Nickel/Bis(oxazoline)-Catalyzed Asymmetric Negishi Arylations of Racemic Secondary Benzylic Electrophiles to Generate Enantioenriched 1,1-Diarylalkanes

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Supporting Information

Table of Contents

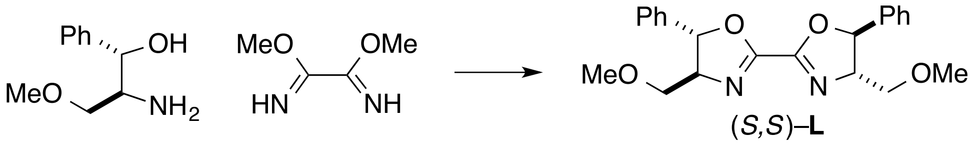
I. General Information

The following reagents were purchased and used as received: $NiBr_2$•diglyme (Aldrich), ZnI_2 (Strem; moisture-sensitive), MsCl (Aldrich), NEt_3 (J.T. Baker), LiI (Strem; moisture-sensitive), and THF (Aldrich; anhydrous and inhibitor-free). The Grignard reagents were purchased (Aldrich) or prepared from the reaction of the aryl iodide with isopropylmagnesium chloride (Aldrich; 2.0 M in THF). CH_2Cl_2 was dried in a solvent-purification system with the aid of activated alumina. All reactions were carried out in oven-dried glassware under an inert atmosphere.

^1H and ^{13}C NMR data were collected on a Varian Inova 500 spectrometer at ambient temperature. HPLC analyses were carried out on an Agilent 1100 Series system with Daicel CHIRALCEL® columns or Daicel CHIRALPAK® columns (I.D. 4.6 mm, column length 250 mm, particle size 3 μm or 5 μm). GC analyses were carried out on an Agilent 6890 Series system with a DB-1 column (I.D. 0.25 mm, column length 30 m) and an Agilent 6850 Series system with a G-TA column (I.D. 0.25 mm, column length 30 m). GC-MS analyses were performed on an Agilent 6980 Series system equipped with an Agilent 5973 Network Mass Selective Detector. SFC analyses were performed on a Thar SFC system equipped with an Agilent 1315B DAD detector using Daicel CHIRALCEL® columns or Daicel CHIRALPAK® columns (I.D. 4.6 mm, column length 250 mm, particle size 3 μm or 5 μm) at 40 °C.

II. Preparation of Materials

These procedures have not been optimized.



(4*S*,4'*S*,5*S*,5'*S*)-4,4'-Bis(methoxymethyl)-5,5'-diphenyl-4,4',5,5'-tetrahydro-2,2'-bioxazole. A solution of (*1S,2S*)-(+)-2-amino-3-methoxy-1-phenyl-1-propanol (Aldrich; 1.0 g, 5.5 mmol) and dimethyl oxalimidate[1] (305 mg, 2.63 mmol; 0.48 equiv) in CH_2Cl_2 (10 mL) in a sealed 20-mL vial was stirred at 55 °C for three days. The solvent was then removed, and the residue was purified by flash chromatography (2% NEt_3 in EtOAc/hexanes 4/6). The purified product was re-dissolved in anhydrous CH_2Cl_2, and then the solvent was removed. The product was dried under vacuum at 50 °C for two days, affording 717 mg (72% yield) of a light-tan viscous oil.

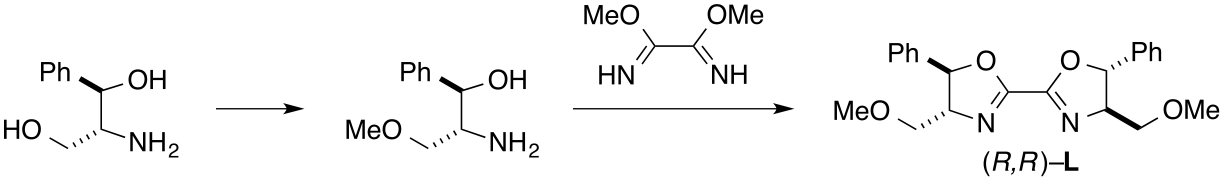
^1H NMR (500 MHz, $CDCl_3$) δ 7.43 – 7.28 (m, 10H), 5.59 (d, J = 7.9 Hz, 2H), 4.44 – 4.36 (m, 2H), 3.74 (dd, J = 9.7, 4.1 Hz, 2H), 3.64 (dd, J = 9.7, 6.4 Hz, 2H), 3.42 (s, 6H).

^{13}C NMR (126 MHz, $CDCl_3$) δ 154.9, 139.3, 128.8, 128.5, 125.9, 84.9, 74.8, 73.3, 59.3.

FT-IR (neat) 3291, 3063, 3033, 2984, 2927, 2891, 2828, 1676, 1620, 1496, 1456, 1382, 1343, 1266, 1224, 1192, 1128, 1011, 957, 915, 847, 759 cm^{-1}.

MS (ESI) *m/z* ($[M + H]^+$) calcd for $C_{22}H_{25}N_2O_4$: 381.2, found: 381.2.

$[\alpha]^{25}_D = -28.0°$ (c = 1.00, $CHCl_3$).



(4*R*,4'*R*,5*R*,5'*R*)-4,4'-Bis(methoxymethyl)-5,5'-diphenyl-4,4',5,5'-tetrahydro-2,2'-bioxazole. A suspension of KH (1.32 g, 33 mmol) in THF was added dropwise to a stirred solution of (*1R,2R*)-2-amino-1-phenylpropane-1,3-diol (Wako; 5.0 g, 30 mmol) in dry THF (90 mL) at r.t. The resulting mixture was stirred at r.t. for 12 h. Next, CH_3I (2.4 mL, 36 mmol) was added dropwise over 2 min. The resulting mixture was stirred for 4 h, and then the reaction was carefully quenched by the addition of brine (50 mL). The reaction mixture was extracted with Et_2O (100 mL x 3), the solvent was removed from the organic extract, and the residue was purified by reverse-phase chromatography, which afforded the desired monomethylated

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(1) This compound was prepared by oxidation of diaminomaleonitrile (Webster, O. W.; Hartter, D. R.; Begland, R. W.; Sheppard, W. A.; Cairncross, A. *J. Org. Chem.* **1972**, *37*, 4133–4136), followed by displacement of cyanide with methoxide (Begland, R. W.; Hartter, D. R. *J. Org. Chem.* **1972**, *37*, 4136–4145).

product (607 mg, 11% yield). The methylated (*R*,*R*)-aminoalcohol was then reacted with dimethyl oxalimidate following the procedure described above for (*S*,*S*)–**L**, which furnished (*R*,*R*)–**L** (412 mg, 69% yield).

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.42 – 7.28 (m, 10H), 5.59 (d, J = 7.8 Hz, 2H), 4.44 – 4.36 (m, 2H), 3.74 (dd, J = 9.7, 4.1 Hz, 2H), 3.64 (dd, J = 9.7, 6.4 Hz, 2H), 3.42 (s, 6H).

^{13}C NMR (126 MHz, $CDCl_3$) δ 154.9, 139.3, 128.8, 128.5, 125.9, 84.9, 74.8, 73.3, 59.3.

FT-IR (neat) 3291, 3063, 3033, 2984, 2927, 2891, 2828, 1677, 1622, 1496, 1456, 1382, 1343, 1266, 1224, 1192, 1123, 1011, 957, 915, 847, 759 cm^{-1}.

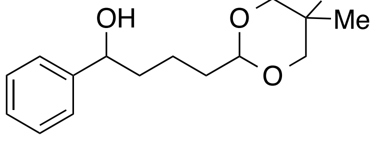
MS (ESI) *m*/*z* ($[M + H]^+$) calcd for $C_{22}H_{25}N_2O_4$: 381.2, found: 381.2.

$[\alpha]^{25}_D = +24.5°$ (c = 1.00, $CHCl_3$).

Preparation of benzylic alcohols. The following alcohols are commercially available: 1-phenylethanol (Aldrich), 1-phenylpropanol (Aldrich), 1-phenylbutanol (TCI), and 1-phenylpentanol (Alfa).

General Procedure A: Reduction of an aryl ketone by $NaBH_4$. A 100-mL round-bottom flask was charged with the ketone (10 mmol) and a mixture of 1,2-dichloroethane/methanol (1:1; 15 mL). $NaBH_4$ (2.0 equiv) was added portionwise to this stirred solution so as to maintain the reaction temperature around r.t. The resulting mixture was stirred at r.t. for 2 h, and then it was transferred to a separatory funnel with the aid of water (20 mL). The aqueous layer was extracted with CH_2Cl_2 (60 mL x 2), and the combined organic layers were washed with brine (20 mL), dried over $MgSO_4$, and concentrated under vacuum to furnish the benzylic alcohol. In most cases, the alcohol was generated in high purity and used without further purification.

General Procedure B: Addition of a Grignard reagent to an aldehyde. A 100-mL round-bottom flask was charged with the aldehyde (10 mmol), the flask was evacuated and backfilled with nitrogen (three cycles), and then THF (dry; 10 mL) was added. The resulting solution was cooled in an ice bath, and then the Grignard reagent (in Et_2O or THF; 1.3 equiv) was added dropwise. Then, the ice bath was removed, and the reaction mixture was stirred at r.t. for 3 h. Next, the reaction mixture was cooled in an ice bath, and the reaction was carefully quenched by the addition of a saturated solution of NH_4Cl (20 mL). The resulting mixture was transferred to a separatory funnel, and the aqueous layer was extracted with Et_2O (50 mL x 3). The combined organic layers were dried over $MgSO_4$ and concentrated under vacuum, and then the residue was purified by column chromatography.



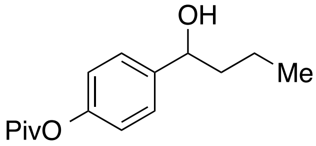
4-(5,5-Dimethyl-1,3-dioxan-2-yl)-1-phenylbutan-1-ol. This compound was prepared according to General Procedure B, using 4-(5,5-dimethyl-1,3-dioxan-2-yl)butanal and phenylmagnesium bromide. The product was obtained as a colorless oil (2.11 g, 80% yield).

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.37 – 7.23 (m, 5H), 4.69 – 4.63 (m, 1H), 4.40 (t, J = 5.0 Hz, 1H), 3.60 – 3.55 (m, 2H), 3.42 – 3.36 (m, 2H), 2.01 (d, J = 3.3 Hz, 1H), 1.89 – 1.62 (m, 4H), 1.64 – 1.49 (m, 1H), 1.50 – 1.36 (m, 1H), 1.17 (s, 3H), 0.71 (s, 3H).

^{13}C NMR (126 MHz, $CDCl_3$) δ 144.8, 128.4, 127.5, 125.9, 102.0, 74.4, 38.9, 34.5, 30.1, 23.0, 21.8, 20.4.

FT-IR (neat) 3435, 2952, 2848, 1603, 1493, 1471, 1453, 1394, 1362, 1311, 1237, 1173, 1133, 1102, 1014, 973, 913, 895, 836, 791, 762 cm^{-1}.

MS (EI) m/z ($[M - H_2O]^+$) calcd for $C_{16}H_{22}O_2$: 246.2, found: 246.1.



4-(1-Hydroxybutyl)phenyl pivalate. This compound was prepared according to General Procedure A, using 4-butyrylphenyl pivalate. The product was obtained as a white solid (2.17 g, 87% yield).

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.38 – 7.30 (m, 2H), 7.07 – 6.99 (m, 2H), 4.71 – 4.64 (m, 1H), 1.89 (d, J = 2.5 Hz, 1H), 1.83 – 1.60 (m, 2H), 1.50 – 1.20 (m, 2H), 1.35 (s, 9H), 0.92 (t, J = 7.4 Hz, 3H).

^{13}C NMR (126 MHz, $CDCl_3$) δ 177.1, 150.3, 142.2, 126.9, 121.4, 73.9, 41.2, 39.1, 27.1, 19.0, 13.9.

FT-IR (neat) 3399, 2959, 2933, 2873, 1752, 1606, 1507, 1480, 1459, 1396, 1279, 1200, 1165, 1118, 1029, 1016, 897, 852 cm^{-1}.

MS (EI) m/z ($[M- H_2O]^+$) calcd for $C_{15}H_{20}O_2$: 232.2, found: 232.0.

III. Stereoconvergent Negishi Arylations

Method A:

Preparation of the nucleophile (for a glovebox-free procedure, see below): In a nitrogen-filled glovebox, isopropylmagnesium chloride (2.0 M in THF; 1.6 mL, 3.2 mmol) was added dropwise over 1 min to a solution of the aryl iodide (3.2 mmol) in dry THF (anhydrous and inhibitor-free in a Sure/Seal bottle from Aldrich) in a 20-mL vial (at –20 °C for aryl iodides that contain potentially reactive functional groups; otherwise, at r.t.). The reaction mixture was stirred at the same temperature for 1 h, and then a solution of ZnI_2 (1.22 g, 3.84 mmol; in 4.5 mL of THF) was added. The resulting suspension was stirred vigorously for 1 h at r.t.

Preparation of the catalyst (half of the material was used for each of two reactions; for a glovebox-free procedure, see below): In a nitrogen-filled glovebox, a 20-mL vial was charged with bis(oxazoline) ligand **L** (70 mg, 0.184 mmol), $NiBr_2\cdot$diglyme (45 mg, 0.126 mmol), and dry CH_2Cl_2 (3.5 mL). The resulting mixture was stirred at r.t. for 30–45 min.

Preparation of the electrophile (conducted without a glovebox): The benzylic alcohol (2.8 mmol), NEt_3 (0.507 mL, 3.64 mmol), and dry CH_2Cl_2 (6.2 mL) were combined in a 20-mL vial. The vial was then flushed with nitrogen and capped. The vial cap was wrapped with electrical tape, and the vial was placed in a cryocool at –15 to –10 °C. The mixture was stirred for 5 min, and then mesyl chloride (0.24 mL, 3.08 mmol) was added in one portion by syringe, which resulted in the immediate precipitation of a white solid. The mixture was stirred at –15 to –10 °C for 30 min, and then it was filtered through an acrodisc into an empty, nitrogen-flushed vial that was capped with a PTFE-lined septum. The filtrate was kept at –15 to –10 °C.

Cross-coupling (for a glovebox-free procedure, see below): In a nitrogen-filled glovebox, a 20-mL vial was charged with LiI (ground; 375 mg, 2.8 mmol) and one-half of the catalyst suspension prepared above (1.75 mL). The vial was tightly sealed with a PTFE-lined septum cap and taken out of the glovebox. The vial cap was wrapped with electrical tape, and then the vial was placed in a cryocool at the indicated temperature (~–40 °C; see below). The solution of the electrophile (1.75 mL, 0.70 mmol) was added by syringe in one portion. After several minutes, the solution of the nucleophile (1.5-1.7 equiv; 3.5-4.0 mL) was added dropwise over one minute, and the septum cap was then covered with grease. The resulting suspension was stirred for 36 h. Next, the reaction was quenched with ethanol (1.5 mL) and stirred for 5 min at the same temperature, before it was allowed to warm to r.t. The mixture was diluted with Et_2O (150 mL) and washed with brine (40 mL). The aqueous phase was extracted with Et_2O (75 mL), and the combined organic layers were dried over $MgSO_4$ and concentrated. The residue was purified by column chromatography (Biotage).

Method B:

Preparation of the nucleophile: Same as Method A.

Preparation of the catalyst: Same as Method A.

Preparation of the electrophile (conducted without a glovebox): Same as Method A, except that dry THF (inhibitor-free; 6.2 mL) was employed as the solvent. Method B was used when the triethylammonium salt did not entirely precipitate from CH_2Cl_2.

Cross-coupling (for a glovebox-free procedure, see below): In a nitrogen-filled glovebox, a 20-mL vial was charged with LiI (ground; 375 mg, 2.8 mmol), CH_2Cl_2 (3.0 mL), and one-half of the catalyst suspension prepared above (1.75 mL). The remainder of the procedure is the same as Method A, except that the electrophile was a solution in THF, rather than CH_2Cl_2.

Gram-scale reaction: The cross-coupling of 1-phenylpropyl mesylate with 4-methoxyphenylzinc iodide (Table 2, Entry 2) was conducted on a 7-mmol scale in a 100-mL round-bottom flask, according to method A. After column chromatography (hexanes → 25% CH_2Cl_2/hexanes), the product was obtained as a colorless oil (1.40 g, 89% yield, 95% ee).

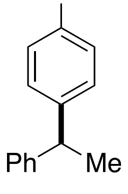
Glovebox-free procedure: The cross-coupling of 1-phenylpropyl mesylate with 4-methoxyphenylzinc iodide (Table 2, Entry 2) was conducted without the use of a glovebox.

Preparation of the nucleophile: A 20-mL vial was charged with the aryl iodide (3.2 mmol), tightly sealed with a PTFE-lined septum cap, and then evacuated/backfilled with nitrogen (three cycles). Dry THF (3.5 mL) was added, followed by the dropwise addition of isopropylmagnesium chloride (2.0 M in THF; 1.6 mL, 3.2 mmol) at r.t. This reaction mixture was stirred for 1 h. In a separate 20-mL vial, a solution of ZnI_2 (1.22 g, 3.84 mmol) in THF (4.5 mL) was prepared in a similar manner under nitrogen, and this solution of ZnI_2 was then added dropwise to the solution of the Grignard reagent. The resulting suspension was stirred vigorously for 1 h.

Preparation of the catalyst: A 20-mL vial was charged with bis(oxazoline) ligand **L** (70 mg, 0.184 mmol) and $NiBr_2$•diglyme (45 mg, 0.126 mmol). The vial was tightly sealed with a PTFE-lined septum cap and then evacuated/backfilled with nitrogen (three cycles). Dry CH_2Cl_2 (3.5 mL) was added, and the suspension was stirred at r.t. for at least 30 min.

Preparation of the electrophile: Same as Method A.

Cross-coupling reaction: A 20-mL vial was charged with LiI (ground; 375 mg, 2.8 mmol), tightly sealed with a PTFE-lined septum cap, and then evacuated/backfilled with nitrogen (three cycles). Next, one-half of the catalyst suspension (1.75 mL) was added by syringe, the vial cap was wrapped with electrical tape, and then the vial was placed in a cryocool at –45 °C. The remainder of the procedure is the same as Method A. After column chromatography (hexanes → 25% CH_2Cl_2/hexanes), the product was obtained as a colorless oil (126 mg, 80% yield; 94% ee).



(*S*)-1-Methoxy-4-(1-phenylethyl)benzene (Table 2, Entry 1). The title compound was prepared according to General Method A: 1-Phenylethyl mesylate (0.70 mmol), 4-methoxyphenylzinc iodide (1.7 equiv), –45 °C. The product was purified by column chromatography (hexanes → 25% CH_2Cl_2/hexanes). Colorless oil. First run: 129 mg (87%; 88% ee). Second run: 131 mg (88%; 88% ee).

The ee was determined by SFC on a CHIRALPAK AD-H column (3% MeOH in CO_2, 2.5 mL/min) with t_r = 2.88 min (major), 3.25 min (minor).

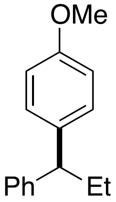
^{1}H NMR (500 MHz, $CDCl_3$) δ 7.33 – 7.10 (m, 7H), 6.88 – 6.78 (m, 2H), 4.11 (q, J = 7.2 Hz, 1H), 3.78 (s, 3H), 1.62 (d, J = 7.2 Hz, 3H).

^{13}C NMR (126 MHz, $CDCl_3$) δ 158.0, 146.9, 138.7, 128.7, 128.5, 127.7, 126.1, 113.9, 55.4, 44.1, 22.2.

FT-IR (neat) 3060, 3026, 2999, 2964, 2930, 2905, 2872, 2833, 1612, 1583, 1511, 1494, 1452, 1373, 1302, 1287, 1246, 1177, 1117, 1035, 1027, 832, 771, 727 cm^{-1}.

MS (EI) *m/z* (M^+) calcd for $C_{15}H_{16}O$: 212.1, found: 212.0.

$[\alpha]^{25}_D$ = +8.7° (c = 1.00, $CHCl_3$).



(*S*)-1-Methoxy-4-(1-phenylpropyl)benzene (Table 2, Entry 2). The title compound was prepared according to General Method A: 1-Phenylpropyl mesylate (0.70 mmol), 4-methoxyphenylzinc iodide (1.7 equiv), –45 °C. The product was purified by column chromatography (hexanes → 25% CH_2Cl_2/hexanes). Colorless oil. First run: 147 mg (93%; 94% ee). Second run: 144 mg (91%; 94% ee).

The ee was determined by SFC on a CHIRALPAK AD-H column (2% MeOH in CO_2, 2.5 mL/min) with t_r = 3.62 min (major), 4.44 min (minor).

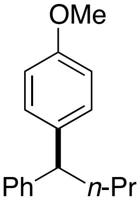
^{1}H NMR (500 MHz, $CDCl_3$) δ 7.30 – 7.12 (m, 7H), 6.84 – 6.80 (m, 2H), 3.77 (s, 3H), 3.74 (t, J = 7.8 Hz, 1H), 2.10 – 1.99 (m, 2H), 0.89 (t, J = 7.3 Hz, 3H).

^{13}C NMR (126 MHz, $CDCl_3$) δ 158.0, 145.7, 137.5, 128.9, 128.5, 128.0, 126.0, 113.9, 55.4, 52.5, 28.9, 13.0.

FT-IR (neat) 3060, 3026, 2959, 2930, 2872, 2833, 1611, 1583, 1511, 1494, 1452, 1377, 1302, 1248, 1177, 1119, 1038, 819, 782, 761, 726 cm^{-1}.

MS (EI) *m/z* (M^+) calcd for $C_{16}H_{18}O$: 226.1, found: 226.1.

$[\alpha]^{25}_D$ = +5.8° (c = 1.00, $CHCl_3$).



(*S*)-1-Methoxy-4-(1-phenylbutyl)benzene (Table 2, Entry 3). The title compound was prepared according to General Method A: 1-Phenylbutyl mesylate (0.70 mmol), 4-methoxyphenylzinc iodide (1.7 equiv), –45 °C. The product was purified by column chromatography (hexanes → 25% CH_2Cl_2/hexanes). Colorless oil. First run: 153 mg (91%; 94% ee). Second run: 150 mg (89%; 94% ee).

The ee was determined by SFC on a CHIRALPAK AD-H column (2% MeOH in CO_2, 2.5 mL/min) with t_r = 3.25 min (major), 3.71 min (minor).

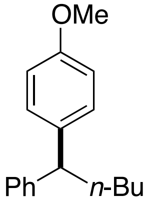
^{1}H NMR (500 MHz, $CDCl_3$) δ 7.32 – 7.12 (m, 7H), 6.87 – 6.77 (m, 2H), 3.86 (t, J = 7.8 Hz, 1H), 3.77 (s, 3H), 2.04 – 1.93 (m, 2H), 1.33 – 1.20 (m, 2H), 0.92 (t, J = 7.4 Hz, 3H).

^{13}C NMR (126 MHz, $CDCl_3$) δ 157.9, 145.9, 137.6, 128.9, 128.5, 127.9, 126.0, 113.9, 55.4, 50.3, 38.3, 21.3, 14.2.

FT-IR (neat) 3060, 3026, 2999, 2955, 2930, 2870, 2833, 1610, 1583, 1511, 1494, 1463, 1452, 1378, 1302, 1249, 1177, 1119, 1067, 1037, 851, 824, 803, 784, 750, 726 cm^{-1}.

MS (EI) *m/z* (M^+) calcd for $C_{17}H_{20}O$: 240.1, found: 240.1.

$[\alpha]^{25}_D$ = +6.4° (c = 1.00, $CHCl_3$).



(*S*)-1-Methoxy-4-(1-phenylpentyl)benzene (Table 2, Entry 4). The title compound was prepared according to General Method A: 1-Phenylpentyl mesylate (0.70 mmol), 4-methoxyphenylzinc iodide (1.7 equiv), –45 °C. The product was purified by column chromatography (hexanes → 25% CH_2Cl_2/hexanes). Colorless oil. First run: 148 mg (83%; 95% ee). Second run: 145 mg (82%; 95% ee).

The ee was determined by HPLC on a CHIRALCEL OJ-H column (2% *i*-PrOH/hexanes, 1.0 mL/min) with t_r = 13.88 min (major), 16.45 min (minor).

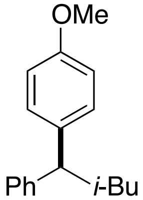
^{1}H NMR (500 MHz, $CDCl_3$) δ 7.30 – 7.12 (m, 7H), 6.85 – 6.79 (m, 2H), 3.83 (t, J = 7.8 Hz, 1H), 3.77 (s, 3H), 2.05 – 1.96 (m, 2H), 1.39 – 1.29 (m, 2H), 1.28 – 1.19 (m, 2H), 0.86 (t, J = 7.3 Hz, 3H).

^{13}C NMR (126 MHz, $CDCl_3$) δ 158.0, 146.0, 137.7, 128.9, 128.5, 127.89, 126.0, 113.9, 55.4, 50.6, 35.8, 30.4, 22.9, 14.2.

FT-IR (neat) 3060, 3026, 2999, 2964, 2930, 2858, 2833, 1611, 1583, 1511, 1494, 1452, 1377, 1302, 1287, 1247, 1177, 1120, 1038, 826, 783, 767, 726 cm^{-1}.

MS (EI) *m/z* (M^+) calcd for $C_{18}H_{22}O$: 254.2, found: 254.2.

$[\alpha]^{25}_D$ = +5.8° (c = 1.00, $CHCl_3$).



(*S*)-1-Methoxy-4-(3-methyl-1-phenylbutyl)benzene (Table 2, Entry 5). The title compound was prepared according to General Method A: 3-Methyl-1-phenylbutyl mesylate (0.70 mmol), 4-methoxyphenylzinc iodide (1.7 equiv), –45 °C. The product was purified by column chromatography (hexanes → 25% CH_2Cl_2/hexanes). Colorless oil. First run: 140 mg (79%; 95% ee). Second run: 131 mg (74%; 95% ee).

The ee was determined by SFC on a CHIRALPAK IC column (2% MeOH in CO_2, 1.5 mL/min) with t_r = 5.90 min (major), 6.21 min (minor).

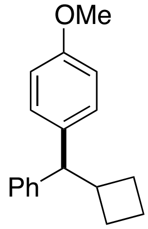
^{1}H NMR (500 MHz, $CDCl_3$) δ 7.32 – 7.11 (m, 7H), 6.87 – 6.77 (m, 2H), 3.97 (t, J = 8.0 Hz, 1H), 3.77 (s, 3H), 1.89 (dd, J = 8.0, 6.9 Hz, 2H), 1.50 – 1.39 (m, 1H), 0.91 (dd, J = 6.6, 0.9 Hz, 6H).

^{13}C NMR (126 MHz, $CDCl_3$) δ 158.0, 145.9, 137.6, 128.9, 128.5, 127.9, 126.0, 113.9, 55.4, 48.1, 45.4, 25.7, 22.8. 22.7.

FT-IR (neat) 3060, 3026, 2953, 2866, 2834, 1611, 1583, 1511, 1494, 1465, 1452, 1383, 1366, 1302, 1249, 1177, 1121, 1070, 1039, 829, 783, 768, 727 cm^{-1}.

MS (EI) *m/z* (M^+) calcd for $C_{18}H_{22}O$: 254.2, found: 254.2.

$[\alpha]^{25}_D$ = +6.0° (c = 1.00, $CHCl_3$).



(*S*)-1-(Cyclobutyl(phenyl)methyl)-4-methoxybenzene (Table 2, Entry 6). The title compound was prepared according to General Method A: Cyclobutyl(phenyl)methyl mesylate (0.70 mmol), 4-methoxyphenylzinc iodide (1.7 equiv), –45 °C. The product was purified by column chromatography (hexanes → 25% CH_2Cl_2/hexanes). Colorless oil. First run: 88 mg (50%; 94% ee). Second run: 90 mg (51%; 94% ee).

The ee was determined by SFC on a CHIRALPAK AD-H column (2% MeOH in CO_2, 2.5 mL/min) with t_r = 5.79 min (major), 7.34 min (minor).

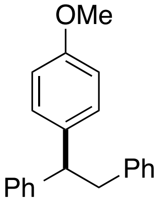
^{1}H NMR (500 MHz, $CDCl_3$) δ 7.29 – 7.06 (m, 7H), 6.85 – 6.76 (m, 2H), 3.81 (d, J = 11.0 Hz, 1H), 3.76 (s, 3H), 3.07 – 2.94 (m, 1H), 2.08 – 1.94 (m, 2H), 1.91 – 1.67 (m, 4H).

^{13}C NMR (126 MHz, $CDCl_3$) δ 157.9, 144.4, 136.2, 129.1, 128.4, 128.1, 126.1, 113.8, 57.6, 55.3, 40.4, 28.1, 28.0, 17.7.

FT-IR (neat) 3060, 3026, 2957, 2833, 1610, 1583, 1511, 1494, 1463, 1302, 1247, 1177, 1131, 1104, 1071, 1037, 804, 723 cm^{-1}.

MS (EI) *m/z* (M^+) calcd for $C_{18}H_{20}O$: 252.1, found: 252.1.

$[\alpha]^{25}_D$ = +1.83° (c = 1.00, $CHCl_3$).



(*S*)-(1-(4-Methoxyphenyl)ethane-1,2-diyl)dibenzene (Table 2, Entry 7). The title compound was prepared according to General Method A: 1,2-Diphenylethyl mesylate (0.70 mmol), 4-methoxyphenylzinc iodide (1.7 equiv), –35 °C. The product was purified by column chromatography (hexanes → 25% CH_2Cl_2/hexanes). White solid. First run: 158 mg (78%; 95% ee). Second run: 163 mg (81%; 95% ee).

The ee was determined by SFC on a CHIRALPAK IC column (3% MeOH in CO_2, 2.5 mL/min) with t_r = 6.70 min (major), 7.13 min (minor).

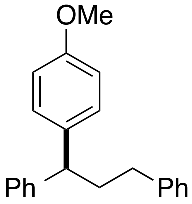
^{1}H NMR (500 MHz, $CDCl_3$) δ 7.30 – 7.06 (m, 10H), 7.03 – 6.97 (m, 2H), 6.82 – 6.74 (m, 2H), 4.19 (t, J = 7.8 Hz, 1H), 3.76 (s, 3H), 3.33 (d, J = 7.8 Hz, 2H).

^{13}C NMR (126 MHz, $CDCl_3$) δ 158.0, 145.0, 140.5, 136.8, 129.2, 129.1, 128.5, 128.2, 128.1, 126.2, 126.0, 113.8, 55.3, 52.4, 42.5.

FT-IR (neat) 3084, 3059, 3026, 3000, 2931, 2835, 1610, 1583, 1510, 1495, 1452, 1302, 1249, 1177, 1110, 1071, 1032, 829 cm^{-1}.

MS (EI) *m/z* ($[M - CH_2C_6H_5]^+$) calcd for $C_{14}H_{13}O$: 197.1, found: 197.0.

$[\alpha]^{25}_D$ = –18.7° (c = 1.00, $CHCl_3$).



(*S*)-(1-(4-Methoxyphenyl)propane-1,3-diyl)dibenzene (Table 2, Entry 8). The title compound was prepared according to General Method A: 1,3-Diphenylpropyl mesylate (0.70 mmol), 4-methoxyphenylzinc iodide (1.7 equiv), –45 °C. The product was purified by column chromatography (hexanes → 25% CH_2Cl_2/hexanes). Colorless oil. First run: 187 mg (89%; 88% ee). Second run: 192 mg (91%; 88% ee).

The ee was determined by SFC on a CHIRALPAK IC column (3% MeOH in CO_2, 2.5 mL/min) with t_r = 7.58 min (major), 8.26 min (minor).

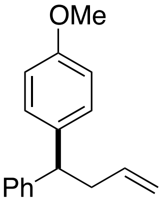
^{1}H NMR (500 MHz, $CDCl_3$) δ 7.32 – 7.11 (m, 12H), 6.89 – 6.79 (m, 2H), 3.88 (t, J = 7.8 Hz, 1H), 3.78 (s, 3H), 2.62 – 2.52 (m, 2H), 2.41 – 2.30 (m, 2H).

^{13}C NMR (126 MHz, $CDCl_3$) δ 158.1, 145.4, 142.3, 137.1, 128.9, 128.593, 128.586, 128.5, 127.9, 126.2, 125.9, 114.0, 55.4, 50.0, 37.6, 34.3.

FT-IR (neat) 3083, 3060, 3025, 3000, 2932, 2860, 2834, 2060, 1947, 1881, 1805, 1753, 1608, 1583, 1515, 1513, 1506, 1495, 1463, 1454, 1441, 1334, 1302, 1247, 1177, 1155, 1111, 1076, 1036, 907, 866, 826, 807, 780, 761, 727 cm^{-1}.

MS (EI) *m/z* (M^+) calcd for $C_{22}H_{22}O$: 302.2, found: 302.1.

$[\alpha]^{25}_D$ = +0.51° (c = 1.00, $CHCl_3$).



(*S*)-1-Methoxy-4-(1-phenylbut-3-en-1-yl)benzene (Table 2, Entry 9). The title compound was prepared according to General Method A: 1-Phenylbut-3-en-1-yl mesylate (0.70 mmol), 4-methoxyphenylzinc iodide (1.7 equiv), –45 °C. The product was purified by column chromatography (hexanes → 25% CH_2Cl_2/hexanes). Colorless oil. First run: 95 mg (57%; 86% ee). Second run: 100 mg (60%; 85% ee).

The ee was determined by SFC on a CHIRALPAK IC column (1% MeOH in CO_2, 2.5 mL/min) with t_r = 5.11 min (major), 5.65 min (minor).

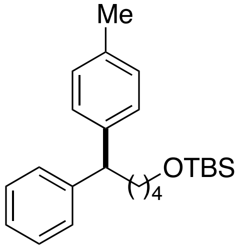
^{1}H NMR (500 MHz, $CDCl_3$) δ 7.33 – 7.10 (m, 7H), 6.88 – 6.77 (m, 2H), 5.77 – 5.66 (m, 1H), 5.06 – 5.00 (m, 1H), 4.97 – 4.93 (m, 1H), 3.97 (t, J = 7.9 Hz, 1H), 3.77 (s, 3H), 2.79 (ddt, J = 8.0, 6.8, 1.3 Hz, 2H).

^{13}C NMR (126 MHz, $CDCl_3$) δ 157.9, 144.9, 136.9, 136.6, 128.8, 128.4, 127.8, 126.1, 116.2, 113.7, 55.2, 50.4, 40.1.

FT-IR (neat) 3060, 3026, 2932, 2833, 1947, 1881, 1608, 1583, 1511, 1494, 1454, 1302, 1247, 1177, 1111, 1076, 1035, 907, 826, 780, 748 cm^{-1}.

MS (EI) *m/z* ($[M – CH_2CH{=}CH_2]^+$) calcd for $C_{14}H_{13}O$: 197.1, found: 197.0.

$[\alpha]^{25}_D$ = +1.25° (c = 1.00, $CHCl_3$).



(*S*)-*t*-Butyldimethyl((5-phenyl-5-(*p*-tolyl)pentyl)oxy)silane (Table 2, Entry 10). The title compound was prepared according to General Method A: 5-((*t*-Butyldimethylsilyl)oxy)-1-phenylpentyl mesylate (0.70 mmol), *p*-tolylzinc iodide (1.7 equiv), –45 °C. The product was purified by column chromatography (hexanes → 25% CH_2Cl_2/hexanes). Colorless oil. First run: 201 mg (78%; 94% ee). Second run: 196 mg (76%; 93% ee).

The ee was determined by SFC on a CHIRALCEL OB-H column (3% MeOH in CO_2, 2.5 mL/min) with t_r = 2.93 min (major), 3.54 min (minor).

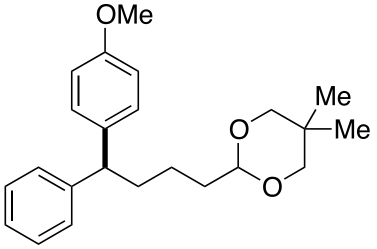
^{1}H NMR (500 MHz, $CDCl_3$) δ 7.30 – 7.18 (m, 4H), 7.21 – 7.04 (m, 5H), 3.85 (t, J = 7.8 Hz, 1H), 3.56 (t, J = 6.6 Hz, 2H), 2.30 (s, 3H), 2.08 – 1.98 (m, 2H), 1.60 – 1.49 (m, 2H), 1.34 – 1.23 (m, 2H), 0.86 (s, 9H), 0.01 (s, 6H).

^{13}C NMR (126 MHz, $CDCl_3$) δ 145.4, 142.2, 135.4, 129.1, 128.3, 127.8, 127.7, 125.9, 63.1, 50.9, 35.5, 32.8, 26.0, 24.3, 21.0, 18.3, –5.3.

FT-IR (neat) 3024, 2928, 2857, 1600, 1512, 1494, 1471, 1462, 1387, 1360, 1255, 1104, 1021, 1005, 835, 774, 720 cm^{-1}.

MS (EI) *m/z* ([M – $(CH_3)_3C]^+$) calcd for $C_{20}H_{27}OSi$: 311.2, found: 311.1.

$[\alpha]^{25}_{D}$ = +4.3° (c = 1.00, $CHCl_3$).



(*S*)-2-(4-(4-Methoxyphenyl)-4-phenylbutyl)-5,5-dimethyl-1,3-dioxane (Table 2, Entry 11). The title compound was prepared according to General Method A: 4-(5,5-Dimethyl-1,3-dioxan-2-yl)-1-phenylbutyl mesylate (0.70 mmol), 4-methoxyphenylzinc iodide (1.7 equiv), –45 °C. The product was purified by column chromatography (hexanes → 10% Et_2O/hexanes). Colorless oil. First run: 204 mg (82%; 92% ee). Second run: 214 mg (86%; 92% ee).

The ee was determined by SFC on a CHIRALCEL OD-H column (5% MeOH in CO_2, 2.5 mL/min) with t_r = 7.50 min (major), 10.40 min (minor).

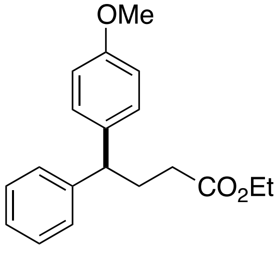
^{1}H NMR (500 MHz, $CDCl_3$) δ 7.31 – 7.09 (m, 7H), 6.91 – 6.78 (m, 2H), 4.35 (t, J = 5.1 Hz, 1H), 3.84 (t, J = 7.8 Hz, 1H), 3.77 (s, 3H), 3.58 – 3.54 (m, 2H), 3.39 – 3.35 (m, 2H), 2.08 – 1.96 (m, 2H), 1.70 – 1.61 (m, 2H), 1.44 – 1.31 (m, 2H), 1.16 (s, 3H), 0.70 (s, 3H).

^{13}C NMR (126 MHz, $CDCl_3$) δ 157.8, 145.5, 137.2, 128.7, 128.4, 127.7, 125.9, 113.7, 102.1, 55.2, 50.5, 35.8, 34.8, 30.1, 23.0, 22.7, 21.8.

FT-IR (neat) 3026, 2951, 2835, 1610, 1583, 1511, 1494, 1463, 1393, 1362, 1302, 1247, 1176, 1131, 1096, 1039, 973, 927, 824, 784, 726 cm^{-1}.

MS (EI) *m/z* (M^+) calcd for $C_{23}H_{30}O_3$: 354.2, found: 354.1.

$[\alpha]^{25}_{D}$ = +0.16° (c = 1.00, $CHCl_3$).



(*S*)-Ethyl 4-(4-methoxyphenyl)-4-phenylbutanoate (Table 2, Entry 12). The title compound was prepared according to General Method B: Ethyl 4-((methylsulfonyl)oxy)-4-phenylbutanoate (0.70 mmol), 4-methoxyphenylzinc iodide (1.7 equiv), –45 °C. The product was purified by column chromatography (hexanes → 10% Et_2O/hexanes). Colorless oil. First run: 176 mg (84%; 94% ee). Second run: 173 mg (83%; 94% ee).

The ee was determined by HPLC on a CHIRALCEL OD-H column (3% *i*-PrOH/hexanes, 1.0 mL/min) with t_r = 10.60 min (minor), 11.53 min (major).

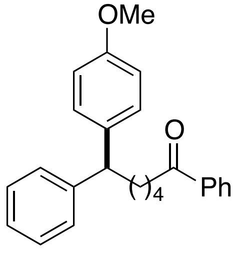
^{1}H NMR (500 MHz, CDCl$_3$) δ 7.32 – 7.12 (m, 7H), 6.86 – 6.77 (m, 2H), 4.10 (q, J = 7.2 Hz, 2H), 3.88 (t, J = 7.8 Hz, 1H), 3.77 (s, 3H), 2.41 – 2.29 (m, 2H), 2.31 – 2.20 (m, 2H), 1.23 (t, J = 7.1 Hz, 3H).

^{13}C NMR (126 MHz, CDCl$_3$) δ 173.5, 158.0, 144.5, 136.3, 128.8, 128.5, 127.7, 126.2, 113.9, 60.3, 55.2, 49.7, 32.8, 30.8, 14.2.

FT-IR (neat) 2963, 2935, 2875, 2835, 1732, 1610, 1583, 1511, 1495, 1452, 1374, 1303, 1249, 1178, 1113, 1035, 827, 784, 765, 727 cm^{-1}.

MS (EI) *m/z* (M$^+$) calcd for $C_{19}H_{22}O_3$: 298.2, found: 298.1.

$[\alpha]^{25}_D$ = +3.2° (c = 1.00, CHCl$_3$).



(*S*)-6-(4-Methoxyphenyl)-1,6-diphenylhexan-1-one (Table 2, Entry 13). The title compound was prepared according to General Method B: 6-Oxo-1,6-diphenylhexyl mesylate (0.70 mmol), 4-methoxyphenylzinc iodide (1.7 equiv), –45 °C. The product was purified by column chromatography (hexanes → 25% CH$_2$Cl$_2$/hexanes). White solid. First run: 221 mg (88%; 94% ee). Second run: 220 mg (88%; 95% ee).

The ee was determined by SFC on a CHIRALPAK AD-H column (7% MeOH in CO$_2$, 2.5 mL/min) with t_r = 8.37 min (major), 13.34 min (minor).

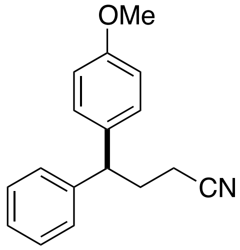
^{1}H NMR (500 MHz, CDCl$_3$) δ 7.96 – 7.89 (m, 2H), 7.59 – 7.50 (m, 1H), 7.49 – 7.40 (m, 2H), 7.32 – 7.11 (m, 7H), 6.85 – 6.78 (m, 2H), 3.86 (t, J = 7.8 Hz, 1H), 3.77 (s, 3H), 2.93 (dd, J = 7.8, 7.0 Hz, 2H), 2.13 – 2.01 (m, 2H), 1.84 – 1.72 (m, 2H), 1.42 – 1.29 (m, 2H).

^{13}C NMR (126 MHz, CDCl$_3$) δ 200.3, 157.8, 145.5, 137.2, 137.0, 132.9, 128.7, 128.5, 128.4, 128.0, 127.7, 126.0, 113.8, 55.2, 50.3, 38.5, 35.7, 27.8, 24.2.

FT-IR (neat) 3058, 3025, 3000, 2933, 2860, 2834, 1683, 1609, 1597, 1581, 1511, 1494, 1463, 1448, 1365, 1302, 1248, 1177, 1034, 827, 753, 727 cm^{-1}.

MS (EI) *m/z* (M$^+$) calcd for $C_{25}H_{26}O_2$: 358.2, found: 358.1.

$[\alpha]^{25}_D$ = +2.0° (c = 1.00, CHCl$_3$).



(*S*)-4-(4-Methoxyphenyl)-4-phenylbutanenitrile (Table 2, Entry 14). The title compound was prepared according to General Method B: 3-Cyano-1-phenylpropyl mesylate (0.70 mmol), 4-methoxyphenylzinc iodide (1.7 equiv), –45 °C. The product was purified by column chromatography (hexanes → 20% Et_2O/hexanes). Colorless oil. First run: 130 mg (74%; 94% ee). Second run: 131 mg (75%; 94% ee).

The ee was determined by SFC on a CHIRALPAK AD-H column (10% MeOH in CO_2, 2.5 mL/min) with t_r = 4.49 min (major), 5.36 min (minor).

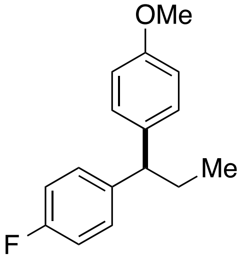
^{1}H NMR (500 MHz, $CDCl_3$) δ 7.35 – 7.10 (m, 7H), 6.90 – 6.80 (m, 2H), 4.01 (t, J = 8.0 Hz, 1H), 3.78 (s, 3H), 2.42 – 2.31 (m, 2H), 2.32 – 2.21 (m, 2H).

^{13}C NMR (126 MHz, $CDCl_3$) δ 158.4, 143.1, 134.8, 128.8, 128.6, 127.6, 126.8, 119.4, 114.2, 55.3, 49.0, 31.2, 15.8.

FT-IR (neat) 3060, 3027, 3002, 2934, 2835, 2244, 1610, 1583, 1506, 1453, 1422, 1303, 1248, 1178, 1113, 1034, 825, 785, 764, 728 cm^{-1}.

MS (EI) *m/z* (M^+) calcd for $C_{17}H_{17}NO$: 251.1, found: 251.1.

$[\alpha]^{25}_D$ = –6.5° (c = 1.00, $CHCl_3$).



(*R*)-1-Fluoro-4-(1-(4-methoxyphenyl)propyl)benzene (Table 2, Entry 15). The title compound was prepared according to General Method A: 1-(4-Fluorophenyl)propyl mesylate (0.70 mmol), 4-methoxyphenylzinc iodide (1.7 equiv), –45 °C. The product was purified by column chromatography (hexanes → 25% CH_2Cl_2/hexanes). Colorless oil. First run: 145 mg (85%; 92% ee). Second run: 150 mg (88%; 93% ee).

The ee was determined by HPLC on a CHIRALCEL OJ-H column (2% *i*-PrOH/hexanes, 1.0 mL/min) with t_r = 13.98 min (minor), 15.48 min (major).

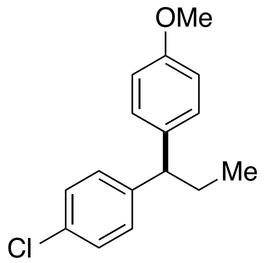
^{1}H NMR (500 MHz, $CDCl_3$) δ 7.19 – 7.09 (m, 4H), 6.98 – 6.92 (m, 2H), 6.85 – 6.80 (m, 2H), 3.77 (s, 3H), 3.72 (t, J = 7.8 Hz, 1H), 2.07 – 1.94 (m, 2H), 0.88 (t, J = 7.3 Hz, 3H).

^{13}C NMR (126 MHz, $CDCl_3$) δ 161.3 (d, J = 243.7 Hz), 158.0, 141.4 (d, J = 3.4 Hz), 137.3, 129.3 (d, J = 8.0 Hz), 128.8, 115.2 (d, J = 21.1 Hz), 113.9, 55.4, 51.7, 29.0, 12.9.

FT-IR (neat) 2961, 2932, 2873, 2834, 1610, 1583, 1506, 1463, 1378, 1302, 1249, 1178, 1158, 1119, 1038, 1015, 825, 781, 737 cm^{-1}.

MS (EI) *m/z* (M^+) calcd for $C_{16}H_{17}FO$: 244.1, found: 244.1.

$[\alpha]^{25}_D$ = +4.8° (c = 1.00, $CHCl_3$).



(*R*)-1-Chloro-4-(1-(4-methoxyphenyl)propyl)benzene (Table 2, Entry 16). The title compound was prepared according to General Method A: 1-(4-Chlorophenyl)propyl mesylate (0.70 mmol), 4-methoxyphenylzinc iodide (1.7 equiv), –45 °C. The product was purified by column chromatography (hexanes → 25% CH_2Cl_2/hexanes). Colorless oil. First run: 162 mg (89%; 90% ee). Second run: 156 mg (86%; 90% ee).

The ee was determined by HPLC on a CHIRALCEL OJ-H column (2% *i*-PrOH/hexanes, 1.0 mL/min) with t_r = 10.87 min (minor), 11.76 min (major).

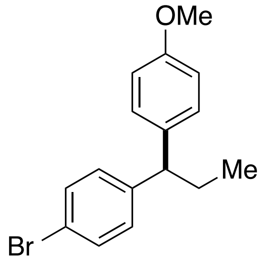
^{1}H NMR (500 MHz, $CDCl_3$) δ 7.28 – 7.20 (m, 2H), 7.17 – 7.08 (m, 4H), 6.86 – 6.79 (m, 2H), 3.77 (s, 3H), 3.72 (t, J = 7.9 Hz, 1H), 2.06 – 1.96 (m, 2H), 0.88 (t, J = 7.3 Hz, 3H).

^{13}C NMR (126 MHz, $CDCl_3$) δ 157.9, 144.1, 136.7, 131.6, 129.1, 128.7, 128.4, 113.8, 55.2, 51.7, 28.6, 12.7.

FT-IR (neat) 2960, 2931, 2873, 2834, 1610, 1583, 1506, 1489, 1407, 1378, 1302, 1249, 1176, 1120, 1092, 1038, 1014, 820, 757 cm^{-1}.

MS (EI) *m/z* (M^+) calcd for $C_{16}H_{17}ClO$: 260.1, found: 260.1.

$[\alpha]^{25}_D$ = +2.8° (c = 1.00, $CHCl_3$).



(*R*)-1-Bromo-4-(1-(4-methoxyphenyl)propyl)benzene (Table 2, Entry 17). The title compound was prepared according to General Method A: 1-(4-Bromophenyl)propyl mesylate (0.70 mmol), 4-methoxyphenylzinc iodide (1.7 equiv), –45 °C. The product was purified by column chromatography (hexanes → 25% CH_2Cl_2/hexanes). Colorless oil. First run: 167 mg (78%; 91% ee). Second run: 170 mg (80%; 91% ee).

The ee was determined by SFC on a CHIRALPAK AD-H column (3% MeOH in CO_2, 2.5 mL/min) with t_r = 7.56 min (minor), 8.87 min (major).

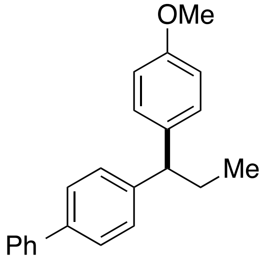
^{1}H NMR (500 MHz, $CDCl_3$) δ 7.42 – 7.33 (m, 2H), 7.16 – 7.03 (m, 4H), 6.86 – 6.77 (m, 2H), 3.77 (s, 3H), 3.70 (t, J = 7.8 Hz, 1H), 2.07 – 1.94 (m, 2H), 0.88 (t, J = 7.3 Hz, 3H).

^{13}C NMR (126 MHz, $CDCl_3$) δ 157.9, 144.6, 136.6, 131.4, 129.6, 128.7, 119.6, 113.8, 55.2, 51.8, 28.6, 12.7.

FT-IR (neat) 2960, 2930, 2872, 2833, 1611, 1583, 1511, 1488, 1463, 1404, 1302, 1249, 1177, 1121, 1075, 1038, 1009, 818, 752 cm^{-1}.

MS (EI) *m/z* (M^+) calcd for $C_{16}H_{17}BrO$: 304.0, found: 303.9.

$[\alpha]^{25}_{D}$ = +0.02° (c = 1.00, $CHCl_3$).



(*S*)-4-(1-(4-Methoxyphenyl)propyl)-1,1'-biphenyl (Table 2, Entry 18). The title compound was prepared according to General Method A: 1-([1,1'-Biphenyl]-4-yl)propyl mesylate (0.70 mmol), 4-methoxyphenylzinc iodide (1.7 equiv), –45 °C. The product was purified by column chromatography (hexanes → 25% CH_2Cl_2/hexanes). Light-tan solid. First run: 165 mg (78%; 92% ee). Second run: 165 mg (78%; 92% ee).

The ee was determined by SFC on a CHIRALPAK IC column (3% MeOH in CO_2, 2.5 mL/min) with t_r = 13.03 min (minor), 13.99 min (major).

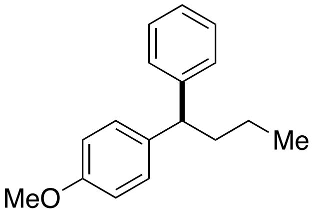
^{1}H NMR (500 MHz, $CDCl_3$) δ 7.60 – 7.37 (m, 6H), 7.37 – 7.24 (m, 3H), 7.24 – 7.15 (m, 2H), 6.88 – 6.79 (m, 2H), 3.79 (t, J = 7.9 Hz, 1H), 3.78 (s, 3H), 2.14 – 2.01 (m, 2H), 0.92 (t, J = 7.3 Hz, 3H).

^{13}C NMR (126 MHz, $CDCl_3$) δ 157.9, 144.7, 141.0, 138.8, 137.2, 128.8, 128.6, 128.2, 127.1, 127.0, 113.8, 55.2, 52.1, 28.8, 12.8.

FT-IR (neat) 3027, 2959, 2930, 2872, 2833, 1611, 1583, 1511, 1486, 1463, 1407, 1377, 1302, 1248, 1177, 1123, 1075, 1038, 1007, 825, 766, 745, 734 cm^{-1}.

MS (EI) *m*/*z* (M^+) calcd for $C_{22}H_{22}O$: 302.2, found: 302.1.

$[\alpha]^{25}_{D}$ = –5.9° (c = 1.00, $CHCl_3$).



(*R*)-1-Methoxy-4-(1-phenylbutyl)benzene (Table 2, Entry 19). The title compound was prepared according to General Method B: 1-(4-Methoxyphenyl)butyl mesylate (0.70 mmol), phenylzinc iodide (1.7 equiv), –45 °C. The product was purified by column chromatography (hexanes → 25% CH_2Cl_2/hexanes). Colorless oil. First run: 157 mg (93%; 94% ee). Second run: 160 mg (95%; 95% ee).

The ee was determined by SFC on a CHIRALCEL AD-H column (3% MeOH in CO_2, 2.5 mL/min) with t_r = 2.91 min (minor), 3.23 min (major).

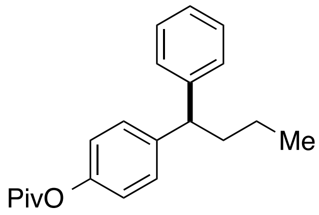
^{1}H NMR (500 MHz, $CDCl_3$) δ 7.32 – 7.10 (m, 7H), 6.86 – 6.77 (m, 2H), 3.86 (t, J = 7.8 Hz, 1H), 3.77 (s, 3H), 2.05 – 1.93 (m, 2H), 1.33 – 1.20 (m, 2H), 0.92 (t, J = 7.4 Hz, 3H).

^{13}C NMR (126 MHz, $CDCl_3$) δ 157.8, 145.7, 137.5, 128.7, 128.3, 127.8, 125.9, 113.7, 55.2, 50.2, 38.1, 21.2, 14.1.

FT-IR (neat) 3060, 3026, 2999, 2955, 2930, 2870, 2833, 1610, 1583, 1511, 1494, 1463, 1452, 1378, 1302, 1249, 1177, 1119, 1067, 1037, 851, 824, 803, 784, 750, 726 cm^{-1}.

MS (EI) *m/z* (M$^+$) calcd for $C_{17}H_{20}O$: 240.1, found: 240.1.

$[\alpha]^{25}_{D}$ = –7.0° (c = 1.00, $CHCl_3$).



(*R*)-4-(1-Phenylbutyl)phenyl pivalate (Table 2, Entry 20). The title compound was prepared according to General Method B: 4-(1-(Mesyloxy)butyl)phenyl pivalate (0.70 mmol), phenylzinc iodide (1.7 equiv), –35 °C. The product was purified by column chromatography (hexanes → 25% CH_2Cl_2/hexanes). Colorless oil. First run: 182 mg (84%; 84% ee). Second run: 180 mg (84%; 84% ee).

The ee was determined by SFC on a CHIRALCEL OB-H column (5% MeOH in CO_2, 2.5 mL/min) with t_r = 2.56 min (minor), 3.75 min (major).

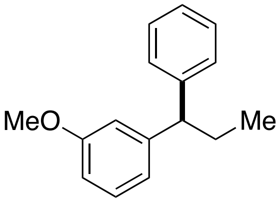
^{1}H NMR (500 MHz, $CDCl_3$) δ 7.31 – 7.11 (m, 7H), 7.01 – 6.93 (m, 2H), 3.91 (t, J = 7.8 Hz, 1H), 2.06 – 1.95 (m, 2H), 1.33 (s, 9H), 1.34 – 1.22 (m, 2H), 0.92 (t, J = 7.4 Hz, 3H).

^{13}C NMR (126 MHz, $CDCl_3$) δ 177.1, 149.2, 145.1, 142.6, 128.7, 128.4, 127.8, 126.0, 121.2, 50.4, 39.0, 37.9, 27.1, 21.1, 14.0.

FT-IR (neat) 3060, 3027, 2958, 2932, 2871, 1750, 1604, 1506, 1479, 1453, 1396, 1368, 1277, 1203, 1167, 1117, 1030, 1018, 895, 794, 753, 730 cm^{-1}.

MS (EI) *m/z* (M$^+$) calcd for $C_{21}H_{26}O_2$: 310.2, found: 310.2.

$[\alpha]^{25}_{D}$ = –3.9° (c = 1.00, $CHCl_3$).



(*R*)-1-Methoxy-3-(1-phenylpropyl)benzene (Table 2, Entry 21). The title compound was prepared according to General Method B: 1-(3-Methoxyphenyl)propyl mesylate (0.70 mmol), phenylzinc iodide (1.7 equiv), –45 °C. The product was purified by column chromatography (hexanes → 25% CH_2Cl_2/hexanes). Colorless oil. First run: 157 mg (93%; 94% ee). Second run: 160 mg (95%; 94% ee).

The ee was determined by SFC on a CHIRALPAK IC column (1% MeOH in CO_2, 2.5 mL/min) with t_r = 4.23 min (major), 4.67 min (minor).

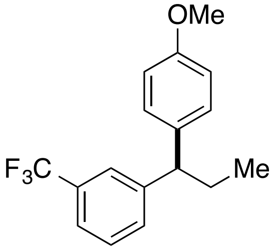
^{1}H NMR (500 MHz, $CDCl_3$) δ 7.33 – 7.12 (m, 6H), 6.87 – 6.77 (m, 2H), 6.71 (ddd, J = 8.2, 2.6, 0.9 Hz, 1H), 3.79 – 3.73 (m, 4H), 2.13 – 2.00 (m, 2H), 0.90 (t, J = 7.3 Hz, 3H).

^{13}C NMR (126 MHz, $CDCl_3$) δ 159.6, 146.8, 145.0, 129.2, 128.3, 127.8, 126.0, 120.4, 114.1, 110.8, 55.1, 53.3, 28.5, 12.8.

FT-IR (neat) 3060, 3026, 2960, 2931, 2873, 2833, 1597, 1583, 1488, 1451, 1436, 1378, 1313, 1288, 1260, 1151, 1049, 874, 775, 758 cm^{-1}.

MS (EI) *m/z* (M^+) calcd for $C_{16}H_{18}O$: 226.1, found: 226.1.

$[\alpha]^{25}_{D}$ = +0.54° (c = 1.00, $CHCl_3$).



(*R*)-1-(1-(4-Methoxyphenyl)propyl)-3-(trifluoromethyl)benzene (Table 2, Entry 22). The title compound was prepared according to General Method A: 1-(3-(Trifluoromethyl)phenyl)propyl mesylate (0.70 mmol), 4-methoxyphenylzinc iodide (1.7 equiv), –35 °C. The product was purified by column chromatography (hexanes → 25% CH_2Cl_2/hexanes). Colorless oil. First run: 125 mg (61%; 89% ee). Second run: 131 mg (64%; 89% ee).

The ee was determined by SFC on a CHIRALCEL OJ-H column (1% MeOH in CO_2, 2.5 mL/min) with t_r = 3.41 min (major), 3.84 min (minor).

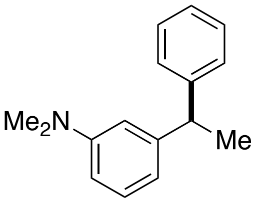
^{1}H NMR (500 MHz, $CDCl_3$) δ 7.51 – 7.33 (m, 4H), 7.20 – 7.09 (m, 2H), 6.90 – 6.80 (m, 2H), 3.81 (t, J = 7.7 Hz, 1H), 3.79 (s, 3H), 2.13 – 2.00 (m, 2H), 0.90 (t, J = 7.3 Hz, 3H).

