Supplementary Information

Expanded Structure-Activity Studies of the Lipoxazolidinone Antibiotics

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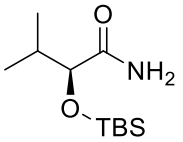
General Information

General information: THF and dichloromethane were purified using an alumina filtration system. Starting materials were purchased from a commercial chemical company and used as received. Reactions were monitored by TLC analysis (pre-coated silica gel 60 F254 plates, 250 mm layer thickness) and visualization was accomplished with a 254 nm UV light and by staining with a KMnO4 solution (1.5 g of $KMnO_4$, 10 g of K_2CO_3, and 1.25 mL of a 10% NaOH solution in 200 mL of water). Reactions were also monitored by LC-MS (2.6 mm C18 50 x 2.10 mm column). Flash chromatography on SiO_2 was used to purify the crude reaction mixtures and performed on a flash system utilizing pre-packed cartridges and linear gradients.

^1H, ^{13}C and NMR spectra were obtained on a 400, 500 or 700 MHz instrument in $CDCl_3$ unless otherwise noted. Chemical shifts were reported in parts per million with the residual solvent peak used as an internal standard ($CDCl_3$ = 7.26 ppm for ^1H and 77.16 ppm for ^{13}C). ^1H NMR spectra were run at 400 MHz and are tabulated as follows: chemical shift, multiplicity (s = singlet, d = doublet, t = triplet, q = quartet, p = pentet, m = multiplet, bs = broad singlet, dt = doublet of triplet, tt = triplet of triplet), number of protons, and coupling constant(s). ^{13}C NMR spectra were run at 100 MHz, 125 MHz or 175 MHz using a proton-decoupled pulse sequence with a d1 of 1 second unless otherwise noted and are tabulated by observed peak. High-resolution mass spectra were obtained on an ion trap mass spectrometer using heated electrospray ionization (HESI). Purity was determined by LC-MS analysis performed on a Shimadzu UHPLC coupled to a UV detector and Shimadzu LCMS-2020 Quadrupole mass spectrometer (ESI-API) using mixtures of HPLC grade MeCN/H_2O (spiked with 0.1% formic acid). The purity of all final compounds was found to be >90% by UV (254 nm).

General procedure for the preparation of O-TBS-α-hydroxy amides from α-amino acids

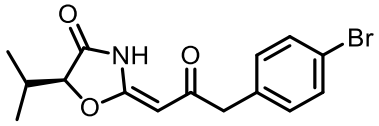
The α-hydroxy acid derivatives were synthesized following a known literature procedure.[1] In brief, the amino acid (10 mmol) was dissolved in 1 M H_2SO_4 (10 mmol) and cooled to 0 ˚C. Then 2 M $NaNO_2$ (20 mmol) was added dropwise and the reaction was allowed to slowly warm to room temperature and stirred overnight followed by addition of another aliquot of 2 M $NaNO_2$ (10 mmol) and the reaction was stirred for a further 24 h at room temperature. The reaction mixture was extracted with EtOAc (7 x 10 mL). The combined organic layers were washed with brine (15 mL), dried ($MgSO_4$), filtered and concentrated. The resulting crude solid was dissolved in DMF (resulting in a 2 M solution) and imidazole (42 mmol) and TBSCl (21 mmol) were added and the reaction was stirred for 24 h at room temperature. The reaction was then diluted with EtOAc and washed with 10% citric acid (15 mL), sat. aq. $NaHCO_3$ (15 mL) and brine (15 mL). The organic layer was dried ($MgSO_4$), filtered, concentrated and purified by flash column chromatography on SiO_2 (20% EtOAc/hexanes). To the resulting TBS protected hydroxy acid (5 mmol) was added *p*-toluenesulfonyl chloride (5 mmol), silica supported ammonium chloride (10 mmol)[2,3] and Et_3N (25 mmol) and the reaction was stirred for 15 minutes at room temperature and then diluted with EtOAc, filtered and concentrated. The residue was purified by flash column chromatography on SiO_2 (20% EtOAc/hexanes).



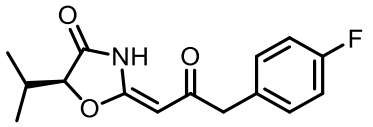
(*S*)-2-((*tert*-Butyldimethylsilyl)oxy)-3-methylbutanamide (8). Yield: 280 mg (30%) of **8** as a white solid. R_f = 0.18 (hexanes:EtOAc, 4:1); $[\alpha]_D$ = -15˚ (*c* = 0.1, dichloromethane); ^{1}H NMR (400 MHz, $CDCl_3$): δ = 7.15 (s, 1 H), 6.30 (s, 1 H), 3.84 (d, *J* = 3.3 Hz, 1 H), 2.03-1.95 (m, 1 H), 0.89 (d, *J* = 7.0 Hz, 3 H), 0.85 (s, 9 H), 0.81 (d, *J* = 7.0 Hz, 3 H), 0.03 (s, 3 H), 0.01 (s, 3 H); ^{13}C NMR (100 MHz, $CDCl_3$): δ = 177.5, 77.9, 32.7, 25.9, 19.4, 18.2, 16.4, -4.9, -5.0; IR (film) 3471, 3205, 3142, 2954, 2926, 1658, 1461 cm^{-1}; HRMS (ESI) *m/z* calculated for $C_{11}H_{26}NO_2Si$ $[M+H]^+$: 232.17273, found: 232.17273.

General procedure for synthesis of 4-oxazolidinones:

Acylated Meldrum's acid derivatives were synthesized following a previously reported procedure.[4] In brief, the carboxylic acid (1 mmol) was dissolved in dichloromethane (0.5 M) and cooled to 0 ˚C. Then 1-ethyl-3-(3-dimethylaminopropyl)carbodiimide (1.1 mmol) and 4-dimethylaminopyridine (0.1 mmol) were added. Then Meldrum's acid (1.01 mmol) was added and the reaction was stirred at room temperature overnight. The insoluble urea was filtered, and the solvent was removed *in vacuo,* redissolved in EtOAc and washed with HCl (15 mL, 1 M) and brine (15 mL), dried ($MgSO_4$), filtered and concentrated *in vacuo*. The crude acylated Meldrum's acid and O-TBS-α-hydroxy amide (0.5 mmol) were dissolved in toluene (2 mL) and stirred at reflux for 1 h. The reaction was cooled to room temperature, concentrated *in vacuo*. The resulting crude imide (0.25 mmol) was dissolved in dichloromethane (2.5 mL) and trifluoroacetic acid (2.5 mL) was added at room temperature. The reaction was allowed to stir for 24 h and then concentrated *in vacuo* and purified by flash column chromatography on SiO_2 (20% EtOAc/hexanes).

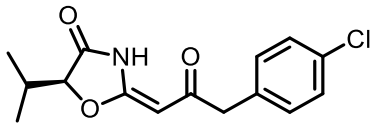


(*S,E*)-2-(3-(4-Bromophenyl)-2-oxopropylidene)-5-isopropyloxazolidin-4-one (6). Yield: 174 mg (51%) of **6** as a white solid: $[\alpha]_D$ = -26˚ (*c* = 0.6, dichloromethane); ^{1}H NMR (400 MHz, $CDCl_3$); δ = 7.46 (m, 2 H), 7.12 (m, 2 H), 5.19 (s, 1 H), 4.47 (d, *J* = 3.9 Hz, 1 H), 3.61 (s, 2 H), 2.28 (m, 1 H), 1.09 (d, *J* = 7.0 Hz, 3 H), 0.95 (d, *J* = 6.9 Hz, 3 H); ^{13}C NMR (125 MHz, $CDCl_3$): δ = 196.9, 172.1, 166.3, 134.5, 132.0, 131.4, 121.2, 83.1, 81.0, 49.2, 30.8, 18.1, 15.9; IR (film) 3211, 2957, 2935, 2863, 1765, 1662, 1578, 1011 cm^{-1}; HRMS (ESI) *m/z* calculated for $C_{15}H_{17}BrNO_3$ $[M+H]^+$: 338.03863, found: 338.03866.

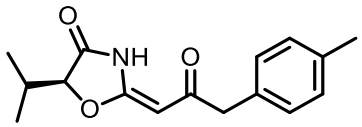


(*S,E*)-2-(3-(4-Fluorophenyl)-2-oxopropylidene)-5-isopropyloxazolidin-4-one (11). Yield: 149 mg (33%) of **11** as an oil: ^{1}H NMR (400 MHz, $CDCl_3$); δ = 7.19 (m, 2 H), 7.02 (m, 2 H), 5.22 (s, 1 H), 4.51 (d, *J* = 3.9 Hz, 1 H), 3.68 (s, 2 H), 2.29 (m, 1 H), 1.09 (d, *J* = 6.9 Hz, 3 H), 0.95 (d, *J* = 6.9 Hz, 3 H); ^{13}C NMR (300 MHz, $CDCl_3$): δ = 198.9, 172.3, 167.0, 163.3, 130.9, 115.5, 83.2,

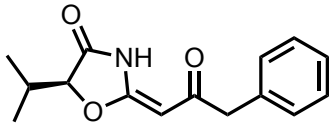
81.3, 48.3, 30.6, 17.8, 15.6; HRMS (ESI) *m/z* calculated for $C_{15}H_{17}FNO_3$ $[M+H]^+$: 278.11870, found: 278.11824.



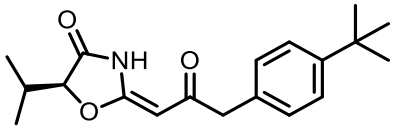
(*S,E*)-2-(3-(4-Chlorophenyl)-2-oxopropylidene)-5-isopropyloxazolidin-4-one (12). Yield: 55 mg (48%) of **12** as an oil: ^{1}H NMR (400 MHz, $CDCl_3$); δ = 7.29 (m, 2 H), 7.17 (m, 2 H), 5.20 (s, 1 H), 4.47 (d, *J* = 3.9 Hz, 1 H), 3.64 (s, 2 H), 2.25 (m, 1 H), 1.09 (d, *J* = 6.9 Hz, 3 H), 0.95 (d, *J* = 6.8 Hz, 3 H); ^{13}C NMR (300 MHz, $CDCl_3$): δ = 197.5, 172.0, 166.4, 130.8, 128.8, 82.9, 80.9, 48.8, 30.5, 17.8, 15.6; HRMS (ESI) *m/z* calculated for $C_{15}H_{17}ClNO_3$ $[M+H]^+$: 294.08915, found: 294.08881.



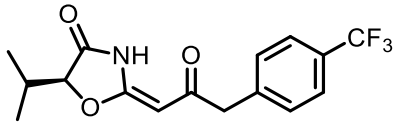
(*S,E*)-5-Isopropyl-2-(2-oxo-3-(*p*-tolyl)propylidene)oxazolidin-4-one (13). Yield: 97 mg (26%) of **13** as a white solid: ^{1}H NMR (400 MHz, $CDCl_3$); δ = 7.12 (m, 4 H), 5.25 (s, 1 H), 4.50 (d, *J* = 3.9 Hz, 1 H), 3.68 (s, 2 H), 2.34 (s, 3H), 2.29 (m, 1 H), 1.10 (d, *J* = 6.9 Hz, 3 H), 0.97 (d, *J* = 6.9 Hz, 3 H); ^{13}C NMR (400 MHz, $CDCl_3$): δ = 200.4, 172.8, 167.5, 137.3, 132.1, 129.9, 83.6, 81.9, 77.3, 49.2, 30.9, 21.5, 16.1; HRMS (ESI) *m/z* calculated for $C_{16}H_{20}NO_3$ $[M+H]^+$: 274.14377, found: 274.14342.



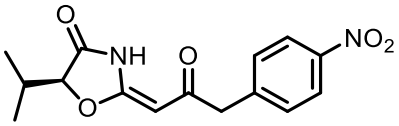
(*S,E*)-5-Isopropyl-2-(2-oxo-3-phenylpropylidene)oxazolidin-4-one (14). Yield: 11 mg (56%) of **14** as an oil: ^{1}H NMR (400 MHz, $CDCl_3$); δ = 7.34-7.23 (m, 5 H), 5.22 (s, 1 H), 4.45 (d, *J* = 3.8 Hz, 1 H), 3.67 (s, 2 H), 2.22 (m, 1 H), 1.09 (d, *J* = 7.0 Hz, 3 H), 0.95 (d, *J* = 6.9 Hz, 3 H); ^{13}C NMR (125 MHz, $CDCl_3$): δ = 197.9, 172.2, 166.1, 135.5, 129.6, 128.9, 127.1, 82.9, 81.1, 50.0, 30.7, 18.1, 15.8; IR (film) 3184, 2957, 2935, 2863, 1765, 1661, 1571, 1014 cm-1; HRMS (ESI) *m/z* calculated for $C_{15}H_{18}NO_3$ [M+H]+: 260.12812, found: 260.12806.



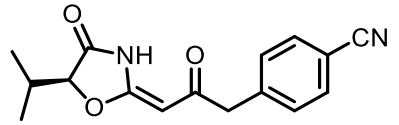
(*S,E*)-2-(3-(4-(tert-Butyl)phenyl)-2-oxopropylidene)-5-isopropyloxazolidin-4-one (15). Yield: 196 mg (38%) of **15** as a white solid: ^{1}H NMR (400 MHz, $CDCl_3$); δ = 7.36 (m, 2 H), 7.17 (m, 2 H), 5.26 (s, 1 H), 4.45 (d, *J* = 3.7 Hz, 1 H), 3.65 (m, 2H), 2.27 (s, 1 H), 1.33 (s, 9 H) 1.10 (d, *J* = 6.8 Hz, 3 H), 0.96 (d, *J* = 6.8 Hz, 3 H); ^{13}C NMR (400 MHz, $CDCl_3$): δ = 198.6, 172.7, 166.4, 150.2, 132.7, 129.6, 126.1, 83.3, 81.6, 49.8, 41.1, 31.9, 31.0, 18.5, 16.2; HRMS (ESI) *m/z* calculated for $C_{19}H_{26}NO_3$ $[M+H]^+$: 316.19072, found: 316.19070.



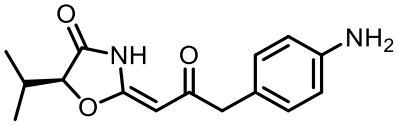
(*S,E*)-5-Isopropyl-2-(2-oxo-3-(4-(trifluoromethyl)phenyl)propylidene)oxazolidin-4-one (16). Yield: 46 mg (46%) of **16** as a white solid: ^{1}H NMR (400 MHz, $CDCl_3$); δ = 7.58 (d, J = 7.6 Hz, 2 H), 7.35 (d, J = 7.6 Hz, 2 H), 5.22 (s, 1 H), 4.47 (d, *J* = 3.3 Hz, 1 H), 3.73 (s, 2 H), 2.26 (m, 1 H), 1.09 (d, *J* = 7.0 Hz, 3 H), 0.95 (d, *J* = 6.7 Hz, 3 H); ^{13}C NMR (300 MHz, $CDCl_3$): δ = 197.2, 172.5, 166.6, 139.9, 130.4, 126.0, 83.4, 81.7, 49.9, 31.0, 18.4, 16.1; HRMS (ESI) *m/z* calculated for $C_{16}H_{17}F_3NO_3$ $[M+H]^+$: 328.11550, found: 328.11501.



(*S,E*)-5-Isopropyl-2-(3-(4-nitrophenyl)-2-oxopropylidene)oxazolidin-4-one (17). Yield: 224 mg (60%) of **17** as a yellow solid: ^{1}H NMR (400 MHz, $CDCl_3$); δ = 8.21 (m, 2 H), 7.42 (m, 2 H) 5.23 (s, 1 H), 4.49 (d, *J* = 3.8 Hz, 1 H), 3.78 (s, 2 H), 2.29 (m, 1 H), 1.11 (d, *J* = 7.0 Hz, 3 H), 0.97 (d, *J* = 7.0 Hz, 3 H); ^{13}C NMR (400 MHz, $CDCl_3$): δ = 195.2, 171.6, 166.1, 146.8, 142.6, 130.2, 123.6, 82.8, 80.7, 48.9, 30.4, 17.7, 15.4; HRMS (ESI) *m/z* calculated for $C_{15}H_{17}N_2O_5$ $[M+H]^+$: 305.11320, found: 305.11315.

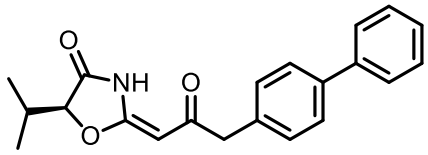


(*S,E*)-4-(3-(5-Isopropyl-4-oxooxazolidin-2-ylidene)-2-oxopropyl)benzonitrile (18). Yield: 215 mg (83%) of **18** as a yellow solid: ^{1}H NMR (400 MHz, $CDCl_3$); δ = 7.56 (d, J = 7.9 Hz, 2 H), 7.32 (d, J = 8.0 Hz, 2H), 5.21 (s, 1 H), 4.48 (d, *J* = 3.7 Hz, 1 H), 3.73 (s, 2 H), 2.21 (m, 1 H), 1.06 (d, *J* = 6.5 Hz, 3 H), 0.90 (d, *J* = 6.5 Hz, 3 H); ^{13}C NMR (300 MHz, $CDCl_3$): δ = 196.0, 172.6, 166.6, 141.2, 132.6, 130.6, 119.1, 110.9, 83.1, 81.3, 49.6, 30.8, 18.1, 15.9; HRMS (ESI) *m/z* calculated for $C_{16}H_{17}N_2O_3$ $[M+H]^+$: 285.12337, found: 285.12328.

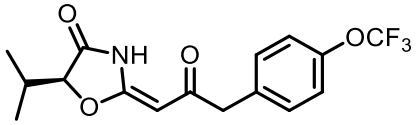


(*S,E*)-2-(3-(4-Aminophenyl)-2-oxopropylidene)-5-isopropyloxazolidin-4-one (19). Yield: 8.2 mg (32%) of **19** as a white solid. A round bottom flask was charged with palladium acetate (0.01 mmol), (*S,E*)-5-isopropyl-2-(3-(4-nitrophenyl)-2-oxopropylidene)oxazolidin-4-one, **17** (0.16 mmol), and dry THF (0.2 M). The flask was sealed and purged with nitrogen. While purging the flask with nitrogen a solution of aqueous KF was added via syringe (0.33 mmol KF, 0.2 mL of degassed water). The nitrogen inlet was replaced with a balloon of nitrogen. PMHS (0.05 mL; 1 mmol of hydride is 0.06mL) was slowly added dropwise via syringe. The reaction was stirred for 2.5 hours under N_3 (g). At that time, the reaction flask was opened to the air, diluted with 5–10 mL of diethyl ether, and stirred for 5 minutes. The layers were separated and the aqueous layer was back extracted with diethyl ether. The combined organics were filtered through a plug of

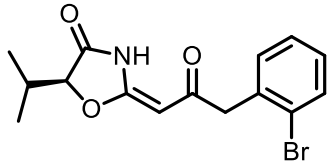
Celite by flushing with EtOAc. The filtrate was concentrated and subjected to reverse phase chromatography (MeOH/H_2O).[5] ^{1}H NMR (400 MHz, $CDCl_3$); δ = 7.02 (m, 2 H), 6.66 (m, 2 H), 5.20 (s, 1 H), 4.44 (d, *J* = 3.9 Hz, 1 H), 3.54 (s, 2 H), 2.27 (m, 1 H), 1.08 (d, *J* = 7.0 Hz, 3 H), 0.95 (d, *J* = 6.9 Hz, 3 H); ^{13}C NMR (300 MHz, $CDCl_3$): δ = 198.7, 172.3, 166.1, 144.9, 130.6, 125.9, 115.9, 82.9, 81.0, 49.3, 30.8, 18.2, 15.9; HRMS (ESI) *m/z* calculated for $C_{15}H_{19}N_2O_3$ $[M+H]^+$: 275.13902; found: 275.13915.



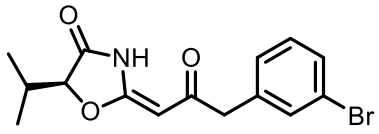
(*S,E*)-2-(3-([1,1'-Biphenyl]-4-yl)-2-oxopropylidene)-5-isopropyloxazolidin-4-one (20). Yield: 6.8 mg (47%) of **20** as an oil: ^{1}H NMR (400 MHz, $CDCl_3$); δ = 7.58 (m, 4 H), 7.43 (m, 2 H), 7.31 (m, 3 H), 5.27 (s, 1 H), 4.47 (d, *J* = 3.8 Hz, 1 H), 3.71 (s, 2 H), 2.28 (m, 1 H), 1.10 (d, *J* = 7.0 Hz, 3 H), 0.97 (d, *J* = 6.9 Hz, 3 H); ^{13}C NMR (125 MHz, $CDCl_3$): δ = 197.5, 171.9, 165.9, 140.7, 139.8, 134.3, 129.8, 128.7, 127.4, 127.2, 127.0, 82.8, 80.9, 49.4, 30.5, 17.9, 15.6; IR (film) 2957, 2935, 2863, 1765, 1661, 1574, 1015 cm-1; HRMS (ESI) *m/z* calculated for $C_{21}H_{22}NO_3$ $[M+H]+$: 336.15942, found: 336.15919.



(*S,E*)-5-Isopropyl-2-(2-oxo-3-(4-(trifluoromethoxy)phenyl)propylidene)oxazolidin-4-one (21). Yield: 9.3 mg (25%) of **21** as a white solid: ^{1}H NMR (400 MHz, $CDCl_3$); δ = 7.32 (m, 2 H), 7.18 (m, 2 H), 5.22 (s, 1 H), 4.47 (d, *J* = 3.3 Hz, 1 H), 3.66 (s, 2 H), 2.28 (m, 1 H), 1.09 (d, *J* = 6.8 Hz, 3 H), 0.96 (d, *J* = 6.7 Hz, 3 H); ^{13}C NMR (300 MHz, $CDCl_3$): δ = 196.8, 172.0, 166.1, 148.2, 134.1, 82.9, 80.9, 48.8, 30.6, 17.8, 15.6; HRMS (ESI) *m/z* calculated for $C_{16}H_{17}F_3NO_4$ $[M+H]^+$: 344.11042, found: 344.11017.

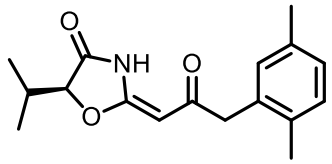


(*S,E*)-2-(3-(2-Bromophenyl)-2-oxopropylidene)-5-isopropyloxazolidin-4-one (22). Yield: 163 mg (40%) of **22** as a white solid: ^{1}H NMR (400 MHz, $CDCl_3$); δ = 7.57 (m, 1 H), 7.30 (m, 2 H), 7.13 (m, 1 H), 5.22 (s, 1 H), 4.47 (d, *J* = 3.9 Hz, 1 H), 3.84 (m, 2 H), 2.26 (s, 1 H), 1.09 (d, *J* = 6.9 Hz, 3 H), 0.96 (d, *J* = 6.9 Hz, 3 H); ^{13}C NMR (400 MHz, $CDCl_3$): δ = 195.5, 172.0, 166.1, 135.5, 132.9, 131.8, 128.8, 127.7, 125.2, 83.5, 81.4, 49.6, 41.4, 30.6, 17.9, 15.7; HRMS (ESI) *m/z* calculated for $C_{15}H_{17}BrNO_3$ $[M+H]^+$: 338.03863, found: 338.03866.

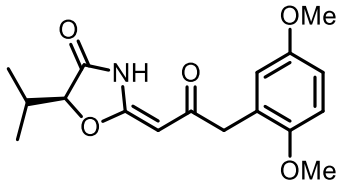


(*S,E*)-2-(3-(3-Bromophenyl)-2-oxopropylidene)-5-isopropyloxazolidin-4-one (23). Yield: 127 mg (38%) of **23** as a yellow solid: ^{1}H NMR (400 MHz, $CDCl_3$); δ = 7.39 (m, 2 H), 7.17 (m, 2 H),

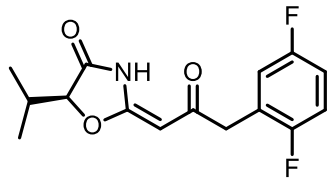
5.20 (s, 1 H), 4.46 (d, *J* = 3.9 Hz, 1 H), 3.63 (m, 2 H), 2.28 (s, 1 H), 1.09 (d, *J* = 6.9 Hz, 3 H), 0.96 (d, *J* = 6.9 Hz, 3 H); ^{13}C NMR (400 MHz, $CDCl_3$): δ = 197.1, 172.5, 166.6, 138.1, 132.9, 130.7, 130.6, 128.6, 83.4, 81.4, 49.7, 31.1, 18.5, 16.2; HRMS (ESI) *m/z* calculated for $C_{15}H_{17}BrNO_3$ $[M+H]^+$: 338.03863, found: 338.03868.



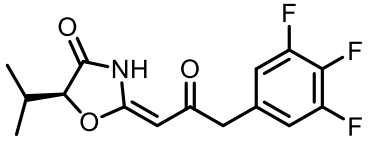
(*S,E*)-2-(3-(2,5-diMethylphenyl)-2-oxopropylidene)-5-isopropyloxazolidin-4-one (24). Yield: 126 mg (39%) of **24** as a white solid: ^{1}H NMR (400 MHz, $CDCl_3$); δ = 7.08 (m, 1 H), 7.03 (m, 2H), 5.17 (s, 1 H), 4.48 (d, *J* = 3.9 Hz, 1 H), 3.68 (m, 2 H), 2.69 (m, 6H), 2.26 (s, 1 H), 1.10 (d, *J* = 6.9 Hz, 3 H), 0.97 (d, *J* = 6.9 Hz, 3 H); ^{13}C NMR (400 MHz, $CDCl_3$): δ = 199.3, 172.6, 166.7, 136.1, 133.9, 131.7, 131.4, 128.7 128.4, 83.3, 81.2, 47.8, 39.2, 30.9, 21.3, 19.6, 18.2, 16.0; HRMS (ESI) *m/z* calculated for $C_{17}H_{22}NO_3$ $[M+H]^+$: 288.15942, found: 288.15985.



(*S,E*)-2-(3-(2,5-diMethoxyphenyl)-2-oxopropylidene)-5-isopropyloxazolidin-4-one (25). Yield: 119 mg (48%) of **25** as a white solid: ^{1}H NMR (400 MHz, $CDCl_3$); δ = 6.78 (m, 3 H), 5.22 (s, 1 H), 4.44 (d, *J* = 3.8 Hz, 1 H), 3.76 (s, 6 H), 3.65 (m, 2 H), 2.25 (m, 1 H), 1.09 (d, *J* = 6.9 Hz, 3 H), 0.96 (d, *J* = 6.9 Hz, 3 H); ^{13}C NMR (300 MHz, $CDCl_3$): δ = 198.4, 172.5, 166.0, 154.0, 152.2, 125.6, 117.7, 113.2, 112.1, 83.2, 81.1, 56.6, 56.2, 44.7, 31.0, 18.4, 16.1; HRMS (ESI) *m/z* calculated for $C_{17}H_{22}NO_5$ $[M+H]^+$: 320.14925, found: 320.14898.

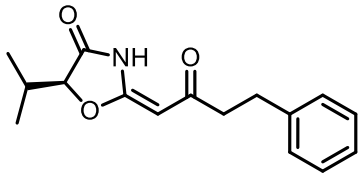


(*S,E*)-2-(3-(2,5-diFluorophenyl)-2-oxopropylidene)-5-isopropyloxazolidin-4-one (26). Yield: 46 mg (16%) of **26** as a white solid: ^{1}H NMR (400 MHz, $CDCl_3$); δ = 6.94 (m, 3 H), 5.25 (s, 1 H), 4.48 (d, *J* = 3.9 Hz, 1 H), 3.69 (s, 2 H), 2.29 (m, 1 H), 1.10 (d, *J* = 6.9 Hz, 3 H), 0.97 (d, *J* = 6.9 Hz, 3 H); ^{13}C NMR (400 MHz, $CDCl_3$): δ = 195.9, 172.5, 166.6, 158.7, 118.5, 116.7, 115.5, 83.4, 81.1, 42.9, 31.1, 18.4, 16.1; HRMS (ESI) *m/z* calculated for $C_{15}H_{16}F_2NO_3$ $[M+H]^+$: 296.10928, found: 296.10924.

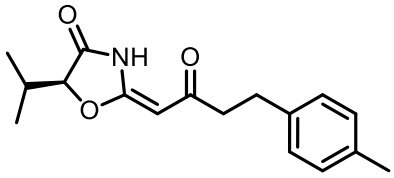


(*S,E*)-5-Isopropyl-2-(2-oxo-3-(3,4,5-trifluorophenyl)propylidene)oxazolidin-4-one (27). Yield: 70 mg (16%) of **27** as a white solid: ^{1}H NMR (400 MHz, $CDCl_3$); δ = 6.88 (m, 2 H), 5.20

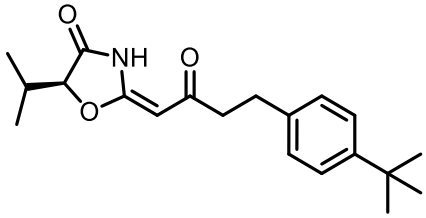
(s, 1 H), 4.48 (d, J = 3.9 Hz, 1 H), 3.59 (m, 2 H), 2.28 (s, 1 H), 1.10 (d, J = 6.9 Hz, 3 H), 0.97 (d, J = 6.9 Hz, 3 H); ^{13}C NMR (400 MHz, $CDCl_3$): δ = 195.6, 171.8, 166.4, 151.9, 150.3, 138.2, 131.5, 83.9, 80.7, 48.5, 30.6, 17.9, 15.7; HRMS (ESI) *m/z* calculated for $C_{15}H_{13}NO_3F_3$ $[M-H]^-$: 312.08530, found: 312.08501.



