SUPPORTING INFORMATION

Asymmetric Synthesis of Polycyclic 3-Fluoroalkylproline Derivatives by Intramolecular Azomethine Ylide Cycloaddition

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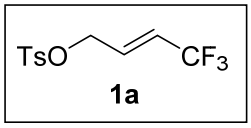
Contents

General methods

Reactions were carried out under a nitrogen atmosphere unless otherwise indicated. Solvents were purified prior to use: THF and PhMe were distilled from sodium, and CH_2Cl_2 was distilled from calcium hydride. The reactions were monitored with the aid of TLC on 0.25 mm precoated silica gel plates. Visualization was carried out with UV light and potassium permanganate stain. Flash column chromatography was performed with the indicated solvents on silica gel 60 (particle size 0.040−0.063 mm). ^{1}H, ^{19}F and ^{13}C NMR spectra were recorded on a 300 MHz spectrometer. Chemical shifts are given in ppm (δ), referenced to the residual proton resonances of the solvents. Coupling constants (J) are given in hertz (Hz). The letters m, s, d, t, and q stand for multiplet, singlet, doublet, triplet, and quartet, respectively. The designation br indicates that the signal is broad. The abbreviations DCM and THF indicate dichloromethane and tetrahydrofuran, respectively. A QTOF mass analyzer system has been used for the HRMS measurements.

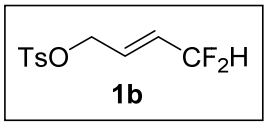
Preparation of tosylates 1

Tosylates **1** were synthesised following a literature procedure[1] from the corresponding crotonates, which were obtained in turn from the corresponding fluorinated oxoesters according to a reported procedure.[2]



1a

(E)-4,4,4-Trifluorobut-2-en-1-yl 4-methylbenzenesulfonate 1a: Starting from commercially available ethyl (*E*)-trifluorocrotonate and following the procedure referred above, **1a** was obtained as a colorless oil in 55% yield (over 2 steps). The spectroscopic data matched those from the literature. ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.85–7.77 (m, 2H), 7.41–7.33 (m, 2H), 6.36-6.25 (m, 1H), 5.96–5.81 (m, 1H), 4.67-4.62 (m, 2H), 2.46 (s, 3H). ^{19}F NMR (282 MHz, $CDCl_3$) δ -64.86–-64.93 (m, 3F). Spectroscopic data are in agreement with those reported in the literature.[1]

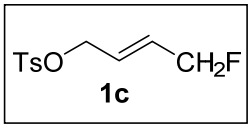


1b

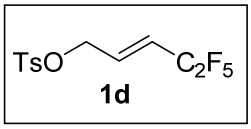
(*E*)-4,4-Difluorobut-2-en-1-yl 4-methylbenzenesulfonate 1b: Starting from ethyl (*E*)-difluorocrotonate and following the procedure referred above, **1b** was obtained as a colorless oil in 3% yield (over 2 steps). The low yield was attributed to the high volatility of the intermediate fluorinated alcohol. ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.84–7.72 (m, 2H), 7.43–7.32 (m, 2H), 6.39–5.66 (m,C*H*=C*H*-CF_2*H*, 3H), 4.71–4.50 (m, 2H), 2.46 (s, 3H). ^{19}F NMR (282 MHz, $CDCl_3$) δ -112.98–-113.33 (m, 2F). ^{13}C NMR (75 MHz, $CDCl_3$) δ 145.4, 132.9, 130.5 (t, *J* = 11.5 Hz),

[1] E. Forcellini, R. Hemelaere, J. Desroches, J.-F. Paquin, *J. Fluorine Chem.* 2015, **180**, 216.
[2] M. Berger, S. Veit, H. P. Niedermann, T. Kappesser, A., Stutz, A. Patent WO2015177179, 2015.

130.2, 128.1, 126.7 (t, J = 24.3 Hz), 113.5 (t, J = 235.6 Hz, $\underline{C}F_2H$), 67.8, 21.8. HRMS (ESI/Q-TOF) m/z: $[M+NH_4]^+$ Calcd for $C_{11}H_{16}F_2NO_3S$ 280.0813; found 280.0817.



(*E*)-4-fluorobut-2-en-1-yl 4-methylbenzenesulfonate 1c: This compound was prepared according to a different route from a reported procedure.[3] Spectroscopic data are in agreement with those from the literature. ^{1}H NMR (300 MHz, Chloroform-*d*) δ 7.84–7.75 (m, 2H), 7.39–7.31 (m, 2H), 6.03–5.69 (m, 2H), 4.93-4.72 (m, 2H), 4.60-4.54 (m, 2H), 2.45 (s, 3H). ^{19}F NMR (282 MHz, $CDCl_3$) δ -217.16–-217.58 (m, 1F).



(*E*)-4,4,5,5,5-Pentafluoropent-2-en-1-yl 4-methylbenzenesulfonate 1d: Starting from ethyl (*E*)-4,4,5,5,5-pentafluoropent-2-enoate and following the procedure referred above, **1c** was obtained as a colorless oil in 53% yield (over 2 steps). ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.84–7.77 (m, 2H), 7.39-7.36 (m, 2H), 6.40-6.30 (m, 1H), 5.93-5.79 (m, 1H), 4.70–4.65 (m, 2H), 2.46 (s, 3H). ^{19}F NMR (282 MHz, $CDCl_3$) δ -85.13 (t, J = 2.0 Hz, 3F), -116.20 (q, J = 2.0 Hz, 2F). ^{13}C NMR (75 MHz, $CDCl_3$) δ 145.7, 134.3 (t, J = 8.9 Hz), 132.6, 131.4-101.9 (m, C_2F_5), 130.2 (2xCH), 128.1 (2xCH), 119.5 (t, J = 23.7 Hz), 67.11, 21.8. HRMS (ESI/Q-TOF) m/z: $[M+H]^+$ Calcd for $C_{15}H_{16}F_3N_2O_5$; found. HRMS (ESI/Q-TOF) m/z: $[M+NH_4]^+$ Calcd for $C_{12}H_{15}F_5NO_3S$ 348.0687; found 348.0688.

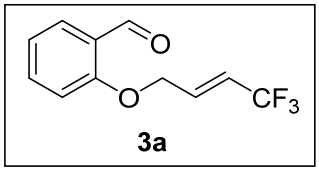
General procedure for the synthesis of starting fluorinated benzaldehydes 3a-p.

This procedure was adapted from the literature procedure.[4] A solution of the corresponding commercially available salicylaldehyde **2a-g** or *N*-(2-formylaryl)-4-methylbenzenesulfonamide **2h-k**[5] (0.78 mmol, 1.1 equiv) and K_2CO_3 (98 mg, 0.71 mmol, 1.0 equiv) in dry acetonitrile (2 mL) in a pressure vial was heated in an oil bath at 60ºC for 10 min. A solution of the corresponding tosylate **1** (200 mg, 0.71 mmol, 1.0 equiv) in dry acetonitrile (2 mL) was added and the resulting mixture was heated at the same temperature for 16 h. Water (4 mL) was added to quench the reaction and the aqueous phase was extracted with ethyl acetate (3x 10 mL). The combined organic phases were washed with brine (30 mL), dried over anhydrous sodium sulfate and concentrated under reduced pressure. The crude was purified by flash chromatography on silica gel [*n*-hexane-EtOAc (10:1)] to afford fluorinated benzaldehydes **3a-p**.

[3] F. Dollé, P. Emond, S. Mavel, S. Demphel, F. Hinnen, Z. Mincheva, W. Saba, H. Valette, S. Chalon, C. Halldin, J. Helfenbein, J. Legaillard, J.-C. Madelmont, J.-B. Deloye, M. Bottlaender, D. Guilloteau. *Bioorg. Med. Chem.* 2006, ***14***, 1115.

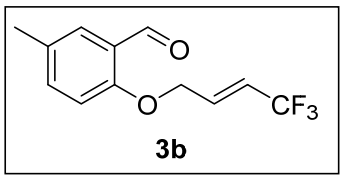
[4] E. Forcellini, R. Hemelaere, J. Desroches, J.-F. Paquin, *J. Fluorine Chem.* 2015, **180**, 216.

[5] M. Giustiniano, S. Pelliccia, L. Sangaletti, F. Meneghetti, J. Amato, E. Novellino, G. C. Tron, *Tetrahedron Lett.* 2017, **58**, 4264.



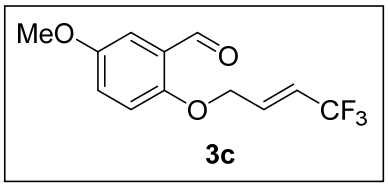
3a

(*E*)-2-[(4,4,4-Trifluorobut-2-en-1-yl)oxy]benzaldehyde (3a): Starting from salicylaldehyde **2a** and tosylate **1a** and following the procedure described above, **3a** was obtained as a white solid (mp = 51-53 ºC) in 85% yield (139 mg). ^{1}H NMR (300 MHz, $CDCl_3$) δ 10.53 (d, *J* = 0.7 Hz, 1H), 7.88 (dd, *J* = 7.7, 1.8 Hz, 1H), 7.57 (ddd, *J* = 8.4, 7.4, 1.8 Hz, 1H), 7.15–7.06 (m, 1H), 6.95 (d, *J* = 8.4 Hz, 1H), 6.66-6.56 (m, 1H), 6.19–6.02 (m, 1H), 4.84–4.73 (m, 2H). ^{19}F NMR (282 MHz, $CDCl_3$) δ -64.46--64.51 (m, 3F). ^{13}C NMR (75 MHz, $CDCl_3$) δ 189.2, 160.0, 136.1, 134.2 (q, *J* = 6.5 Hz), 129.4, 125.3, 121.8, 120.5, 120.2 (q, 34.4 Hz), 118.2 (q, *J* = 275. Hz, CF_3), 116.4, 112.6, 66.2. HRMS (ESI/Q-TOF) m/z: $[M+Me]^+$ Calcd for $C_{12}H_{12}F_3O_2$ 245.0784; found 245.0786. (Methanol was used for sample preparation).



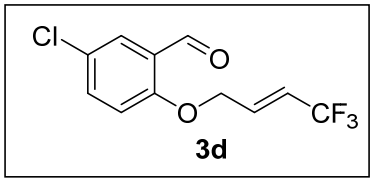
3b

(*E*)-5-Methyl-2-[(4,4,4-trifluorobut-2-en-1-yl)oxy]benzaldehyde (3b): Starting from 5-methylsalicylaldehyde **2b** and tosylate **1a** and following the procedure described above, **3b** was obtained as a white solid (mp = 50-52 ºC) in 78% yield (136 mg). ^{1}H NMR (300 MHz, $CDCl_3$) δ 10.50 (s, 1H), 7.67 (d, *J* = 2.2 Hz, 1H), 7.36 (ddd, *J* = 8.5, 2.2, 0.6 Hz, 1H), 6.84 (d, *J* = 8.5 Hz, 1H), 6.67–6.53 (m, 1H), 6.20–6.00 (m, 1H), 4.81–4.69 (m, 2H), 2.33 (s, 3H). ^{19}F NMR (282 MHz, $CDCl_3$) δ -64.44--64.497 (m, 3F). ^{13}C NMR (75 MHz, $CDCl_3$) δ 189.4, 158.2, 136.7, 134.4 (d, *J* = 6.4 Hz), 131.4), 129.3, 125.0, 121.7 (d, *J* = 273.5 Hz).120.1 (d, *J* = 34.6 Hz), 112.7, 66.4, 20.4. HRMS (ESI/Q-TOF) m/z: $[M+H]^+$ Calcd for $C_{12}H_{12}F_3O_2$ 245.0784; found 245.0786.



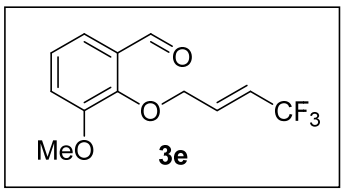
3c

(*E*)-5-Chloro-2-[(4,4,4-trifluorobut-2-en-1-yl)oxy]benzaldehyde (3c): Starting from 5-chlorosalicylaldehyde **2c** and tosylate **1a** and following the procedure described above, **3c** was obtained as a white solid (mp = 33-35 ºC) in 93% yield (174 mg). ^{1}H NMR (300 MHz, $CDCl_3$) δ 10.39 (s, 1H), 7.76 (d, *J* = 2.7 Hz, 1H), 7.44 (dd, *J* = 8.9, 2.7 Hz, 1H), 6.84 (d, *J* = 8.9 Hz, 1H), 6.57-6.47 (m, 1H), 6.10–5.91 (m, 1H), 4.75–4.66 (m, 2H). ^{19}F NMR (282 MHz, $CDCl_3$) δ -64.53--64.58 (m, 3F). ^{13}C NMR (75 MHz, $CDCl_3$) δ 187.8, 158.5, 135.6, 133.7 (q, *J* = 6.4 Hz), 128.9, 127.6, 126.3 (q, *J* = 274.1 Hz, CF_3), 126.2, 120.5 (q, *J* = 34.7 Hz), 66.6. HRMS (ESI/Q-TOF) m/z: $[M+Me]^+$ Calcd for $C_{12}H_{11}ClF_3O_2$ 279.0394; found 279.0393. (Methanol was used for sample preparation.



