 10000 9000 8000 7000 6000 5000 4000 3000 2000 1000 0 -1000

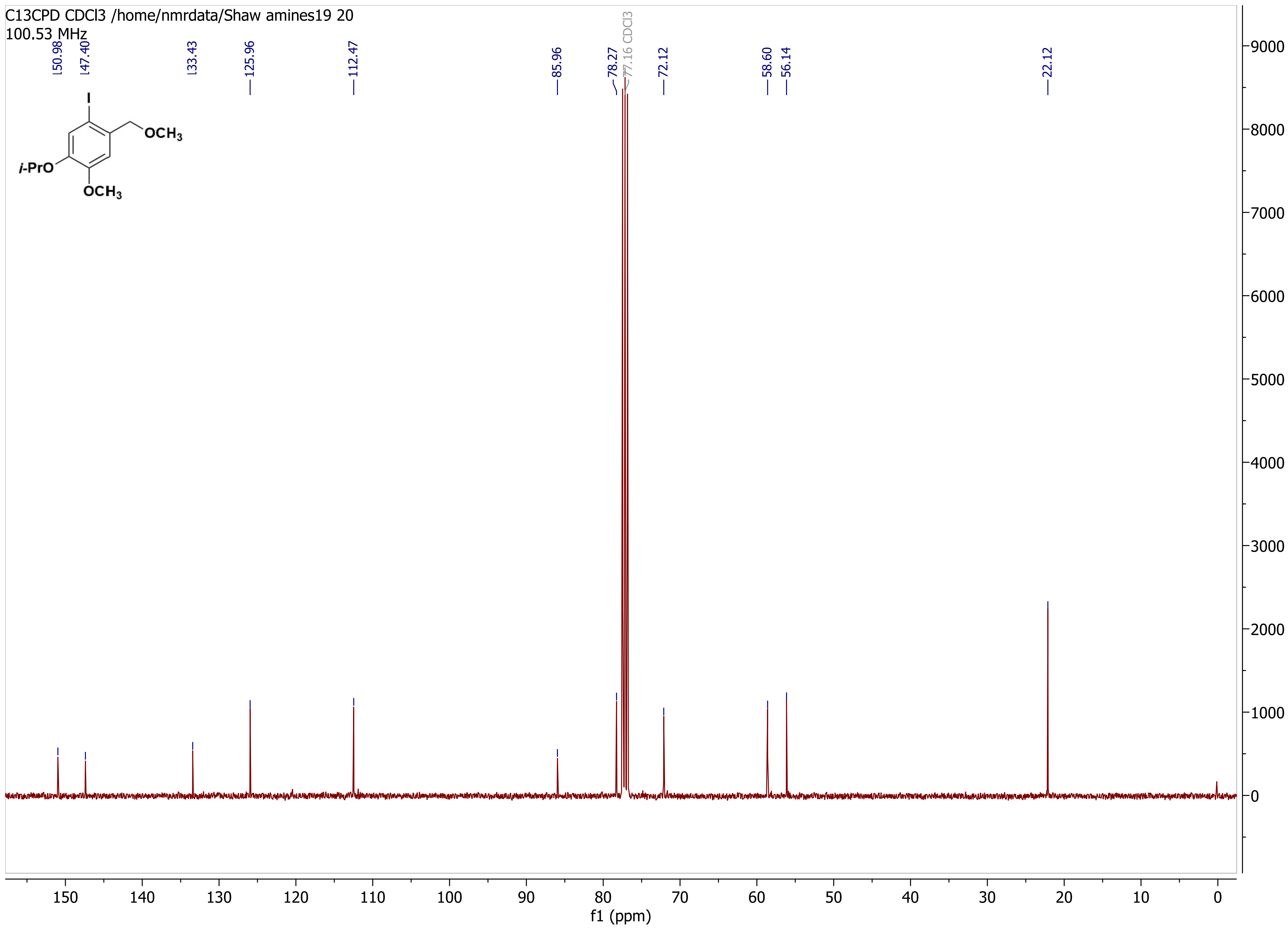
C13CPD CDCl3 {D:\nmrdata\Shaw} amines19 45
100.53 MHz