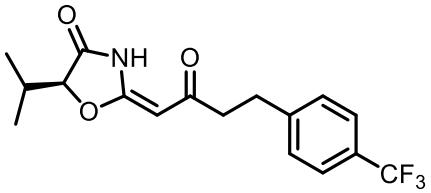
(*S,E*)-5-Isopropyl-2-(2-oxo-4-phenylbutylidene)oxazolidin-4-one (28). Yield: 300 mg (56%) of **28** as a white solid: ^{1}H NMR (400 MHz, $CDCl_3$); δ = 7.31 (m, 2 H), 7.22 (m, 3 H). 5.36 (s, 1 H), 4.58 (d, J = 3.8 Hz, 1 H), 2.98 (m, 2H), 2.78 (m, 2 H), 2.33 (m, 1 H), 1.14 (d, J = 6.9 Hz, 3 H), 1.00 (d, J = 6.9 Hz, 3 H); ^{13}C NMR (400 MHz, $CDCl_3$): δ = 199.7, 177.9, 165.9, 141.4, 128.6, 126.4, 83.1, 81.8, 44.6, 36.0, 31.4, 18.3, 16.0; HRMS (ESI) *m/z* calculated for $C_{16}H_{20}NO_3$ $[M+H]^+$: 274.14377, found: 274.14358.



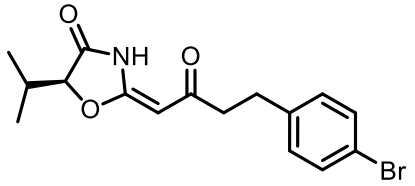
(*S,E*)-5-Isopropyl-2-(2-oxo-7-phenylheptylidene)oxazolidin-4-one (29). Yield: 226 mg (42%) of **29** as an oil: ^{1}H NMR (400 MHz, $CDCl_3$); δ = 7.09 (m, 4 H), 5.25 (s, 1 H), 4.47 (d, J = 3.8 Hz, 1 H), 2.93 (m, 2 H), 2.70 (m, 2 H), 2.31 (s, 3 H), 2.27 (m, 1 H), 1.11 (d, J = 6.9 Hz, 3 H), 0.97 (d, J = 6.9 Hz, 3 H); ^{13}C NMR (400 MHz, $CDCl_3$): δ = 199.7, 172.6, 165.9, 138.4, 129.6, 128.6, 83.1, 81.7, 44.9, 35.9, 30.7, 21.4, 18.4, 16.0; HRMS (ESI) *m/z* calculated for $C_{17}H_{22}NO_3$ $[M+H]^+$: 288.15942, found: 288.15941.



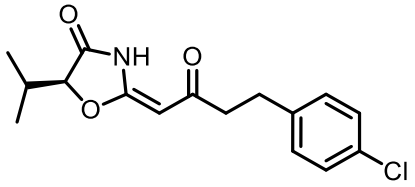
(*S,E*)-2-(4-(4-(tert-Butyl)phenyl)-2-oxobutylidene)-5-isopropyloxazolidin-4-oneone (30). Yield: 125 mg (46%) of **30** as a white solid: ^{1}H NMR (400 MHz, $CDCl_3$); δ = 7.31 (m, 2 H), 7.14 (m, 2 H), 5.27 (s, 1 H), 4.48 (d, J = 3.4 Hz, 1 H), 2.91 (m, 2 H), 2.72 (m, 2 H), 2.28 (s, 1 H), 1.31 (s, 9 H), 1.11 (d, J = 6.9 Hz, 3 H), 0.98 (d, J = 6.9 Hz, 3 H); ^{13}C NMR (400 MHz, $CDCl_3$): δ = 199.8, 172.7, 165.9, 149.4, 138.5, 128.4, 125.9, 83.2, 81.7, 44.9, 34.9, 31.9, 30.9, 18.5, 16.1; HRMS (ESI) *m/z* calculated for $C_{20}H_{28}NO_3$ $[M+H]^+$: 330.20637, found: 330.20679.



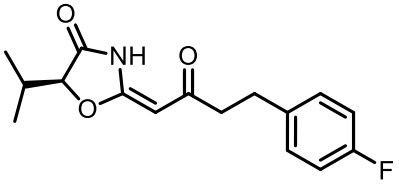
(*S*,*E*)-5-Isopropyl-2-(2-oxo-4-(4-(trifluoromethyl)phenyl)butylidene)oxazolidin-4-one (31). Yield: 91 mg (19%) of **31** as a white solid: ^{1}H NMR (400 MHz, $CDCl_3$); δ = 7.53 (d, J = 8.4 Hz, 2 H), 7.31 (d, J = 8.4, 2 H), 5.26 (s, 1 H), 4.51 (d, *J* = 3.8 Hz, 1 H), 2.99 (m, 2H), 2.75 (m, 2 H), 2.29 (m, 1 H), 1.11 (d, *J* = 6.9 Hz, 3 H), 0.97 (d, *J* = 6.9 Hz, 3 H); ^{13}C NMR (400 MHz, $CDCl_3$): δ = 198.9, 172.6, 166.0, 145.8, 129.2, 125.9, 83.3, 81.7, 44.2, 31.1, 18.5, 16.1; HRMS (ESI) *m/z* calculated for $C_{17}H_{19}F_3NO_3$ $[M+H]^+$: 342.13115, found: 342.13068.



(*S*,*E*)-2-(4-(4-Bromophenyl)-2-oxobutylidene)-5-isopropyloxazolidin-4-one (32). Yield: 68 mg (24%) of **32** as a white solid: ^{1}H NMR (400 MHz, $CDCl_3$); δ = 7.40 (d, J = 8.5 Hz, 2 H), 7.08 (d, J = 8.5 Hz, 2 H), 5.23 (s, 1 H), 4.49 (d, *J* = 3.9 Hz, 1 H), 2.89 (m, 2 H), 2.69 (m, 2 H), 2.32 (m, 1 H), 1.11 (d, *J* = 6.9 Hz, 3 H), 0.97 (d, *J* = 6.9 Hz, 3 H); ^{13}C NMR (300 MHz, $CDCl_3$): δ = 199.9, 177.9, 165.9, 141.4, 128.7, 126.5, 83.1, 81.8, 44.6, 36.0, 31.4, 18.3, 15.9; HRMS (ESI) *m/z* calculated for $C_{16}H_{19}BrNO_3$ $[M+H]^+$: 352.05428, found: 352.05410.

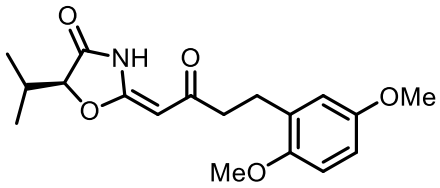


(*S*,*E*)-2-(4-(4-Chlorophenyl)-2-oxobutylidene)-5-isopropyloxazolidin-4-one (33). Yield: 113 mg (34%) of **33** as a white solid ^{1}H NMR (400 MHz, $CDCl_3$); δ = 7.22 (m, 2 H), 7.12 (m, 2 H), 5.23 (s, 1 H), 4.48 (d, *J* = 3.5 Hz, 1 H), 2.91 (m, 2 H), 2.65 (m, 2H), 2.28 (s, 1 H), 1.09 (d, *J* = 6.9 Hz, 3 H), 0.97 (d, *J* = 6.9 Hz, 3 H); ^{13}C NMR (400 MHz, $CDCl_3$): δ = 199.4, 172.9, 166.0, 139.9, 130.1, 128.9, 83.2, 81.8, 44.4, 35.8, 30.4, 18.5, 16.0; HRMS (ESI) *m/z* calculated for $C_{16}H_{19}ClNO_3$ $[M+H]^+$: 308.10480, found: 308.10503.

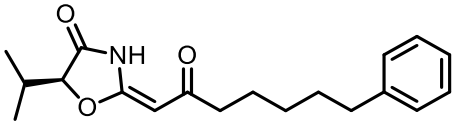


(*S*,*E*)-2-(4-(4-Fluorophenyl)-2-oxobutylidene)-5-isopropyloxazolidin-4-one (34). Yield: 197 mg (37%) of **34** as a white solid: ^{1}H NMR (400 MHz, $CDCl_3$); δ = 7.14 (m, 2 H), 6.97 (m, 2H), 5.23 (s, 1 H), 4.48 (d, *J* = 3.8 Hz, 1 H), 2.94 (m, 2 H), 2.67 (m, 2H), 2.29 (s, 1 H), 1.11 (d, *J* = 6.9 Hz, 3 H), 0.97 (d, *J* = 6.9 Hz, 3 H); ^{13}C NMR (400 MHz, $CDCl_3$): δ = 199.3, 172.7, 165.9, 137.2,

130.2, 115.6, 83.2, 81.7, 44.8, 30.6, 18.5, 16.1; HRMS (ESI) *m/z* calculated for $C_{16}H_{19}FNO_3$ $[M+H]^+$: 292.13435, found: 292.13414.



(*S*,*E*)-2-(4-(2,5-diMethoxyphenyl)-2-oxobutylidene)-5-isopropyloxazolidin-4-one (35). Yield: 54 mg (16%) of **35** as an oil: ^{1}H NMR (400 MHz, $CDCl_3$); δ = 6.72 (m, 3H), 5.26 (s, 1 H), 4.46 (d, *J* = 3.8 Hz, 1 H), 3.77 (s, 6 H), 2.88 (m, 2 H), 2.69 (m, 2H), 2.27 (m, 1 H), 1.09 (d, *J* = 6.9 Hz, 3 H), 0.95 (d, *J* = 6.9 Hz, 3 H); ^{13}C NMR (300 MHz, $CDCl_3$): δ = 199.5, 172.1, 165.1, 153.2, 151.5, 130.4, 116.1, 110.9, 82.5, 81.0, 55.5, 42.6, 30.4, 26.0, 17.8, 15.4; HRMS (ESI) *m/z* calculated for $C_{18}H_{24}NO_5$ $[M+H]^+$: 334.16490, found: 334.16466.



(*S*,*E*)-5-Isopropyl-2-(2-oxo-7-phenylheptylidene)oxazolidin-4-one (36). Yield: 117 mg (49%) of **36** as an oil: ^{1}H NMR (400 MHz, $CDCl_3$); δ = 7.28 (m, 2 H), 7.17 (m, 3 H), 5.35 (s, 1 H), 4.58 (d, *J* = 3.9 Hz, 1 H), 2.60 (m, 2 H), 2.43 (m, 2 H), 2.31 (m, 1 H), 1.65 (m, 4 H), 1.40 (m, 2 H), 1.14 (d, *J* = 6.9 Hz, 3 H), 1.00 (d, *J* = 6.9 Hz, 3 H); ^{13}C NMR (400 MHz, $CDCl_3$): δ = 200.9, 172.8, 165.9, 143.0, 128.8, 126.1, 83.1, 81.6, 43.3, 36.2, 31.7, 31.0, 29.4, 25.6, 18.4, 16.1; HRMS (ESI) *m/z* calculated for $C_{19}H_{26}NO_3$ $[M+H]^+$: 316.19072, found: 316.19081.

Biological data, bacterial strains and assay protocols

General information

Methicillin-resistant *Staphylococcus aureus* (MRSA) strains were obtained from the ATCC (33591) and colonies were grown on solid media as instructed. *Escherichia coli* strains were obtained from Dr. Alexander Mankin (University of Illinois Chicago) and colonies were grown on solid media as instructed.

Mueller-Hinton broth (MHB, 211443-BD) and tryptic soy broth (TSB, Remel: R455052) were purchased from Fisher Scientific. Tryptic soy agar (TSA, cat. # 22091) and Linezolid (cat. # P70014) were purchased from Sigma-Aldrich. All assays were run in duplicate and repeated at least two separate times for MIC assays. All compounds were dissolved in molecular biology grade DMSO as 10 mM stock solutions. Optical densities were measured using a Thermo Scientific Genesys 20 spectrophotometer.

Broth microdilution method for determination of minimum inhibitory concentration (MIC)[6]

MSSA and MRSA were grown in MHB for 6-8 h; this culture was used to inoculate fresh MHB (5 x 10^5 CFU/mL). *E. coli* was grown in LB for 6-8 h; this culture was use to inoculate fresh MHB. The resulting bacterial suspension was aliquoted (1 mL) into 1.5 mL tubes and compound was added from a 10 mM DMSO stock to achieve the desired initial starting concentration (typically 128 μg/mL). Linezolid (from a 10 mM DMSO stock) was used as a positive control.

Inoculated media not treated with compound served as the negative control. Rows 2-12 of a 96-well microtiter plate were filled at 100 µL/well from the remaining inoculated media. The samples containing test compounds and linezolid were then aliquoted (200 µL) into the corresponding first row wells of the microtiter plate (two wells for each compound and two negative controls). Row 1 wells were mixed 6 to 8 times, then 100 µL was transferred to row 2. Row 2 wells were mixed 6 to 8 times, followed by a 100 µL transfer from row 2 to row 3. This procedure was repeated to serially dilute the rest of the rows of the microtiter plate. The plate was then covered and sealed with GLAD Press'n Seal® and incubated under stationary conditions at 37 °C. After 16 h, minimum inhibitory concentration (MIC) values were recorded as the lowest concentration of compound at which no visible growth of bacteria was observed.

A549 Cell Toxicity

Cell toxicity studies were performed by Dr. Melanie Cushion's lab (University of Cincinnati College of Medicine) as part of a NIAID contract. Compound Preparation: Compounds were stored at -80 °C without exposure to light. Just prior to testing, the compounds were solubilized in DMSO for a 20 mg/mL stock solution. Unused portions were stored at -20 °C. ATP quench control assay indicated that these compounds did not interfere with the luciferin/luciferase reaction at ≤ 100µg/mL concentrations. A549 Toxicity assay: Cultured cells were plated at $2x10^5$/mL and grown to confluent monolayers. Media were removed and replaced with fresh media containing controls and test compound dilutions. Triplicate assays of 3-time points (24, 48, 72 hours) with triplicate wells were tested for viability. Media was aspirated from the wells, adherent cells were lysed with 0.1 M NaOH, and a portion of the lysate was assayed for ATP using the Perkin Elmer ATP-liteM luciferin-luciferase assay. Compounds between 10.1 and 99.9 µg/mL are considered to be mildly toxic.

Table S1. A549 Toxicity Results average of 3 assays.

A549 toxicity tests of KRR_35 and 21 resulted in toxicity measurements of moderate (9.86 µg/ml) and mild (14.19 µg/ml) respectively in cultured cells after 72 hours exposure.

***A549* %reduction in ATP/media control**

	24 hour	48 hour	72 hour
Antimycin A 75µg/ml	25+/-0.115	44+/-0.077	46+/-0.123
5 100µg/ml	100+/-0.002	100+/-0.0007	100+/-0.003
10µg/ml	11 +/-0.054	37 +/-0.234	34 +/-0.232
1µg/ml	0	0	0
0.1µg/ml	0	0	0
IC50			9.86ug/ml
21 100µg/ml	74+/-0.156	88 +/-0.089	91+/-0.081
10µg/ml	4 +/-0.108	23+/-0.220	30+/-0.180
1µg/ml	0	0	0
0.1µg/ml	0	0	0
IC50			14.19ug/ml

References

[1] Nakajima, M.; Watanabe B.; Han, L.; Shimizu, B.; Wada, K.; Fukuyama, K.; Suzuki, H.; Hiratake, J. *Bioorg. Med. Chem.* **2014**, *22*, 1176.

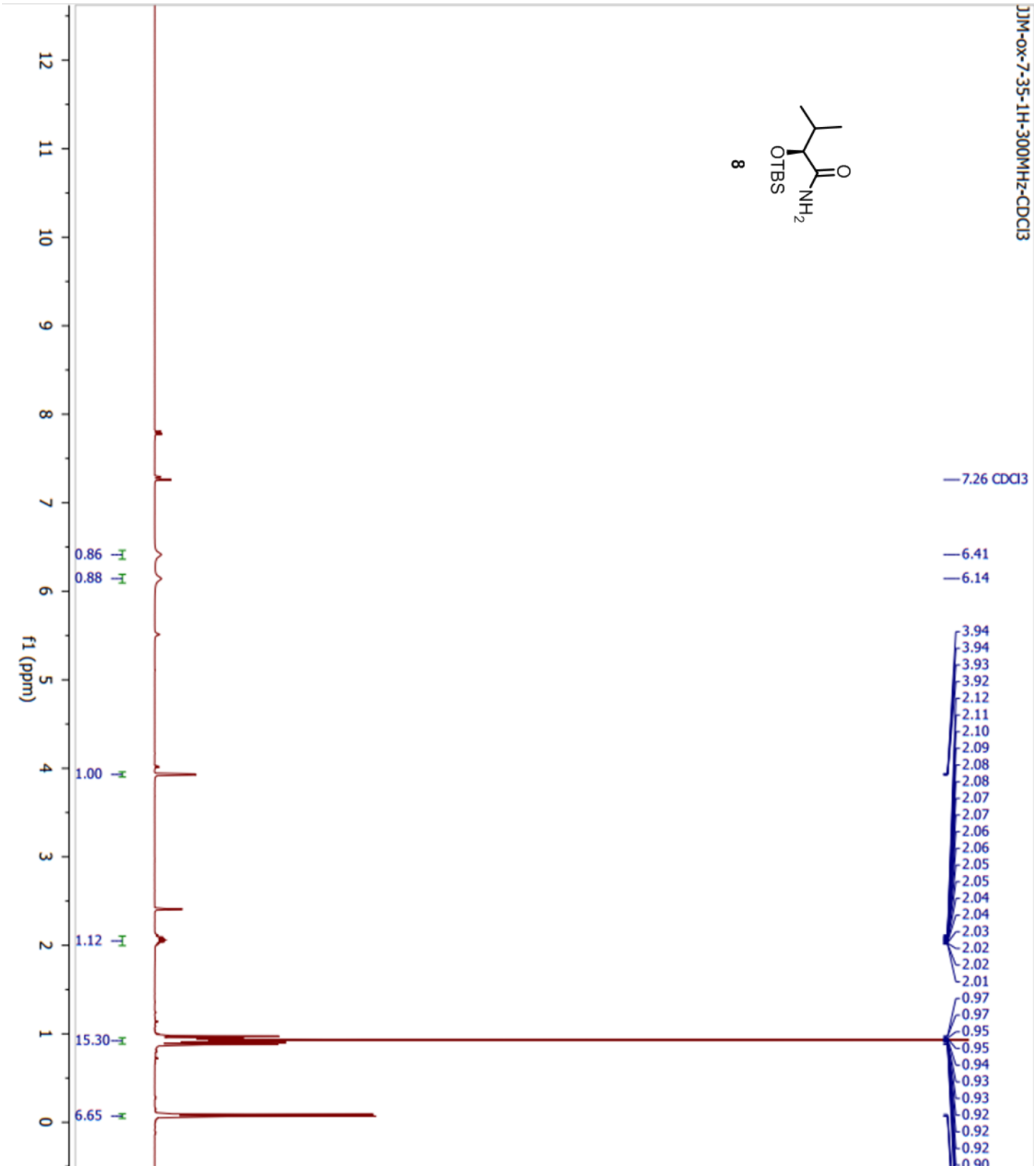
[2] Khalafi-Nezhad, A.; Parhami, A.; Rad, M. N. S.; Zarea, A. *Tetrahedron Lett.* **2005**, *46*, 6879.

[3] Silica gel (5.0 g) was mixed with a solution of ammonium chloride (20 mmol) in water (5.0 mL). Evaporation of water under reduced pressure gave a dry white powder, which was used as the amine source.

[4] Knoth, T; Warburg, K.; Katzka, C.; Rai, A.; Wolf, A.; Brockmeyer, A.; Janning, P.; Reubold, T. F.; Eschenburg, S.; Manstein, D.J.; Huebel, K.; Kaiser, M.; Waldmann, H. *Angew. Chem. Int. Ed.* **2009**, *48*, 7240.

[5] Rahaim, R.J.; Maleczka, R.E. *Org. Lett*. **2005**, *7*, 5087.

[6] Clinical Laboratory and Standards Institute (CLSI). *Methods for Dilution Antimicrobial Susceptibility Tests for Bacteria That Grow Aerobically; Approved Standard—Tenth Edition*. CLSI document M07-A10 [ISBN 1-56238-988-2]. CLSI, 950 West Valley Road, Suite 2500, Wayne, Pennsylvania 19087 USA, 2015.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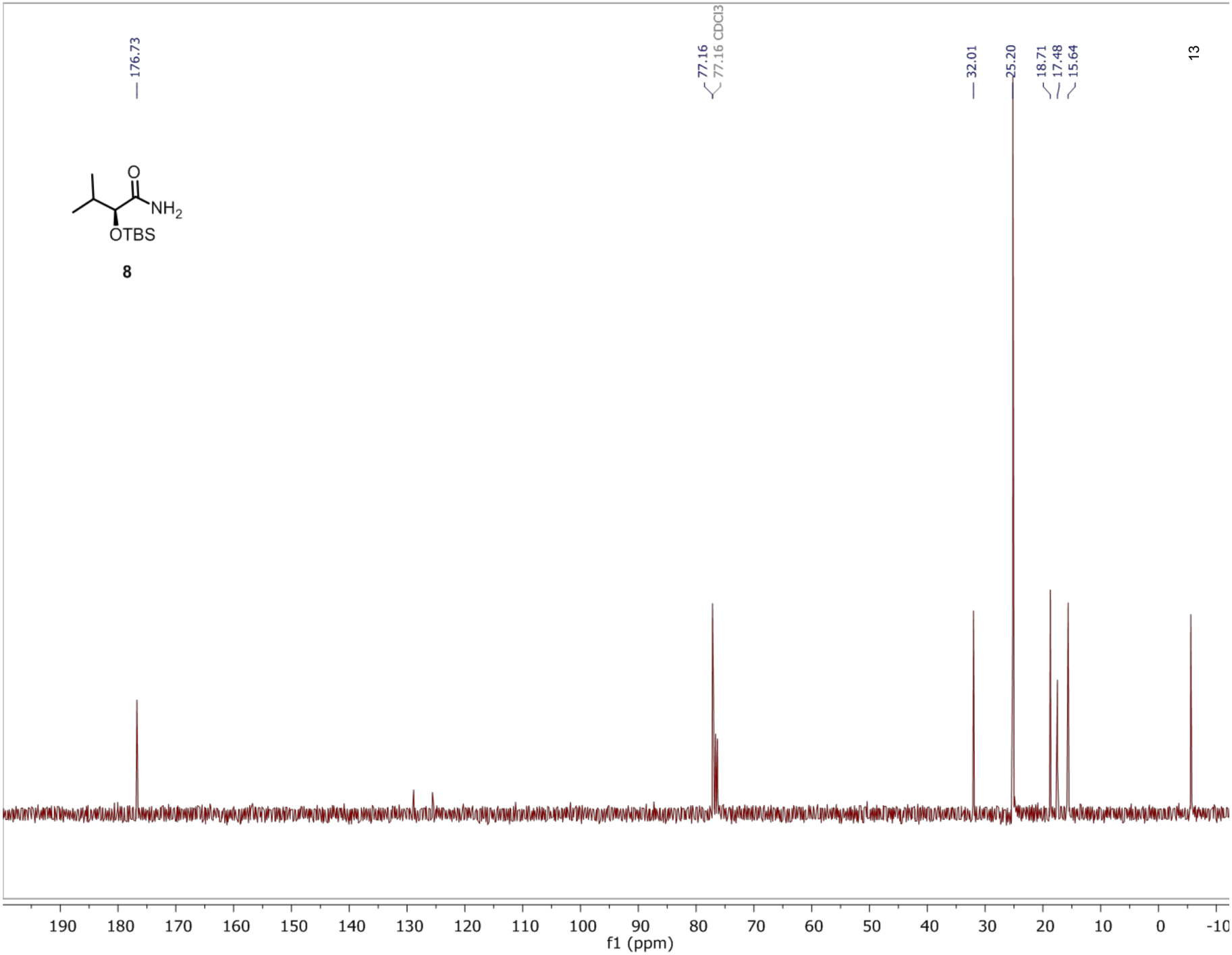
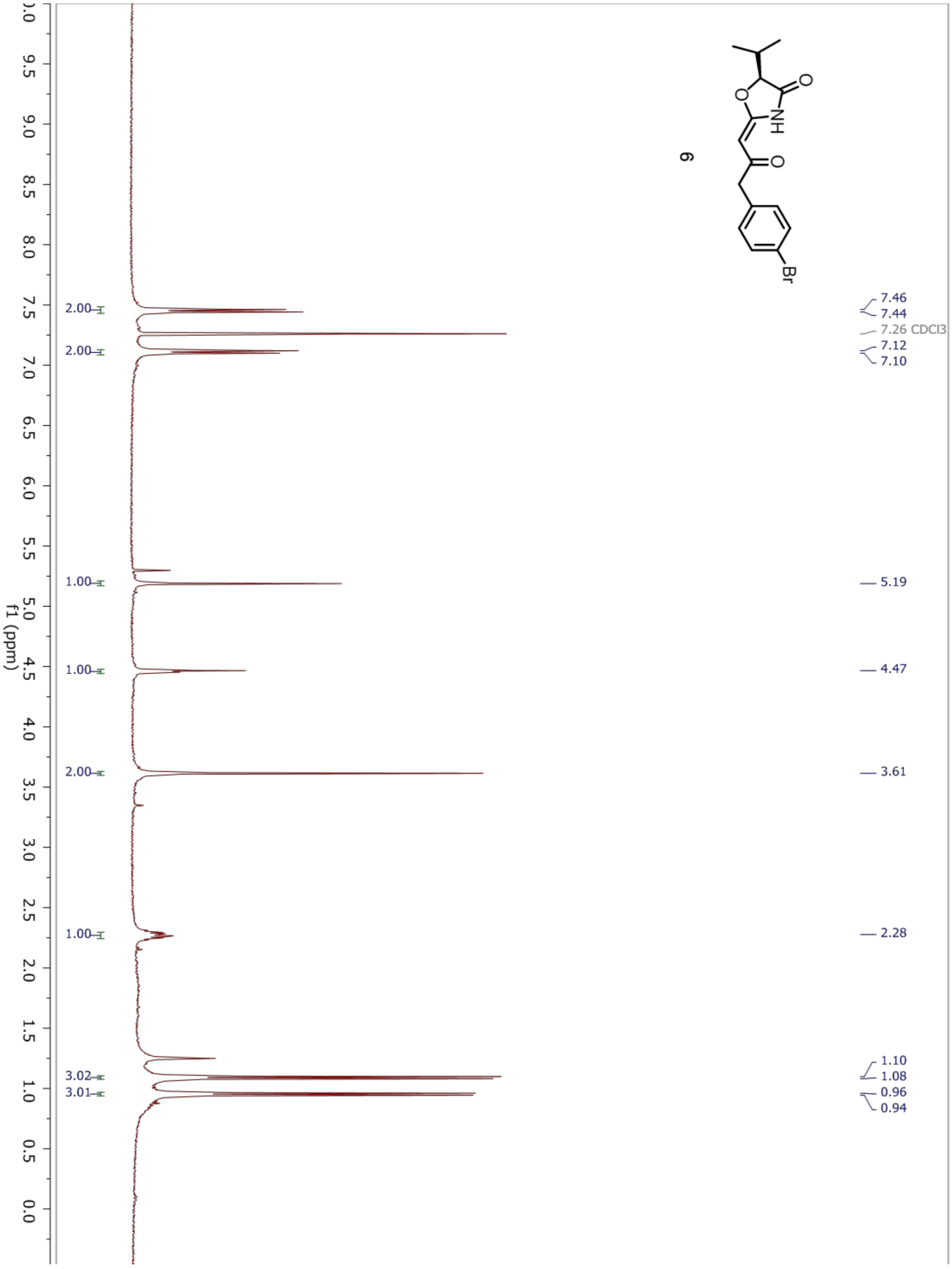
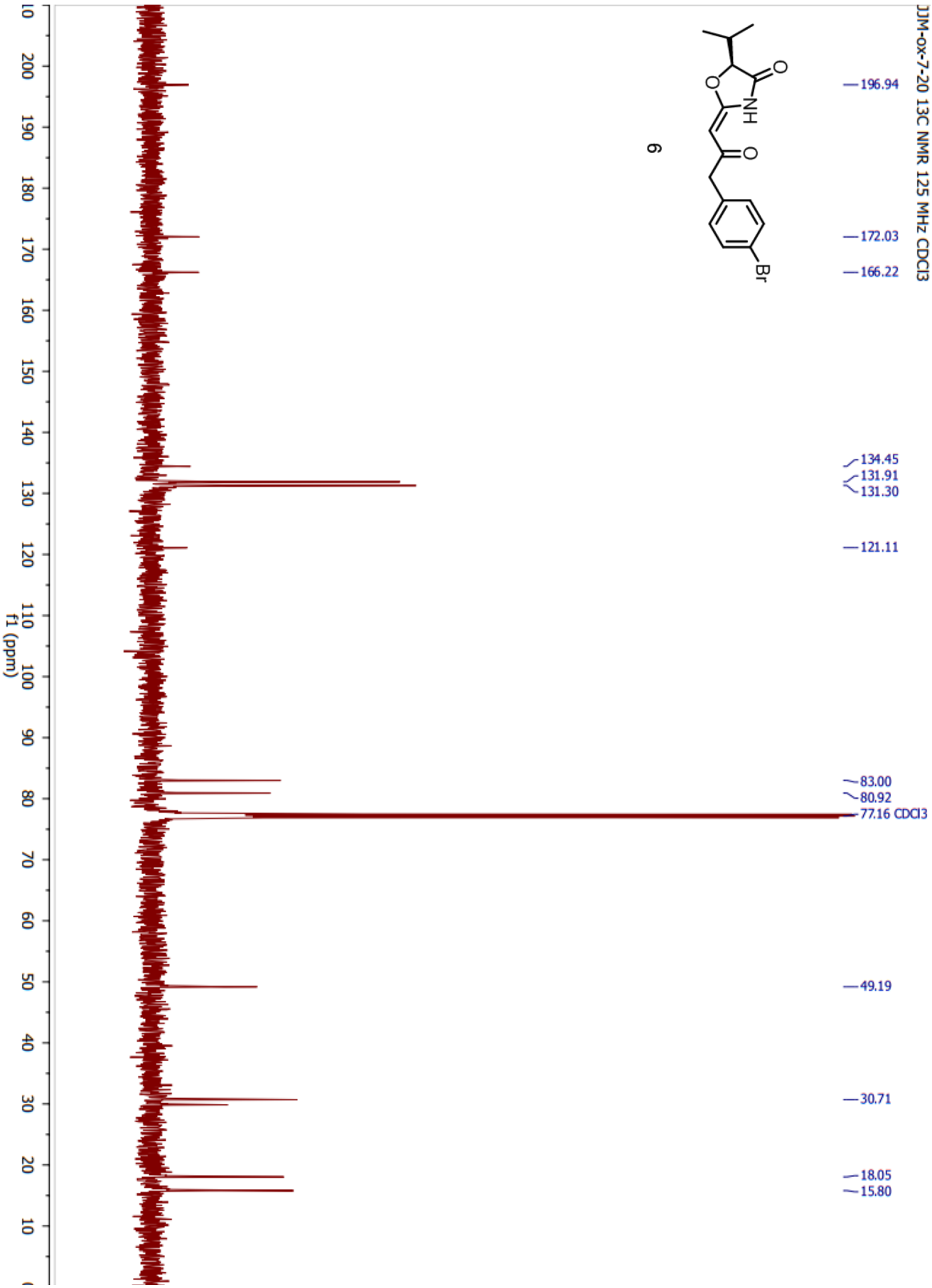
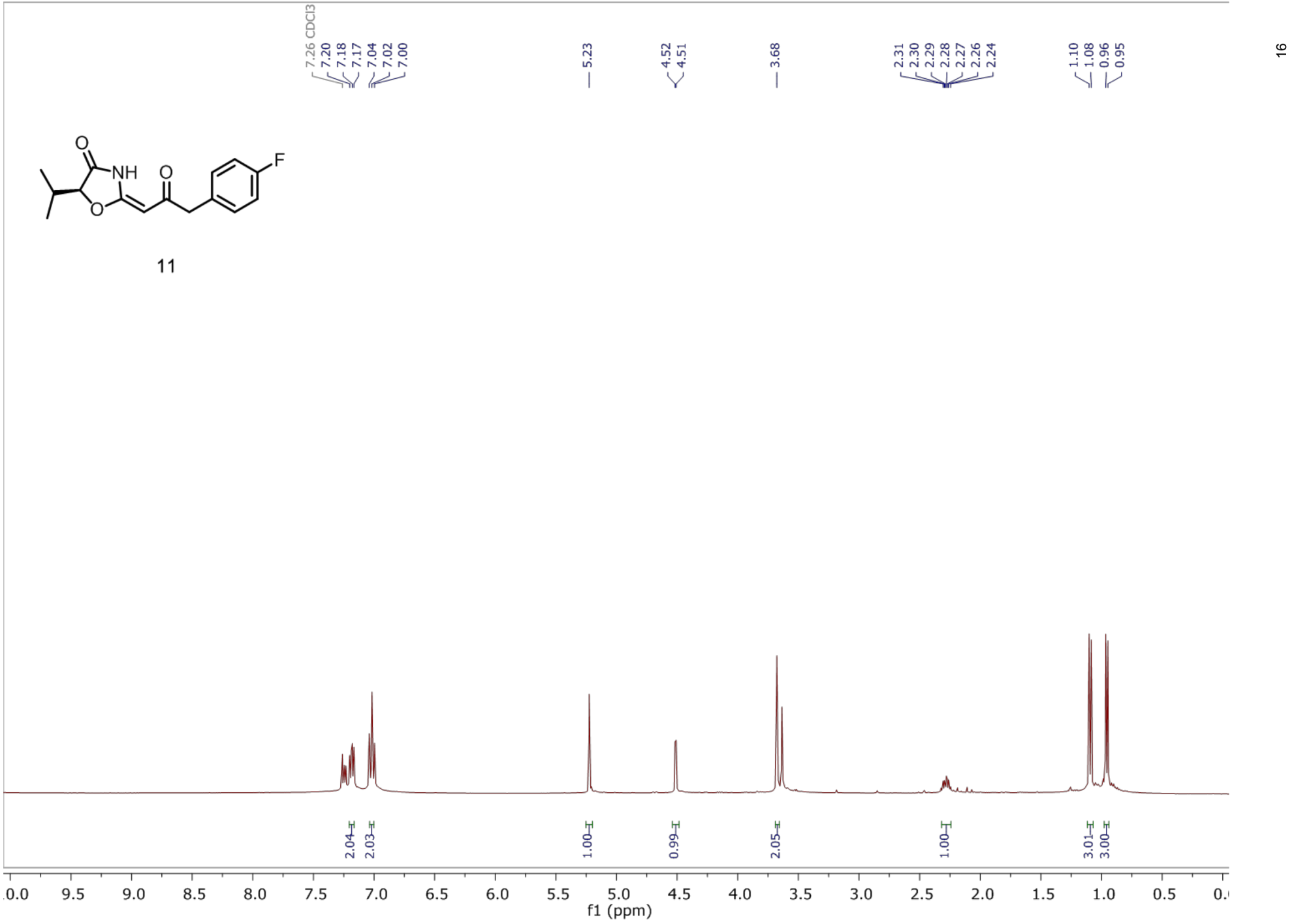
TEZ-02-20-13C-NMR-100MHz-CDCl3-03-02-2016