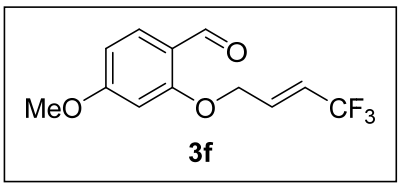
3d

(*E*)-5-Methoxy-2-[(4,4,4-trifluorobut-2-en-1-yl)oxy]benzaldehyde (3d): Starting from 5-methoxysalicylaldehyde **2d** and tosylate **1a** and following the procedure described above, **3d** was obtained as a white solid (mp = 55-57 ºC) in 69% yield (127 mg). ^{1}H NMR (300 MHz, $CDCl_3$) δ 10.50 (s, 1H), 7.36 (d, *J* = 3.3 Hz, 1H), 7.13 (dd, *J* = 9.0, 3.3 Hz, 1H), 6.90 (d, *J* = 9.0 Hz, 1H), 6.64-6.54 (m, 1H), 6.14–6.00 (m, 1H), 4.78–4.70 (m, 2H), 3.82 (s, 3H). ^{19}F NMR (282 MHz, $CDCl_3$) δ -64.45--64.50 (m, 3F). ^{13}C NMR (75 MHz, $CDCl_3$) δ 189.1, 155.0, 154.6, 134.6 (q, *J* = 6.3 Hz), 127.6 (q, *J* = 275.3 Hz, CF_3), 125.8, 123.6, 120.2 (q, *J* = 34.5 Hz), 114.8, 111.2, 67.1, 56.1. HRMS (ESI/Q-TOF) m/z: $[M+Me]^+$ Calcd for $C_{13}H_{14}F_3O_3$ 275.0878; found 275.0888. (Methanol was used for sample preparation).



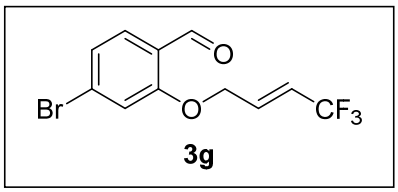
3e

(*E*)-3-methoxy-2-((4,4,4-trifluorobut-2-en-1-yl)oxy)benzaldehyde (3e): Starting from 3-methoxysalicylaldehyde **2e** and tosylate **1a** and following the procedure described above, **3e** was obtained as a white solid in 86% yield (160 mg). The product could not be separated from the excess of 3-methoxysalicylaldehyde and was used as a mixture in the subsequent step. The given yield has already been corrected considering the purity of the product. ^{1}H NMR (500 MHz, $CDCl_3$) δ 10.4 (s, 1H), 7.44 (dd, *J* = 6.5, 2.9 Hz, 1H), 7.19–7.17 (m, 2H), 6.60-6.54 (m, 1H), 6.16–6.06 (m, 1H), 4.76 (m, 2H), 3.90 (s, 3H). ^{19}F NMR (471 MHz, $CDCl_3$) δ -64.41--64.42 (m, 3F).



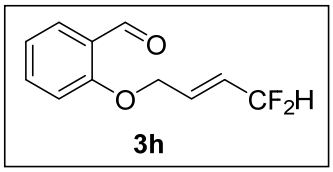
3f

(*E*)-4-methoxy-2-((4,4,4-trifluorobut-2-en-1-yl)oxy)benzaldehyde (3f): Starting from salicylaldehyde **2f** and tosylate **1a** and following the procedure described above, **3f** was obtained as a light yellow solid (mp=59-61 °C) in 82% yield (152 mg). ^{1}H NMR (300 MHz, $CDCl_3$) δ 10.35 (s, 1H), 7.85 (d, *J* = 8.7 Hz, 1H), 6.66–6.52 (m, 2H), 6.40 (d, *J* = 2.2 Hz, 1H), 6.18-6.04 (m, 1H), 4.78-4.72 (m, 2H), 3.88 (s, 3H).^{19}F NMR (282 MHz, $CDCl_3$) δ -64.47--64.52 (m, 3F). ^{13}C NMR (75 MHz, $CDCl_3$) δ 187.8, 166.2, 161.7, 134.0 (q, *J* = 6.4 Hz), 131.5, 122.8 (q, *J* = 269.4 Hz, CF_3), 120.2 (q, *J* = 34.5 Hz), 106.5, 99.3, 66.2. HRMS (ESI/Q-TOF) m/z: $[M+H]^+$ Calcd for $C_{12}H_{12}F_3O_3$ 261.0733; found 261.0735.



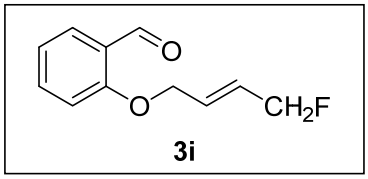
3g

(*E*)-4-bromo-2-((4,4,4-trifluorobut-2-en-1-yl)oxy)benzaldehyde (3g): Starting from salicylaldehyde **2g** and tosylate **1a** and following the procedure described above, **3g** was obtained as a white solid (mp=89-91 °C) in 55% yield (121 mg). ^{1}H NMR (300 MHz, $CDCl_3$) δ 10.45 (d, *J* = 0.7 Hz, 1H), 7.74 (d, *J* = 8.3 Hz, 1H), 7.28-7.24 (m, 1H), 7.13 (d, *J* = 1.6 Hz, 1H), 6.66–6.53 (m, 1H), 6.17-6.03 (m, 1H), 4.83–4.73 (m, 2H). ^{19}F NMR (282 MHz, $CDCl_3$) δ -64.54--64.58 (m, 3F). ^{13}C NMR (75 MHz, $CDCl_3$) δ 188.2, 160.1, 133.5 (q, *J* = 6.4 Hz), 130.7, 130.5, 125.4, 124.1, 123.4 (q, *J* = 275.4 Hz, CF_3), 120.6 (q, *J* = 34.7 Hz), 116.3, 66.6. HRMS (ESI/Q-TOF) m/z: $[M+H]^+$ Calcd for $C_{11}H_9BrF_3O_2$ 308.9733; found 308.9732.



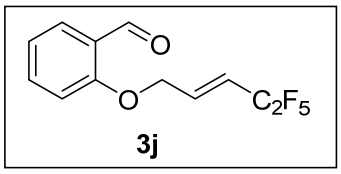
3h

(*E*)-2-[(4,4-Difluorobut-2-en-1-yl)oxy]benzaldehyde (3h): Starting from salicylaldehyde **2a** and tosylate **1b** and following the procedure described above, **3h** was obtained as a colorless oil in 69% yield (104 mg). ^{1}H NMR (300 MHz, $CDCl_3$) δ 10.54 (d, *J* = 0.7 Hz, 1H), 7.87 (dd, *J* = 7.7, 1.8 Hz, 1H), 7.56 (ddd, *J* = 8.4, 7.4, 1.8 Hz, 1H), 7.13–7.04 (m, 1H), 6.95 (d, *J* = 8.4 Hz, 1H), 6.41–5.90 (m, C*H*=C*H*-CF_2*H*, 3H), 4.78-4.73 (m, 2H). ^{19}F NMR (282 MHz, $CDCl_3$) δ -112.11–-112.51 (m, 2F). ^{13}C NMR (75 MHz, $CDCl_3$) δ 189.4, 160.4, 136.1, 132.8 (t, *J* = 11.4 Hz), 129.1, 125.3, 125.3 (t, *J* = 24.2 Hz), 121.6, 114.1 (t, *J* = 235.2 Hz, *C*F_2H), 112.7, 66.9. HRMS (ESI/Q-TOF) m/z: $[M+H]^+$ Calcd for $C_{11}H_{11}F_2O_2$ 213.0722; found 213.0722.



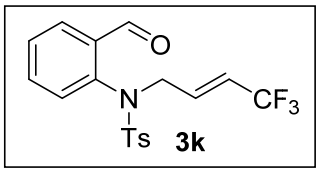
3i

(*E*)-2-((4-fluorobut-2-en-1-yl)oxy)benzaldehyde (3i): Starting from salicylaldehyde **2a** and tosylate **1c** and following the procedure described above, **3i** was obtained as a colorless oil in 71% yield (98 mg). ^{1}H NMR (300 MHz, Chloroform-*d*) δ 10.53 (d, *J* = 0.8 Hz, 1H), 7.85 (dd, *J* = 7.7, 1.8 Hz, 1H), 7.54 (ddd, *J* = 8.4, 7.3, 1.9 Hz, 1H), 7.10–7.00 (m, 1H), 7.00–6.93 (m, 1H), 6.41–5.89 (m, 2H), 5.08–4.80 (m, 2H), 4.73-4.67 (dt, *J* = 4.9, 2.4 Hz, 2H). ^{19}F NMR (282 MHz, Chloroform-*d*) δ -215.01–-215.61 (m, 1F). ^{13}C NMR (75 MHz, Chloroform-*d*) δ 189.7, 160.8, 136.0, 128.8, 128.3 (d, *J* = 6.2 Hz), 128.1 (d, *J* = 11.2 Hz), 125.3, 121.2, 112.8, 82.4 (d, *J* = 164.9 Hz, *C*H_2F), 68.0. HRMS (ESI/Q-TOF) m/z: $[M+H]^+$ Calcd for $C_{11}H_{12}FO_2$ 195.0816; found 195.0820.



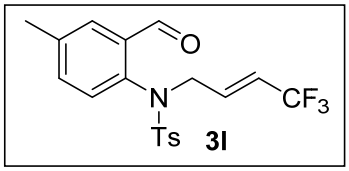
3j

(*E*)-2-[(4,4,5,5,5-Pentafluoropent-2-en-1-yl]oxy)benzaldehyde (3j): Starting from salicylaldehyde **2a** and tosylate **1d** and following the procedure described above, **3j** was obtained as a colorless oil in 63% yield (125 mg). ^{1}H NMR (300 MHz, $CDCl_3$) δ 10.53 (d, *J* = 0.7 Hz, 1H), 7.88 (dd, *J* = 7.7, 1.8 Hz, 1H), 7.57 (ddd, *J* = 8.4, 7.4, 1.8 Hz, 1H), 7.16–7.07 (m, 1H), 6.95 (d, *J* = 8.4 Hz, 1H), 6.72–6.59 (m, 1H), 6.15-6.02 (m, 1H), 4.88–4.76 (m, 2H). ^{19}F NMR (282 MHz, $CDCl_3$) δ -85.11 (t, *J* = 1.8 Hz, 3F), -115.83--115.91 (m, 2F). ^{13}C NMR (75 MHz, $CDCl_3$) δ 189.3, 160.1, 136.5 (t, *J* = 9.2 Hz), 136.2, 129.5, 125.4, 122.0, 121.3-116.3 (m, C_2F_5), 118.6 (t, *J* = 23.8 Hz), 112.7, 66.7. HRMS (ESI/Q-TOF) m/z: $[M+H]^+$ Calcd for $C_{12}H_{10}F_5O_2$ 281.0595; found 281.0594.



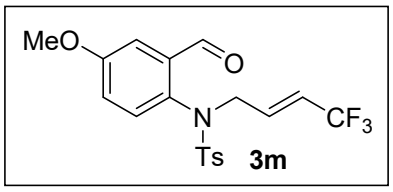
3k

(*E*)-N-(2-Formylphenyl)-4-methyl-*N*-(4,4,4-trifluorobut-2-en-1-yl)benzenesulfonamide (3k): Starting from *N*-(2-formylphenyl)-4-methylbenzenesulfonamide **2h** and tosylate **1a** and following the procedure described above, **3k** was obtained as a white solid (mp = 99-101 ºC) in 83% yield (225 mg). ^{1}H NMR (300 MHz, $CDCl_3$) δ 10.29 (d, *J* = 0.5 Hz, 1H), 8.06–7.95 (m, 1H), 7.55–7.44 (m, 4H), 7.32-7.28 (m, 2H), 6.84–6.73 (m, 1H), 6.40–6.26 (m, 1H), 5.76–5.59 (m, 1H), 4.61-3.97 (m, 2H, CH_2), 2.45 (s, 3H). ^{19}F NMR (282 MHz, $CDCl_3$) δ -64.73--64.77 (m, 3F). ^{13}C NMR (75 MHz, $CDCl_3$) δ 189.5, 144.9, 141.0, 135.8, 134.6, 134.4, 134.1 (d, *J* = 6.4 Hz), 131.6 (q, *J* = 272.5 Hz, CF_3), 130.1, 129.5 (q, *J* = 11.6 Hz), 128.6, 128.2, 123.1 (q, *J* = 34.5 Hz), 52.3, 21.9. HRMS (ESI/Q-TOF) m/z: $[M+H]^+$ Calcd for $C_{18}H_{17}F_3NO_3S$ 384.0876; found 384.0876.

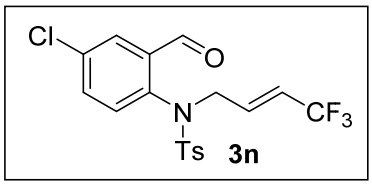


3l

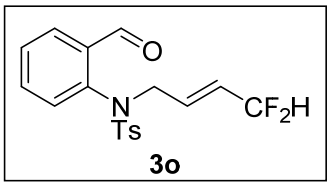
(*E*)-*N*-(2-Formyl-4-methylphenyl)-4-methyl-*N*-(4,4,4-trifluorobut-2-en-1-yl) benzenesulfonamide (3l): Starting from *N*-(2-formyl-4-methylphenyl)-4-methylbenzenesulfonamide **2i** and tosylate **1a** and following the procedure described above, **3l** was obtained as a white solid (mp = 70-72 ºC) in 83% yield (233 mg). ^{1}H NMR (300 MHz, $CDCl_3$) δ 10.24 (s, 1H), 7.79 (d, *J* = 2.1 Hz, 1H), 7.53–7.43 (m, 2H), 7.35–7.27 (m, 3H), 6.67 (d, *J* = 8.1 Hz, 1H), 6.38-6.26 (m, 1H), 5.76–5.60 (m, 1H), 4.60-3.95 (m, 2H, CH_2), 2.45 (s, 3H), 2.42 (s, 3H). ^{19}F NMR (282 MHz, $CDCl_3$) δ -64.69--64.73 (m, 3F). ^{13}C NMR (75 MHz, $CDCl_3$) δ 189.8, 144.8, 139.8, 138.4, 135.4, 134.5, 134.2 (q, *J* = 6.4 Hz), 130.1, 129.9, 128.6 (q, *J* = 275.6 Hz, CF_3), 128.4, 128.2, 123.0 (q, *J* = 34.4 Hz), 52.4, 21.9, 21.3. HRMS (ESI/Q-TOF) m/z: $[M+H]^+$ Calcd for $C_{19}H_{19}F_3NO_3S$ 398.1032; found 398.1040.