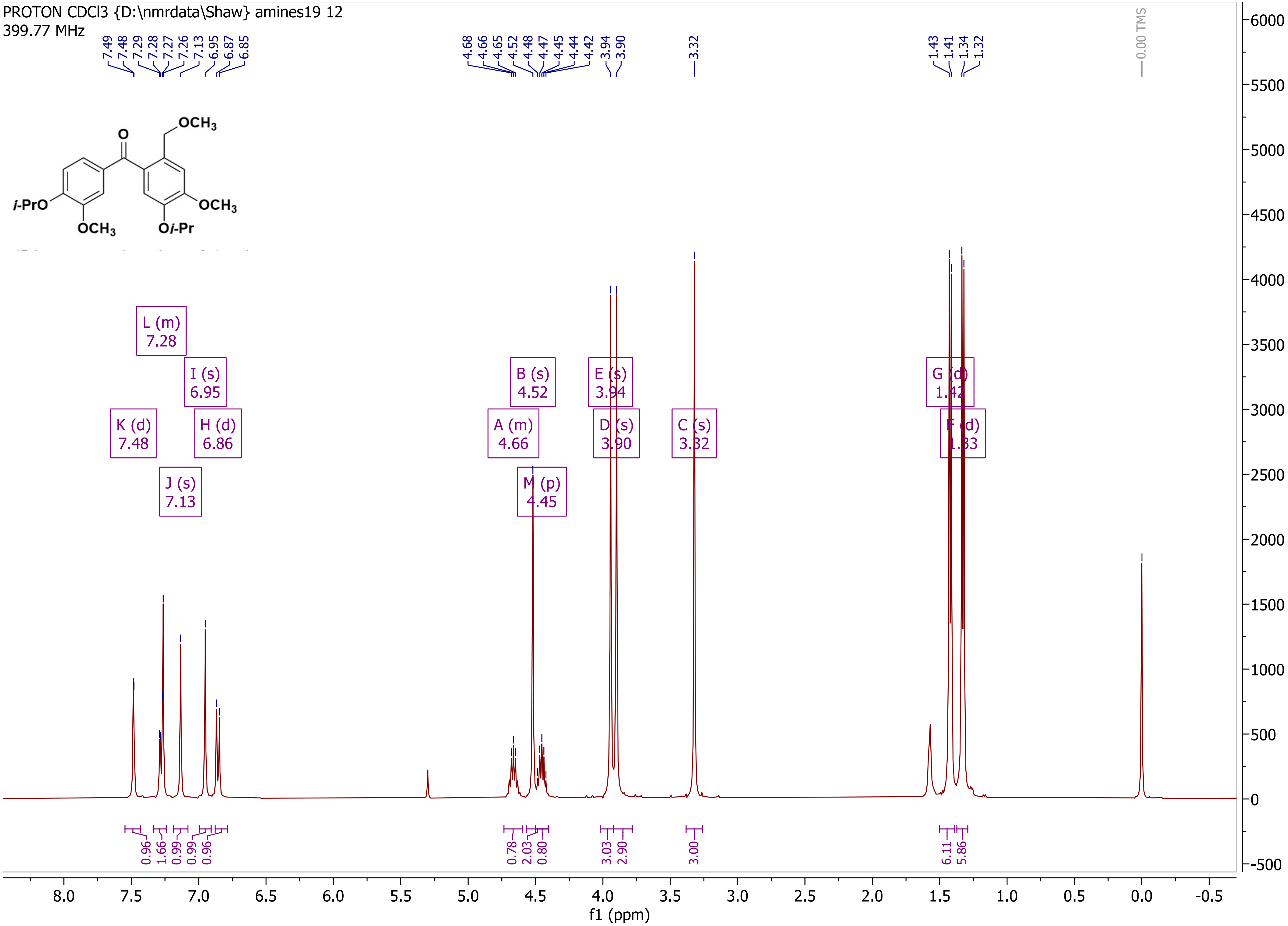

PROTON CDCl3 {D:\nmrdata\Shaw} amines19 32
399.77 MHz
7.39 7.38 7.38 7.37 7.36 7.36 7.36 7.34 7.34 7.33 7.32 7.32 7.32 7.31 7.31 7.30 7.30 7.29 7.28 7.28 7.27 7.26 7.26 7.24 7.24 7.23 7.23 7.22 7.22 7.22 7.22 7.21 7.20 7.19 7.19 7.18 7.17 7.16 7.15 7.15 7.07 7.06 7.05 7.05 5.81 5.81 4.84 4.25 4.23 4.22 4.20 4.03 4.01 4.01 4.00 3.99 3.98 3.97 3.96 3.95 3.94 3.93 3.92 3.91 3.91 3.90 3.88 3.80 1.22 1.20 1.18 1.03 1.02 1.00
0.00 TMS
Ph
CO2Et
CO2Et
O
OCH3
20d
I (m) 7.34
H (dd) 7.06
J (m) 7.22
G (d) 5.81
A (s) 4.84
B (q) 4.22
C (m) 3.96
D (s) 3.80
E (t) 1.20
F (t) 1.02
3.36
5.32
0.96
1.00
1.00
1.85
1.79
2.58
2.61
2.47
f1 (ppm)


C13CPD CDCl3 {D:\nmrdata\Shaw} amines19 32
100.53 MHz
167.94
166.25
139.55
136.02
131.80
130.09
129.45
129.16
128.30
128.26
127.40
127.29
126.03
99.01
84.19
77.16 CDCl3
62.50
62.01
56.90
47.48
14.14
13.87
Ph
CO2Et
CO2Et
O
OCH3
20d
f1 (ppm)