JJM-ox-7-20-1H-400MHz-CDCl3
6
O
NH
O
O
Br
7.46
7.44
7.26 CDCl3
7.12
7.10
5.19
4.47
3.61
2.28
1.10
1.08
0.96
0.94
2.00
2.00
1.00
1.00
2.00
1.00
3.02
3.01
f1 (ppm)


JJM-ox-7-20 13C NMR 125 MHz CDCl3
6
NH
O
O
O
Br
196.94
172.03
166.22
134.45
131.91
131.30
121.11
83.00
80.92
77.16 CDCl3
49.19
30.71
18.05
15.80
f1 (ppm)

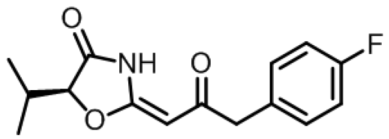
KR0612A_1H_CDCl3_400MHz_11_21_17



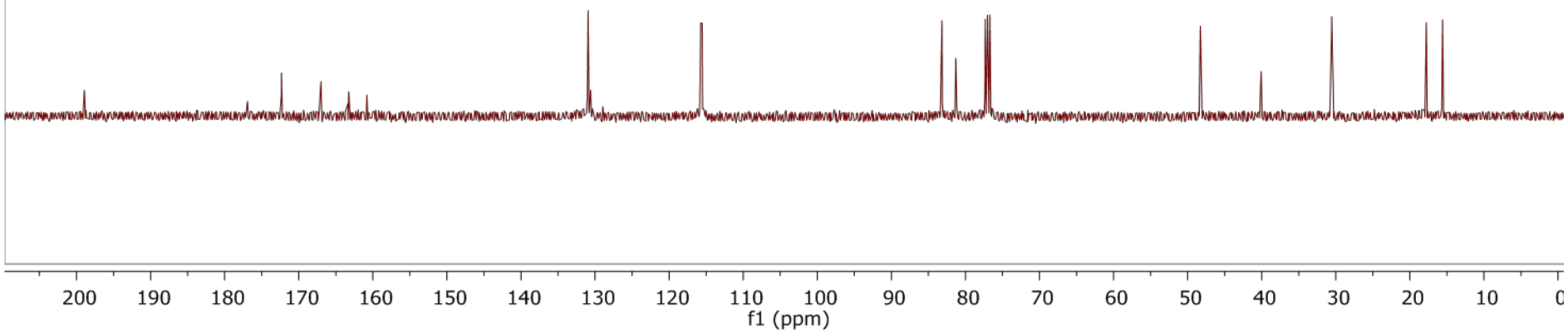
11

KR0612A_13C_CDCl3_400MHz_11_27_17

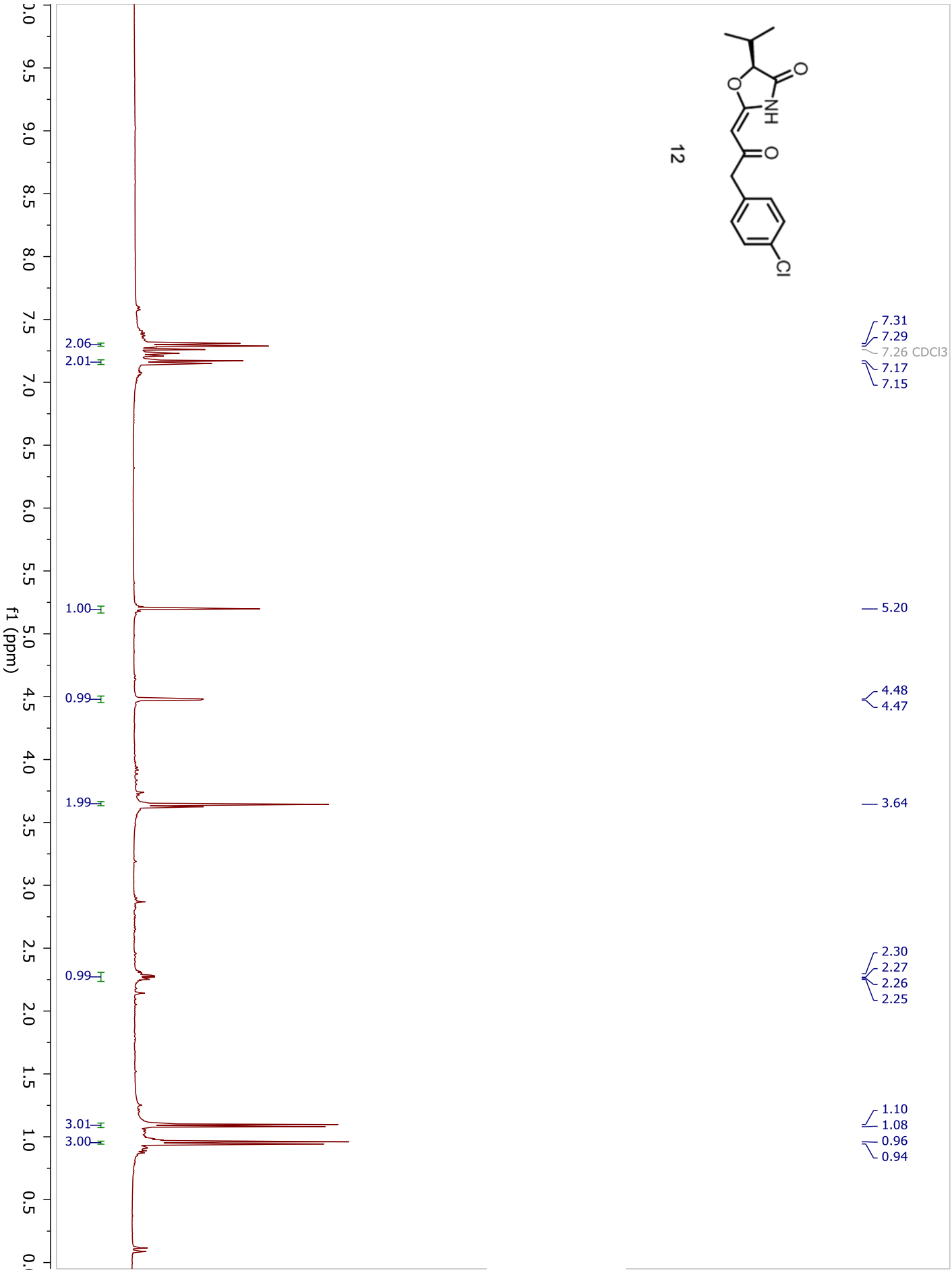
198.95
172.34
167.01
163.25
130.93
115.53
83.16
81.31
76.70 CDCl3
48.29
30.55
17.78
15.59



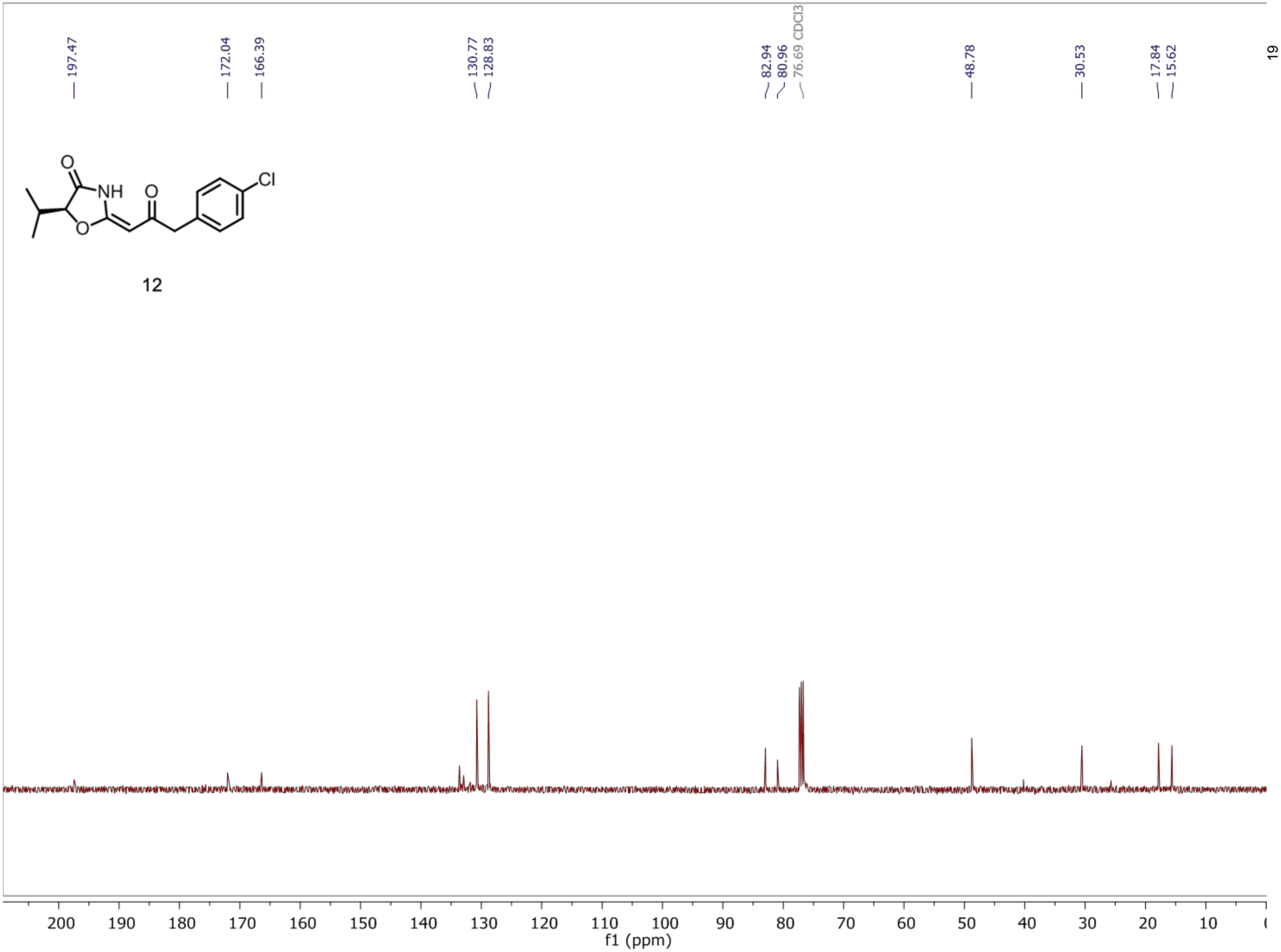
11



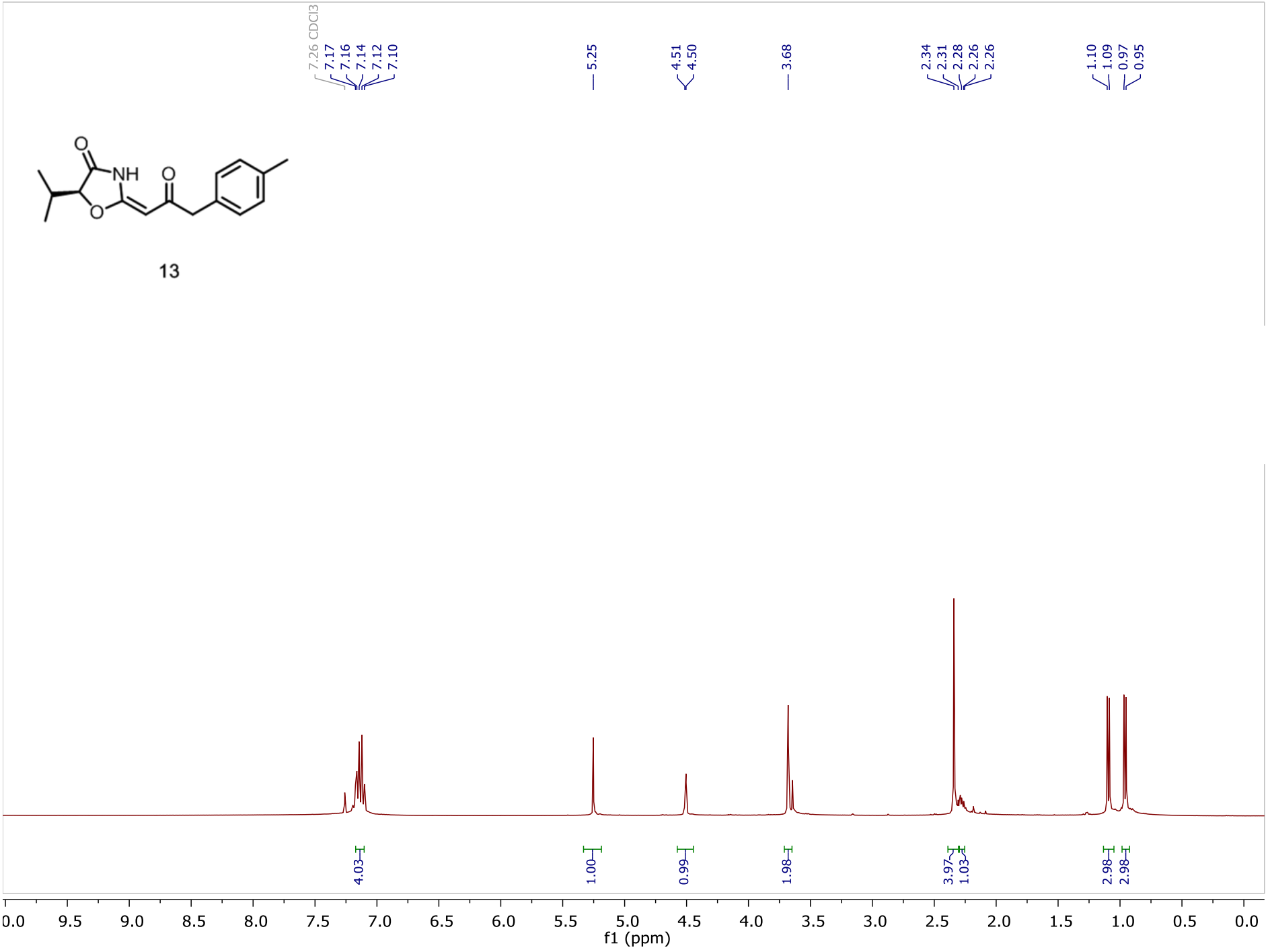
17

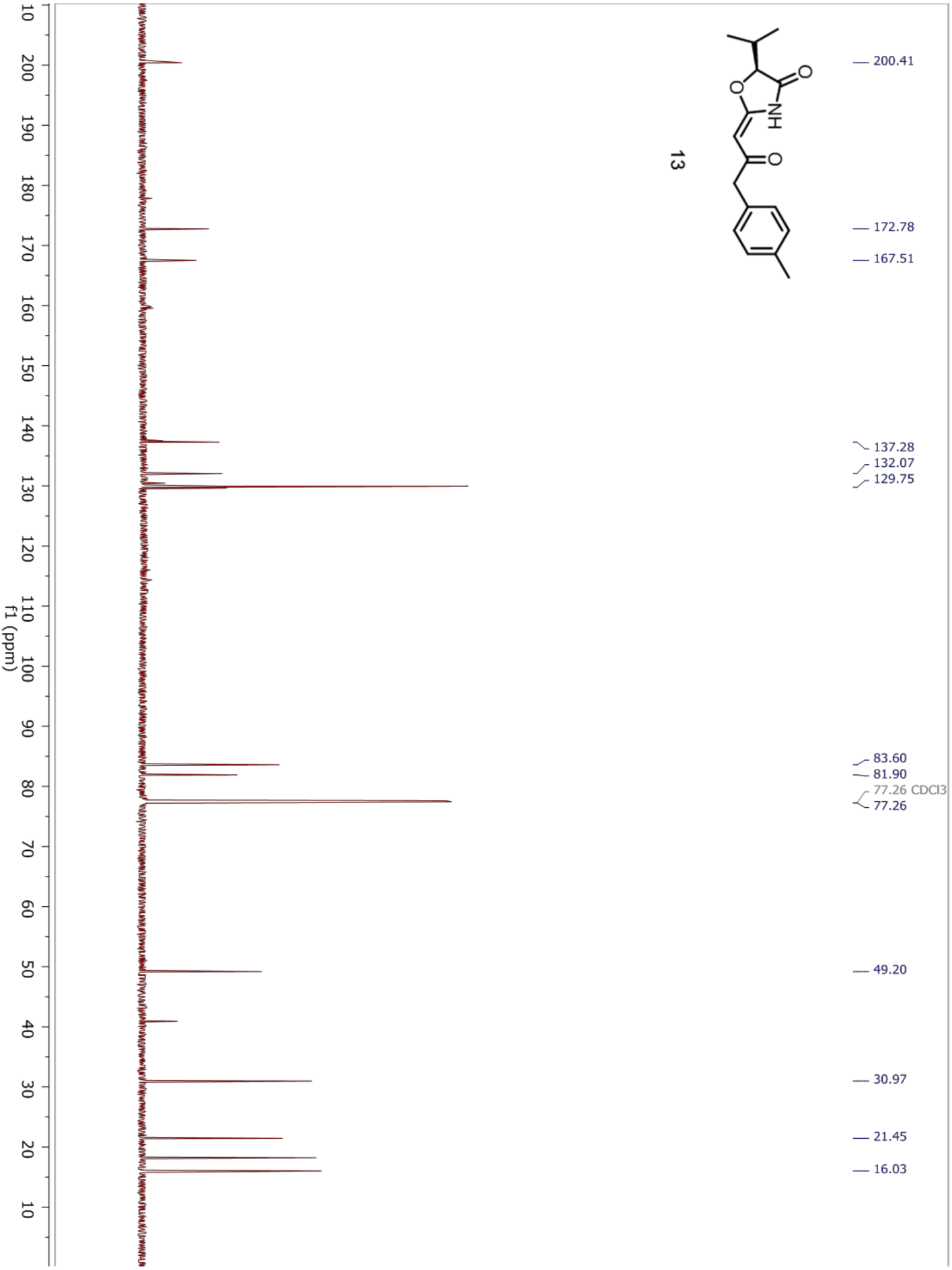

KR0613A_1H_CDCl3_400MHz_11_21_17
12
NH
O
O
O
Cl
7.31
7.29
7.26 CDCl3
7.17
7.15
5.20
4.48
4.47
3.64
2.30
2.27
2.26
2.25
1.10
1.08
0.96
0.94
2.06
2.01
1.00
0.99
1.99
0.99
3.01
3.00
f1 (ppm)