(*E*)-*N*-(2-Formyl-4-methoxyphenyl)-4-methyl-*N*-(4,4,4-trifluorobut-2-en-1-yl) benzenesulfonamide (3m): Starting from *N*-(2-formyl-4-methoxyphenyl)-4-methylbenzenesulfonamide **2j** and tosylate **1a** and following the procedure described above, **3m** was obtained as a white solid (mp = 81-83 ºC) in 88% yield (258 mg). ^{1}H NMR (300 MHz, $CDCl_3$) δ 10.24 (s, 1H), 7.52–7.42 (m, 3H), 7.29 (d, *J* = 8.0 Hz, 2H), 7.01 (dd, *J* = 8.8, 3.1 Hz, 1H), 6.65 (d, *J* = 8.8 Hz, 1H), 6.37-6.27 (m, 1H), 5.76–5.61 (m, 1H), 4.58-4.44 (m, 1H, CH_2), 4.21–3.97 (m, 1H, CH_2), 3.87 (s, 3H), 2.45 (s, 3H). ^{19}F NMR (282 MHz, $CDCl_3$) δ -64.68--64.72 (m, 3F). ^{13}C NMR (75 MHz, $CDCl_3$) δ 189.4, 159.8, 144.7, 136.7, 134.3, 134.0 (q, *J* = 6.4 Hz), 133.6, 130.0, 129.6, 128.1, 122.9 (q, *J* = 34.5 Hz), 122.1 (q, *J* = 269.9 Hz, CF_3), 121.8, 111.6, 55.9, 52.3, 21.8. HRMS (ESI/Q-TOF) m/z: $[M+H]^+$ Calcd for $C_{19}H_{19}F_3NO_4S$ 414.0981; found 414.0982.

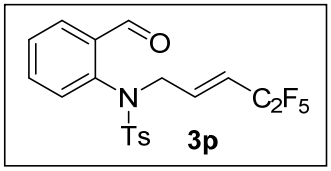


(*E*)-*N*-(4-Chloro-2-formylphenyl)-4-methyl-*N*-(4,4,4-trifluorobut-2-en-1-yl) benzenesulfonamide (3n): Starting from *N*-(4-chloro-2-formylphenyl)-4-methylbenzenesulfonamide **2k** and tosylate **1a** and following the procedure described above, **3n** was obtained as a white solid (mp = 98-100 ºC in 75% yield (222 mg). ^{1}H NMR (300 MHz, $CDCl_3$) δ 10.23 (s, 1H), 7.96 (d, *J* = 2.5 Hz, 1H), 7.49-7.44 (m, 3H), 7.30-7.33 (m, 2H), 6.70 (d, *J* = 8.5 Hz, 1H), 6.43–6.18 (m, 1H), 5.86–5.60 (m, 1H), 4.34 (m, 2H, CH_2), 2.46 (s, 3H). ^{19}F NMR (282 MHz, $CDCl_3$) δ -64.73--64.77 (m, 3F). ^{13}C NMR (75 MHz, $CDCl_3$) δ 188.0, 145.1, 139.2, 136.9, 135.8, 134.3, 133.9, 133.6 (q, *J* = 6.5 Hz), 130.1, 129.7, 129.3, 128.2 (q, *J* = 270.8 Hz, CF_3), 128.1, 123.3 (q, *J* = 34.4 Hz), 52.1, 21.8. HRMS (ESI/Q-TOF) m/z: $[M+H]^+$ Calcd for $C_{18}H_{16}F_3ClNO_3S$ 418.0486; found 418.0487.



(*E*)-N-(4,4-difluorobut-2-en-1-yl)-N-(2-formylphenyl)-4-methylbenzenesulfonamide (3o): Starting from salicylaldehyde **2h** and tosylate **1b** and following the procedure described above, **3o** was obtained as a white solid (mp=114-116 °C) in 55% yield (143 mg). ^{1}H NMR (300 MHz, $CDCl_3$) δ 10.33 (d, *J* = 0.5 Hz, 1H), 8.07–7.95 (m, 1H), 7.56–7.43 (m, 4H), 7.32-7.27 (m, 2H), 6.82–6.72 (m, 1H), 6.22–5.73 (m, 2H, C*H*=CH-CF_2*H*), 5.73–5.51 (m, 1H), 4.70-3.85 (m, 2H, CH_2). ^{19}F NMR (282 MHz, $CDCl_3$) δ -112.20--112.46 (m, 2F). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 189.7, 144.7, 141.1, 135.8, 134.4, 134.3, 132.5 (t, *J* = 11.4 Hz), 130.0 (2xCH),

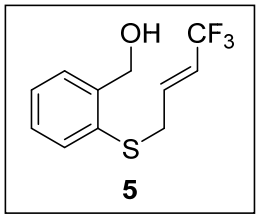
129.2, 128.1 (2xCH), 128.0 (t, J = 24.4 Hz), 113.6 (t, J = 235.2 Hz, CF_2H), 52.7, 21.8. HRMS (ESI/Q-TOF) m/z: $[M+H]^+$ Calcd for $C_{18}H_{18}F_2NO_3S$ 366.0970; found 366.0969.



3p

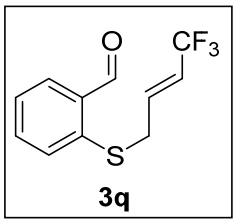
(*E*)-N-(2-Formylphenyl)-4-methyl-N-(4,4,5,5,5-pentafluoropent-2-en-1-yl) benzenesulfonamide (3p): Starting from *N*-(2-formylphenyl)-4-methylbenzenesulfonamide **2h** and tosylate **1d** and following the procedure described above, **3p** was obtained as a white solid (mp = 69-71 ºC) in 83% yield (255 mg). ^{1}H NMR (300 MHz, $CDCl_3$) δ 10.29 (s, 1H), 8.05–7.96 (m, 1H), 7.54–7.45 (m, 4H), 7.30 (d, J = 8.0 Hz, 2H), 6.83–6.72 (m, 1H), 6.45–6.28 (m, 1H), 5.69-5.57 (m, 1H), 4.65-4.05 (m, 2H, CH_2), 2.45 (s, 3H). ^{19}F NMR (282 MHz, $CDCl_3$) δ -85.29 (t, J = 1.7 Hz, 3F), -116.16–-116.37 (m, 2F). ^{13}C NMR (75 MHz, $CDCl_3$) δ 189.4, 144.8, 140.7, 136.1 (t, J = 9.8 Hz), 135.7, 134.4, 134.3, 130.0, 129.5, 129.3, 128.5, 128.1, 125.3-117.9 (m, C_2F_5), 121.7 (t, J = 23.8 Hz), 52.5, 21.8. HRMS (ESI/Q-TOF) m/z: $[M+H]^+$ Calcd for $C_{19}H_{17}F_5NO_3S$ 434.0844; found 434.0846.

Synthesis of (*E*)-2-((4,4,4-trifluorobut-2-en-1-yl)thio)benzaldehyde (3q): This synthesis was adapted from the literature procedure.[6]



5

(*E*)-[2-(4,4,4-Trifluorobut-2-en-1-yl)thio]phenyl)methanol (5): Starting from (2-mercaptophenyl)methanol[7] **4** and tosylate **1a** and following the procedure described above, **5** was obtained as a yellow oil in 71% yield (125 mg). ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.50–7.44 (m, 1H), 7.43–7.38 (m, 1H), 7.35–7.30 (m, 2H), 6.48-6.36 (m, 1H), 5.65–5.43 (m, 1H), 4.83 (d, J = 6.3 Hz, 2H), 3.65–3.46 (m, 2H), 2.02 (t, J = 6.3 Hz, 1H, O*H*). ^{19}F NMR (282 MHz, $CDCl_3$) δ -64.18–-64.27 (m, 3F). ^{13}C NMR (75 MHz, $CDCl_3$) δ 142.4, 135.1 (q, J = 6.6 Hz), 132.8, 132.5, 129.9 (q, J = 286.5 Hz, CF_3), 128.9, 128.6, 128.3, 120.9 (q, J = 33.9 Hz), 63.9, 35.8.



3q

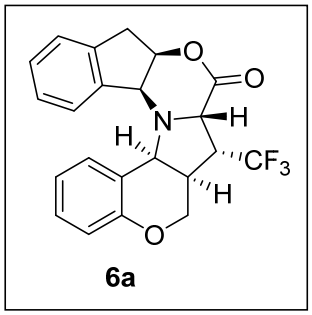
The intermediate alcohol **5** was redissolved in 5 mL DCM and PCC (162 mg, 0.75 mmol, 1.5 equiv) was added in one portion. The resulting mixture was stirred for 2 h at room temperature and then it was filtered through a short pad of silica gel affording **3q** as a light yellow solid (mp

[6] I. Piel, M. Steinmetz, K. Hirano, R. Fröhlich, S. Grimme, F. Glorius, *Angew. Chem. Int. Ed.* 2011, **50**, 4983.
[7] M. Li,J. L. Petersen, J. M. Hoover, *Org. Lett* 2017, **19**, 638.

= 31-33 ºC) in 58% yield (71 mg). ^{1}H NMR (300 MHz, $CDCl_3$) δ 10.38 (s, 1H), 7.93–7.85 (m, 1H), 7.55 (td, *J* = 7.6, 1.6 Hz, 1H), 7.42-7.36 (m, 2H), 6.53–6.36 (m, 1H), 5.76-5.67 (m, 1H), 3.74–3.57 (m, 2H). ^{19}F NMR (282 MHz, $CDCl_3$) δ -64.32 (s, 3F). ^{13}C NMR (75 MHz, $CDCl_3$) δ 191.7, 139.1, 134.9, 134.5 (q, *J* = 6.5 Hz), 134.2, 132.6, 129.8, 126.8, 122.5 (q, *J* = 269.6 Hz, CF_3), 121.8 (q, *J* = 34.0 Hz), 34.3. HRMS (ESI/Q-TOF) m/z: $[M+H]^+$ Calcd for $C_{11}H_{10}F_3OS$ 247.0399; found 247.0400.

General procedure for the asymmetric intramolecular dipolar cycloaddition of substrates 3 and azomethine ylide precursor IV

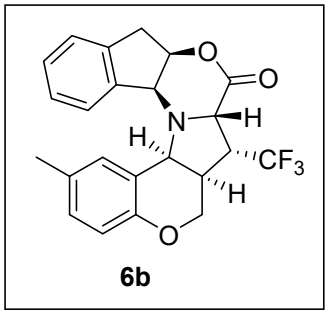
A solution of the corresponding fluorinated benzaldehyde **3, 7** (0.10 mmol, 1.0 equiv) and morpholinone **IV**[8] (28 mg, 0.15 mmol, 1.5 equiv) in toluene (3 mL) was heated at 120 ºC for 16 h in a pressure vial. The solvent was removed under reduced pressure and the crude was purified by flash chromatography on silica gel [*n*-hexane-EtOAc (10:1 to 4:1)] to afford **6, 8**. The diastereomeric ratio (d.r.) was determined by ^{19}F-NMR of the crude mixture. Major diastereoisomers were characterised as follows.



6a

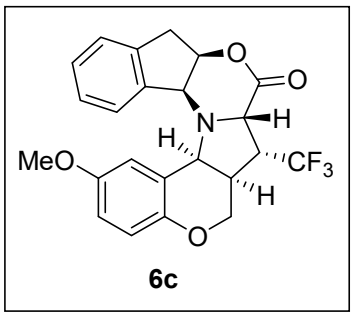
(9a*R*,14b*S*)-17-(Trifluoromethyl)-7,7a,9a,14b-tetrahydro-10*H*,16*H*-7,16-methanobenzo[*b*]indeno[1',2':5,6][1,4]oxazino[4,3-*e*][1,5]oxazocin-8(6*H*)-one (6a): Starting from **3a**, **6a** was obtained as a white solid (mp = 75-77 ºC) in 73% yield (29 mg). $[\alpha]_D^{25}$ = -62.7 (c 1.0; $CHCl_3$). ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.37–7.27 (m, 2H), 7.25–7.15 (m, 3H), 7.00 (dd, *J* = 7.6, 1.7 Hz, 1H), 6.96–6.83 (m, 2H), 5.55–5.42 (m, 1H), 4.54 (d, *J* = 4.9 Hz, 1H), 4.49 (d, *J* = 7.2 Hz, 1H), 4.28 (dd, *J* = 11.4, 5.6 Hz, 1H), 4.20 (dd, *J* = 11.4, 3.6 Hz, 1H), 4.09 (d, *J* = 8.9 Hz, 1H), 3.43–3.17 (m, 3H), 3.05-2.98 (m, 1H). ^{19}F NMR (282 MHz, $CDCl_3$) δ -63.64 (d, *J* = 10.1 Hz, 3F). ^{13}C NMR (75 MHz, $CDCl_3$) δ 165.7, 155.7, 139.3, 139.3, 130.1, 129.6, 129.3, 127.6, 126.2 (q, *J* = 278.7 Hz, CF_3), 126.0, 125.2, 121.7, 121.2, 117.6, 81.2, 66.0, 58.2, 57.8, 56.4, 48.0 (q, *J* = 29.0 Hz), 38.9, 37.1. HRMS (ESI/Q-TOF) m/z: $[M+H]^+$ Calcd for $C_{22}H_{19}F_3NO_3$ 402.1312; found 402.1310.