^{13}C NMR (126 MHz, $CDCl_3$) δ 158.1, 146.5, 136.2, 131.27 – 131.16 (m), 130.6 (q, J = 31.8 Hz), 128.80 – 128.71 (m), 124.4 (q, J = 3.8 Hz), 124.3 (q, J = 272.1 Hz), 122.9 (q, J = 3.8 Hz), 113.9, 55.2, 52.2, 28.6, 12.7.

FT-IR (neat) 2963, 2933, 2875, 2836, 1611, 1584, 1512, 1486, 1443, 1377, 1251, 1177, 1163, 1124, 1074, 1038, 900, 828, 802, 765, 735 cm^{-1}.

MS (EI) *m/z* (M^+) calcd for $C_{17}H_{17}F_3O$: 294.1, found: 294.1.

$[\alpha]^{25}_{D}$ = +6.1° (c = 1.00, $CHCl_3$).



(*R*)-*N,N*-Dimethyl-3-(1-phenylethyl)aniline (Table 2, Entry 23). The title compound was prepared according to General Method B: 1-(3-(Dimethylamino)phenyl)ethyl mesylate (0.70 mmol), phenylzinc iodide (1.7 equiv), –45 °C. The product was purified by column chromatography (hexanes → 25% CH_2Cl_2/hexanes). Light-tan oil. First run: 135 mg (86%; 92% ee). Second run: 140 mg (89%; 92% ee).

The ee was determined by HPLC on a CHIRALCEL OD-H column (2% *i*-PrOH/hexanes, 1.0 mL/min) with t_r = 5.94 min (major), 6.95 min (minor).

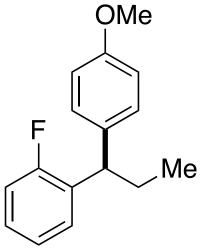
^{1}H NMR (500 MHz, $CDCl_3$) δ 7.33 – 7.21 (m, 4H), 7.23 – 7.11 (m, 2H), 6.64 – 6.55 (m, 3H), 4.11 (q, J = 7.2 Hz, 1H), 2.92 (s, 6H), 1.64 (d, J = 7.2 Hz, 3H).

^{13}C NMR (126 MHz, $CDCl_3$) δ 150.7, 147.2, 146.6, 129.0, 128.2, 127.6, 125.8, 116.1, 112.3, 110.5, 45.2, 40.7, 21.9.

FT-IR (neat) 3060, 3025, 2965, 2929, 2872, 2801, 1682, 1597, 1578, 1495, 1450, 1436, 1351, 1231, 1177, 1154, 1061, 1028, 995, 958, 849, 766 cm^{-1}.

MS (EI) *m/z* (M^+) calcd for $C_{16}H_{19}N$: 225.2, found: 225.1.

$[\alpha]^{25}_D$ = +10.7° (c = 1.00, $CHCl_3$).



(*R*)-1-Fluoro-2-(1-(4-methoxyphenyl)propyl)benzene (Table 2, Entry 24). The title compound was prepared according to General Method A: 1-(2-Fluorophenyl)propyl mesylate (0.70 mmol), 4-methoxyphenylzinc iodide (1.7 equiv), –45 °C. The product was purified by column chromatography (hexanes → 25% CH_2Cl_2/hexanes). Colorless oil. First run: 114 mg (67%; 80% ee). Second run: 111 mg (65%; 81% ee).

The ee was determined by HPLC on a CHIRALCEL OJ-H column (1% *i*-PrOH/hexanes, 0.5 mL/min) with t_r = 31.87 min (minor), 35.53 min (major).

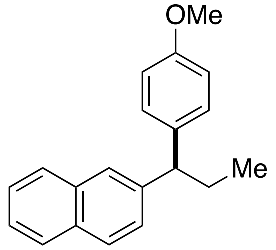
^{1}H NMR (500 MHz, $CDCl_3$) δ 7.28 – 7.03 (m, 5H), 6.98 (ddd, J = 10.4, 8.1, 1.3 Hz, 1H), 6.86 – 6.79 (m, 2H), 4.11 (t, J = 7.8 Hz, 1H), 3.77 (s, 3H), 2.10 – 1.98 (m, 2H), 0.91 (t, J = 7.3 Hz, 3H).

^{13}C NMR (126 MHz, $CDCl_3$) δ 160.7 (d, J = 244.6 Hz), 157.9, 136.1, 132.4 (d, J = 14.8 Hz), 128.8, 128.4 (d, J = 4.8 Hz), 127.4 (d, J = 8.4 Hz), 124.0 (d, J = 3.4 Hz), 115.3 (d, J = 22.9 Hz), 113.7, 55.2, 44.5 (d, J = 2.3 Hz), 27.8, 12.6.

FT-IR (neat) 2962, 2932, 2873, 2834, 1610, 1583, 1511, 1488, 1455, 1378, 1302, 1250, 1178, 1121, 1072, 1036, 825, 777, 756 cm^{-1}.

MS (EI) *m/z* (M^+) calcd for $C_{16}H_{17}FO$: 244.1, found: 244.1.

$[\alpha]^{25}_D$ = +6.0° (c = 1.00, $CHCl_3$).



(*R*)-2-(1-(4-Methoxyphenyl)propyl)naphthalene (Table 2, Entry 25). The title compound was prepared according to General Method A: 1-(Naphthalen-2-yl)propyl mesylate (0.70 mmol), 4-methoxyphenylzinc iodide (1.7 equiv), –45 °C. The product was purified by column chromatography (hexanes → 25% CH_2Cl_2/hexanes). Colorless oil. First run: 155 mg (80%; 92% ee). Second run: 149 mg (77%; 90% ee).

The ee was determined by SFC on a CHIRALPAK IC column (3% MeOH in CO_2, 2.5 mL/min) with t_r = 8.11 min (major), 9.19 min (minor).

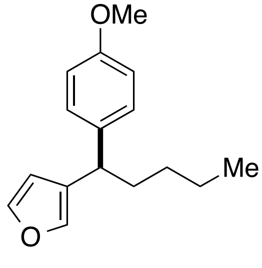
^{1}H NMR (500 MHz, $CDCl_3$) δ 7.82 – 7.66 (m, 4H), 7.49 – 7.37 (m, 2H), 7.32 (dd, J = 8.5, 1.8 Hz, 1H), 7.24 – 7.14 (m, 2H), 6.86 – 6.77 (m, 2H), 3.91 (t, J = 7.7 Hz, 1H), 3.77 (s, 3H), 2.23 – 2.06 (m, 2H), 0.93 (t, J = 7.3 Hz, 3H).

^{13}C NMR (126 MHz, $CDCl_3$) δ 157.8, 142.9, 137.2, 133.5, 132.1, 128.9, 127.9, 127.7, 127.5, 126.8, 125.8, 125.7, 125.2, 113.7, 55.2, 52.4, 28.5, 12.8.

FT-IR (neat) 2959, 2930, 2872, 2833, 1609, 1583, 1510, 1462, 1302, 1249, 1178, 1118, 1037, 816, 745 cm^{-1}.

MS (EI) *m/z* (M^+) calcd for $C_{20}H_{20}O$: 276.2, found: 276.1.

$[\alpha]^{25}_D$ = –10.7° (c = 1.00, $CHCl_3$).



(*R*)-3-(1-(4-Methoxyphenyl)pentyl)furan (Table 2, Entry 26). The title compound was prepared according to General Method B: 1-(Furan-3-yl)pentyl mesylate (0.70 mmol), 4-methoxyphenylzinc iodide (1.7 equiv), –45 °C. The product was purified by column chromatography (hexanes → 25% CH_2Cl_2/hexanes). Colorless oil. First run: 152 mg (89%; 93% ee). Second run: 149 mg (87%; 92% ee).

The ee was determined by SFC on a CHIRALCEL AS-H column (1% MeOH in CO_2, 2.5 mL/min) with t_r = 2.70 min (major), 3.05 min (minor).

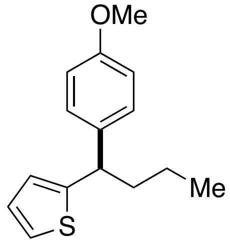
^{1}H NMR (500 MHz, $CDCl_3$) δ 7.33 (t, J = 1.7 Hz, 1H), 7.19 (dt, J = 1.8, 1.0 Hz, 1H), 7.18 – 7.07 (m, 2H), 6.87 – 6.78 (m, 2H), 6.21 (dd, J = 1.9, 0.9 Hz, 1H), 3.79 (s, 3H), 3.68 (t, J = 7.7 Hz, 1H), 1.99 – 1.77 (m, 2H), 1.42 – 1.13 (m, 4H), 0.86 (t, J = 7.2 Hz, 3H).

^{13}C NMR (126 MHz, $CDCl_3$) δ 157.9, 142.8, 138.6, 136.9, 129.8, 128.6, 113.7, 110.4, 55.2, 41.5, 35.8, 30.0, 22.6, 14.0.

FT-IR (neat) 2997, 2955, 2930, 2858, 2834, 1611, 1584, 1507, 1464, 1441, 1378, 1302, 1247, 1176, 1159, 1114, 1065, 1037, 873, 835, 788, 764, 727 cm^{-1}.

MS (EI) *m*/*z* (M^+) calcd for $C_{16}H_{20}O_2$: 244.1, found: 244.1.

$[\alpha]^{25}_D = -32.6°$ (c = 1.00, $CHCl_3$).



(*R*)-2-(1-(4-Methoxyphenyl)butyl)thiophene (Table 2, Entry 27). The title compound was prepared according to General Method B: 1-(Thiophen-2-yl)butyl mesylate (0.70 mmol), 4-methoxyphenylzinc iodide (1.7 equiv), –45 °C. The product was purified by column chromatography (hexanes → 25% CH_2Cl_2/hexanes). Colorless oil. First run: 94 mg (54%; 83% ee). Second run: 92 mg (53%; 82% ee).

The ee was determined by SFC on a CHIRALPAK IC column (2% MeOH in CO_2, 2.5 mL/min) with t_r = 6.11 min (major), 6.63 min (minor).

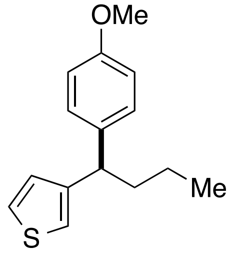
^{1}H NMR (500 MHz, $CDCl_3$) δ 7.22 – 7.09 (m, 3H), 6.95 – 6.77 (m, 4H), 4.09 (t, J = 7.6 Hz, 1H), 3.79 (s, 3H), 2.12 – 1.92 (m, 2H), 1.39 – 1.22 (m, 2H), 0.92 (t, J = 7.4 Hz, 3H).

^{13}C NMR (126 MHz, $CDCl_3$) δ 158.1, 150.5, 136.9, 128.6, 126.4, 123.4, 123.2, 113.8, 55.2, 45.7, 39.7, 21.0, 13.9.

FT-IR (neat) 3067, 2997, 2955, 2930, 2870, 2833, 1610, 1584, 1508, 1463, 1440, 1378, 1302, 1247, 1177, 1116, 1036, 827, 778, 758 cm^{-1}.

MS (EI) *m*/*z* (M^+) calcd for $C_{15}H_{18}OS$: 246.1, found: 246.0.

$[\alpha]^{25}_D = -9.1°$ (c = 1.00, $CHCl_3$).



(*R*)-3-(1-(4-Methoxyphenyl)butyl)thiophene (Table 2, Entry 28). The title compound was prepared according to General Method B: 1-(Thiophen-3-yl)butyl mesylate (0.70 mmol), 4-methoxyphenylzinc iodide (1.7 equiv), –45 °C. The product was purified by column chromatography (hexanes → 25% CH_2Cl_2/hexanes). Colorless oil. First run: 160 mg (93%; 94% ee). Second run: 161 mg (93%; 94% ee).

The ee was determined by SFC on a CHIRALPAK AD-H column (3% MeOH in CO_2, 2.5 mL/min) with t_r = 3.76 min (minor), 4.29 min (major).

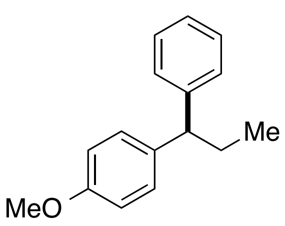
^{1}H NMR (500 MHz, CDCl$_3$) δ 7.21 (dd, J = 5.0, 2.9 Hz, 1H), 7.17 – 7.08 (m, 2H), 6.96 (dt, J = 2.9, 1.1 Hz, 1H), 6.89 (dd, J = 5.0, 1.3 Hz, 1H), 6.85 – 6.80 (m, 2H), 3.92 (t, J = 7.9 Hz, 1H), 3.78 (s, 3H), 2.08 – 1.86 (m, 2H), 1.34 – 1.20 (m, 2H), 0.91 (t, J = 7.3 Hz, 3H).

^{13}C NMR (126 MHz, CDCl$_3$) δ 157.9, 146.8, 137.1, 128.7, 127.7, 125.2, 119.7, 113.7, 55.2, 45.8, 38.5, 21.0, 14.0.

FT-IR (neat) 3101, 2997, 2955, 2930, 2870, 2833, 1610, 1584, 1510, 1463, 1440, 1378, 1302, 1246, 1177, 1113, 1036, 829, 788, 757, 743 cm^{-1}.

MS (EI) *m/z* (M$^+$) calcd for $C_{15}H_{18}OS$: 246.1, found: 246.1.

$[\alpha]^{25}_{D}$ = –36.0° (c = 1.00, CHCl$_3$).



(*R*)-1-Methoxy-4-(1-phenylpropyl)benzene (Table 3, Entry 1). The title compound was prepared according to General Method B: 1-(4-Methoxyphenyl)propyl mesylate (0.70 mmol), phenylzinc iodide (1.7 equiv; prepared at r.t.), –40 °C, 48 h. The product was purified by column chromatography (hexanes → 25% CH$_2$Cl$_2$/hexanes). Colorless oil. First run: 150 mg (95%; 94% ee). Second run: 152 mg (96%; 94% ee).

The ee was determined by SFC on a CHIRALPAK AD-H column (2% MeOH in CO$_2$, 2.5 mL/min) with t_r = 3.67 min (minor), 4.37 min (major).

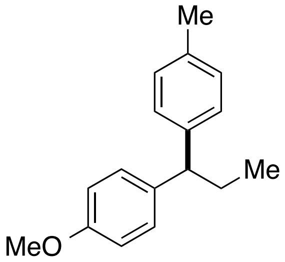
^{1}H NMR (500 MHz, CDCl$_3$) δ 7.33 – 7.10 (m, 7H), 6.86 – 6.77 (m, 2H), 3.77 (s, 3H), 3.74 (t, J = 7.8 Hz, 1H), 2.10 – 1.98 (m, 2H), 0.89 (t, J = 7.3 Hz, 3H).

^{13}C NMR (126 MHz, CDCl$_3$) δ 157.8, 145.6, 137.3, 128.7, 128.3, 127.8, 125.9, 113.7, 55.2, 52.4, 28.7, 12.8.

FT-IR (neat) 3060, 3026, 2959, 2930, 2872, 2833, 1611, 1583, 1509, 1494, 1463, 1452, 1377, 1302, 1248, 1177, 1119, 1038, 819, 782, 761, 726 cm^{-1}.

MS (EI) *m/z* (M$^+$) calcd for $C_{16}H_{18}O$: 226.1, found: 226.1.

$[\alpha]^{25}_{D}$ = –6.5° (c = 1.00, CHCl$_3$).



(*R*)-1-Methoxy-4-(1-(*p*-tolyl)propyl)benzene (Table 3, Entry 2). The title compound was prepared according to General Method B: 1-(4-Methoxyphenyl)propyl mesylate (0.70 mmol), *p*-tolylzinc iodide (1.5 equiv; prepared by the dropwise addition of *p*-tolylmagnesium bromide (3.2 mL, 1.0 M) to a solution of ZnI$_2$ (1.22 g) in dry THF (3.3 mL), with the resulting white suspension stirred vigorously at r.t. for 1 h before adding it to the reaction), –40 °C, 48 h. The product was purified by column chromatography (hexanes → 25% CH_2Cl_2/hexanes). Colorless oil. First run: 152 mg (91%; 94% ee). Second run: 152 mg (91%; 93% ee).

The ee was determined by SFC on a CHIRALCEL OB-H column (3% MeOH in CO_2, 2.5 mL/min) with t_r = 8.74 min (major), 11.17 min (minor).

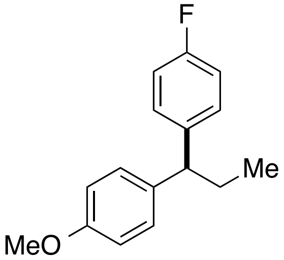
^{1}H NMR (500 MHz, $CDCl_3$) δ 7.17 – 7.05 (m, 6H), 6.87 – 6.76 (m, 2H), 3.77 (s, 3H), 3.71 (t, J = 7.6 Hz, 1H), 2.30 (s, 3H), 2.08 – 1.96 (m, 2H), 0.88 (t, J = 7.3 Hz, 3H).

^{13}C NMR (126 MHz, $CDCl_3$) δ 157.7, 142.6, 137.6, 135.3, 129.0, 128.7, 127.6, 113.7, 55.2, 51.9, 28.8, 21.0, 12.8.

FT-IR (neat) 3000, 2958, 2930, 2872, 2833, 1610, 1583, 1508, 1462, 1377, 1301, 1248, 1177, 1122, 1038, 809, 770, 736, 716 cm^{-1}.

MS (EI) *m/z* (M^+) calcd for $C_{17}H_{20}O$: 240.1, found: 240.1.

$[\alpha]^{25}_D$ = +1.56° (c = 1.00, $CHCl_3$).



(*S*)-1-Fluoro-4-(1-(4-methoxyphenyl)propyl)benzene (Table 3, Entry 3). The title compound was prepared according to General Method B: 1-(4-Methoxyphenyl)propyl mesylate (0.70 mmol), 4-fluorophenylzinc iodide (1.7 equiv; prepared at –20 °C and then r.t.), –40 °C. The product was purified by column chromatography (hexanes → 25% CH_2Cl_2/hexanes). Colorless oil. First run: 160 mg (94%; 94% ee). Second run: 164 mg (96%; 94% ee).

The ee was determined by HPLC on a CHIRALCEL OJ-H column (2% *i*-PrOH/hexanes, 1.0 mL/min) with t_r = 14.11 min (major), 15.98 min (minor).

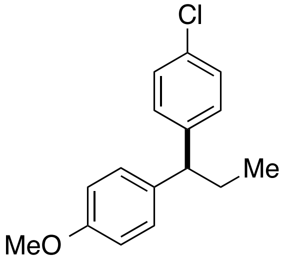
^{1}H NMR (500 MHz, $CDCl_3$) δ 7.20 – 7.08 (m, 4H), 7.01 – 6.91 (m, 2H), 6.86 – 6.79 (m, 2H), 3.77 (s, 3H), 3.72 (t, J = 7.8 Hz, 1H), 2.07 – 1.94 (m, 2H), 0.88 (t, J = 7.3 Hz, 3H).

^{13}C NMR (126 MHz, $CDCl_3$) δ 161.2 (d, J = 243.7 Hz), 157.9, 141.2 (d, J = 2.6 Hz), 137.1 (d, J = 0.7 Hz), 129.1 (d, J = 7.7 Hz), 128.7, 115.0 (d, J = 21.0 Hz), 113.8, 55.2, 51.6, 28.9, 12.7.

FT-IR (neat) 2961, 2932, 2873, 2834, 1610, 1583, 1508, 1463, 1441, 1378, 1302, 1249, 1178, 1158, 1119, 1038, 1014, 825, 781, 737 cm^{-1}.

MS (EI) *m/z* (M^+) calcd for $C_{16}H_{17}FO$: 244.1, found: 244.1.

$[\alpha]^{25}_D$ = –5.7° (c = 1.00, $CHCl_3$).



(*S*)-1-Chloro-4-(1-(4-methoxyphenyl)propyl)benzene (Table 3, Entry 4). The title compound was prepared according to General Method B: 1-(4-Methoxyphenyl)propyl mesylate (0.70 mmol), 4-chlorophenylzinc iodide (1.7 equiv; prepared at –20 °C and then r.t.), –40 °C. The product was purified by column chromatography (hexanes → 25% CH_2Cl_2/hexanes). Colorless oil. First run: 174 mg (95%; 94% ee). Second run: 172 mg (94%; 94% ee).

The ee was determined by HPLC on a CHIRALCEL OJ-H column (2% *i*-PrOH/hexanes, 1.0 mL/min) with t_r = 11.11 min (major), 12.07 min (minor).

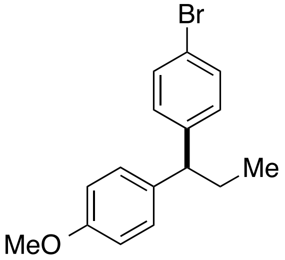
^{1}H NMR (500 MHz, $CDCl_3$) δ 7.28 – 7.21 (m, 2H), 7.16 – 7.08 (m, 4H), 6.87 – 6.77 (m, 2H), 3.77 (s, 3H), 3.72 (t, J = 7.8 Hz, 1H), 2.07 – 1.94 (m, 2H), 0.88 (t, J = 7.3 Hz, 3H).

^{13}C NMR (126 MHz, $CDCl_3$) δ 157.9, 144.1, 136.7, 131.6, 129.1, 128.7, 128.4, 113.8, 55.2, 51.7, 28.6, 12.7.

FT-IR (neat) 2960, 2931, 2873, 2834, 1610, 1583, 1511, 1490, 1462, 1407, 1378, 1302, 1249, 1176, 1120, 1092, 1038, 1014, 820, 757 cm^{-1}.

MS (EI) *m*/*z* (M^+) calcd for $C_{16}H_{17}ClO$: 260.1, found: 260.1.

$[\alpha]^{25}_D$ = –1.37° (c = 1.00, $CHCl_3$).



(*S*)-1-Bromo-4-(1-(4-methoxyphenyl)propyl)benzene (Table 3, Entry 5). The title compound was prepared according to General Method B: 1-(4-Methoxyphenyl)propyl mesylate (0.70 mmol), 4-bromophenylzinc iodide (1.7 equiv; prepared at –20 °C and then r.t.), –45 °C. The product was purified by column chromatography (hexanes → 25% CH_2Cl_2/hexanes). Colorless oil. First run: 180 mg (84%; 94% ee). Second run: 191 mg (89%; 94% ee).

The ee was determined by SFC on a CHIRALPAK AD-H column (3% MeOH in CO_2, 2.5 mL/min) with t_r = 7.59 min (major), 9.20 min (minor).

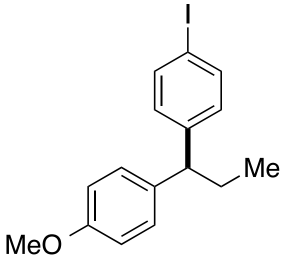
^{1}H NMR (500 MHz, $CDCl_3$) δ 7.43 – 7.34 (m, 2H), 7.16 – 7.04 (m, 4H), 6.87 – 6.77 (m, 2H), 3.77 (s, 3H), 3.70 (t, J = 7.8 Hz, 1H), 2.07 – 1.94 (m, 2H), 0.88 (t, J = 7.3 Hz, 3H).

^{13}C NMR (126 MHz, $CDCl_3$) δ 157.9, 144.6, 136.6, 131.4, 129.6, 128.7, 119.7, 113.8, 55.2, 51.8, 28.6, 12.7.

FT-IR (neat) 2960, 2930, 2872, 2833, 1611, 1583, 1511, 1488, 1463, 1440, 1404, 1302, 1249, 1177, 1121, 1075, 1038, 1009, 818, 752 cm^{-1}.

MS (EI) *m*/*z* (M^+) calcd for $C_{16}H_{17}BrO$: 304.0, found: 304.0.

$[\alpha]^{25}_{D}$ = –0.17° (c = 1.00, $CHCl_3$).



(*S*)-1-Iodo-4-(1-(4-methoxyphenyl)propyl)benzene (Table 3, Entry 6). The title compound was prepared according to General Method B: 1-(4-Methoxyphenyl)propyl mesylate (0.70 mmol), 4-iodophenylzinc iodide (1.5 equiv; prepared at –20 °C and then r.t.), –45 °C. The product was purified by column chromatography (hexanes → 25% CH_2Cl_2/hexanes). Colorless oil. First run: 165 mg (67%; 94% ee). Second run: 161 mg (65%; 94% ee).

The ee was determined by HPLC on a CHIRALPAK AD-H column (1% *i*-PrOH/hexanes, 1.0 mL/min) with t_r = 7.65 min (minor), 8.34 min (major).

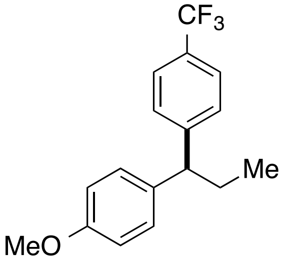
^{1}H NMR (500 MHz, $CDCl_3$) δ 7.61 – 7.53 (m, 2H), 7.15 – 7.05 (m, 2H), 7.01 – 6.92 (m, 2H), 6.86 – 6.77 (m, 2H), 3.77 (s, 3H), 3.68 (t, J = 7.8 Hz, 1H), 2.06 – 1.93 (m, 2H), 0.88 (t, J = 7.3 Hz, 3H).

^{13}C NMR (126 MHz, $CDCl_3$) δ 157.9, 145.3, 137.4, 136.6, 129.9, 128.7, 113.8, 91.1, 55.2, 51.9, 28.5, 12.7.

FT-IR (neat) 2958, 2929, 2871, 2832, 1611, 1583, 1511, 1483, 1462, 1400, 1302, 1248, 1177, 1122, 1037, 1005, 809, 749 cm^{-1}.

MS (EI) *m/z* (M^+) calcd for $C_{16}H_{17}IO$: 352.0, found: 352.0.

$[\alpha]^{25}_{D}$ = –0.87° (c = 1.00, $CHCl_3$).



(*R*)-1-Methoxy-4-(1-(4-(trifluoromethyl)phenyl)propyl)benzene (Table 3, Entry 7). The title compound was prepared according to General Method B: 1-(4-Methoxyphenyl)propyl mesylate (0.70 mmol), 4-trifluoromethylphenylzinc iodide (1.7 equiv; prepared at –20 °C and then r.t.), –40 °C. The product was purified by column chromatography (hexanes → 25% CH_2Cl_2/hexanes). Colorless oil. First run: 201 mg (98%; 94% ee). Second run: 202 mg (98%; 94% ee).

The ee was determined by SFC on a CHIRALCEL OB-H column (1% MeOH in CO_2, 2.5 mL/min) with t_r = 6.22 min (minor), 8.89 min (major).

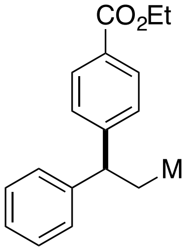
^{1}H NMR (500 MHz, $CDCl_3$) δ 7.56 – 7.49 (m, 2H), 7.38 – 7.28 (m, 2H), 7.18 – 7.09 (m, 2H), 6.89 – 6.80 (m, 2H), 3.81 (t, J = 7.8 Hz, 1H), 3.78 (s, 3H), 2.13 – 1.99 (m, 2H), 0.90 (t, J = 7.3 Hz, 3H).

^{13}C NMR (126 MHz, $CDCl_3$) δ 158.1, 149.7 (d, J = 1.4 Hz), 136.2, 128.7, 128.2 (q, J = 33.3 Hz), 128.1, 125.3 (q, J = 3.7 Hz), 124.3 (q, J = 272.4 Hz), 113.9, 55.2, 52.2, 28.5, 12.7.

FT-IR (neat) 3034, 3001, 2963, 2934, 2876, 2836, 1617, 1584, 1510, 1464, 1442, 1417, 1379, 1325, 1303, 1250, 1178, 1163, 1122, 1067, 1038, 1018, 825 cm^{-1}.

MS (EI) *m/z* (M^+) calcd for $C_{17}H_{17}F_3O$: 294.1, found: 294.1.

$[\alpha]^{25}_{D}$ = –5.4° (c = 1.00, $CHCl_3$).



(*S*)-Ethyl 4-(1-phenylpropyl)benzoate (Table 3, Entry 8). The title compound was prepared according to General Method A: 1-Phenylpropyl mesylate (0.70 mmol), 4-ethoxycarbonylphenylzinc iodide (1.7 equiv; prepared at –20 °C and then r.t.), –40 °C. The product was purified by column chromatography (hexanes → 5% Et_2O/hexanes). Colorless oil. First run: 170 mg (91%; 93% ee). Second run: 171 mg (91%; 93% ee).

The ee was determined by chiral SFC on a CHIRALPAK IC column (3% MeOH in CO_2, 2.5 mL/min) with t_r = 6.63 min (major), 7.52 min (minor).

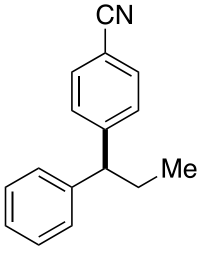
^{1}H NMR (500 MHz, $CDCl_3$) δ 8.00 – 7.90 (m, 2H), 7.34 – 7.13 (m, 7H), 4.35 (q, J = 7.1 Hz, 2H), 3.85 (t, J = 7.8 Hz, 1H), 2.15 – 2.03 (m, 2H), 1.37 (t, J = 7.1 Hz, 3H), 0.90 (t, J = 7.3 Hz, 3H).

^{13}C NMR (126 MHz, $CDCl_3$) δ 166.6, 150.4, 144.2, 129.7, 128.5, 128.4, 127.89, 127.85, 126.3, 60.7, 53.2, 28.3, 14.3, 12.7.

FT-IR (neat) 3060, 3026, 2964, 2932, 2874, 1720, 1716, 1610, 1575, 1493, 1463, 1452, 1416, 1366, 1309, 1276, 1179, 1107, 1020, 865, 842, 775, 756, 736 cm^{-1}.

MS (EI) *m/z* (M^+) calcd for $C_{18}H_{20}O_2$: 268.1, found: 268.1.

$[\alpha]^{25}_{D}$ = +0.52° (c = 1.00, $CHCl_3$).



(*S*)-4-(1-Phenylpropyl)benzonitrile (Table 3, Entry 9). The title compound was prepared according to General Method A: 1-Phenylpropyl mesylate (0.70 mmol), 4-cyanophenylzinc iodide (1.7 equiv; prepared at –20 °C and then r.t.), –40 °C. The product was purified by column chromatography (hexanes → 5% Et_2O/hexanes). Colorless oil. First run: 129 mg (83%; 92% ee). Second run: 129 mg (83%; 92% ee).

The ee was determined by SFC on a CHIRALPAK AD-H column (3% MeOH in CO_2, 2.5 mL/min) with t_r = 4.94 min (major), 5.74 min (minor).

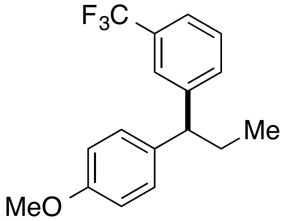
^{1}H NMR (500 MHz, $CDCl_3$) δ 7.61 – 7.53 (m, 2H), 7.37 – 7.14 (m, 7H), 3.85 (t, J = 7.8 Hz, 1H), 2.16 – 1.99 (m, 2H), 0.90 (t, J = 7.3 Hz, 3H).

^{13}C NMR (126 MHz, $CDCl_3$) δ 150.8, 143.4, 132.2, 128.67, 128.64, 127.8, 126.6, 119.0, 109.9, 53.3, 28.2, 12.6.

FT-IR (neat) 3061, 3027, 2964, 2931, 2874, 2227, 1606, 1502, 1492, 1452, 1414, 1380, 1176, 1123, 1020, 859, 841, 818, 763, 730 cm^{-1}.

MS (EI) *m/z* (M^+) calcd for $C_{16}H_{15}N$: 221.1, found: 221.1.

$[\alpha]^{25}_D$ = +0.07° (c = 1.00, $CHCl_3$).



(*S*)-1-(1-(4-Methoxyphenyl)propyl)-3-(trifluoromethyl)benzene (Table 3, Entry 10). The title compound was prepared according to General Method B: 1-(4-Methoxyphenyl)propyl mesylate (0.70 mmol), 3-trifluoromethylphenylzinc iodide (1.7 equiv; prepared at –20 °C and then r.t.), –40 °C. The product was purified by column chromatography (hexanes → 25% CH_2Cl_2/hexanes). Colorless oil. First run: 196 mg (95%; 94% ee). Second run: 200 mg (97%; 94% ee).

The ee was determined by SFC on a CHIRALCEL OB-H column (1% MeOH in CO_2, 2.5 mL/min) with t_r = 3.92 min (minor), 4.51 min (major).

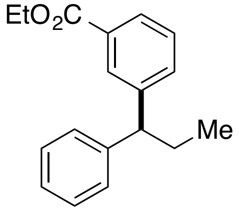
^{1}H NMR (500 MHz, $CDCl_3$) δ 7.50 – 7.33 (m, 4H), 7.17 – 7.08 (m, 2H), 6.89 – 6.79 (m, 2H), 3.80 (t, J = 7.7 Hz, 1H), 3.78 (s, 3H), 2.11 – 2.00 (m, 2H), 0.89 (t, J = 7.3 Hz, 3H).

^{13}C NMR (126 MHz, $CDCl_3$) δ 158.1, 146.5, 136.2, 131.2 (q, J = 1.3 Hz), 130.6 (q, J = 31.8 Hz), 128.76, 128.75, 124.4 (q, J = 3.8 Hz), 124.3 (q, J = 272.8 Hz), 122.9 (q, J = 3.9 Hz), 113.9, 55.2, 52.2, 28.7, 12.7.

FT-IR (neat) 3034, 3001, 2963, 2934, 2876, 2836, 1611, 1584, 1512, 1464, 1443, 1328, 1251, 1179, 1163, 1124, 1074, 1038, 900, 828, 802, 765, 735 cm^{-1}.

MS (EI) *m/z* (M^+) calcd for $C_{17}H_{17}F_3O$: 294.1, found: 294.1.

$[\alpha]^{25}_D$ = –7.5° (c = 1.00, $CHCl_3$).



(*S*)-Ethyl 3-(1-phenylpropyl)benzoate (Table 3, Entry 11). The title compound was prepared according to General Method A: 1-Phenylpropyl mesylate (0.70 mmol), 3-ethoxycarbonylphenylzinc iodide (1.7 equiv; prepared at –20 °C and then r.t.), –40 °C. The product was purified by column chromatography (hexanes → 5% Et_2O/hexanes). Colorless oil. First run: 170 mg (90%; 94% ee). Second run: 173 mg (93%; 93% ee).

The ee was determined by SFC on a CHIRALPAK IC column (2% MeOH in CO_2, 2.5 mL/min) with t_r = 6.31 min (minor), 6.81 min (major).

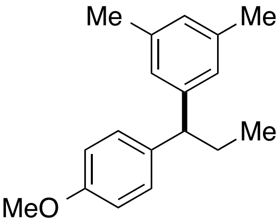
^{1}H NMR (500 MHz, $CDCl_3$) δ 7.95 (td, J = 1.8, 0.9 Hz, 1H), 7.86 (dt, J = 7.6, 1.5 Hz, 1H), 7.43 – 7.39 (m, 1H), 7.38 – 7.14 (m, 6H), 4.37 (q, J = 7.2 Hz, 2H), 3.85 (t, J = 7.8 Hz, 1H), 2.17 – 2.04 (m, 2H), 1.39 (t, J = 7.1 Hz, 3H), 0.90 (t, J = 7.3 Hz, 3H).

^{13}C NMR (126 MHz, $CDCl_3$) δ 166.8, 145.5, 144.6, 132.5, 130.5, 129.0, 128.5, 128.4, 127.8, 127.3, 126.2, 60.9, 53.1, 28.5, 14.3, 12.7.

FT-IR (neat) 3061, 3026, 2963, 2932, 2873, 1720, 1602, 1586, 1494, 1463, 1452, 1391, 1367, 1278, 1185, 1104, 1084, 1025, 767, 752 cm^{-1}.

MS (EI) *m/z* (M^+) calcd for $C_{18}H_{20}O_2$: 268.1, found: 268.1.

$[\alpha]^{25}_D$ = +3.3° (c = 1.00, $CHCl_3$).



(*S*)-1-(1-(4-Methoxyphenyl)propyl)-3,5-dimethylbenzene (Table 3, Entry 12). The title compound was prepared according to General Method B: 1-(4-Methoxyphenyl)propyl mesylate (0.70 mmol), 3,5-dimethylphenylzinc iodide (1.7 equiv; prepared at r.t.), –40 °C. The product was purified by column chromatography (hexanes → 25% CH_2Cl_2/hexanes). Colorless oil. First run: 153 mg (86%; 93% ee). Second run: 154 mg (87%; 92% ee).

The ee was determined by HPLC on a CHIRALCEL OJ-H column (2% *i*-PrOH/hexanes, 1.0 mL/min) with t_r = 7.67 min (minor), 10.68 min (major).

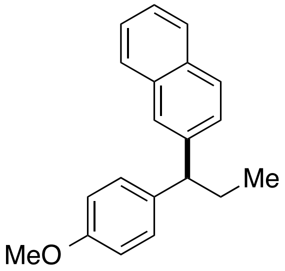
^{1}H NMR (500 MHz, $CDCl_3$) δ 7.19 – 7.11 (m, 2H), 6.86 – 6.77 (m, 5H), 3.77 (s, 3H), 3.66 (t, J = 7.8 Hz, 1H), 2.27 (d, J = 0.7 Hz, 6H), 2.07 – 1.95 (m, 2H), 0.88 (t, J = 7.3 Hz, 3H).

^{13}C NMR (126 MHz, $CDCl_3$) δ 157.7, 145.5, 137.6, 137.5, 128.7, 127.6, 125.6, 113.7, 55.2, 52.3, 28.8, 21.4, 12.9.

FT-IR (neat) 2958, 2930, 2872, 2833, 1608, 1583, 1511, 1462, 1376, 1302, 1248, 1177, 1118, 1038, 826, 798, 745 cm^{-1}.

MS (EI) *m/z* (M^+) calcd for $C_{18}H_{22}O$: 254.2, found: 254.1.

$[\alpha]^{25}_{D}$ = –1.61° (c = 1.00, $CHCl_3$).



(*S*)-2-(1-(4-Methoxyphenyl)propyl)naphthalene (Table 3, Entry 13). The title compound was prepared according to General Method B: 1-(4-Methoxyphenyl)propyl mesylate (0.70 mmol), 2-naphthylzinc iodide (1.7 equiv; prepared by the dropwise addition of 2-naphthylmagnesium bromide (6.8 mL, 0.47 M) to a solution of ZnI_2 (1.22 g) in dry THF (3.3 mL), with the resulting white suspension stirred vigorously at r.t. for 1 h before adding it to the reaction), –30 °C. The product was purified by column chromatography (hexanes → 25% CH_2Cl_2/hexanes). Colorless oil. First run: 178 mg (92%; 92% ee). Second run: 181 mg (94%; 92% ee).

The ee was determined by SFC on a CHIRALPAK IC column (3% MeOH in CO_2, 2.5 mL/min) with t_r = 8.20 min (minor), 9.11 min (major).

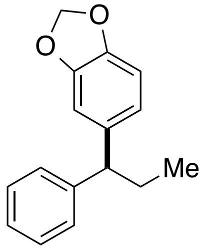
^{1}H NMR (500 MHz, $CDCl_3$) δ 7.83 – 7.67 (m, 4H), 7.49 – 7.37 (m, 2H), 7.32 (dd, J = 8.5, 1.8 Hz, 1H), 7.25 – 7.14 (m, 2H), 6.88 – 6.78 (m, 2H), 3.92 (t, J = 7.7 Hz, 1H), 3.77 (s, 3H), 2.23 – 2.06 (m, 2H), 0.94 (t, J = 7.3 Hz, 3H).

^{13}C NMR (126 MHz, $CDCl_3$) δ 157.8, 143.0, 137.2, 133.5, 132.1, 128.9, 127.9, 127.7, 127.5, 126.8, 125.8, 125.7, 125.2, 113.7, 55.2, 52.4, 28.5, 12.8.

FT-IR (neat) 3053, 2959, 2930, 2872, 2833, 1632, 1609, 1583, 1510, 1462, 1440, 1376, 1302, 1248, 1177, 1118, 1038, 826, 816, 745 cm^{-1}.

MS (EI) *m/z* (M^+) calcd for $C_{20}H_{20}O$: 276.1, found: 276.1.

$[\alpha]^{25}_{D}$ = +12.4° (c = 1.00, $CHCl_3$).



(*S*)-5-(1-Phenylpropyl)benzo[*d*][1,3]dioxole (Table 3, Entry 14). The title compound was prepared according to General Method A: 1-Phenylpropyl mesylate (0.70 mmol), benzo[d][1,3]dioxol-5-ylzinc iodide (1.7 equiv; prepared at r.t.), –40 °C. The product was purified by column chromatography (hexanes → 25% CH_2Cl_2/hexanes). Colorless oil. First run: 147 mg (88%; 94% ee). Second run: 145 mg (86%; 94% ee).

The ee was determined by SFC on a CHIRALPAK IC column (2% MeOH in CO_2, 1.0 mL/min) with t_r = 9.59 min (minor), 9.93 min (major).

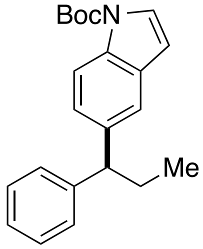
^{1}H NMR (500 MHz, $CDCl_3$) δ 7.34 – 7.13 (m, 5H), 6.77 – 6.66 (m, 3H), 5.90 (q, J = 1.5 Hz, 2H), 3.71 (t, J = 7.8 Hz, 1H), 2.10 – 1.94 (m, 2H), 0.89 (t, J = 7.3 Hz, 3H).

^{13}C NMR (126 MHz, $CDCl_3$) δ 147.6, 145.7, 145.2, 139.2, 128.4, 127.7, 126.0, 120.8, 108.2, 108.0, 100.8, 52.9, 28.6, 12.7.

FT-IR (neat) 3060, 3025, 2961, 2930, 2873, 2775, 1601, 1502, 1486, 1438, 1377, 1363, 1245, 1185, 1103, 1040, 935, 862, 808, 762 cm^{-1}.

MS (EI) *m/z* (M^+) calcd for $C_{16}H_{16}O_2$: 240.1, found: 240.1.

$[\alpha]^{25}_D$ = +11.1° (c = 1.00, $CHCl_3$).



(*S*)-*t*-Butyl 5-(1-phenylpropyl)-1*H*-indole-1-carboxylate (Table 3, Entry 15). The title compound was prepared according to General Method A: 1-Phenylpropyl mesylate (0.70 mmol), 1-(*t*-butoxycarbonyl)-1*H*-indol-5-ylzinc iodide (1.7 equiv; prepared at –20 °C and then r.t.), –40 °C. The product was purified by column chromatography (hexanes → 25% CH_2Cl_2/hexanes). Colorless oil. First run: 182 mg (78%; 93% ee). Second run: 179 mg (76%; 93% ee).

The ee was determined by chiral SFC on a CHIRALCEL IC column (2% MeOH in CO_2, 2.5 mL/min) with t_r = 8.84 min (major), 9.82 min (minor).

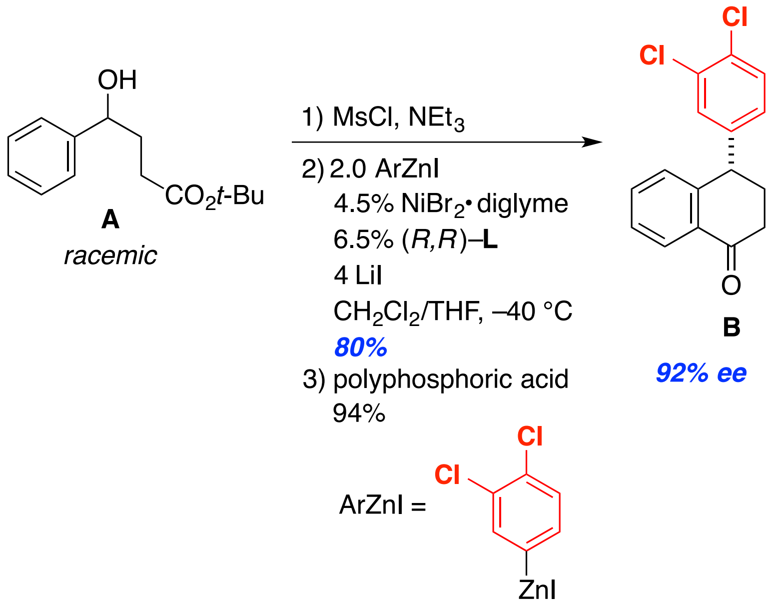
^{1}H NMR (500 MHz, $CDCl_3$) δ 8.01 (d, J = 8.5 Hz, 1H), 7.56 (d, J = 3.5 Hz, 1H), 7.45 – 7.39 (m, 1H), 7.30 – 7.12 (m, 6H), 6.51 (dd, J = 3.7, 0.8 Hz, 1H), 3.89 (t, J = 7.8 Hz, 1H), 2.13 (pentet, J = 7.3 Hz, 2H), 1.65 (s, 9H), 0.92 (t, J = 7.3 Hz, 3H).

^{13}C NMR (126 MHz, $CDCl_3$) δ 145.7, 139.6, 130.7, 128.3, 127.9, 126.0, 125.9, 124.6, 119.8, 115.0, 107.3, 83.5, 81.0, 53.0, 28.8, 28.2, 27.9, 12.9.

FT-IR (neat) 3060, 3025, 2973, 2931, 2873, 1735, 1601, 1580, 1537, 1470, 1370, 1352, 1291, 1254, 1212, 1163, 1132, 1083, 1040, 1023, 884, 846, 809, 767, 726 cm^{-1}.

MS (ESI) *m/z* ($[M + H]^+$) calcd for $C_{22}H_{26}NO_2$: 336.2, found: 336.2.

$[\alpha]^{25}_D$ = +11.4° (c = 1.00, $CHCl_3$).



Gram-scale synthesis of (*S*)-sertraline tetralone (eq 3).

(*R*)-*t*-Butyl 4-(3,4-dichlorophenyl)-4-phenylbutanoate [147189-42-2]. The title compound was prepared according to General Method A, using $NiBr_2$•diglyme (4.5%) and (*R*,*R*)-**L** (6.5%): *t*-Butyl 4-((methylsulfonyl)oxy)-4-phenylbutanoate (4.9 mmol), 3,4-dichlorophenylzinc iodide (2.0 equiv), –40 °C, 60 h. The product was purified by column chromatography (hexanes → 5% Et_2O/hexanes). Colorless oil. 1.43 g (80%, 92% ee).

The ee was determined by HPLC on a CHIRALCEL OD-H column (1% *i*-PrOH/hexanes, 1.0 mL/min) with t_r = 7.29 min (major), 8.41 min (minor).

(*S*)-Sertraline tetralone. A 20-mL vial was charged with (*R*)-*t*-butyl 4-(3,4-dichlorophenyl)-4-phenylbutanoate (1.43 g, 3.92 mmol) and polyphosphoric acid (7.0 mL). The resulting mixture was heated at 85 °C for 3 h under an atmosphere of nitrogen. Next, the mixture was allowed to cool to r.t., and then it was diluted with water (120 mL). The mixture was extracted with EtOAc (100 mL x 3). The combined organic layers were washed with saturated $NaHCO_3$ (100 mL) and brine (100 mL), dried over $MgSO_4$, and concentrated. The residue was purified by flash chromatography (hexanes → 15% Et_2O/hexanes), which provided (*S*)-sertraline tetralone as a light-tan solid (1.07 g, 94% yield, 92% ee).

The ee was determined by HPLC on a CHIRALCEL OD-H column (2% *i*-PrOH/hexanes, 1.0 mL/min) with t_r = 14.78 min (major), 17.45 min (minor).

^{1}H NMR (500 MHz, $CDCl_3$) δ 8.12 (dd, J = 7.7, 1.7 Hz, 1H), 7.53 – 7.33 (m, 3H), 7.22 (d, J = 2.1 Hz, 1H), 7.00 – 6.89 (m, 2H), 4.27 (dd, J = 8.1, 4.6 Hz, 1H), 2.81 – 2.36 (m, 3H), 2.35 – 2.14 (m, 1H).

^{13}C NMR (126 MHz, $CDCl_3$) δ 197.3, 144.8, 144.0, 133.9, 132.8, 132.7, 131.0, 130.6, 130.5, 129.3, 127.9, 127.5, 127.4, 44.5, 36.5, 31.7.

FT-IR (neat) 3354, 3062, 3026, 2951, 2867, 1686, 1597, 1560, 1468, 1452, 1399, 1329, 1284, 1253, 1235, 1200, 1133, 1112, 1030, 924, 880, 847, 823, 774, 729, 721, 710 cm^{-1}.

MS (EI) *m*/*z* (M^+) calcd for $C_{16}H_{12}Cl_2O$: 290.0, found: 290.0.

$[\alpha]^{25}_D$ = +61.2° (c = 1.00, benzene). Lit.[2] $[\alpha]^{25}_D$ = +63.8° (c = 1.16, benzene; 94% ee).

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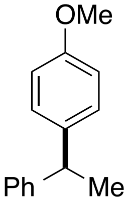
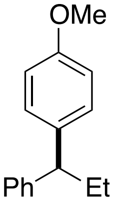
(2) Roesner, S.; Casatejada, J. M.; Elford, T. G.; Sonawane, R. P.; Aggarwal, V. K. *Org. Lett.* **2011**, *13*, 5740–5743.

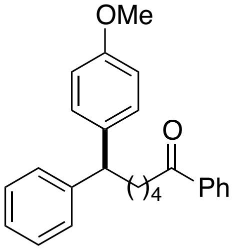
IV. Assignment of Absolute Configuration



(*S*)-1-Methoxy-4-(1-phenylethyl)benzene: Product from Table 2, Entry 1, run with (*S*,*S*)-L. To determine the absolute stereochemistry, the optical rotation of this compound was compared with a literature value: $[\alpha]^{25}_{D}$ = +8.7° (c = 1.0, $CHCl_3$; 88% ee); lit.[3] $[\alpha]^{20}_{D}$ = +5.0° (c = 0.8, $CHCl_3$; 96% ee).



(*S*)-1-Methoxy-4-(1-phenylpropyl)benzene: Product from Table 2, Entry 2, run with (*S*,*S*)-L. To determine the absolute stereochemistry, the optical rotation of this compound was compared with a literature value: $[\alpha]^{25}_{D}$ = +5.8° (c = 1.0, $CHCl_3$; 94% ee); lit.[4] $[\alpha]^{23}_{D}$ = +5.0° (c = 1.0, $CDCl_3$; 77% ee).



(*S*)-6-(4-Methoxyphenyl)-1,6-diphenylhexan-1-one: Product from Table 2, Entry 13, run with (*S*,*S*)-L. Crystals suitable for X-ray crystallography were grown in hexanes.

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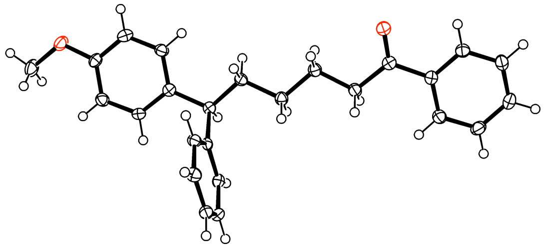
(3) Nave, S.; Sonawane, R. P.; Elford, T. G.; Aggarwal, V. K. *J Am Chem. Soc.* **2010**, *132*, 17096–17098.

(4) Tolstoy, P.; Engman, M.; Paptchikhine, A.; Bergquist, J.; Church, T. L.; Leung, A. W.-M.; Andersson, P. G. *J. Am. Chem. Soc.* **2009**, *131*, 8855–8860.



A. Crystal Data

Empirical Formula	$C_{25}H_{26}O_2$	
Formula Weight	358.64	
Crystal Color, Habit	colorless, block	
Crystal Dimensions	0.20 X 0.10 X 0.10 mm	
Crystal System	orthorhombic	
Lattice Type	Primitive	
Lattice Parameters	a = 5.42580(10) Å	α = 90°
	b = 8.18170(10) Å	β = 90°
	c = 43.389(3) Å	γ = 90°
	V = 1926.13(14) $Å^3$	
Space Group	$P2_12_12_1$	
Z value	4	
D_{calc}	1.236 g/cm^3	
F_{000}	768.00	
μ(CuKα)	0.597 mm^{-1}	

B. Intensity Measurements

Diffractometer	Rigaku Saturn944+ CCD
Radiation	CuKα (λ = 1.54187 Å)
Detector Aperture	94 mm x 94 mm
$2\theta_{max}$	136.46°
No. of Reflections Measured	Total: 64719 Unique: 3533 (R_{int} = 0. 0721) Friedel pairs: 1422
Corrections	Lorentz-polarization, Absorption (trans. factors: 0.890 - 0.943)

C. Structure Solution and Refinement

Structure Solution	Direct Methods
Refinement	Full-matrix least-squares on F^2
Function Minimized	$\Sigma\, w\, (Fo^2 - Fc^2)^2$
Least Squares Weights	$w = 1/\,[\,\sigma^2\,(Fo^2) + (0.0538 \cdot P)^2 + 0.3123 \cdot P\,]$ where $P = (\mathrm{Max}(Fo^2,0) + 2Fc^2)/3$
No. Observations (All reflections)	3533

No. Variables	245
Reflection/Parameter Ratio	14.42
Residuals: R1 (I>2.00σ(I))	0.0352
Residuals: R (All reflections)	0.0360
Residuals: wR2 (All reflections)	0.0949
Goodness of Fit Indicator	1.144
Max Shift/Error in Final Cycle	0.001
Flack parameter	0.0(2)
Hooft parameter	0.01(8)
Maximum peak in Final Diff. Map	0.527 $e^-/Å^3$
Minimum peak in Final Diff. Map	-0.524 $e^-/Å^3$

D. Experimental Details

The crystal sample was mounted in a Hampton Research loop with immersion oil. All measurements were made on a Rigaku Saturn944+ CCD diffractometer with filtered Cu-Kα radiation at a temperature of –180 °C. The structure was solved by direct methods[5] and expanded using Fourier techniques. The non-hydrogen atoms were refined anisotropically. Hydrogen atoms were refined using the riding model. The absolute structure was deduced based on the Flack parameter, 0.0(2).[6] The Hooft absolute structure parameter y = 0.01(8)[7] was calculated using PLATON,[8] and confirms the assigned absolute configuration.

Table 1. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$ x 10^3). Ueq is defined as 1/3 of the trace of the orthogonalised U_{IJ} tensor.

atom	x	y	z	U_{eq}
O2	-3021(2)	-2247.2(15)	-2132.1(2)	28.4(3)
O1	6644(2)	326.6(14)	-4395.1(2)	28.6(3)
C1	4958(3)	-194.1(18)	-4553.6(3)	19.9(3)
C9	2739(3)	-938.8(18)	-4057.9(3)	21.2(3)
C13	-2024(3)	-2591.8(17)	-3085.6(3)	18.2(3)
C11	527(3)	-1854.1(17)	-3567.6(3)	19.1(3)
C10	639(3)	-1920.7(18)	-3919.4(3)	20.6(3)
C12	-1778(3)	-2690.5(18)	-3436.2(3)	18.1(3)
C16	-2790(3)	-2413.4(18)	-2445.9(3)	21.2(3)
C18	-3956(3)	-3414.2(18)	-2943.3(3)	21.3(3)
C2	5067(3)	4.3(17)	-4897.8(3)	19.0(3)
C8	2756(3)	-1014.0(19)	-4408.9(3)	21.7(3)
C14	-470(3)	-1672.8(19)	-2897.4(3)	22.1(3)
C25	-168(3)	-5585.3(18)	-3451.8(3)	20.1(3)
C7	3264(3)	-640.7(19)	-5093.2(3)	23.3(3)
C6	3408(3)	-364(2)	-5408.5(3)	26.8(3)

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(5) Sheldrick, G.M. *Acta Cryst.* **2008**, A64, 112–122.

(6) Flack, H. D. *Acta Cryst.* **1983**, A39, 876–881.

(7) Hooft, R. W. W.; Straver, L. H.; Spek, A.L. *J. Appl. Cryst.* **2008**, 41, 96–103.

(8) (a) Spek, A. L. *PLATON, A Multipurpose Crystallographic Tool*; Utrecht University, Utrecht, The Netherlands, 2010. (b) Spek, A. L. *Acta Cryst.* **2009**, D65, 148–155.