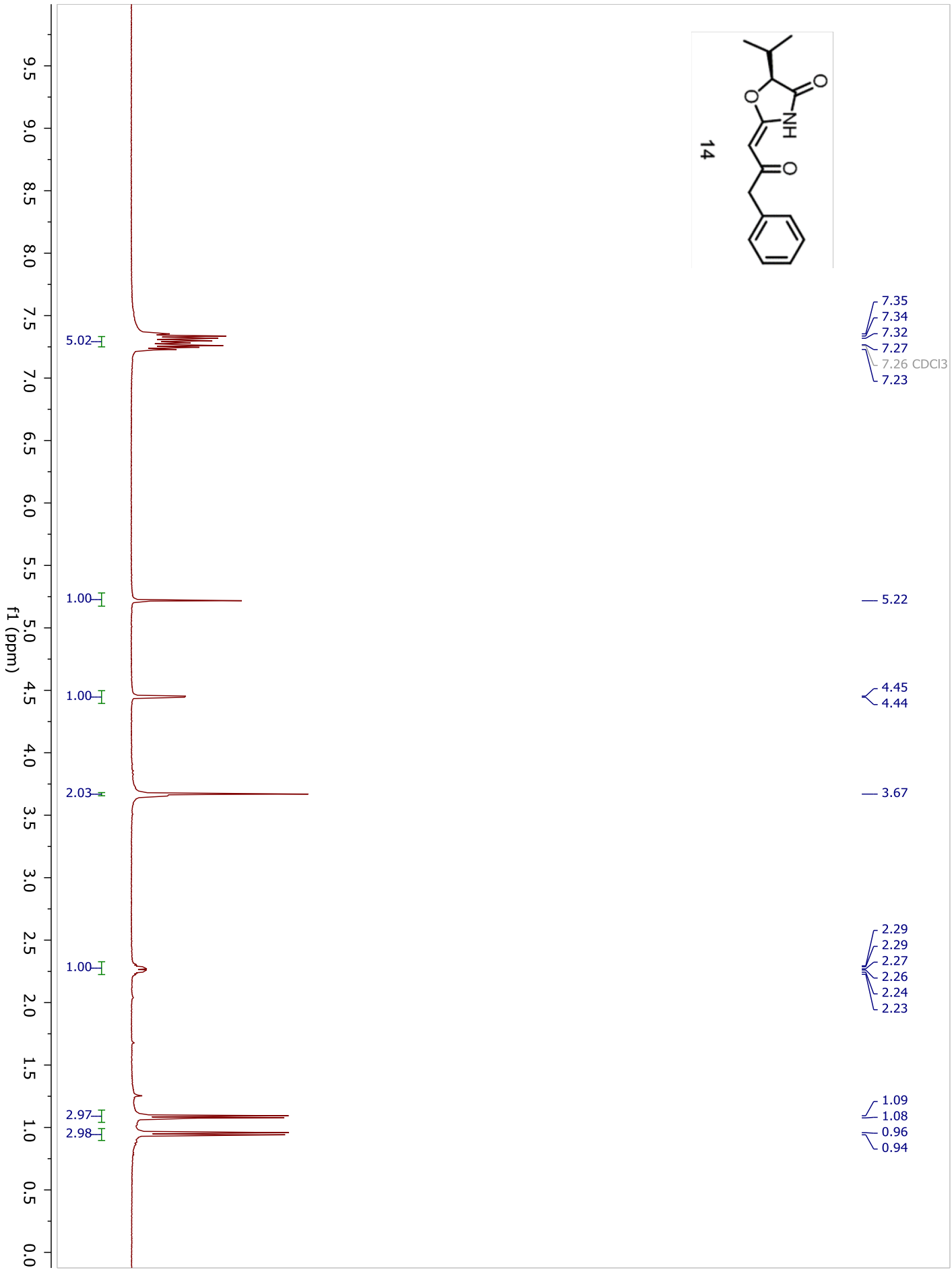
KR0613A_13C_CDCl3_400MHz_11_29_17

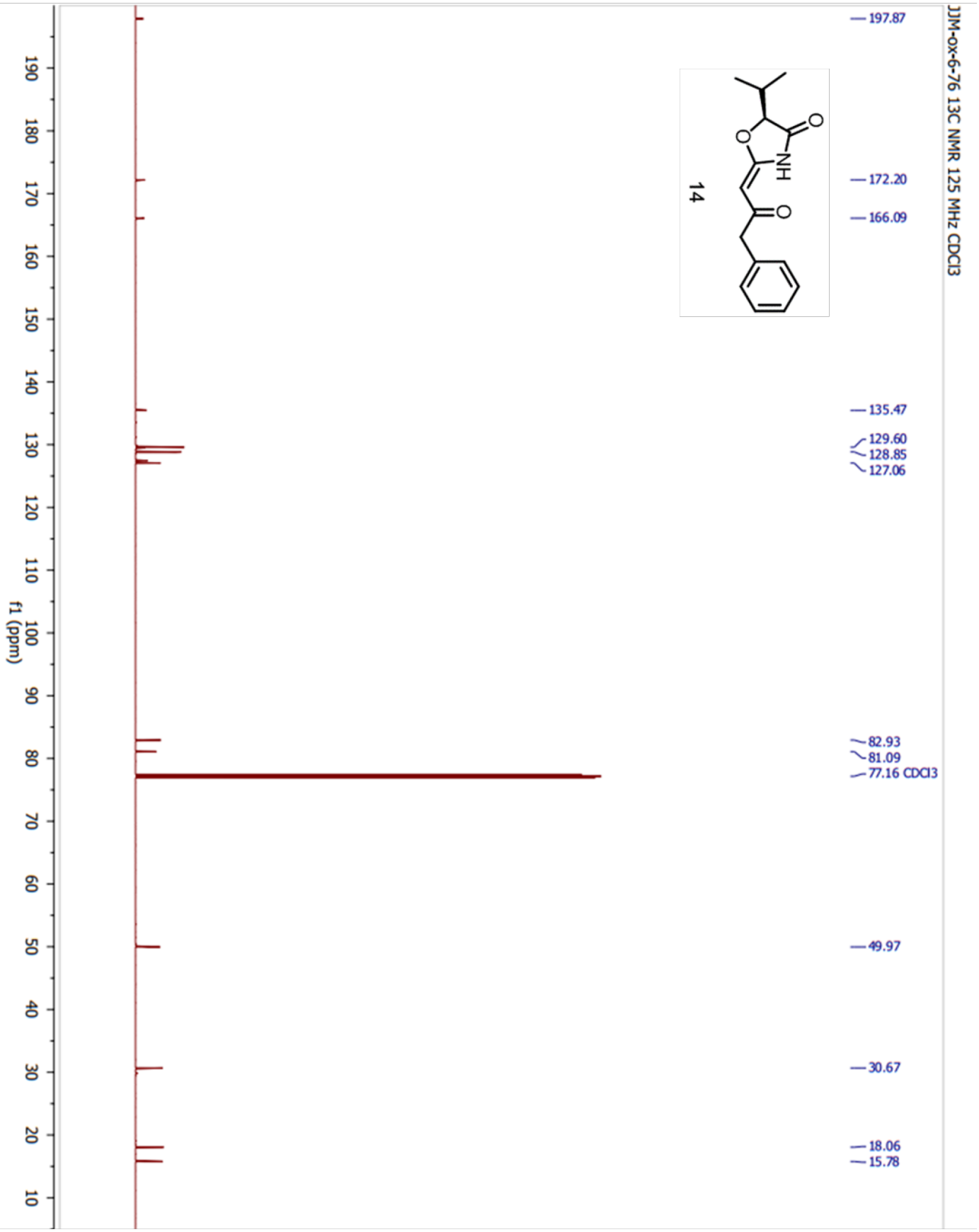


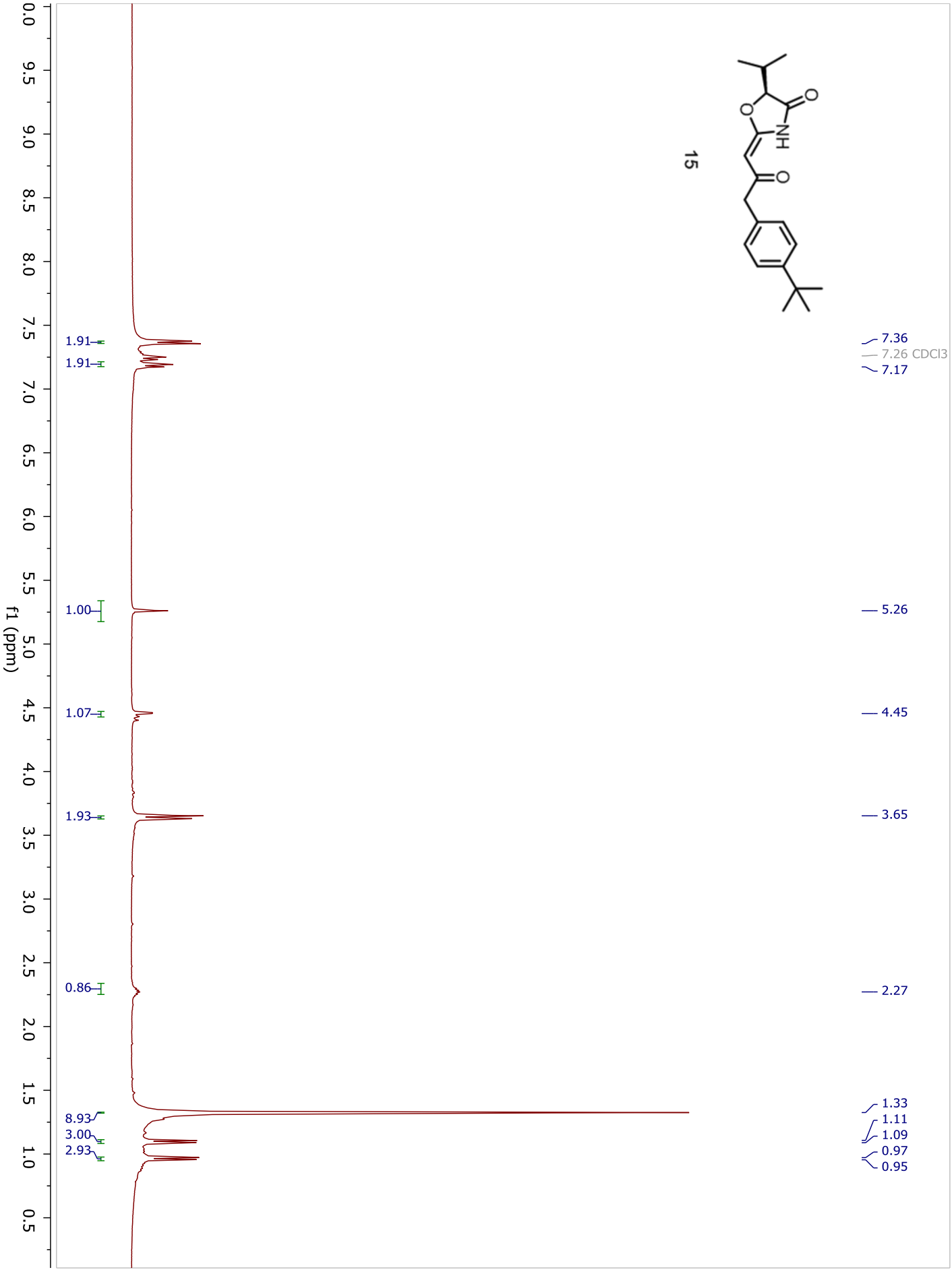
KR0620A_1H_CDCl3_400MHz_11_21_17



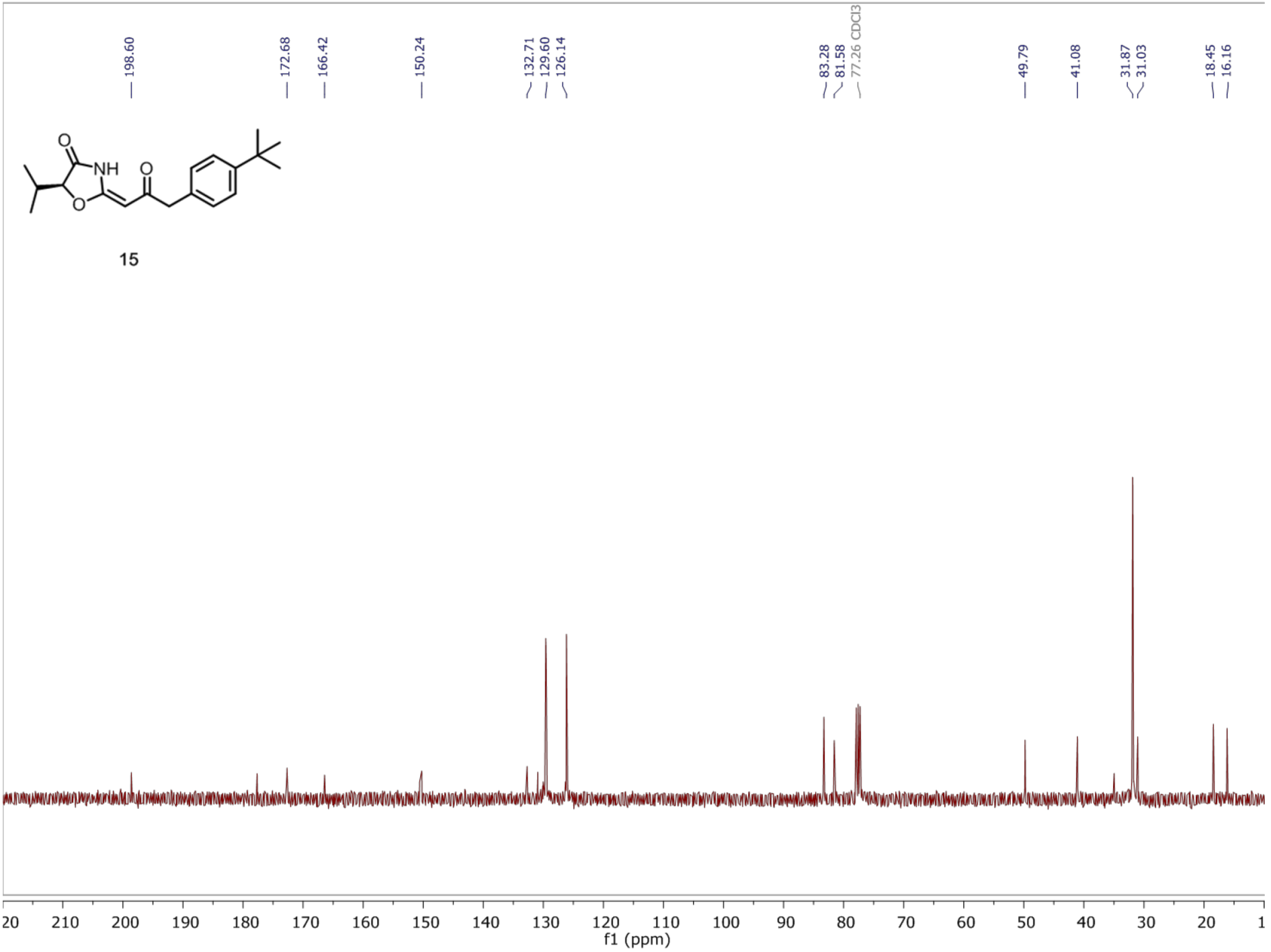

KR0620A.2.fid
13
NH
O
O
O
200.41
172.78
167.51
137.28
132.07
129.75
83.60
81.90
77.26 CDCl3
77.26
49.20
30.97
21.45
16.03
f1 (ppm)
10
20
30
40
50
60
70
80
90
100
110
120
130
140
150
160
170
180
190
200
10


JJM-ox-6-76-1H-400MHz-CDCl3
14
NH
O
O
O
f1 (ppm)
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
5.02
1.00
1.00
2.03
1.00
2.97
2.98
7.35
7.34
7.32
7.27
7.26 CDCl3
7.23
5.22
4.45
4.44
3.67
2.29
2.29
2.27
2.26
2.24
2.23
1.09
1.08
0.96
0.94

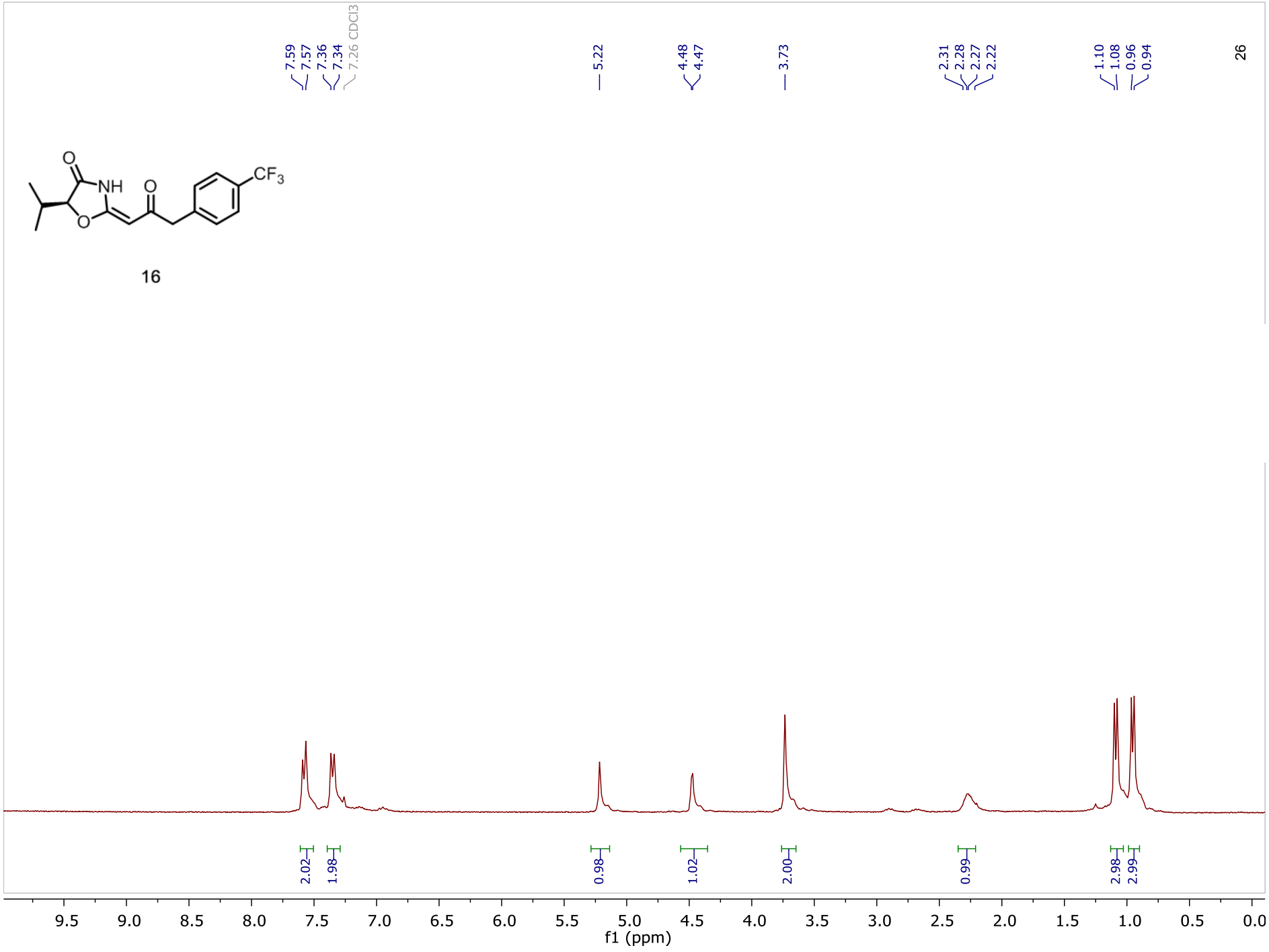

JJM-ox-6-76 13C NMR 125 MHz CDCl3
14
197.87
172.20
166.09
135.47
129.60
128.85
127.06
82.93
81.09
77.16 CDCl3
49.97
30.67
18.06
15.78
f1 (ppm)


KR0668A_1H_CDCl3_400MHz_2_19_18
15
f1 (ppm)
0.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
1.91
1.91
1.00
1.07
1.93
0.86
8.93
3.00
2.93
7.36
7.26 CDCl3
7.17
5.26
4.45
3.65
2.27
1.33
1.11
1.09
0.97
0.95

KR0668A_13C_CDCl3_400MHz_2_19_18



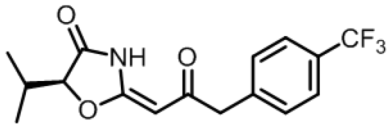
KR0614X2A_1H_CDCl3_300MHz_1_22_1



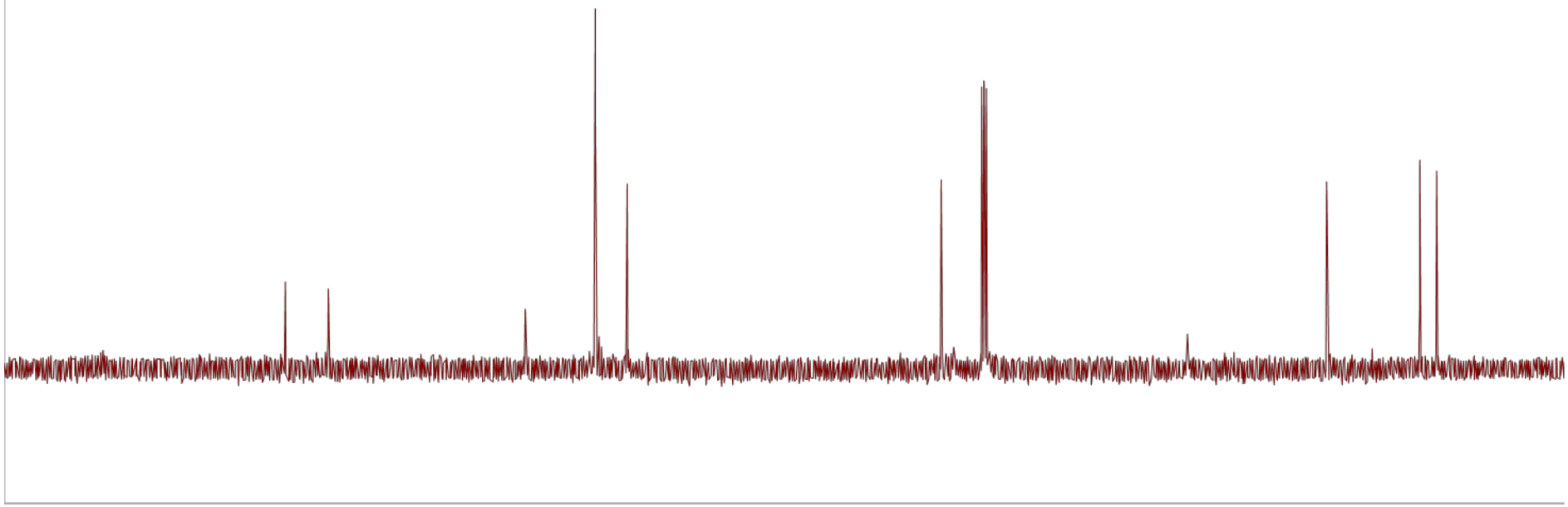
KR0614x2A_13C_400MHz_CDCl3_01_03_18

197.21
172.46
166.62
139.88
130.35
126.03
83.40
81.71
77.26 CDCl3
49.99
31.06
18.41
16.12

27



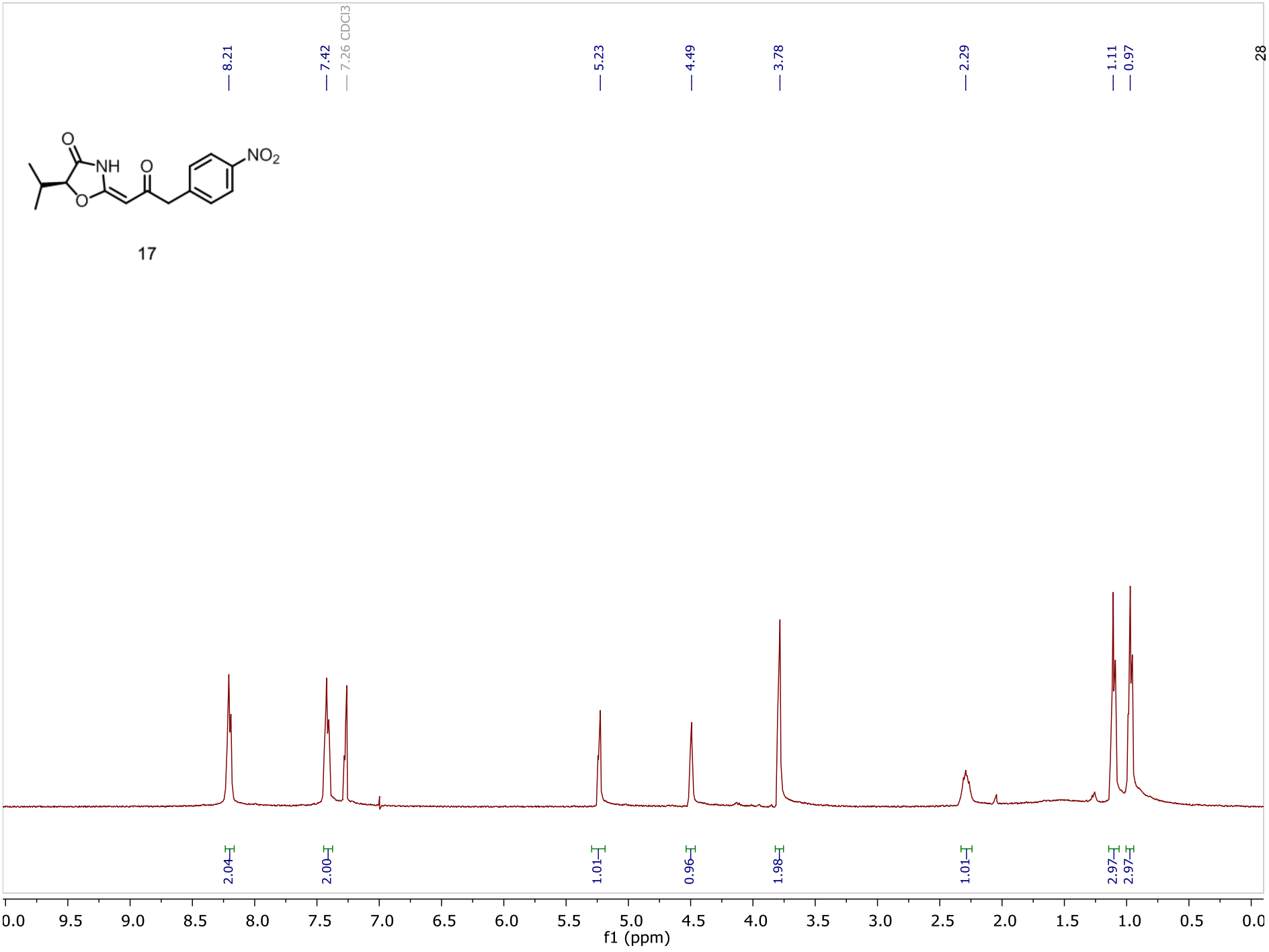
16

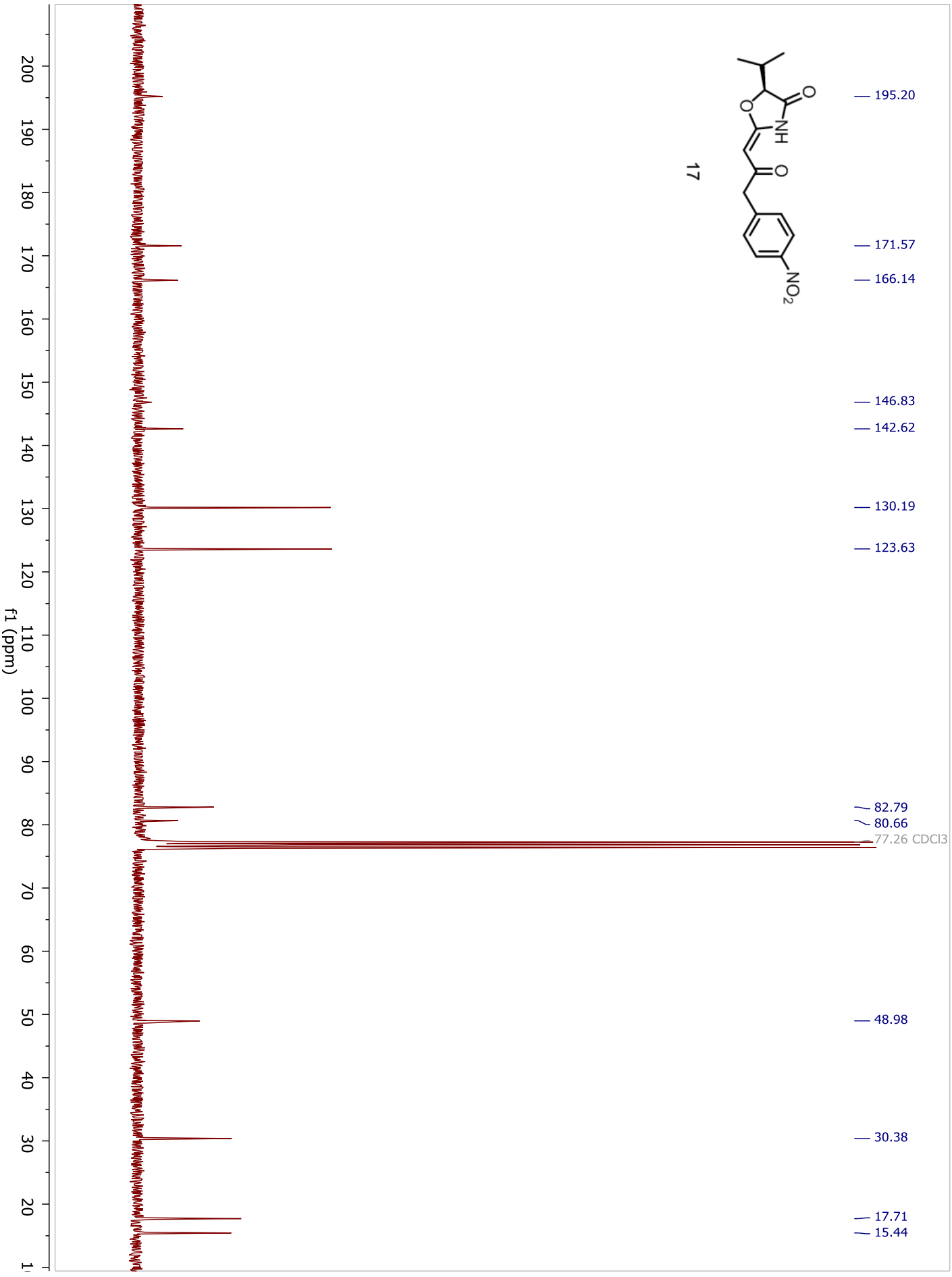


210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0

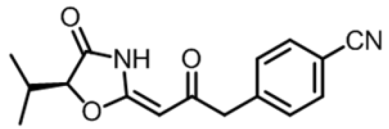
f1 (ppm)

KR0431A_1H_CDCl3_400MHz_5_15_17



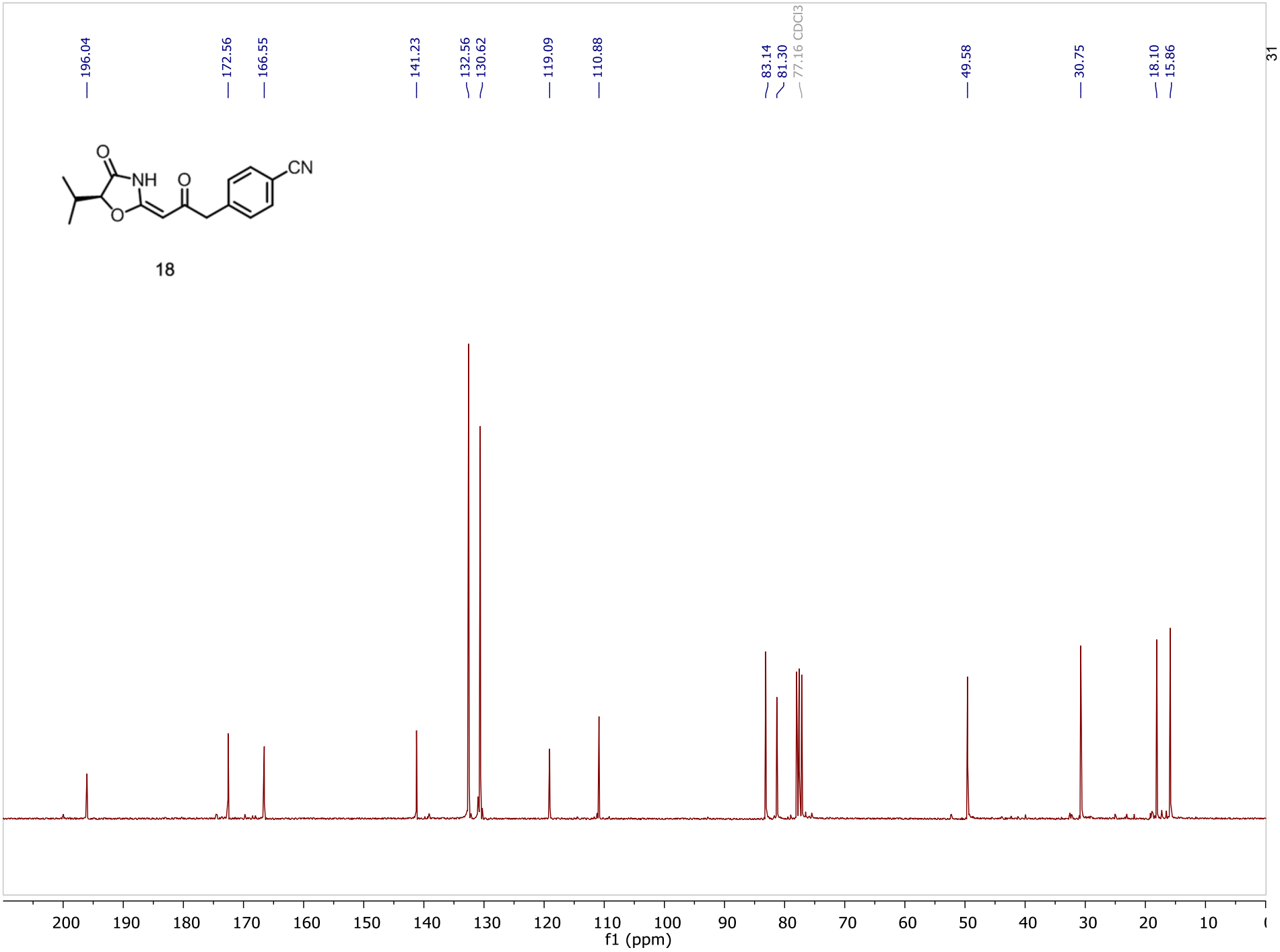

KR0431A_13C_CDCl3_300MHz_10_14_17
17
195.20
171.57
166.14
146.83
142.62
130.19
123.63
82.79
80.66
77.26 CDCl3
48.98
30.38
17.71
15.44
f1 (ppm)