[8] N. Shimada, Y. Abe, S. Yokoshima, T. Fukuyama, *Angew. Chem. Int. Ed.* 2012, **51**, 11824.



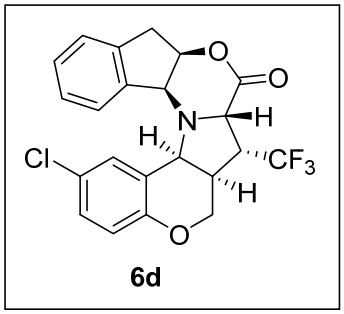
6b

(9a*R*,14b*S*)-2-Methyl-17-(trifluoromethyl)-7,7a,9a,14b-tetrahydro-10*H*,16*H*-7,16-methanobenzo[*b*]indeno[1',2':5,6][1,4]oxazino[4,3-*e*][1,5]oxazocin-8(6*H*)-one (6b): Starting from **3b**, **6b** was obtained as a white solid (mp = 38-40 ºC) in 88% yield (37 mg). $[\alpha]_D^{25}$ = -47.4 (c 1.0; $CHCl_3$). ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.36–7.28 (m, 2H), 7.28–7.20 (m, 2H), 7.01 (dd, *J* = 8.3, 2.1 Hz, 1H), 6.82 (d, *J* = 8.3 Hz, 1H), 6.78 (d, *J* = 2.1 Hz, 1H), 5.50 (ddd, *J* = 5.3, 4.9, 4.2 Hz, 1H), 4.56 (d, *J* = 4.9 Hz, 1H), 4.44 (d, *J* = 7.3 Hz, 1H), 4.25 (dd, *J* = 11.4, 5.6 Hz, 1H), 4.14 (dd, *J* = 11.4, 3.6 Hz, 1H), 4.09 (d, *J* = 8.8 Hz, 1H), 3.44 – 3.16 (m, 3H), 3.03-2.95 (m, 1H), 2.21 (s, 3H). ^{19}F NMR (282 MHz, $CDCl_3$) δ -63.55 (d, *J* = 10.1 Hz, 3F). ^{13}C NMR (75 MHz, $CDCl_3$) δ 165.8, 153.5, 139.3, 139.3, 131.0, 130.3, 130.1, 129.3, 127.6, 126.2 (q, *J* = 278.6 Hz, CF_3), 126.0, 125.2, 121.0, 117.3, 81.2, 66.1, 58.3, 57.9, 56.5, 47.9 (q, *J* = 28.9 Hz), 38.9, 37.3 (q, *J* = 1.9 Hz), 20.8. HRMS (ESI/Q-TOF) m/z: $[M+H]^+$ Calcd for $C_{23}H_{21}F_3NO_3$ 416.1468; found 416.1471.



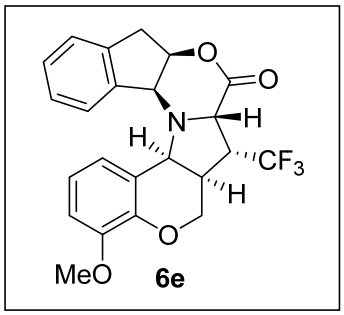
6c

(9a*R*,14b*S*)-2-Methoxy-17-(trifluoromethyl)-7,7a,9a,14b-tetrahydro-10*H*,16*H*-7,16-methanobenzo[*b*]indeno[1',2':5,6][1,4]oxazino[4,3-*e*][1,5]oxazocin-8(6*H*)-one (6c): Starting from **3c**, **6c** was obtained as a white solid (mp = 45-47 ºC) in 75% yield (32 mg). $[\alpha]_D^{25}$ = -46.0 (c 1.0; $CHCl_3$). ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.35–7.18 (m, 4H), 6.84 (d, *J* = 8.9 Hz, 1H), 6.76 (dd, *J* = 8.9, 3.0 Hz, 1H), 6.45 (d, *J* = 3.0 Hz, 1H), 5.43 (dt, *J* = 10.0, 5.0 Hz, 1H), 4.59–4.42 (m, 2H), 4.26 (dd, *J* = 11.5, 4.7 Hz, 1H), 4.12 (dd, *J* = 11.5, 3.3 Hz, 1H), 4.07 (d, *J* = 8.8 Hz, 1H), 3.64 (s, 3H), 3.50–3.20 (m, 3H), 3.05-2.98 (m, 1H). ^{19}F NMR (282 MHz, $CDCl_3$) δ -63.62 (d, *J* = 10.2 Hz, 3F). ^{13}C NMR (75 MHz, $CDCl_3$) δ 165.6, 154.2, 149.8, 139.4, 139.4, 129.4, 127.5, 126.2 (q, *J* = 278.9 Hz, CF_3), 126.0, 125.3, 122.4, 118.1, 114.9, 114.7, 81.2, 66.3, 58.2, 58.1, 56.7, 55.7, 48.2 (q, *J* = 28.8 Hz), 38.7, 37.4. HRMS (ESI/Q-TOF) m/z: $[M+H]^+$ Calcd for $C_{23}H_{21}F_3NO_4$ 432.1417; found 432.1413.



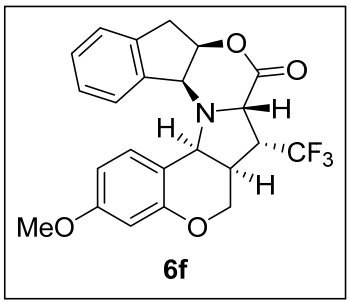
6d

(9a*R*,14b*S*)-2-Chloro-17-(trifluoromethyl)-7,7a,9a,14b-tetrahydro-10*H*,16*H*-7,16-methanobenzo[*b*]indeno[1',2':5,6][1,4]oxazino[4,3-*e*][1,5]oxazocin-8(6*H*)-one (6d): Starting from **3d**, **6d** was obtained as a white solid (mp = 46-48 ºC) in 71% yield (31 mg). $[\alpha]_D^{25}$ = -31.0 (c 1.0; $CHCl_3$). ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.39–7.30 (m, 2H), 7.29–7.21 (m, 2H), 7.15 (dd, *J* = 8.7, 2.5 Hz, 1H), 6.92 (d, *J* = 2.5 Hz, 1H), 6.85 (d, *J* = 8.7 Hz, 1H), 5.44 (dt, *J* = 9.8, 4.9 Hz, 1H), 4.50–4.43 (m, 2H), 4.29 (dd, *J* = 11.5, 5.1 Hz, 1H), 4.18 (dd, *J* = 11.5, 3.4 Hz, 1H), 4.08 (d, *J* = 8.9 Hz, 1H), 3.46–3.22 (m, 3H), 3.07–2.98 (m, 1H). ^{19}F NMR (282 MHz, $CDCl_3$) δ -63.61 (d, *J* = 10.1 Hz, 3F). ^{13}C NMR (75 MHz, $CDCl_3$) δ 165.4, 154.3, 139.4, 139.0, 129.7, 129.6, 129.4, 127.6, 126.5, 126.1, 126.1 (q, *J* = 278.7 Hz, CF_3), 125.2, 123.0, 119.0, 81.2, 66.1, 58.1, 57.7, 56.6, 56.6, 48.0 (q, *J* = 28.9 Hz), 38.8, 37.0 (q, *J* = 1.9 Hz). HRMS (ESI/Q-TOF) m/z: $[M+H]^+$ Calcd for $C_{22}H_{18}ClF_3NO_3$ 436.0922; found 436.0924.



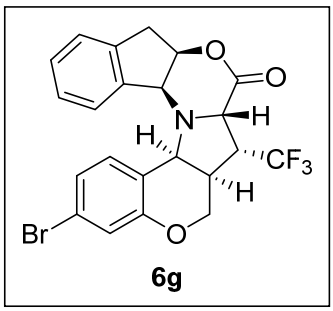
6e

(9a*R*,14b*S*)-4-Methoxy-17-(trifluoromethyl)-7,7a,9a,14b-tetrahydro-10*H*,16*H*-7,16-methanobenzo[*b*]indeno[1',2':5,6][1,4]oxazino[4,3-*e*][1,5]oxazocin-8(6*H*)-one (6e): Starting from **3e**, **6e** was obtained as a yellow solid (mp = 42-44 ºC) in 67% yield (29 mg). $[\alpha]_D^{25}$ = -61.4 (c 1.0; $CHCl_3$). ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.32-7.30 (m, 2H), 7.25–7.20 (m, 2H), 6.88–6.77 (m, 2H), 6.60 (dd, *J* = 6.6, 2.5 Hz, 1H), 5.50–5.42 (m, 1H), 4.53 (d, *J* = 4.9 Hz, 1H), 4.50 (d, *J* = 7.3 Hz, 1H), 4.38 (dd, *J* = 11.4, 5.5 Hz, 1H), 4.25 (dd, *J* = 11.4, 3.5 Hz, 1H), 4.08 (d, *J* = 8.8 Hz, 1H), 3.89 (s, 3H), 3.41–3.22 (m, 3H), 3.06–2.97 (m, 1H). ^{19}F NMR (282 MHz, $CDCl_3$) δ -63.65 (d, *J* = 10.1 Hz, 3F). ^{13}C NMR (75 MHz, $CDCl_3$) δ 165.6, 148.7, 145.1, 139.3, 139.3, 129.3, 127.6, 126.1 (q, *J* = 278.6 Hz, CF_3), 125.9, 125.2, 122.0, 121.5, 121.3, 111.1, 81.2, 66.4, 58.2, 57.7, 56.4, 56.1, 47.9 (q, *J* = 28.9 Hz), 38.8, 37.1. HRMS (ESI/Q-TOF) m/z: $[M+H]^+$ Calcd for $C_{23}H_{21}F_3NO_4$ 432.1417; found 432.1424.



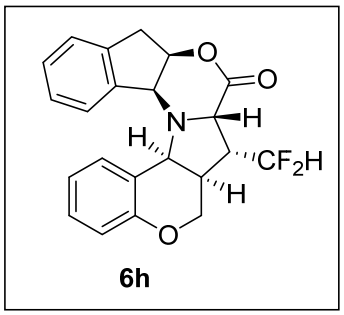
6f

(6a*R*,7*R*,7a*S*,9a*R*,14b*S*,15a*S*)-3-methoxy-7-(trifluoromethyl)-6a,7,7a,9a,14b,15a-hexahydro-6*H*,8*H*,10*H*-chromeno[3',4':4,5]pyrrolo[1,2-d]indeno[2,1-b][1,4]oxazin-8-one (6f): Starting from **3f**, **6f** was obtained as a light yellow solid (mp=108-110 °C) in 77% yield (33 mg). $[\alpha]_D^{25}$ = -68.9° (c 1.0; $CHCl_3$). ^{1}H NMR (300 MHz, Chloroform-*d*) δ 7.36–7.24 (m, 2H), 7.27–7.19 (m, 2H), 6.90 (d, *J* = 8.1 Hz, 1H), 6.53–6.41 (m, 2H), 5.48 (td, *J* = 5.3, 4.1 Hz, 1H), 4.52 (d, *J* = 4.9 Hz, 1H), 4.41 (d, *J* = 7.0 Hz, 1H), 4.25 (dd, *J* = 11.3, 6.1 Hz, 1H), 4.18 (dd, *J* = 11.3, 3.9 Hz, 1H), 4.09 (d, *J* = 8.9 Hz, 1H), 3.76 (s, 3H), 3.43–3.11 (m, 3H), 2.96 (qd, *J* = 6.3, 3.8 Hz, 1H). ^{19}F NMR (282 MHz, Chloroform-*d*) δ -63.70 (d, *J* = 10.2 Hz, 3F). ^{13}C NMR (75 MHz, Chloroform-*d*) δ 165.7, 160.7, 156.6, 139.3, 130.8, 130.3, 129.3, 127.6, 126.2 (d, *J* = 278.6 Hz, CF_3), 126.0, 125.1, 113.0, 108.9, 101.9, 81.2, 66.1, 58.0, 57.5, 56.3, 55.5, 48.0 (q, *J* = 29.0 Hz), 38.9, 37.0 (q, *J* = 2.2 Hz). HRMS (ESI/Q-TOF) m/z: $[M+H]^+$ Calcd for $C_{23}H_{21}F_3NO_4$ 432.1417; found 432.1418. The minor diastereoisomer was isolated in a mixed fraction with the major one. The ^{1}H NMR signals given next were inferred from the spectrum of the mixture. ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.73–7.66 (m, 1H), 7.44–7.32 (m, 3H), 7.30–7.22 (m, 1H), 6.57–6.48 (m, 2H), 5.12 (ddd, *J* = 5.7, 4.2, 1.7 Hz, 1H), 4.98 (d, *J* = 5.7 Hz, 1H), 4.56 (d, *J* = 5.2 Hz, 1H), 4.19–4.09 (m, 1H), 3.96 (dd, *J* = 11.0 Hz, 11.0 Hz, 1H), 3.79 (s, 3H), 3.65 (d, *J* = 6.2 Hz, 1H), 3.26–3.09 (m, 2H), 2.91–2.73 (m, 1H), 2.67 (dtd, *J* = 11.3, 5.1, 2.1 Hz, 1H). ^{19}F NMR (282 MHz, $CDCl_3$) δ -69.78 (d, *J* = 9.4 Hz, 3F).