C4	7125(3)	1176.5(19)	-5338.1(3)	24.0(3)
C20	-1923(3)	-4452.0(17)	-3546.6(3)	17.3(3)
C23	-2030(3)	-7675.9(18)	-3765.9(3)	22.5(3)
C5	5326(3)	552(2)	-5530.2(3)	24.7(3)
C15	-837(3)	-1584(2)	-2581.6(3)	24.4(3)
C17	-4363(3)	-3340(2)	-2627.7(3)	22.7(3)
C22	-3818(3)	-6575.5(19)	-3856.6(3)	22.0(3)
C24	-214(3)	-7176.0(18)	-3561.1(3)	23.0(3)
C3	7001(3)	911.4(18)	-5022.4(3)	21.9(3)
C21	-3763(3)	-4974.4(18)	-3748.3(3)	19.4(3)
C19	-5116(3)	-3005(2)	-1992.7(3)	32.5(4)

Table 2. Atomic coordinates and U_{eq} of hydrogen atoms

atom	x	y	z	U_{eq}
H9A	4293	-1356	-3980	25
H9B	2592	192	-3993	25
H11A	546	-721	-3502	23
H11B	1982	-2380	-3484	23
H10A	807	-3052	-3983	25
H10B	-906	-1515	-4002	25
H12	-3207	-2120	-3523	22
H18	-5015	-4038	-3064	26
H8A	2724	-2151	-4472	26
H8B	1268	-499	-4486	26
H14	840	-1108	-2985	27
H25	1052	-5271	-3313	24
H7	1972	-1253	-5012	28
H6	2212	-796	-5539	32
H4	8423	1777	-5421	29
H23	-2042	-8740	-3841	27
H5	5401	745	-5741	30
H15	227	-967	-2460	29
H17	-5673	-3903	-2539	27
H22	-5062	-6905	-3990	26
H24	982	-7915	-3497	28
H3	8210	1340	-4894	26
H21	-4972	-4241	-3811	23
H19A	-6592	-2618	-2090	49
H19B	-5162	-2737	-1777	49
H19C	-5003	-4169	-2017	49

Table 3. Bond lengths (Å)

atom	atom	distance
O2	C16	1.3743(16)
O2	C19	1.429(2)

atom	atom	distance
C18	C17	1.388(2)
C2	C7	1.398(2)

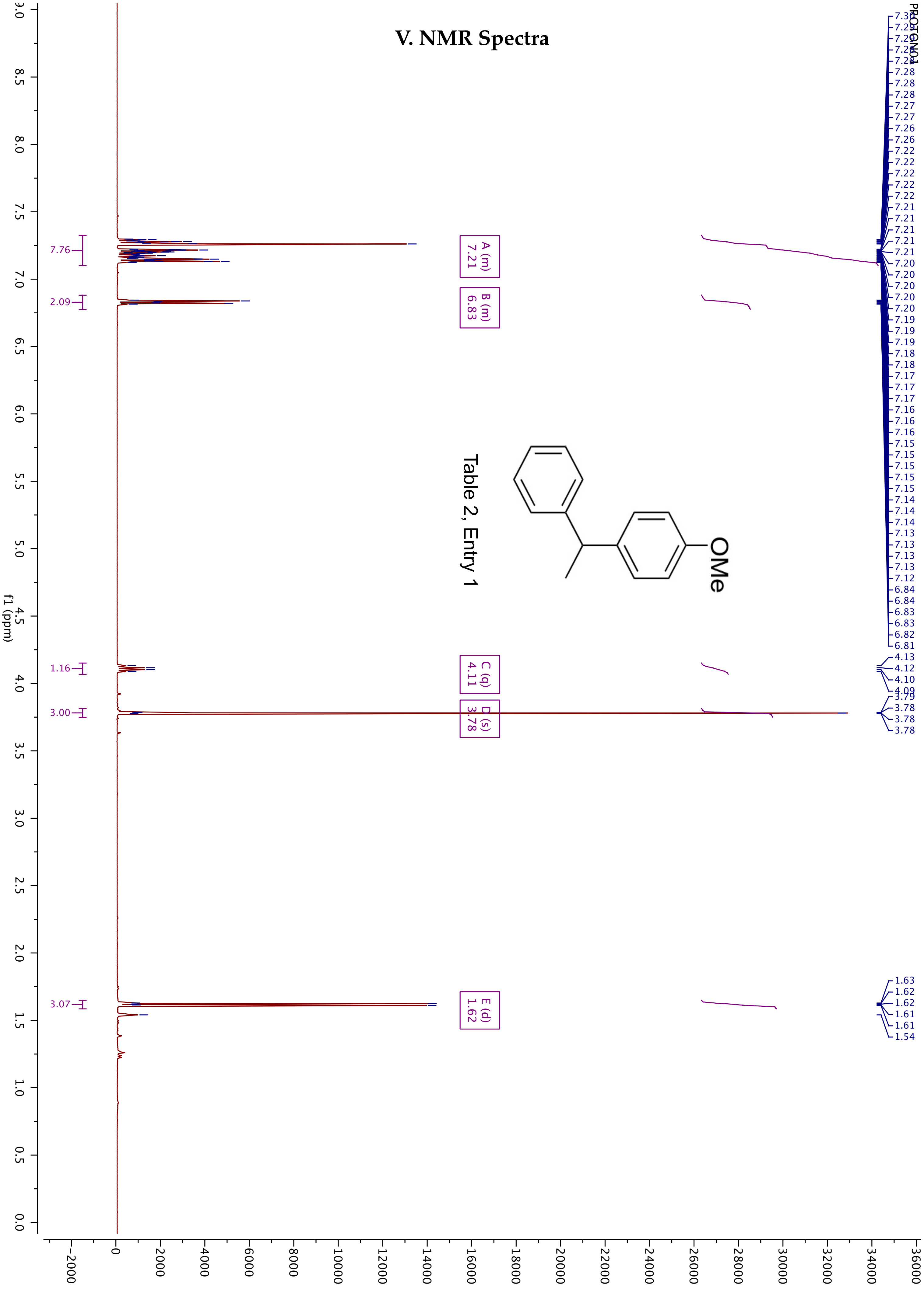
O1	C1	1.2213(18)
C1	C2	1.5031(18)
C1	C8	1.507(2)
C9	C10	1.518(2)
C9	C8	1.5243(19)
C13	C12	1.5293(18)
C13	C18	1.390(2)
C13	C14	1.394(2)
C11	C10	1.5285(18)
C11	C12	1.5356(19)
C12	C20	1.521(2)
C16	C15	1.389(2)
C16	C17	1.387(2)

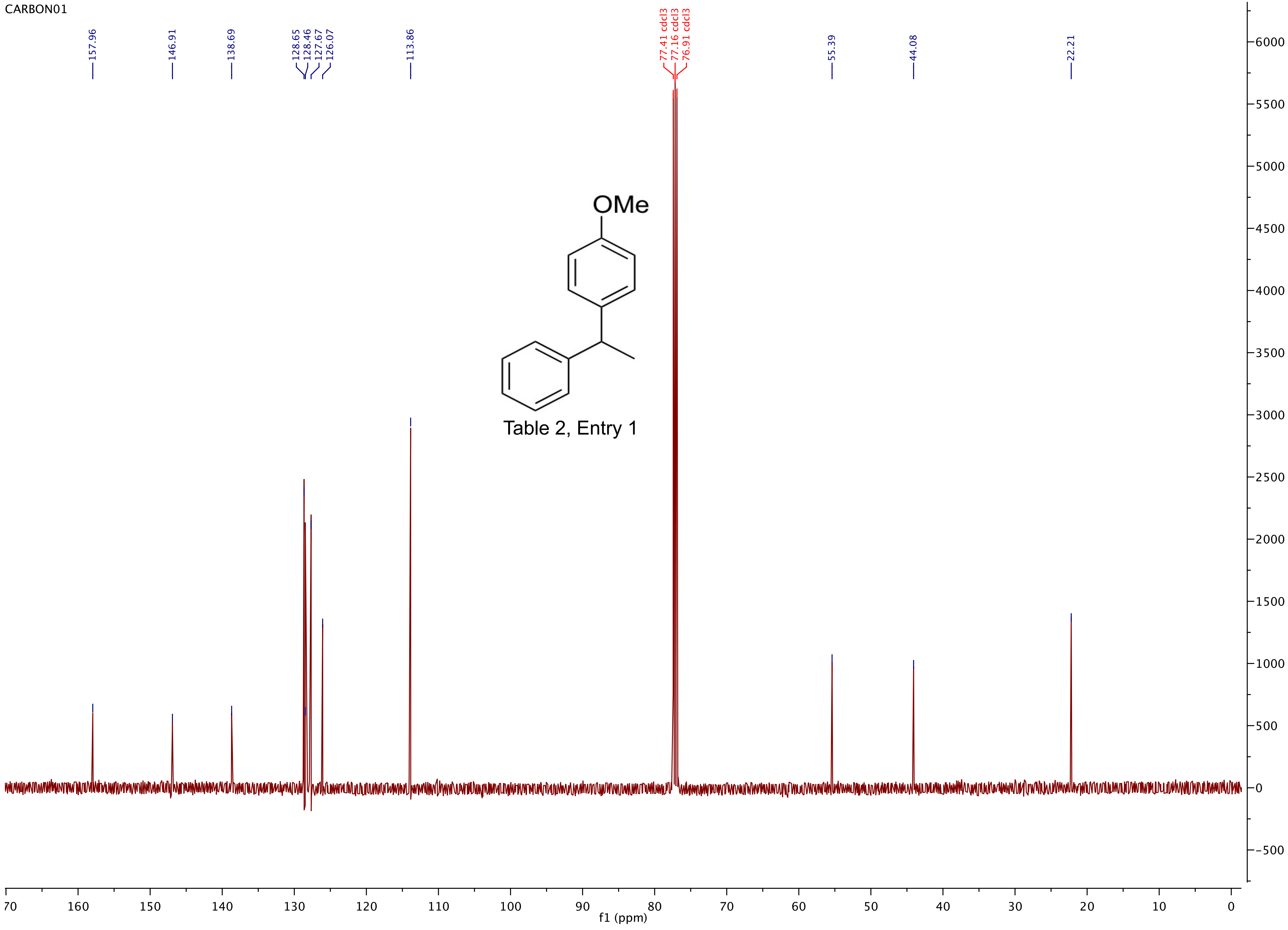
C2	C3	1.394(2)
C14	C15	1.386(2)
C25	C20	1.391(2)
C25	C24	1.385(2)
C7	C6	1.389(2)
C6	C5	1.387(2)
C4	C5	1.382(2)
C4	C3	1.389(2)
C20	C21	1.395(2)
C23	C22	1.381(2)
C23	C24	1.389(2)
C22	C21	1.392(2)

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

atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
O2	28.1(6)	39.5(7)	17.7(5)	-5.4(4)	1.0(4)	-3.0(5)
O1	25.9(6)	37.8(7)	22.1(5)	2.4(4)	-3.0(4)	-8.4(5)
C1	20.2(7)	18.1(7)	21.5(7)	0.6(5)	-1.4(6)	3.2(6)
C9	22.6(7)	19.3(7)	21.7(7)	1.6(5)	-0.4(6)	0.2(6)
C13	19.1(7)	15.4(7)	20.3(7)	-0.9(5)	-0.2(5)	3.5(6)
C11	21.4(7)	15.2(7)	20.8(7)	0.5(5)	0.0(6)	-0.2(6)
C10	22.1(7)	19.1(7)	20.6(7)	1.0(5)	0.7(5)	0.5(6)
C12	18.1(7)	17.3(7)	18.8(6)	0.4(5)	-0.4(5)	1.3(6)
C16	21.4(7)	24.6(8)	17.8(6)	-2.7(6)	-0.2(6)	4.3(7)
C18	21.9(7)	20.6(7)	21.3(7)	-2.8(6)	-2.0(6)	-3.5(6)
C2	19.4(7)	18.2(7)	19.4(7)	0.1(5)	0.8(6)	2.9(6)
C8	20.2(7)	23.5(8)	21.4(7)	2.4(6)	0.2(6)	-1.6(6)
C14	19.9(7)	22.5(7)	24.0(7)	-2.0(6)	0.9(6)	-4.0(6)
C25	20.2(7)	18.0(7)	22.0(7)	0.7(5)	-1.7(6)	-2.0(6)
C7	22.4(7)	23.6(8)	23.8(7)	-0.2(6)	1.8(6)	-1.5(7)
C6	25.7(8)	32.7(9)	22.2(7)	-4.9(6)	-3.6(6)	-1.8(7)
C4	26.9(8)	21.9(7)	23.3(7)	1.6(6)	6.1(6)	-0.2(7)
C20	19.2(7)	17.9(7)	14.8(6)	0.4(5)	4.0(5)	-2.3(6)
C23	27.8(8)	19.5(7)	20.2(6)	-2.4(5)	3.0(6)	-2.7(7)
C5	30.9(8)	25.7(8)	17.5(7)	0.3(6)	2.0(6)	4.0(7)
C15	23.0(7)	26.1(8)	24.2(7)	-5.8(6)	-4.0(6)	-0.6(7)
C17	22.0(7)	22.5(8)	23.5(7)	-1.3(6)	3.0(6)	-1.9(6)
C22	24.4(7)	25.4(8)	16.2(6)	-1.9(6)	-1.7(6)	-4.3(7)
C24	23.0(7)	18.8(7)	27.1(7)	0.8(6)	-0.9(6)	1.8(6)
C3	22.0(7)	20.8(7)	22.8(7)	-0.6(5)	-0.9(6)	0.1(7)
C21	20.0(7)	21.3(7)	16.9(6)	1.6(5)	-0.2(5)	1.5(6)
C19	29.4(8)	48.2(10)	20.0(7)	-0.3(7)	5.2(7)	0.4(8)

V. NMR Spectra

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126.07
113.86
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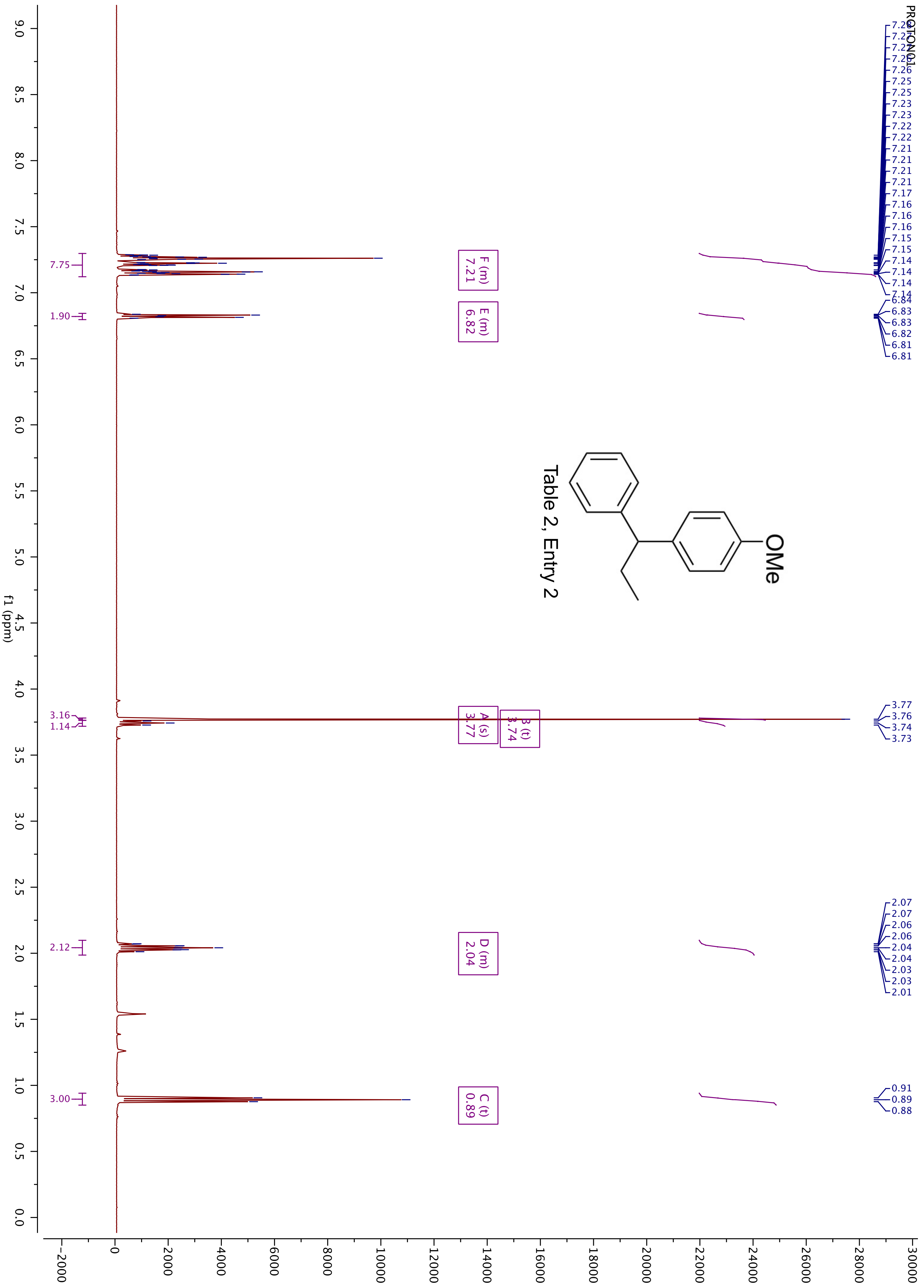
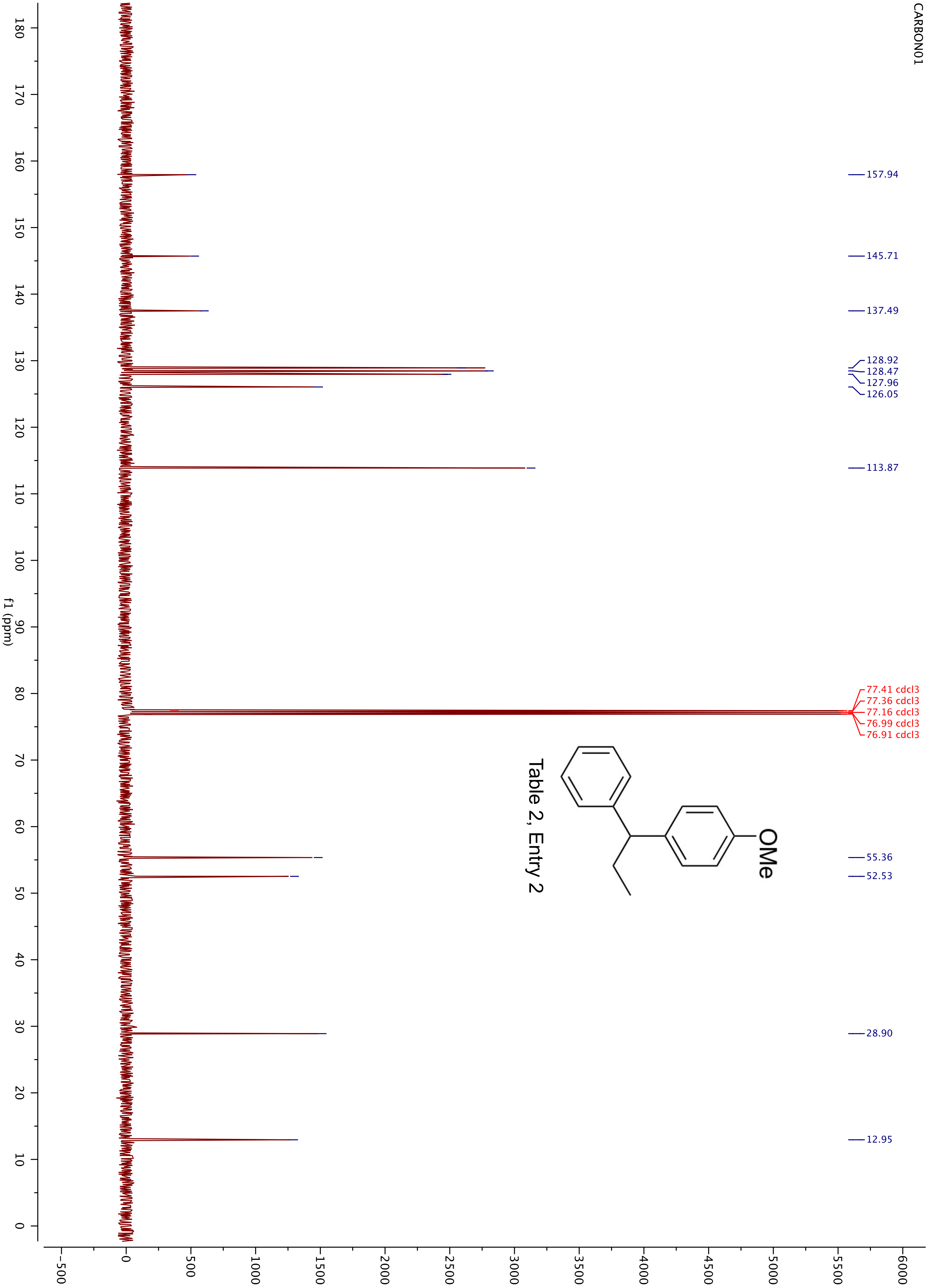
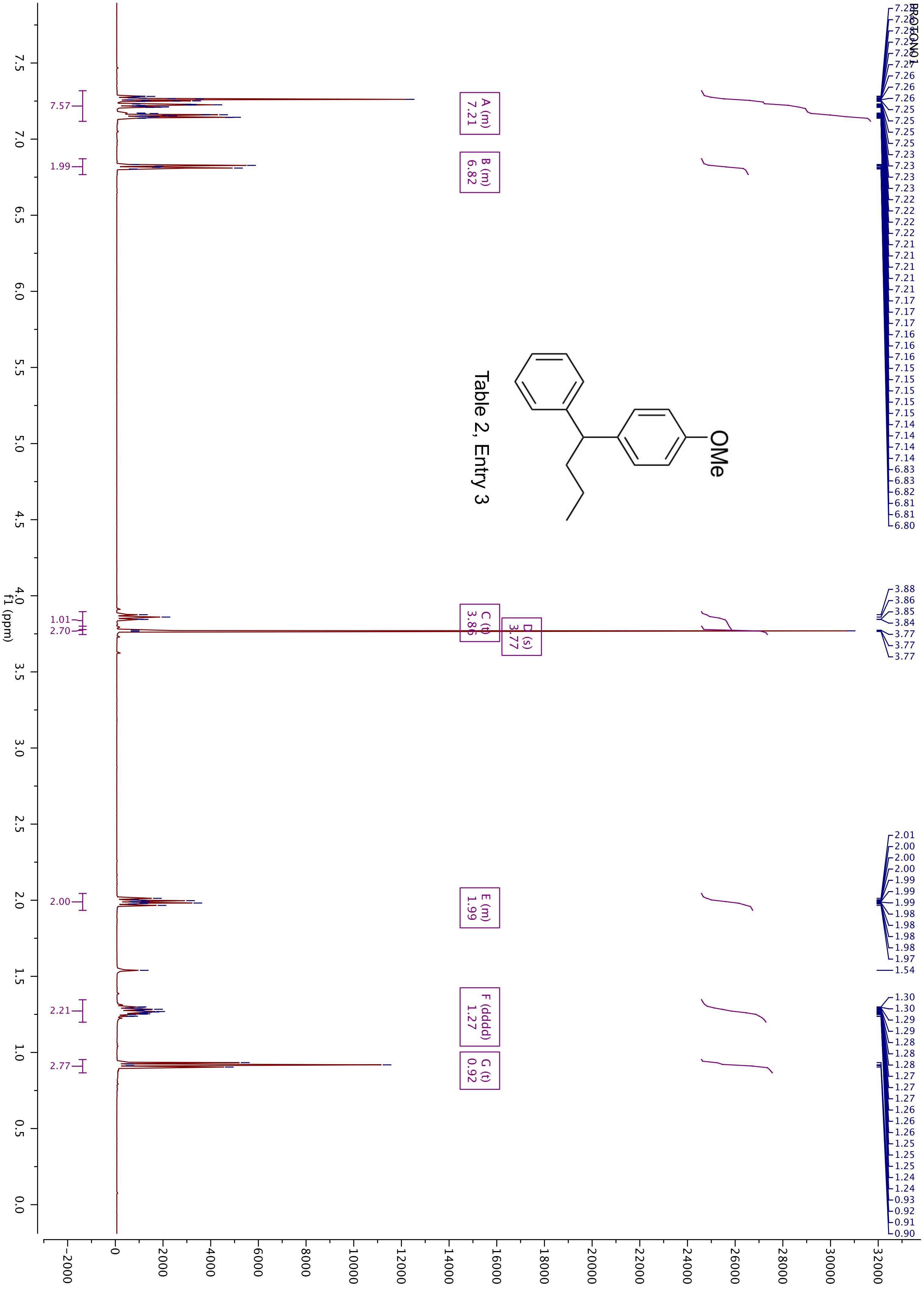
77.16 cdcl3
76.91 cdcl3
55.39
44.08
22.21
OMe
Table 2, Entry 1
6000
5500
5000
4500
4000
3500
3000
2500
2000
1500
1000
500
0
−500
70
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


PROTON01
7.28
7.27
7.27
7.26
7.26
7.25
7.25
7.23
7.23
7.22
7.22
7.21
7.21
7.21
7.21
7.17
7.16
7.16
7.16
7.15
7.15
7.14
7.14
7.14
7.14
6.84
6.83
6.83
6.82
6.81
6.81
3.77
3.76
3.74
3.73
2.07
2.07
2.06
2.06
2.04
2.04
2.03
2.03
2.01
0.91
0.89
0.88
OMe
Table 2, Entry 2
F (m)
7.21
E (m)
6.82
A (s)
3.77
B (t)
3.74
D (m)
2.04
C (t)
0.89
7.75
1.90
3.16
1.14
2.12
3.00
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
f1 (ppm)
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-2000
0
2000
4000
6000
8000
10000
12000
14000
16000
18000
20000
22000
24000
26000
28000
30000


CARBON01
Table 2, Entry 2
OMe
157.94
145.71
137.49
128.92
128.47
127.96
126.05
113.87
77.41 cdcl3
77.36 cdcl3
77.16 cdcl3
76.99 cdcl3
76.91 cdcl3
55.36
52.53
28.90
12.95
f1 (ppm)
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-500
0
500
1000
1500
2000
2500
3000
3500
4000
4500
5000
5500
6000


PROTON01
Table 2, Entry 3
OMe
A (m) 7.21
B (m) 6.82
C (t) 3.86
D (s) 3.77
E (m) 1.99
F (dddd) 1.27
G (t) 0.92
7.57
1.99
1.01
2.70
2.00
2.21
2.77
f1 (ppm)
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
-2000
0
2000
4000
6000
8000
10000
12000
14000
16000
18000
20000
22000
24000
26000
28000
30000
32000
7.27
7.26
7.26
7.26
7.25
7.25
7.25
7.25
7.23
7.23
7.23
7.23
7.22
7.22
7.22
7.22
7.21
7.21
7.21
7.21
7.21
7.17
7.17
7.17
7.16
7.16
7.16
7.15
7.15
7.15
7.15
7.15
7.14
7.14
7.14
7.14
6.83
6.83
6.82
6.81
6.81
6.80
3.88
3.86
3.85
3.84
3.77
3.77
3.77
2.01
2.00
2.00
2.00
1.99
1.99
1.99
1.98
1.98
1.98
1.98
1.97
1.54
1.30
1.30
1.29
1.29
1.28
1.28
1.28
1.27
1.27
1.27
1.26
1.26
1.26
1.25
1.25
1.25
1.24
1.24
0.93
0.92
0.91
0.90

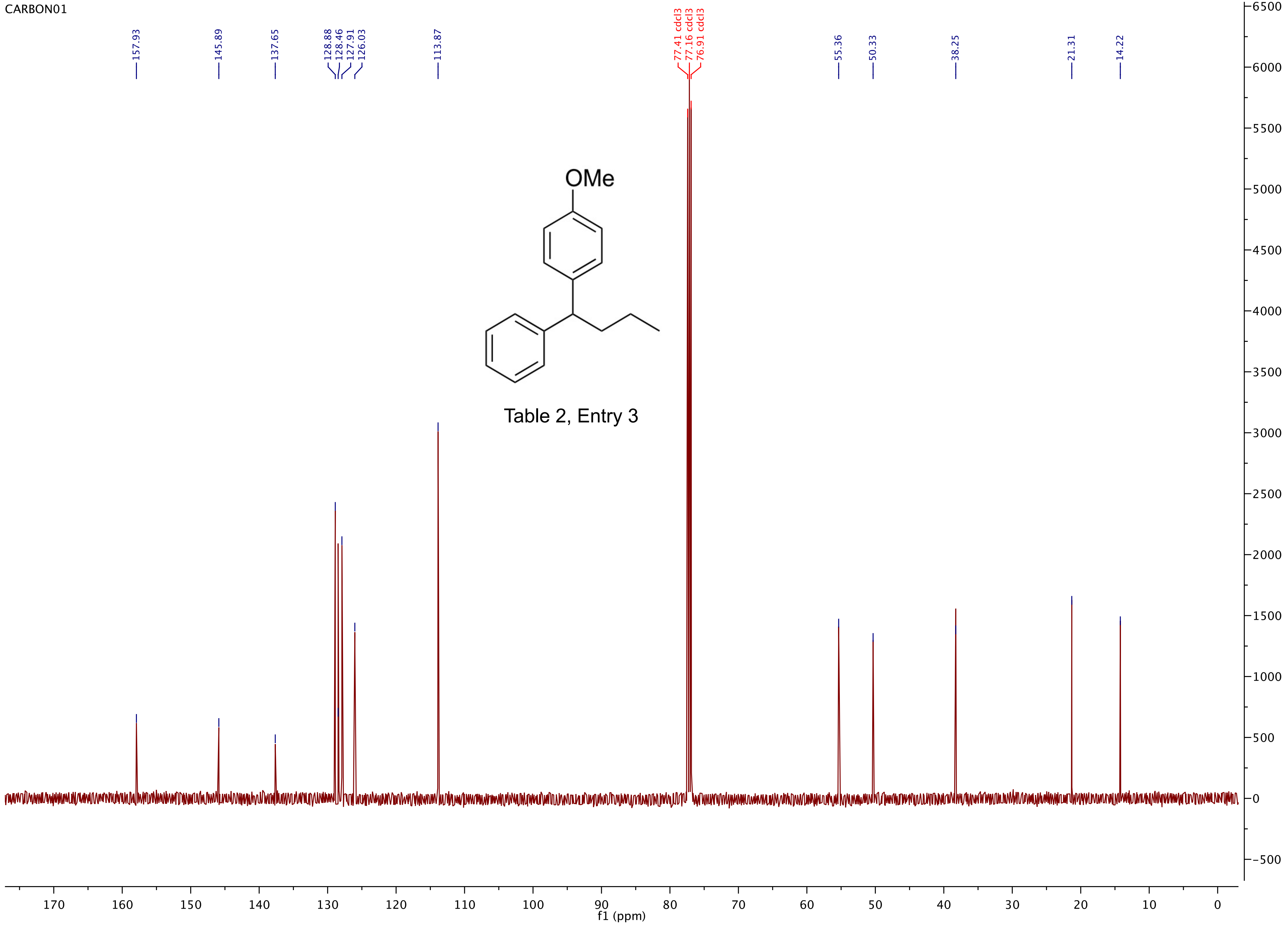


Table 2, Entry 3

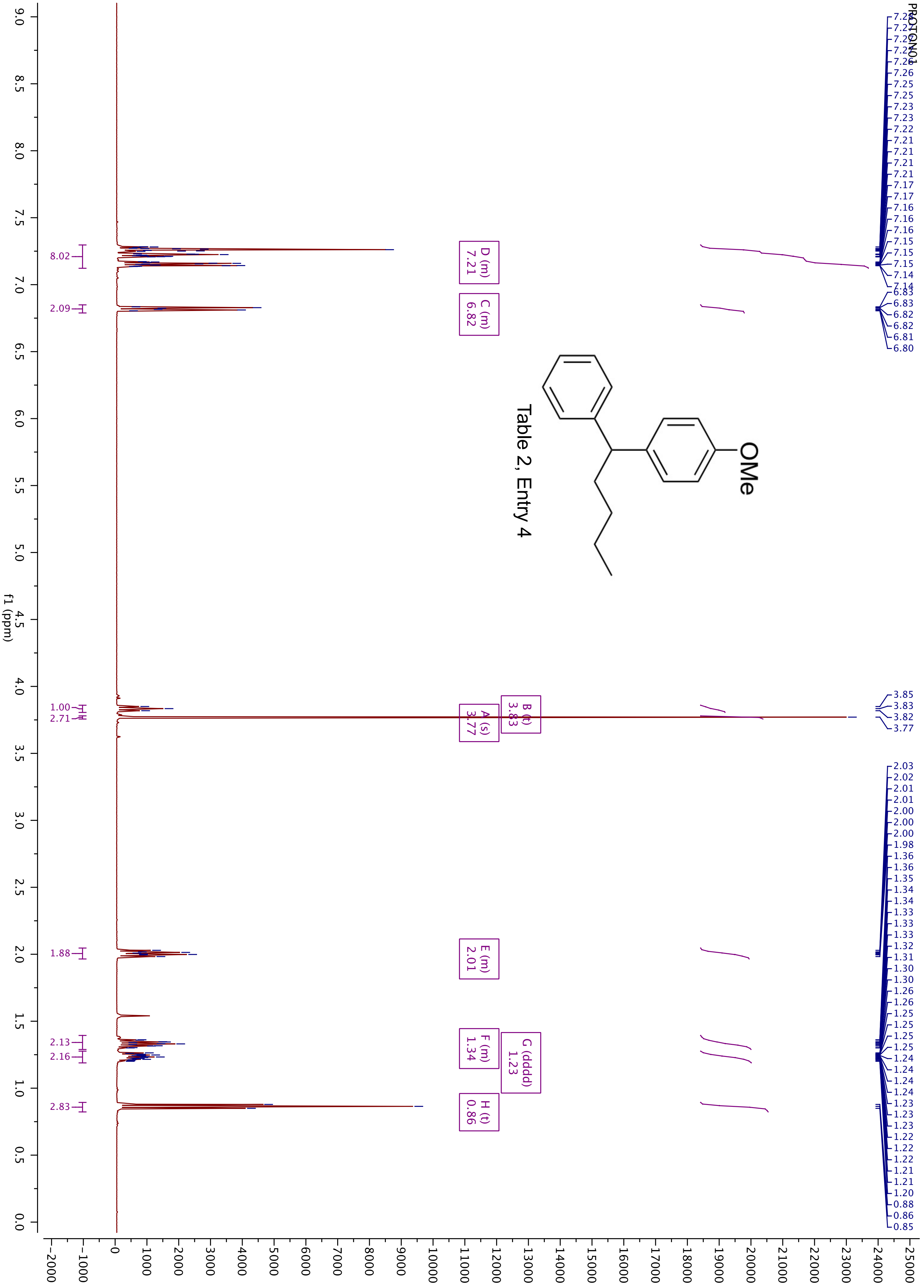


Table 2, Entry 4

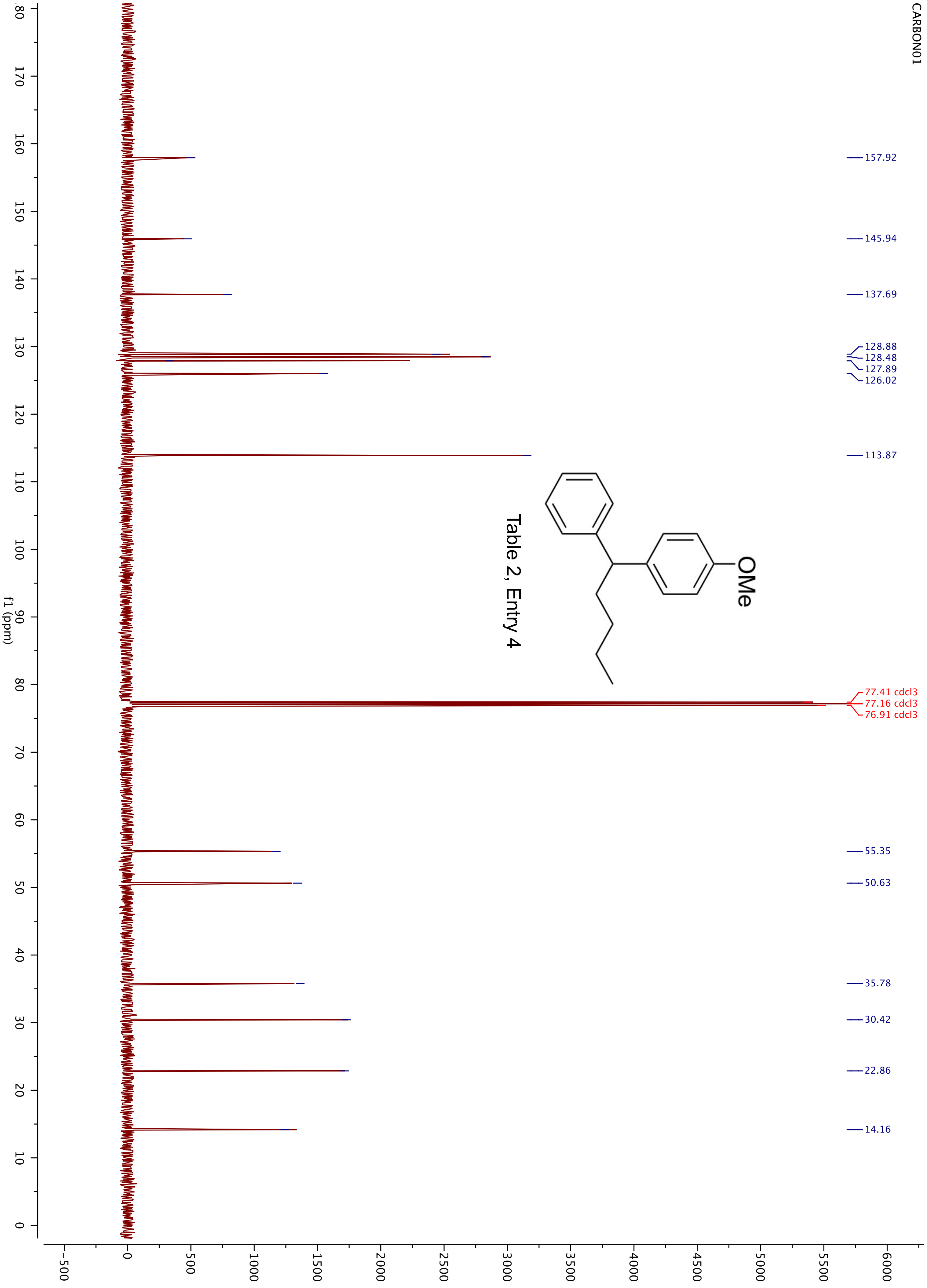
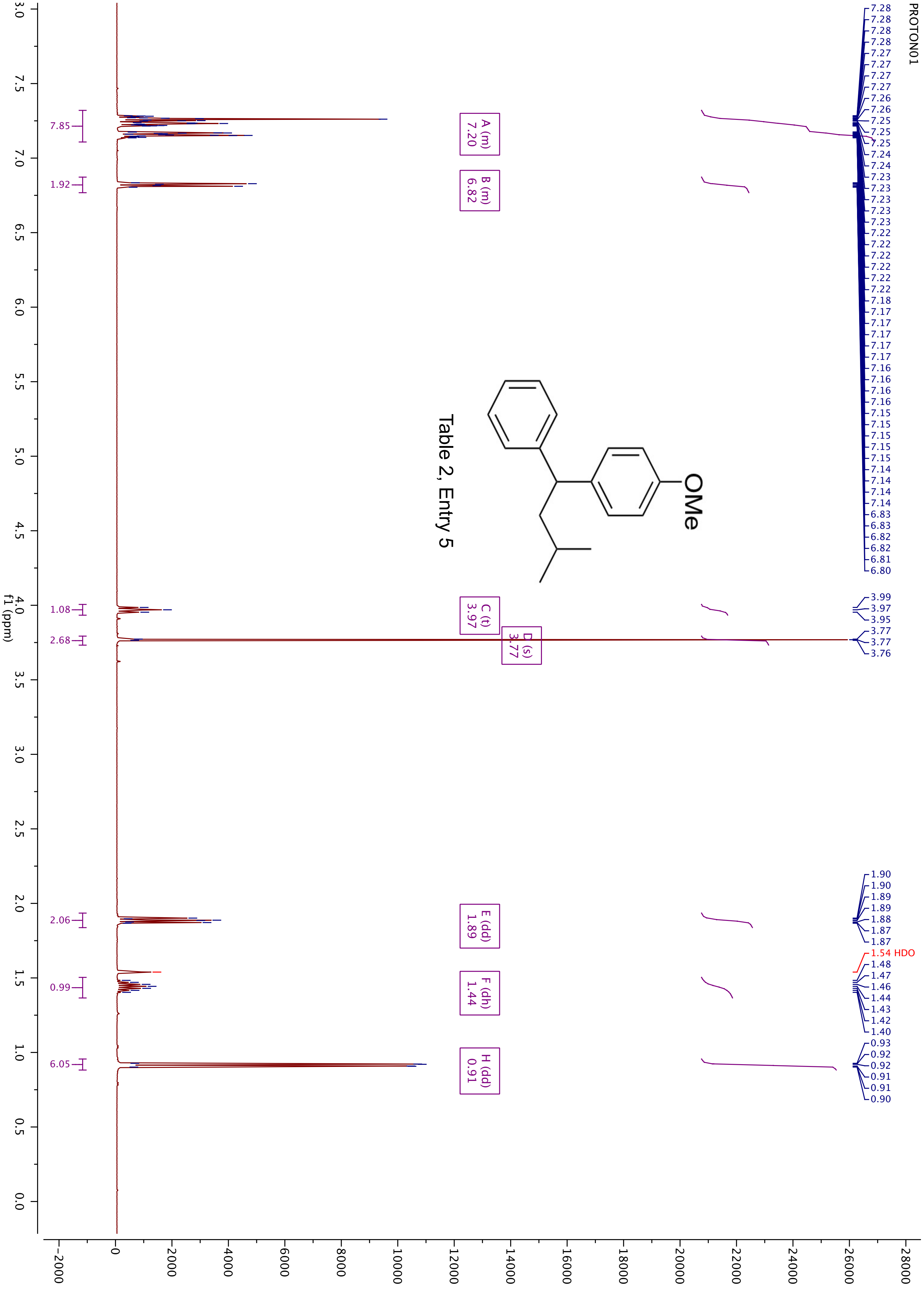
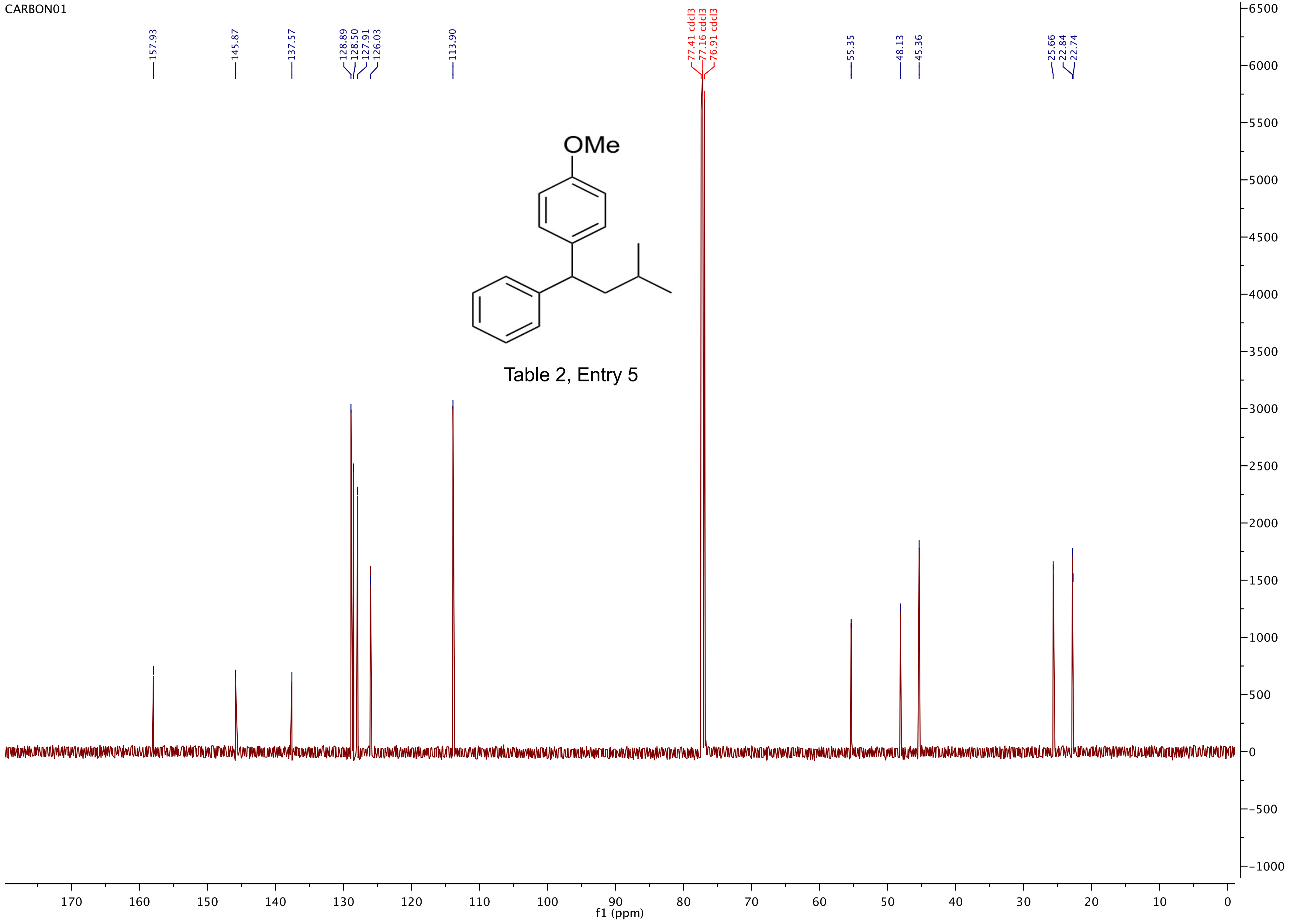
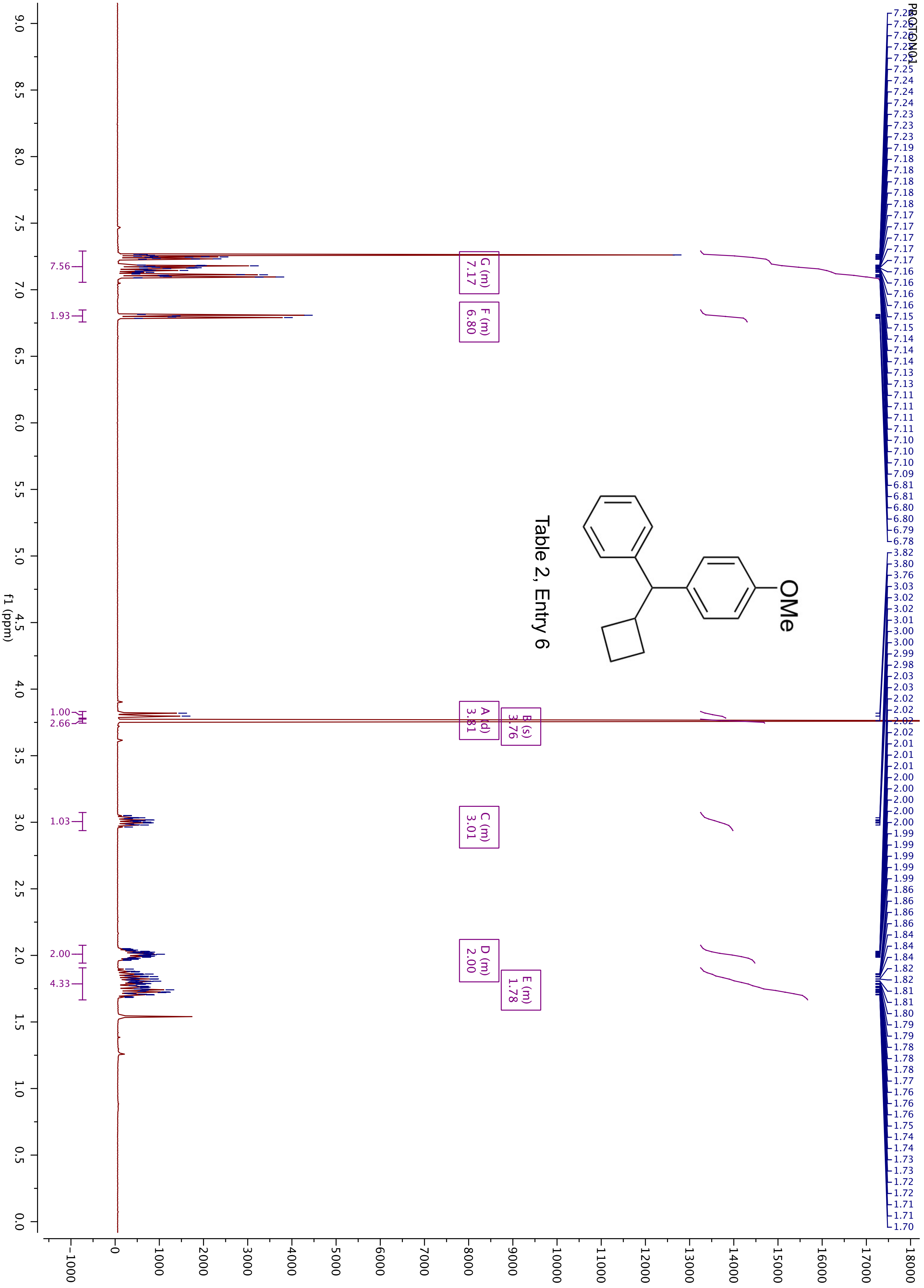
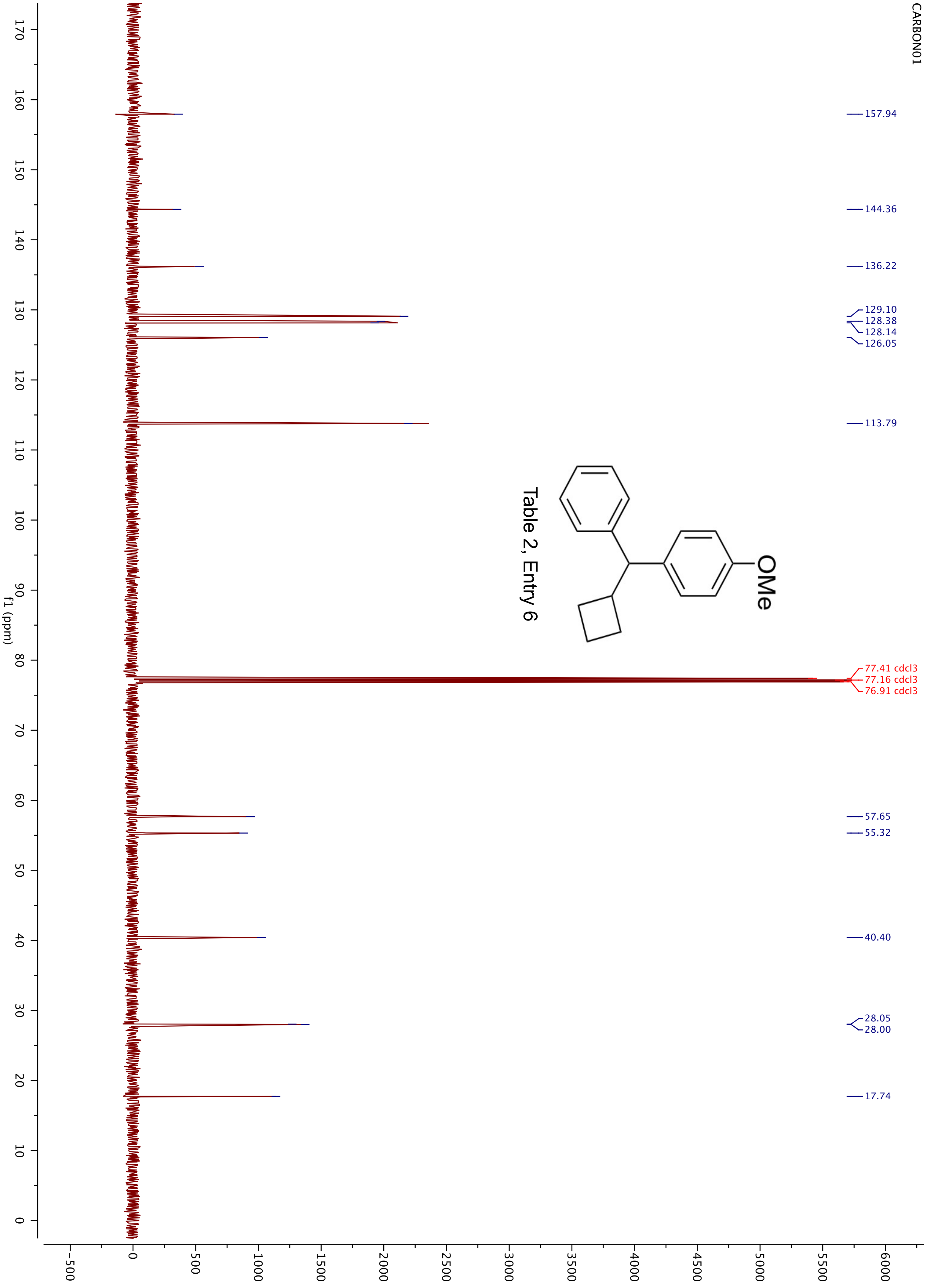


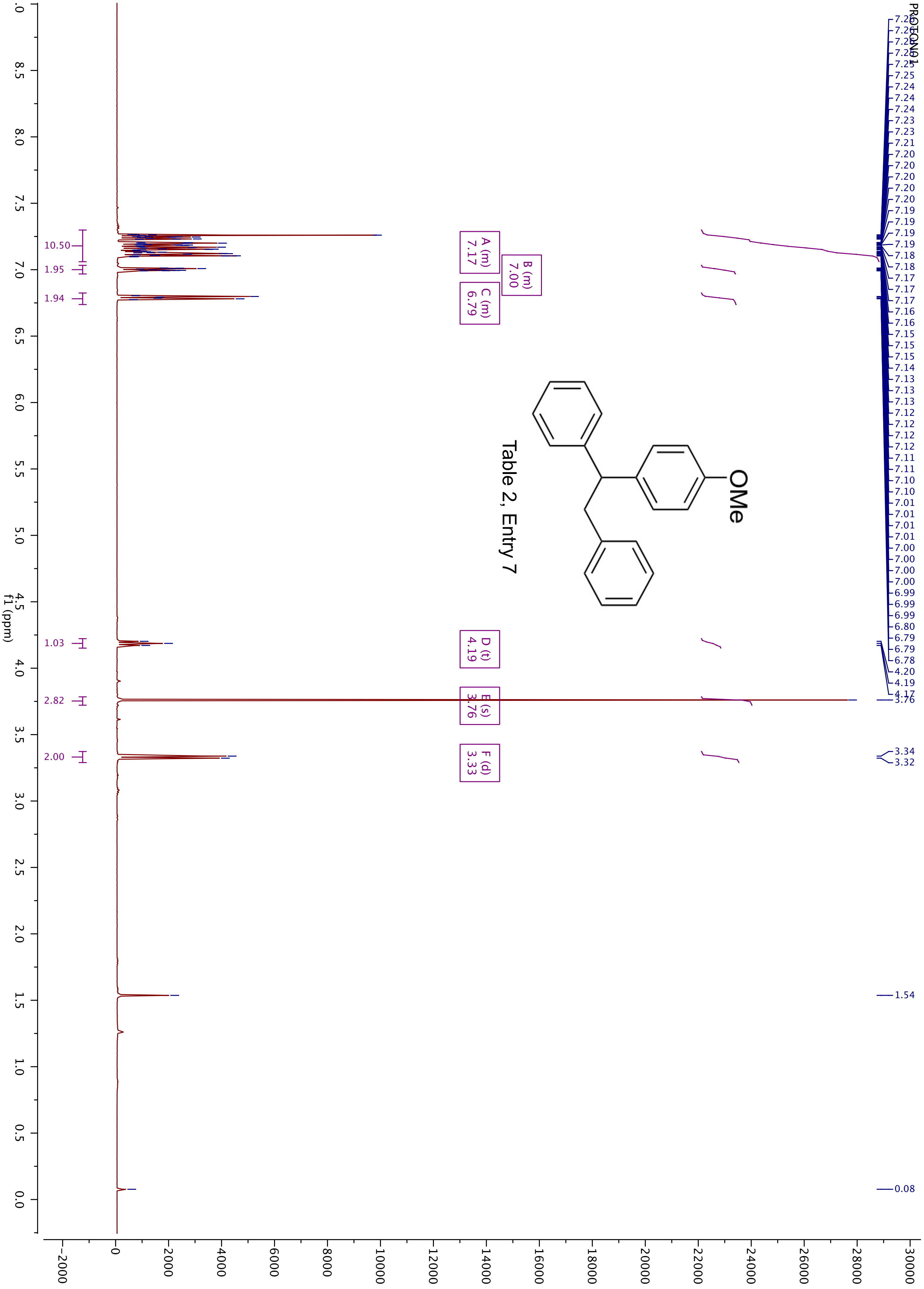
Table 2, Entry 4


PROTON01
Table 2, Entry 5
OMe
A (m) 7.20
B (m) 6.82
C (t) 3.97
D (s) 3.77
E (dd) 1.89
F (dh) 1.44
H (dd) 0.91
7.85
1.92
1.08
2.68
2.06
0.99
6.05
7.28 7.28 7.28 7.28 7.27 7.27 7.27 7.27 7.26 7.26 7.25 7.25 7.25 7.24 7.24 7.23 7.23 7.23 7.23 7.23 7.22 7.22 7.22 7.22 7.22 7.22 7.18 7.17 7.17 7.17 7.17 7.17 7.16 7.16 7.16 7.16 7.15 7.15 7.15 7.15 7.15 7.14 7.14 7.14 7.14 6.83 6.83 6.82 6.82 6.81 6.80
3.99 3.97 3.95
3.77 3.77 3.76
1.90 1.90 1.89 1.89 1.88 1.87 1.87
1.54 HDO
1.48 1.47 1.46 1.44 1.43 1.42 1.40
0.93 0.92 0.92 0.91 0.91 0.90
f1 (ppm)
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
-2000 0 2000 4000 6000 8000 10000 12000 14000 16000 18000 20000 22000 24000 26000 28000


CARBON01
157.93
145.87
137.57
128.89
128.50
127.91
126.03
113.90
77.41 cdcl3
77.16 cdcl3
76.91 cdcl3
55.35
48.13
45.36
25.66
22.84
22.74
OMe
Table 2, Entry 5
6500
6000
5500
5000
4500
4000
3500
3000
2500
2000
1500
1000
500
0
−500
−1000
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


PROTON01
7.26
7.26
7.26
7.25
7.25
7.25
7.24
7.24
7.24
7.23
7.23
7.23
7.19
7.18
7.18
7.18
7.18
7.18
7.17
7.17
7.17
7.17
7.17
7.16
7.16
7.16
7.16
7.15
7.15
7.14
7.14
7.14
7.13
7.13
7.11
7.11
7.11
7.11
7.10
7.10
7.10
7.09
6.81
6.81
6.80
6.80
6.79
6.78
3.82
3.80
3.76
3.03
3.02
3.02
3.01
3.00
3.00
2.99
2.98
2.03
2.03
2.02
2.02
2.02
2.02
2.02
2.01
2.01
2.01
2.00
2.00
2.00
2.00
2.00
1.99
1.99
1.99
1.99
1.99
1.86
1.86
1.86
1.86
1.84
1.84
1.84
1.82
1.82
1.81
1.81
1.80
1.79
1.79
1.78
1.78
1.78
1.77
1.76
1.76
1.76
1.75
1.74
1.74
1.73
1.73
1.72
1.72
1.71
1.71
1.70
OMe
Table 2, Entry 6
G (m) 7.17
F (m) 6.80
A (d) 3.81
B (s) 3.76
C (m) 3.01
D (m) 2.00
E (m) 1.78
7.56
1.93
1.00
2.66
1.03
2.00
4.33
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)
-1000
0
1000
2000
3000
4000
5000
6000
7000
8000
9000
10000
11000
12000
13000
14000
15000
16000
17000
18000


CARBON01
Table 2, Entry 6
OMe
157.94
144.36
136.22
129.10
128.38
128.14
126.05
113.79
77.41 cdcl3
77.16 cdcl3
76.91 cdcl3
57.65
55.32
40.40
28.05
28.00
17.74
f1 (ppm)
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-500
0
500
1000
1500
2000
2500
3000
3500
4000
4500
5000
5500
6000


PROTON01
Table 2, Entry 7
OMe
A (m) 7.17
B (m) 7.00
C (m) 6.79
D (t) 4.19
E (s) 3.76
F (d) 3.33
10.50
1.95
1.94
1.03
2.82
2.00
7.25
7.25
7.24
7.24
7.24
7.23
7.23
7.21
7.20
7.20
7.20
7.20
7.20
7.19
7.19
7.19
7.19
7.18
7.18
7.17
7.17
7.17
7.16
7.16
7.15
7.15
7.15
7.14
7.13
7.13
7.13
7.12
7.12
7.12
7.12
7.11
7.11
7.10
7.10
7.01
7.01
7.01
7.01
7.00
7.00
7.00
7.00
6.99
6.99
6.99
6.80
6.79
6.79
6.78
4.20
4.19
4.17
3.76
3.34
3.32
1.54
0.08
f1 (ppm)
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
-2000
0
2000
4000
6000
8000
10000
12000
14000
16000
18000
20000
22000
24000
26000
28000
30000