KR0444A_1H_CDCl3_400MHz_5_15_17

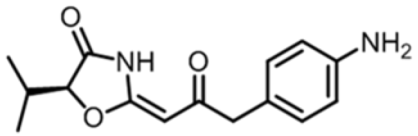


18

KR0444A_13C_CDCl3_300MHz_10_12_17

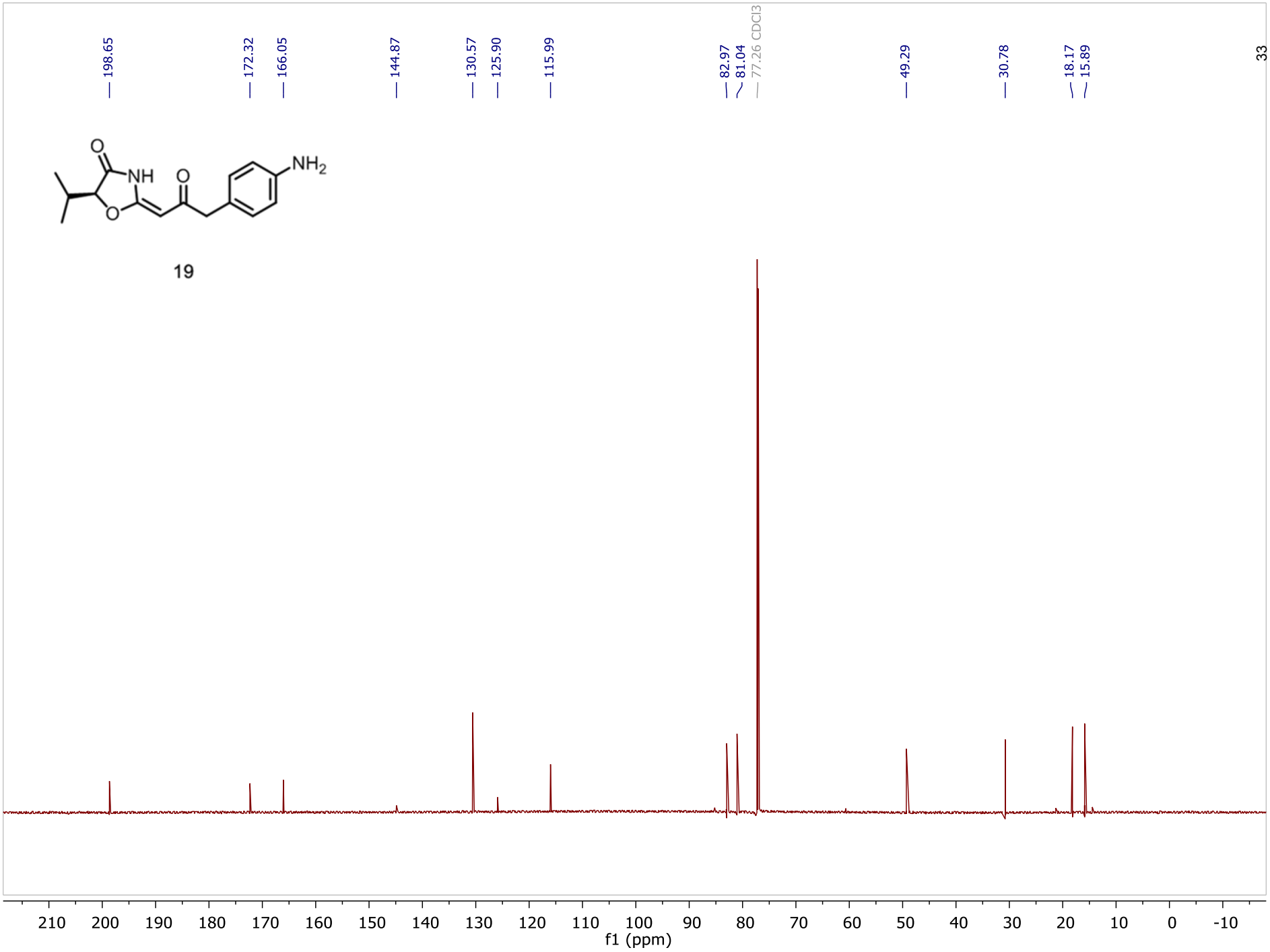


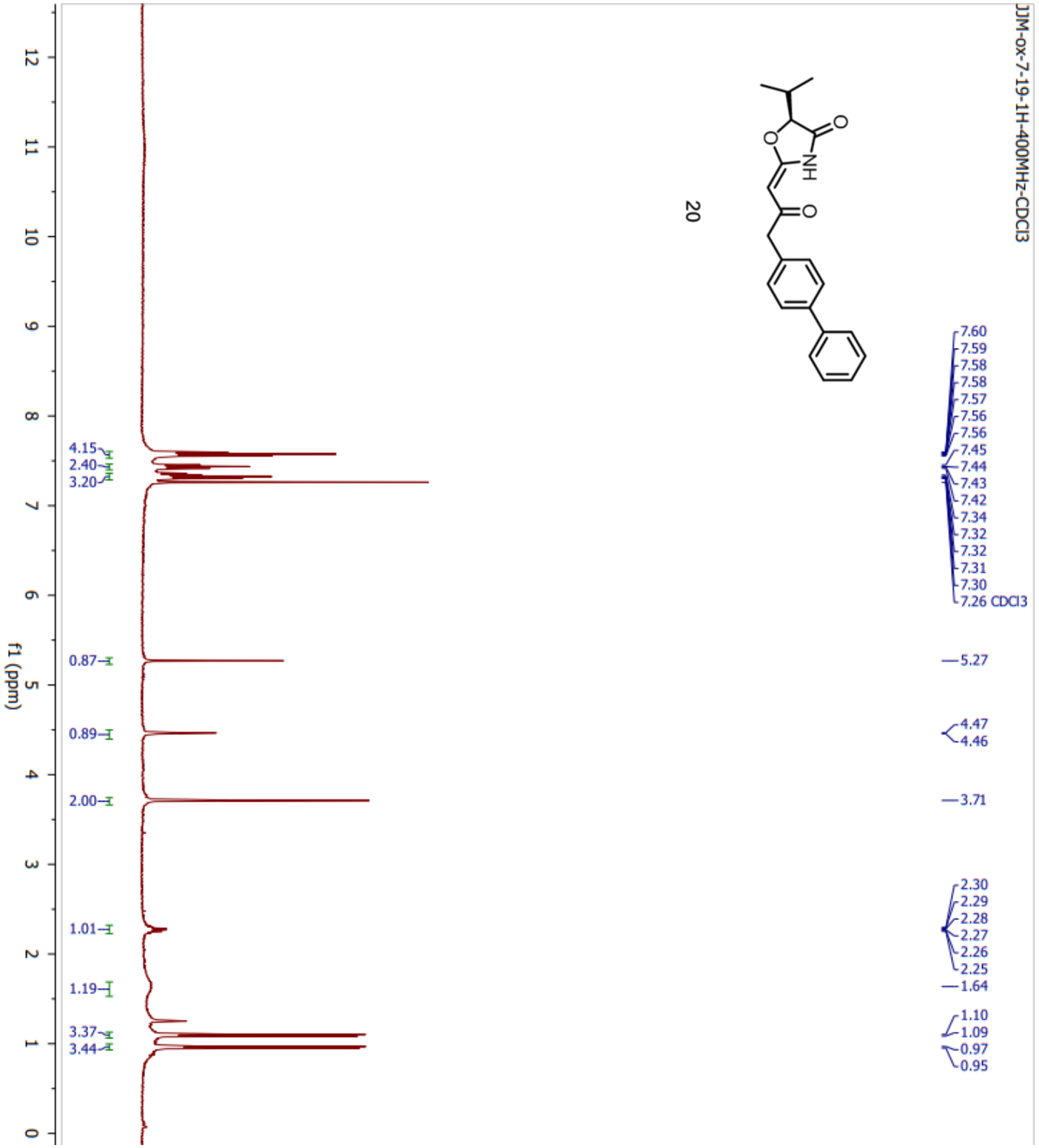
KR0542_1H_CDCl3_400MHz_8_31_17



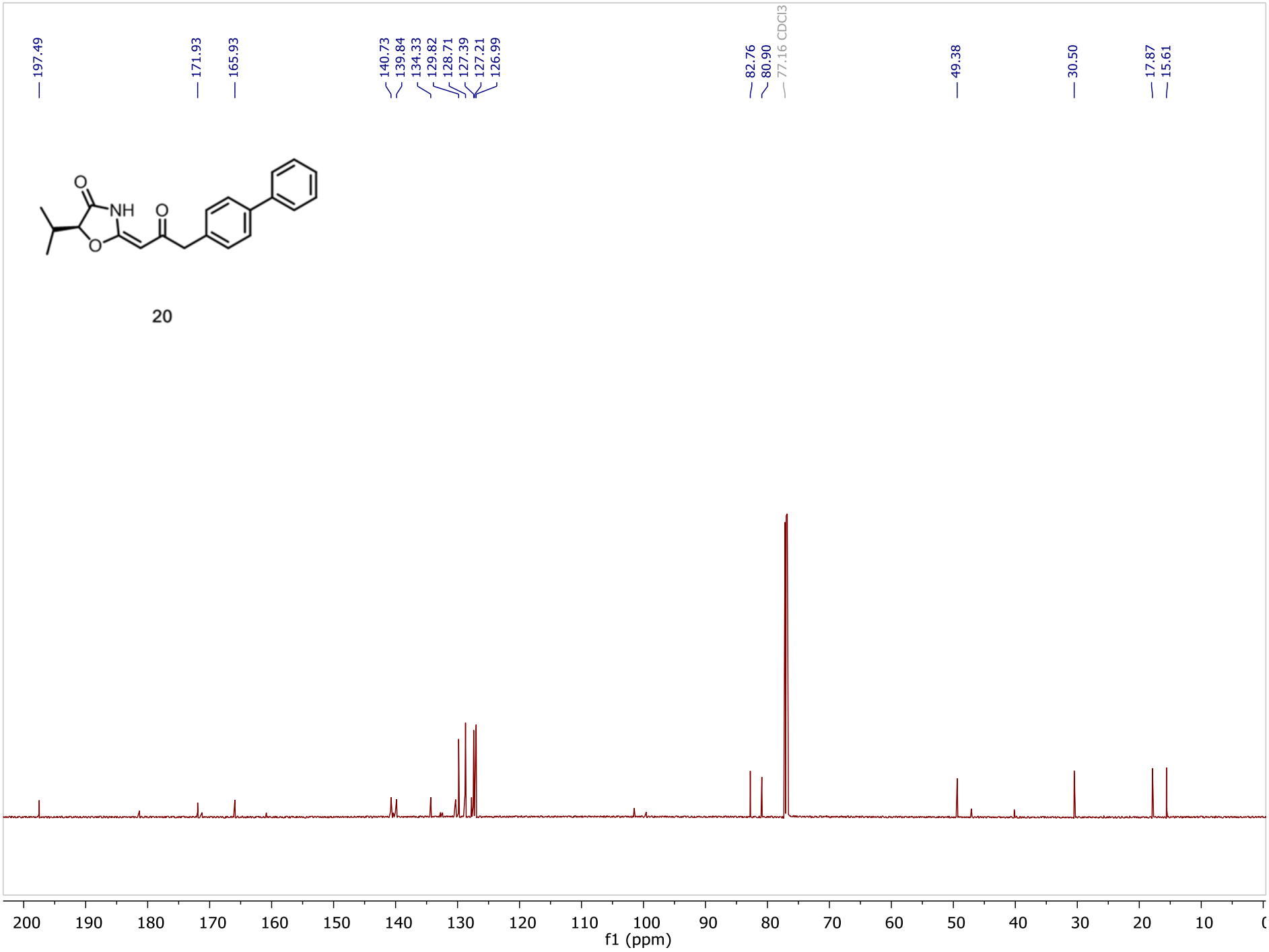
19

KR0542X2_f11_13C_CDCl3_700MHz_2_09_19.1.fid

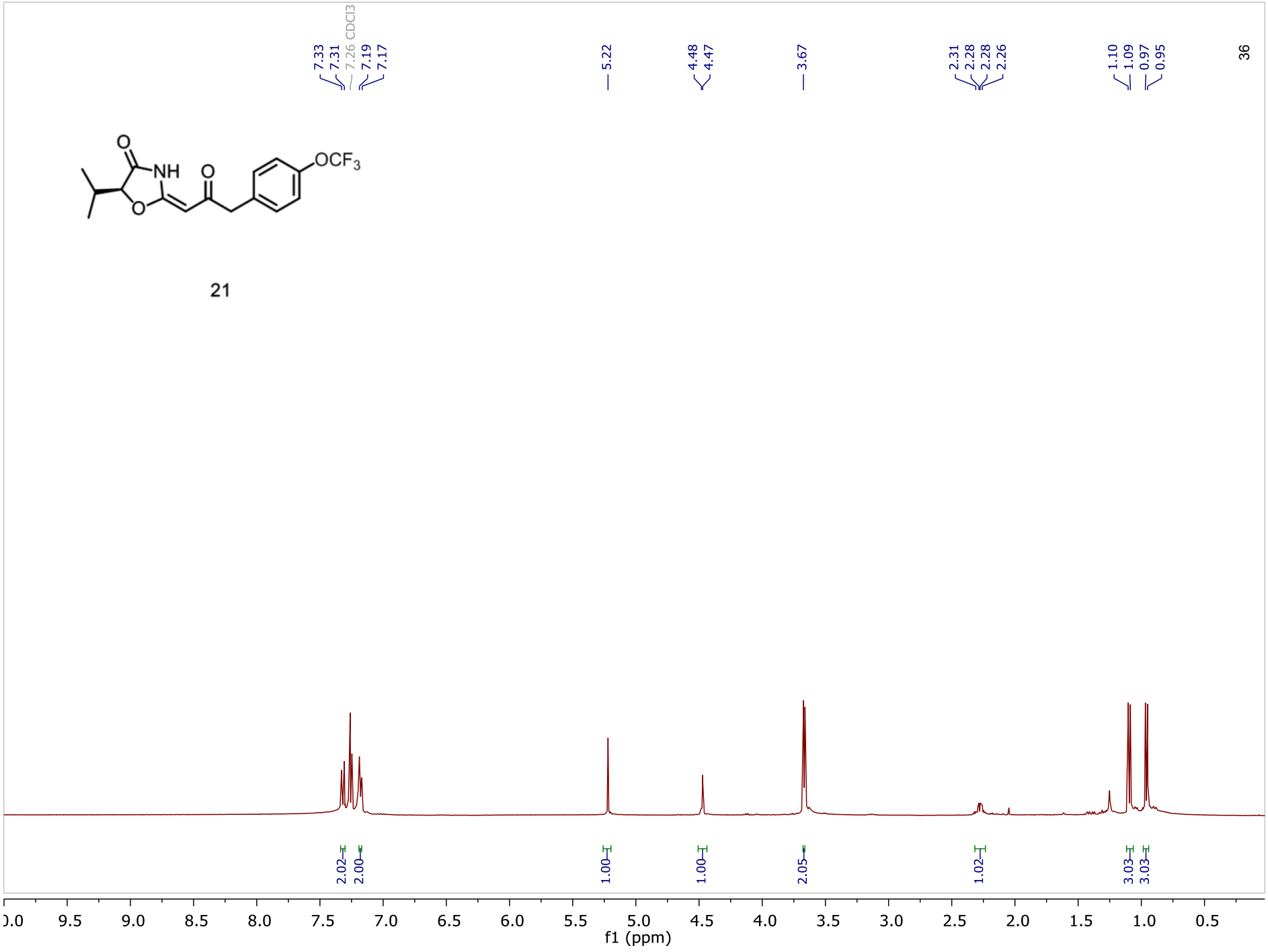



JJM-ox-7-19-1H-400MHz-CDCl3
20
NH
O
O
O
f1 (ppm)
0 1 2 3 4 5 6 7 8 9 10 11 12
4.15
2.40
3.20
0.87
0.89
2.00
1.01
1.19
3.37
3.44
7.60
7.59
7.58
7.58
7.57
7.56
7.56
7.45
7.44
7.43
7.42
7.34
7.32
7.32
7.31
7.30
7.26 CDCl3
5.27
4.47
4.46
3.71
2.30
2.29
2.28
2.27
2.26
2.25
1.64
1.10
1.09
0.97
0.95

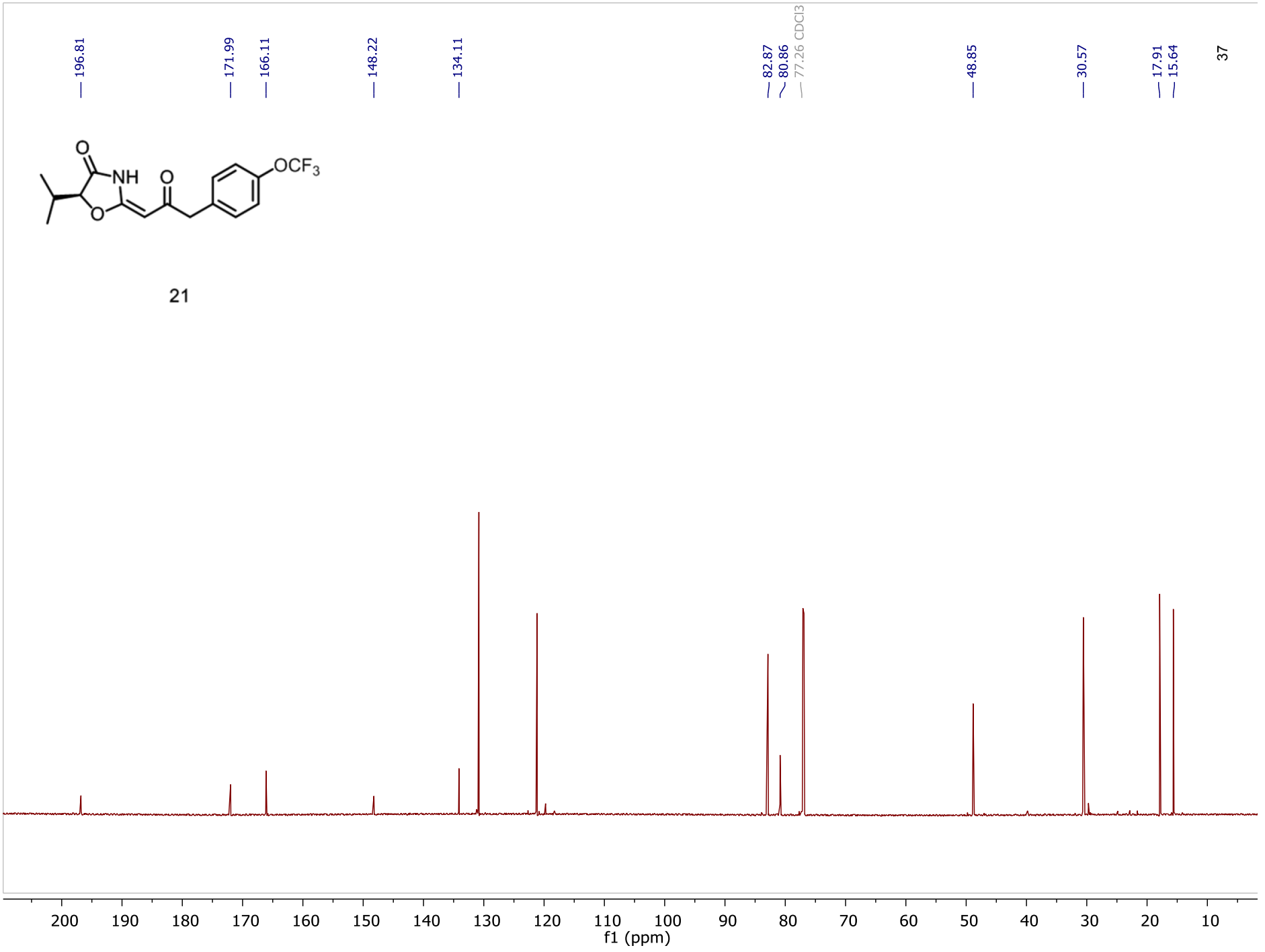
KR0872A_13C_CDCl3_700MHz_2_18_19.1.fid



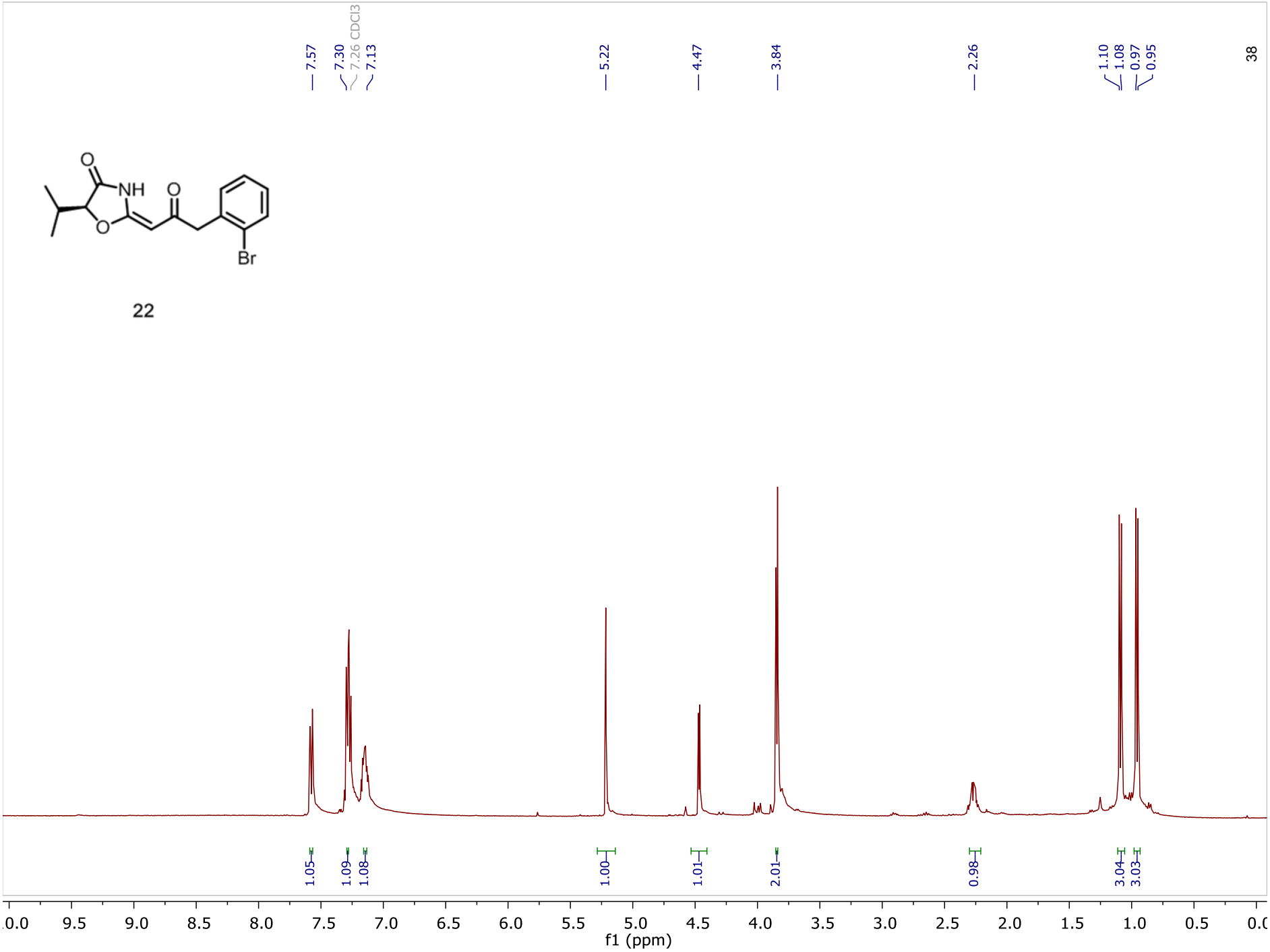
KR0615AA_1H_CDCl3_400MHz_11_21_17



KR0615x2A.2.fid

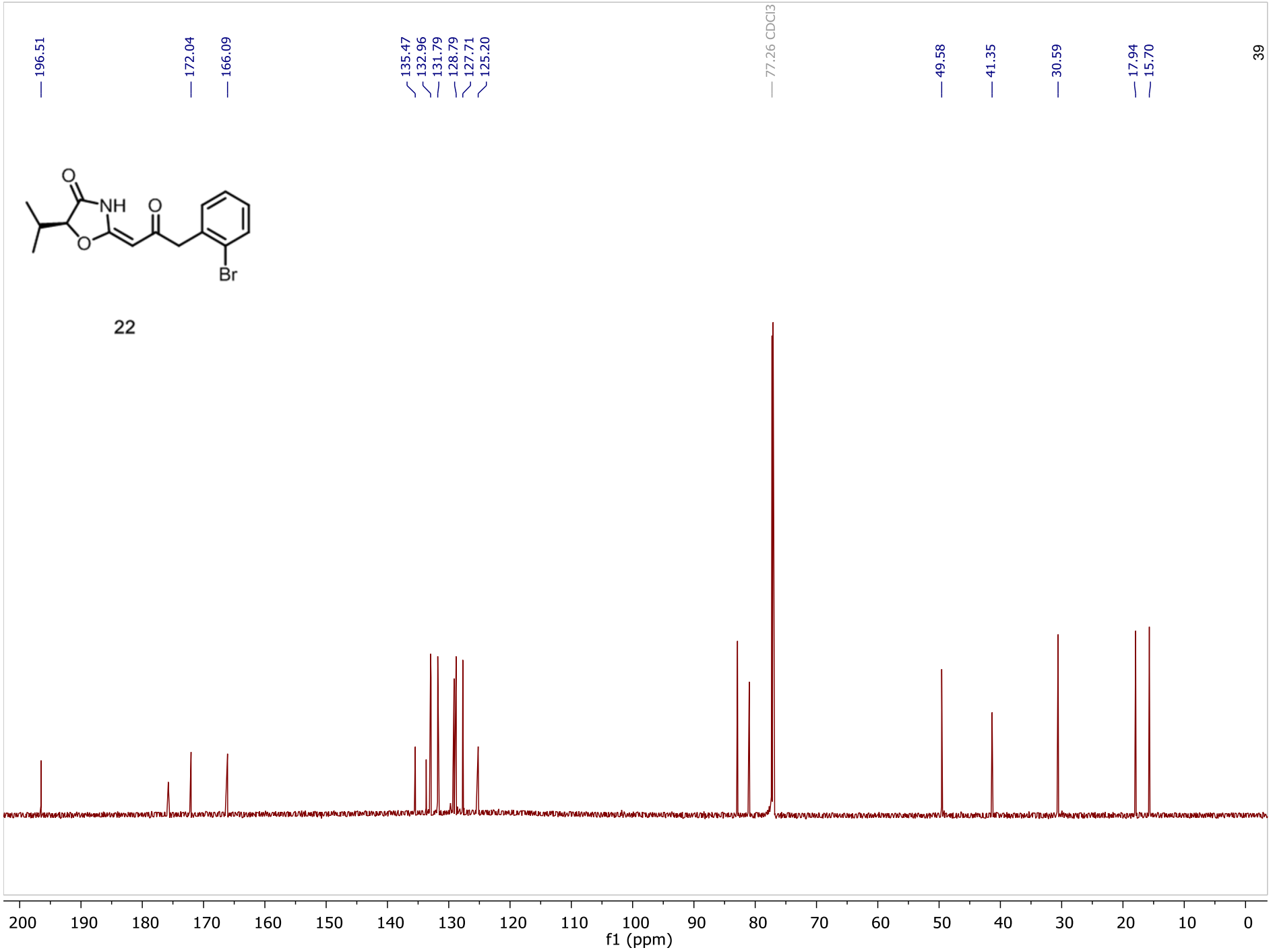


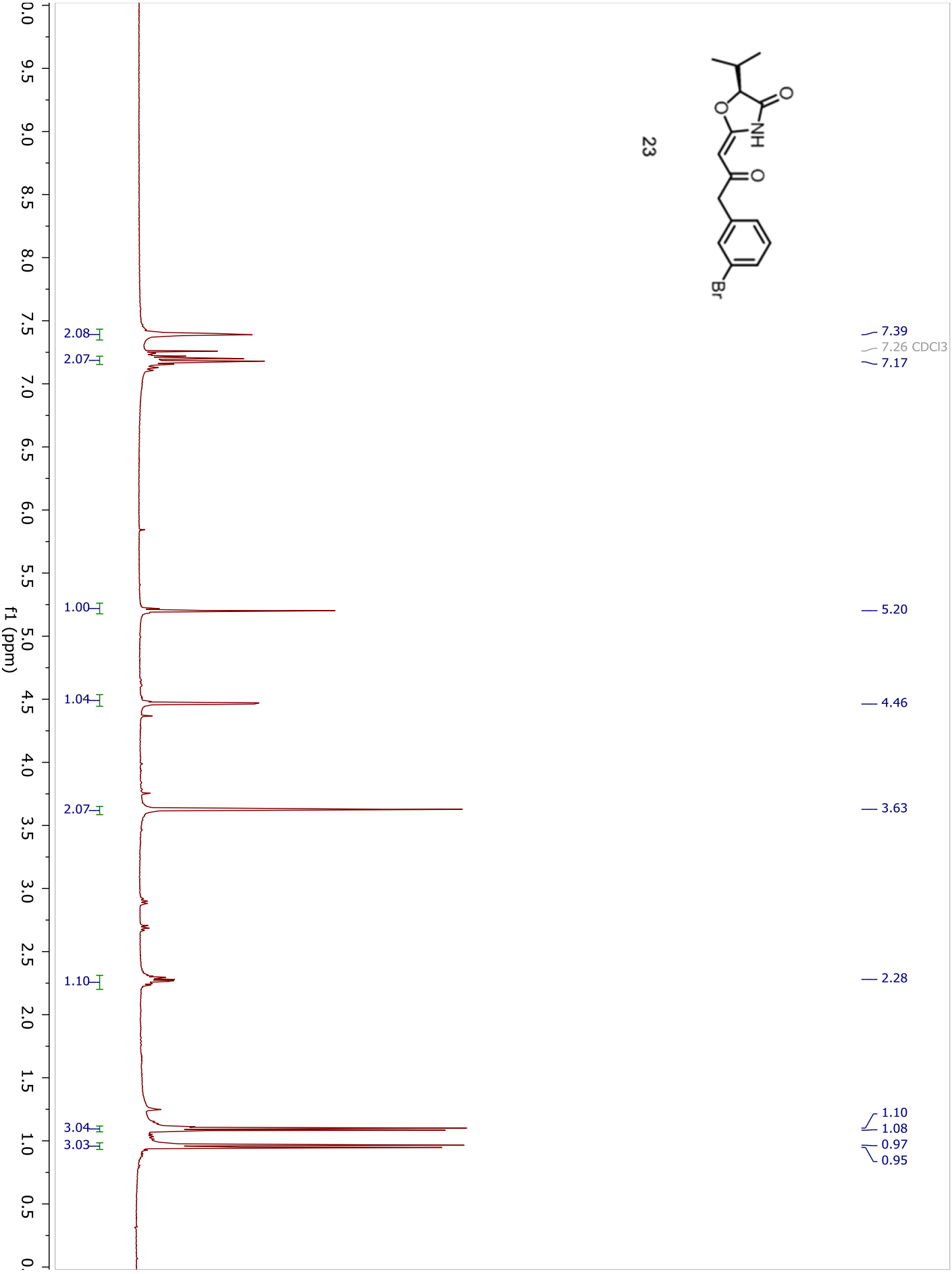
KR0652A_1H_400MHz_CDCl3_12-18-17



22

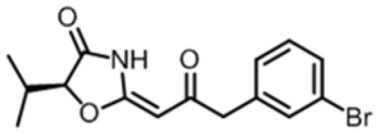
KR0652.2.fid


196.51
172.04
166.09
135.47
132.96
131.79
128.79
127.71
125.20
77.26 CDCl3
49.58
41.35
30.59
17.94
15.70
39
O
NH
O
O
Br
22
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