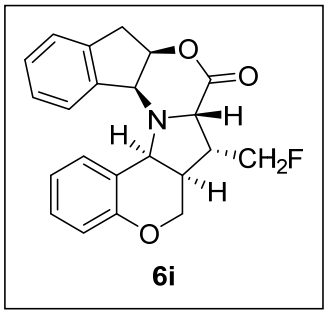
6g

(6a*R*,7*R*,7a*S*,9a*R*,14b*S*,15a*S*)-3-bromo-7-(trifluoromethyl)-6a,7,7a,9a,14b,15a-hexahydro-6*H*,8*H*,10*H*-chromeno[3',4':4,5]pyrrolo[1,2-d]indeno[2,1-b][1,4]oxazin-8-one (6g): Starting from **3g**, **6g** was obtained as a white solid (mp=88-90 °C) in 60% yield (29 mg). $[\alpha]_D^{25}$ = -57.7° (c 1.0; $CHCl_3$). ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.36–7.28 (m, 2H), 7.27–7.18 (m, 2H), 7.10 (d, *J* = 2.0 Hz, 1H), 7.01 (dd, *J* = 8.2, 2.0 Hz, 1H), 6.83 (d, *J* = 8.2, 1H), 5.45 (dt, *J* = 5.6, 4.5 Hz, 1H), 4.47 (d, *J* = 4.5 Hz, 1H), 4.44 (d, *J* = 7.2 Hz, 1H), 4.27 (dd, *J* = 11.5, 5.6 Hz, 1H), 4.19 (dd, *J* = 11.5, 3.6 Hz, 1H), 4.08 (d, *J* = 8.9 Hz, 1H), 3.49–3.17 (m, 3H), 3.01 (tdd, *J* = 6.8, 5.6, 3.6 Hz, 1H). ^{19}F NMR (282 MHz, $CDCl_3$) δ -63.67 (d, *J* = 10.0 Hz, 3F). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 165.4, 156.3, 139.3, 139.1, 131.2, 129.5, 127.7, 126.1, 126.1 (d, *J* = 278.7 Hz, CF_3), 125.1, 125.0, 122.7, 120.8, 120.3, 81.2, 66.1, 58.2, 57.5, 56.5, 48.1 (q, *J* = 29.0 Hz), 38.8, 36.9 (d, *J* = 2.3 Hz), 36.9. HRMS (ESI/Q-TOF) m/z: $[M+Me]^+$ Calcd for $C_{22}H_{18}BrF_3NO_3$ 480.0417; found 480.0409.



6h

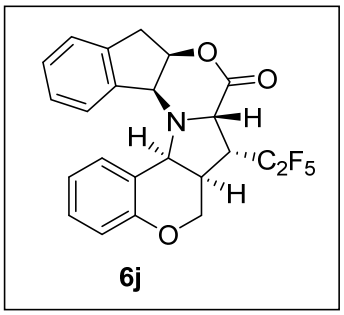
(9a*R*,14b*S*)-17-(Difluoromethyl)-7,7a,9a,14b-tetrahydro-10*H*,16*H*-7,16-methanobenzo[*b*]indeno[1',2':5,6][1,4]oxazino[4,3-*e*][1,5]oxazocin-8(6*H*)-one (6h): Starting from **3h**, **6h** was obtained as a white solid (mp = 69-71 ºC) in 68% yield (26 mg). $[\alpha]_D^{25}$ = -94.3 (c 1.0; $CHCl_3$). ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.32–7.17 (m, 5H), 7.12 (dd, *J* = 7.6, 1.6 Hz, 1H), 6.97 (dd, *J* = 8.3, 1.1 Hz, 1H), 6.92 (td, *J* = 7.4, 1.2 Hz, 1H), 6.44 (td, *J* = 56.1, 3.0 Hz, 1H), 5.64 (td, *J* = 4.7, 2.2 Hz, 1H), 4.75 (d, *J* = 4.7 Hz, 1H), 4.29–4.12 (m, 3H), 4.07 (d, *J* = 9.5 Hz, 1H), 3.38–3.20 (m, 2H), 2.97-2.89 (m, 1H), 2.79-2.62 (m, 1H). ^{19}F NMR (282 MHz, $CDCl_3$) δ -118.65 (ddd, *J* = 285.9, 56.1, 6.3 Hz), -125.12 (ddd, *J* = 285.9, 56.1, 29.3 Hz). ^{13}C NMR (75 MHz, $CDCl_3$) δ 168.2, 155.6, 139.0, 138.9, 130.9, 129.8, 129.1, 127.7, 126.0, 124.7, 120.9, 120.5, 117.7, 115.64 (dd, *J* = 241.3, 238.7 Hz, CF_2H), 80.8, 66.4, 58.0, 57.6, 55.5 (dd, *J* = 6.8, 2.1 Hz), 45.4 (dd, *J* = 22.1, 22.1 Hz,), 39.2, 34.8 (dd, *J* = 3.9, 2.4 Hz). HRMS (ESI/Q-TOF) m/z: $[M+H]^+$ Calcd for $C_{22}H_{20}F_2NO_3$ 384.1406; found 384.1404.



6i

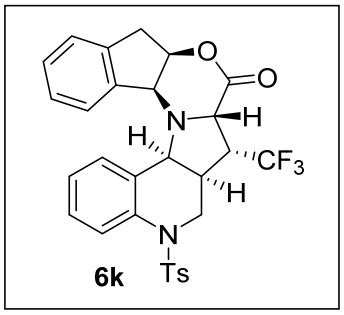
(6a*R*,7*R*,7a*S*,9a*R*,14b*S*,15a*S*)-7-(fluoromethyl)-6a,7,7a,9a,14b,15a-hexahydro-6*H*,8*H*,10*H*-chromeno[3',4':4,5]pyrrolo[1,2-*d*]indeno[2,1-*b*][1,4]oxazin-8-one (6i): Starting from **3i**, **6i** was obtained in 72% overall yield as a 62:38 mixture of two diastereoisomers which were separated by flash column chromatography. Major diastereoisomer: light yellow oil (127 mg, 49% yield). $[\alpha]_D^{25}$ = -85.0° (c 1.0; $CHCl_3$). ^{1}H NMR (300 MHz, Chloroform-*d*) δ 7.31–7.19 (m, 5H), 7.15 (dd, *J* = 7.6, 1.7 Hz, 1H), 6.99–6.87 (m, 2H), 5.63 (td, *J* = 4.5, 1.7 Hz, 1H), 4.85 (d, *J* = 4.3 Hz, 1H), 4.76 (d, *J* = 4.5 Hz, 1H), 4.69 (d, *J* = 4.6 Hz, 1H), 4.32–4.13 (m, 3H), 4.02 (d, *J* = 9.3 Hz, 1H), 3.41–3.05 (m, 2H), 2.75–2.44 (m, 2H).^{19}F NMR (282 MHz, Chloroform-*d*) δ -221.22 (td, *J* = 46.9, 31.0 Hz). ^{13}C NMR (75 MHz, Chloroform-*d*) δ 168.8, 155.3, 139.1, 139.0, 131.0, 129.6, 128.9, 127.5, 126.0, 124.7, 120.7, 117.6, 83.5 (d, *J* = 166.8 Hz, CH_2F), 80.7, 66.1, 58.5, 57.4 (d, *J* = 1.4 Hz), 55.7 (d, *J* = 5.8 Hz), 42.5 (d, *J* = 19.9 Hz), 39.3, 39.0 (d, *J* = 1.9 Hz). Minor diastereoisomer: light yellow oil (60 mg, 23% yield). $[\alpha]_D^{25}$ = +111.8° (c 1.0; $CHCl_3$). ^{1}H NMR (300 MHz, Chloroform-*d*) δ 7.82–7.68 (m, 1H), 7.43–7.24 (m, 5H), 7.00 (dd, *J* = 8.3, 1.2 Hz, 1H), 6.92 (td, *J* = 7.4, 1.3 Hz, 1H), 5.13 (ddd, *J* = 5.4, 4.4, 1.1 Hz, 1H), 5.00 (d, *J* = 5.1 Hz, 1H), 4.83–4.65 (m, 1H), 4.68–4.49 (m, 1H), 4.50 (d, *J* = 5.6 Hz, 1H), 4.14 (dd, *J* = 10.7, 5.1 Hz,

1H), 3.95 (t, *J* = 11.1 Hz, 1H), 3.49 (d, *J* = 7.7 Hz, 1H), 3.23–3.02 (m, 2H), 2.58-2.49 (m, 1H), 2.32–2.11 (m, 1H). ^{19}F NMR (282 MHz, Chloroform-*d*) δ -226.68 (td, *J* = 47.2, 30.7 Hz). ^{13}C NMR (75 MHz, Chloroform-*d*) δ 169.5, 155.6, 141.8, 137.5, 130.8, 129.8, 129.0, 127.6, 126.9, 125.5, 120.6, 117.9, 84.2 (d, *J* = 169.7 Hz, CH_2F), 66.1, 59.7, 56.2, 55.7 (d, *J* = 5.4 Hz), 43.1 (d, *J* = 19.0 Hz), 38.3, 36.9 (d, *J* = 2.2 Hz). HRMS (ESI/Q-TOF) m/z: $[M+H]^+$ Calcd for $C_{22}H_{21}FNO_3$ 366.1500; found 366.1508.



6j

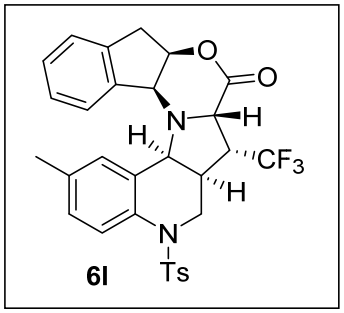
(9a*R*,14b*S*)-17-(Perfluoroethyl)-7,7a,9a,14b-tetrahydro-10*H*,16*H*-7,16-methanobenzo[*b*]indeno[1',2':5,6][1,4]oxazino[4,3-*e*][1,5]oxazocin-8(6*H*)-one (6j): Starting from **3j**, **6j** was obtained as a white solid (mp = 40-42 ºC) in 75% yield (34 mg). $[\alpha]_D^{25}$ = -22.5 (c 1.0; $CHCl_3$). ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.46–7.14 (m, 5H), 7.08–6.83 (m, 3H), 5.50 (ddd, *J* = 5.3, 5.3, 5.3 Hz, 1H), 4.50 (d, *J* = 5.2 Hz, 1H), 4.46 (d, *J* = 7.4 Hz, 1H), 4.28–4.12 (m, 2H), 4.08 (d, *J* = 8.1 Hz, 1H), 3.41–3.31 (m, 2H), 3.30-3.13 (m, 1H), 3.11–2.97 (m, 1H). ^{19}F NMR (282 MHz, $CDCl_3$) δ -82.32 (s, 3F), -109.46 (dd, *J* = 272.1, 9.1 Hz, 1F), -116.14 (dd, *J* = 272.1, 26.2 Hz, 1F). ^{13}C NMR (75 MHz, $CDCl_3$) δ 165.4, 156.1, 139.4, 139.4, 130.2, 129.6, 129.4, 127.7, 125.9, 125.3, 121.8, 121.2, 120.9-111.5 (m, C_2F_5), 117.6, 81.2, 66.5, 58.5, 57.8 (d, *J* = 3.0 Hz), 57.3, 46.5 (dd, *J* = 22.9, 21.9 Hz, <u>C</u>H-C_2F_5), 39.0, 36.3. HRMS (ESI/Q-TOF) m/z: $[M+H]^+$ Calcd for $C_{23}H_{19}F_5NO_3$ 452.1280; found 452.1277.



6k

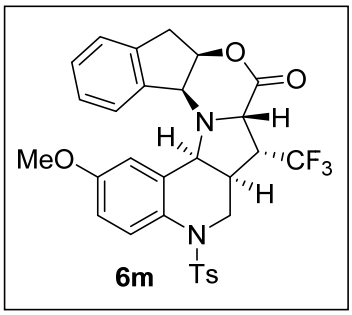
(9a*R*,14b*S*)-5-Tosyl-17-(trifluoromethyl)-5,7,7a,9a,14b,16-hexahydro-10*H*-7,16-methanobenzo[*f*]indeno[1',2':5,6][1,4]oxazino[4,3-*a*][1,5]diazocin-8(6*H*)-one (6k): Starting from **3k**, **6k** was obtained as a white solid (mp = 81-83 ºC) in 70% yield (39 mg). $[\alpha]_D^{25}$ = -11.3 (c 1.0; $CHCl_3$). ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.78–7.68 (m, 2H), 7.56 (dd, *J* = 8.1, 1.1 Hz, 1H), 7.37–7.13 (m, 9H), 5.48 (td, *J* = 4.9, 1.7 Hz, 1H), 4.41 (d, *J* = 5.0 Hz, 1H), 4.06 (d, *J* = 7.7 Hz, 1H), 3.99 (d, *J* = 9.0 Hz, 1H), 3.89–3.72 (m, 2H), 3.36–3.13 (m, 3H), 3.02-2.93 (m, 1H), 2.46 (s, 3H). ^{19}F NMR (282 MHz, $CDCl_3$) δ -63.45 (d, *J* = 9.5 Hz, 3F). ^{13}C NMR (75 MHz, $CDCl_3$) δ 165.5, 144.3, 139.1, 139.0, 138.5, 137.9, 130.2, 129.7, 129.3, 129.3 (q, *J* = 275.0 Hz,

CF_3), 129.0, 127.9, 127.2, 125.9, 125.6, 125.0, 124.0, 80.6, 59.5, 59.2, 56.3, 49.6, 48.9 (q, *J* = 29.1 Hz), 40.1, 39.4, 21.7. HRMS (ESI/Q-TOF) m/z: $[M+H]^+$ Calcd for $C_{29}H_{26}F_3N_2O_4S$ 555.1560; found 555.1563.