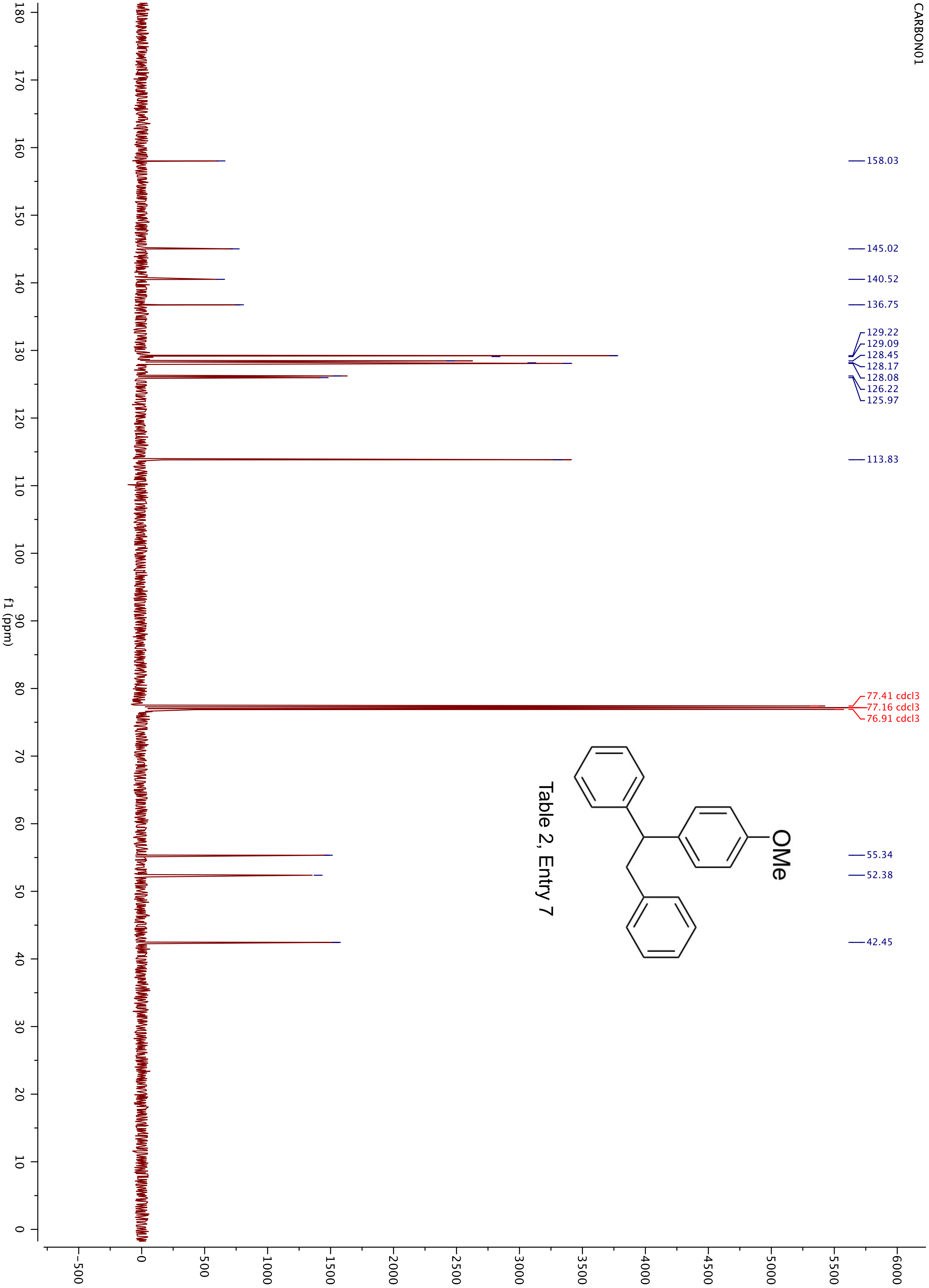
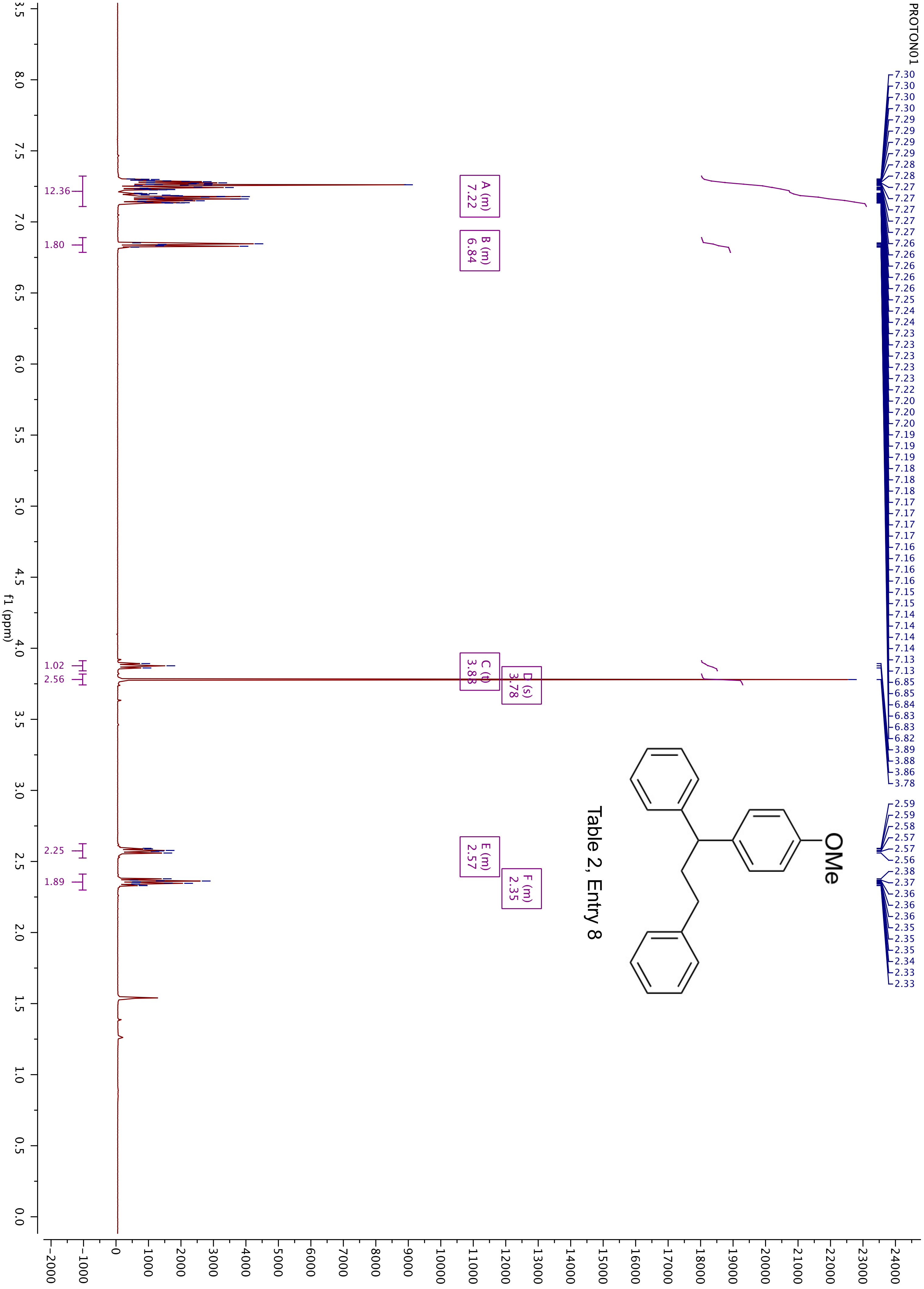


Table 2, Entry 7


PROTON01
7.30
7.30
7.30
7.30
7.29
7.29
7.29
7.29
7.28
7.28
7.27
7.27
7.27
7.27
7.27
7.26
7.26
7.26
7.26
7.26
7.25
7.24
7.24
7.23
7.23
7.23
7.23
7.23
7.22
7.20
7.20
7.20
7.19
7.19
7.19
7.18
7.18
7.18
7.17
7.17
7.17
7.17
7.16
7.16
7.16
7.16
7.15
7.15
7.14
7.14
7.14
7.14
7.13
7.13
6.85
6.85
6.84
6.83
6.83
6.82
3.89
3.88
3.86
3.78
2.59
2.59
2.58
2.57
2.57
2.56
2.38
2.37
2.36
2.36
2.36
2.35
2.35
2.35
2.34
2.33
2.33
A (m)
7.22
B (m)
6.84
C (t)
3.88
D (s)
3.78
E (m)
2.57
F (m)
2.35
12.36
1.80
1.02
2.56
2.25
1.89
OMe
Table 2, Entry 8
f1 (ppm)
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
-2000
-1000
0
1000
2000
3000
4000
5000
6000
7000
8000
9000
10000
11000
12000
13000
14000
15000
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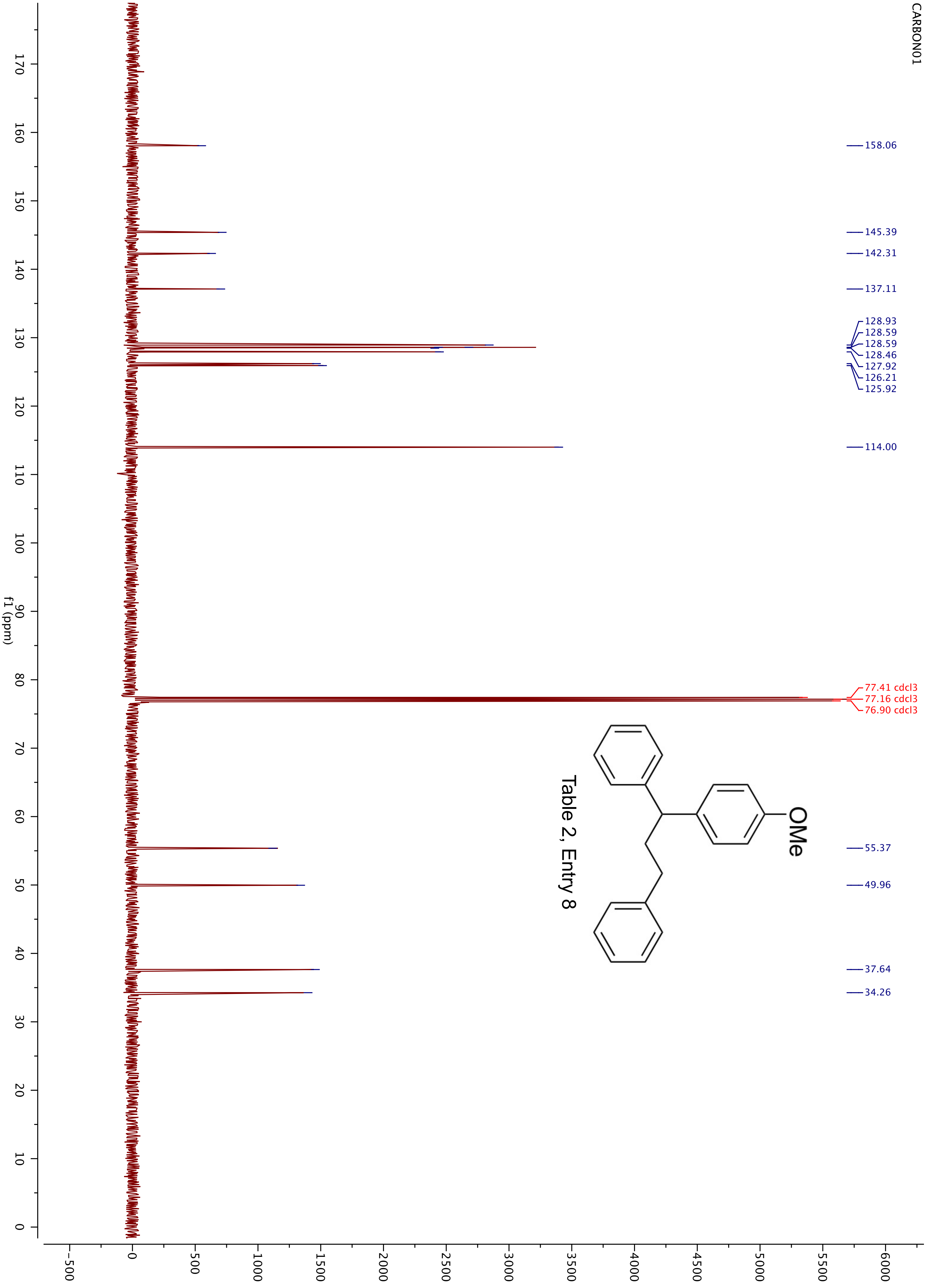
20000
21000
22000
23000
24000


CARBON01
158.06
145.39
142.31
137.11
128.93
128.59
128.59
128.46
127.92
126.21
125.92
114.00
77.41 cdcl3
77.16 cdcl3
76.90 cdcl3
55.37
49.96
37.64
34.26
OMe
Table 2, Entry 8
f1 (ppm)
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-500
0
500
1000
1500
2000
2500
3000
3500
4000
4500
5000
5500
6000

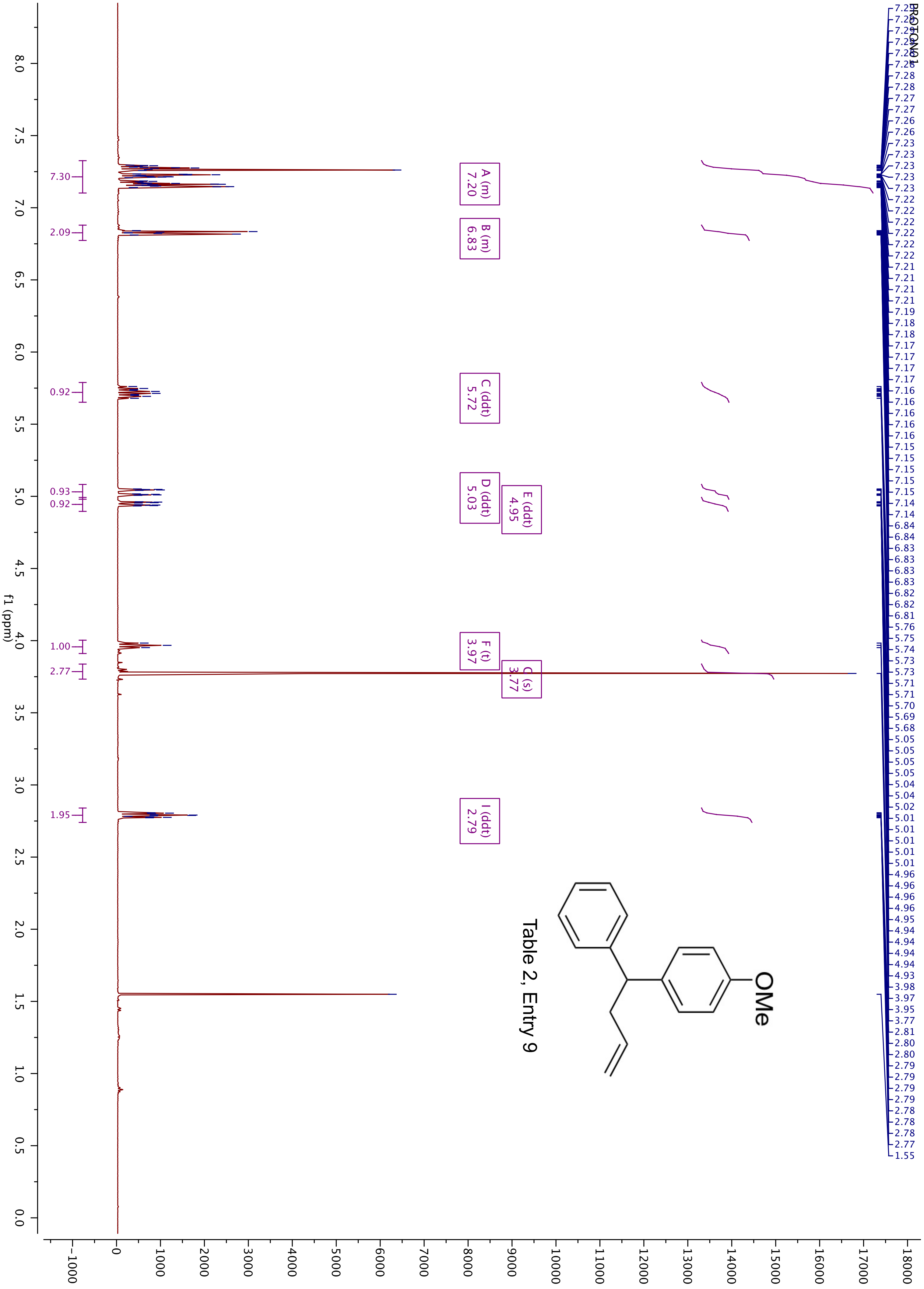
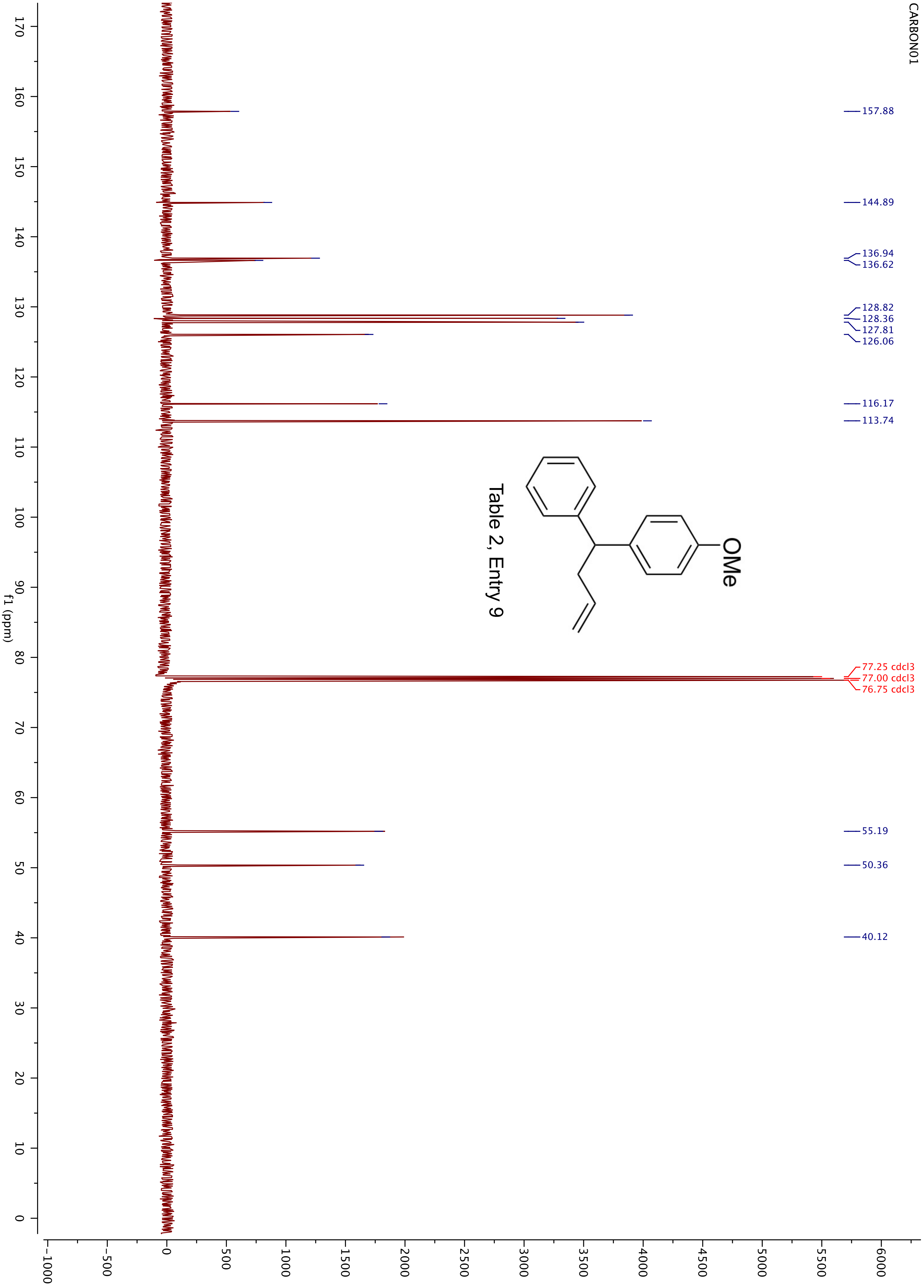


Table 2, Entry 9


CARBON01
Table 2, Entry 9
OMe
157.88
144.89
136.94
136.62
128.82
128.36
127.81
126.06
116.17
113.74
77.25 cdcl3
77.00 cdcl3
76.75 cdcl3
55.19
50.36
40.12
f1 (ppm)
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-1000
-500
0
500
1000
1500
2000
2500
3000
3500
4000
4500
5000
5500
6000

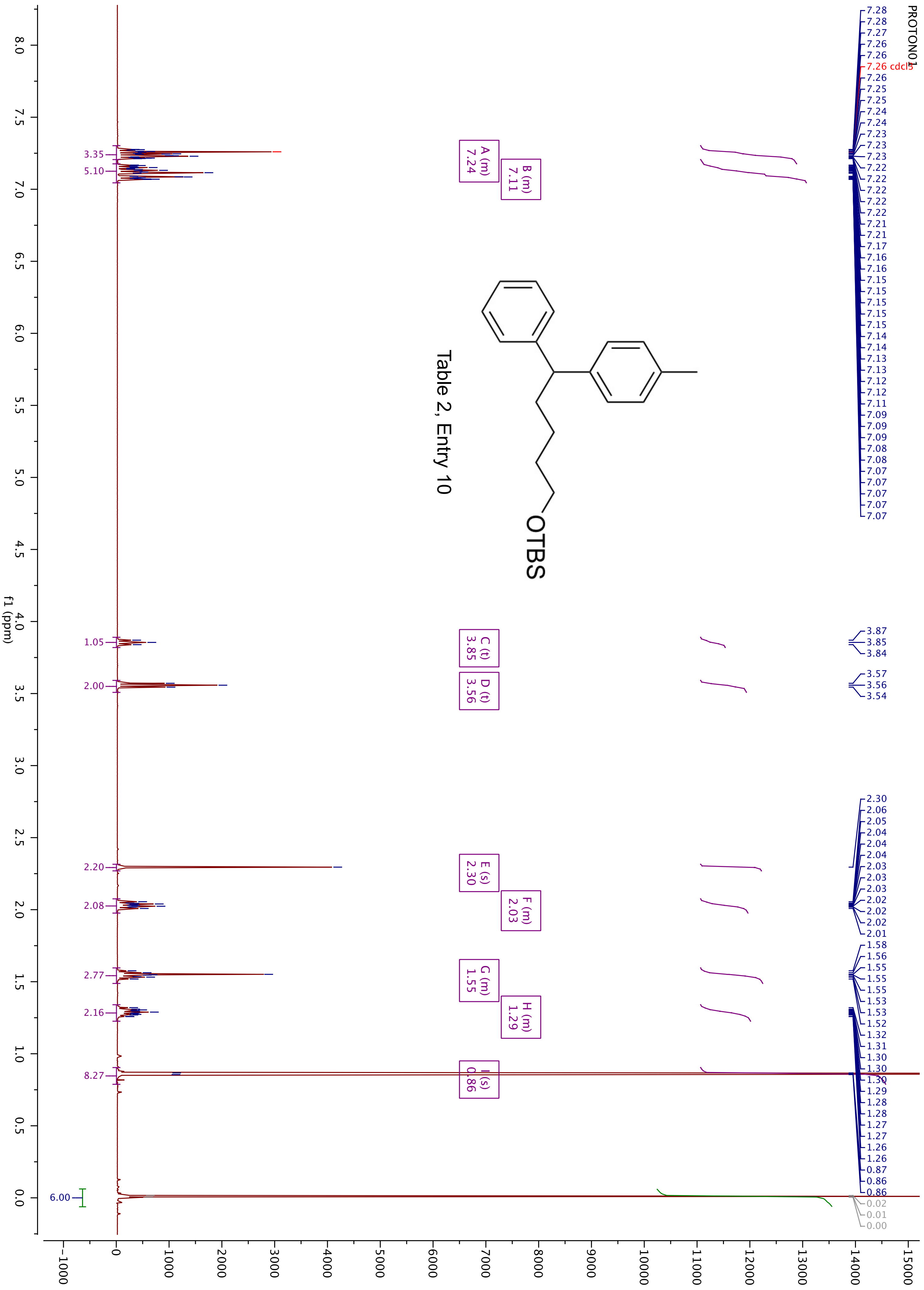
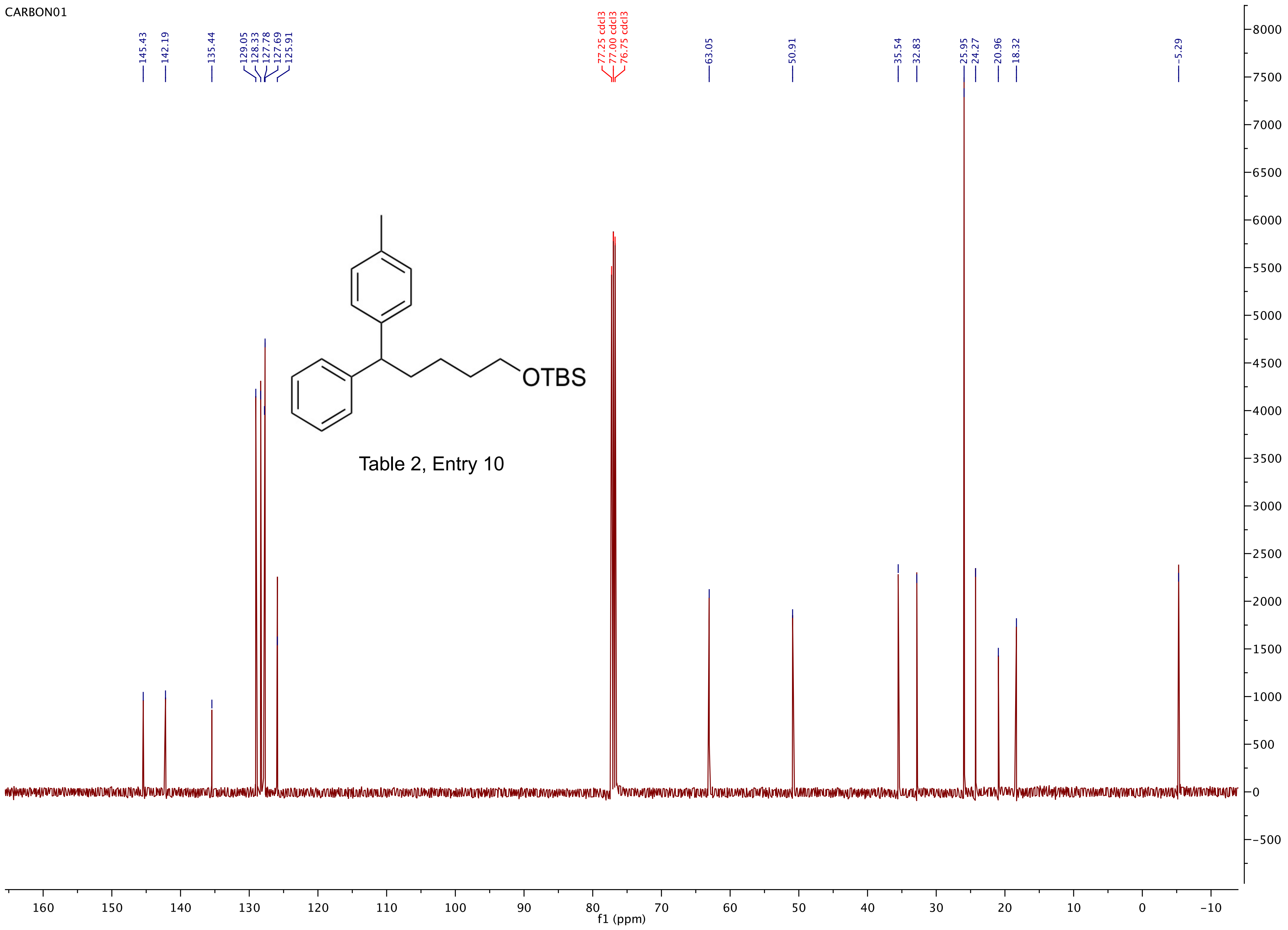


Table 2, Entry 10


CARBON01
145.43
142.19
135.44
129.05
128.33
127.78
127.69
125.91
77.25 cdcl3
77.00 cdcl3
76.75 cdcl3
63.05
50.91
35.54
32.83
25.95
24.27
20.96
18.32
-5.29
OTBS
Table 2, Entry 10
f1 (ppm)
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
8000
7500
7000
6500
6000
5500
5000
4500
4000
3500
3000
2500
2000
1500
1000
500
0
-500

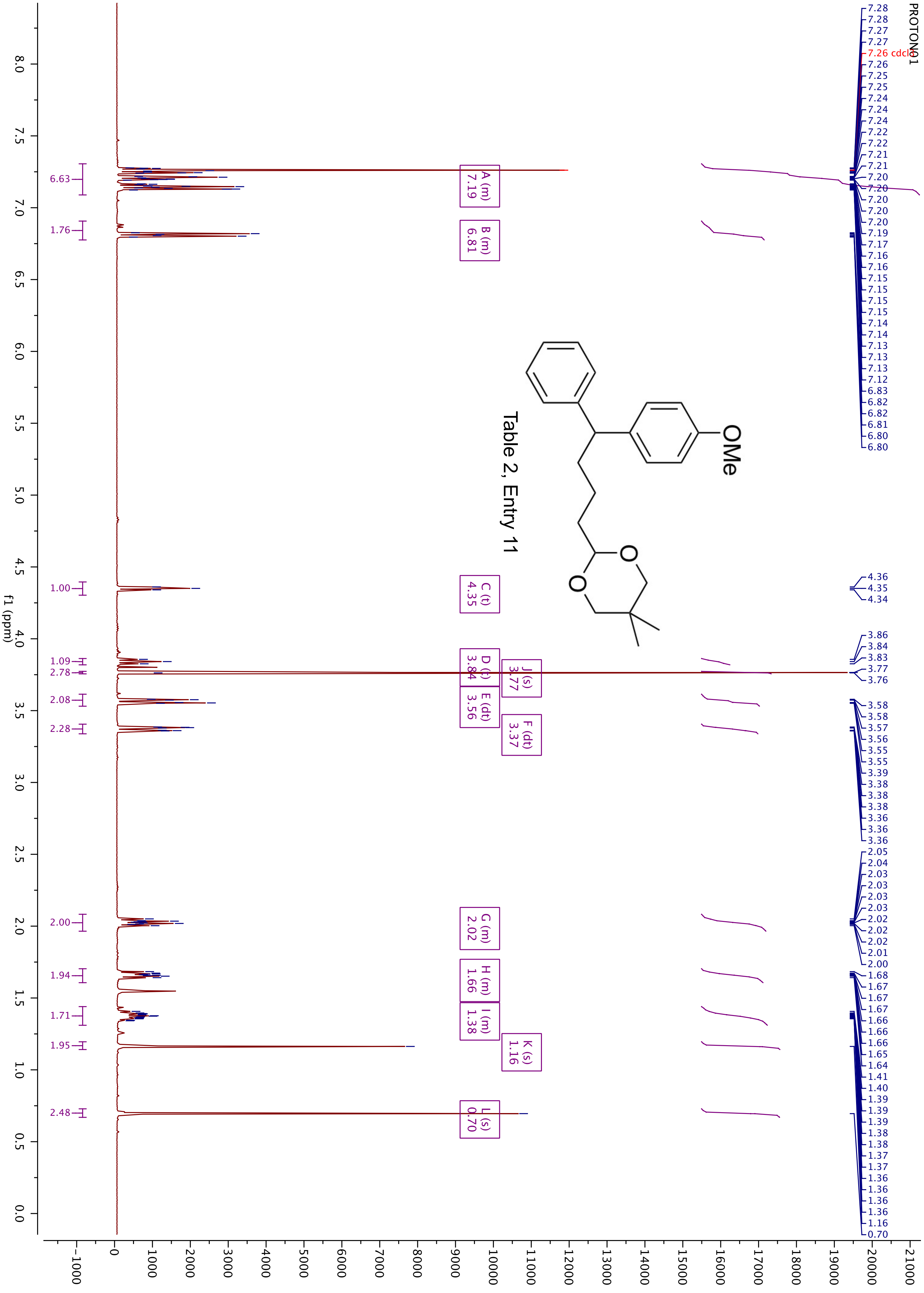
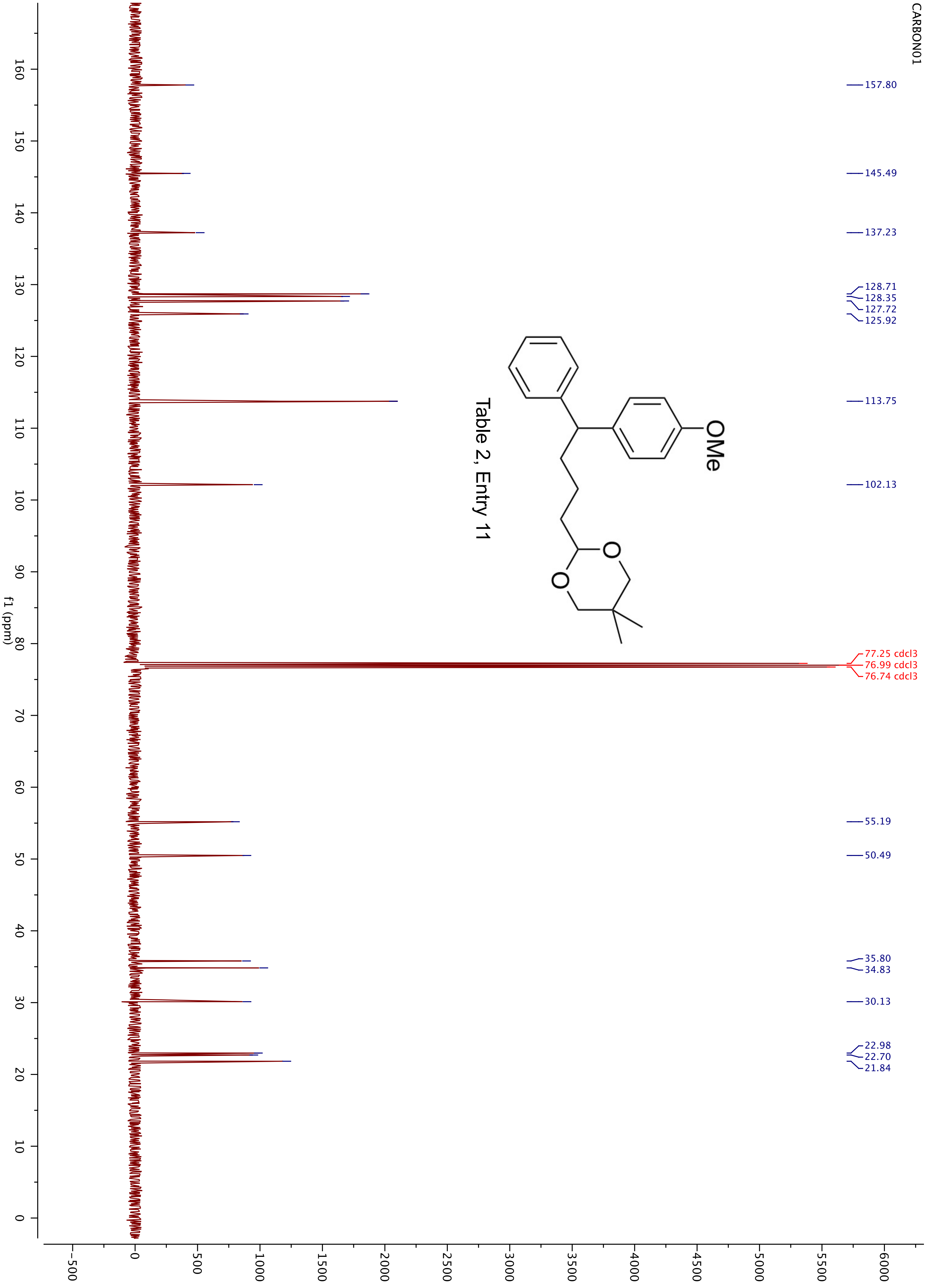
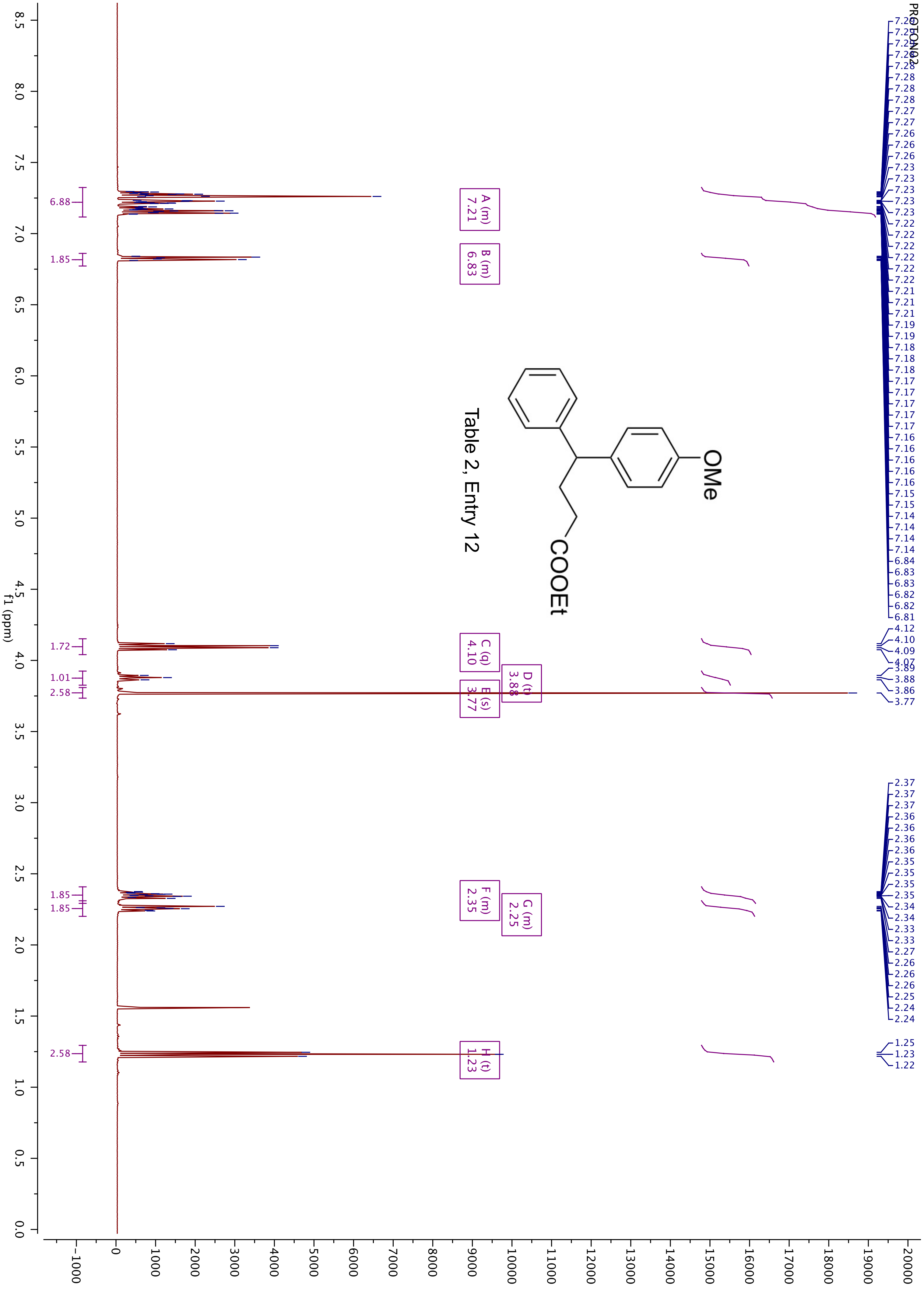


Table 2, Entry 11


CARBON01
Table 2, Entry 11
OMe
O
O
157.80
145.49
137.23
128.71
128.35
127.72
125.92
113.75
102.13
77.25 cdcl3
76.99 cdcl3
76.74 cdcl3
55.19
50.49
35.80
34.83
30.13
22.98
22.70
21.84
f1 (ppm)
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-500
0
500
1000
1500
2000
2500
3000
3500
4000
4500
5000
5500
6000


PROTON02
Table 2, Entry 12
OMe
COOEt
A (m) 7.21
B (m) 6.83
C (q) 4.10
D (t) 3.88
E (s) 3.77
F (m) 2.35
G (m) 2.25
H (t) 1.23
6.88
1.85
1.72
1.01
2.58
1.85
1.85
2.58
7.29
7.29
7.29
7.29
7.28
7.28
7.28
7.28
7.27
7.27
7.26
7.26
7.26
7.23
7.23
7.23
7.23
7.23
7.22
7.22
7.22
7.22
7.22
7.22
7.21
7.21
7.21
7.19
7.19
7.18
7.18
7.18
7.17
7.17
7.17
7.17
7.17
7.16
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7.16
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7.16
7.15
7.15
7.14
7.14
7.14
7.14
6.84
6.83
6.83
6.82
6.82
6.81
4.12
4.10
4.09
4.07
3.89
3.88
3.86
3.77
2.37
2.37
2.37
2.36
2.36
2.36
2.36
2.35
2.35
2.35
2.35
2.34
2.34
2.33
2.33
2.27
2.26
2.26
2.26
2.25
2.24
2.24
1.25
1.23
1.22
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)
-1000
0
1000
2000
3000
4000
5000
6000
7000
8000
9000
10000
11000
12000
13000
14000
15000
16000
17000
18000
19000
20000

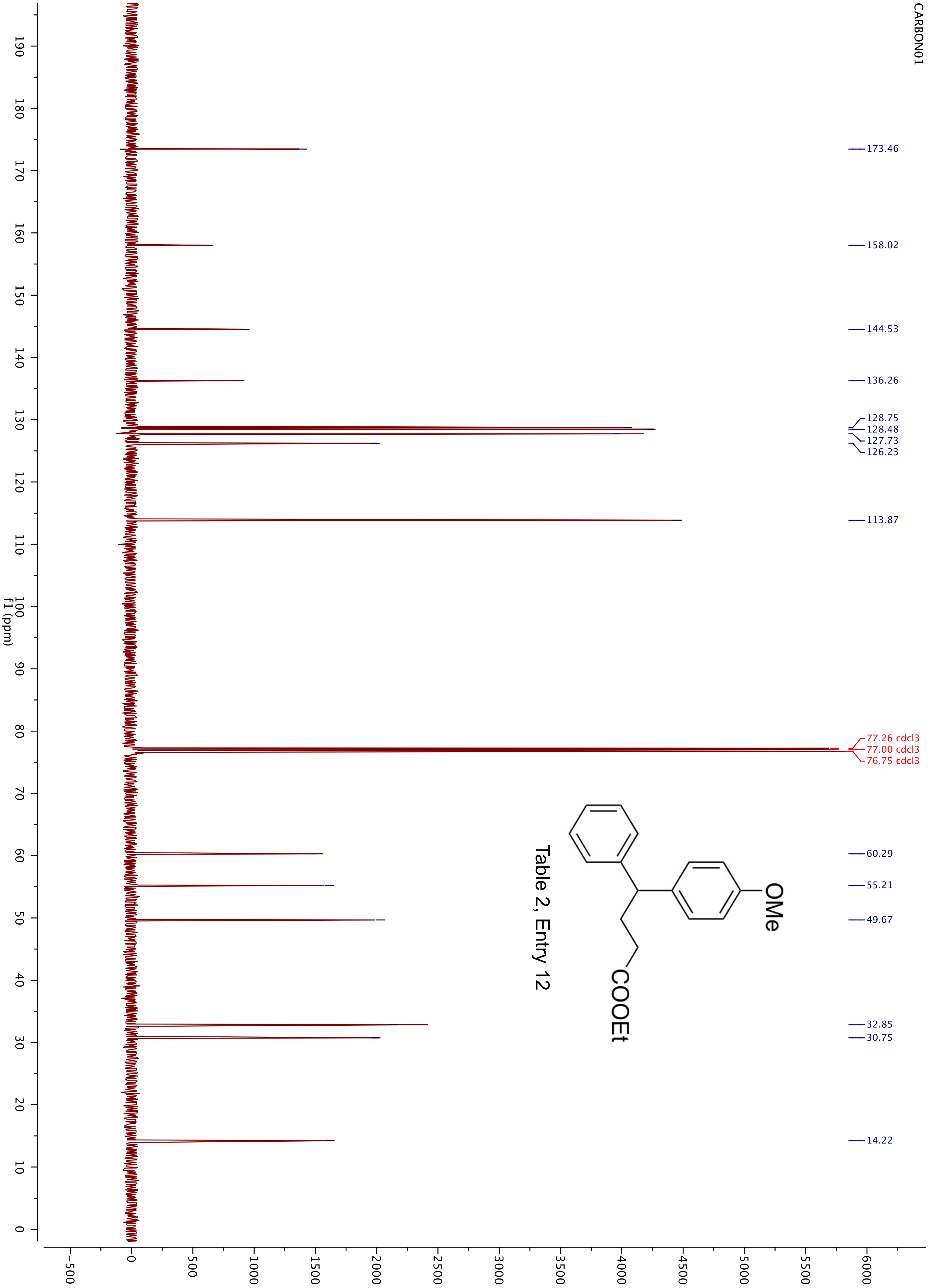
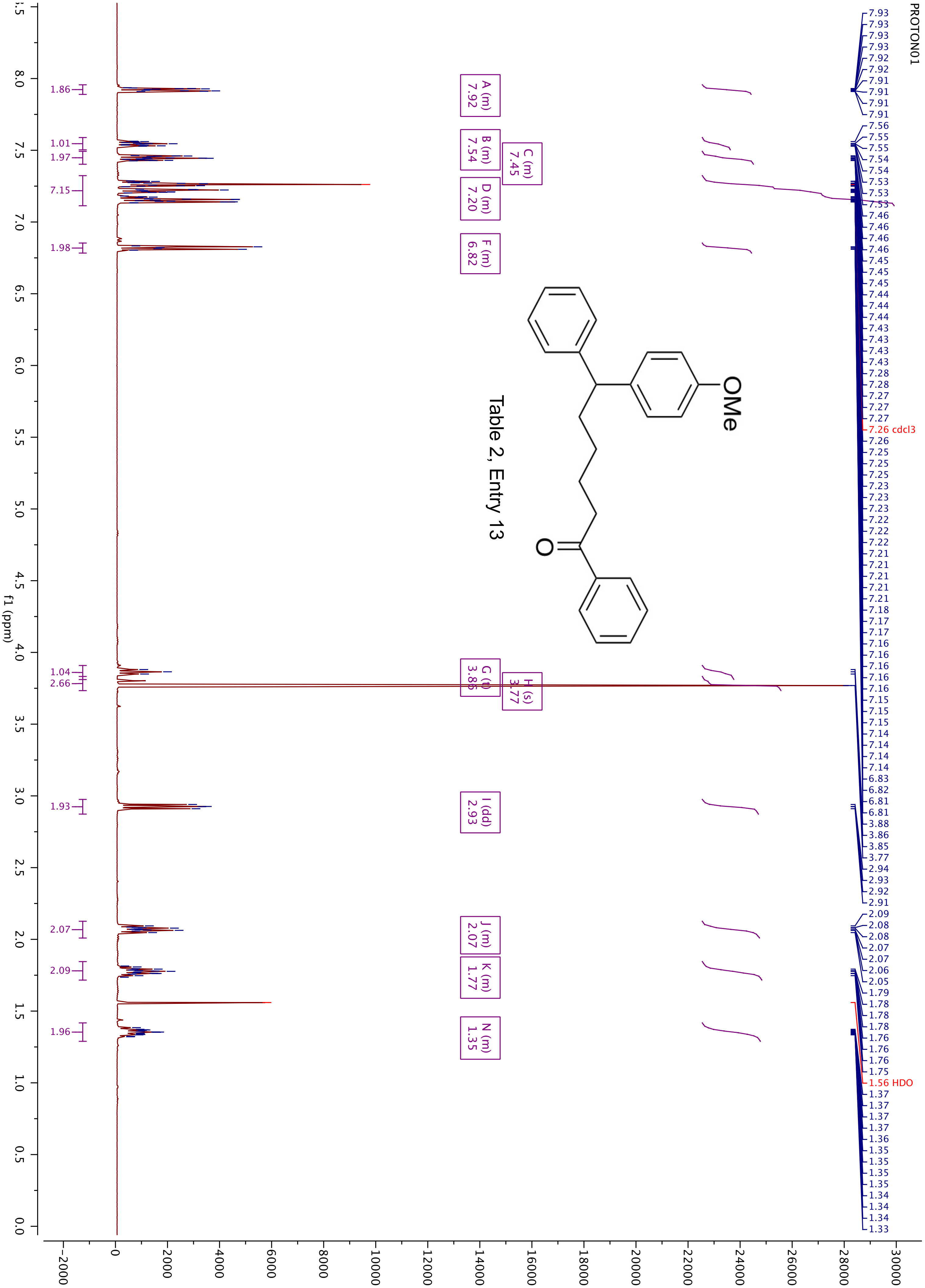


Table 2, Entry 12


PROTON01
Table 2, Entry 13
OMe
O
A (m) 7.92
B (m) 7.54
C (m) 7.45
D (m) 7.20
F (m) 6.82
G (t) 3.86
H (s) 3.77
I (dd) 2.93
J (m) 2.07
K (m) 1.77
N (m) 1.35
1.86
1.01
1.97
7.15
1.98
1.04
2.66
1.93
2.07
2.09
1.96
7.93
7.93
7.93
7.93
7.92
7.92
7.91
7.91
7.91
7.91
7.56
7.55
7.55
7.54
7.54
7.53
7.53
7.53
7.46
7.46
7.46
7.46
7.45
7.45
7.45
7.44
7.44
7.44
7.43
7.43
7.43
7.43
7.28
7.28
7.27
7.27
7.27
7.26 cdcl3
7.26
7.25
7.25
7.25
7.23
7.23
7.23
7.22
7.22
7.22
7.21
7.21
7.21
7.21
7.21
7.18
7.17
7.17
7.16
7.16
7.16
7.16
7.16
7.15
7.15
7.15
7.14
7.14
7.14
7.14
6.83
6.82
6.81
6.81
3.88
3.86
3.85
3.77
2.94
2.93
2.92
2.91
2.09
2.08
2.08
2.07
2.07
2.06
2.05
1.79
1.78
1.78
1.78
1.76
1.76
1.76
1.75
1.56 HDO
1.37
1.37
1.37
1.37
1.36
1.35
1.35
1.35
1.35
1.34
1.34
1.34
1.33
f1 (ppm)
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
-2000
0
2000
4000
6000
8000
10000
12000
14000
16000
18000
20000
22000
24000
26000
28000
30000

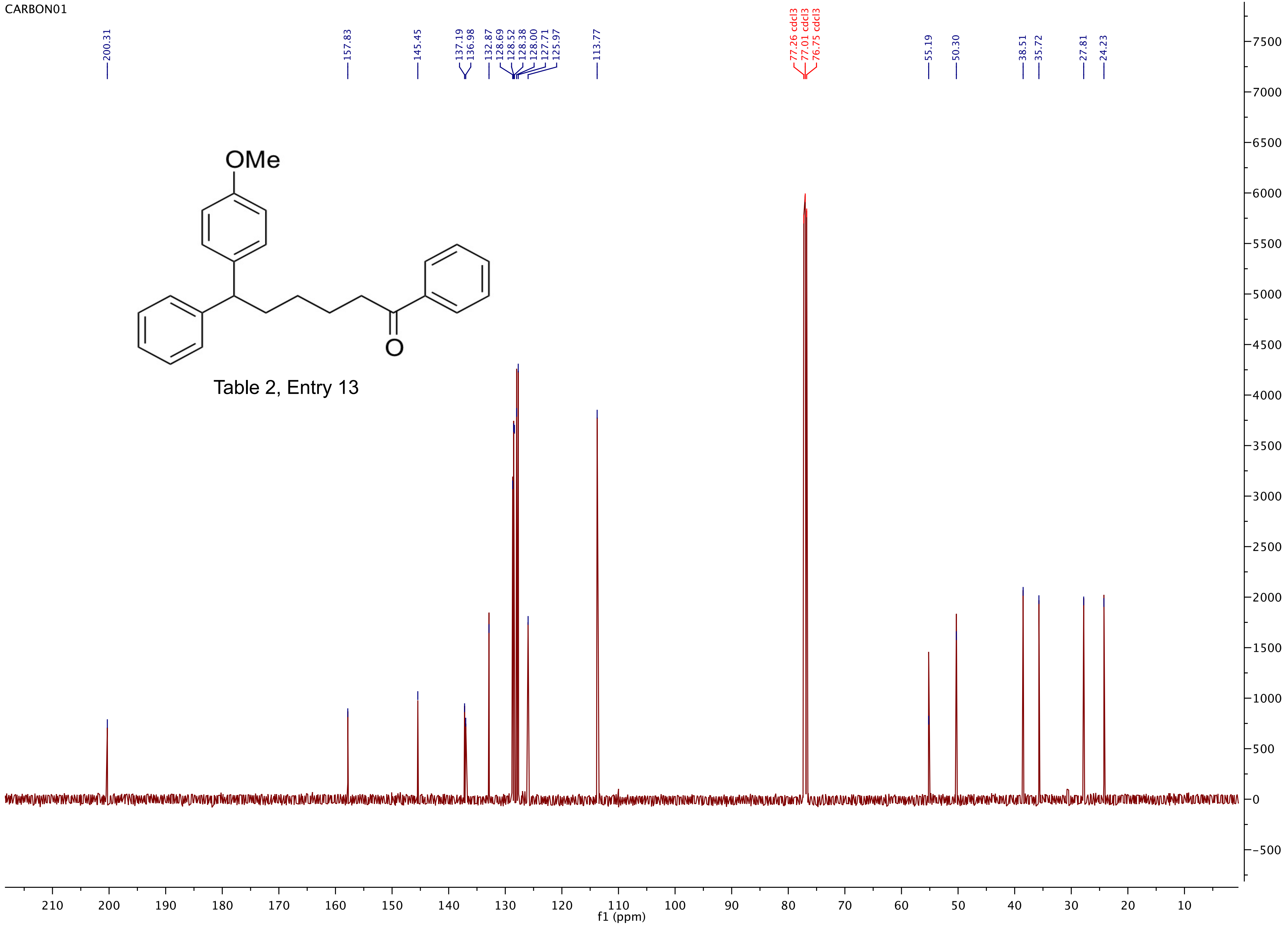
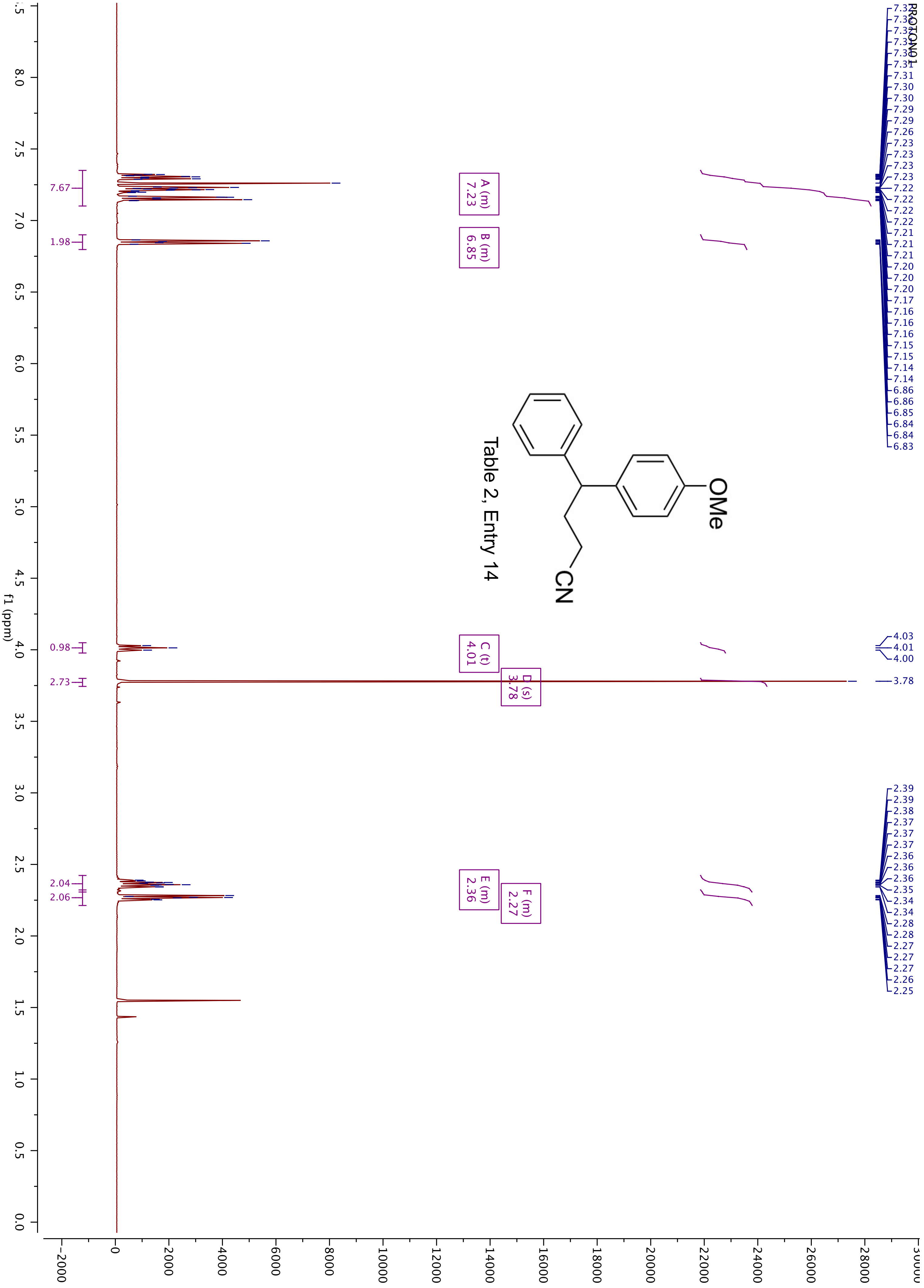
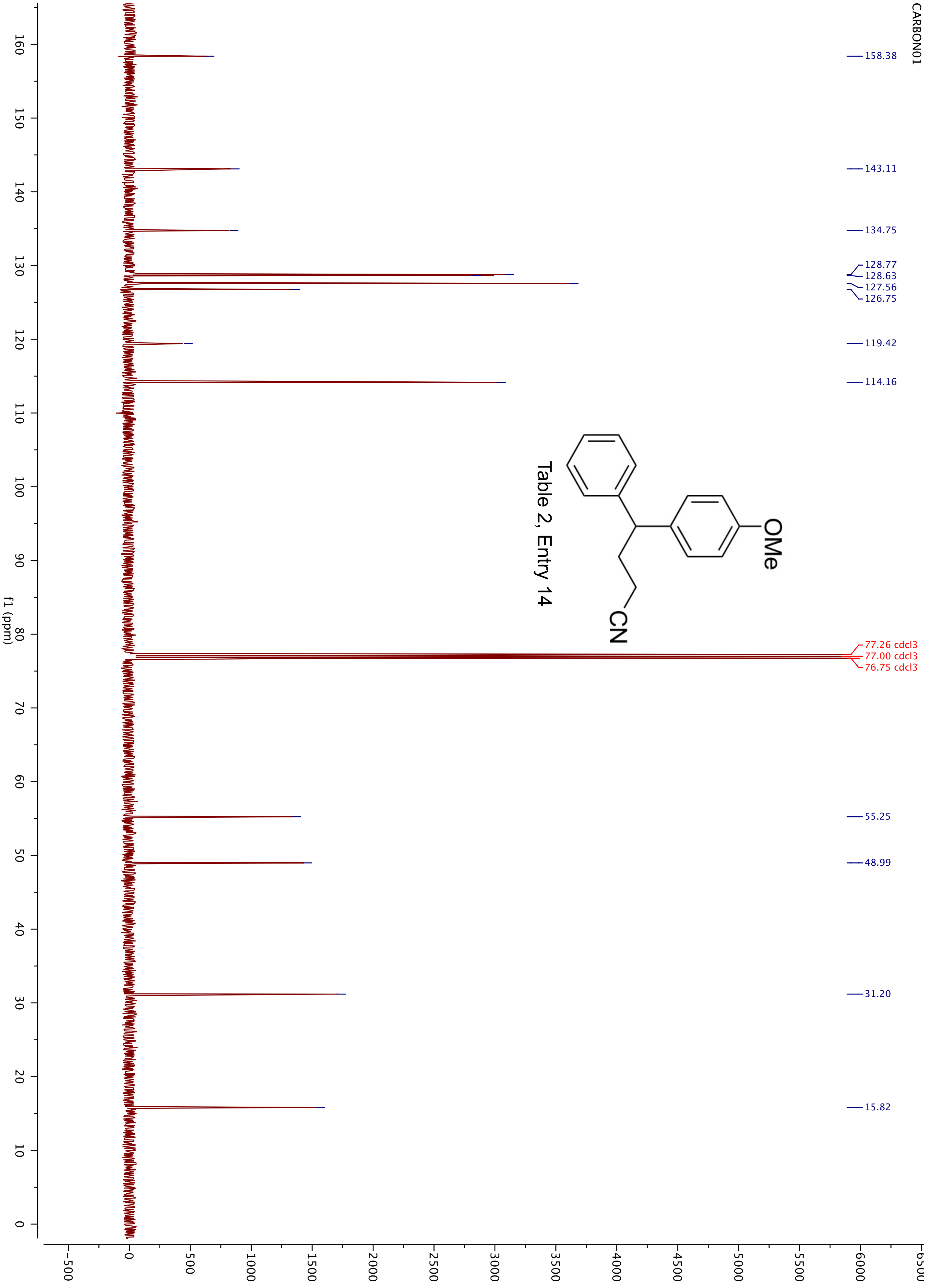


Table 2, Entry 13


PROTON01
Table 2, Entry 14
OMe
CN
A (m) 7.23
B (m) 6.85
C (t) 4.01
D (s) 3.78
E (m) 2.36
F (m) 2.27
7.67
1.98
0.98
2.73
2.04
2.06
7.32
7.32
7.32
7.31
7.31
7.31
7.31
7.30
7.30
7.29
7.29
7.26
7.23
7.23
7.23
7.23
7.22
7.22
7.22
7.22
7.21
7.21
7.21
7.20
7.20
7.20
7.17
7.16
7.16
7.16
7.15
7.15
7.14
7.14
6.86
6.86
6.85
6.84
6.84
6.83
4.03
4.01
4.00
3.78
2.39
2.39
2.38
2.37
2.37
2.37
2.36
2.36
2.36
2.35
2.34
2.34
2.28
2.28
2.27
2.27
2.27
2.26
2.25
f1 (ppm)
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
-2000
0
2000
4000
6000
8000
10000
12000
14000
16000
18000
20000
22000
24000
26000
28000
30000


CARBON01
158.38
143.11
134.75
128.77
128.63
127.56
126.75
119.42
114.16
77.26 cdcl3
77.00 cdcl3
76.75 cdcl3
55.25
48.99
31.20
15.82
OMe
CN
Table 2, Entry 14
f1 (ppm)
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-500
0
500
1000
1500
2000
2500
3000
3500
4000
4500
5000
5500
6000
6500