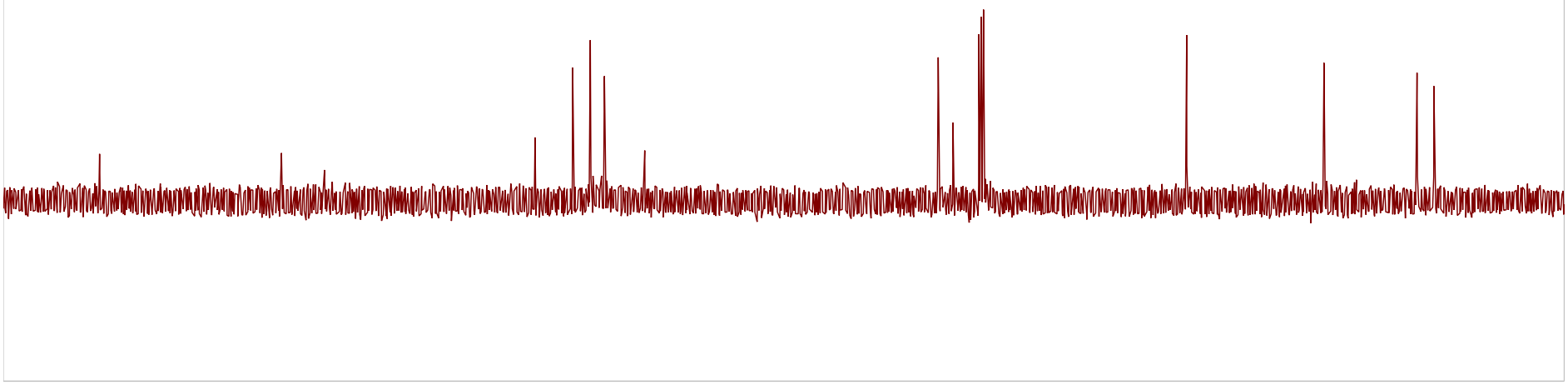

KR0653A_1H_400MHz_CDCl3_3_2_18
23
NH
O
O
O
Br
f1 (ppm)
0.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
2.08
2.07
1.00
1.04
2.07
1.10
3.04
3.03
7.39
7.26 CDCl3
7.17
5.20
4.46
3.63
2.28
1.10
1.08
0.97
0.95

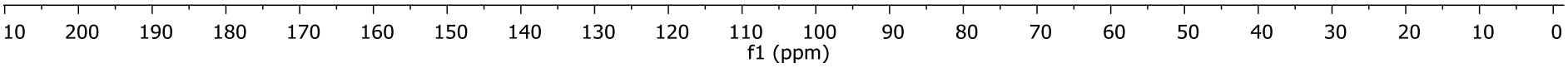
KR0653A_13C_400MHz_CDCl3_3_2_18

197.13
172.47
166.63
138.08
132.97
130.71
130.58
128.67
123.20
83.40
81.40
77.26 CDCl3
49.70
31.08
18.47
16.18

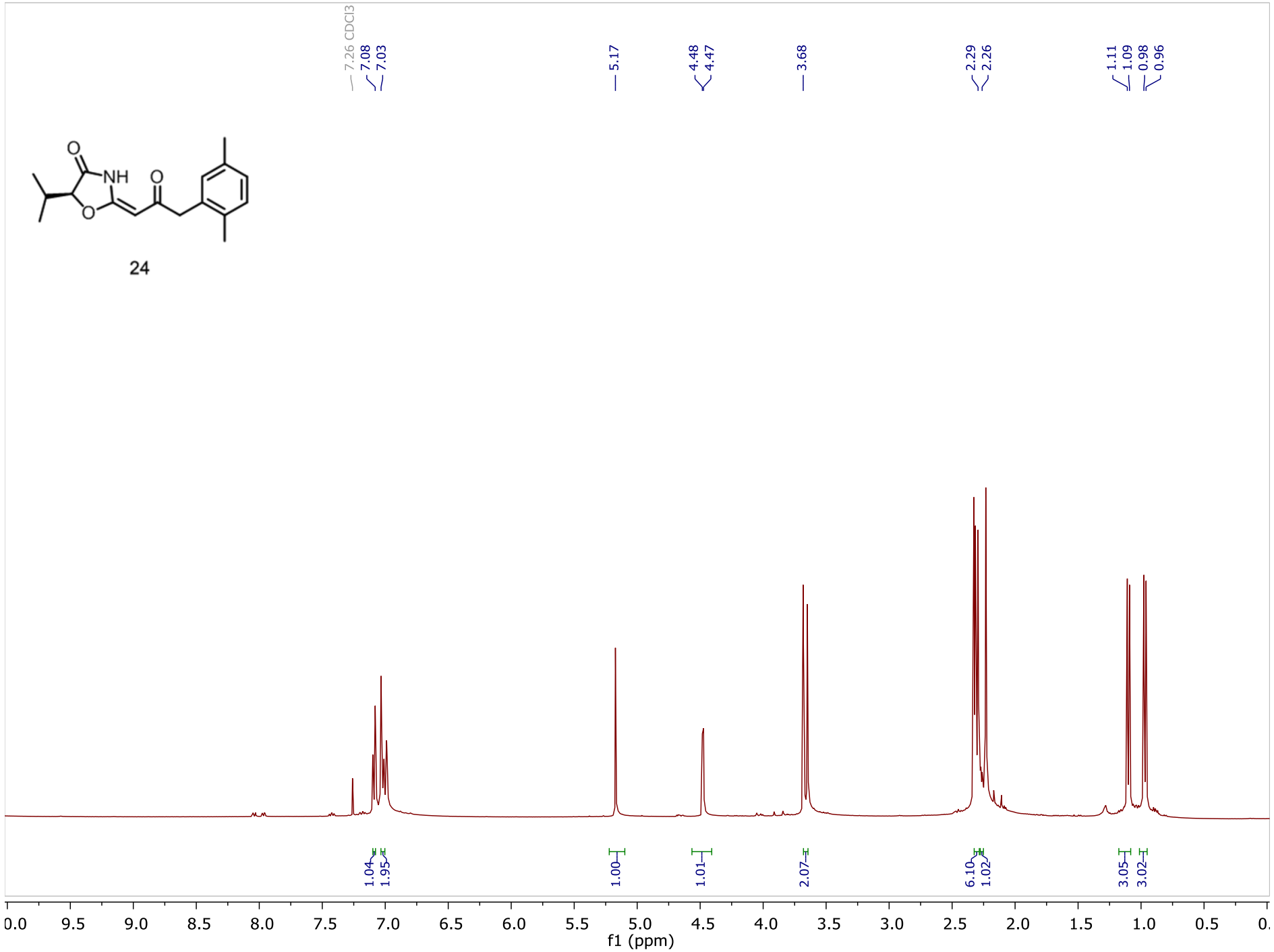


23

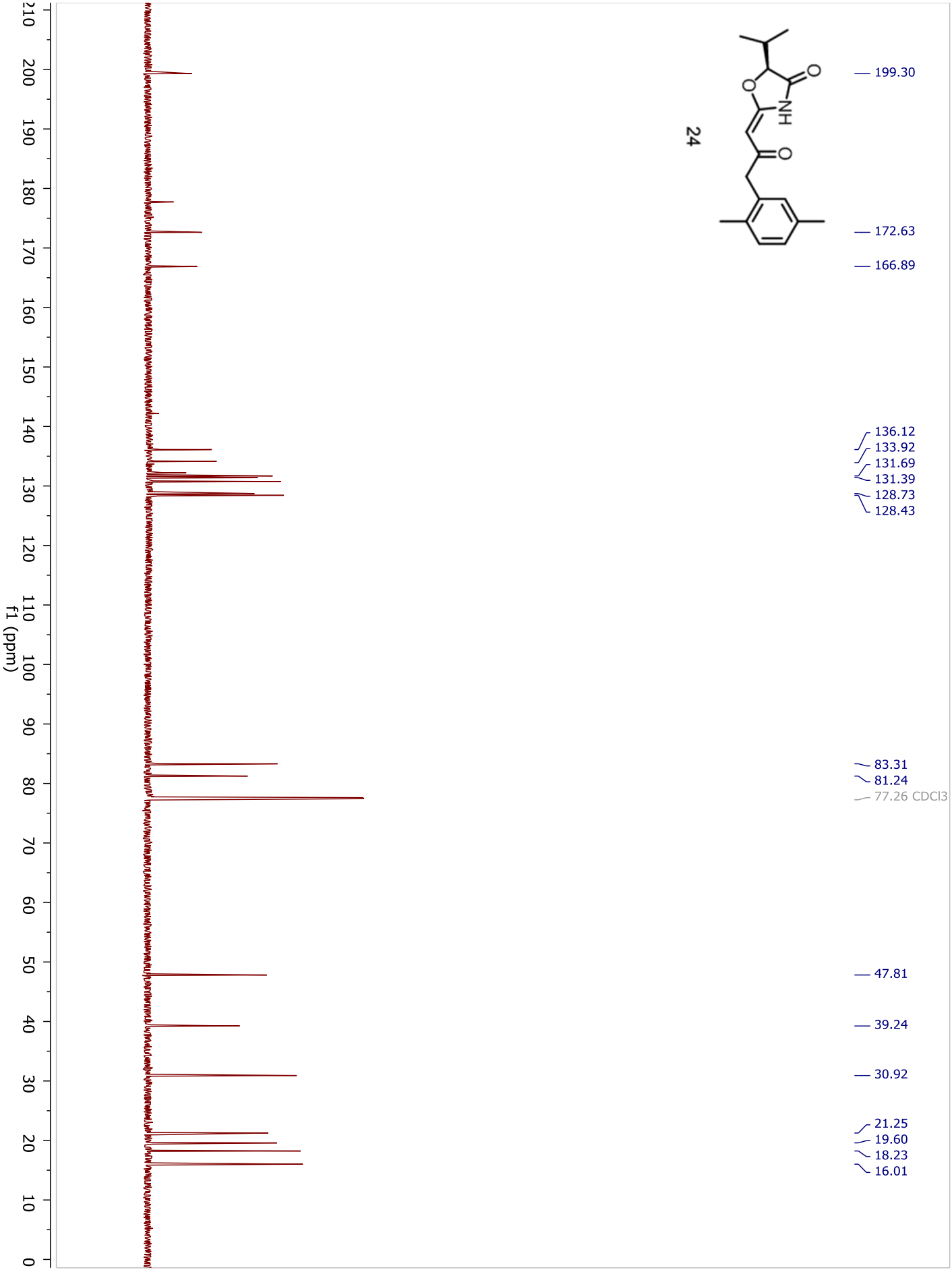


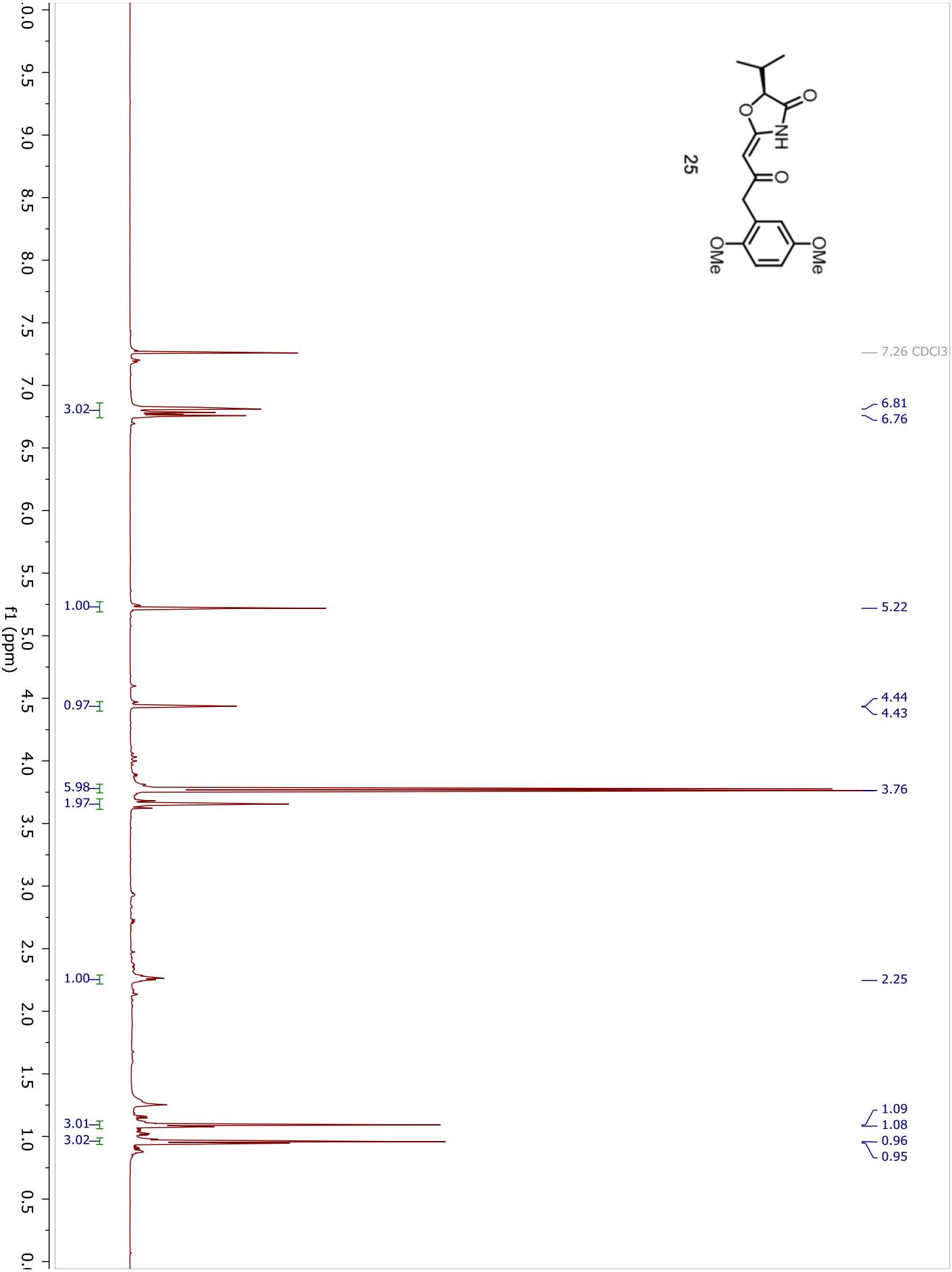


KR0664AA_1H_CDCl3_400MHz_1_22_18

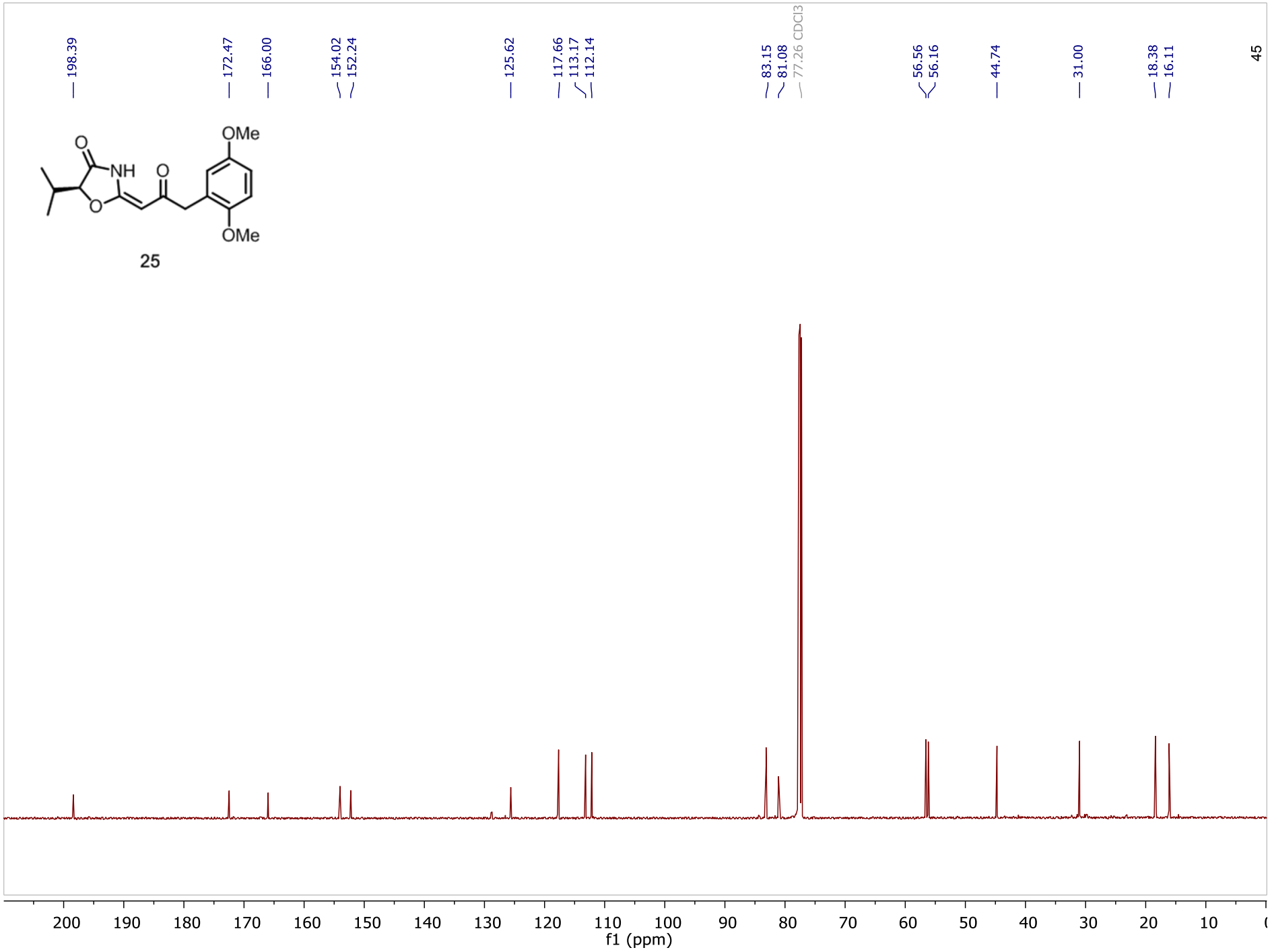


24

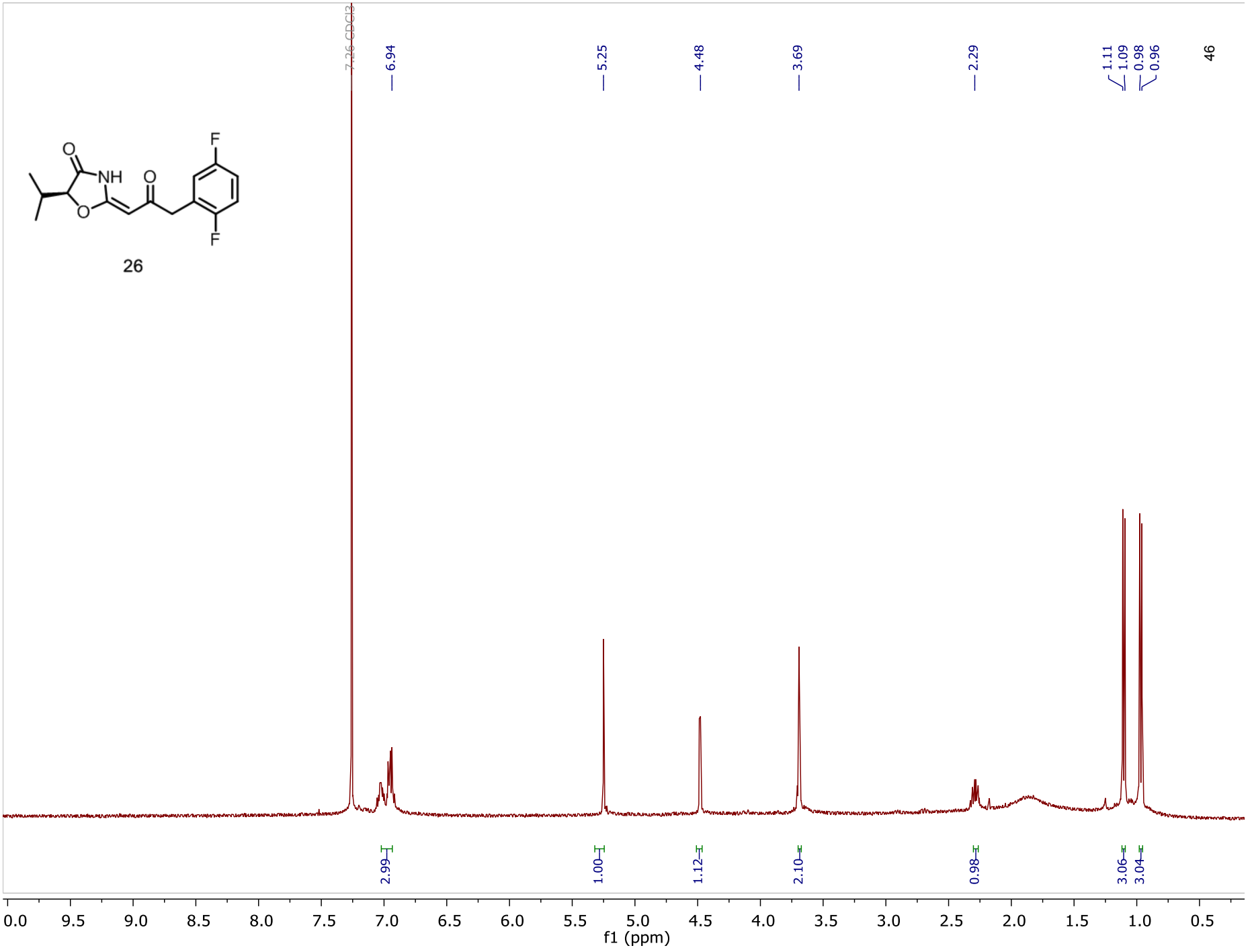

KR0664A.2.fid
24
199.30
172.63
166.89
136.12
133.92
131.69
131.39
128.73
128.43
83.31
81.24
77.26 CDCl3
47.81
39.24
30.92
21.25
19.60
18.23
16.01
f1 (ppm)


Jun06-2018-616X2A.10.fid
25
NH
O
OMe
OMe
f1 (ppm)
7.26 CDCl3
6.81
6.76
5.22
4.44
4.43
3.76
2.25
1.09
1.08
0.96
0.95
3.02
1.00
0.97
5.98
1.97
1.00
3.01
3.02

Jun06-2018-616X2A.11.fid



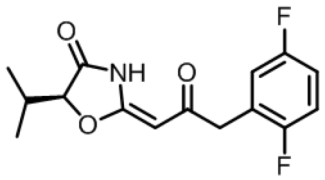
KR0617A_1H_CDCl3_400MHz_12_18_17



26

KR0617x2A_13C_400MHz_CDCl3_3_2_18

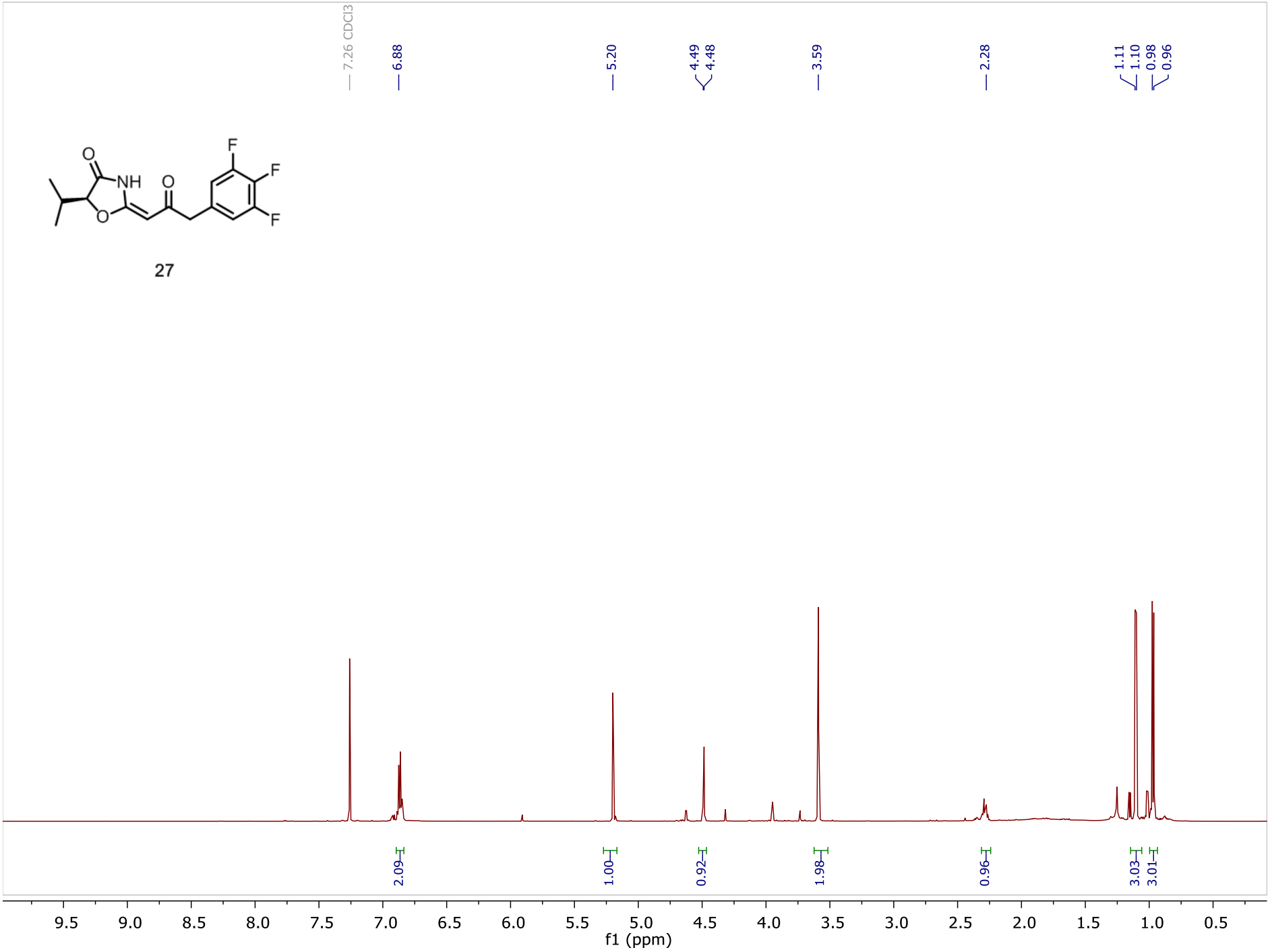
195.98
172.47
166.61
160.22
158.74
118.41
116.66
115.51
83.40
81.08
77.26 CDCl3
42.97
31.06
18.43
16.13
47



26

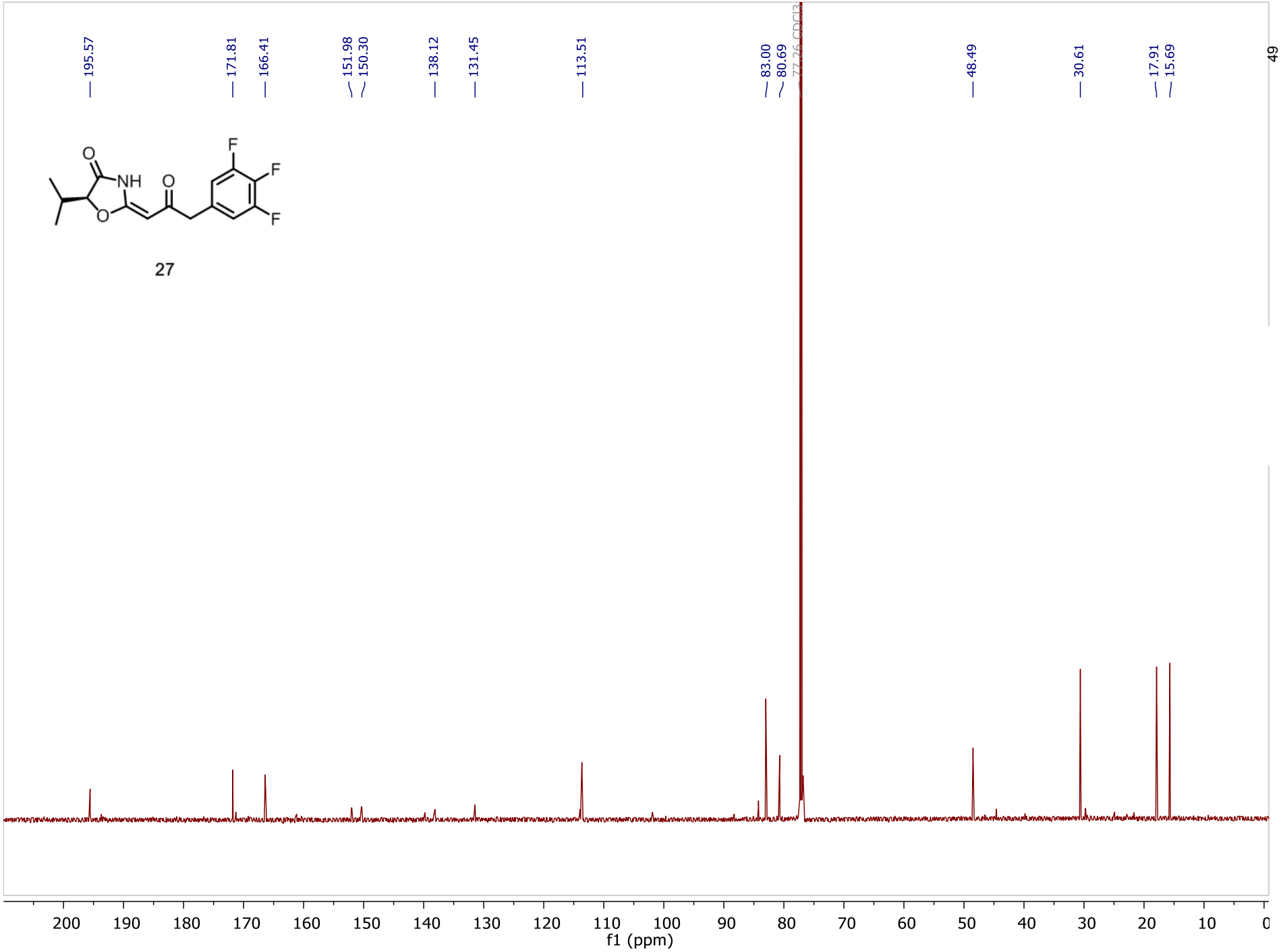
f1 (ppm)