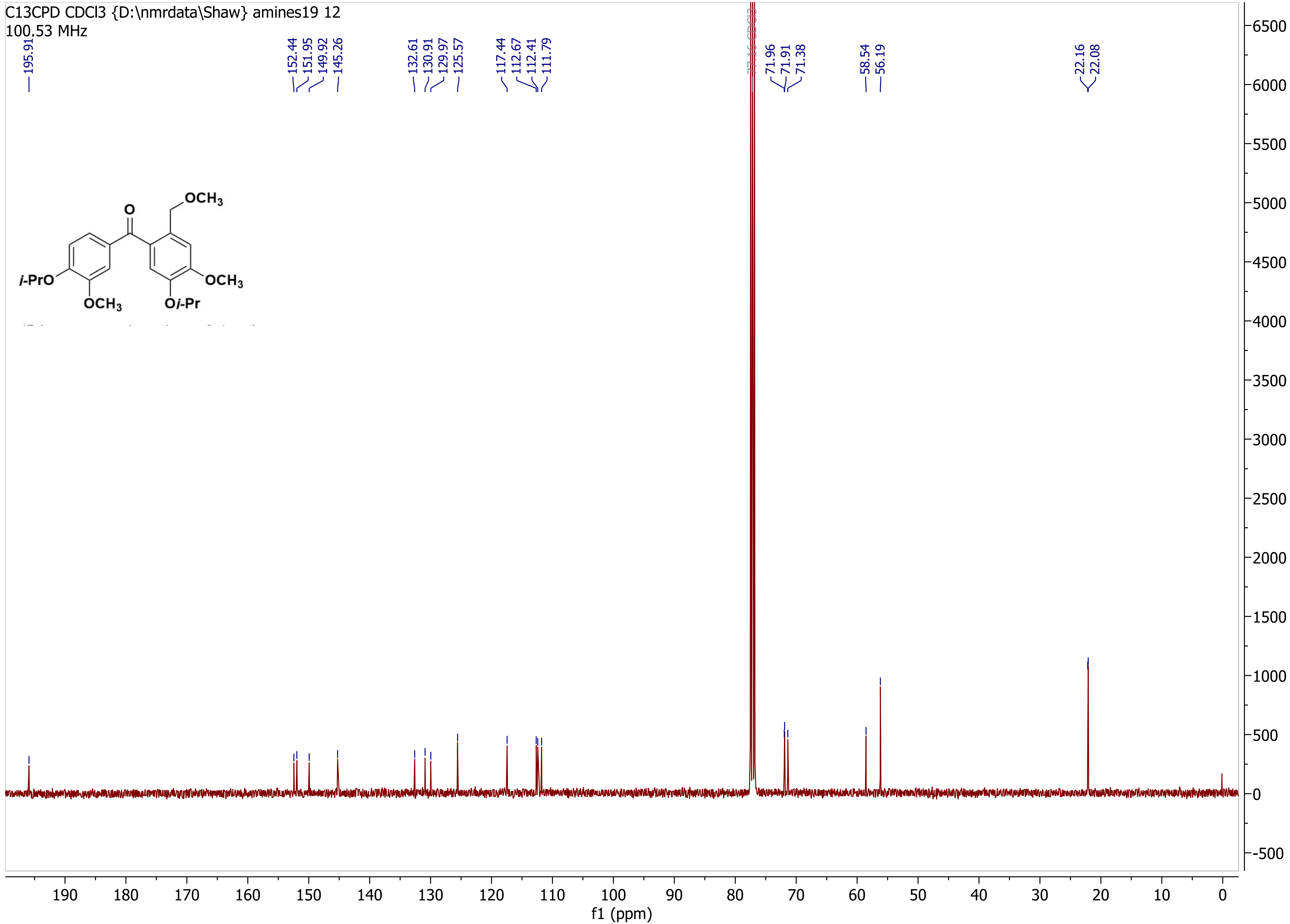

PROTON CDCl3 /home/nmrdata/Shaw amines19 15
399.77 MHz
7.27
6.97
4.52
4.51
4.50
4.49
4.49
4.47
4.46
4.38
3.85
3.46
1.36
1.35
0.00 TMS
I
OCH3
i-PrO
OCH3
G (s) 7.27
F (s) 6.97
B (s) 4.38
A (dt) 4.49
C (s) 3.85
D (s) 3.46
E (d) 1.35
0.96
0.99
1.09
2.09
2.81
3.00
6.09
f1 (ppm)