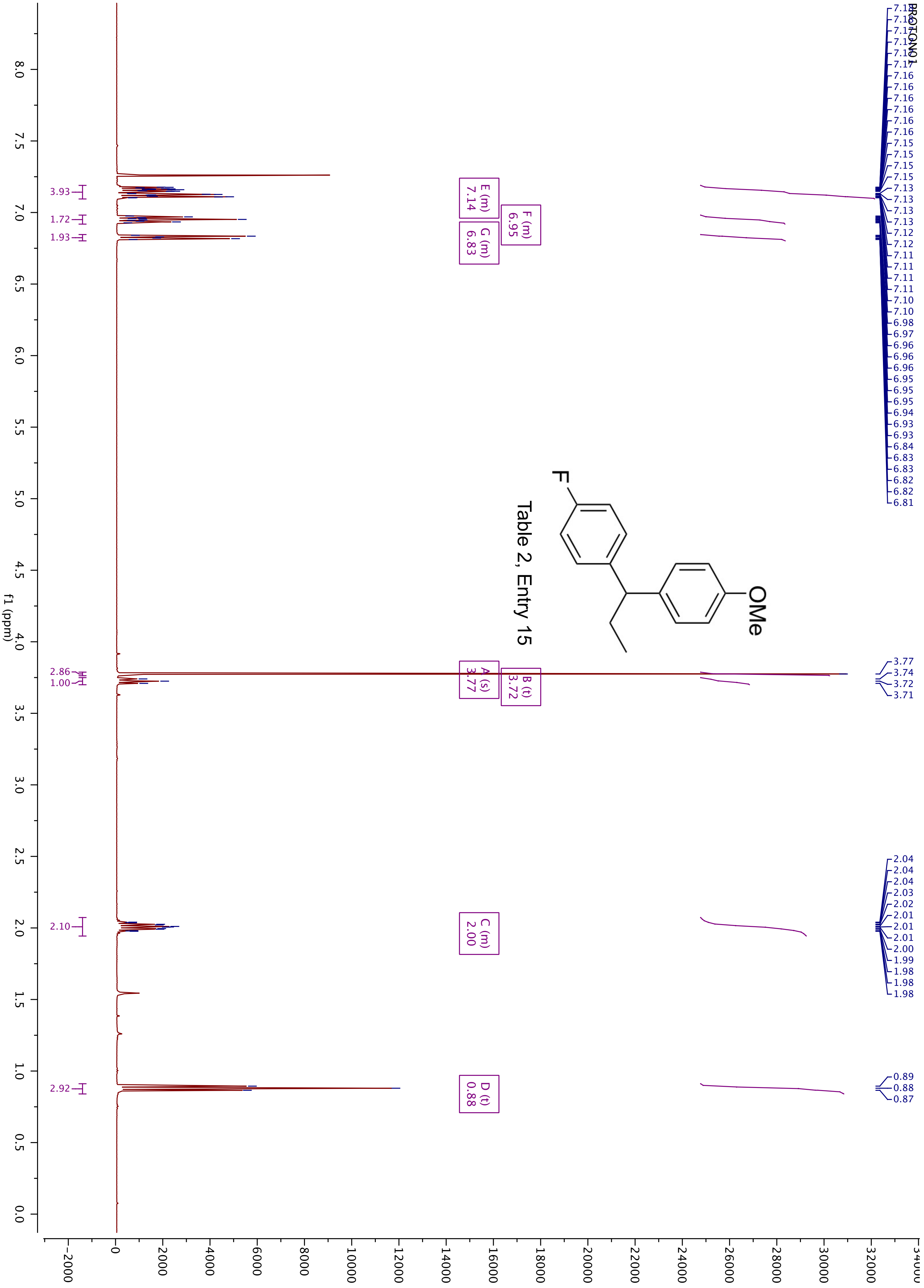
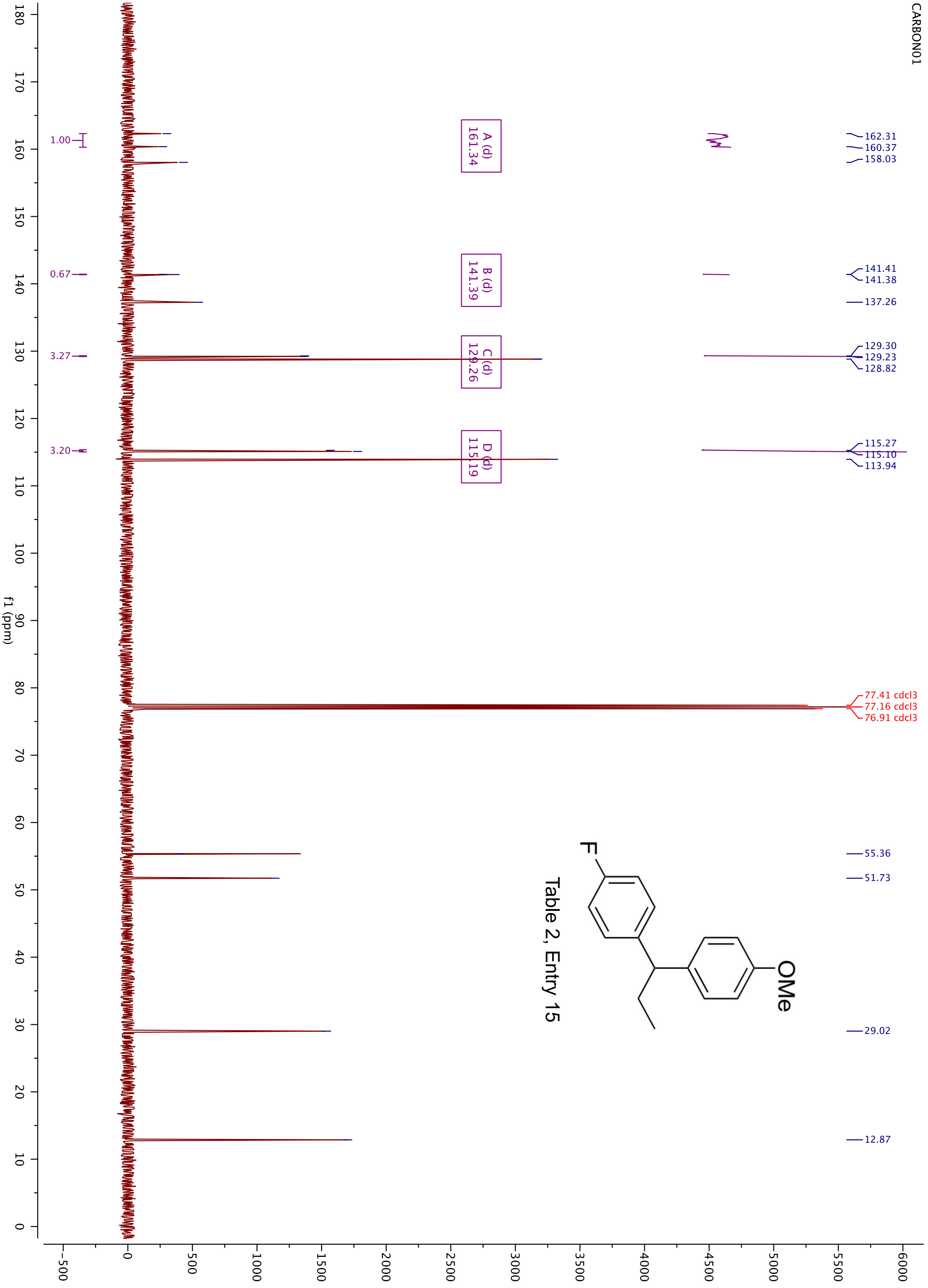


Table 2, Entry 15


CARBON01
Table 2, Entry 15
F
OMe
A (d) 161.34
B (d) 141.39
C (d) 129.26
D (d) 115.19
1.00
0.67
3.27
3.20
162.31
160.37
158.03
141.41
141.38
137.26
129.30
129.23
128.82
115.27
115.10
113.94
77.41 cdcl3
77.16 cdcl3
76.91 cdcl3
55.36
51.73
29.02
12.87
f1 (ppm)
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-500
0
500
1000
1500
2000
2500
3000
3500
4000
4500
5000
5500
6000

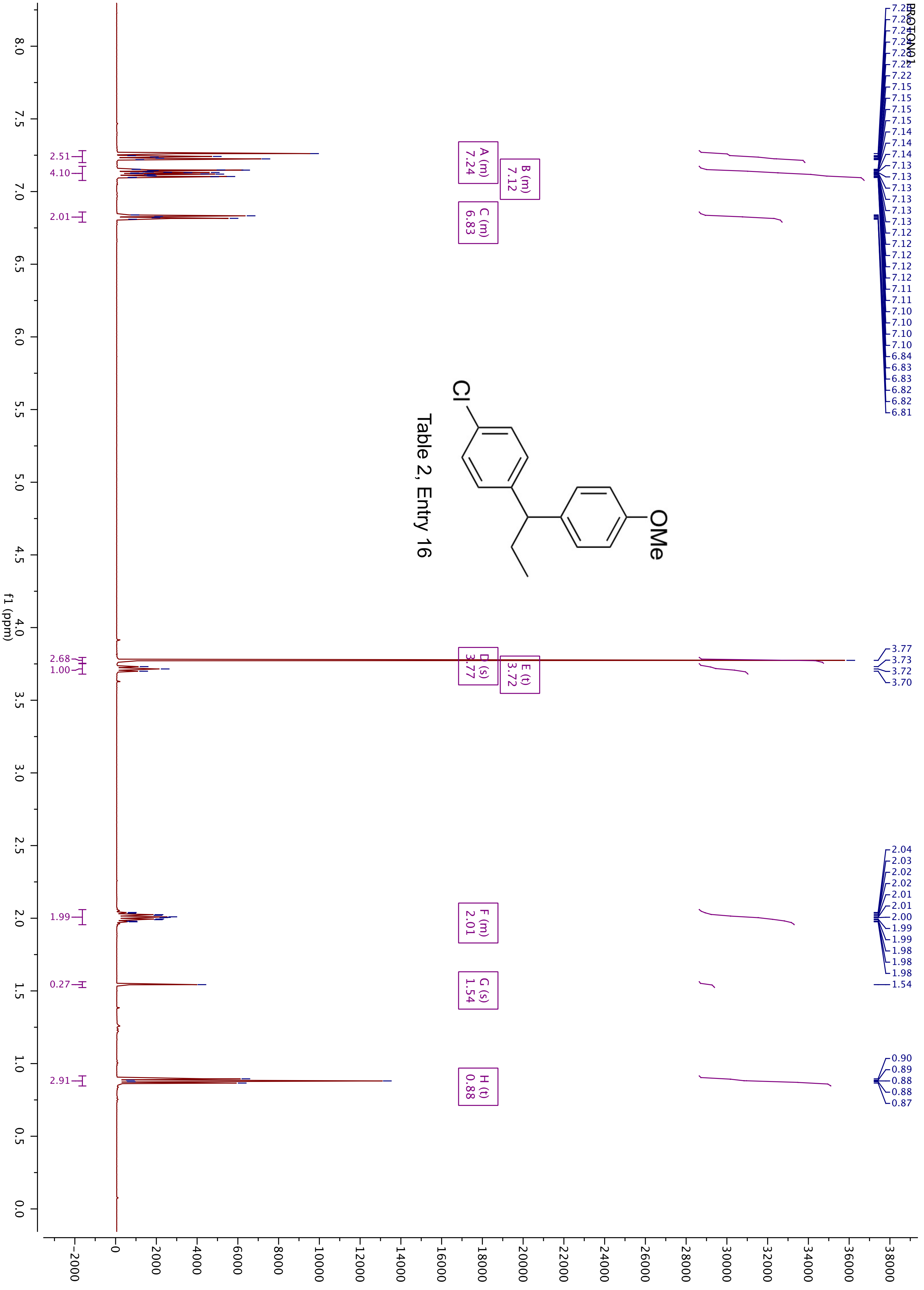


Table 2, Entry 16

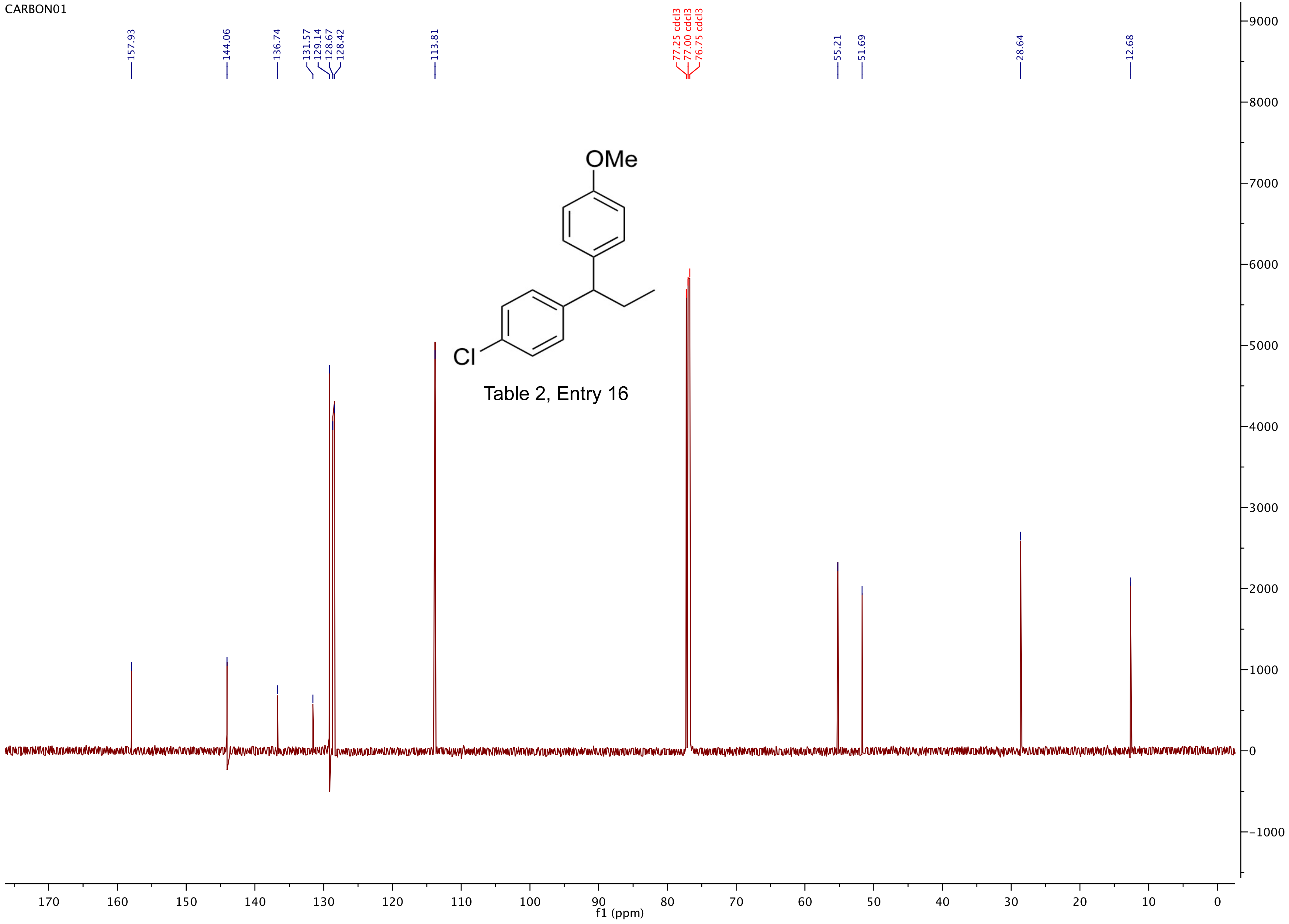


Table 2, Entry 16

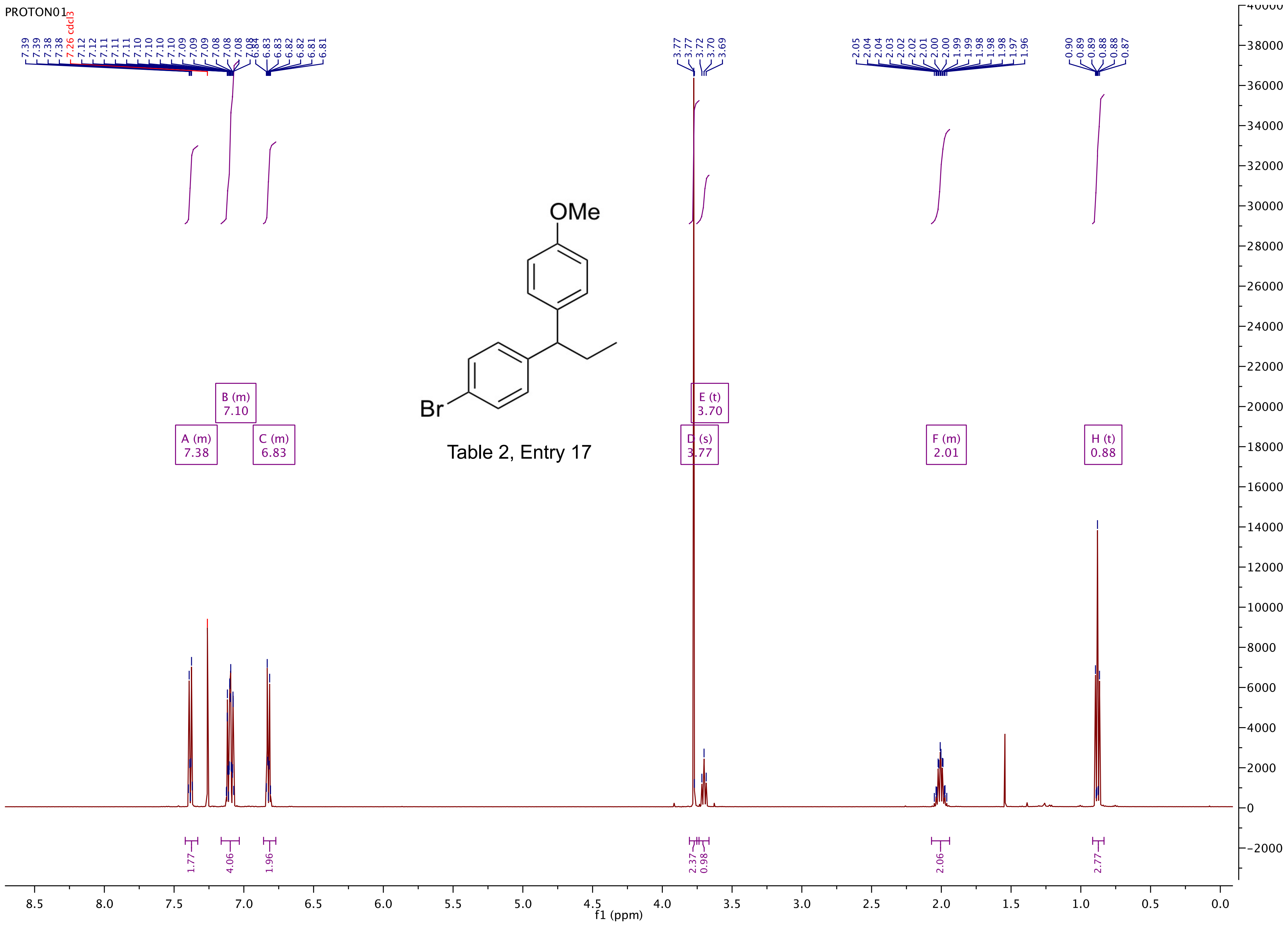


Table 2, Entry 17

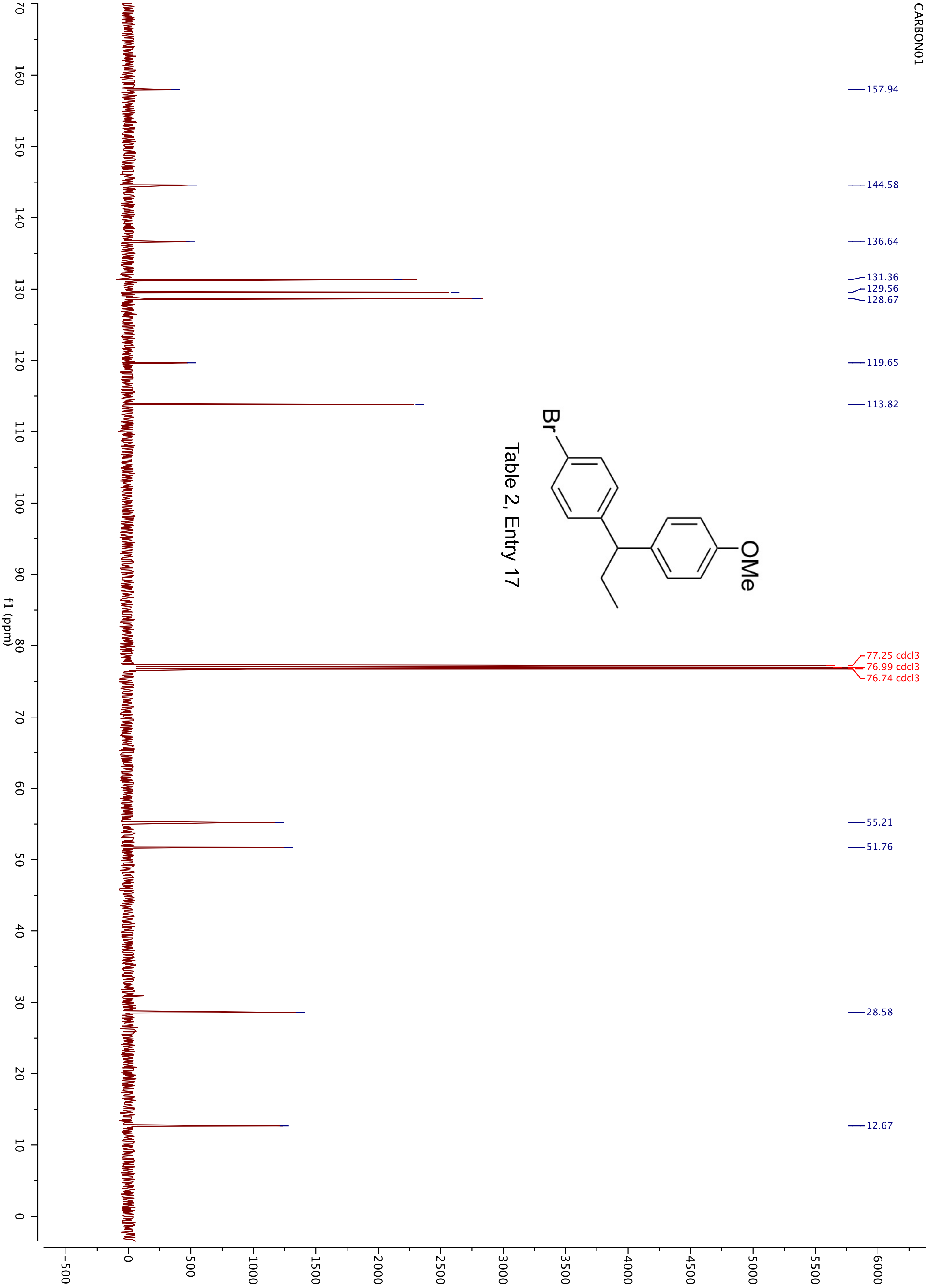
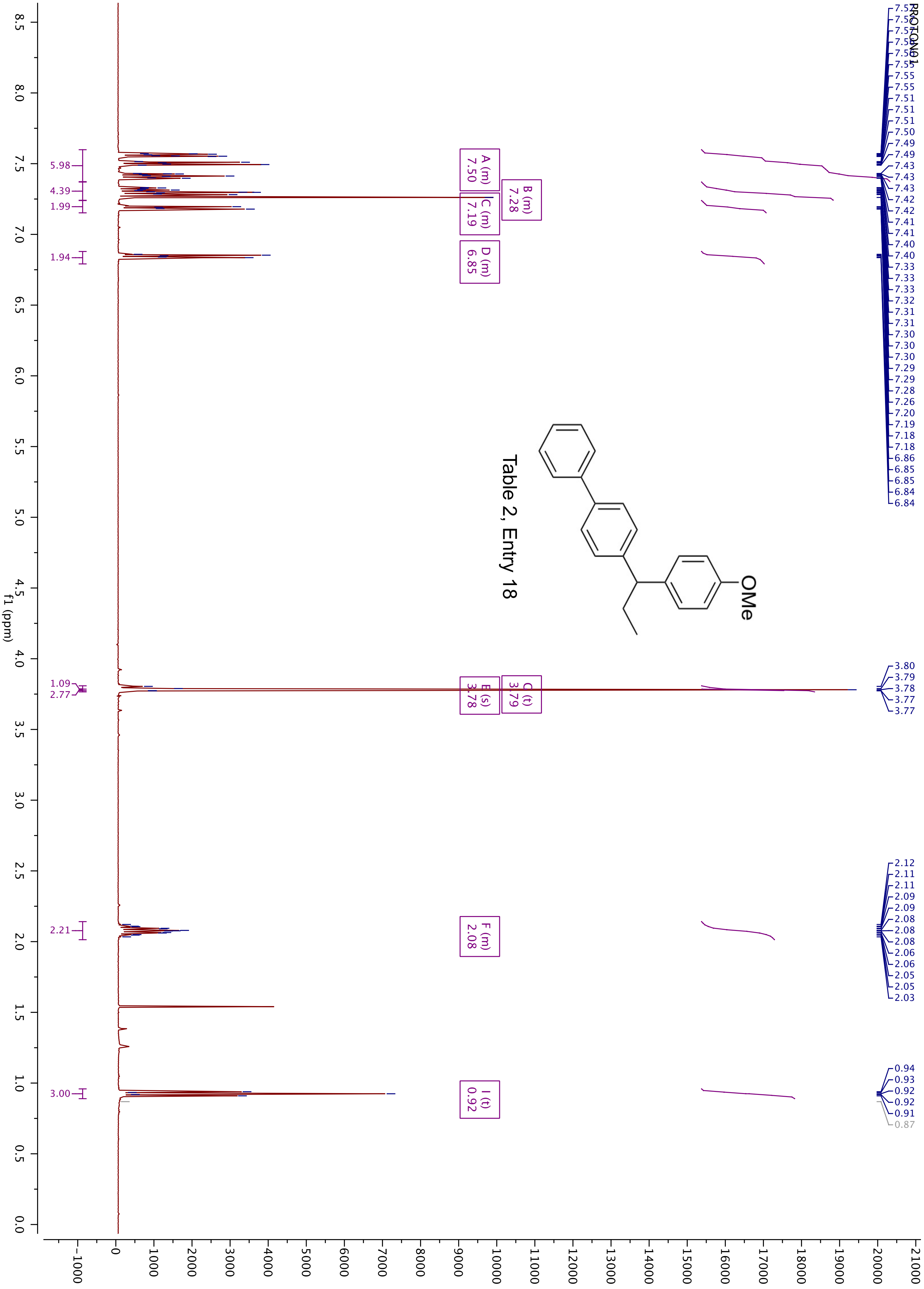
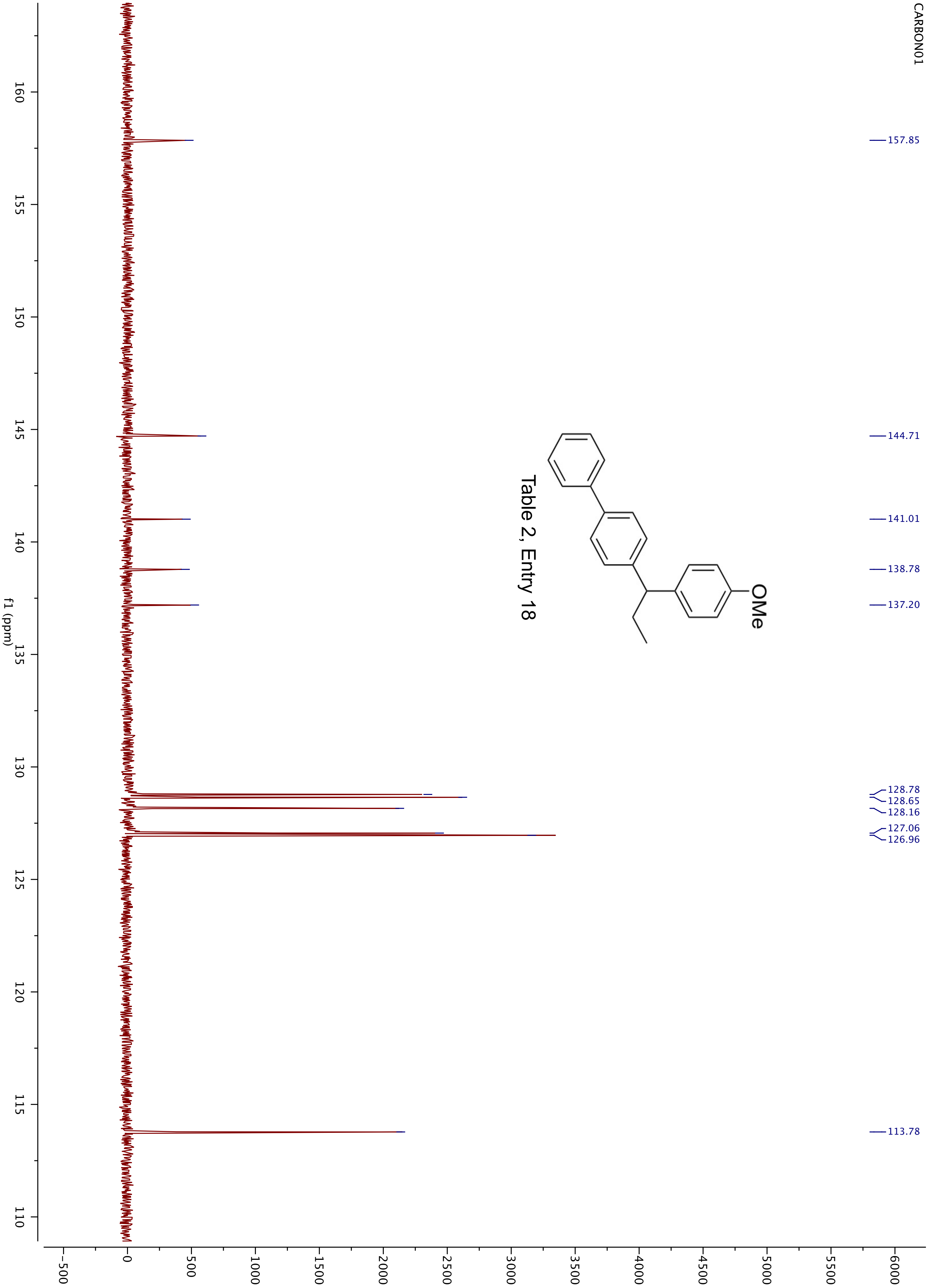
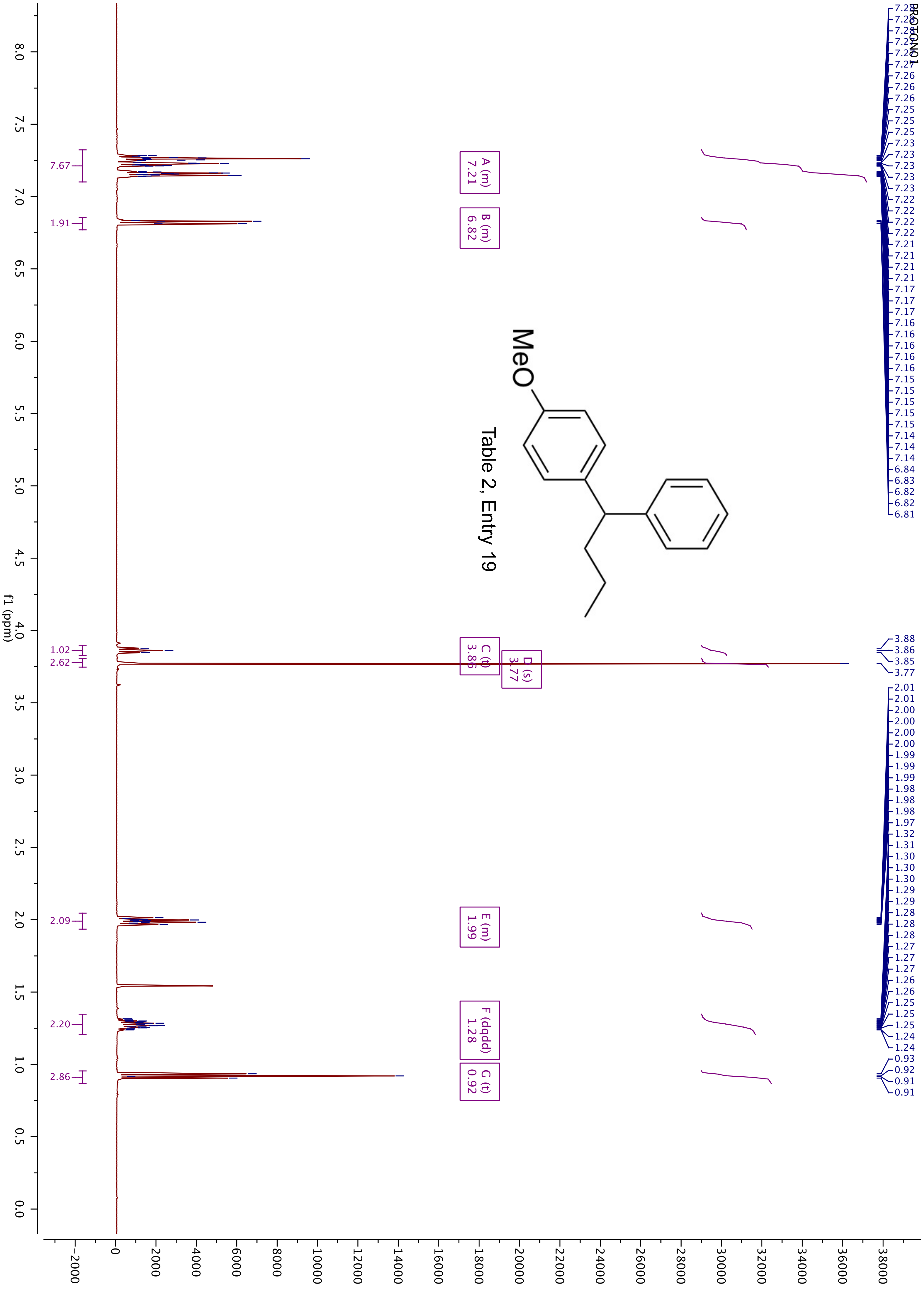
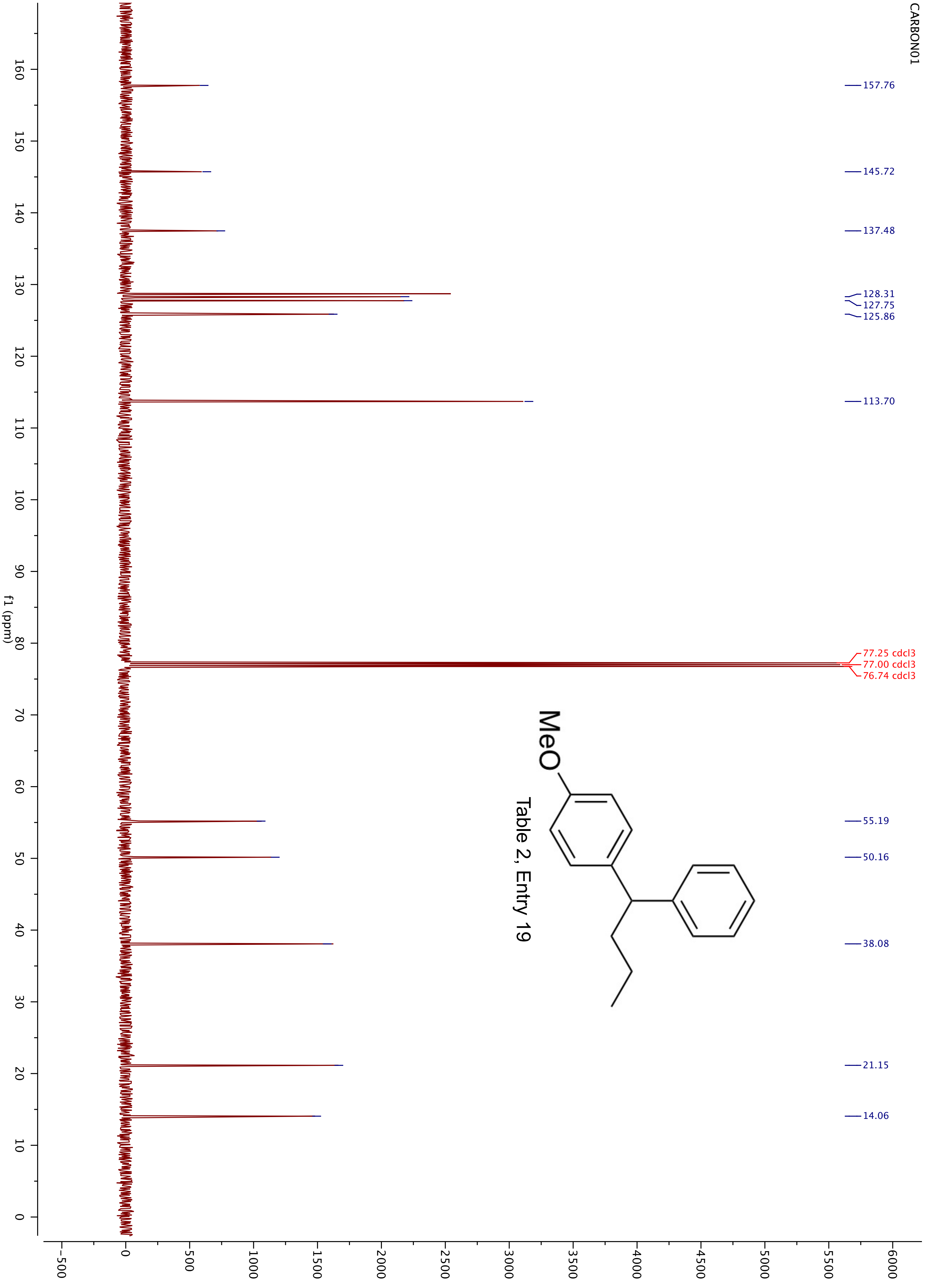


Table 2, Entry 17


PROTON01
Table 2, Entry 18
OMe
A (m) 7.50
B (m) 7.28
C (m) 7.19
D (m) 6.85
C (t) 3.79
E (s) 3.78
F (m) 2.08
I (t) 0.92
5.98
4.39
1.99
1.94
1.09
2.77
2.21
3.00
7.52
7.51
7.51
7.50
7.50
7.55
7.55
7.55
7.51
7.51
7.51
7.50
7.49
7.49
7.43
7.43
7.43
7.42
7.42
7.41
7.41
7.40
7.40
7.33
7.33
7.33
7.32
7.31
7.31
7.30
7.30
7.30
7.29
7.29
7.28
7.26
7.20
7.19
7.18
7.18
6.86
6.85
6.85
6.84
6.84
3.80
3.79
3.78
3.77
3.77
2.12
2.11
2.11
2.09
2.09
2.08
2.08
2.08
2.06
2.06
2.05
2.05
2.03
0.94
0.93
0.92
0.92
0.91
0.87
f1 (ppm)
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
-1000
0
1000
2000
3000
4000
5000
6000
7000
8000
9000
10000
11000
12000
13000
14000
15000
16000
17000
18000
19000
20000
21000


CARBON01
Table 2, Entry 18
OMe
157.85
144.71
141.01
138.78
137.20
128.78
128.65
128.16
127.06
126.96
113.78
f1 (ppm)
160
155
150
145
140
135
130
125
120
115
110
-500
0
500
1000
1500
2000
2500
3000
3500
4000
4500
5000
5500
6000


PROTON01
7.28
7.28
7.28
7.27
7.27
7.27
7.26
7.26
7.26
7.25
7.25
7.25
7.23
7.23
7.23
7.23
7.23
7.22
7.22
7.22
7.22
7.21
7.21
7.21
7.21
7.17
7.17
7.17
7.16
7.16
7.16
7.16
7.16
7.15
7.15
7.15
7.15
7.15
7.14
7.14
7.14
6.84
6.83
6.82
6.82
6.81
3.88
3.86
3.85
3.77
2.01
2.01
2.00
2.00
2.00
2.00
1.99
1.99
1.99
1.98
1.98
1.98
1.97
1.32
1.31
1.30
1.30
1.30
1.29
1.29
1.28
1.28
1.28
1.27
1.27
1.27
1.26
1.26
1.25
1.25
1.25
1.24
1.24
0.93
0.92
0.91
0.91
MeO
Table 2, Entry 19
A (m) 7.21
B (m) 6.82
C (t) 3.85
D (s) 3.77
E (m) 1.99
F (dqdd) 1.28
G (t) 0.92
7.67
1.91
1.02
2.62
2.09
2.20
2.86
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)
-2000
0
2000
4000
6000
8000
10000
12000
14000
16000
18000
20000
22000
24000
26000
28000
30000
32000
34000
36000
38000


CARBON01
157.76
145.72
137.48
128.31
127.75
125.86
113.70
77.25 cdcl3
77.00 cdcl3
76.74 cdcl3
55.19
50.16
38.08
21.15
14.06
MeO
Table 2, Entry 19
f1 (ppm)
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-500
0
500
1000
1500
2000
2500
3000
3500
4000
4500
5000
5500
6000

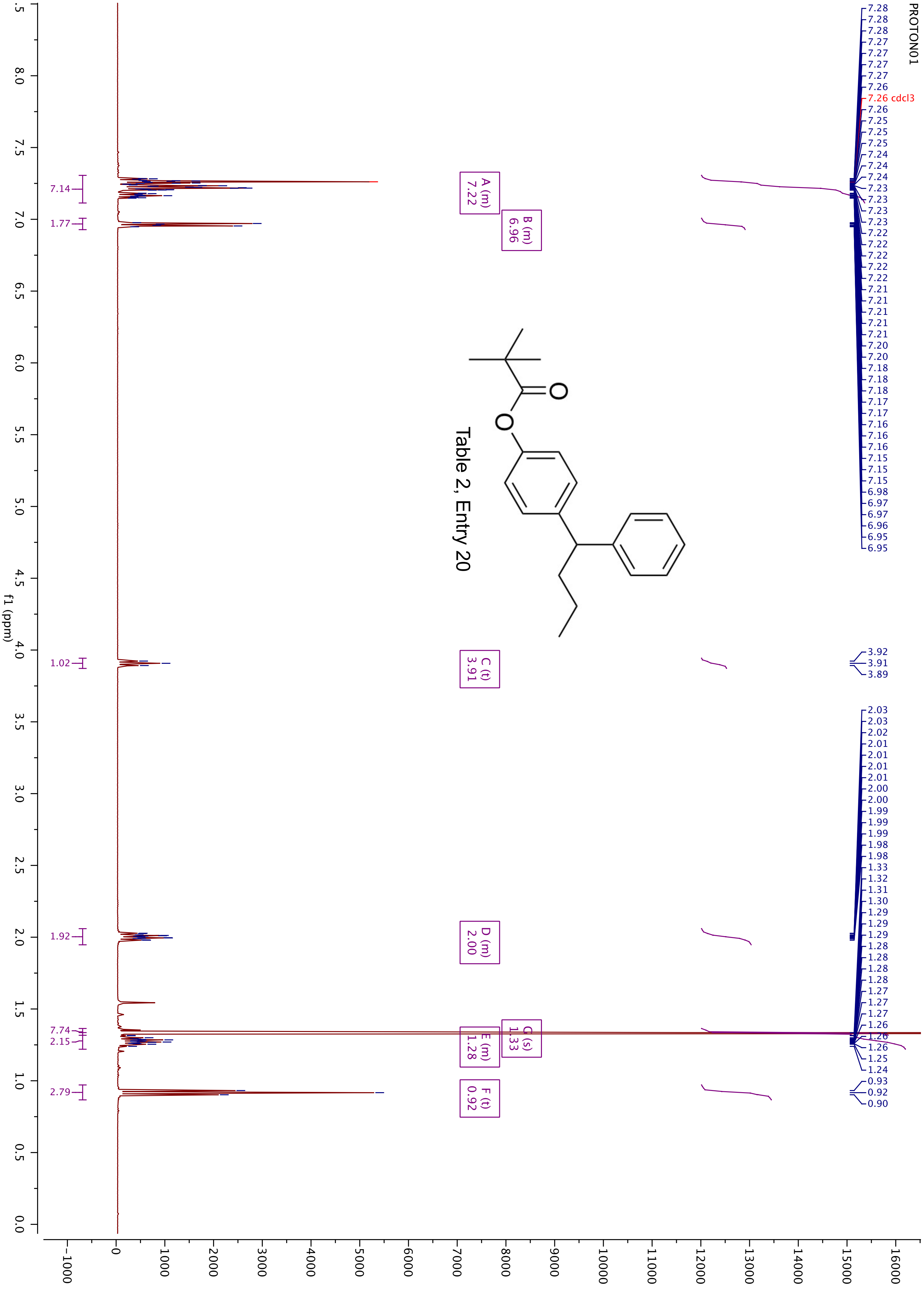
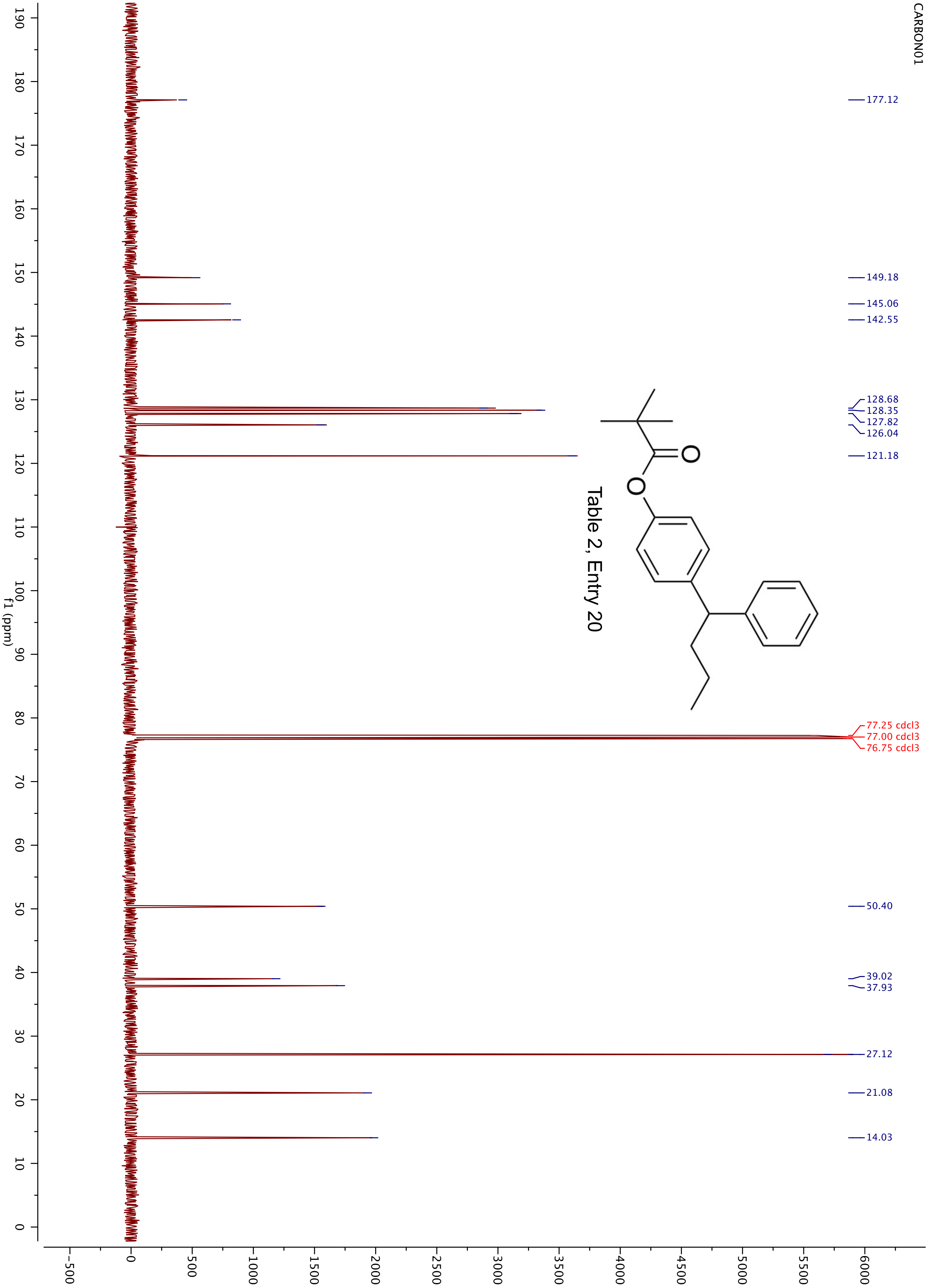
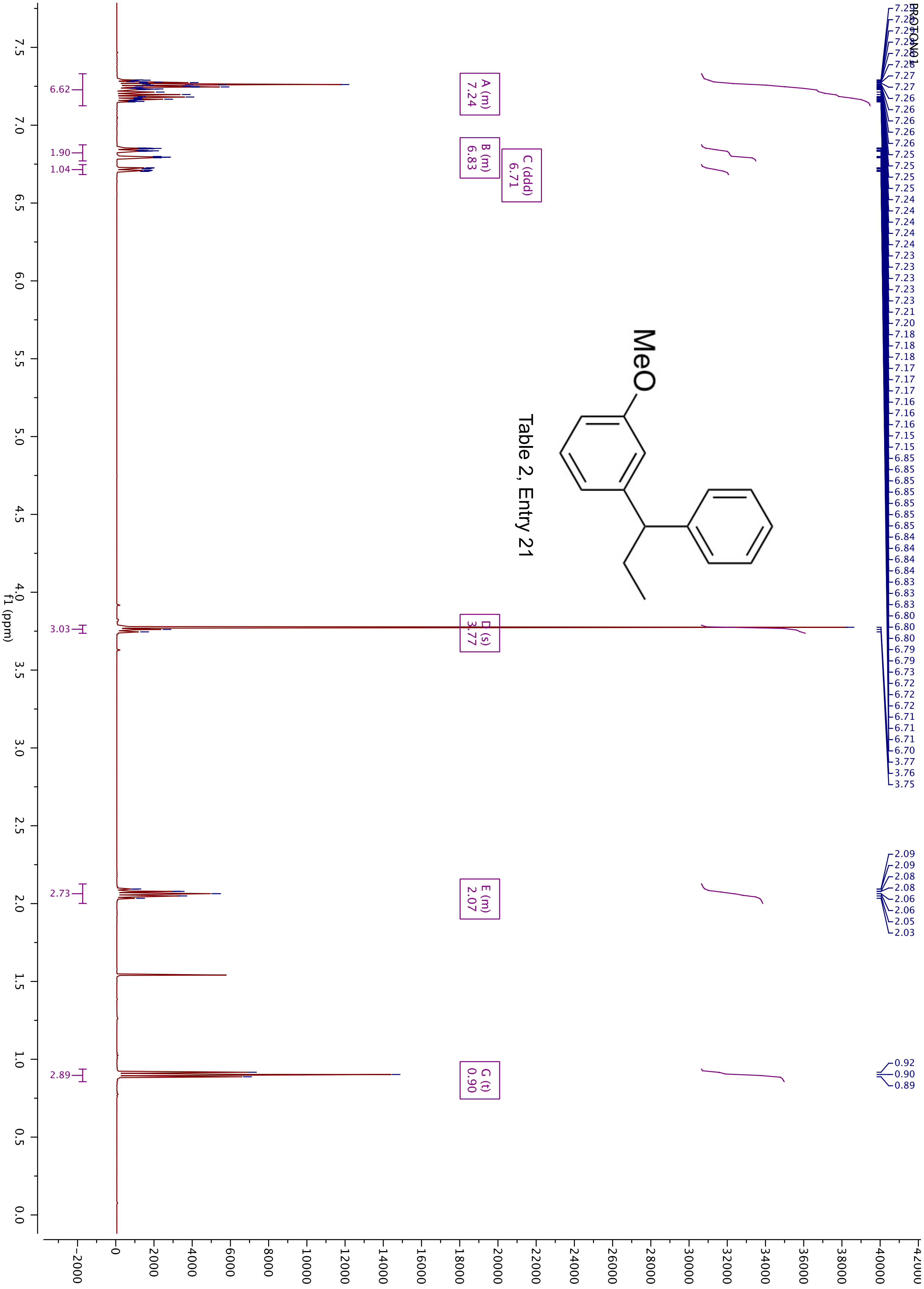


Table 2, Entry 20


CARBON01
Table 2, Entry 20
177.12
149.18
145.06
142.55
128.68
128.35
127.82
126.04
121.18
77.25 cdcl3
77.00 cdcl3
76.75 cdcl3
50.40
39.02
37.93
27.12
21.08
14.03
f1 (ppm)
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-500
0
500
1000
1500
2000
2500
3000
3500
4000
4500
5000
5500
6000


PROTON01
Table 2, Entry 21
MeO
A (m) 7.24
B (m) 6.83
C (ddd) 6.71
D (s) 3.77
E (m) 2.07
G (t) 0.90
6.62
1.90
1.04
3.03
2.73
2.89
7.29 7.29 7.29 7.28 7.28 7.28 7.27 7.27 7.26 7.26 7.26 7.26 7.26 7.25 7.25 7.25 7.25 7.24 7.24 7.24 7.24 7.24 7.23 7.23 7.23 7.23 7.23 7.21 7.20 7.18 7.18 7.18 7.17 7.17 7.17 7.16 7.16 7.16 7.15 7.15 6.85 6.85 6.85 6.85 6.85 6.85 6.85 6.84 6.84 6.84 6.84 6.83 6.83 6.83 6.80 6.80 6.80 6.79 6.79 6.73 6.72 6.72 6.72 6.71 6.71 6.71 6.70 3.77 3.76 3.75
2.09 2.09 2.08 2.08 2.06 2.06 2.05 2.03
0.92 0.90 0.89
f1 (ppm)
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
-2000 0 2000 4000 6000 8000 10000 12000 14000 16000 18000 20000 22000 24000 26000 28000 30000 32000 34000 36000 38000 40000 42000