Jun06-2018-670AAA.10.fid

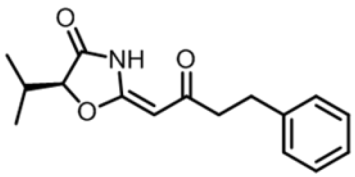


27

Jun06-2018-670AAA.11.fid

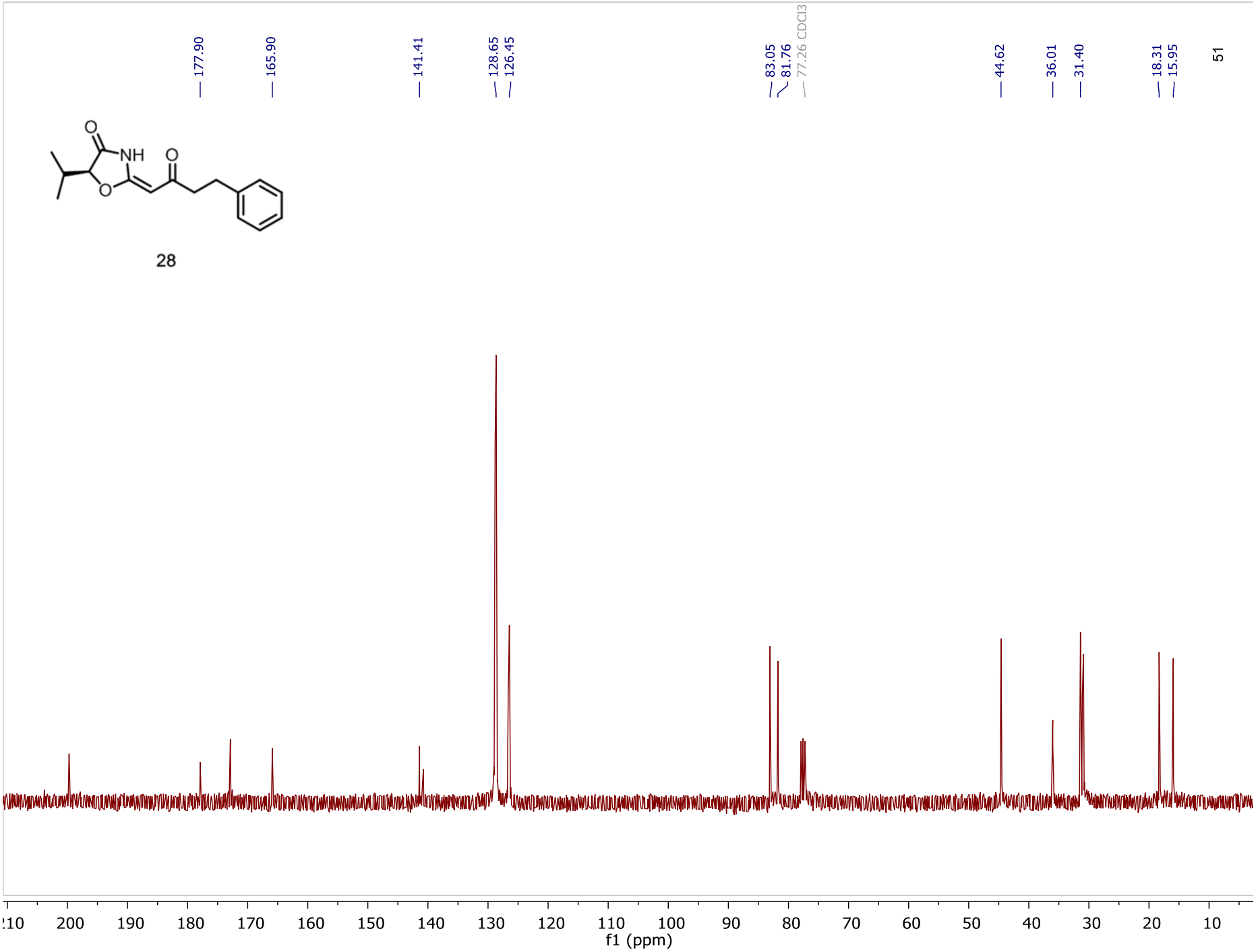


KR0634A_1H_CDCl3_400MHz_11_21_17

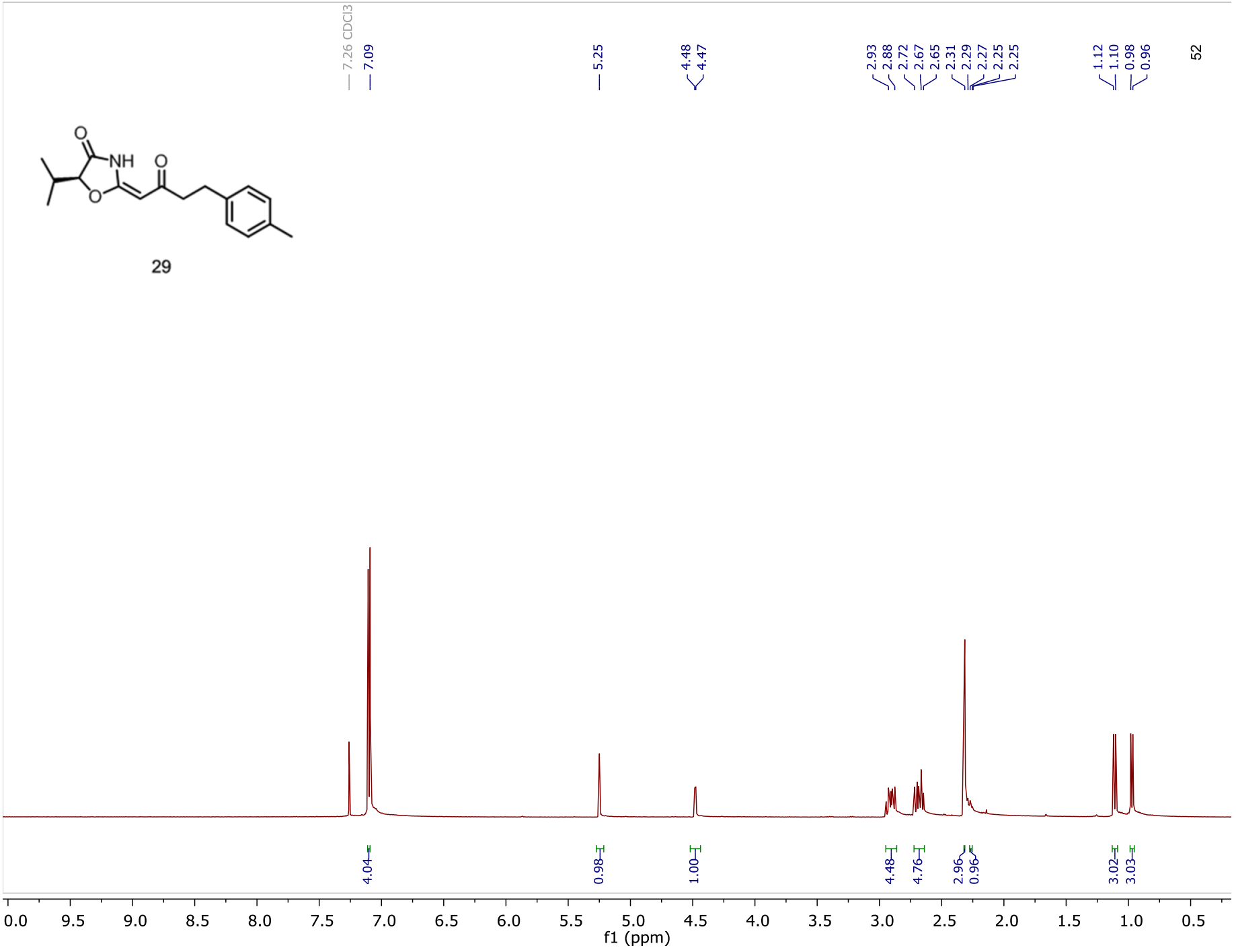


28

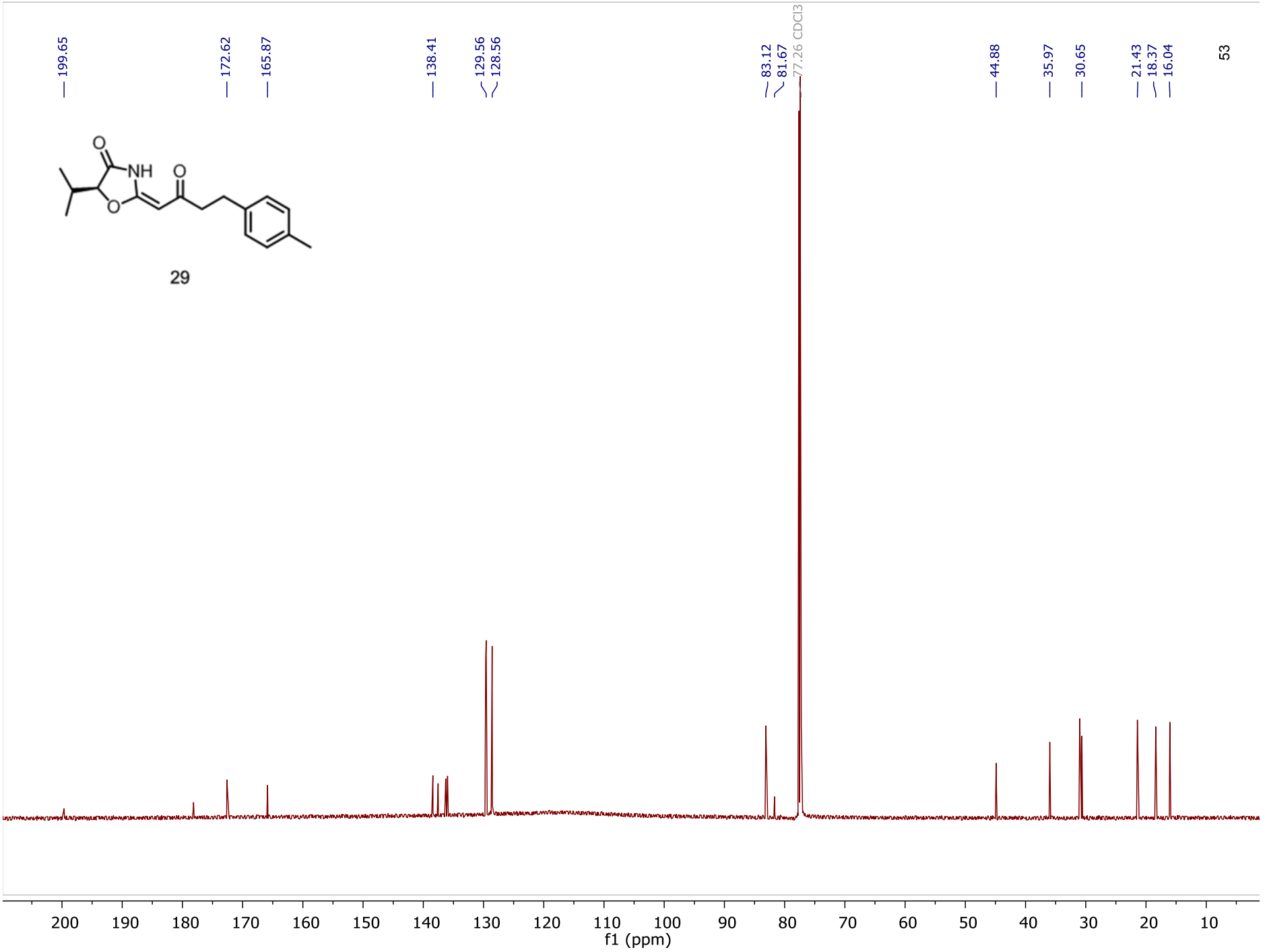
KR0634A_13C_CDCl3_400MHz_2_19_18



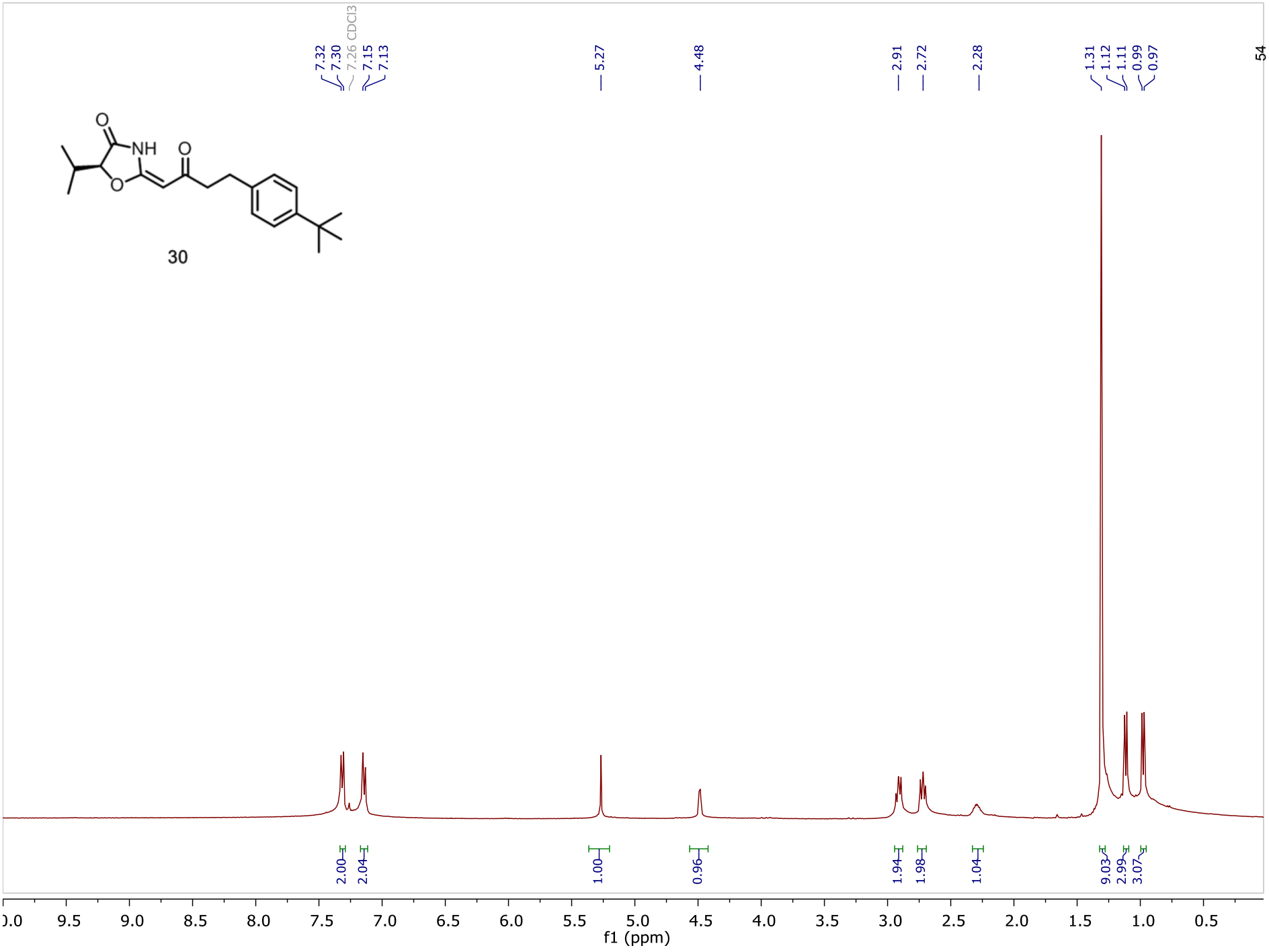
KR0650A_1H_400MHz_CDCl3_12-18-17

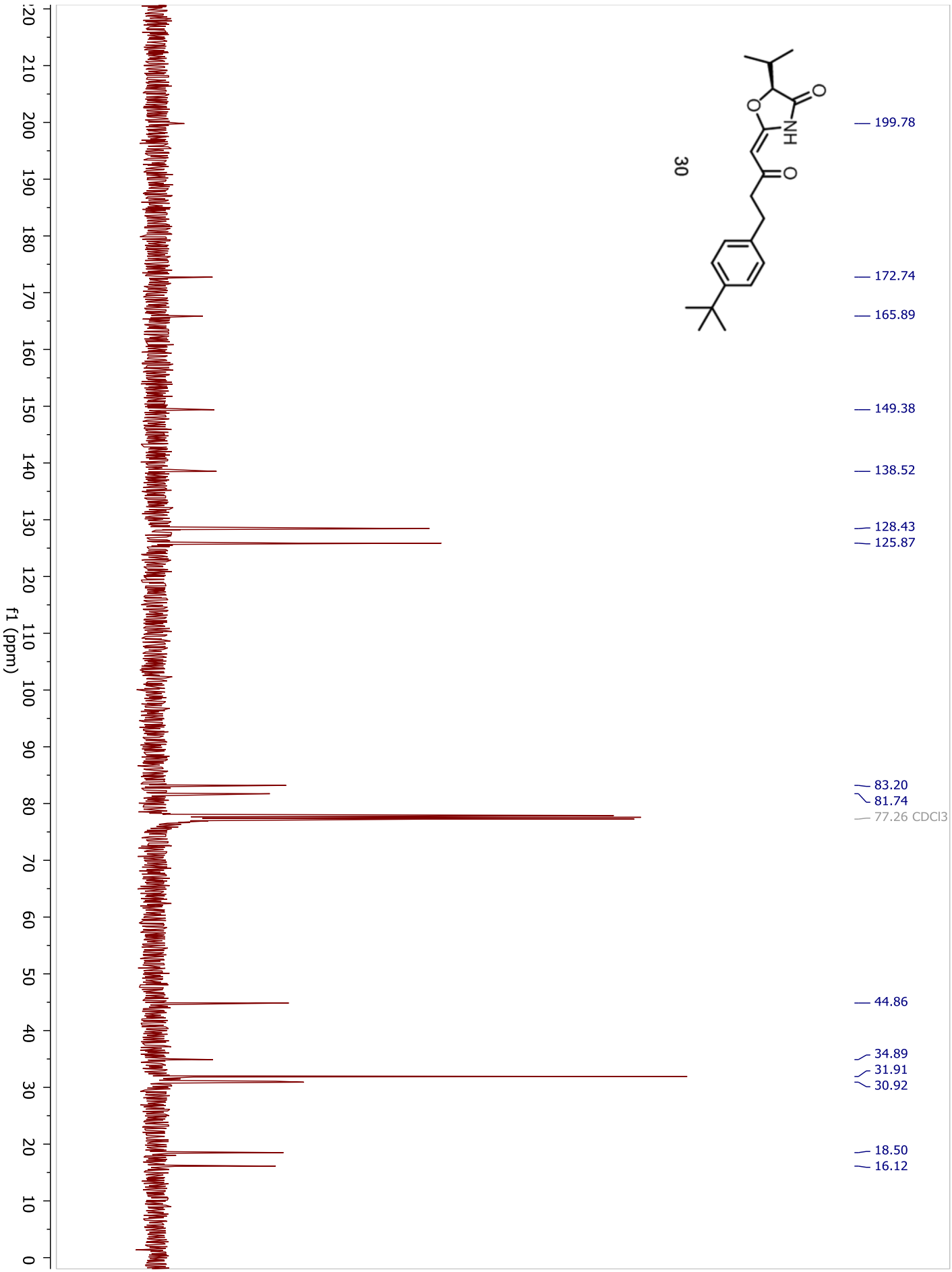


KR0650A.2.fid

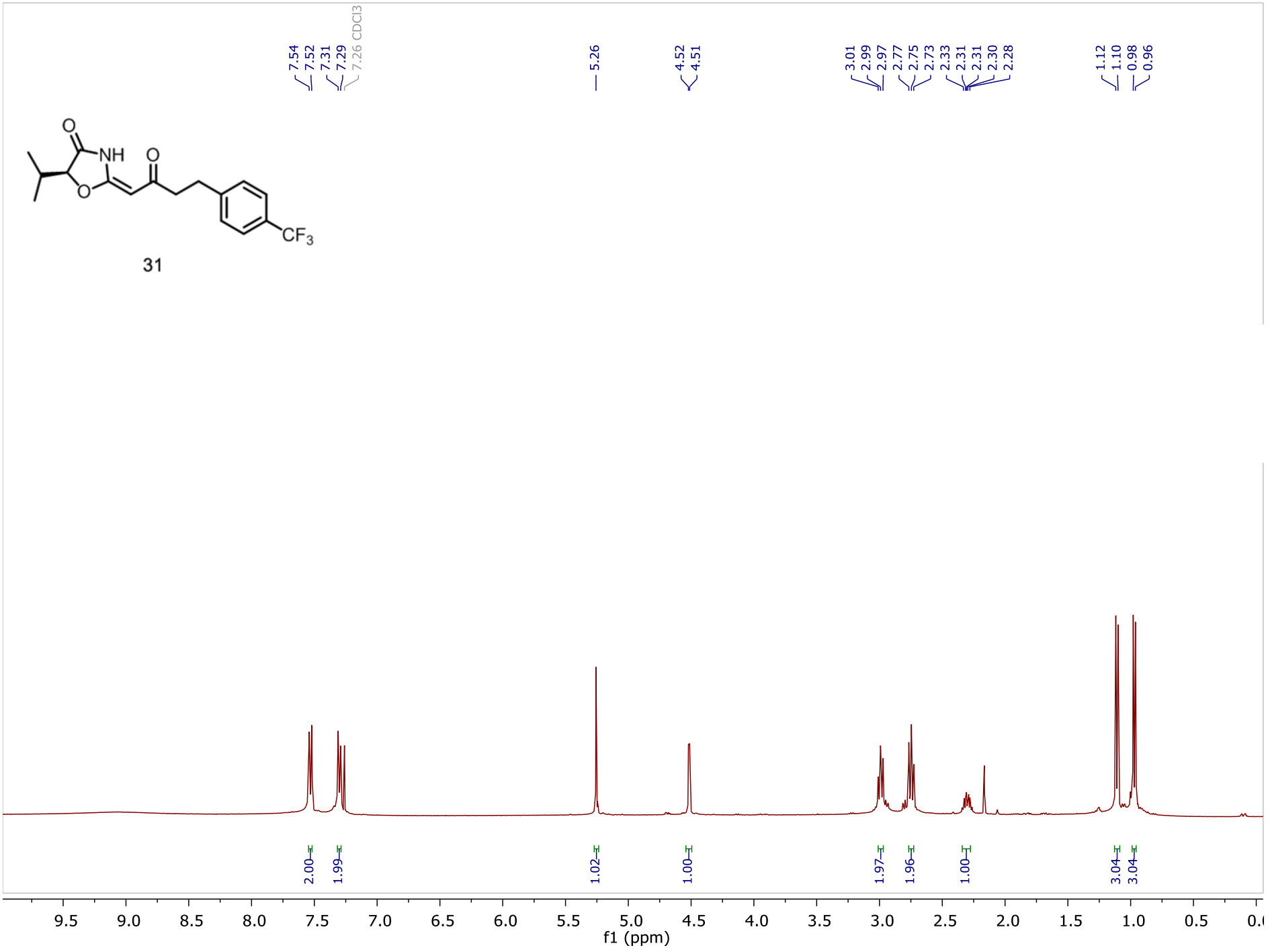


KR0673A_1H_400MHz_CDCl3_01_03_18



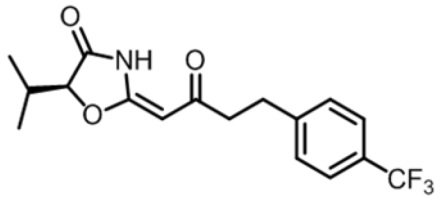

KR0673A_13C_400MHz_CDCl3_01_03_18
f1 (ppm)
0
10
20
30
40
50
60
70
80
90
100
110
120
130
140
150
160
170
180
190
200
210
220
30
O
O
NH
O
199.78
172.74
165.89
149.38
138.52
128.43
125.87
83.20
81.74
77.26 CDCl3
44.86
34.89
31.91
30.92
18.50
16.12

KR0621A_1H_CDCl3_400MHz_11_18_17

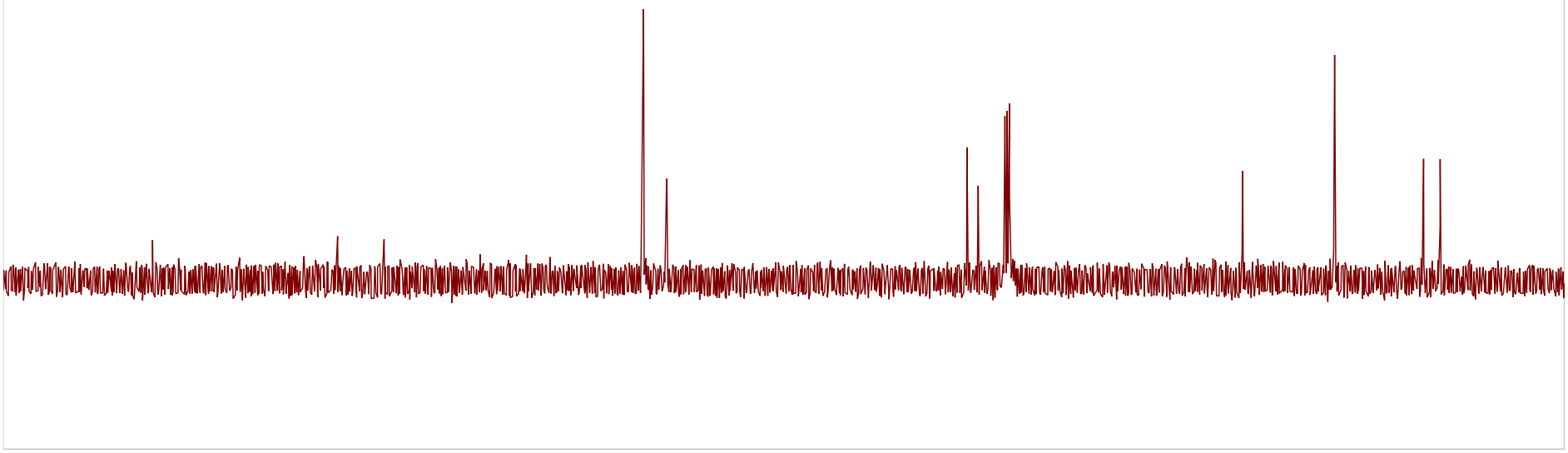


KR0621A_13C_CDCl3_400MHz_2_19_18

198.88
172.61
166.02
145.82
129.19
125.88
83.29
81.69
77.26 CDCl3
44.16
31.10
18.47
16.12