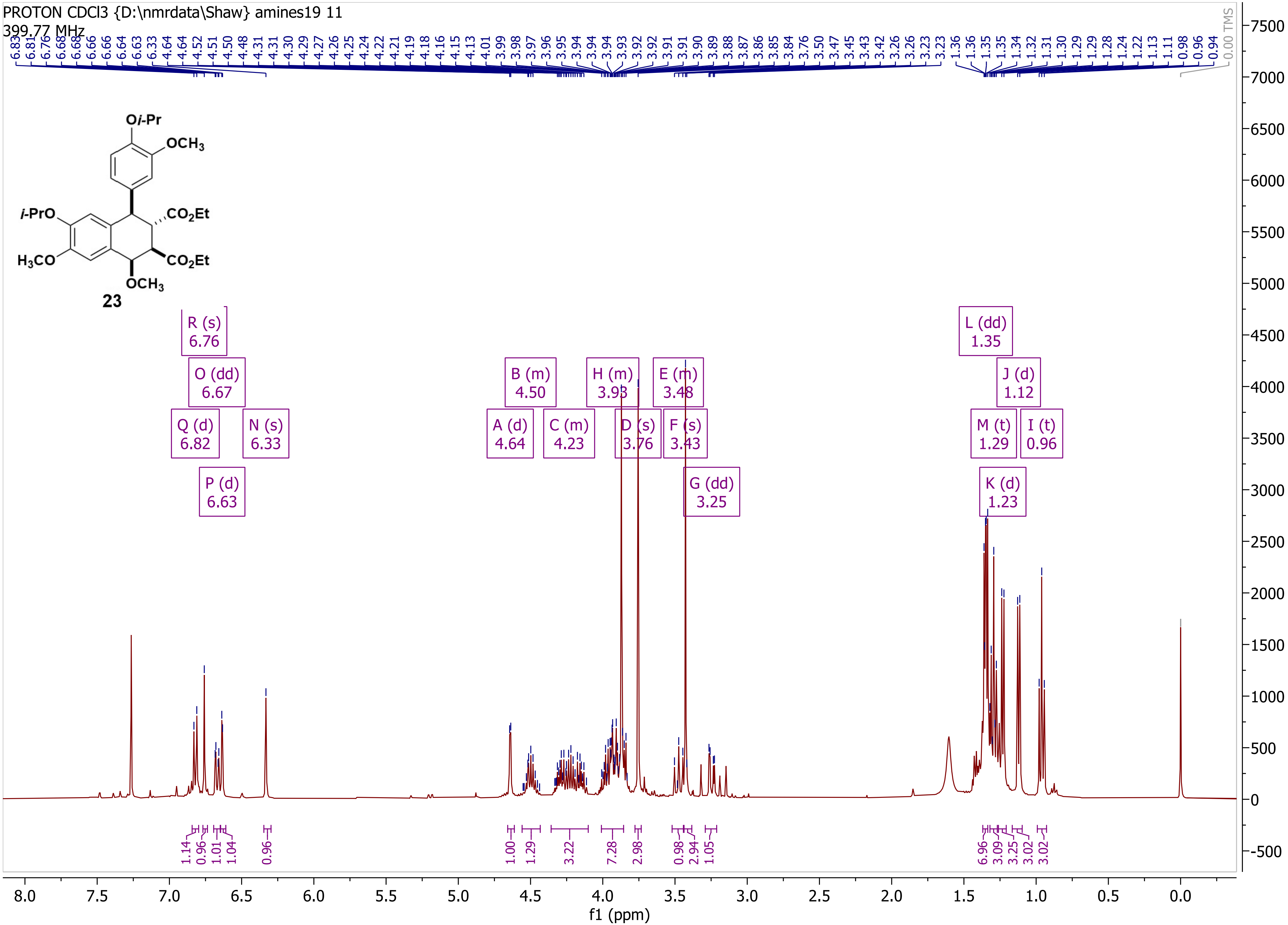


C13CPD CDCl3 /home/nmrdata/Shaw amines19 20
100.53 MHz
150.98
147.40
133.43
125.96
112.47
85.96
78.27
77.16 CDCl3
72.12
58.60
56.14
22.12
I
OCH3
i-PrO
OCH3
f1 (ppm)