6l

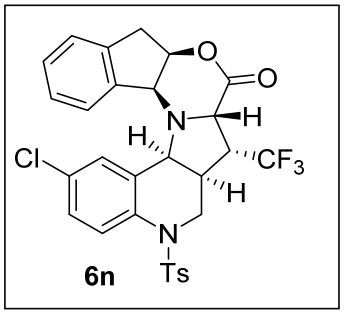
(9a*R*,14b*S*)-2-Methyl-5-tosyl-17-(trifluoromethyl)-5,7,7a,9a,14b,16-hexahydro-10*H*-7,16-methanobenzo[*f*]indeno[1',2':5,6][1,4]oxazino[4,3-*a*][1,5]diazocin-8(6*H*)-one (6l): Starting from **3l**, **6l** was obtained as a white solid (mp = 74-76 ºC) in 67% yield (38 mg). $[\alpha]_D^{25}$ = +17.1 (c 1.0; $CHCl_3$). ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.69–7.62 (m, 2H), 7.36 (d, *J* = 8.2 Hz, 1H), 7.26 (d, *J* = 8.0 Hz, 2H), 7.22–7.14 (m, 4H), 7.04 (dd, *J* = 8.3, 1.7 Hz, 1H), 6.93 (s, 1H), 5.39 (td, *J* = 4.9, 1.8 Hz, 1H), 4.36 (d, *J* = 5.0 Hz, 1H), 3.97 (d, *J* = 7.7 Hz, 1H), 3.83 (d, *J* = 9.0 Hz, 1H), 3.77 (dd, *J* = 14.0, 6.0 Hz, 1H), 3.65 (dd, *J* = 14.0, 5.4 Hz, 1H), 3.32–3.05 (m, 3H), 2.95–2.79 (m, 1H), 2.39 (s, 3H), 2.23 (s, 3H). ^{19}F NMR (282 MHz, $CDCl_3$) δ -63.46 (d, *J* = 9.5 Hz, 3F). ^{13}C NMR (126 MHz, Chloroform-*d*) δ 165.5, 144.1, 139.0, 138.6, 138.0, 136.4, 135.6, 130.1, 129.7, 129.6, 129.6, 129.3, 127.9, 127.2, 125.9, 125.7 (q, *J* = 278.1 Hz, CF_3), 125.0, 124.1, 80.6, 59.5, 59.4, 56.3, 49.6, 49.1 (q, *J* = 29.3 Hz), 40.1, 39.4, 21.7, 21.2. HRMS (ESI/Q-TOF) m/z: $[M+H]^+$ Calcd for $C_{30}H_{28}F_3N_2O_4S$ 569.1716; found 569.1700.



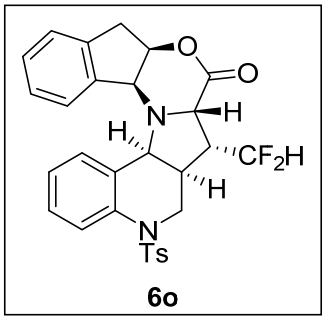
6m

(9a*R*,14b*S*)-2-Methoxy-5-tosyl-17-(trifluoromethyl)-5,7,7a,9a,14b,16-hexahydro-10*H*-7,16-methanobenzo[*f*]indeno[1',2':5,6][1,4]oxazino[4,3-*a*][1,5]diazocin-8(6*H*)-one (6m): Starting from **3m**, **6m** was obtained as a white solid (mp = 63-65 ºC) in 76% yield (44 mg). $[\alpha]_D^{25}$ = +37.1 (c 1.0; $CHCl_3$). ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.67 (d, *J* = 8.3 Hz, 2H), 7.46 (d, *J* = 8.8 Hz, 1H), 7.33 (d, *J* = 8.3 Hz, 2H), 7.29–7.19 (m, 4H), 6.83 (dd, *J* = 8.8, 2.9 Hz, 1H), 6.76 (d, *J* = 2.9 Hz, 1H), 5.33 (td, *J* = 5.0, 2.1 Hz, 1H), 4.41 (d, *J* = 4.9 Hz, 1H), 4.11–3.98 (m, 2H), 3.73 (s, 3H), 3.69 (d, *J* = 9.2 Hz, 1H), 3.52 (dd, *J* = 14.3, 6.7 Hz, 1H), 3.28 (dd, *J* = 17.1, 2.0 Hz, 1H), 3.23–3.03 (m, 2H), 3.02–2.88 (m, 1H), 2.46 (s, 3H). ^{19}F NMR (282 MHz, $CDCl_3$) δ -63.53 (d, *J* = 9.3 Hz, 3F). ^{13}C NMR (75 MHz, $CDCl_3$) δ 165.5, 157.8, 144.2, 139.1, 138.5, 137.9, 132.3, 131.1, 130.2, 129.5, 128.0, 127.4, 126.5, 126.1, 125.6 (q, *J* = 278.0 Hz, CF_3), 125.0, 114.3,

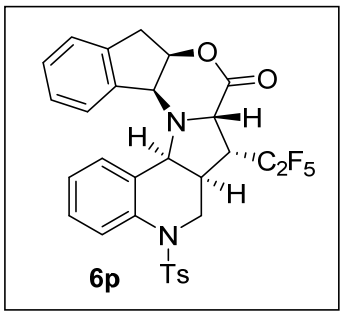
113.4, 80.8, 60.0, 59.4, 56.5, 55.7, 49.9 (q, *J* = 29.4 Hz), 49.3, 39.7, 39.3, 21.8. HRMS (ESI/Q-TOF) m/z: $[M+H]^+$ Calcd for $C_{30}H_{28}F_3N_2O_5S$ 585.1666; found 585.1642.



(9a*R*,14b*S*)-2-Chloro-5-tosyl-17-(trifluoromethyl)-5,7,7a,9a,14b,16-hexahydro-10*H*-7,16-methanobenzo[*f*]indeno[1',2':5,6][1,4]oxazino[4,3-*a*][1,5]diazocin-8(6*H*)-one (6n): Starting from **3n**, **6n** was obtained as a white solid (mp = 95-97 ºC) in 51% yield (30 mg). $[\alpha]_D^{25}$ = +48.0 (c 1.0; $CHCl_3$). ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.79–7.66 (m, 2H), 7.51 (d, *J* = 8.7 Hz, 1H), 7.35 (d, *J* = 8.0 Hz, 2H), 7.32 – 7.20 (m, 5H), 7.17 (d, *J* = 2.4 Hz, 1H), 5.40 (td, *J* = 4.9, 2.1 Hz, 1H), 4.39 (d, *J* = 4.9 Hz, 1H), 4.04 (d, *J* = 7.6 Hz, 1H), 3.92 (dd, *J* = 14.2, 6.1 Hz, 1H), 3.83 (d, *J* = 9.2 Hz, 1H), 3.64 (dd, *J* = 14.2, 6.0 Hz, 1H), 3.33-3.07 (m, 3H), 3.04-2.94 (m, 1H), 2.47 (s, 3H). ^{19}F NMR (282 MHz, $CDCl_3$) δ -63.47 (d, *J* = 9.3 Hz, 3F). ^{13}C NMR (75 MHz, $CDCl_3$) δ 165.2, 144.6, 139.0, 138.2, 137.5, 137.3, 132.0, 131.4, 130.3, 129.5, 129.0, 128.7, 128.0, 127.2, 126.1, 125.8, 125.5 (q, *J* = 278.1 Hz, CF_3), 124.9, 80.7, 59.6, 59.1, 56.4, 49.3 (q, *J* = 29.3 Hz), 49.2, 40.0, 39.3, 21.7. HRMS (ESI/Q-TOF) m/z: $[M+H]^+$ Calcd for $C_{29}H_{25}ClF_3N_2O_4S$ 589.1170; found 589.1144.

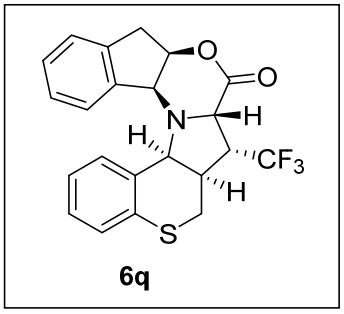


(6a*S*,7*R*,7a*S*,9a*R*,14b*S*,15a*S*)-7-(difluoromethyl)-5-tosyl-5,6,6a,7,7a,9a,14b,15a-octahydro-8*H*,10*H*-indeno[1'',2'':5',6'][1,4]oxazino[4',3':1,5]pyrrolo[3,2-c]quinolin-8-one (6o): Starting from **3o**, **6o** was obtained as a white solid (mp=82-84 °C) in 77% yield (41 mg). $[\alpha]_D^{25}$ = -30.3° (c 1.0; $CHCl_3$). ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.75–7.61 (m, 3H), 7.38–7.26 (m, 3H), 7.28–7.13 (m, 6H), 6.37 (ddd, *J* = 56.8, 54.7, 4.8 Hz, 1H, $CF_2\underline{H}$), 5.48 (td, *J* = 4.6, 1.8 Hz, 1H), 4.50 (d, *J* = 5.0 Hz, 1H), 3.96 (d, *J* = 7.9 Hz, 1H), 3.92–3.83 (m, 2H), 3.74 (dd, *J* = 13.9, 6.2 Hz, 1H), 3.32–3.10 (m, 2H), 2.94–2.60 (m, 2H), 2.43 (s, 3H). ^{19}F NMR (282 MHz, $CDCl_3$) δ -115.19 (ddd, *J* = 289.5, 54.7, 7.5 Hz, 1F), -122.63 (ddd, *J* = 289.5, 56.8, 21.4 Hz, 1F). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 167.9, 144.1, 138.9, 138.8, 138.6, 137.7, 130.1 (2xCH), 129.5, 129.3, 129.1, 128.9, 127.9, 127.2 (2xCH), 125.8, 125.3, 124.9, 124.2, 116.2 (t, *J* = 240.7, CF_2H), 80.3, 59.4, 58.9, 56.2 (dd, *J* = 5.8, 3.9 Hz), 49.5 (d, *J* = 2.1 Hz), 47.6 (t, *J* = 22.7 Hz), 39.4, 38.4 (d, *J* = 5.3 Hz), 21.7. HRMS (ESI/Q-TOF) m/z: $[M+H]^+$ Calcd for $C_{29}H_{27}F_2N_2O_4S$ 537.1654; found 537.1655.



6p

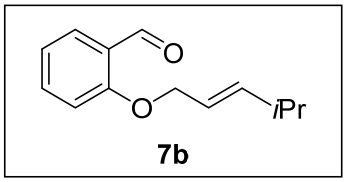
(9a*R*,14b*S*)-17-(Perfluoroethyl)-5-tosyl-5,7,7a,9a,14b,16-hexahydro-10*H*-7,16-methanobenzo[*f*]indeno[1',2':5,6][1,4]oxazino[4,3-*a*][1,5]diazocin-8(6*H*)-one (6p): Starting from **3p**, **6p** was obtained as a white solid (mp = 37-39 ºC) in 77% yield (47 mg). $[\alpha]_D^{25}$ = +11.9 (c 1.0; $CHCl_3$). ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.70–7.60 (m, 2H), 7.43 (d, *J* = 7.9 Hz, 1H), 7.31–7.25 (m, 2H), 7.25–7.14 (m, 4H), 7.13–7.01 (m, 2H), 5.40 (td, *J* = 5.1, 3.3 Hz, 1H), 4.23 (d, *J* = 5.4 Hz, 1H), 3.97 (d, *J* = 7.1 Hz, 1H), 3.93 (d, *J* = 9.0 Hz, 1H), 3.69 (d, *J* = 5.4 Hz, 1H), 3.41–3.11 (m, 3H), 3.06-2.97 (m, 1H), 2.40 (s, 3H). ^{19}F NMR (282 MHz, $CDCl_3$) δ -82.60 (s, 3F), -112.65 (dd, *J* = 272.7, 13.1 Hz, 1F), -114.33 (dd, *J* = 272.7, 20.9 Hz, 1F). ^{13}C NMR (75 MHz, $CDCl_3$) δ 165.0, 144.0, 139.4, 138.9, 138.7, 138.1, 130.0, 129.5, 129.4, 129.2, 129.0, 127.9, 126.9, 125.6, 125.6, 125.1, 123.8, 118.2 (qt, *J* = 287.1, 36.6 Hz, $\underline{C}F_2$), 113.9 (ddq, *J* = 261.4, 254.3, 37.5 Hz, $\underline{C}F_3$), 80.5, 60.1, 58.4, 57.0, 49.9, 46.0, 39.9, 39.3, 21.6. HRMS (ESI/Q-TOF) m/z: $[M+H]^+$ Calcd for $C_{30}H_{26}F_5N_2O_4S$ 605.1528; found 605.1510.