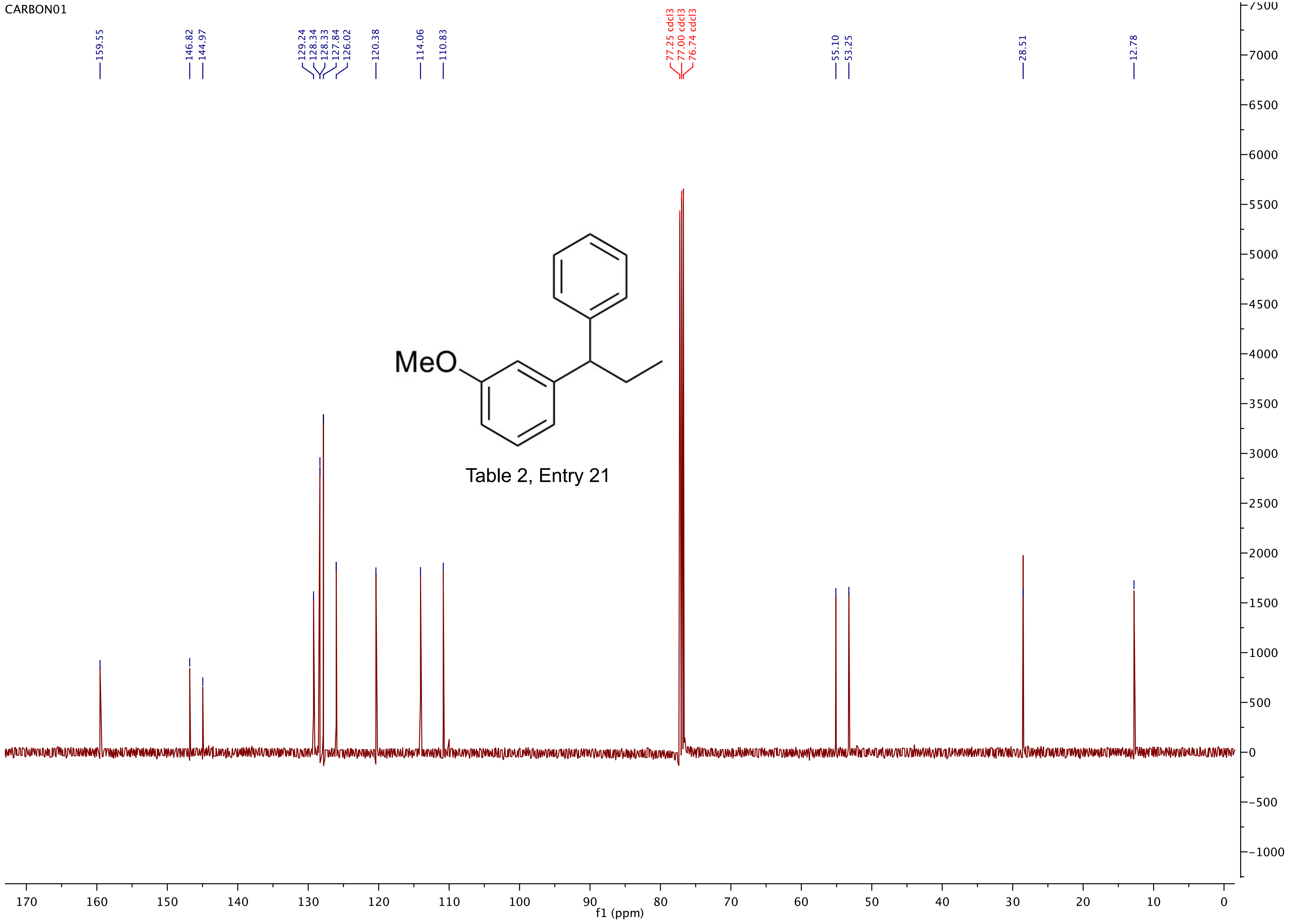


Table 2, Entry 21

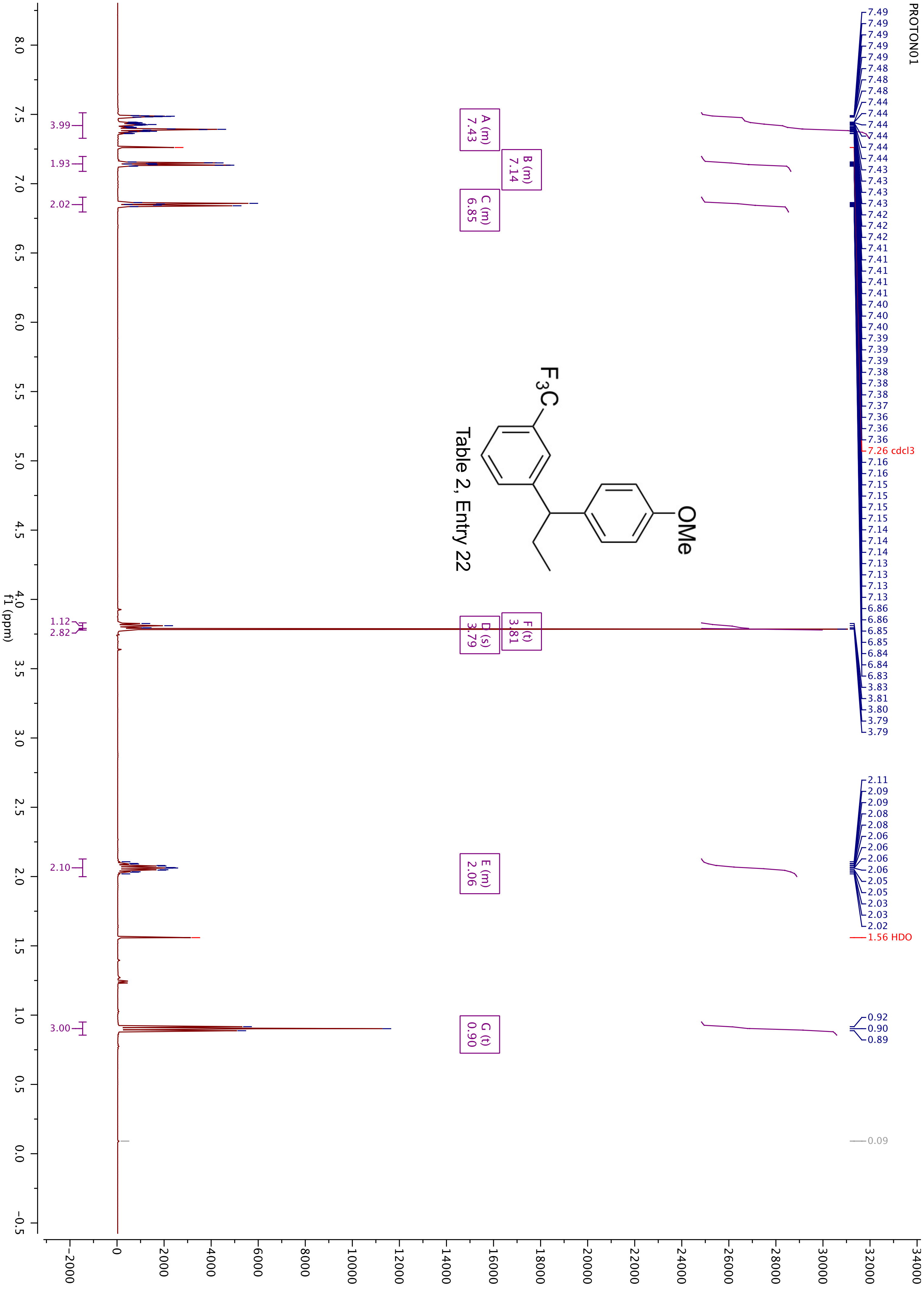


Table 2, Entry 22

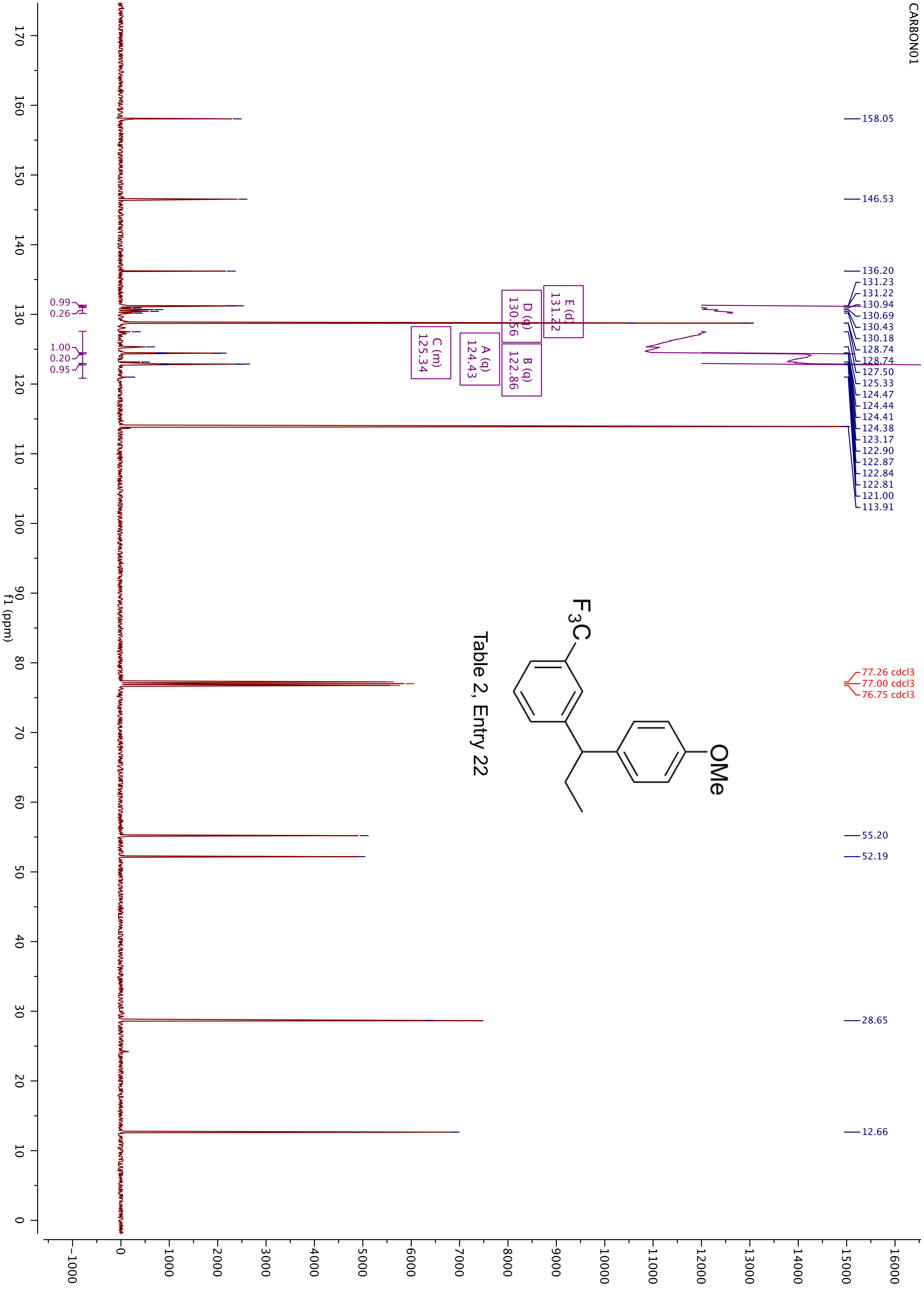


Table 2, Entry 22

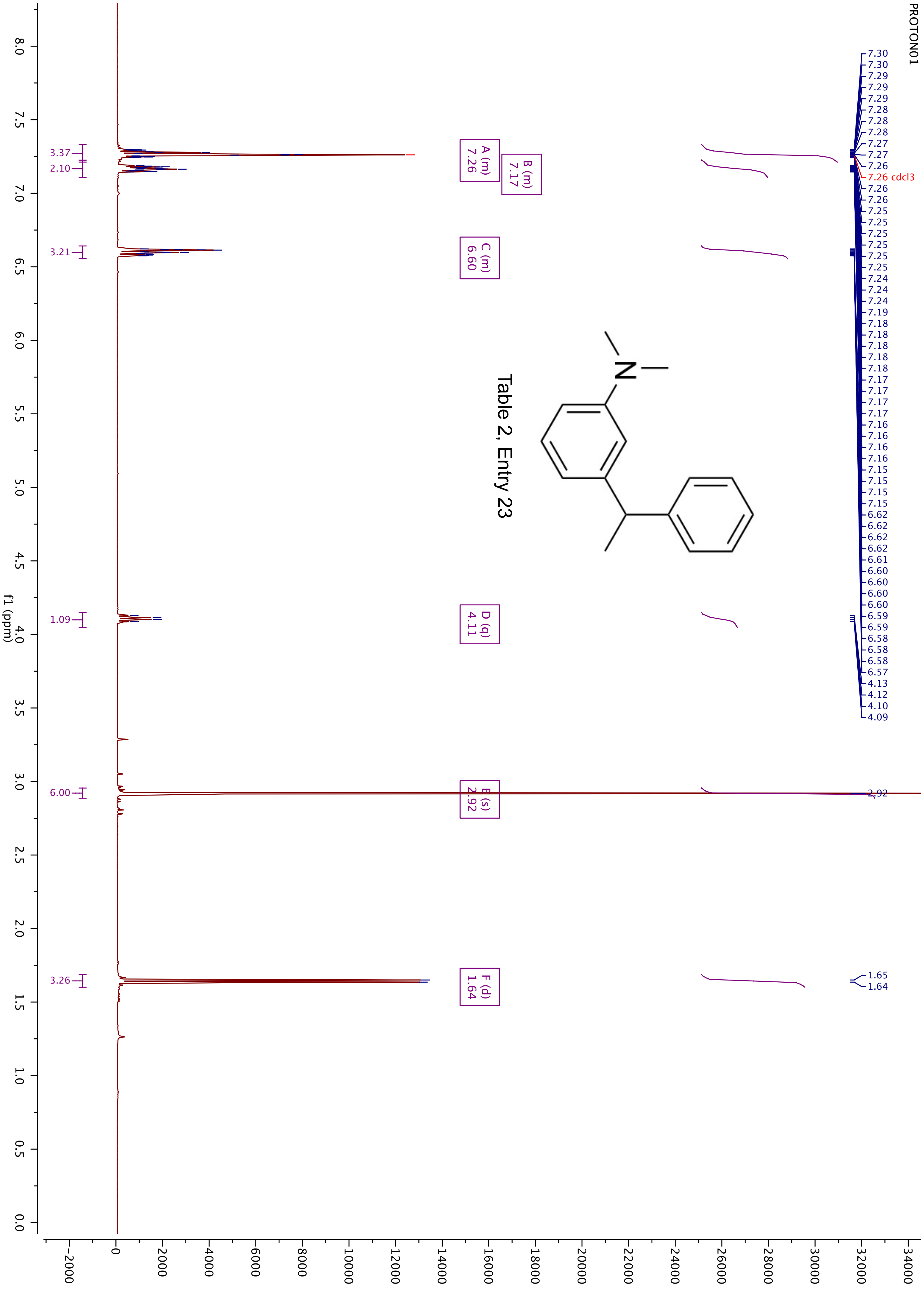
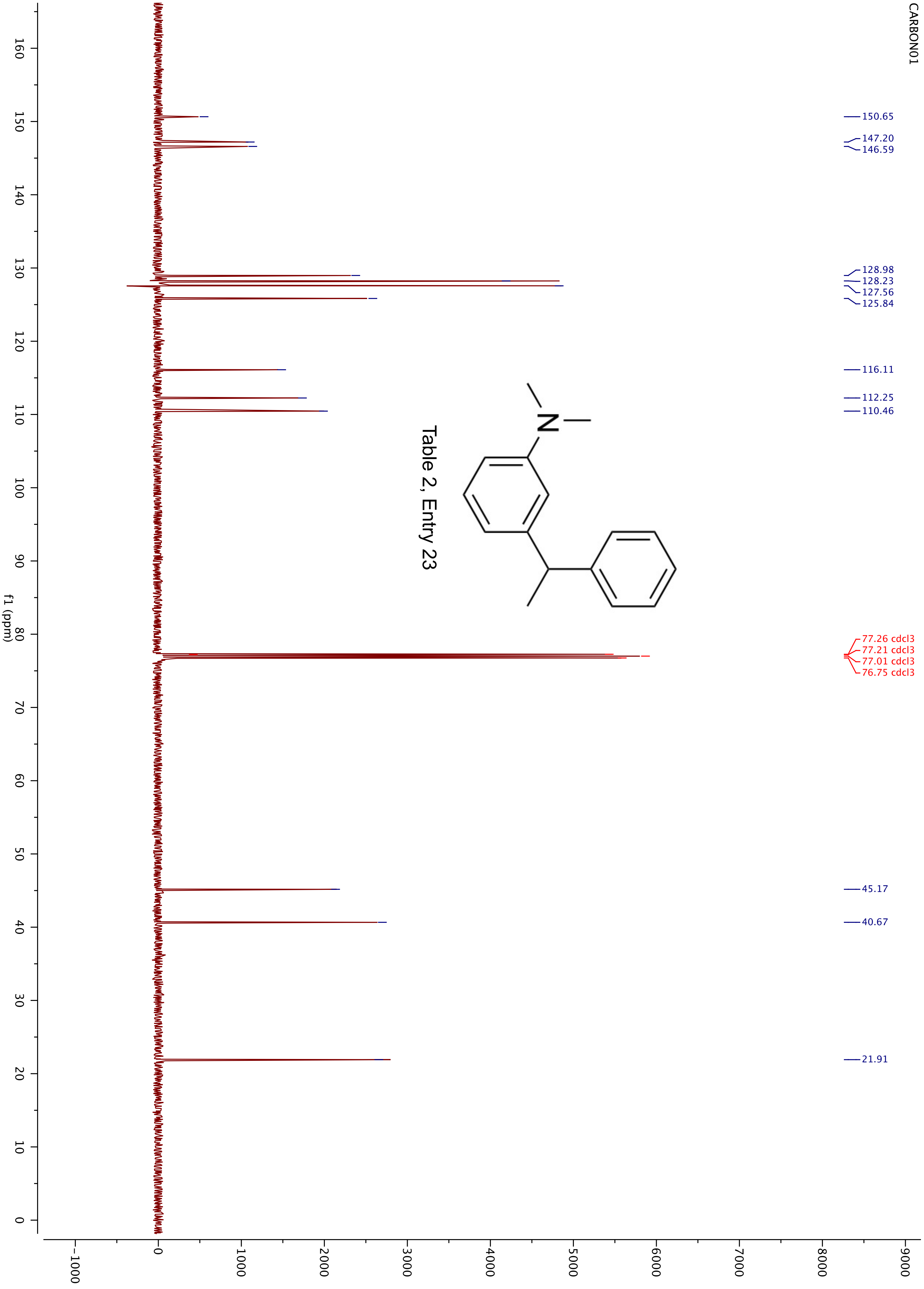


Table 2, Entry 23


CARBON01
Table 2, Entry 23
N
150.65
147.20
146.59
128.98
128.23
127.56
125.84
116.11
112.25
110.46
77.26 cdcl3
77.21 cdcl3
77.01 cdcl3
76.75 cdcl3
45.17
40.67
21.91
f1 (ppm)
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-1000
0
1000
2000
3000
4000
5000
6000
7000
8000
9000

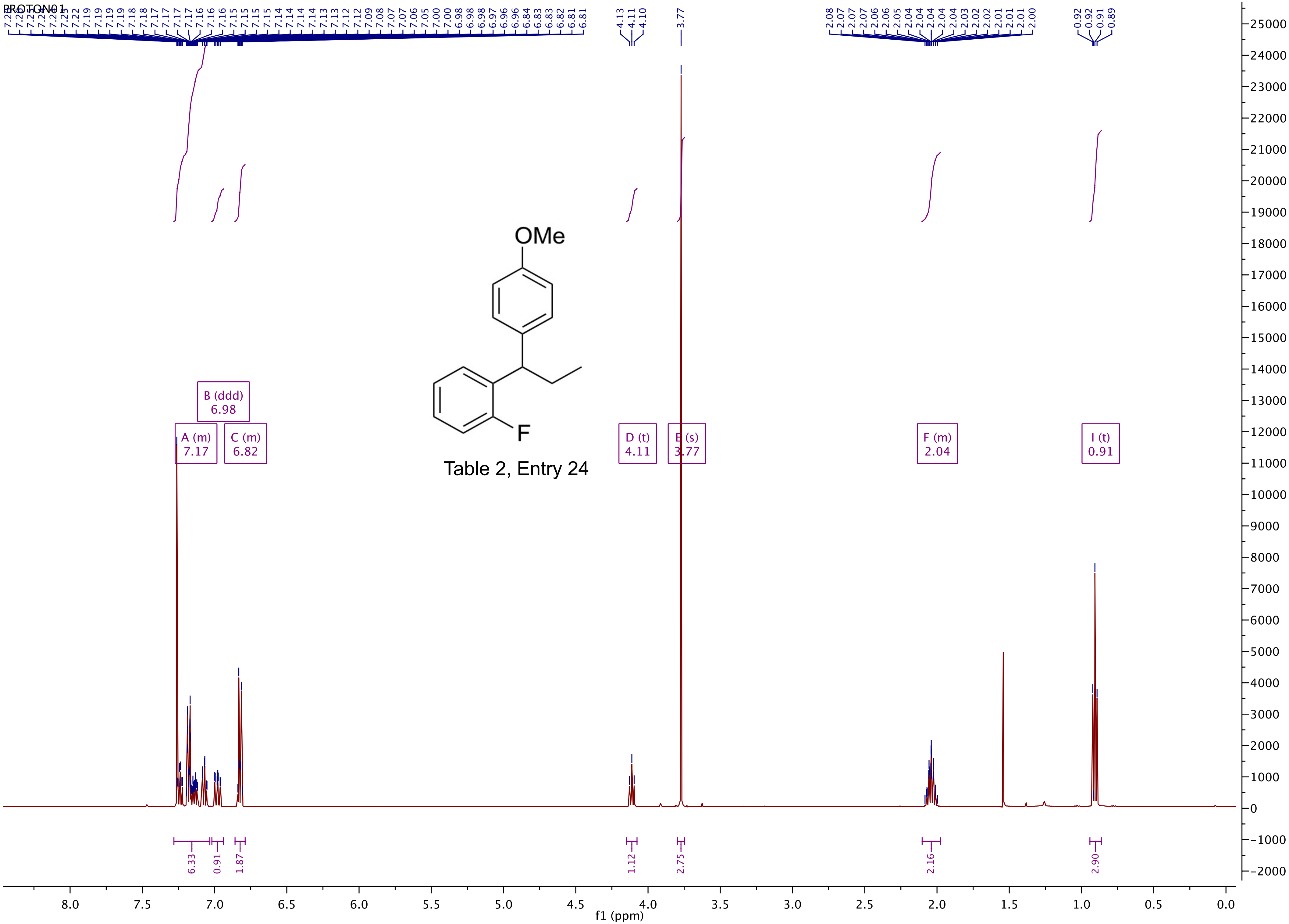


Table 2, Entry 24

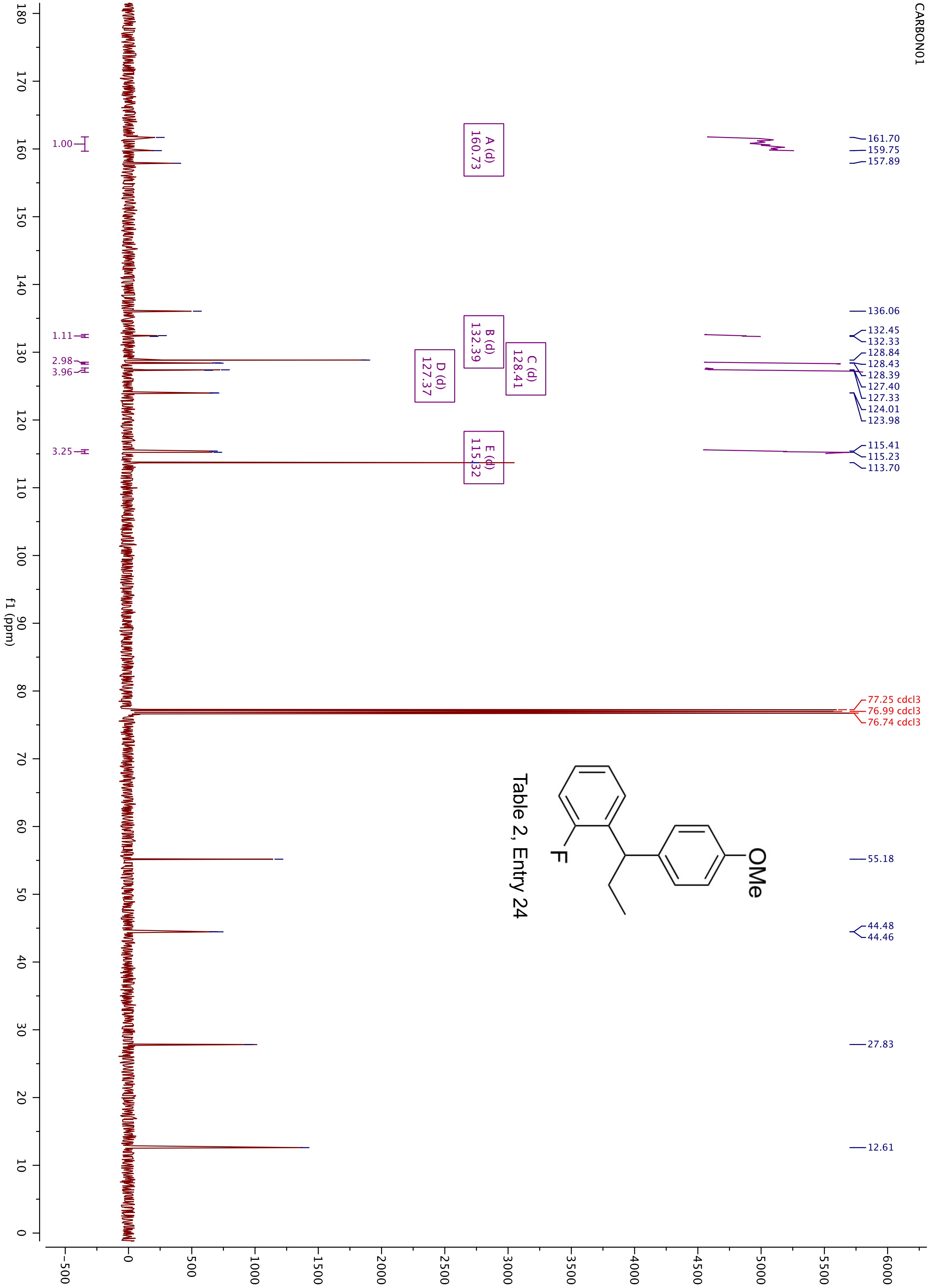
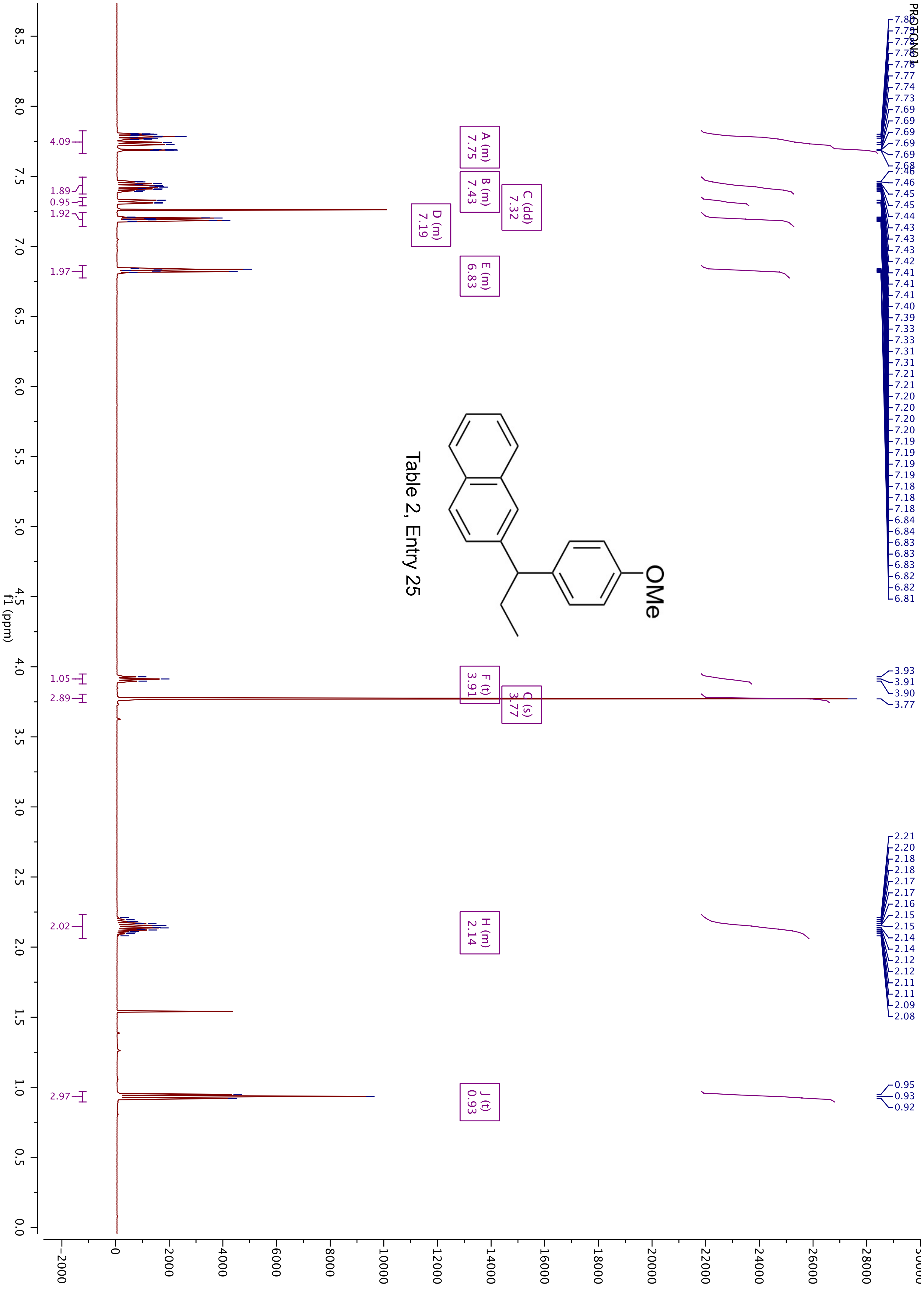
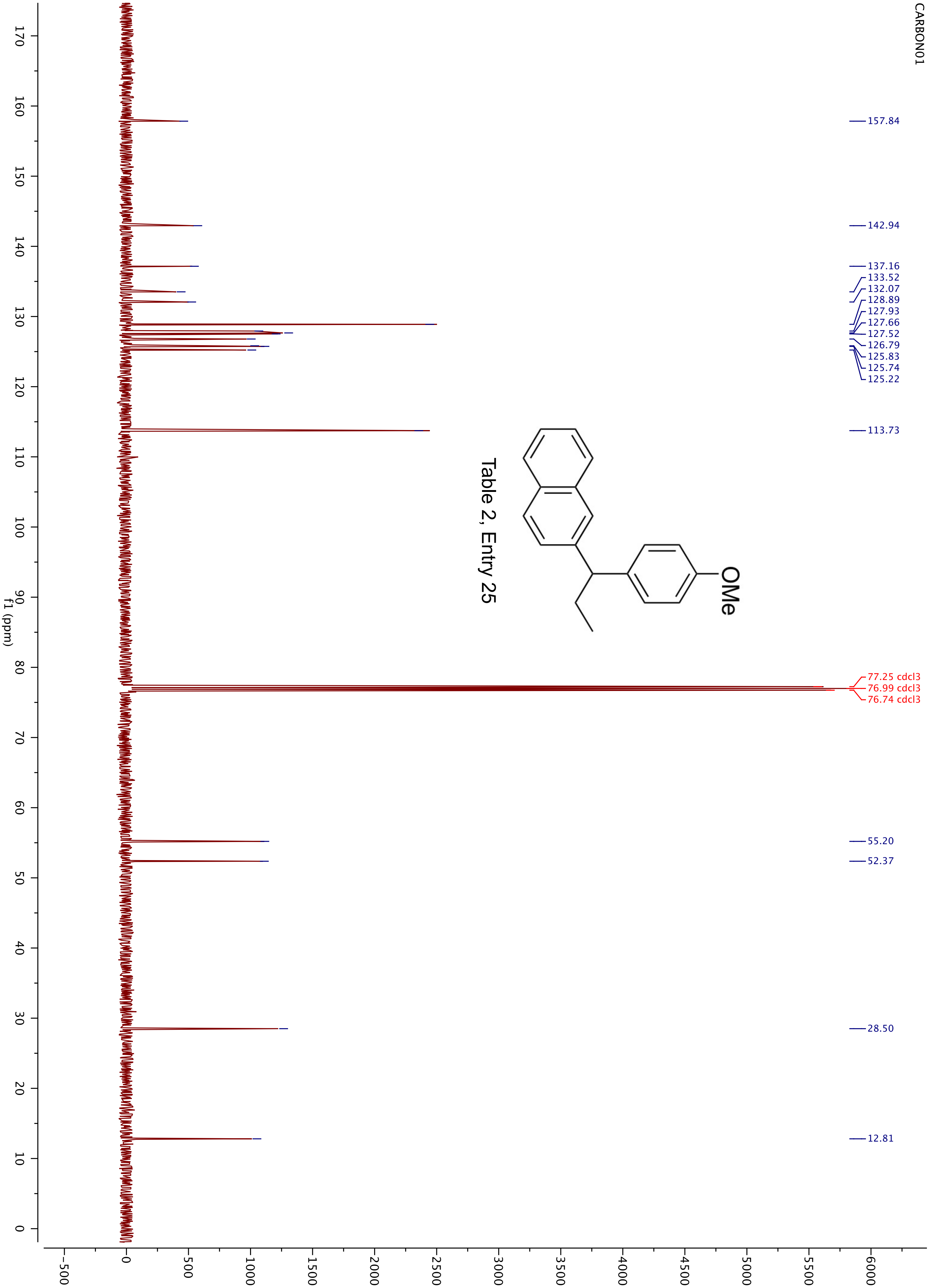
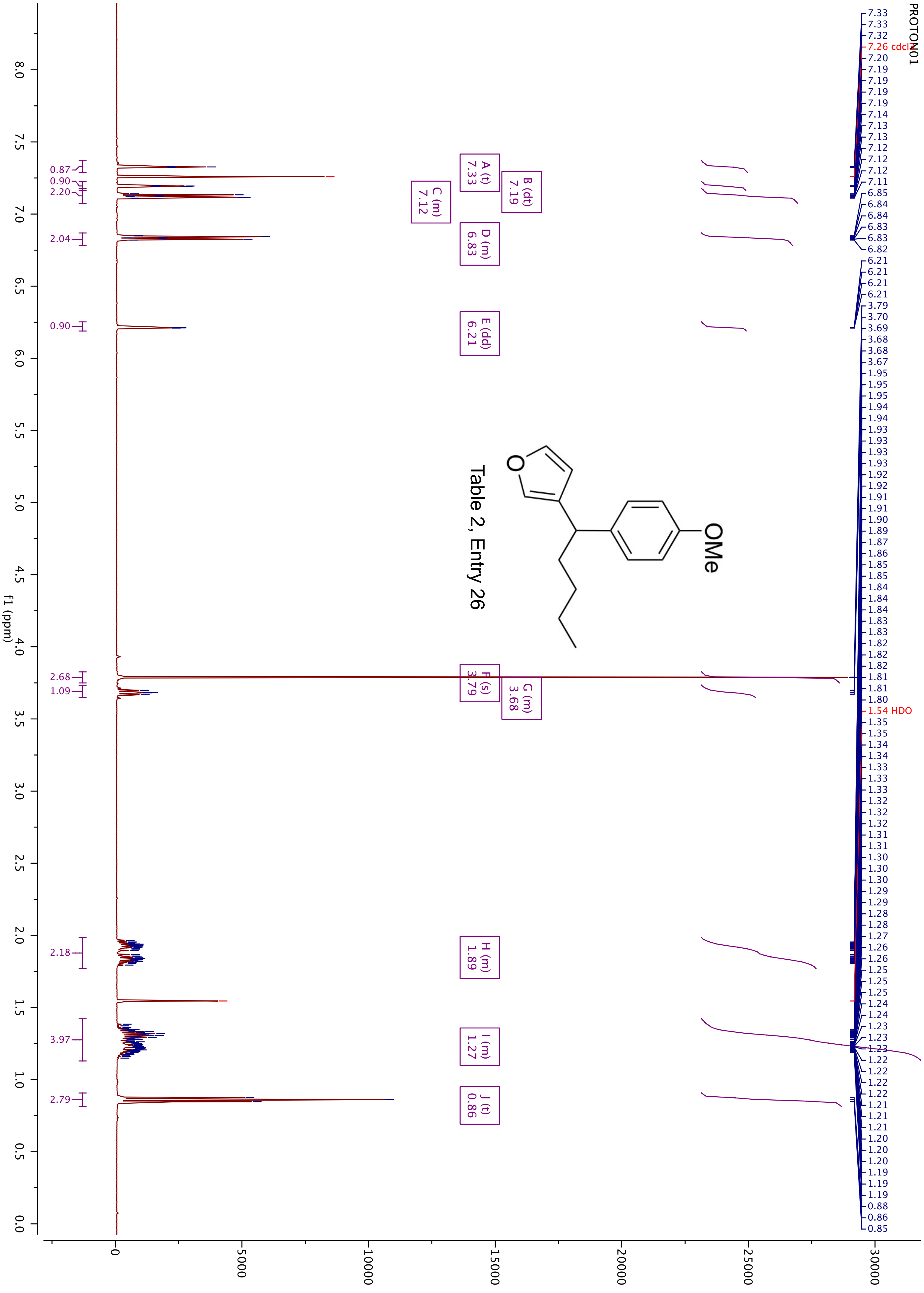
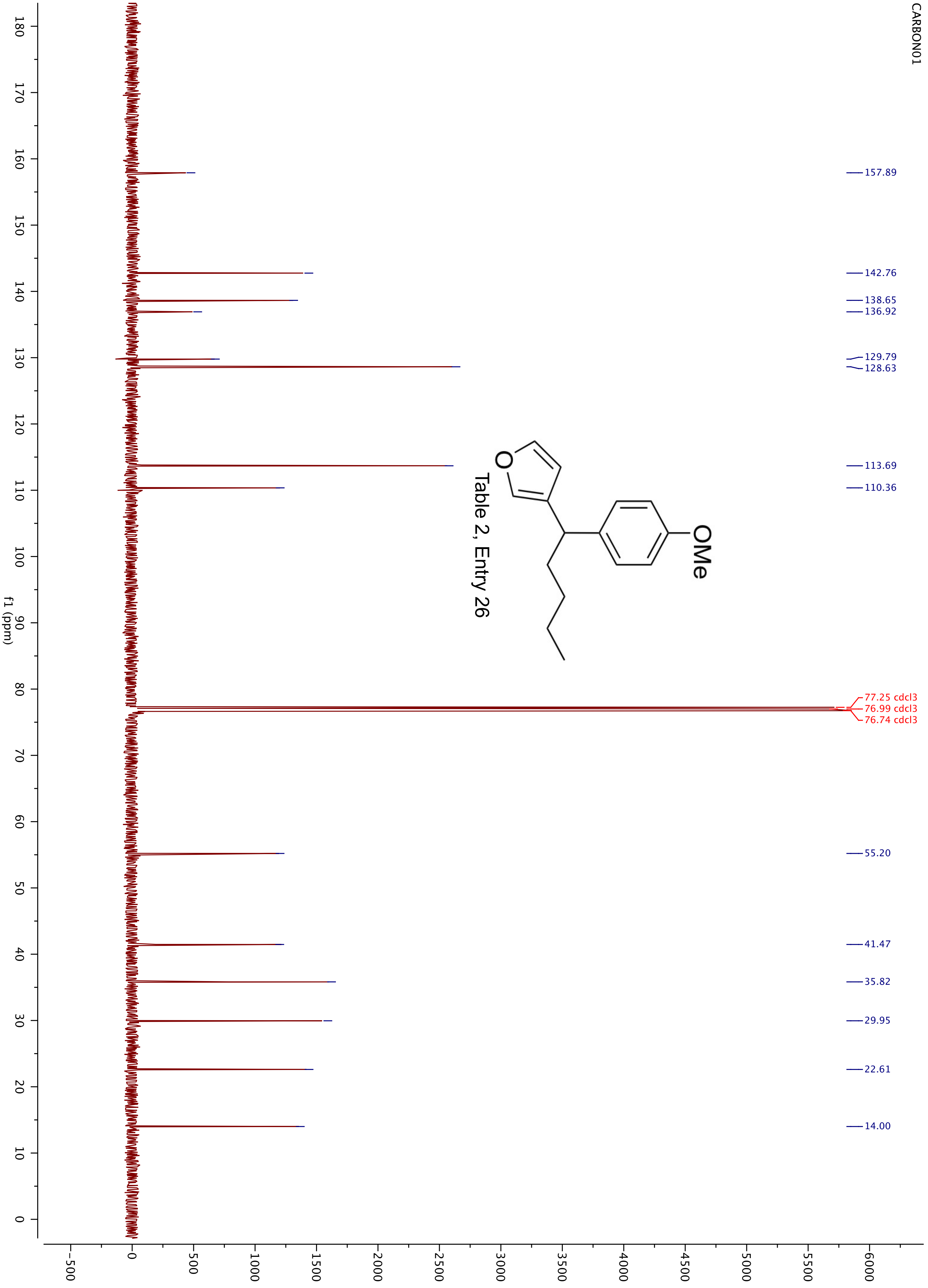


Table 2, Entry 24


PROTON01
Table 2, Entry 25
OMe
A (m) 7.75
B (m) 7.43
C (dd) 7.32
D (m) 7.19
E (m) 6.83
F (t) 3.91
G (s) 3.77
H (m) 2.14
J (t) 0.93
4.09
1.89
0.95
1.92
1.97
1.05
2.89
2.02
2.97
7.80 7.79 7.79 7.78 7.78 7.77 7.74 7.73 7.69 7.69 7.69 7.69 7.69 7.68 7.46 7.46 7.45 7.45 7.44 7.43 7.43 7.43 7.42 7.41 7.41 7.41 7.40 7.39 7.33 7.33 7.31 7.31 7.21 7.21 7.20 7.20 7.20 7.20 7.19 7.19 7.19 7.19 7.18 7.18 7.18 6.84 6.84 6.83 6.83 6.83 6.82 6.82 6.81
3.93 3.91 3.90 3.77
2.21 2.20 2.18 2.18 2.17 2.17 2.16 2.15 2.15 2.14 2.14 2.12 2.12 2.11 2.11 2.09 2.08
0.95 0.93 0.92
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)
-2000 0 2000 4000 6000 8000 10000 12000 14000 16000 18000 20000 22000 24000 26000 28000


CARBON01
Table 2, Entry 25
OMe
157.84
142.94
137.16
133.52
132.07
128.89
127.93
127.66
127.52
126.79
125.83
125.74
125.22
113.73
77.25 cdcl3
76.99 cdcl3
76.74 cdcl3
55.20
52.37
28.50
12.81
f1 (ppm)
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-500
0
500
1000
1500
2000
2500
3000
3500
4000
4500
5000
5500
6000

PROTON01
Table 2, Entry 26
OMe
O
A (t) 7.33
B (dt) 7.19
C (m) 7.12
D (m) 6.83
E (dd) 6.21
F (s) 3.79
G (m) 3.68
H (m) 1.89
I (m) 1.27
J (t) 0.86
0.87
0.90
2.20
2.04
0.90
2.68
1.09
2.18
3.97
2.79
7.33
7.33
7.32
7.26 cdcl3
7.20
7.19
7.19
7.19
7.19
7.14
7.13
7.13
7.12
7.12
7.12
7.11
6.85
6.84
6.84
6.83
6.83
6.82
6.21
6.21
6.21
6.21
3.79
3.70
3.69
3.68
3.68
3.67
1.95
1.95
1.95
1.94
1.94
1.93
1.93
1.93
1.93
1.92
1.92
1.91
1.91
1.90
1.89
1.87
1.86
1.85
1.85
1.84
1.84
1.84
1.83
1.83
1.82
1.82
1.82
1.81
1.81
1.80
1.54 HDO
1.35
1.35
1.34
1.34
1.33
1.33
1.33
1.32
1.32
1.32
1.31
1.31
1.30
1.30
1.30
1.29
1.29
1.28
1.28
1.27
1.26
1.26
1.25
1.25
1.25
1.24
1.24
1.23
1.23
1.23
1.22
1.22
1.22
1.22
1.21
1.21
1.21
1.20
1.20
1.20
1.19
1.19
1.19
0.88
0.86
0.85
f1 (ppm)
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
5000
10000
15000
20000
25000
30000


CARBON01
Table 2, Entry 26
O
OMe
157.89
142.76
138.65
136.92
129.79
128.63
113.69
110.36
77.25 cdcl3
76.99 cdcl3
76.74 cdcl3
55.20
41.47
35.82
29.95
22.61
14.00
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)
-500
0
500
1000
1500
2000
2500
3000
3500
4000
4500
5000
5500
6000

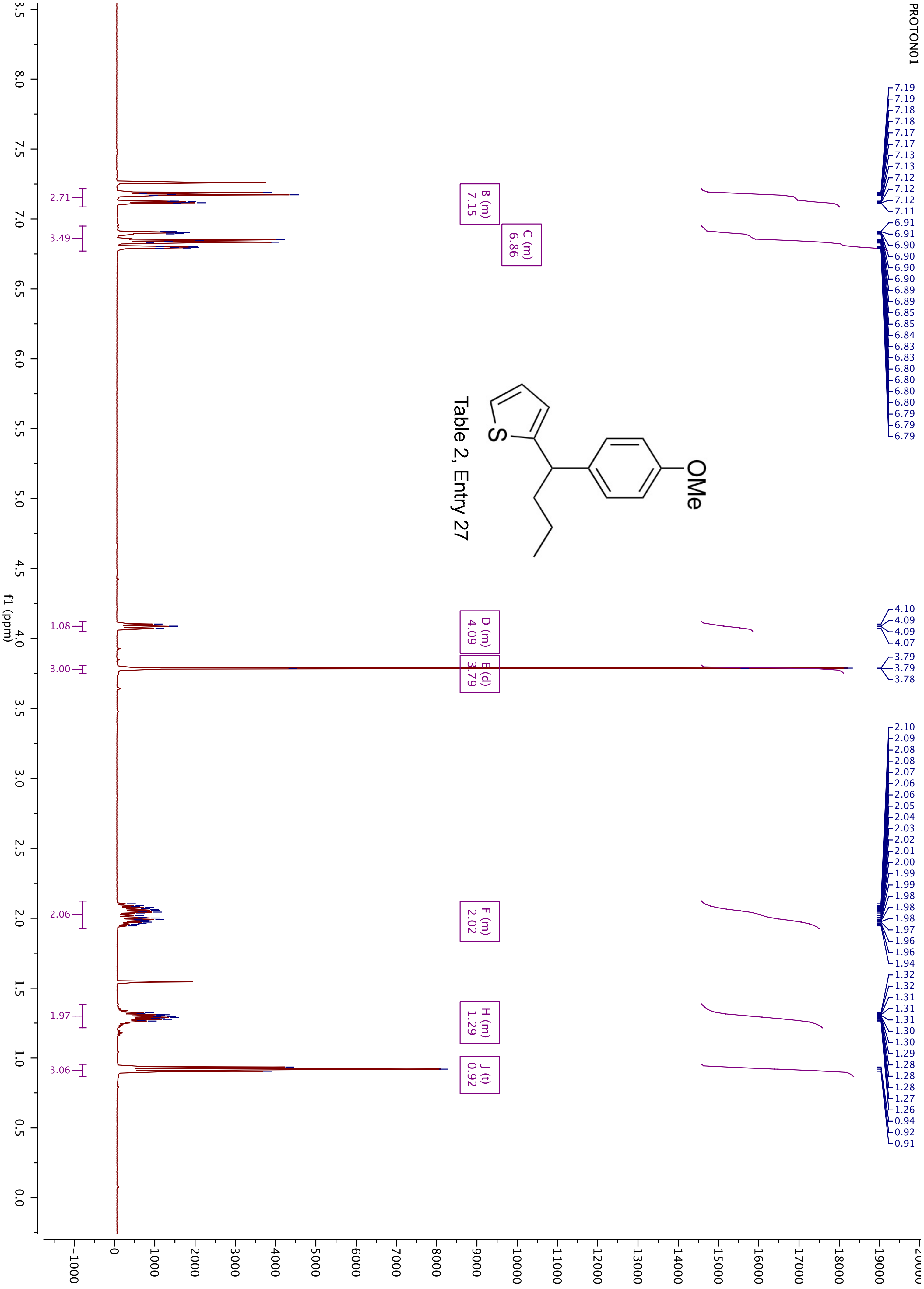
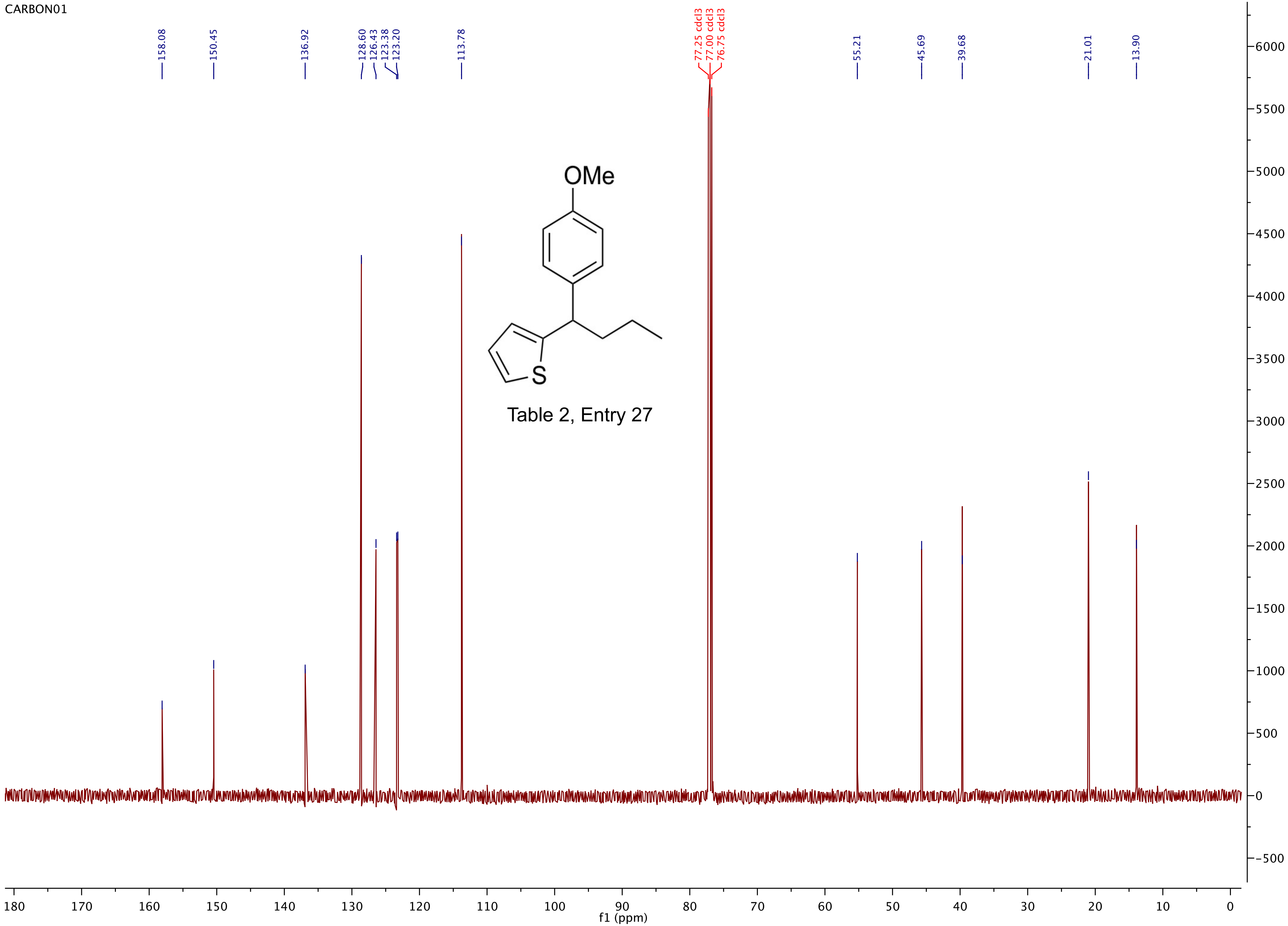


Table 2, Entry 27


CARBON01
158.08
150.45
136.92
128.60
126.43
123.38
123.20
113.78
77.25 cdcl3
77.00 cdcl3
76.75 cdcl3
55.21
45.69
39.68
21.01
13.90
OMe
S
Table 2, Entry 27
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)
6000
5500
5000
4500
4000
3500
3000
2500
2000
1500
1000
500
0
-500

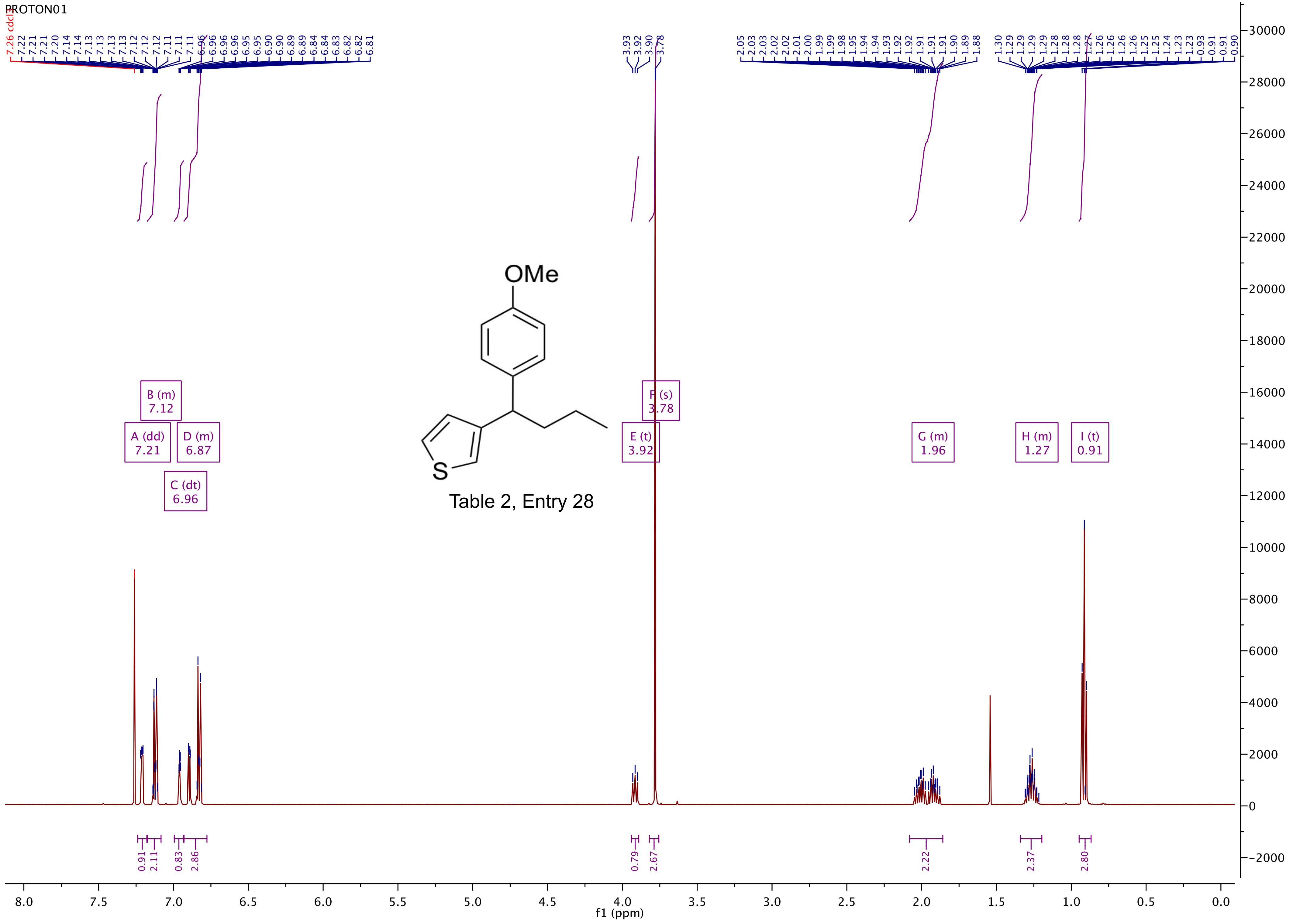
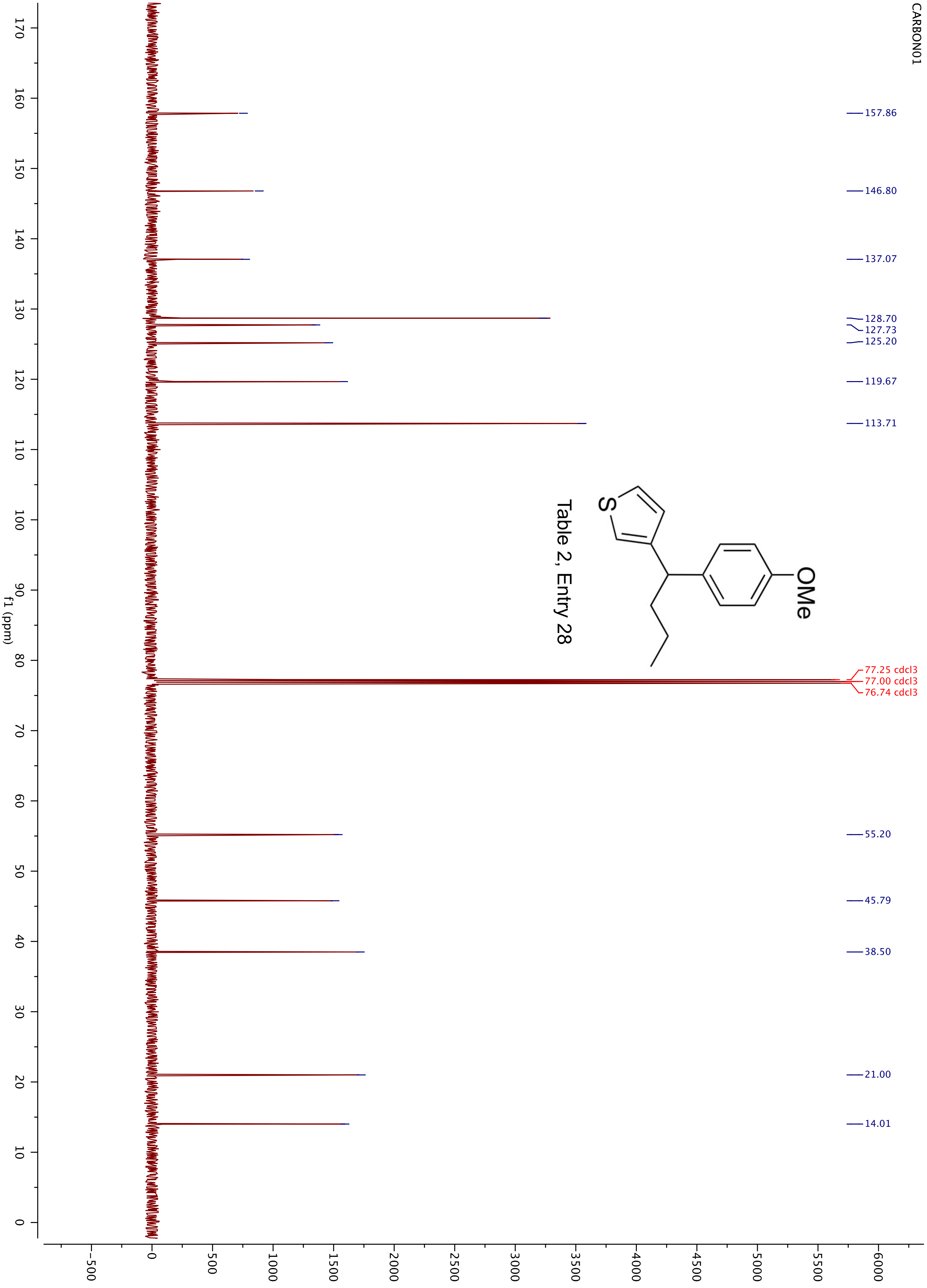


Table 2, Entry 28


CARBON01
157.86
146.80
137.07
128.70
127.73
125.20
119.67
113.71
77.25 cdcl3
77.00 cdcl3
76.74 cdcl3
55.20
45.79
38.50
21.00
14.01
Table 2, Entry 28
S
OMe
f1 (ppm)
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-500
0
500
1000
1500
2000
2500
3000
3500
4000
4500
5000
5500
6000

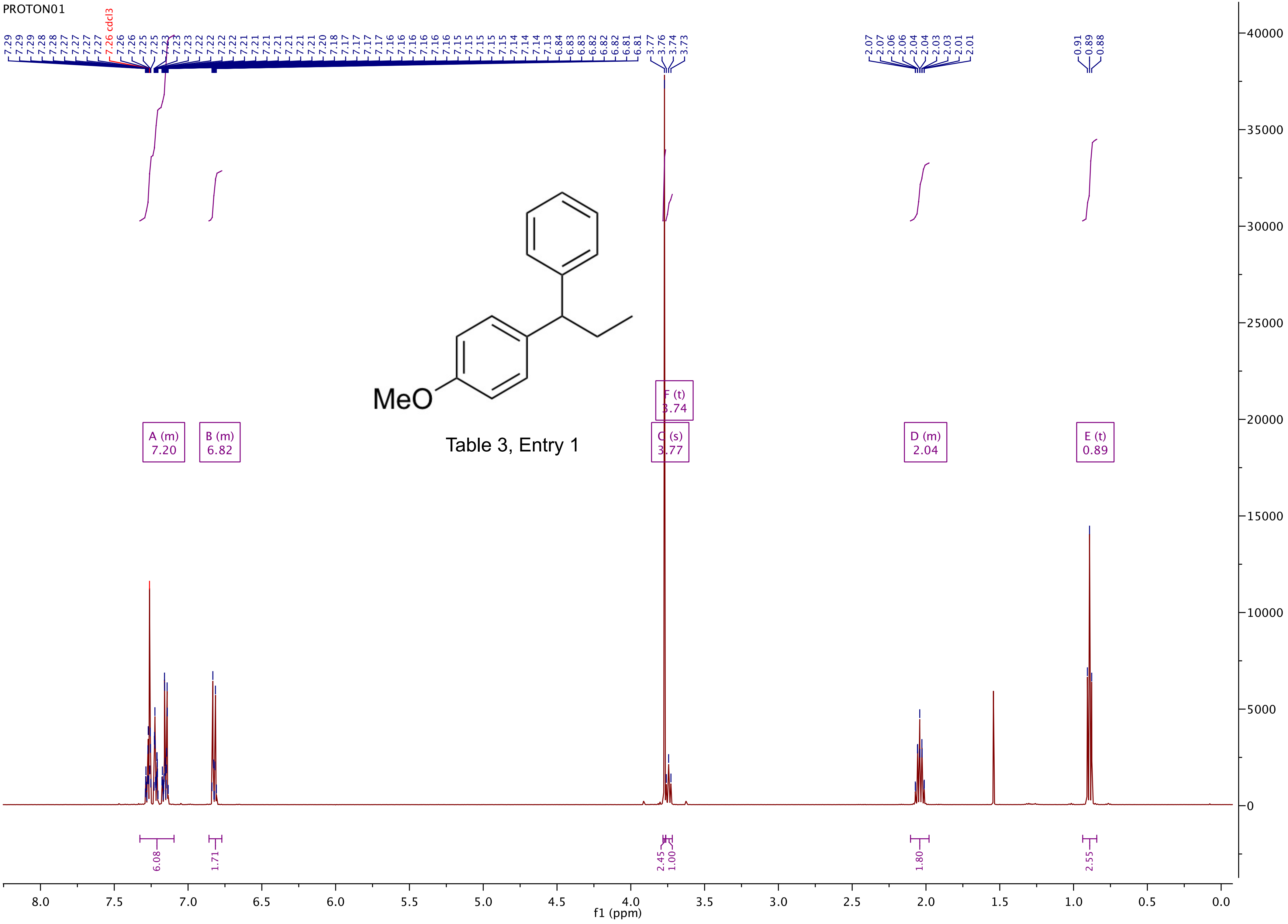
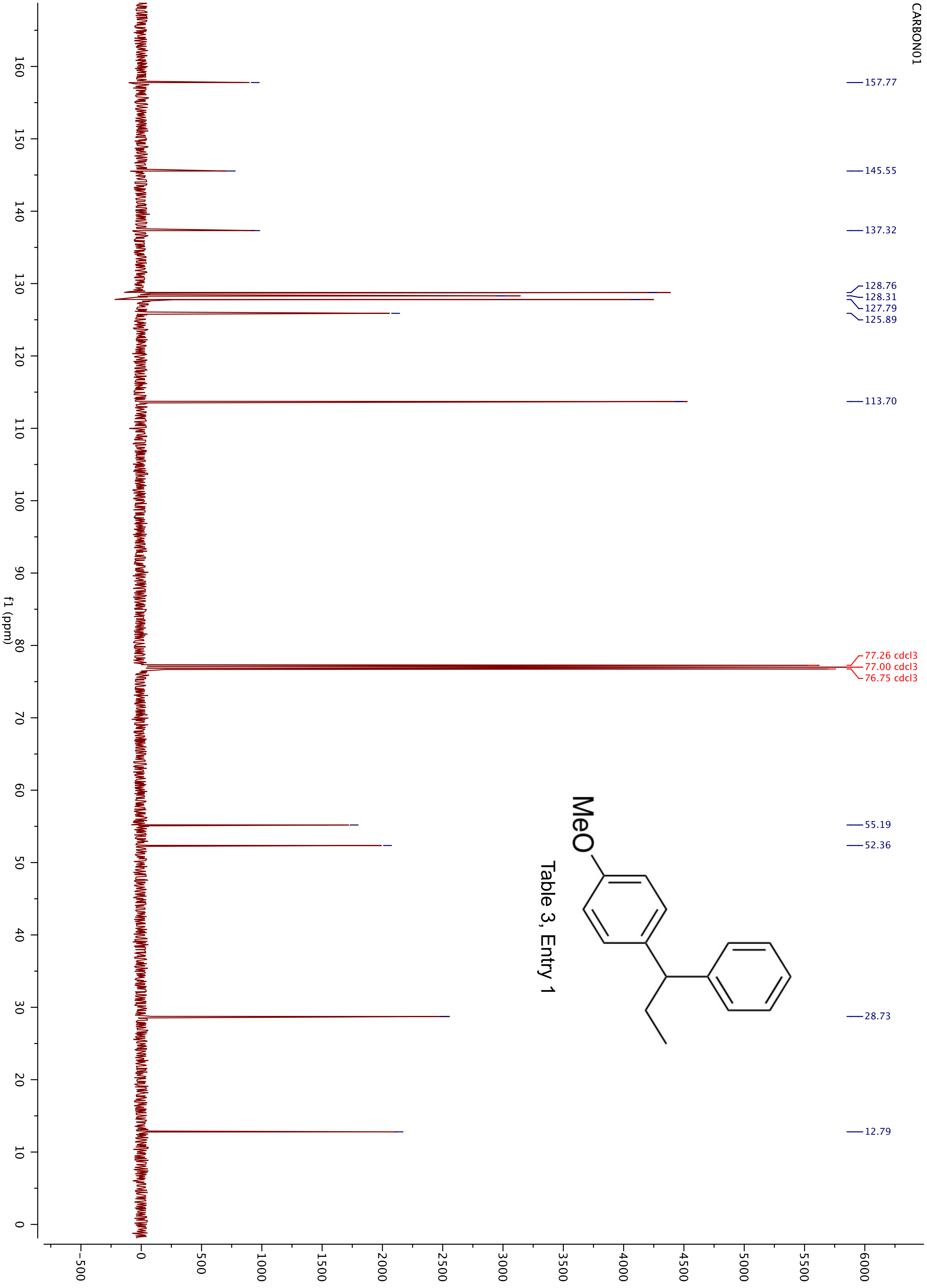