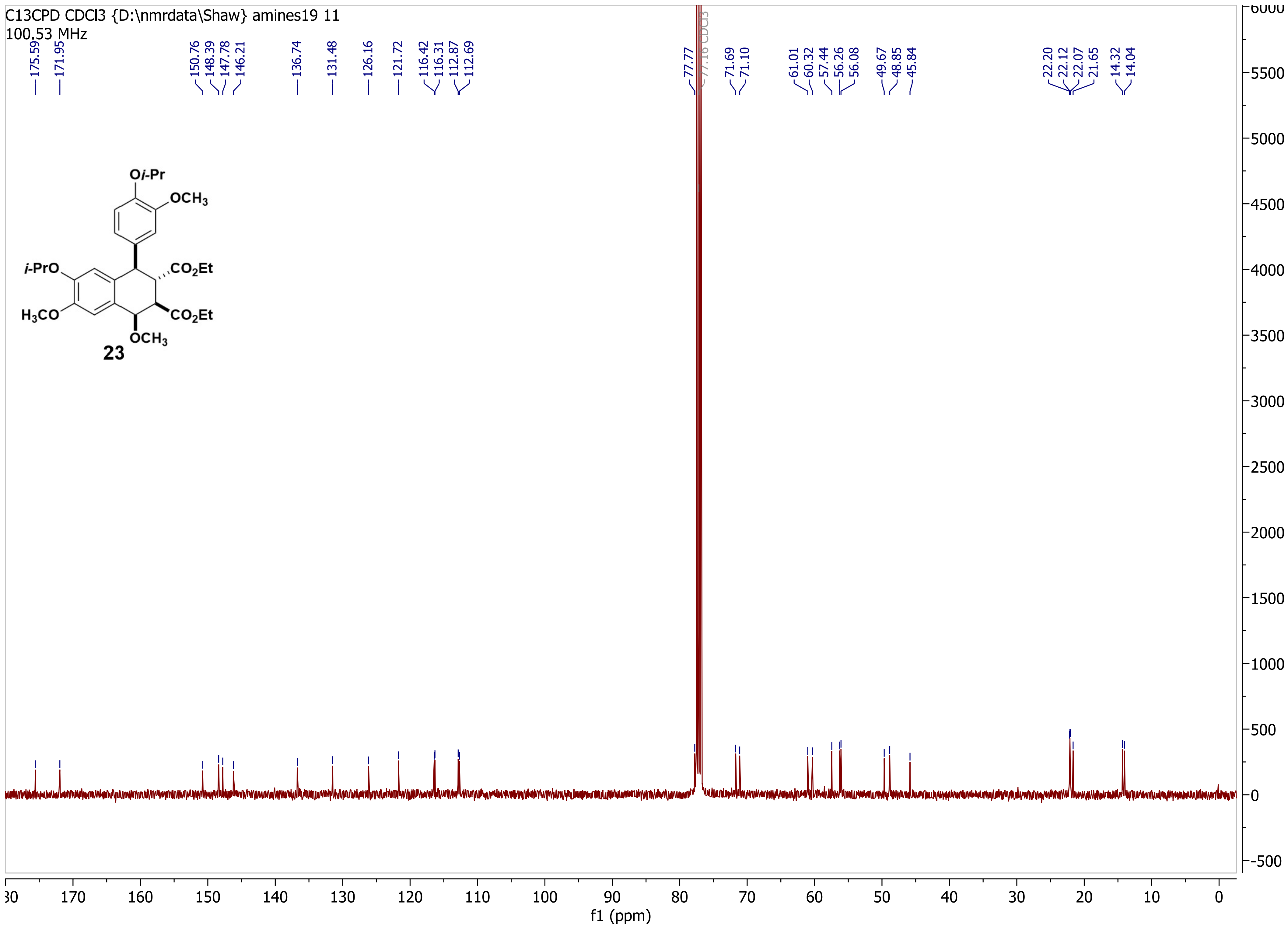


PROTON CDCl3 {D:\nmrdata\Shaw} amines19 12
399.77 MHz
7.49 7.48 7.29 7.28 7.27 7.26 7.13 6.95 6.87 6.85
4.68 4.66 4.65 4.52 4.48 4.47 4.45 4.44 4.42 3.94 3.90
3.32
1.43 1.41 1.34 1.32
0.00 TMS
L (m) 7.28
I (s) 6.95
K (d) 7.48
H (d) 6.86
J (s) 7.13
B (s) 4.52
A (m) 4.66
M (p) 4.45
E (s) 3.94
D (s) 3.90
C (s) 3.32
G (d) 1.42
F (d) 1.33
0.96 1.66 0.99 0.99 0.96
0.78 2.03 0.80
3.03 2.90
3.00
6.11 5.86
f1 (ppm)

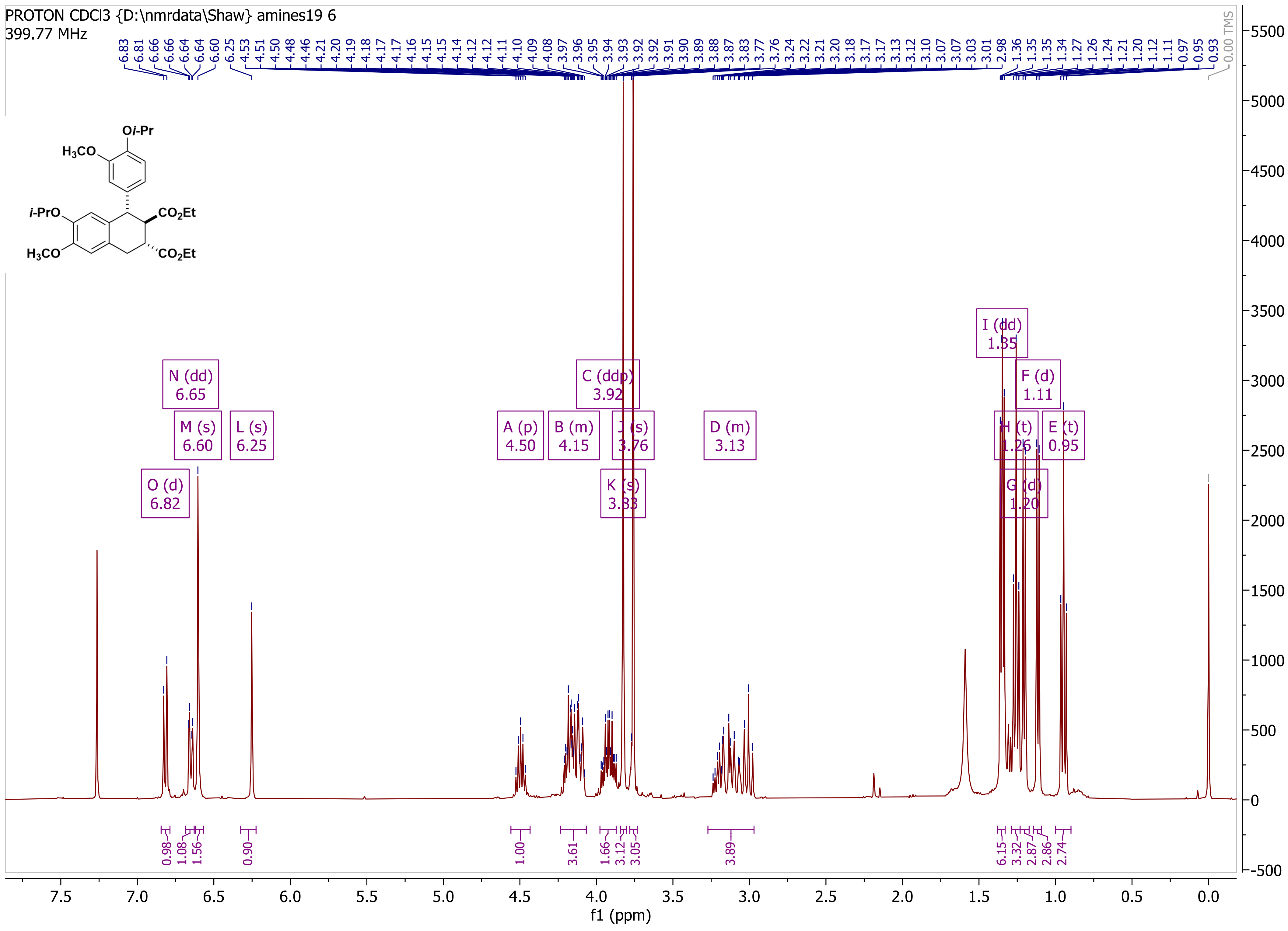

C13CPD CDCl3 {D:\nmrdata\Shaw} amines19 12
100.53 MHz
195.91
152.44
151.95
149.92
145.26
132.61
130.91
129.97
125.57
117.44
112.67
112.41
111.79
77.16 CDCl3
71.96
71.91
71.38
58.54
56.19
22.16
22.08
OCH3
O
i-PrO
OCH3
OCH3
Oi-Pr
f1 (ppm)
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
6500 6000 5500 5000 4500 4000 3500 3000 2500 2000 1500 1000 500 0 -500