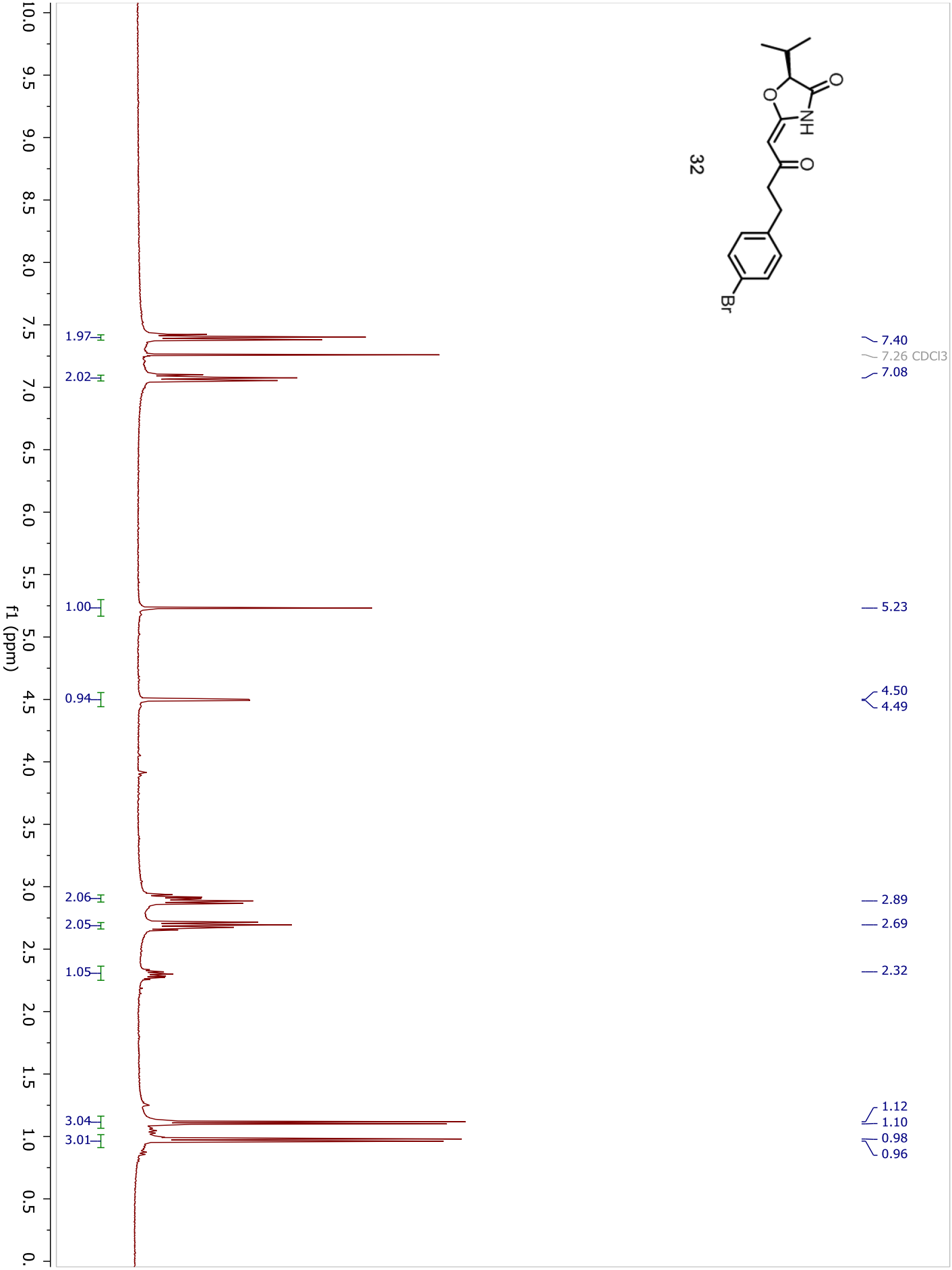


31

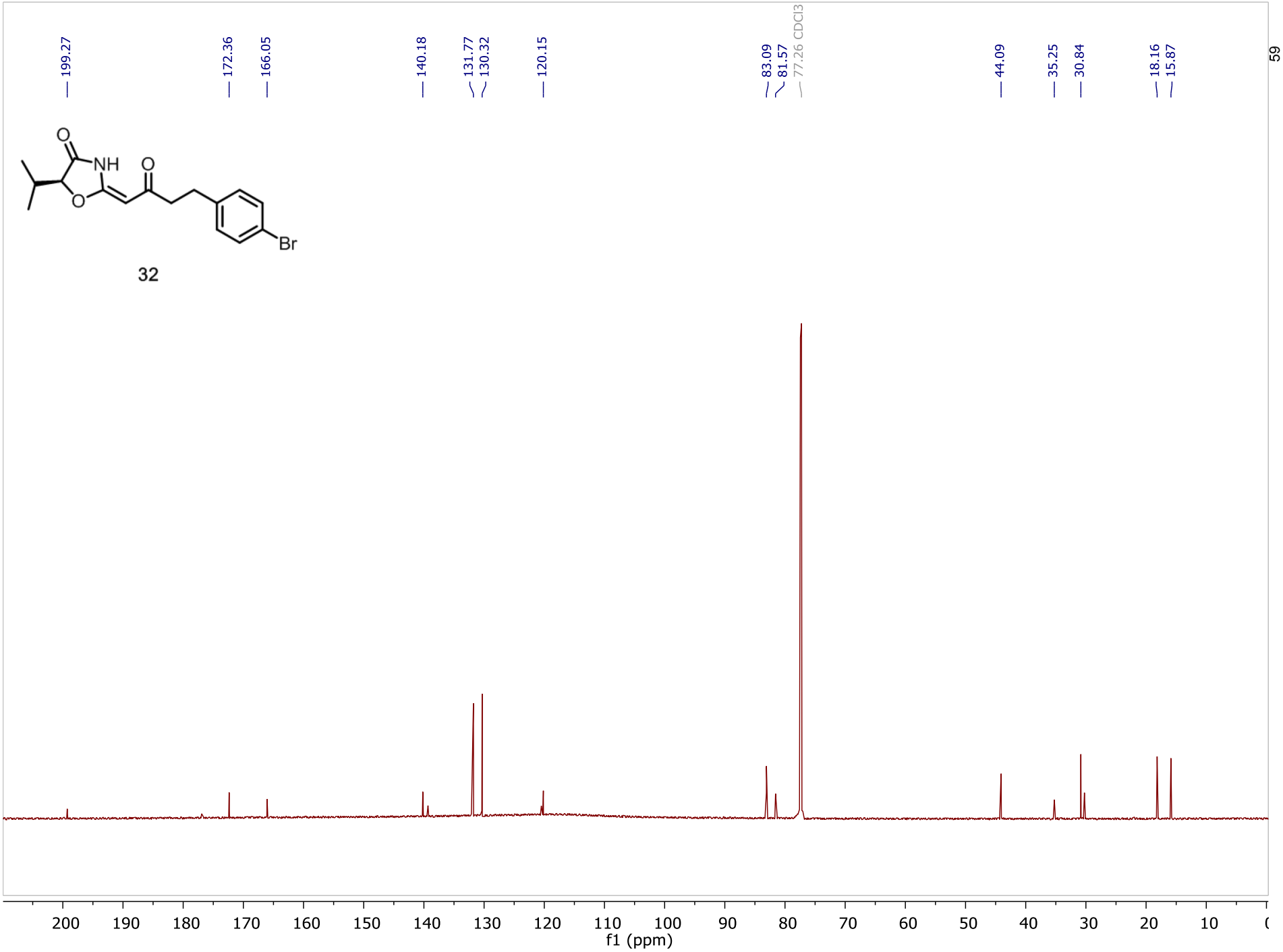


20 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0

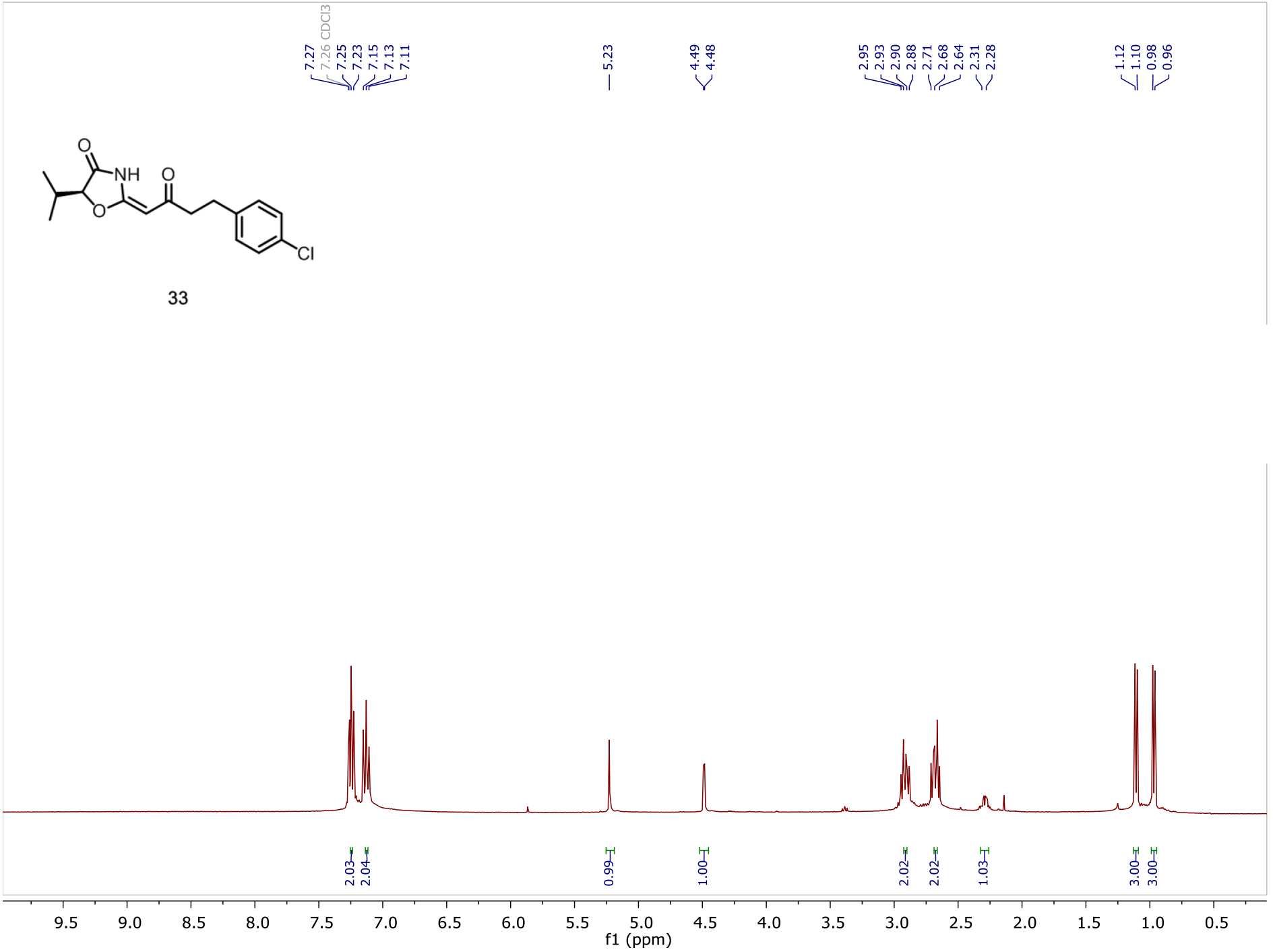
f1 (ppm)


KR0660A_1H_CDCl3_400MHz_12_18_17
32
Br
O
NH
O
O
f1 (ppm)
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.
1.97
2.02
1.00
0.94
2.06
2.05
1.05
3.04
3.01
7.40
7.26 CDCl3
7.08
5.23
4.50
4.49
2.89
2.69
2.32
1.12
1.10
0.98
0.96

KR0660A.2.fid

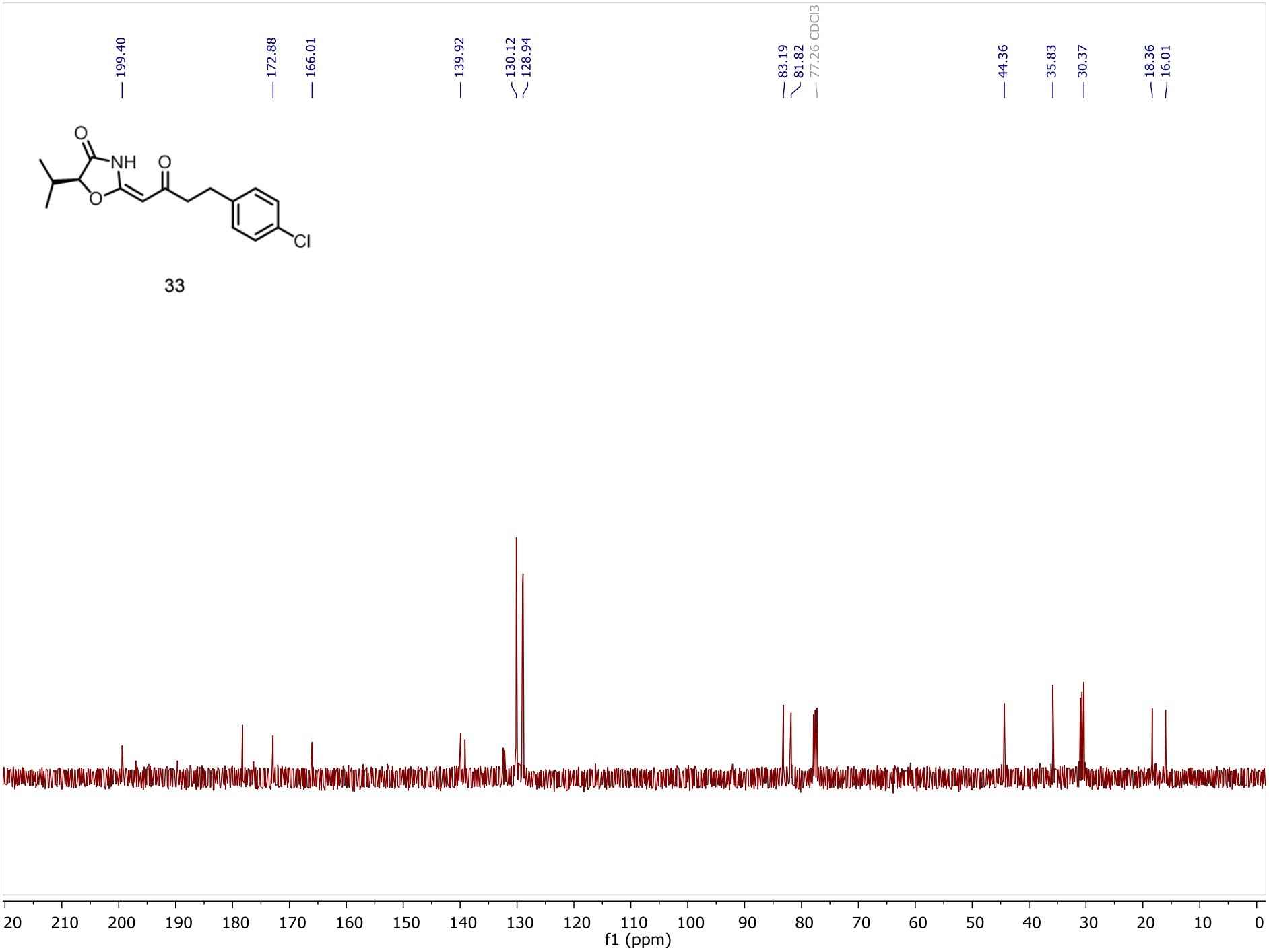


KR0654A_1H_400MHz_CDCl3_12-18-17

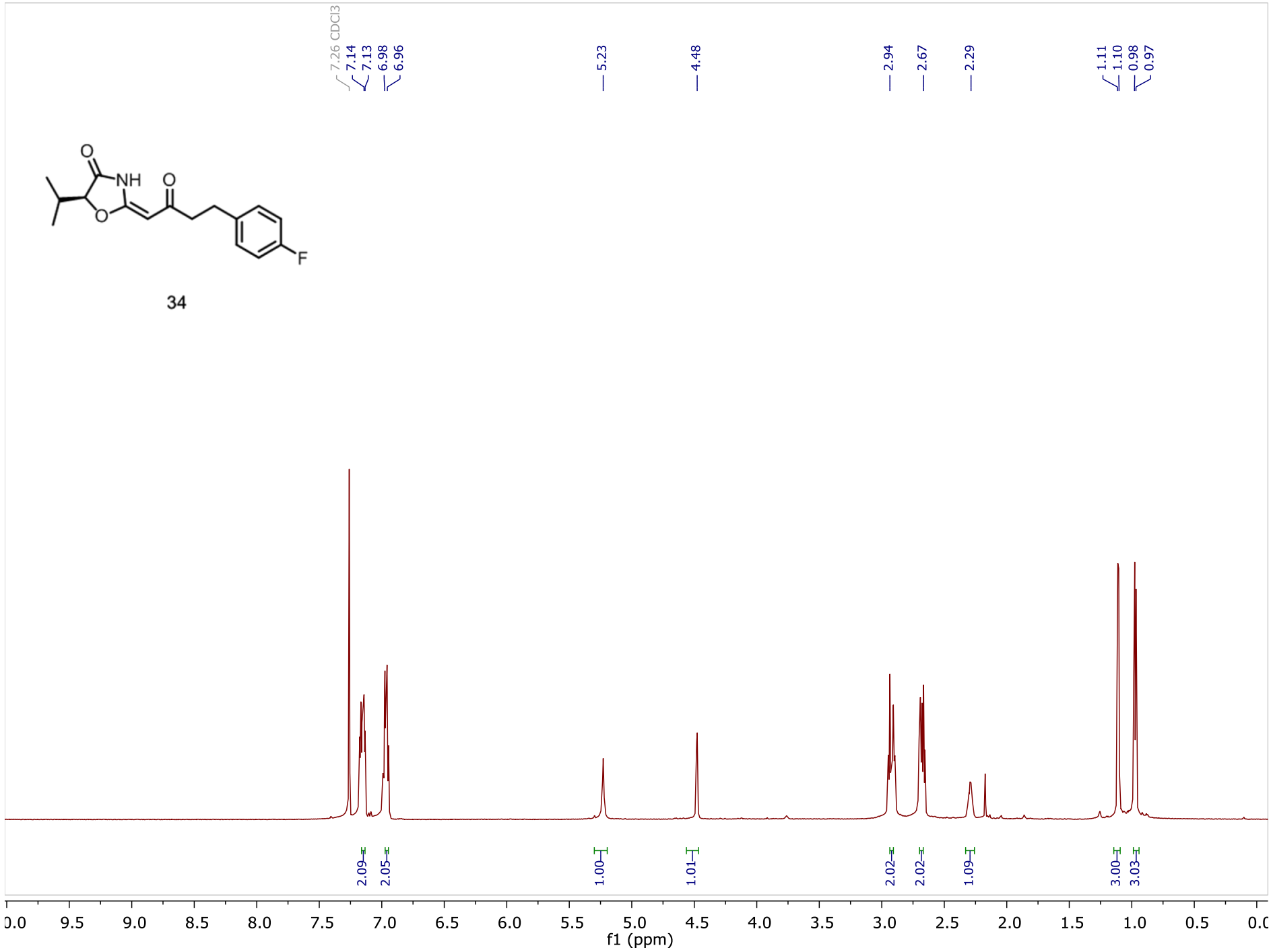


33

KR0654A_13C_400MHz_CDCl3_3_2_18



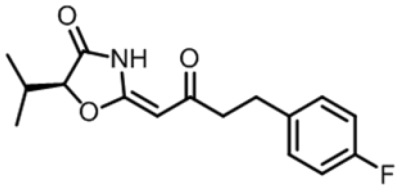
KR0651A.1.fid



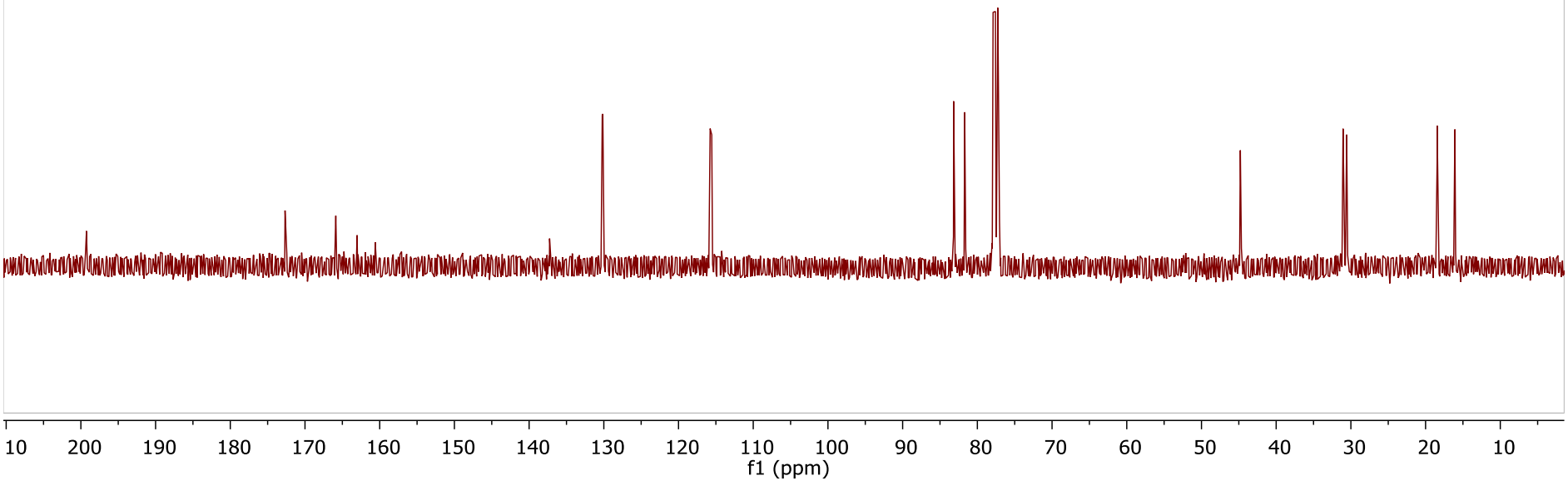
34

KR0651A_13C_400MHz_CDCl3_01_03_18

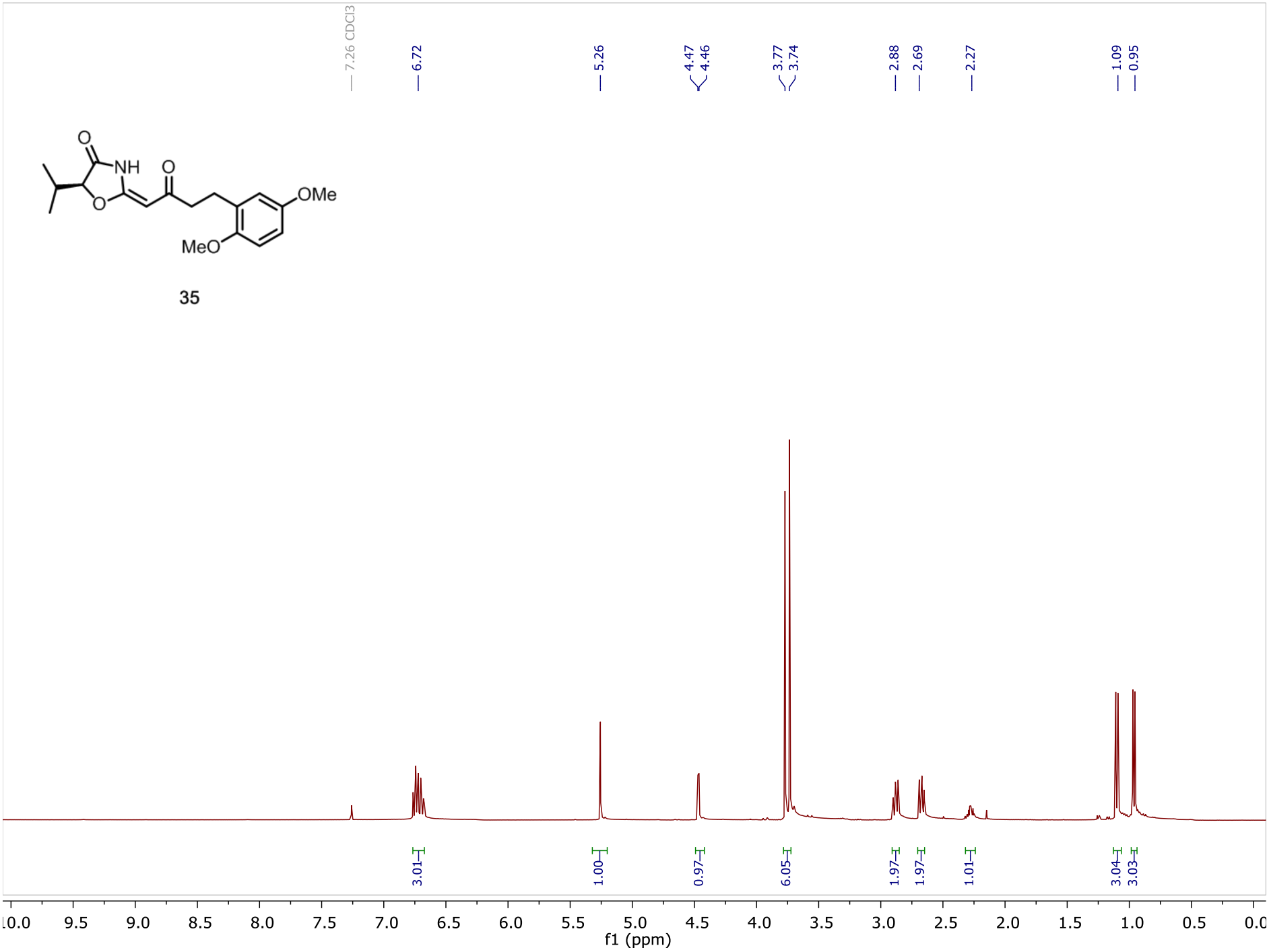
199.25
172.67
165.88
137.23
130.21
115.55
83.18
81.70
77.26 CDCl3
44.80
30.57
18.45
16.08



34

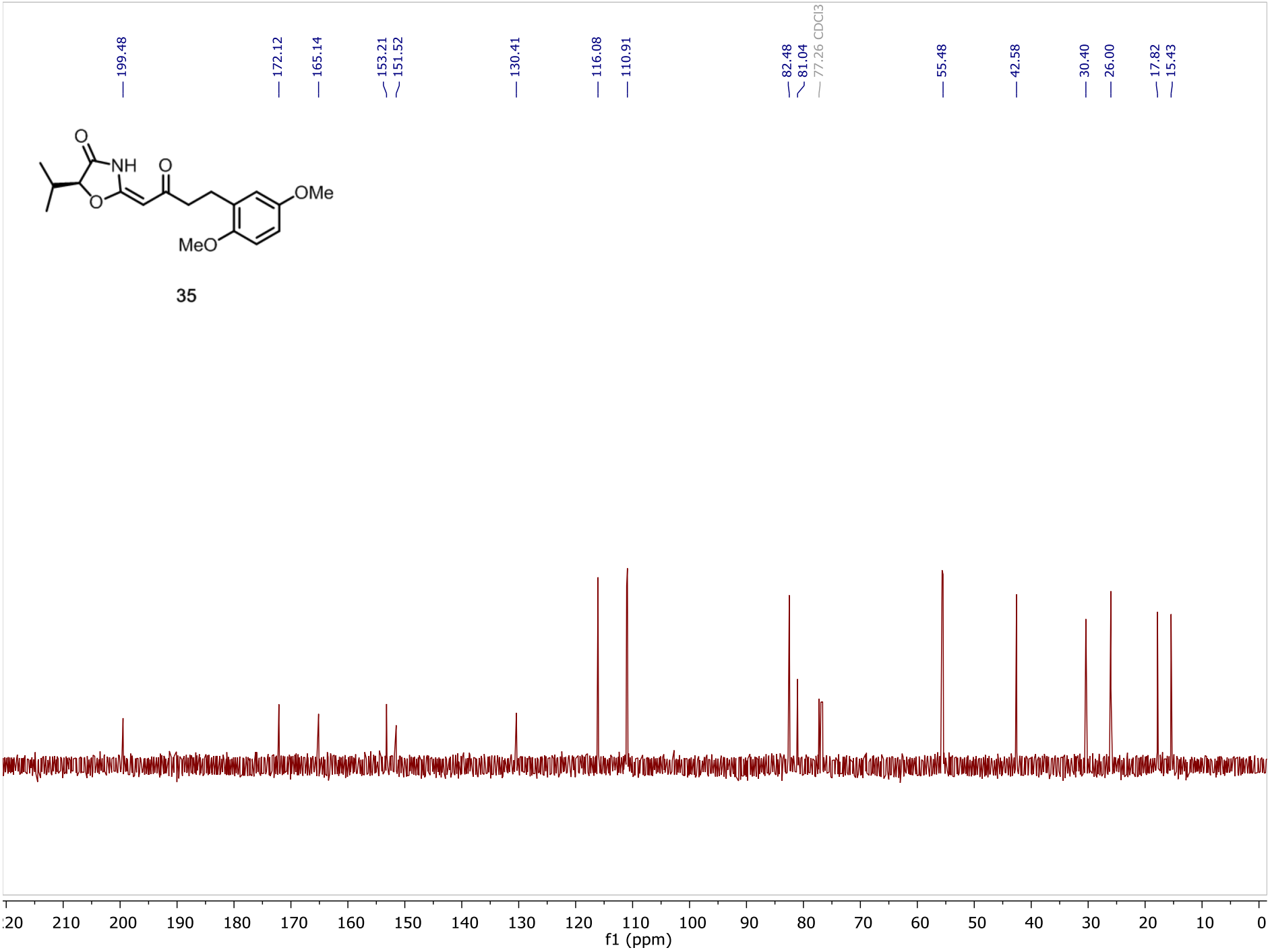


KR0629A_1H_CDCl3_400MHz_11_21_17

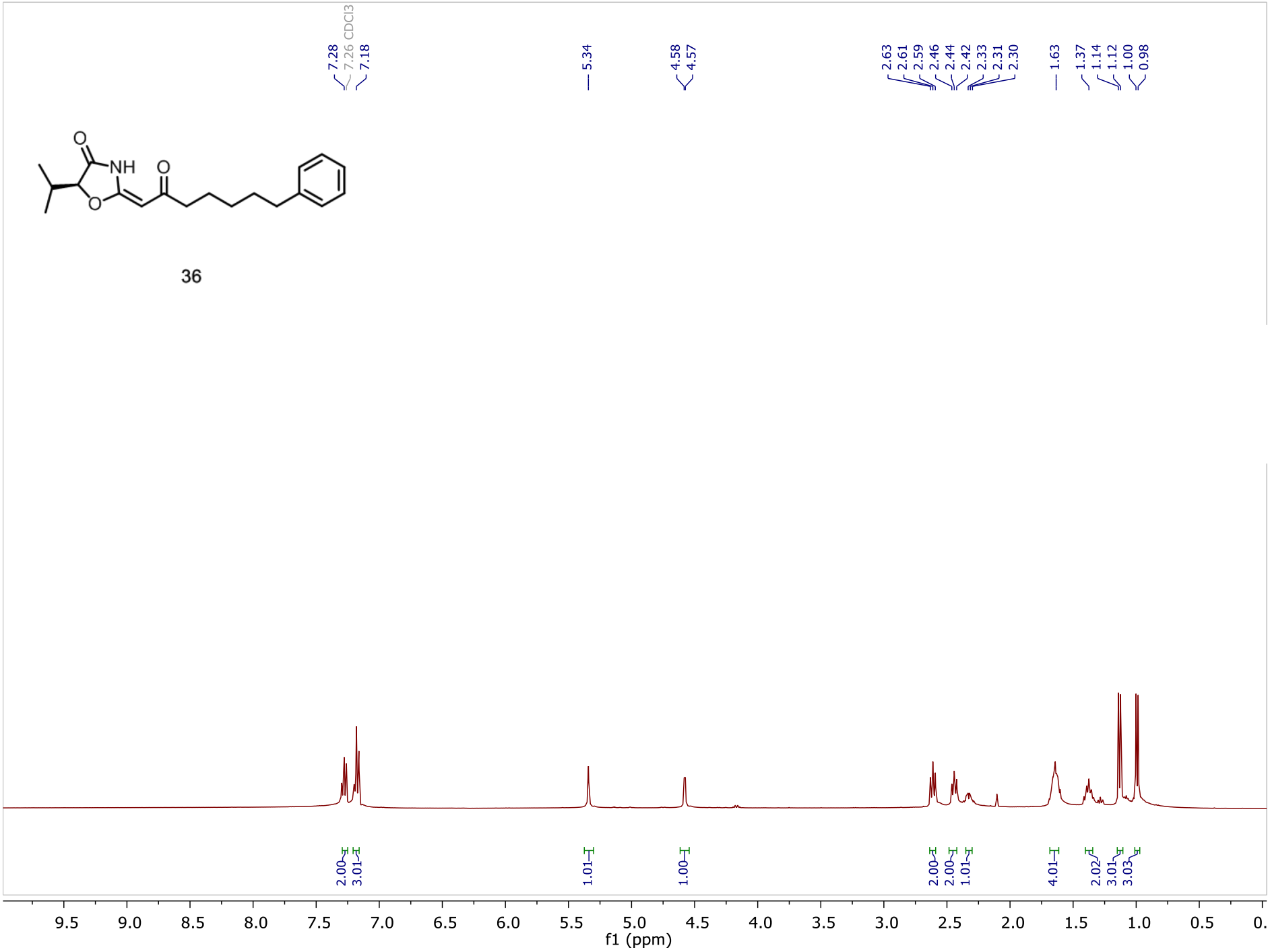


35

KR0629A_13C_CDCl3_400MHz_2_19_18



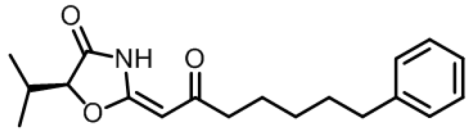
KR0635A_1H_CDCl3_400MHz_11_21_17



36

KR0635A_13C_CDCl3_400MHz_2_19_18

200.88
172.81
165.90
143.00
128.83
126.09
83.08
81.64
77.26 CDCl3
43.27
36.20
31.72
31.00
29.41
25.56
18.43
16.08



36