Table 3, Entry 1


CARBON01
157.77
145.55
137.32
128.76
128.31
127.79
125.89
113.70
77.26 cdcl3
77.00 cdcl3
76.75 cdcl3
55.19
52.36
28.73
12.79
MeO
Table 3, Entry 1
f1 (ppm)
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-500
0
500
1000
1500
2000
2500
3000
3500
4000
4500
5000
5500
6000

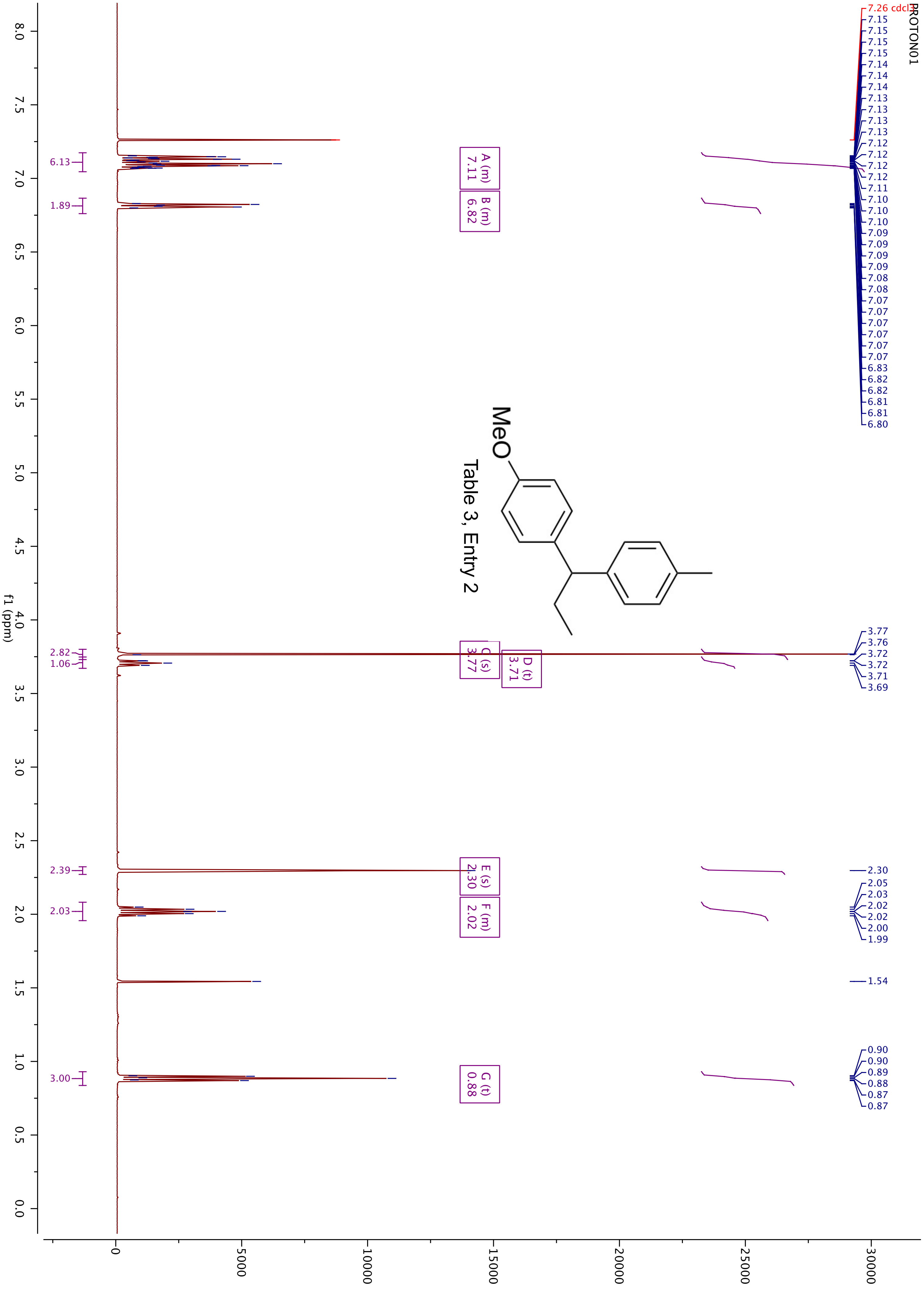


Table 3, Entry 2

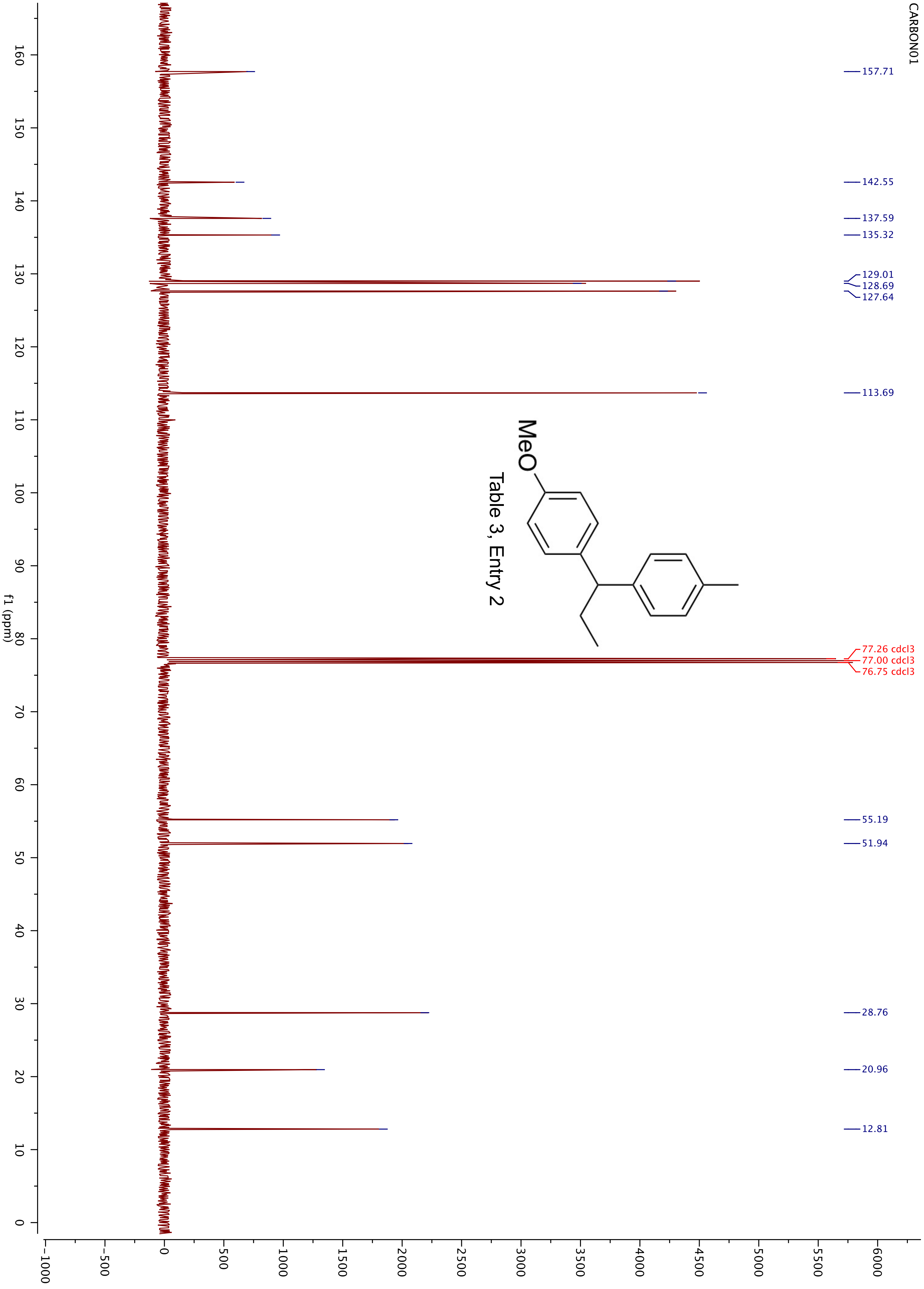
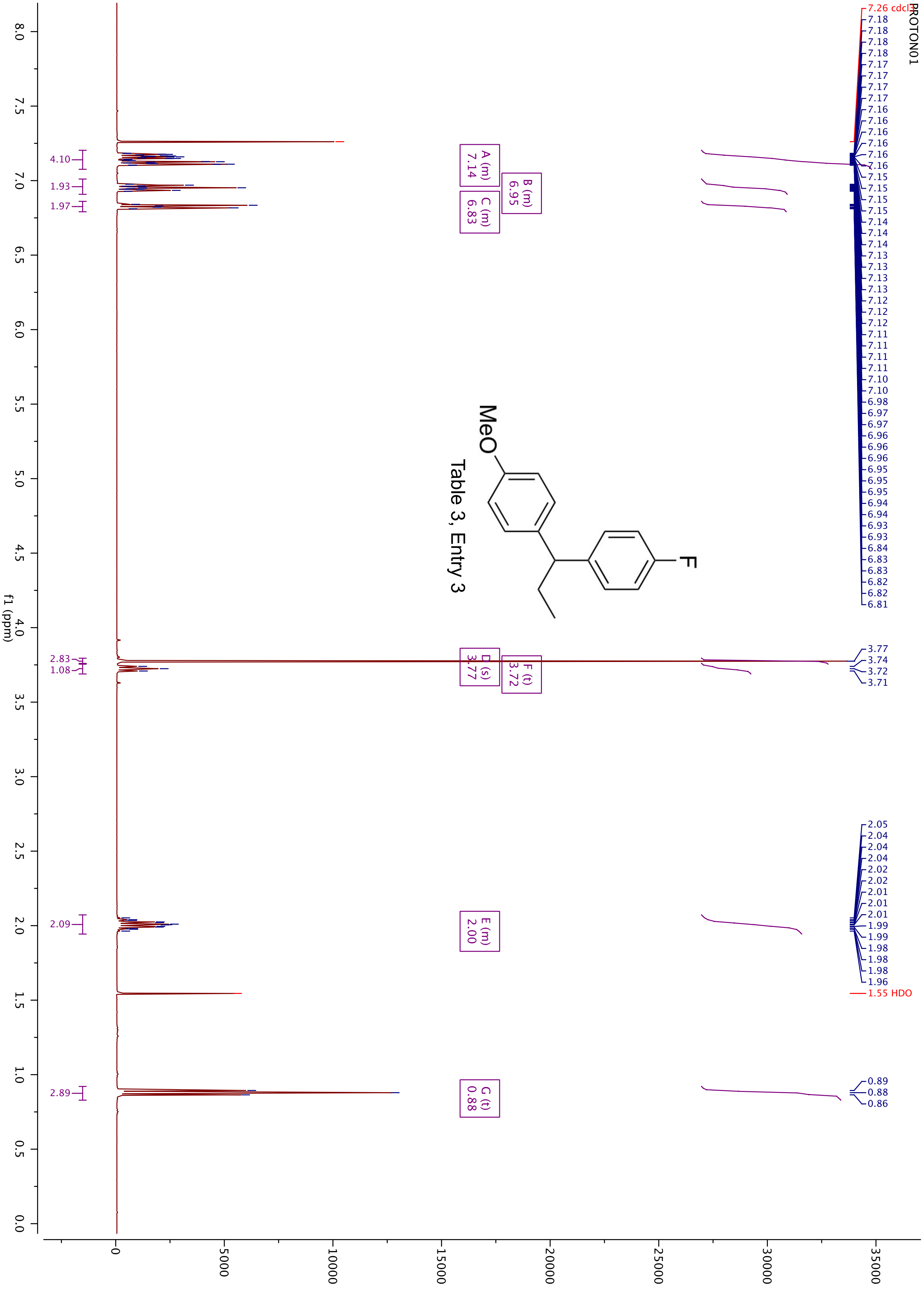


Table 3, Entry 2


PROTON01
7.26 cdcl3
7.18
7.18
7.18
7.18
7.17
7.17
7.17
7.17
7.16
7.16
7.16
7.16
7.16
7.16
7.15
7.15
7.15
7.15
7.14
7.14
7.14
7.13
7.13
7.13
7.13
7.12
7.12
7.12
7.11
7.11
7.11
7.11
7.10
7.10
6.98
6.97
6.97
6.96
6.96
6.96
6.95
6.95
6.95
6.94
6.94
6.93
6.93
6.84
6.83
6.83
6.82
6.82
6.81
3.77
3.74
3.72
3.71
2.05
2.04
2.04
2.04
2.02
2.02
2.01
2.01
2.01
1.99
1.99
1.98
1.98
1.98
1.96
1.55 HDO
0.89
0.88
0.86
A (m)
7.14
B (m)
6.95
C (m)
6.83
D (s)
3.77
F (t)
3.72
E (m)
2.00
G (t)
0.88
4.10
1.93
1.97
2.83
1.08
2.09
2.89
MeO
F
Table 3, Entry 3
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)
0
5000
10000
15000
20000
25000
30000
35000

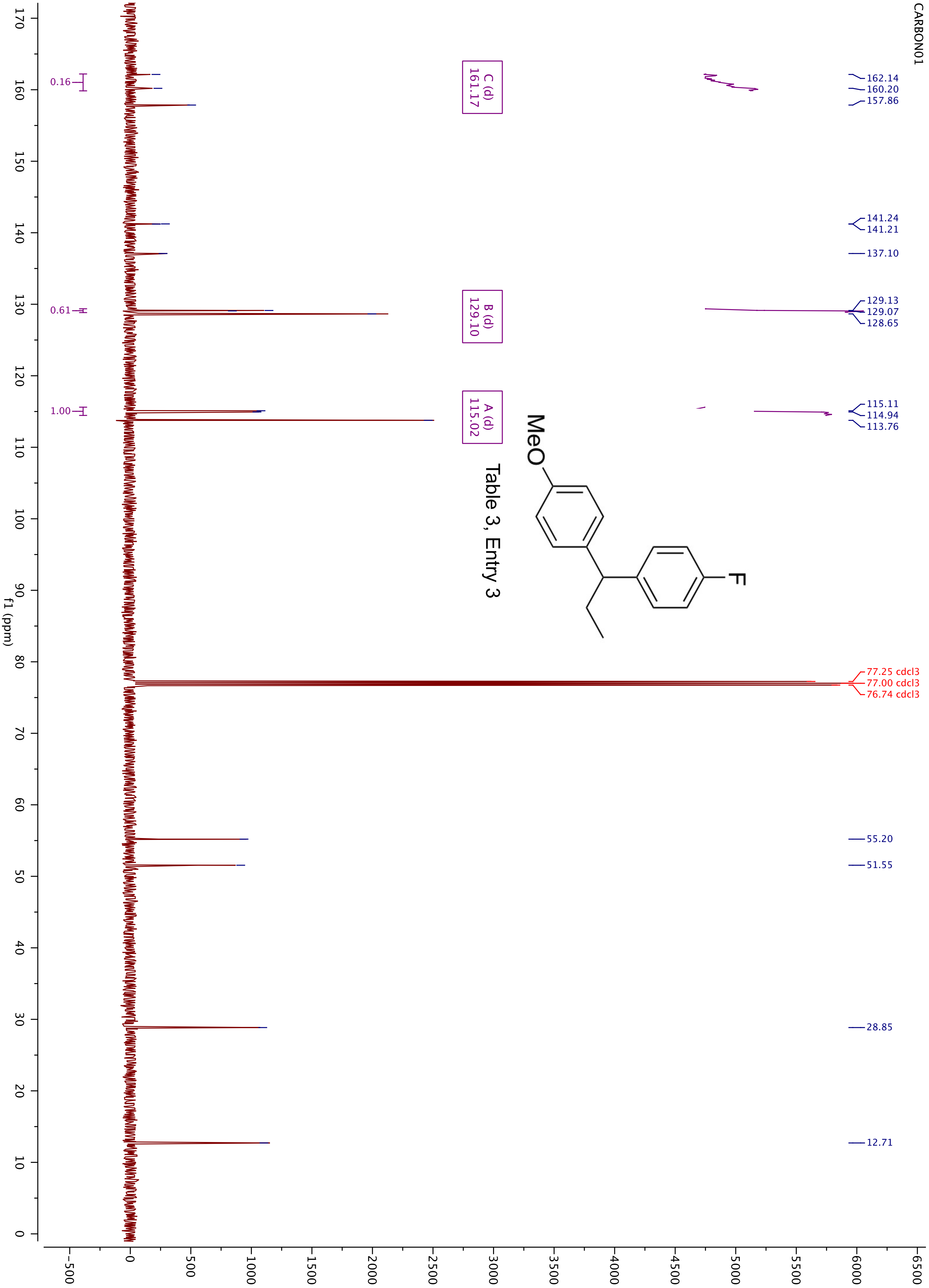


Table 3, Entry 3

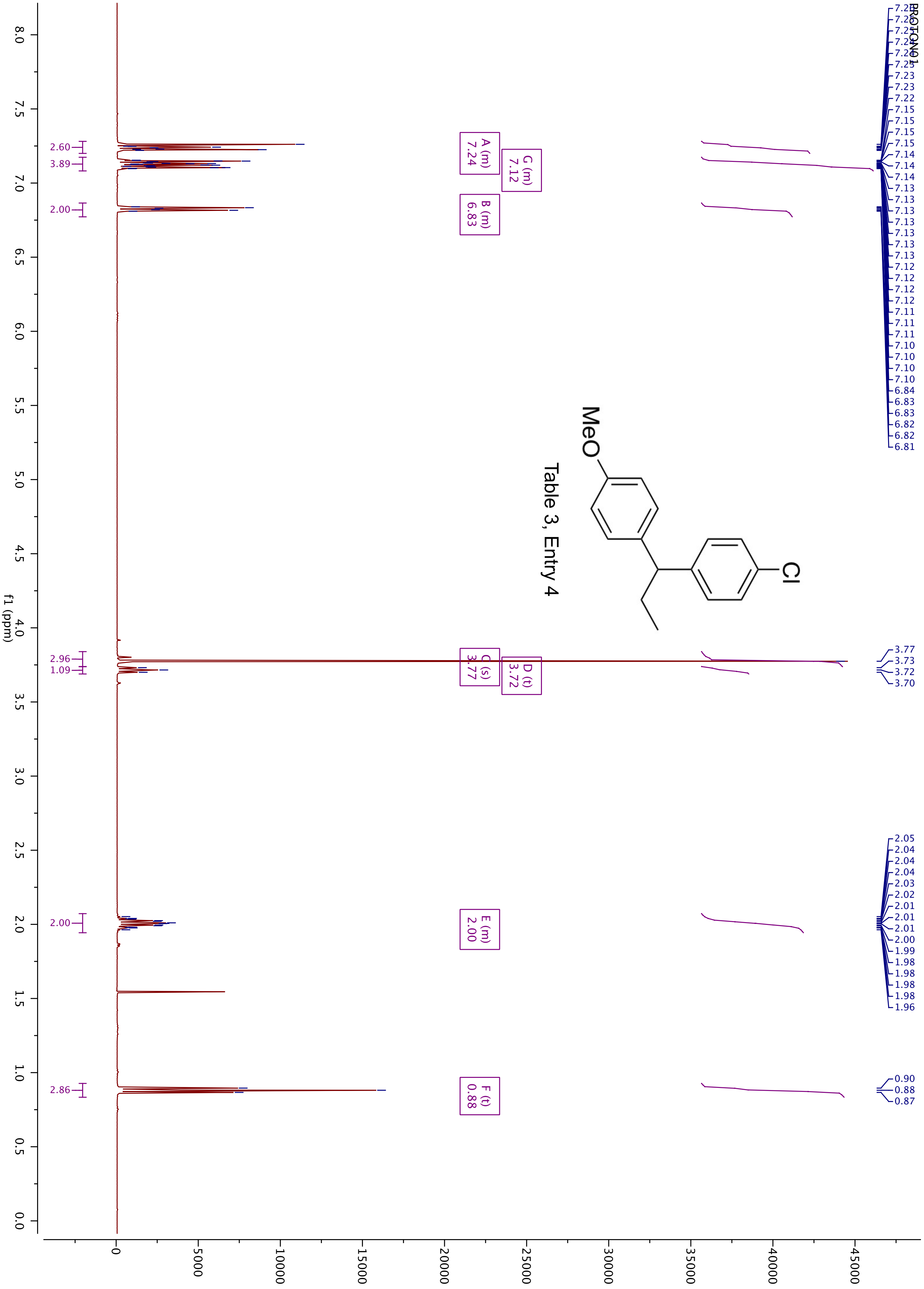
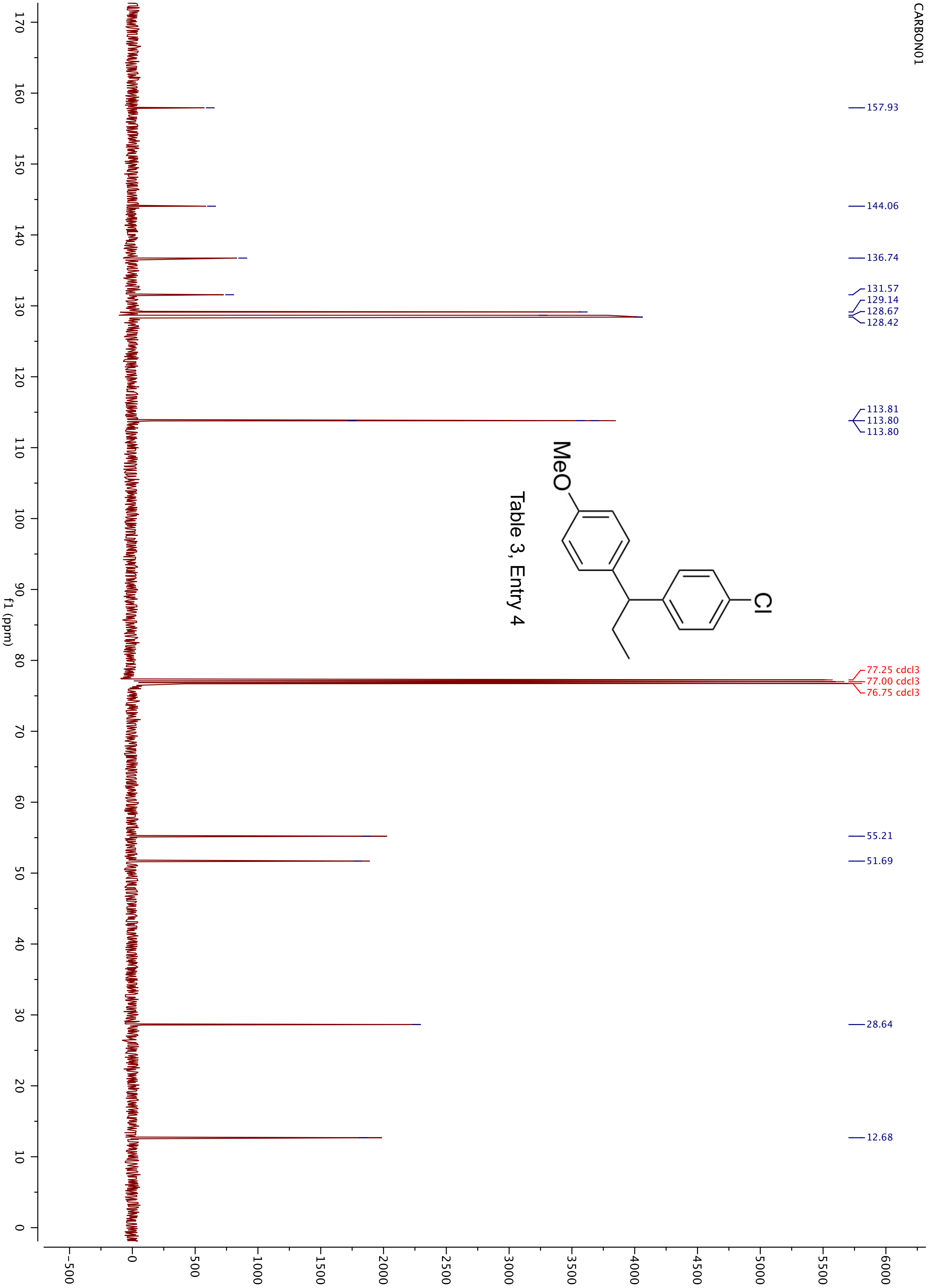
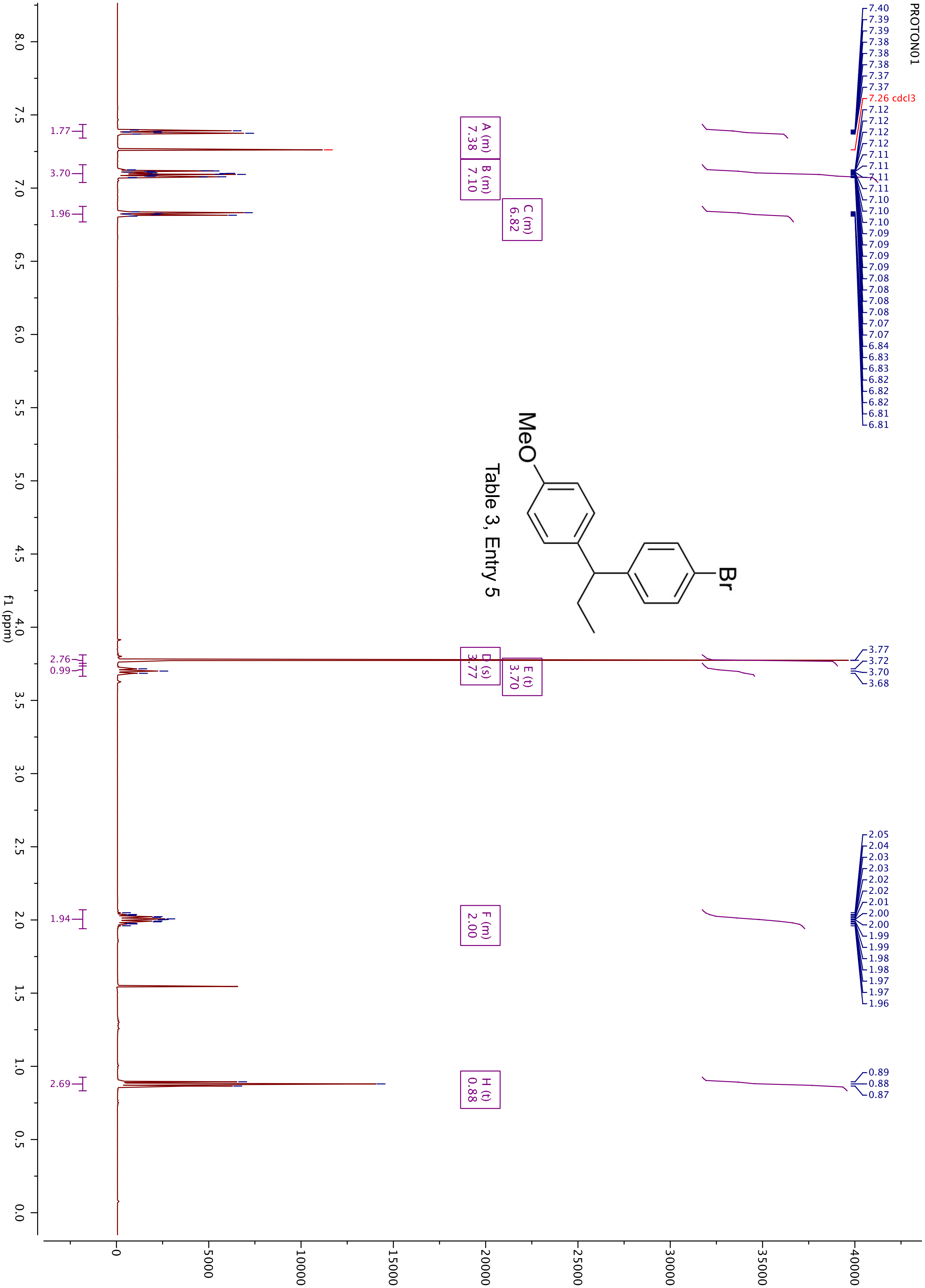
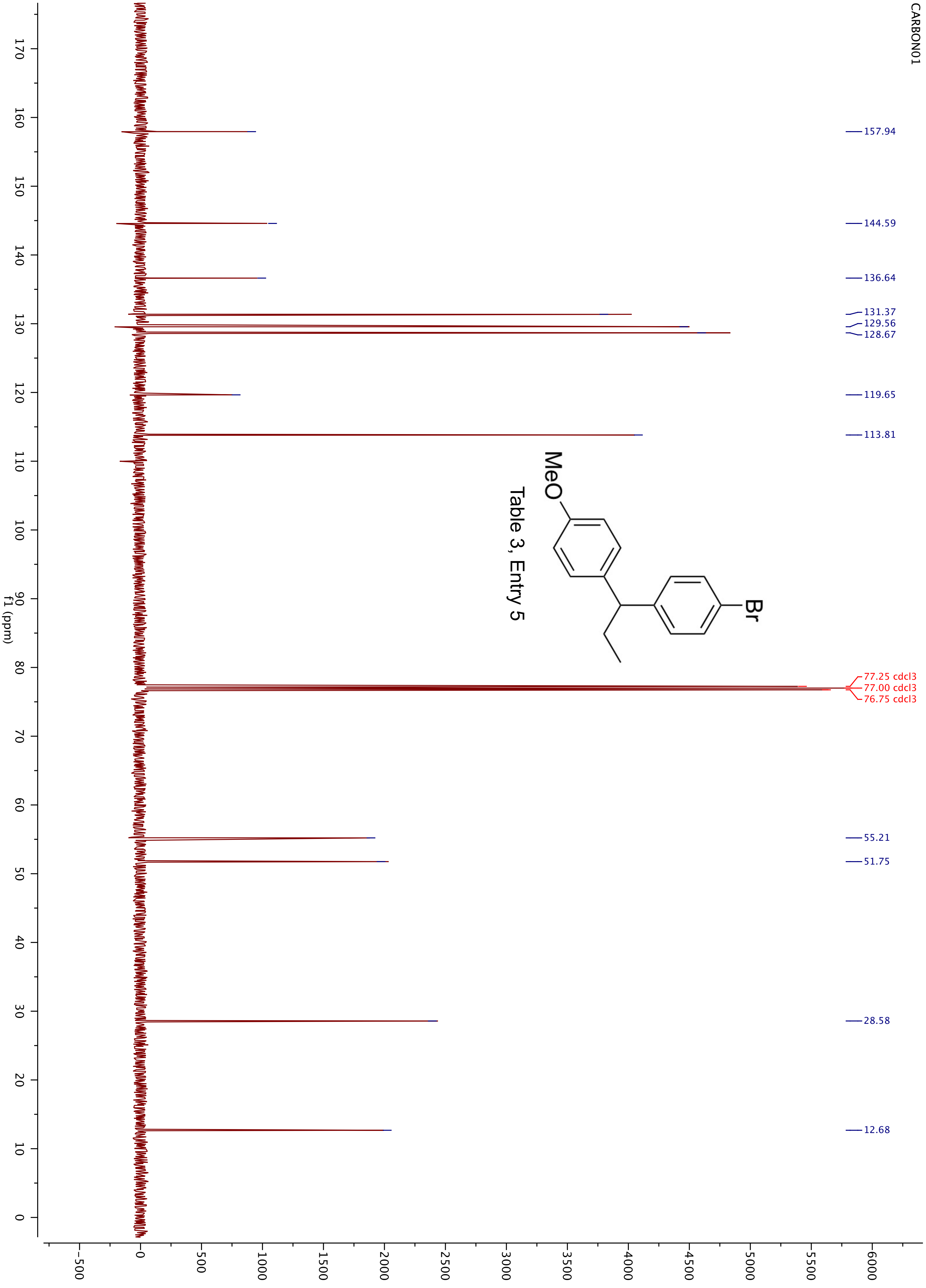


Table 3, Entry 4


CARBON01
157.93
144.06
136.74
131.57
129.14
128.67
128.42
113.81
113.80
113.80
77.25 cdcl3
77.00 cdcl3
76.75 cdcl3
55.21
51.69
28.64
12.68
MeO
Cl
Table 3, Entry 4
f1 (ppm)
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-500
0
500
1000
1500
2000
2500
3000
3500
4000
4500
5000
5500
6000


PROTON01
Table 3, Entry 5
MeO
Br
7.40
7.39
7.39
7.38
7.38
7.38
7.37
7.37
7.26 cdcl3
7.12
7.12
7.12
7.12
7.11
7.11
7.11
7.11
7.10
7.10
7.10
7.09
7.09
7.09
7.09
7.08
7.08
7.08
7.08
7.07
7.07
6.84
6.83
6.83
6.82
6.82
6.82
6.81
6.81
3.77
3.72
3.70
3.68
2.05
2.04
2.03
2.03
2.02
2.02
2.01
2.00
2.00
1.99
1.99
1.98
1.98
1.97
1.97
1.96
0.89
0.88
0.87
A (m) 7.38
B (m) 7.10
C (m) 6.82
D (s) 3.77
E (t) 3.70
F (m) 2.00
H (t) 0.88
1.77
3.70
1.96
2.76
0.99
1.94
2.69
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)
0
5000
10000
15000
20000
25000
30000
35000
40000


CARBON01
157.94
144.59
136.64
131.37
129.56
128.67
119.65
113.81
77.25 cdcl3
77.00 cdcl3
76.75 cdcl3
55.21
51.75
28.58
12.68
MeO
Br
Table 3, Entry 5
f1 (ppm)
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-500
0
500
1000
1500
2000
2500
3000
3500
4000
4500
5000
5500
6000

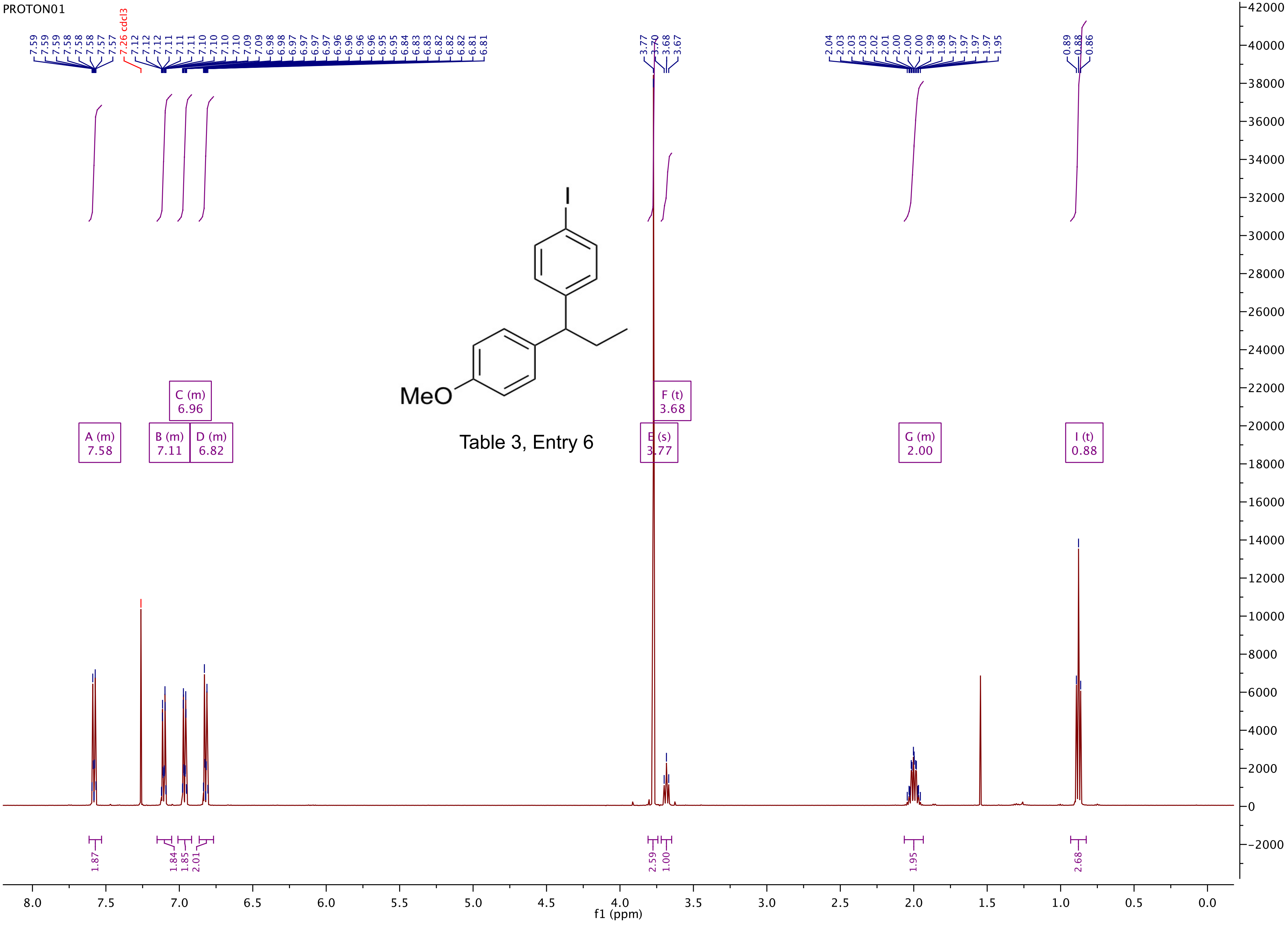


Table 3, Entry 6

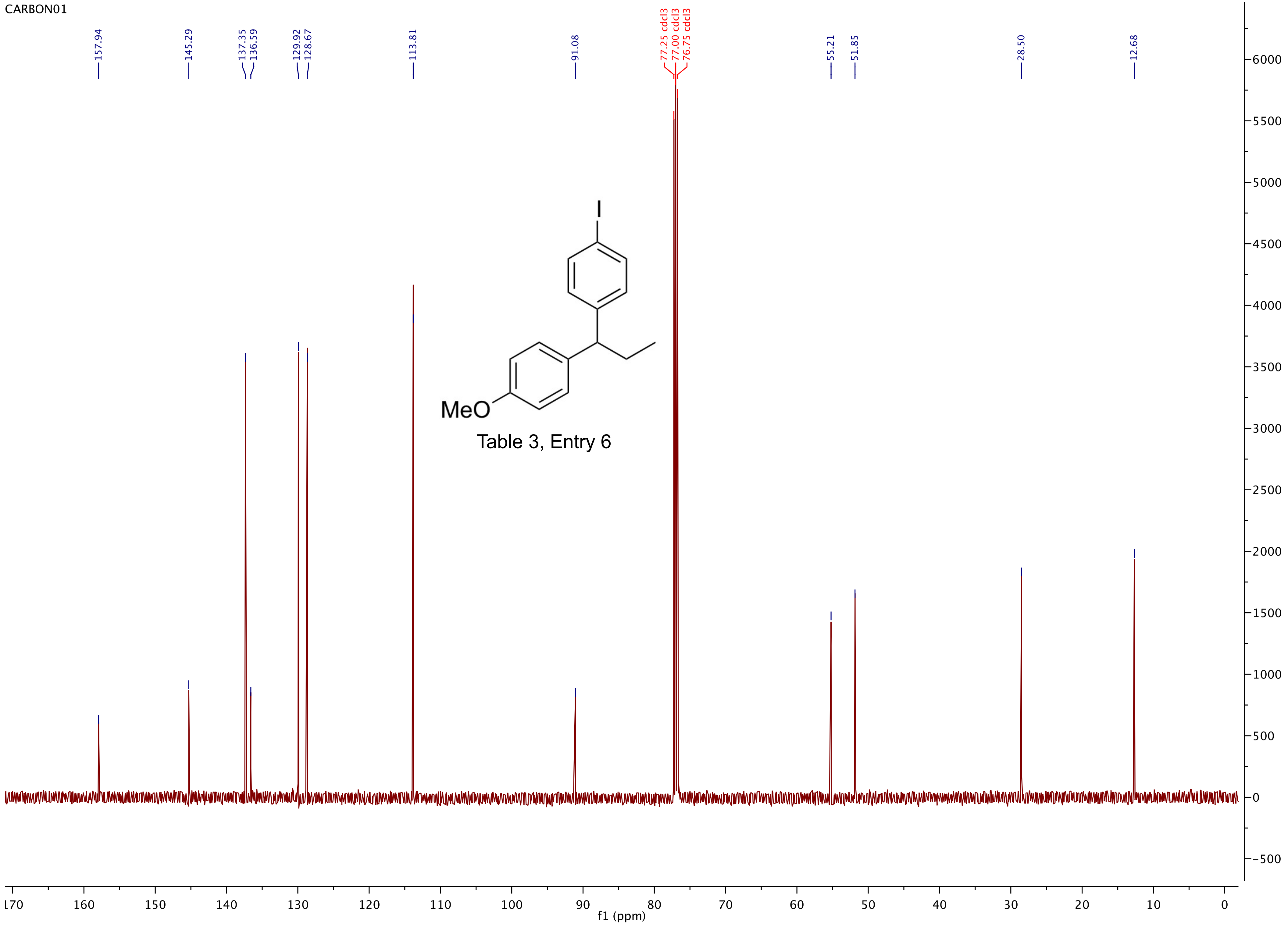


Table 3, Entry 6

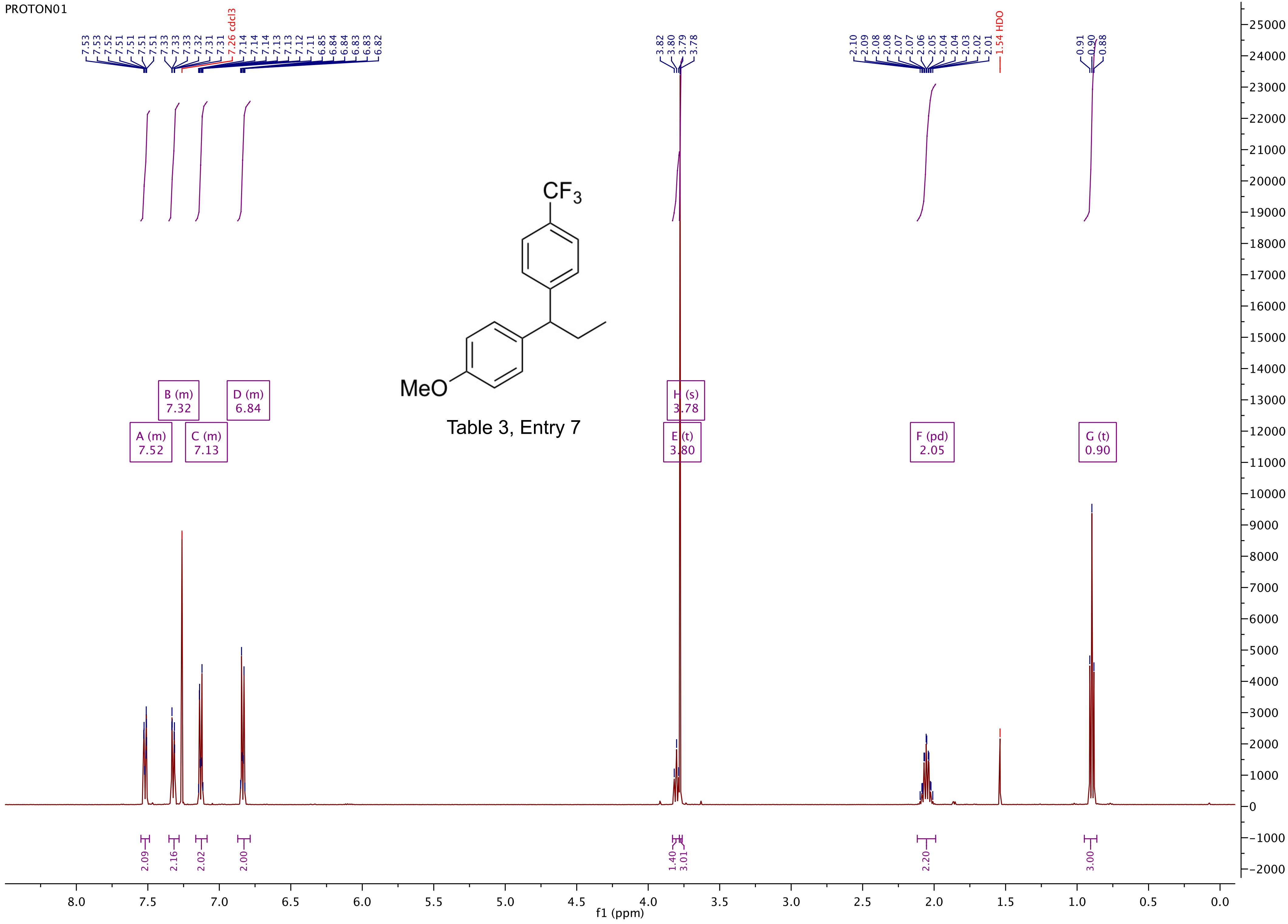
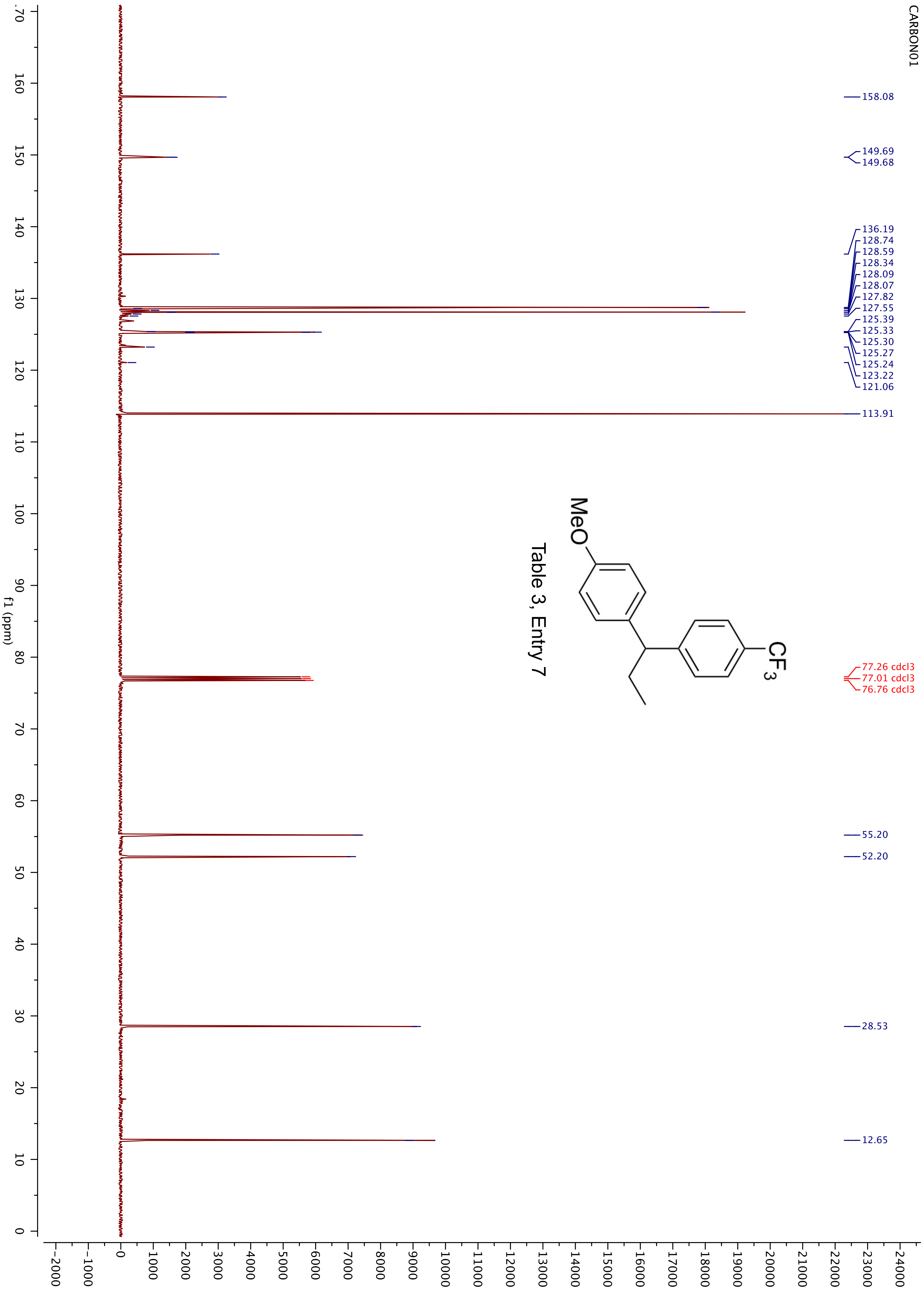
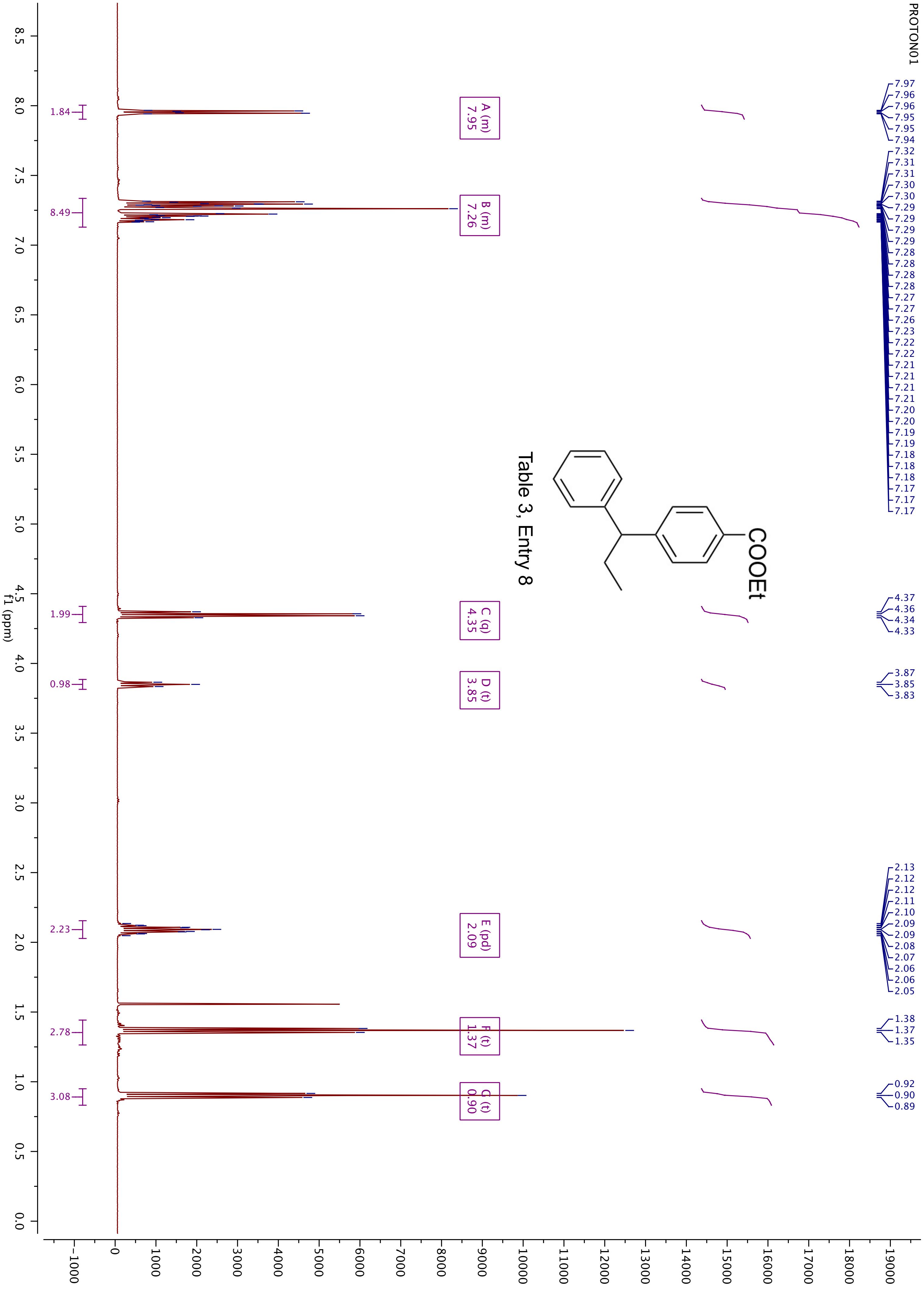


Table 3, Entry 7


CARBON01
Table 3, Entry 7
MeO
CF3
158.08
149.69
149.68
136.19
128.74
128.59
128.34
128.09
128.07
127.82
127.55
125.39
125.33
125.30
125.27
125.24
123.22
121.06
113.91
77.26 cdcl3
77.01 cdcl3
76.76 cdcl3
55.20
52.20
28.53
12.65
f1 (ppm)
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-2000
-1000
0
1000
2000
3000
4000
5000
6000
7000
8000
9000
10000
11000
12000
13000
14000
15000
16000
17000
18000
19000
20000
21000
22000
23000
24000


PROTON01
Table 3, Entry 8
COOEt
7.97
7.96
7.96
7.95
7.95
7.94
7.32
7.31
7.31
7.30
7.30
7.29
7.29
7.29
7.29
7.28
7.28
7.28
7.28
7.27
7.27
7.26
7.23
7.22
7.22
7.21
7.21
7.21
7.21
7.20
7.20
7.19
7.19
7.18
7.18
7.18
7.17
7.17
7.17
4.37
4.36
4.34
4.33
3.87
3.85
3.83
2.13
2.12
2.12
2.11
2.10
2.09
2.09
2.08
2.07
2.06
2.06
2.05
1.38
1.37
1.35
0.92
0.90
0.89
A (m) 7.95
B (m) 7.26
C (q) 4.35
D (t) 3.85
E (pd) 2.09
F (t) 1.37
G (t) 0.90
1.84
8.49
1.99
0.98
2.23
2.78
3.08
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)
-1000
0
1000
2000
3000
4000
5000
6000
7000
8000
9000
10000
11000
12000
13000
14000
15000
16000
17000
18000
19000