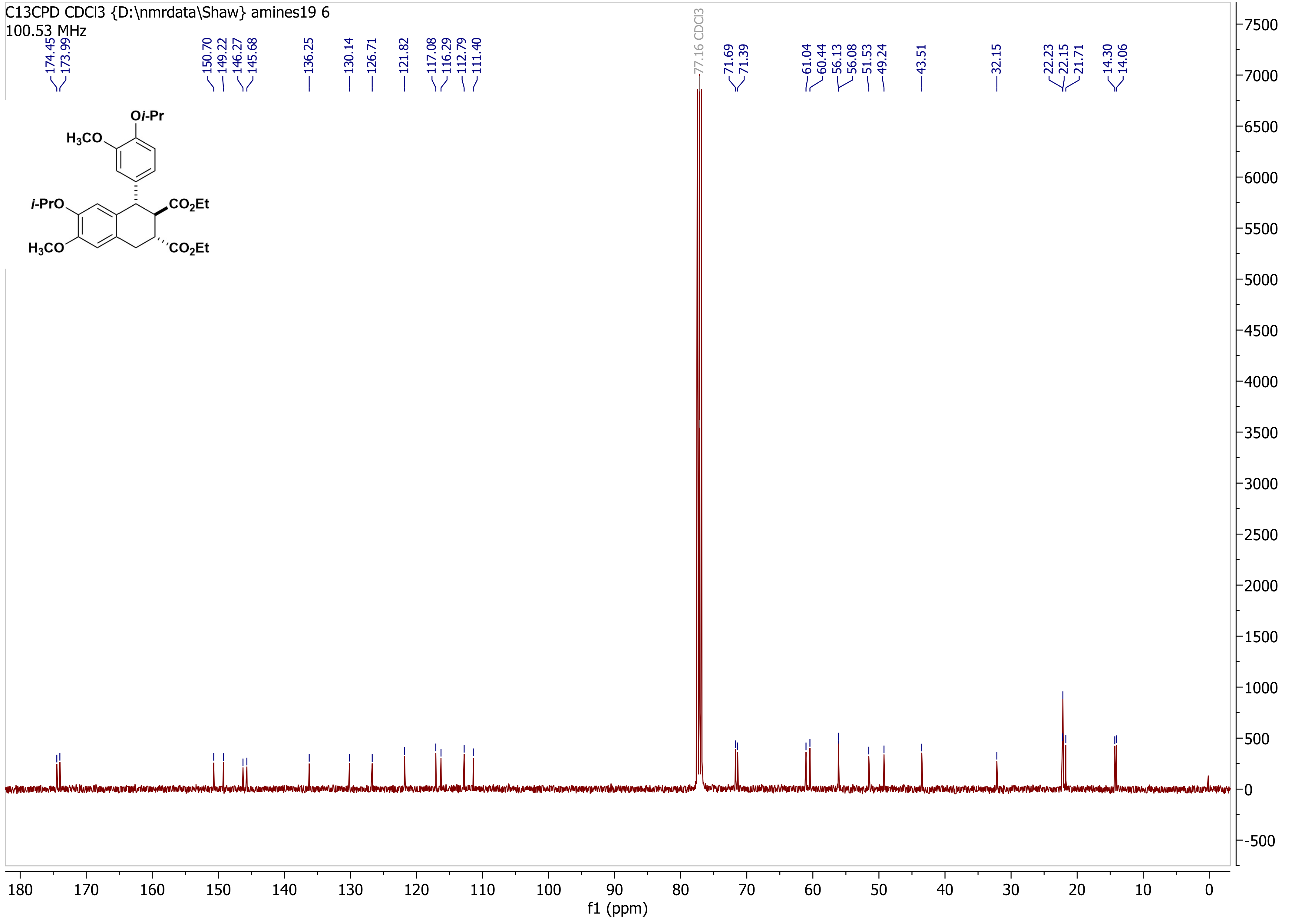
PROTON CDCl3 {D:\nmrdata\Shaw} amines19 11
399.77 MHz
6.83 6.81 6.76 6.68 6.68 6.66 6.66 6.64 6.63 6.33 4.64 4.64 4.52 4.51 4.50 4.48 4.31 4.31 4.30 4.29 4.27 4.26 4.25 4.24 4.22 4.21 4.19 4.18 4.16 4.15 4.13 4.01 3.99 3.98 3.97 3.96 3.95 3.94 3.94 3.94 3.93 3.92 3.92 3.91 3.91 3.90 3.89 3.88 3.87 3.86 3.85 3.84 3.76 3.50 3.47 3.45 3.43 3.42 3.26 3.23 3.23 1.36 1.36 1.35 1.35 1.34 1.32 1.31 1.30 1.29 1.29 1.28 1.24 1.22 1.13 1.11 0.98 0.96 0.94
0.00 TMS
Oi-Pr
OCH3
i-PrO
CO2Et
H3CO
CO2Et
OCH3
23
R (s) 6.76
O (dd) 6.67
Q (d) 6.82
N (s) 6.33
P (d) 6.63
B (m) 4.50
A (d) 4.64
C (m) 4.23
H (m) 3.93
D (s) 3.76
E (m) 3.48
F (s) 3.43
G (dd) 3.25
L (dd) 1.35
J (d) 1.12
M (t) 1.29
I (t) 0.96
K (d) 1.23
1.14 0.96 1.01 1.04 0.96 1.00 1.29 3.22 7.28 2.98 0.98 2.94 1.05 6.96 3.09 3.25 3.02 3.02
f1 (ppm)