6q

(9a*R*,14b*S*)-17-(Trifluoromethyl)-7,7a,9a,14b-tetrahydro-10*H*,16*H*-7,16-methanobenzo[*b*]indeno[1',2':5,6][1,4]oxazino[4,3-*e*][1,5]thiazocin-8(6*H*)-one (6q): Starting from **3q**, **6q** was obtained as a yellow thick oil in 79% yield (33 mg). $[\alpha]_D^{25}$ = -15.8 (c 1.0; $CHCl_3$). ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.42 (dd, *J* = 7.5, 1.5 Hz, 1H), 7.34–7.13 (m, 7H), 5.61 (td, *J* = 5.1, 2.0 Hz, 1H), 4.41-4.37 (m, 2H), 4.12 (d, *J* = 7.1 Hz, 1H), 3.55–3.34 (m, 2H), 3.30 (dd, *J* = 17.2, 2.0 Hz, 1H), 3.21 (dd, *J* = 17.2, 5.0 Hz, 1H), 3.03 (dd, *J* = 13.6, 4.6 Hz, 1H), 2.77 (dd, *J* = 13.6, 3.9 Hz, 1H). ^{19}F NMR (282 MHz, $CDCl_3$) δ -62.33 (d, *J* = 9.0 Hz, 3F). ^{13}C NMR (75 MHz, $CDCl_3$) δ 165.8, 139.2, 138.8, 137.4, 134.7, 130.4, 130.4, 129.2, 128.1, 127.8, 126.2, 125.9, 125.9 (q, *J* = 277.9 Hz, CF_3). 125.0, 80.6, 62.5, 59.1, 56.5 (q, *J* = 1.8 Hz), 48.0 (q, *J* = 29.0 Hz), 41.0, 39.4, 33.7. HRMS (ESI/Q-TOF) m/z: $[M+H]^+$ Calcd for $C_{22}H_{19}F_3NO_2S$ 418.1083; found 418.1078.

Synthesis of (*E*)-2-((4-methylpent-2-en-1-yl)oxy)benzaldehyde (7b):



7b

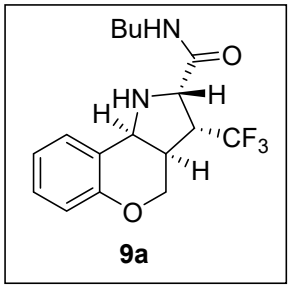
A solution of salicylaldehyde **2a** (0.14 mL, 1.35 mmol, 1.1 equiv) and K_2CO_3 (187 mg, 1.35 mmol, 1.0 equiv) in dry acetonitrile (3 mL) in a pressure vial was heated in an oil bath at 60 °C for 10 min. A solution of the (*E*)-1-bromo-4-methylpent-2-ene (prepared according to a literature procedure)[9] (200 mg, 1.23 mmol, 1.0 equiv) in dry acetonitrile (3 mL) was added and the resulting mixture was heated at the same temperature for 16 h. Water (4 mL) was added to quench the reaction and the aqueous phase was extracted with ethyl acetate (3x 10 mL). The combined organic phases were washed with brine (30 mL), dried over anhydrous sodium sulfate and concentrated under reduced pressure. The crude was purified by flash chromatography on silica gel [*n*-hexane-EtOAc (30:1)] to afford non-fluorinated benzaldehyde **7b** as a colorless oil in 28% yield (70 mg). ^{1}H NMR (300 MHz, Chloroform-*d*) δ 10.53 (d, *J* = 0.8 Hz, 1H), 7.84 (dd, *J* = 7.7, 1.8 Hz, 1H), 7.52 (ddd, *J* = 8.4, 7.3, 1.8 Hz, 1H), 7.10–6.89 (m, 2H), 5.85 (ddt, *J* = 15.6, 6.4, 1.2 Hz, 1H), 5.66 (dtd, *J* = 15.6, 5.8, 1.2 Hz, 1H), 4.60 (dt, *J* = 5.8, 1.2 Hz, 2H), 2.49–2.27 (m, 1H), 1.03 (d, *J* = 6.8 Hz, 6H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 190.1, 161.4, 143.0, 135.9, 128.5, 125.3, 121.2, 120.8, 113.2, 69.6, 31.0, 22.2. HRMS (ESI/Q-TOF) m/z: $[M+H]^+$ Calcd for $C_{13}H_{17}O_2$ 205.1223; found 205.1221.

Further derivatisation and removal of the chiral auxiliary.

Synthesis of amides 9

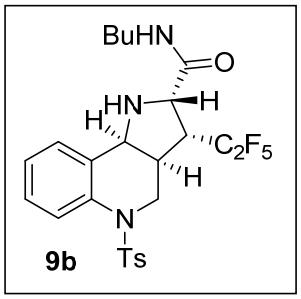
To a solution of **6** (0.10 mmol, 1.0 equiv) in THF (1 mL), n-butylamine (0.02 mL, 0.20 mmol, 2.0 equiv) was added and the resulting mixture was stirred at room temperature for 16 h. A saturated NH_4Cl solution (2 mL) was added, the organic phase was separated and the aqueous phase was extracted with ethyl acetate (3x5 mL). The combined organic phases were washed with brine (20 mL) and dried over anhydrous sodium sulfate and the solvent was removed under vacuum. The crude amide was redissolved in 1 mL of a water/acetonitrile mixture (1/1) and to the resulting solution ammonium cerium (IV) nitrate (110 mg, 0.20 mmol, 2.0 equiv) was added. After 1 h at room temperature, the reaction was quenched with saturated sodium bicarbonate (2 mL), extracted with ethyl acetate (3x 5 mL), dried over sodium sulfate and concentrated under reduced pressure. The crude was purified by flash chromatography on silica gel [*n*-hexane-EtOAc (1:1) to pure EtOAc] to afford compounds **9**.

[9] D. J. Vyas, M. Oestreich *Chem. Commun.* 2010, **46**, 568.



9a

***N*-Butyl-11-(trifluoromethyl)-3,4,5,6-tetrahydro-2*H*-3,6-methanobenzo[*b*][1,5]oxazocine-4-carboxamide (9a):** Starting from **6a**, **9a** was obtained as a white solid (mp = 103-105 ºC) in 59% yield (20 mg). $[\alpha]_D^{25}$ = +23.1 (c 1.0; $CHCl_3$). ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.23 (dd, *J* = 7.6, 1.5 Hz, 1H), 7.17 (td, *J* = 8.2, 1.5 Hz, 1H), 6.98 (td, *J* = 7.6, 1.1 Hz, 1H), 6.96 (br s, 1H), 6.86 (dd, *J* = 8.2, 1.1 Hz, 1H), 4.61 (d, *J* = 7.3 Hz, 1H), 4.14 (dd, *J* = 11.5, 3.2 Hz, 1H), 4.02 (dd, *J* = 11.5, 5.2 Hz, 1H), 3.83 (d, *J* = 8.5 Hz, 1H), 3.41–3.11 (m, 3H), 2.97–2.83 (m, 1H), 1.95 (br s, 1H), 1.60–1.42 (m, 2H), 1.43–1.26 (m, 2H), 0.93 (t, *J* = 7.2 Hz, 3H). ^{19}F NMR (282 MHz, $CDCl_3$) δ -65.82 (d, *J* = 9.9 Hz, 3F). ^{13}C NMR (75 MHz, $CDCl_3$) δ 169.2, 155.0, 129.1, 128.9, 126.76 (q, *J* = 279.9 Hz, CF_3), 124.1, 122.4, 117.5, 66.0, 60.0, 54.1, 47.5 (q, *J* = 27.0 Hz), 39.2, 39.1 (q, *J* = 1.9 Hz), 31.4, 20.2, 13.9. HRMS (ESI/Q-TOF) m/z: $[M+H]^+$ Calcd for $C_{17}H_{22}F_3N_2O_2$ 343.1628; found 343.1620.



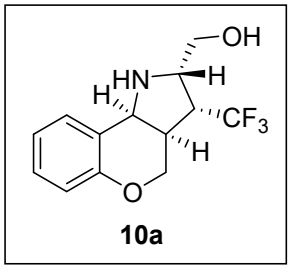
9b

***N*-Butyl-11-(perfluoroethyl)-1-tosyl-1,2,3,4,5,6-hexahydro-3,6-methanobenzo[*b*][1,5] diazocine-4-carboxamide (9b):** Starting from **6p**, **9b** was obtained as a white solid (mp = 42-44 ºC) in 77% yield (42 mg). $[\alpha]_D^{25}$ =-74.0 (c 1.0; $CHCl_3$). ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.73–7.65 (m, 1H), 7.51–7.42 (m, 2H), 7.34–7.26 (m, 2H), 7.25–7.16 (m, 3H), 6.51 (t, *J* = 5.5 Hz, 1H), 4.25 (d, *J* = 7.7 Hz, 1H), 4.17 (dd, *J* = 14.0, 5.4 Hz, 1H), 3.89 (d, *J* = 7.1 Hz, 1H), 3.32–3.12 (m, 3H), 3.01–2.77 (m, 1H), 2.73–2.56 (m, 1H), 2.39 (s, 3H), 1.98 (br s, 1H), 1.57–1.39 (m, 2H), 1.41–1.18 (m, 2H), 0.91 (t, *J* = 7.2 Hz, 3H). ^{19}F NMR (282 MHz, $CDCl_3$) δ -82.47 (s, 3F), -112.04 (dd, *J* = 273.5, 8.2 Hz, 1F), -120.11 (dd, *J* = 273.5, 25.7 Hz, 1F). ^{13}C NMR (75 MHz, $CDCl_3$) δ 169.7, 144.4, 136.9, 136.3, 131.4, 130.0, 129.1, 128.2, 127.0, 126.4, 124.8, 123.3-111.9 (m, C_2F_5), 60.6, 55.6, 47.9 (t, *J* = 20.3 Hz), 47.8, 39.3, 37.4, 31.3, 21.7, 20.2, 13.8. HRMS (ESI/Q-TOF) m/z: $[M+H]^+$ Calcd for $C_{25}H_{29}F_5N_3O_3S$ 546.1795; found 546.1821

Synthesis of amino alcohols 10.

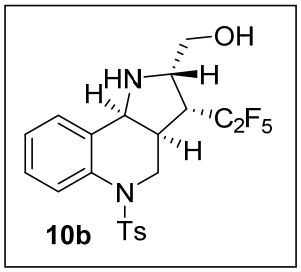
To a solution of **6** (0.10 mmol, 1.0 equiv) in THF (1 mL), lithium aluminum hydride (8 mg, 0.20 mmol, 2.0 equiv) was carefully added and the resulting mixture was stirred at room temperature for 16 h. A saturated NH_4Cl solution (2 mL) was added dropwise, the organic phase was separated and the aqueous phase was extracted with ethyl acetate (3x5 mL). The combined

organic phases were washed with brine (20 mL) and dried over anhydrous sodium sulfate and the solvent was removed under vacuum. The crude amino alcohol was redissolved in 1 mL of a water/acetonitrile mixture (1/1) and to the resulting solution ammonium cerium (IV) nitrate (110 mg, 0.20 mmol, 2.0 equiv) was added. After 1 h at room temperature, the reaction was quenched with saturated sodium bicarbonate (2 mL), extracted with ethyl acetate (3x 5 mL), dried over sodium sulfate and concentrated under reduced pressure. The crude was purified by flash chromatography on silica gel [*n*-hexane-EtOAc (1:1) to pure EtOAc] to afford compounds **10**.



10a

[11-(Trifluoromethyl)-3,4,5,6-tetrahydro-2*H*-3,6-methanobenzo[*b*][1,5]oxazocin-4-yl] methanol (10a): Starting from **6a**, **10a** was obtained as a white solid (mp = 53-55 ºC) in 61% yield (17 mg). $[\alpha]_D^{25}$ =+88.1 (c 1.0; $CHCl_3$). ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.30 (dd, *J* = 7.6, 1.5 Hz, 1H), 7.23–7.14 (m, 1H), 6.99 (td, *J* = 7.6, 1.2 Hz, 1H), 6.89 (dd, *J* = 8.2, 1.2 Hz, 1H), 4.43 (d, *J* = 7.3 Hz, 1H), 4.19–4.10 (m, 1H), 3.95 (dd, *J* = 11.4, 5.1 Hz, 1H), 3.74–3.45 (m, 3H), 2.94–2.76 (m, 2H). ^{19}F NMR (282 MHz, $CDCl_3$) δ -64.24 (d, *J* = 9.8 Hz, 3F). ^{13}C NMR (75 MHz, $CDCl_3$) δ 155.2, 129.5, 129.0, 127.0 (q, *J* = 278.9 Hz, CF_3), 124.1, 122.4, 117.5, 66.4, 60.31 (q, *J* = 3.1 Hz), 59.0, 53.5, 47.08 (q, *J* = 26.9 Hz), 39.71 (q, *J* = 1.7 Hz). HRMS (ESI/Q-TOF) m/z: $[M+H]^+$ Calcd for $C_{13}H_{15}F_3NO_2$ 274.1049; found 274.1044.