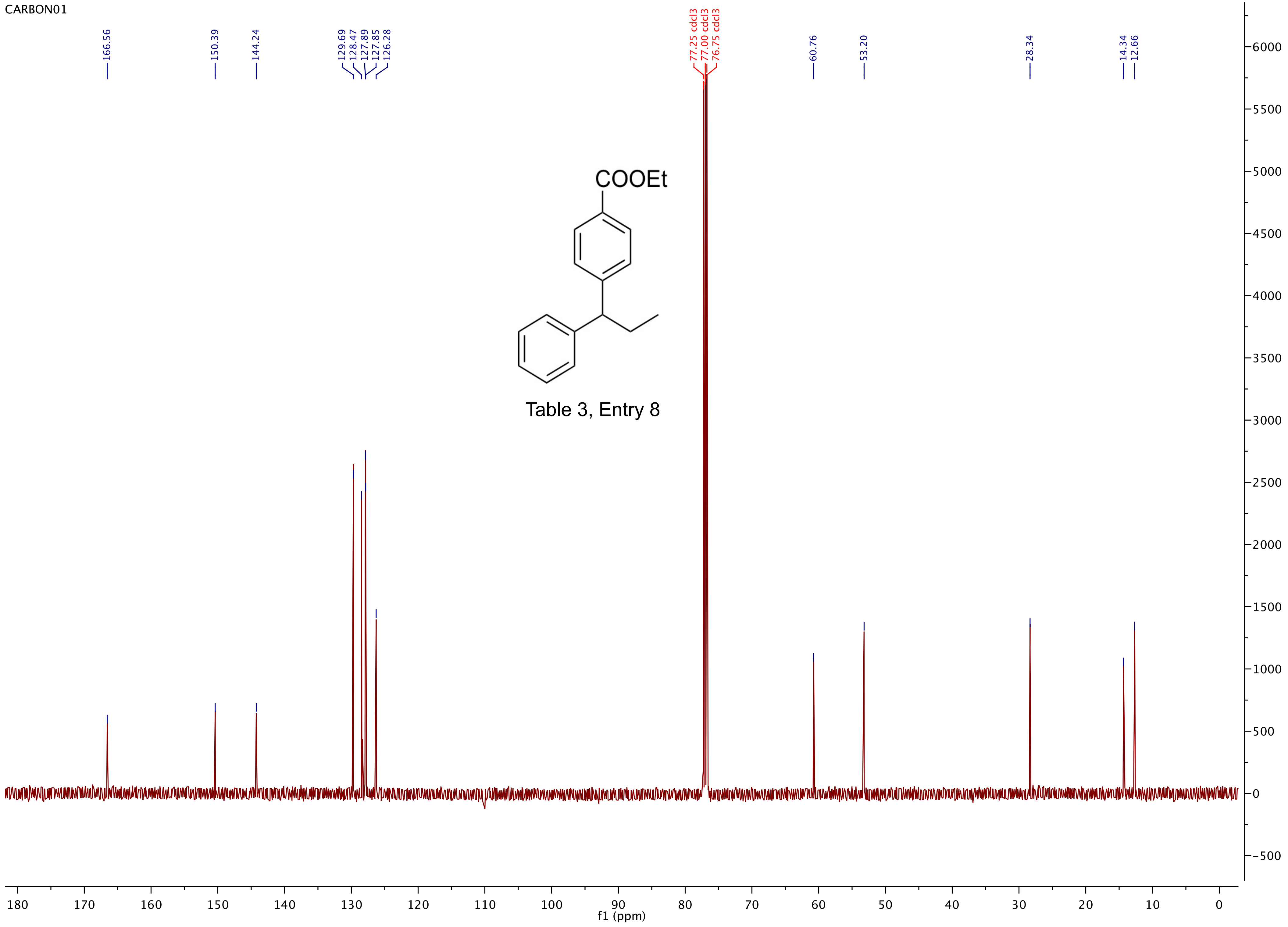


Table 3, Entry 8

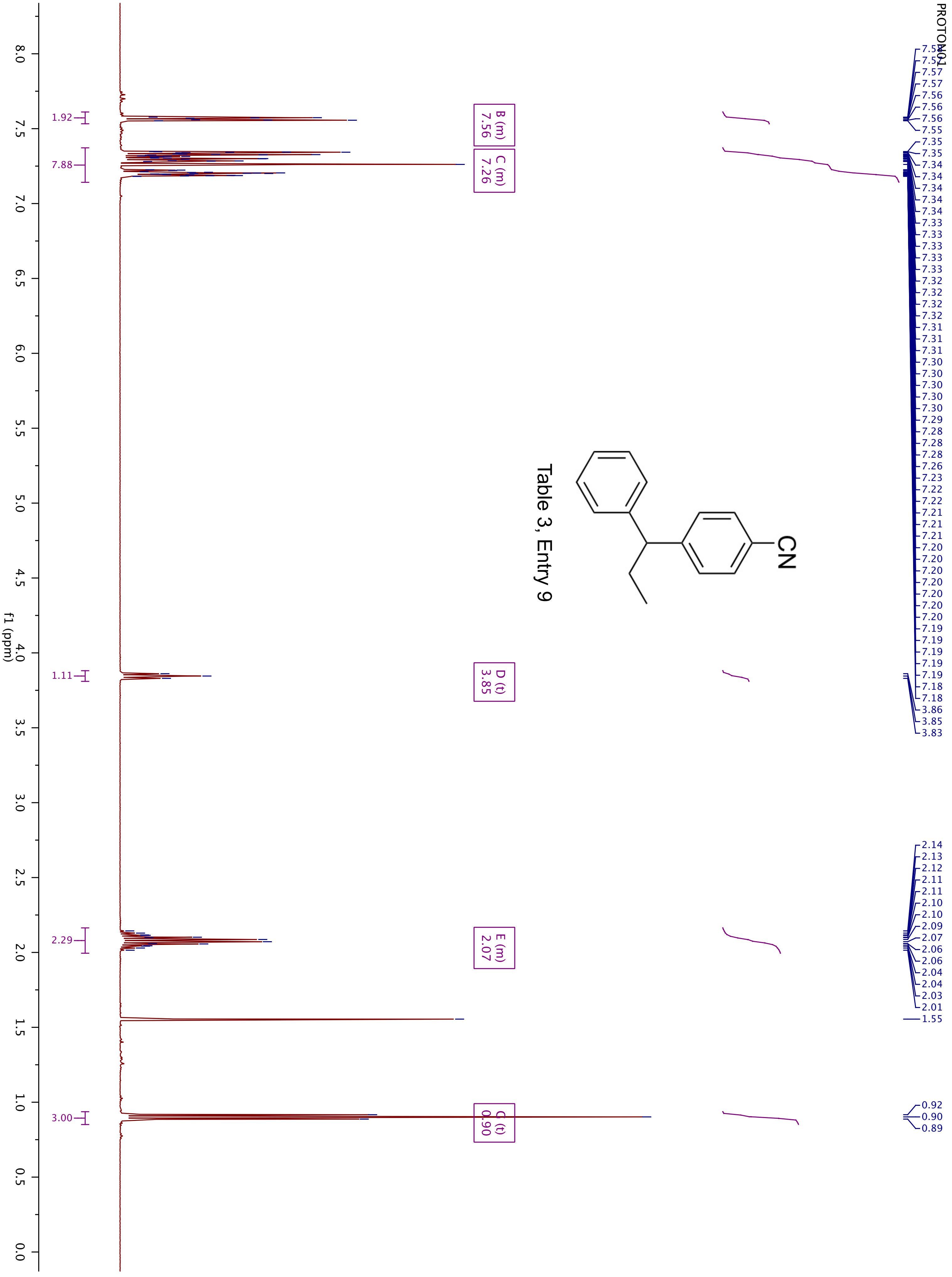


Table 3, Entry 9

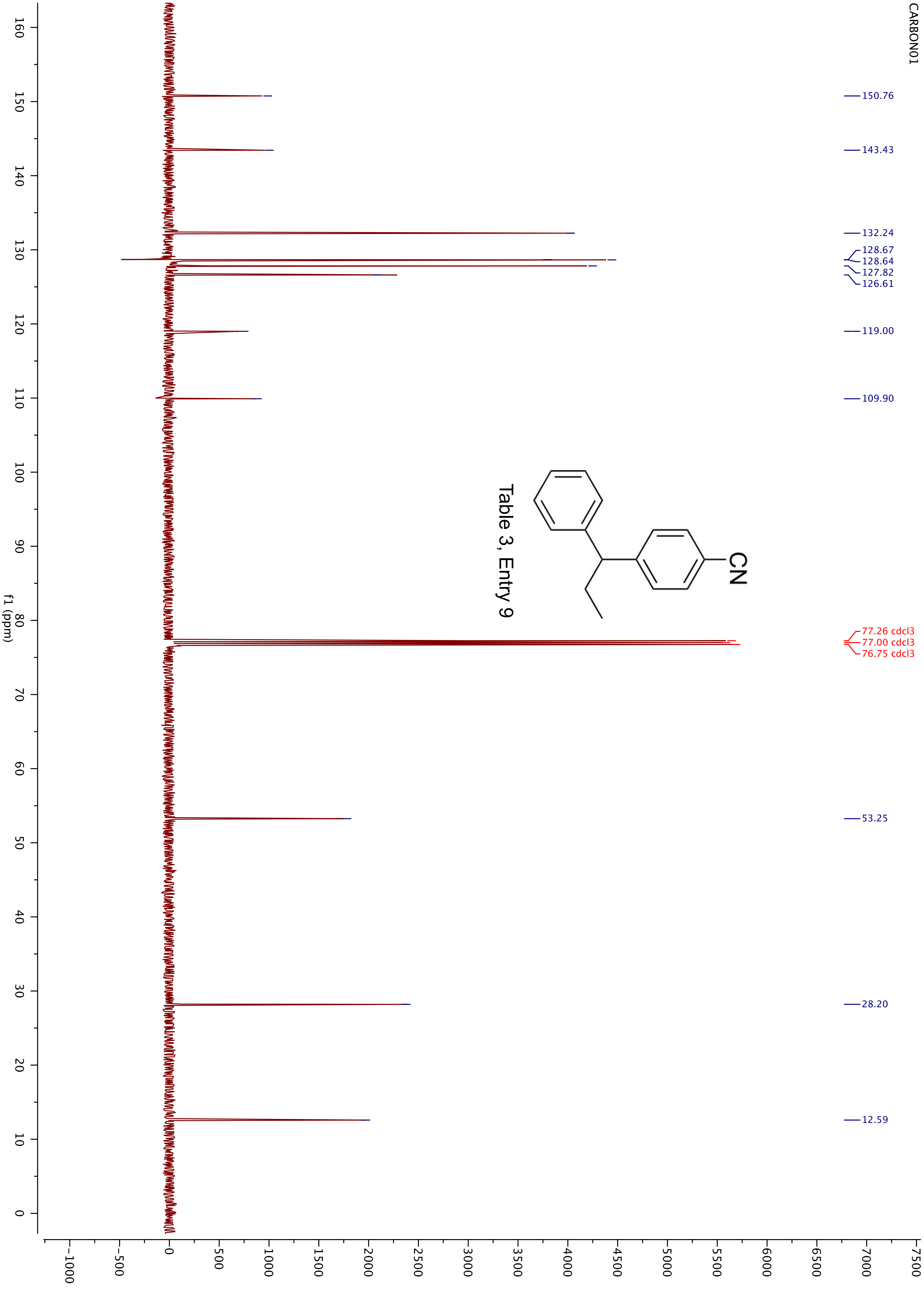
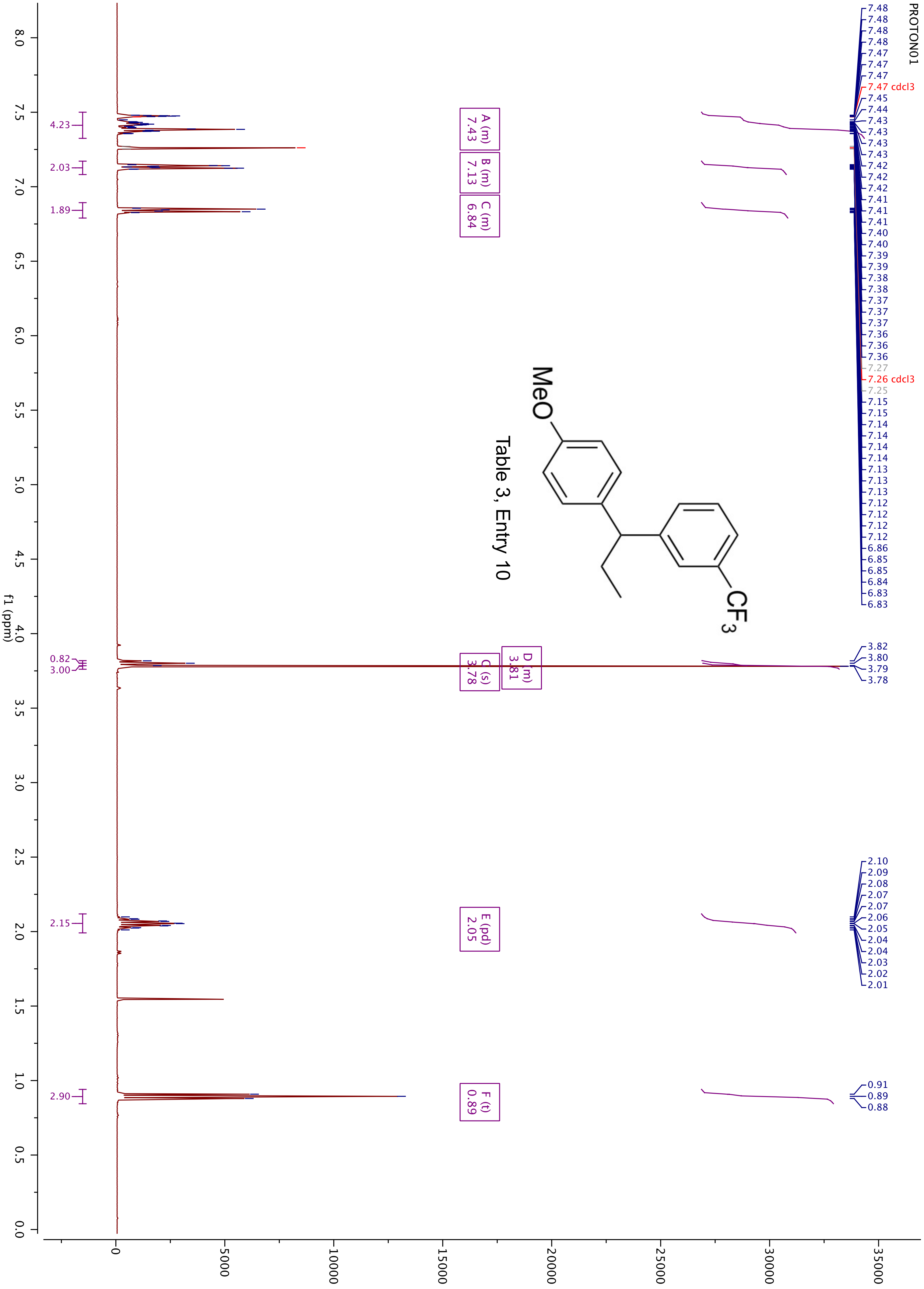


Table 3, Entry 9


PROTON01
Table 3, Entry 10
MeO
CF3
7.48
7.48
7.48
7.48
7.47
7.47
7.47
7.47 cdcl3
7.45
7.44
7.43
7.43
7.43
7.43
7.42
7.42
7.42
7.41
7.41
7.41
7.40
7.40
7.39
7.39
7.38
7.38
7.37
7.37
7.37
7.36
7.36
7.36
7.27
7.26 cdcl3
7.25
7.15
7.15
7.14
7.14
7.14
7.14
7.13
7.13
7.13
7.12
7.12
7.12
7.12
6.86
6.85
6.85
6.84
6.83
6.83
3.82
3.80
3.79
3.78
2.10
2.09
2.08
2.07
2.07
2.06
2.05
2.04
2.04
2.03
2.02
2.01
0.91
0.89
0.88
A (m) 7.43
B (m) 7.13
C (m) 6.84
D (m) 3.81
C (s) 3.78
E (pd) 2.05
F (t) 0.89
4.23
2.03
1.89
0.82
3.00
2.15
2.90
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)
0
5000
10000
15000
20000
25000
30000
35000

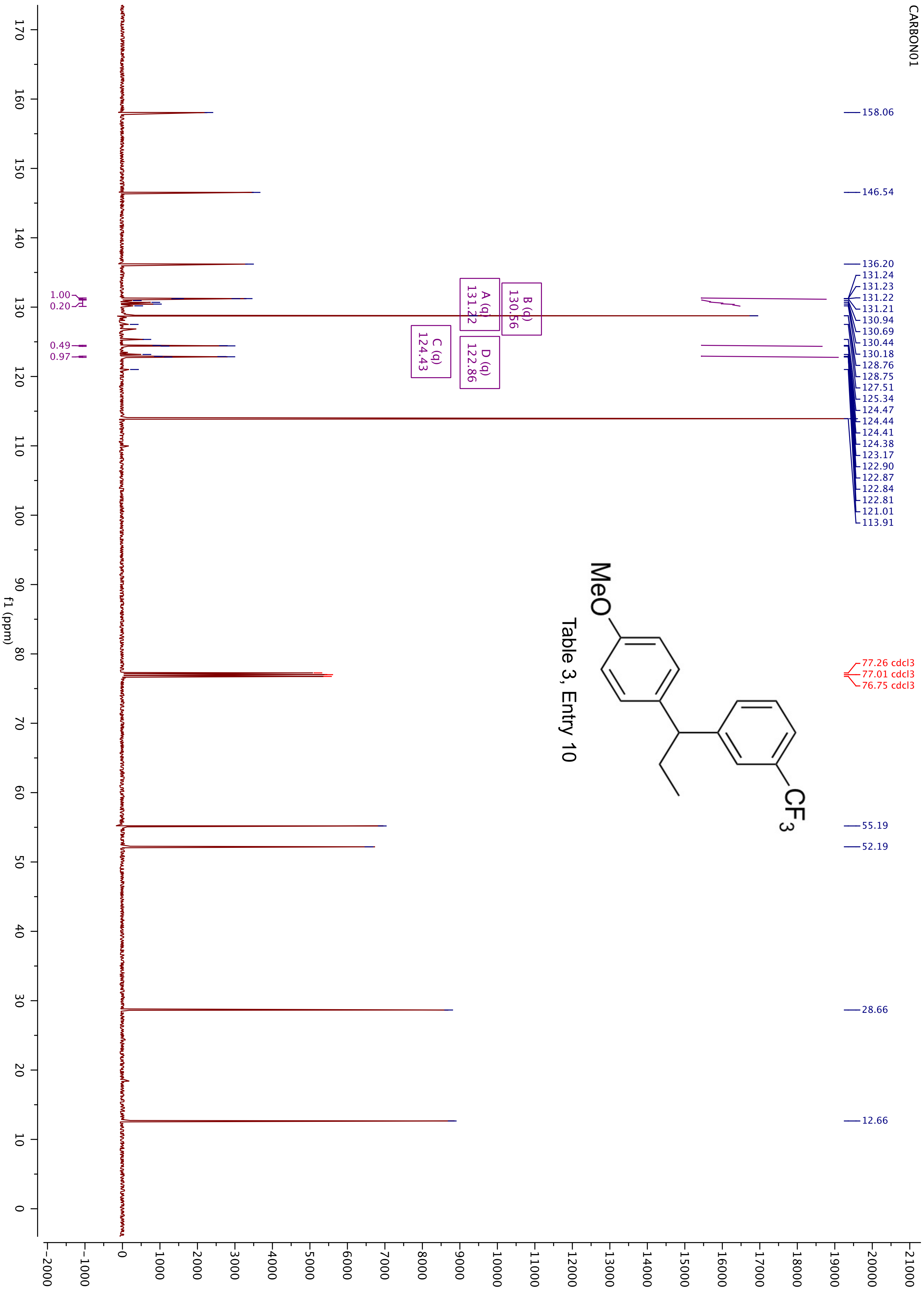


Table 3, Entry 10

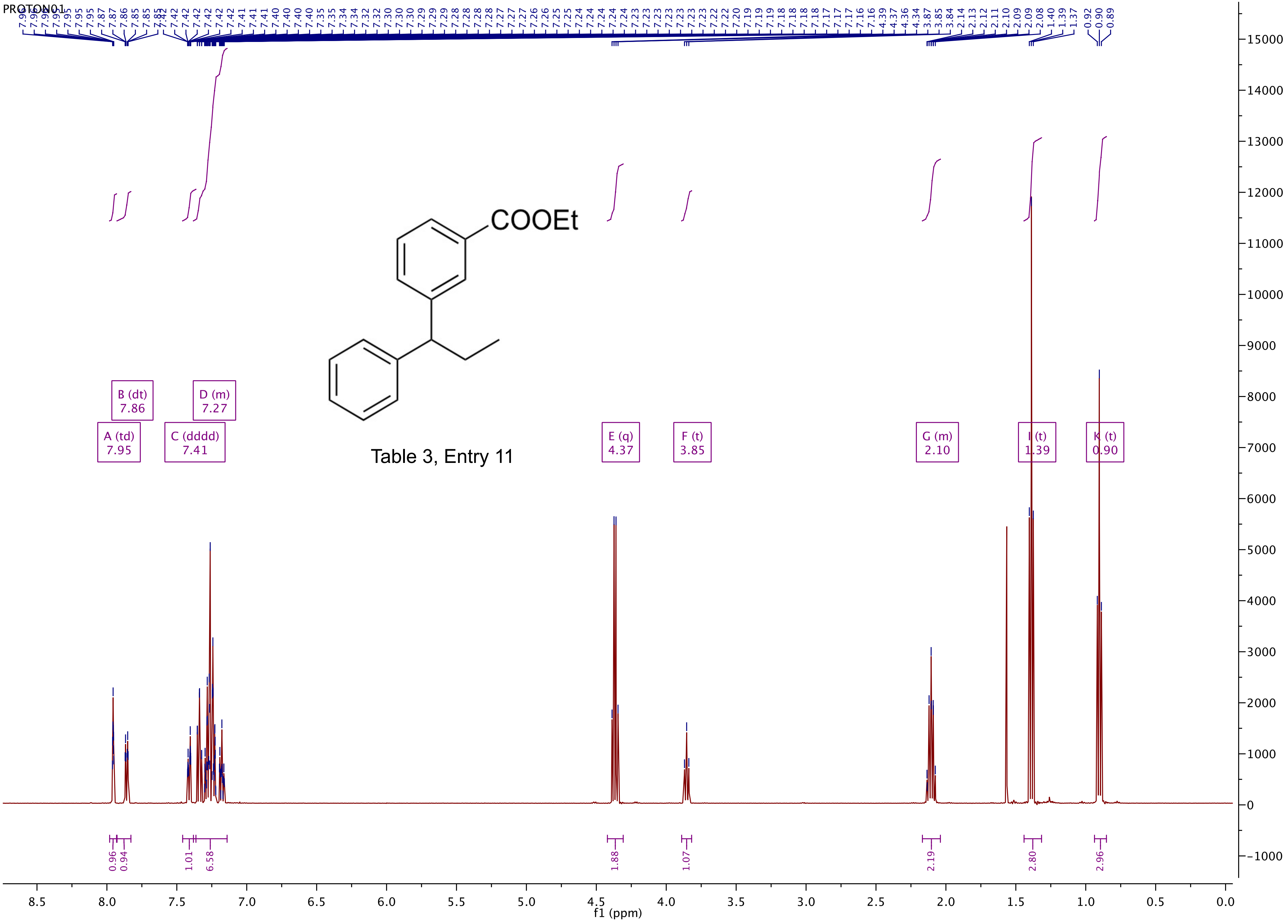
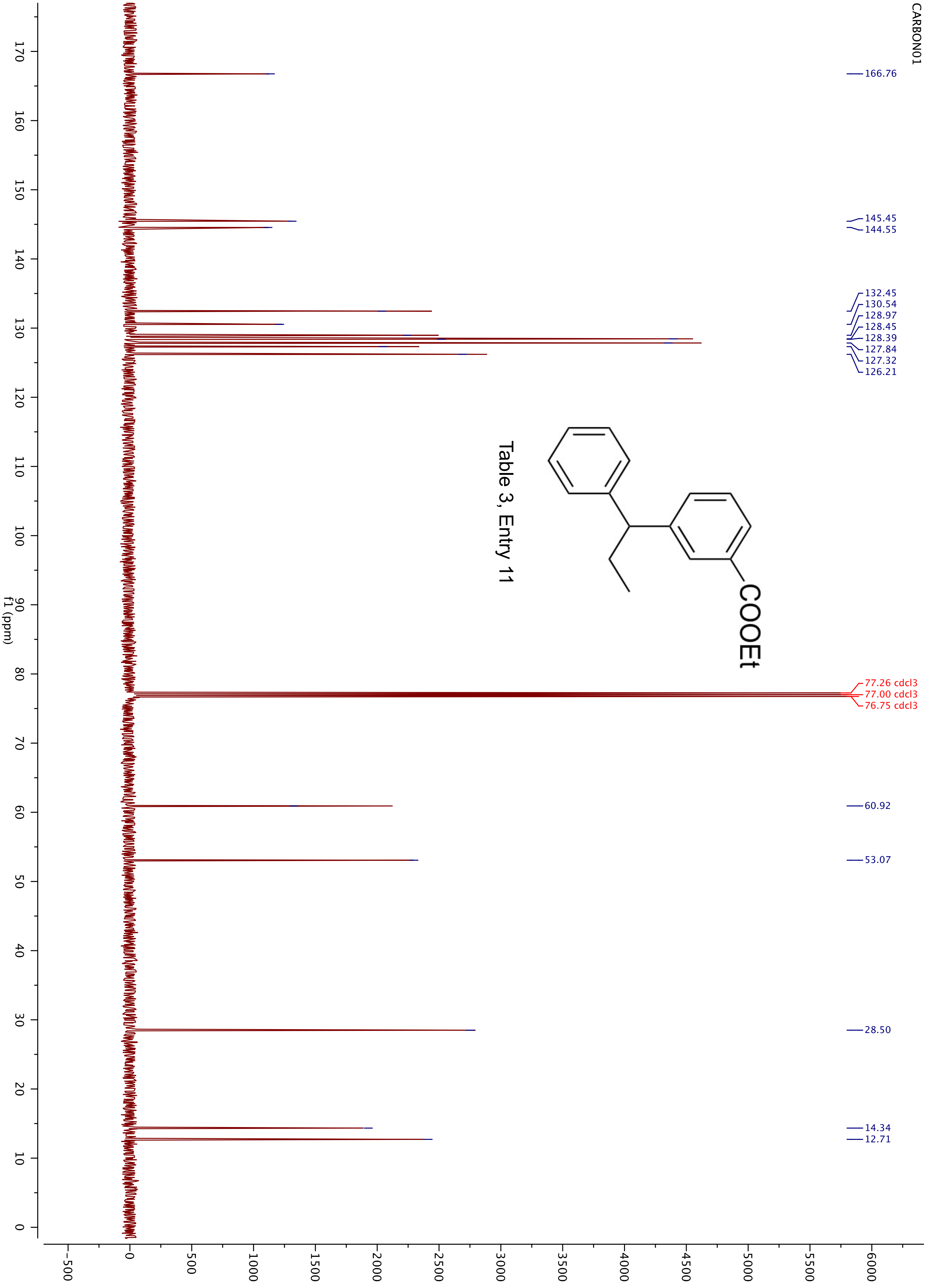


Table 3, Entry 11


CARBON01
Table 3, Entry 11
COOEt
166.76
145.45
144.55
132.45
130.54
128.97
128.45
128.39
127.84
127.32
126.21
77.26 cdcl3
77.00 cdcl3
76.75 cdcl3
60.92
53.07
28.50
14.34
12.71
f1 (ppm)
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-500
0
500
1000
1500
2000
2500
3000
3500
4000
4500
5000
5500
6000

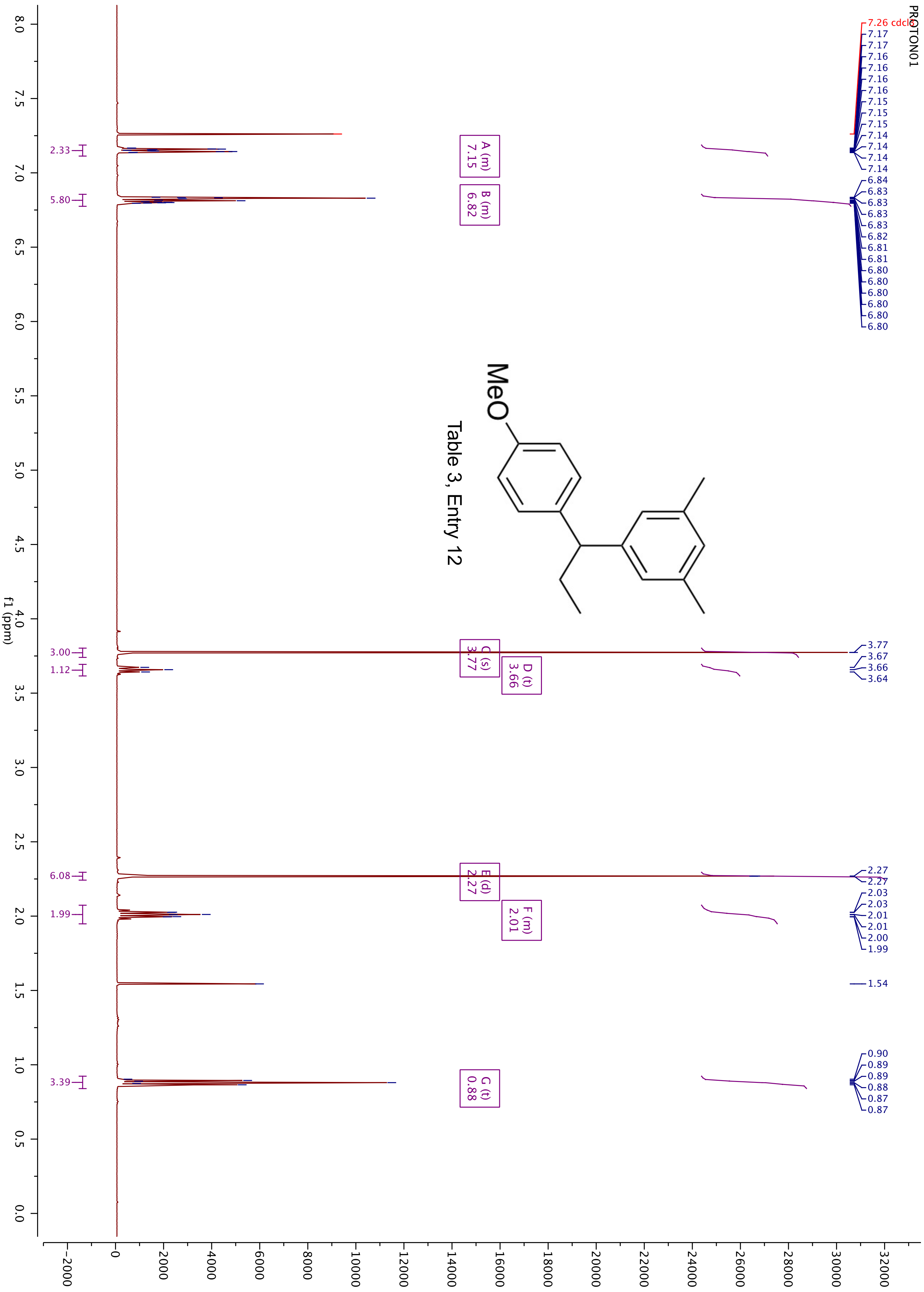
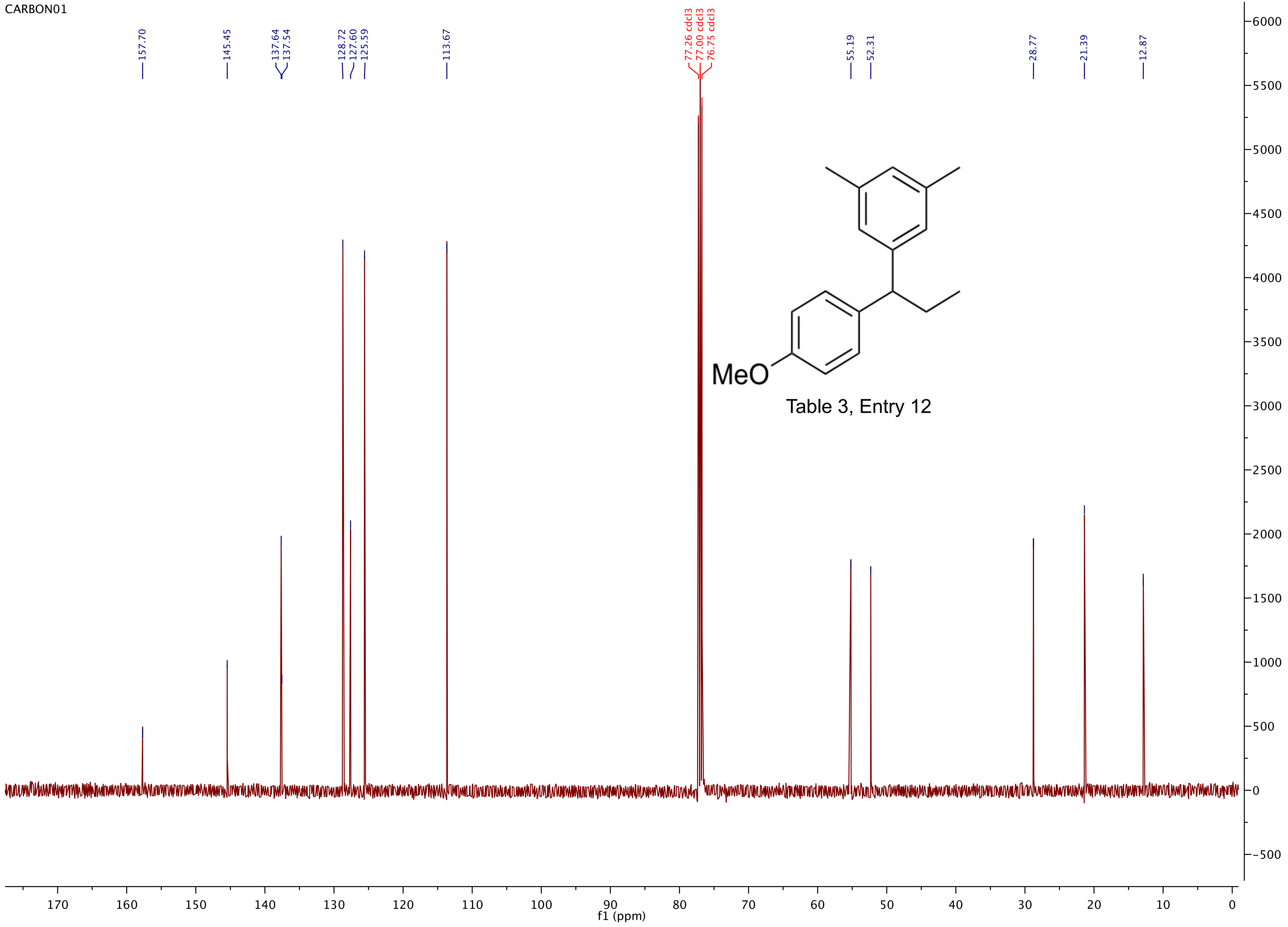


Table 3, Entry 12



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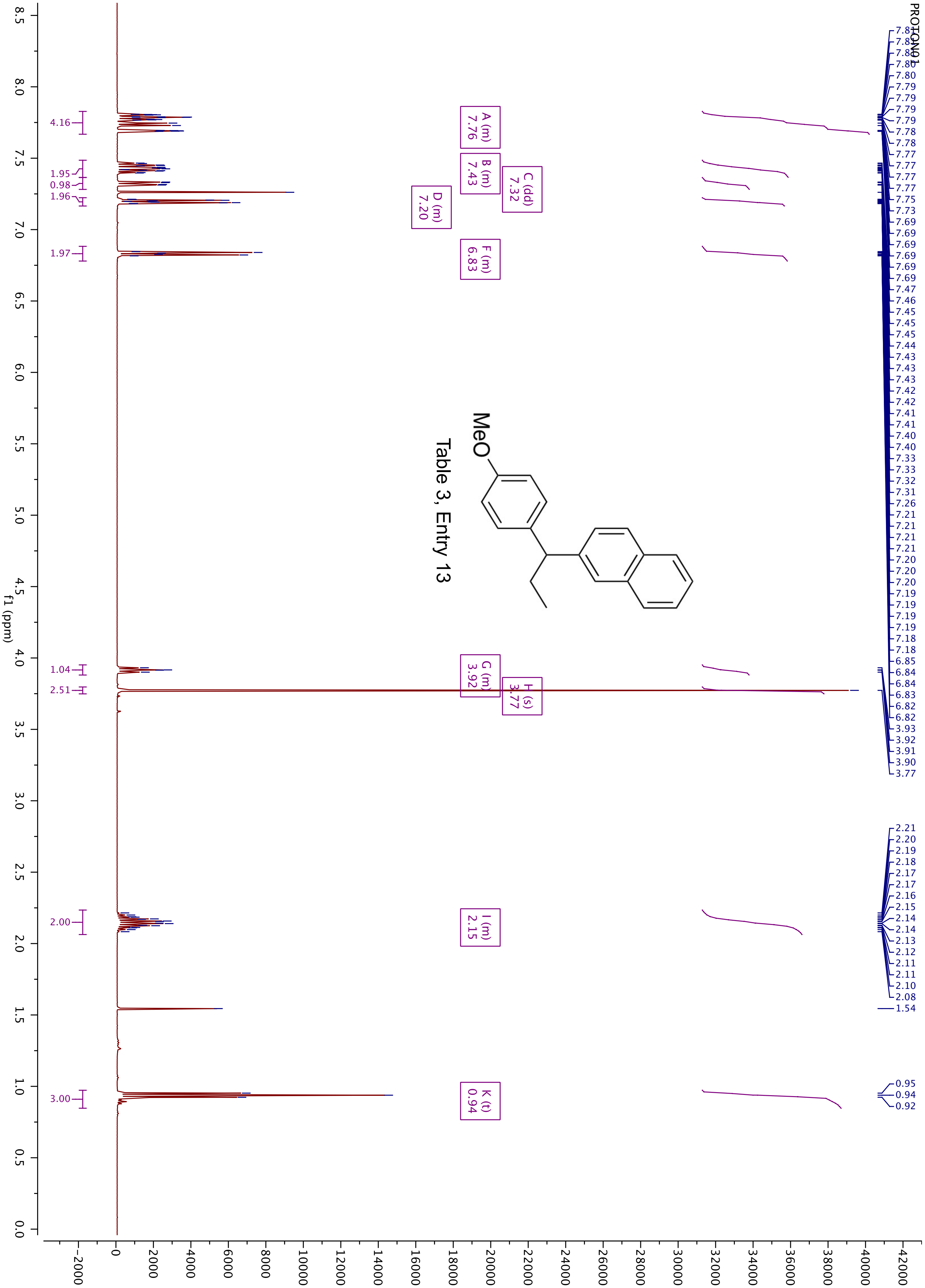

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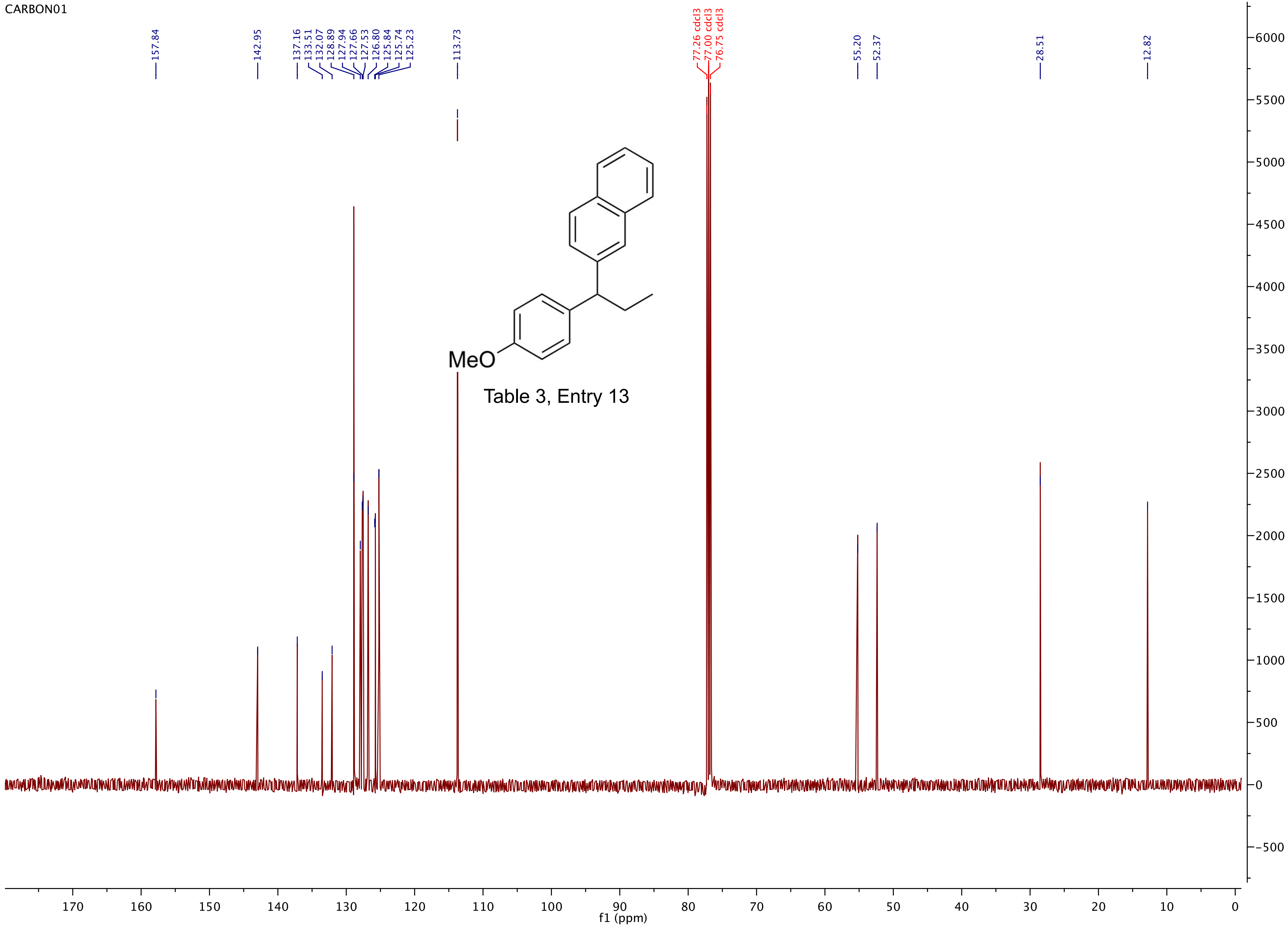

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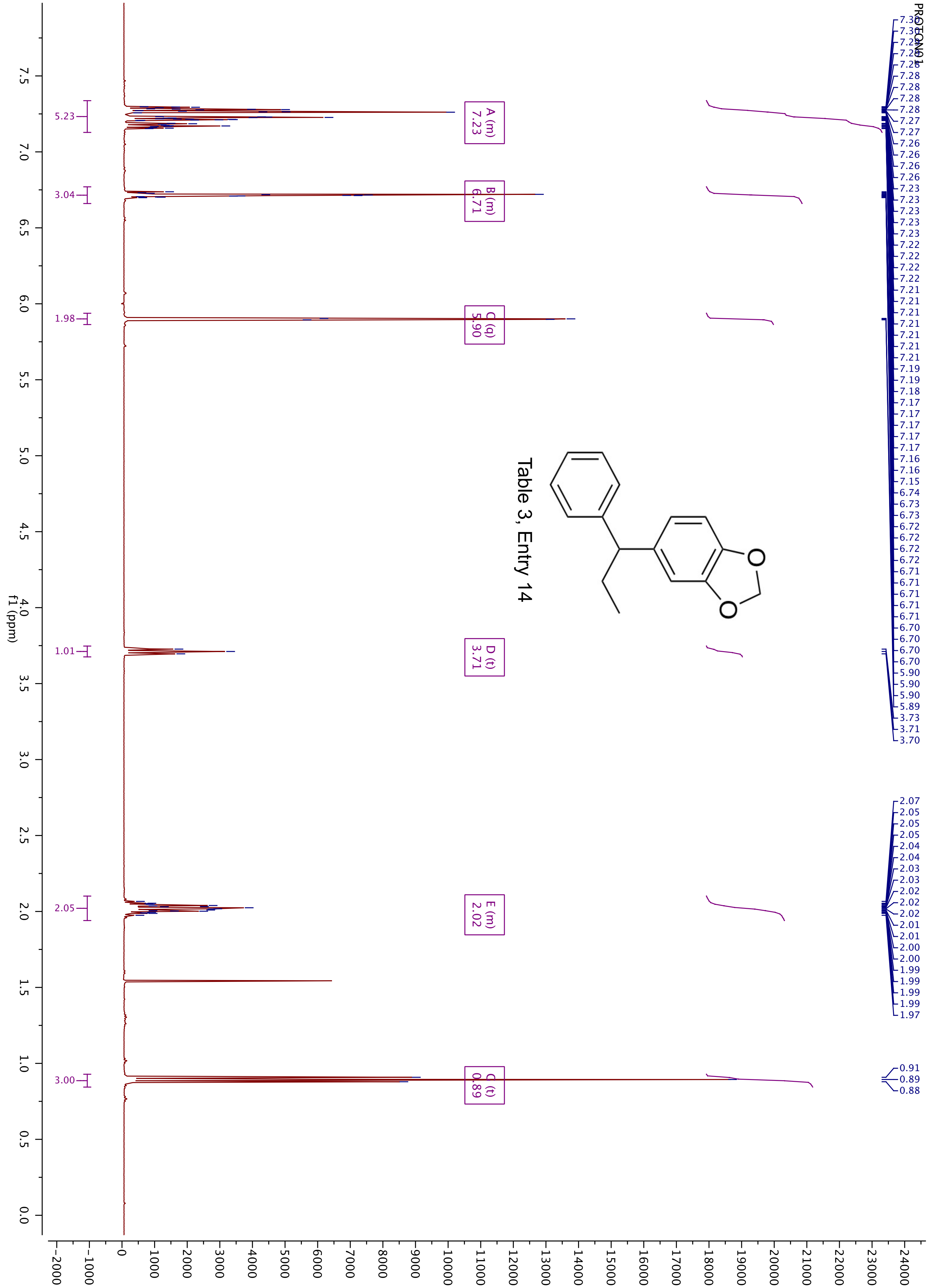
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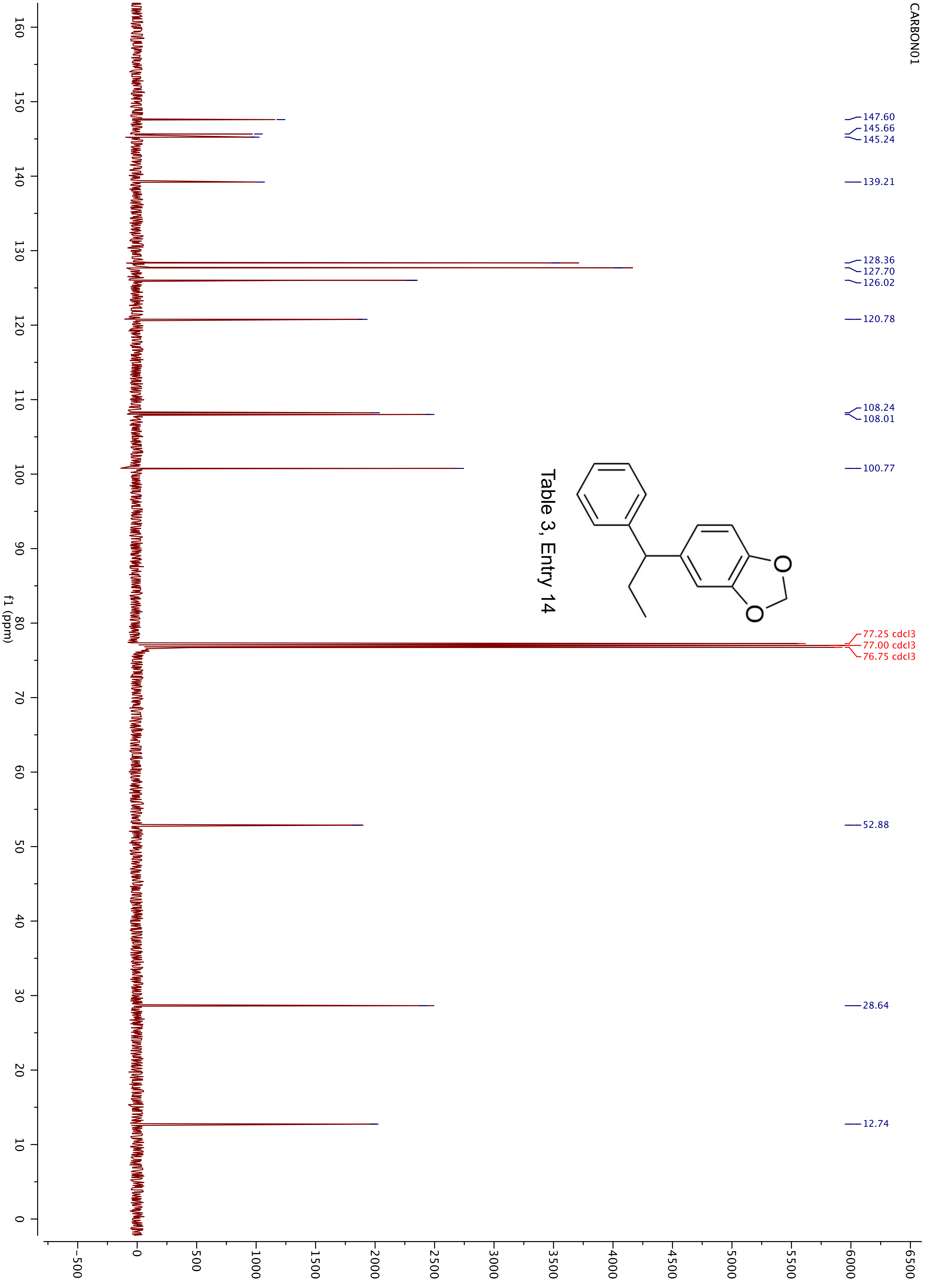

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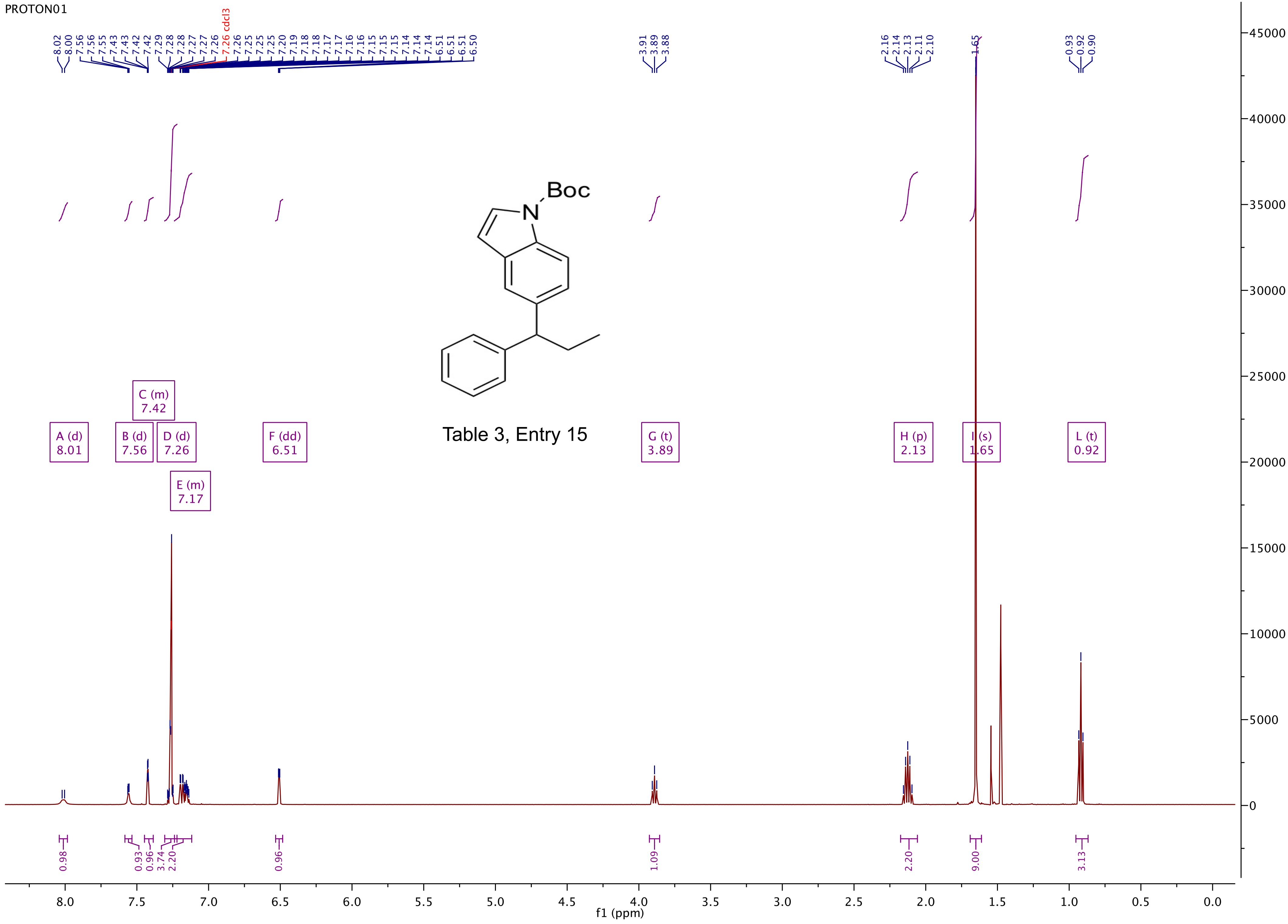

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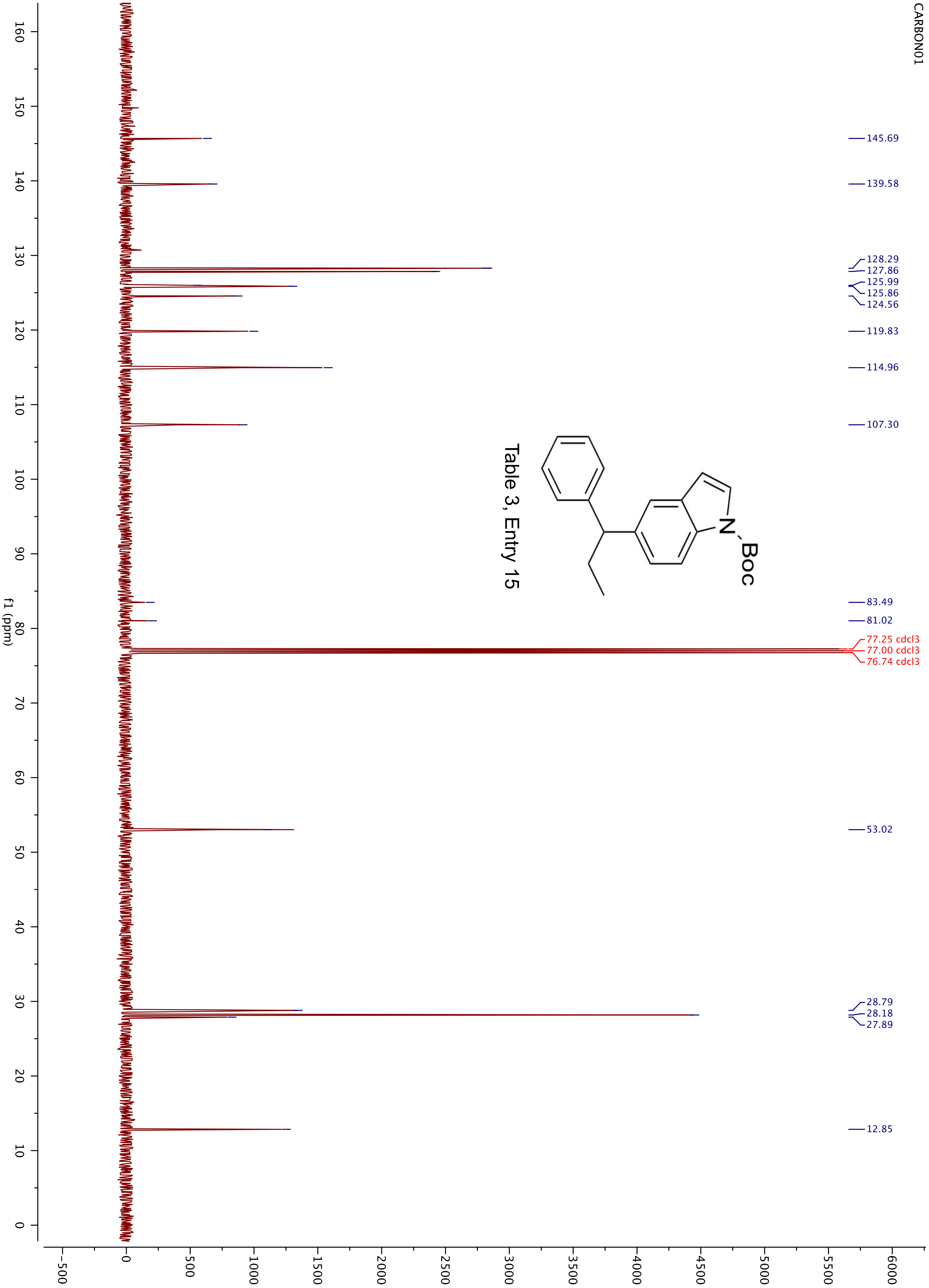
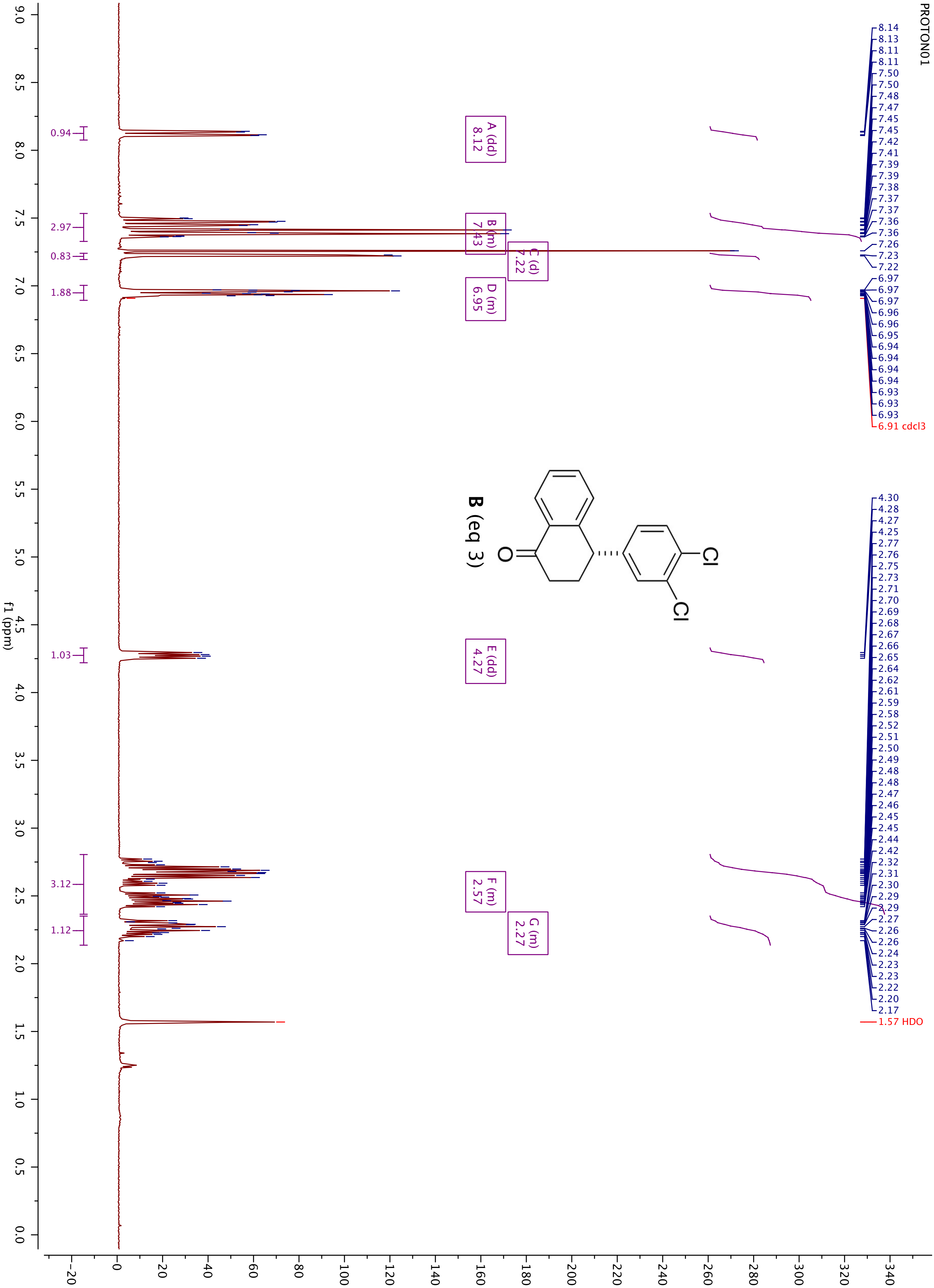
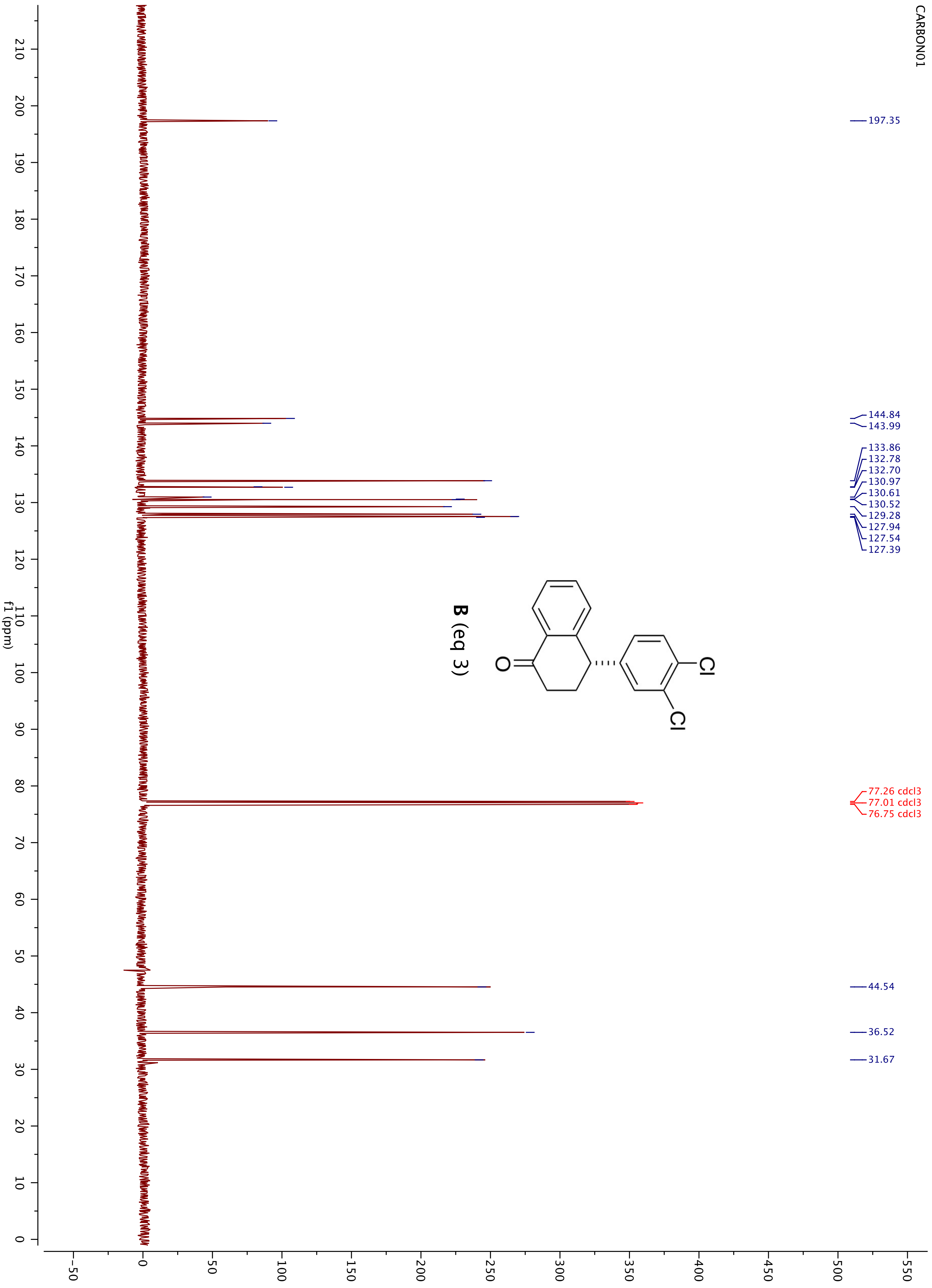

CARBON01
Table 3, Entry 15
N
Boc
145.69
139.58
128.29
127.86
125.99
125.86
124.56
119.83
114.96
107.30
83.49
81.02
77.25 cdcl3
77.00 cdcl3
76.74 cdcl3
53.02
28.79
28.18
27.89
12.85
f1 (ppm)
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-500
0
500
1000
1500
2000
2500
3000
3500
4000
4500
5000
5500
6000


PROTON01
B (eq 3)
Cl
Cl
O
A (dd) 8.12
B (m) 7.43
C (d) 7.22
D (m) 6.95
E (dd) 4.27
F (m) 2.57
G (m) 2.27
0.94
2.97
0.83
1.88
1.03
3.12
1.12
8.14
8.13
8.11
8.11
7.50
7.50
7.48
7.47
7.45
7.45
7.42
7.41
7.39
7.39
7.38
7.37
7.37
7.36
7.36
7.26
7.23
7.22
6.97
6.97
6.97
6.96
6.96
6.95
6.94
6.94
6.94
6.94
6.93
6.93
6.93
6.91 cdcl3
4.30
4.28
4.27
4.25
2.77
2.76
2.75
2.73
2.71
2.70
2.69
2.68
2.67
2.66
2.65
2.64
2.62
2.61
2.59
2.58
2.52
2.51
2.50
2.49
2.48
2.48
2.47
2.46
2.45
2.45
2.44
2.42
2.32
2.31
2.30
2.29
2.29
2.27
2.26
2.26
2.24
2.23
2.23
2.22
2.20
2.17
1.57 HDO
f1 (ppm)
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
-20
0
20
40
60
80
100
120
140
160
180
200
220
240
260
280
300
320
340


CARBON01
197.35
144.84
143.99
133.86
132.78
132.70
130.97
130.61
130.52
129.28
127.94
127.54
127.39
77.26 cdcl3
77.01 cdcl3
76.75 cdcl3
44.54
36.52
31.67
O
Cl
Cl
f1 (ppm)
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-50
0
50
100
150
200
250
300
350
400
450
500
550

B (eq 3)