C13CPD CDCl3 {D:\nmrdata\Shaw} amines19 11
100.53 MHz
175.59
171.95
150.76
148.39
147.78
146.21
136.74
131.48
126.16
121.72
116.42
116.31
112.87
112.69
77.77
77.16 CDCl3
71.69
71.10
61.01
60.32
57.44
56.26
56.08
49.67
48.85
45.84
22.20
22.12
22.07
21.65
14.32
14.04
Oi-Pr
OCH3
i-PrO
CO2Et
H3CO
CO2Et
OCH3
23
f1 (ppm)

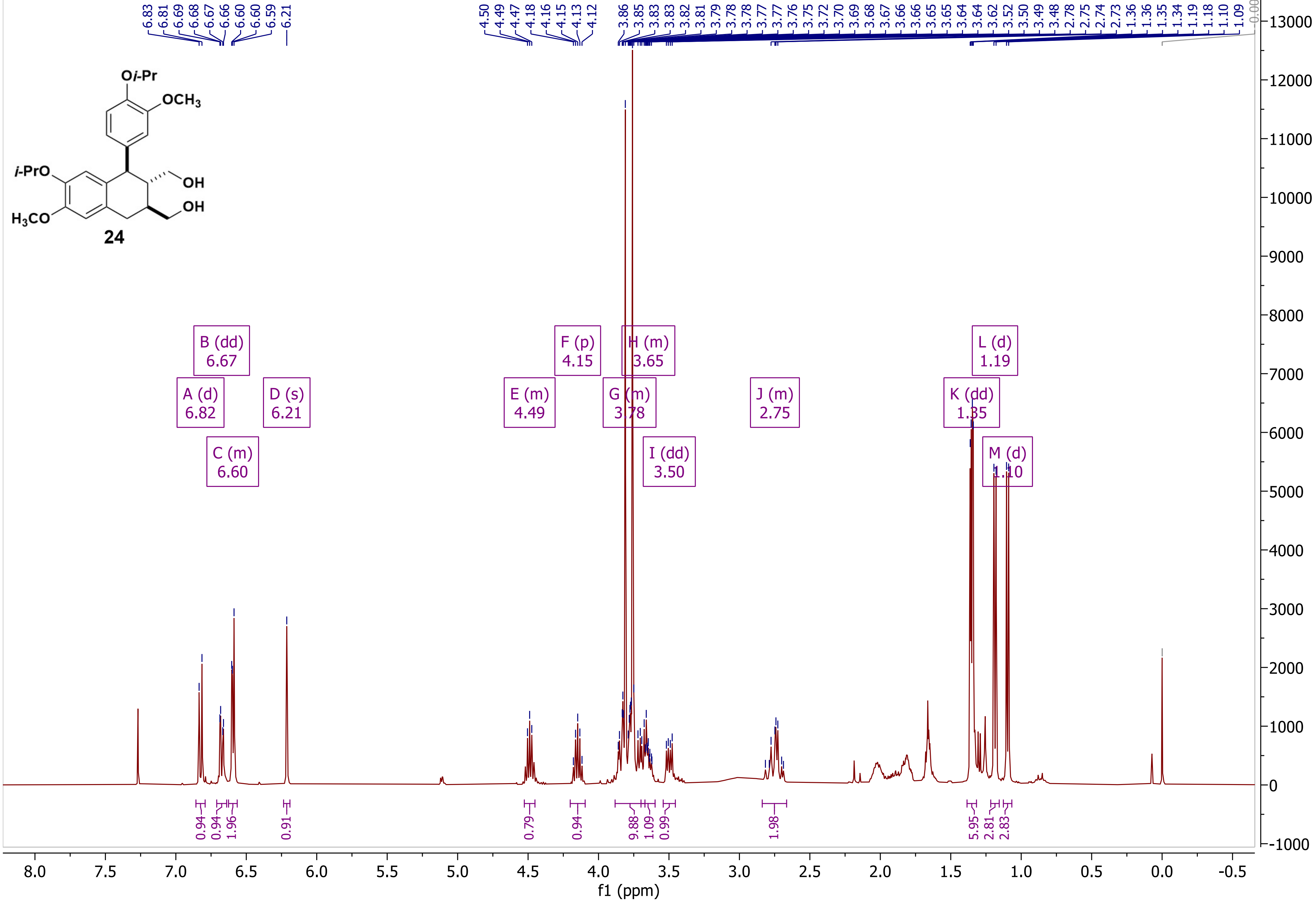


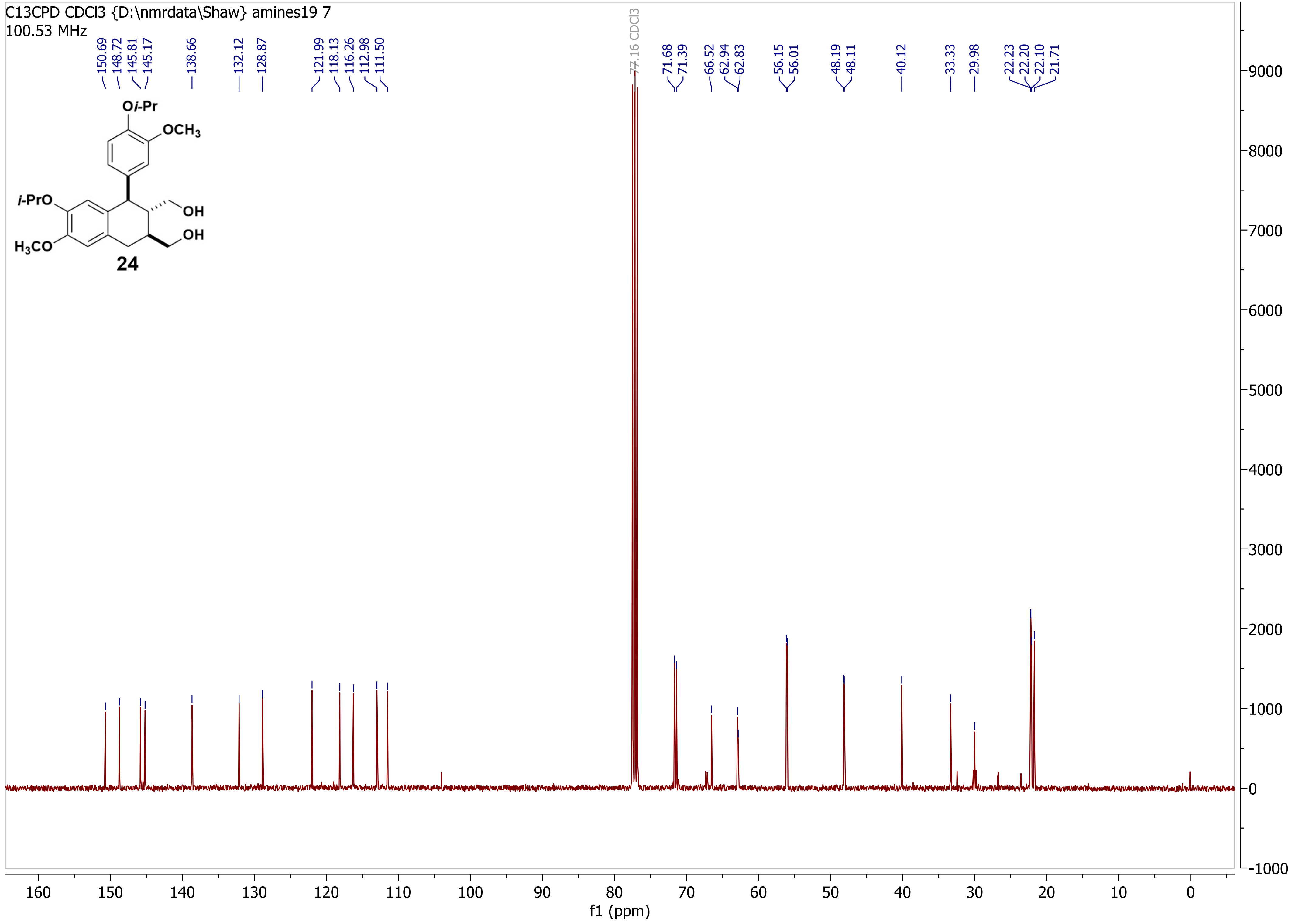
PROTON CDCl3 {D:\nmrdata\Shaw} amines19 6
399.77 MHz
N (dd) 6.65
M (s) 6.60
L (s) 6.25
O (d) 6.82
A (p) 4.50
B (m) 4.15
C (ddp) 3.92
J (s) 3.76
K (s) 3.83
D (m) 3.13
I (dd) 1.35
F (d) 1.11
H (t) 1.26
E (t) 0.95
G (d) 1.20
f1 (ppm)



C13CPD CDCl3 {D:\nmrdata\Shaw} amines19 6
100.53 MHz
174.45
173.99
150.70
149.22
146.27
145.68
136.25
130.14
126.71
121.82
117.08
116.29
112.79
111.40
77.16 CDCl3
71.69
71.39
61.04
60.44
56.13
56.08
51.53
49.24
43.51
32.15
22.23
22.15
21.71
14.30
14.06
Oi-Pr
H3CO
i-PrO
CO2Et
H3CO
CO2Et
f1 (ppm)

PROTON CDCl3 {D:\nmrdata\Shaw} amines19 7
399.77 MHz




C13CPD CDCl3 {D:\nmrdata\Shaw} amines19 7
100.53 MHz
150.69
148.72
145.81
145.17
138.66
132.12
128.87
121.99
118.13
116.26
112.98
111.50
77.16 CDCl3
71.68
71.39
66.52
62.94
62.83
56.15
56.01
48.19
48.11
40.12
33.33
29.98
22.23
22.20
22.10
21.71
Oi-Pr
OCH3
i-PrO
H3CO
OH
OH
24
f1 (ppm)