10b

[11-(Perfluoroethyl)-1-tosyl-1,2,3,4,5,6-hexahydro-3,6-methanobenzo[*b*][1,5]diazocin-4-yl]methanol (10b): Starting from **6p**, **10b** was obtained as a white solid (mp = 46-48 ºC) in 81% yield (39 mg). $[\alpha]_D^{25}$ =+8.2 (c 1.0; $CHCl_3$). ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.59 (dd, *J* = 8.1, 1.3 Hz, 1H), 7.46–7.39 (m, 2H), 7.34 (dd, *J* = 7.6, 1.3 Hz, 1H), 7.29–7.20 (m, 1H), 7.19–7.09 (m, 3H), 4.15 (dd, *J* = 14.1, 5.6 Hz, 1H), 3.76 (d, *J* = 8.5 Hz, 1H), 3.51 (ddd, *J* = 11.5, 7.2, 4.3 Hz, 2H), 3.28 (ddd, *J* = 11.5, 7.0, 2.1 Hz, 1H), 2.99 (dd, *J* = 14.1, 10.1 Hz, 1H), 2.64–2.37 (m, 2H), 2.34 (s, 3H). ^{19}F NMR (282 MHz, $CDCl_3$) δ -83.79 (s, 3F), -114.57 (dd, *J* = 274.7, 19.2 Hz, 1F), -116.50 (dd, *J* = 274.5, 16.3 Hz, 1F). ^{13}C NMR (75 MHz, $CDCl_3$) δ 144.4, 137.1, 136.9, 130.3, 130.0, 129.2, 128.4, 127.1, 126.5, 125.4, 119.7-110.4 (m, C_2F_5), 60.1, 58.7–58.2 (m), 53.9, 48.7, 48.5, 38.1, 21.7. HRMS (ESI/Q-TOF) m/z: $[M+H]^+$ Calcd for $C_{21}H_{22}F_5N_2O_3S$ 477.1243; found 477.1260.

X-Ray structure of 6a[10]

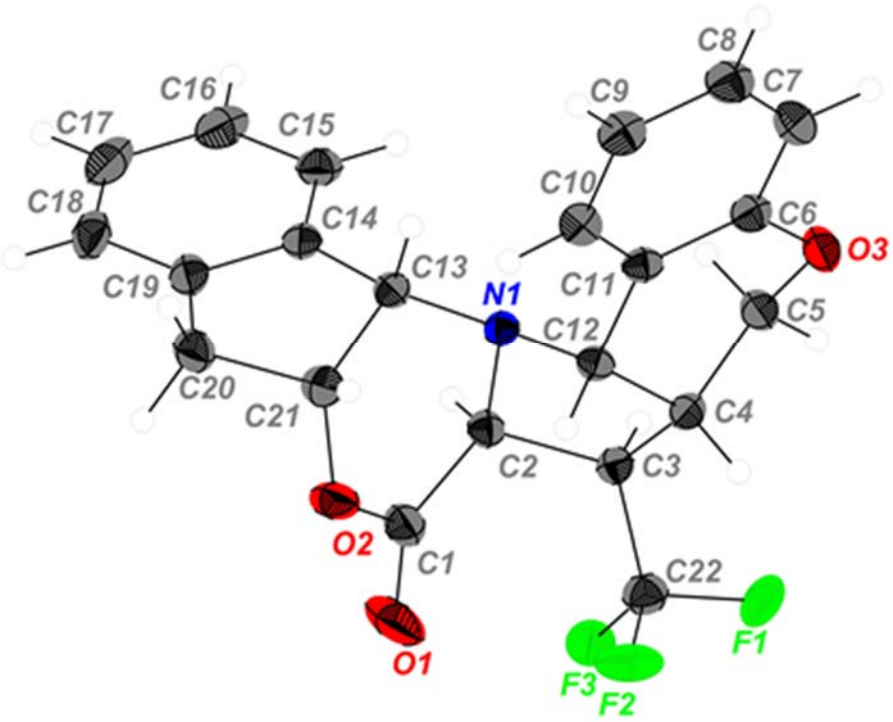


Figure S1. Ortep diagram for compound **6a**

[10] CCDC 1899383 contains the supplementary crystallographic data of compound **6a**. These data can be obtained free of charge at www.ccdc.cam.ac.uk/conts/retrieving.html [or from the Cambridge Crystallographic Data Centre, 12 Union Road, Cambridge CB2 1EZ, UK; fax: (internat.) +44(1223)336-033, e-mail: deposit@ccdc.cam.ac.uk].

Computational Methods

All of the calculations were performed using the Gaussian09 program.[11] Computations were done using B3LYP functional[12] in conjuction with Grimme's dispersion correction.[13] Standard basis sets def2SVP and def2TZVP were employed.[14] Geometry full optimizations were made at B3LYP-D3BJ/def2SVP level and then single point calculations at B3LYP-D3BJ/def2TZVP level were carried out in order to obtain more accurate values of the energies. Solvent effects (toluene) were considered using the PCM model.[15] The nature of stationary points was defined on the basis of calculations of normal vibrational frequencies (force constant Hessian matrix). The optimizations were carried out using the Berny analytical gradient optimization method.[16] Minimum energy pathways for the reactions studied were found by gradient descent of transition states in the forward and backward direction of the transition vector (IRC analysis),[17] using using the Hratchian-Schlegel algorithm.[18] Analytical second derivatives of the energy were calculated to classify the nature of every stationary point, to determine the harmonic vibrational frequencies, and to provide zero-point vibrational energy corrections. The thermal and entropic contributions to the free energies were also obtained from the vibrational frequency calculations, using the unscaled frequencies. NCI (non-covalent interactions) were computed using the methodology previously described.[19] Data were obtained with the NCIPLOT program.[20] A density cutoff of ρ=0.1 a.u. was applied and the pictures were created for an

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isosurface value of s=0.4 and colored in the [-0.02,0.02] a.u. sign(λ_2)ρ range using VMD software.[21] Structural representations were generated using CYLView.[22]

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Approaches studied

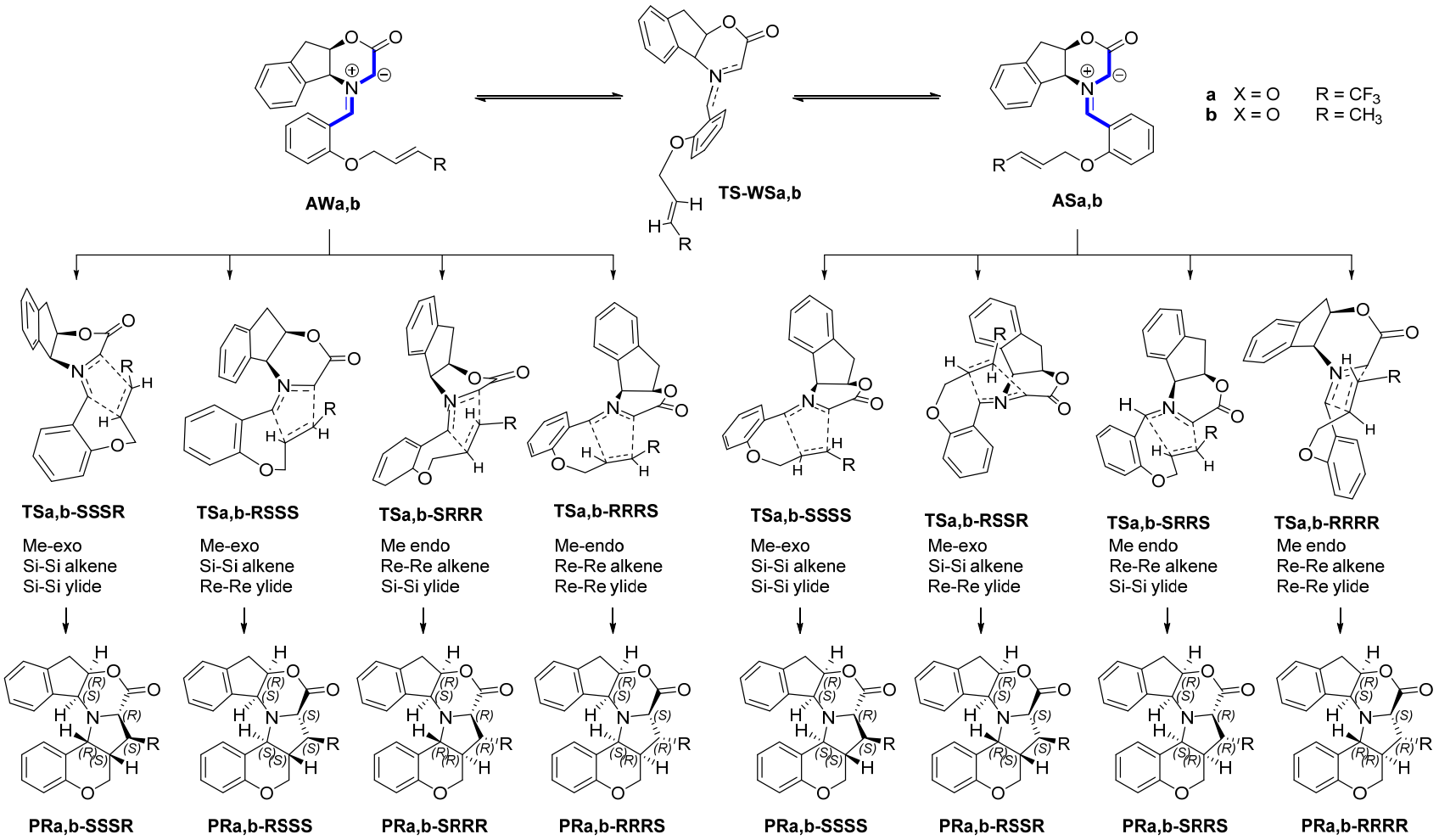

Figure S1 Approaches considered for the intramolecular cycloaddition of azomethine ylides.

Energy Values

Table S1 Calculated (B3LYP-D3BJ/def2TZVP/PCM=toluene//B3LYP-D3BJ/def2SVP) absolute (hartrees) and relative (kcal/mol) energies for the intramolecular cycloaddition of the azomethine ylide derived from 3a and IV.

	E_0	ΔE_0[a]	G	ΔG[a]	im. freq	%[b]
AWa	-1429.383117	0.0	-1429.439121	0.0		
ASa	-1429.378491	2.9	-1429.433866	3.3		
TS-WSa	-1429.365027	11.4	-1429.420814	11.5	-44.4	
TSa-RRRR	-1429.350423	20.5	-1429.401690	23.5	-356.3	0.0
TSa-RSSR	-1429.364022	12.0	-1429.415886	14.6	-243.2	9.0
TSa-SRRS	-1429.365290	11.2	-1429.418069	13.2	-277.7	91.0
TSa-SSSS	-1429.353454	18.6	-1429.405921	20.8	-355.1	0.0
TSa-RRRS	-1429.295365	55.1	-1429.347784	57.3	-180.6	0.0
TSa-RSSS	-1429.357805	15.9	-1429.409191	18.8	-375.5	0.0
TSa-SRRR	-1429.315701	42.3	-1429.370171	43.3	-256.5	0.0
TSa-SSSR	-1429.314283	43.2	-1429.368104	44.6	-142.8	0.0
PRa-RRRR	-1429.431657	-30.5	-1429.483230	-27.7		
PRa-RRRS	-1429.447725	-40.5	-1429.498639	-37.3		
PRa-RSSR	-1429.432097	-30.7	-1429.483179	-27.6		
PRa-RSSS	-1429.422902	-25.0	-1429.473628	-21.7		
PRa-SRRR	-1429.426440	-27.2	-1429.478486	-24.7		
PRa-SRRS	-1429.437830	-34.3	-1429.489983	-31.9		
PRa-SSSR	-1429.441904	-36.9	-1429.495100	-35.1		
PRa-SSSS	-1429.437424	-34.1	-1429.490844	-32.5		

[a] referred to **AWa**. [b] % abundance according to Boltzmann distribution

Table S2 Calculated (B3LYP-D3BJ/def2TZVP/PCM=toluene//B3LYP-D3BJ/def2SVP) absolute (hartrees) and relative (kcal/mol) energies for the intramolecular cycloaddition of the azomethine ylide derived from 7 and IV.

	E_0	ΔE_0[a]	G	ΔG[a]	im. freq	%[b]
AWb	-1131.498183	0.0	-1131.552321	0.0		
ASb	-1131.492855	3.3	-1131.544041	5.2		
TS-WSb	-1131.479465	11.7	-1131.535213	10.7	-40.2	
TSb-RRRR	-1131.458744	24.7	-1131.507087	28.4	-415.3	0.0
TSb-RSSR	-1131.476805	13.4	-1131.525129	17.1	-336.0	35.9
TSb-SRRS	-1131.476433	13.6	-1131.525630	16.7	-334.0	61.0
TSb-SSSS	-1131.463061	22.0	-1131.512105	25.2	-413.1	0.0
TSb-RRRS	-1131.417883	50.4	-1131.465298	54.6	-330.5	0.0
TSb-RSSS	-1131.474769	14.7	-1131.522827	18.5	-369.2	3.1
TSb-SRRR	-1131.428292	43.9	-1131.479921	45.4	-371.6	0.0
TSb-SSSR	-1131.423960	46.6	-1131.474964	48.5	-241.6	0.0
PRb-RRRR	-1131.543232	-28.3	-1131.591394	-24.5		
PRb-RRRS	-1131.557753	-37.4	-1131.605362	-33.3		
PRb-RSSR	-1131.549325	-32.1	-1131.597904	-28.6		
PRb-RSSS	-1131.537287	-24.5	-1131.585195	-20.6		
PRb-SRRR	-1131.540951	-26.8	-1131.589845	-23.5		
PRb-SRRS	-1131.552472	-34.1	-1131.600238	-30.1		
PRb-SSSR	-1131.555497	-36.0	-1131.604795	-32.9		
PRb-SSSS	-1131.550506	-32.8	-1131.599607	-29.7		

[a] referred to **AWa**. [b] % abundance according to Boltzmann distribution

Energy Profiles

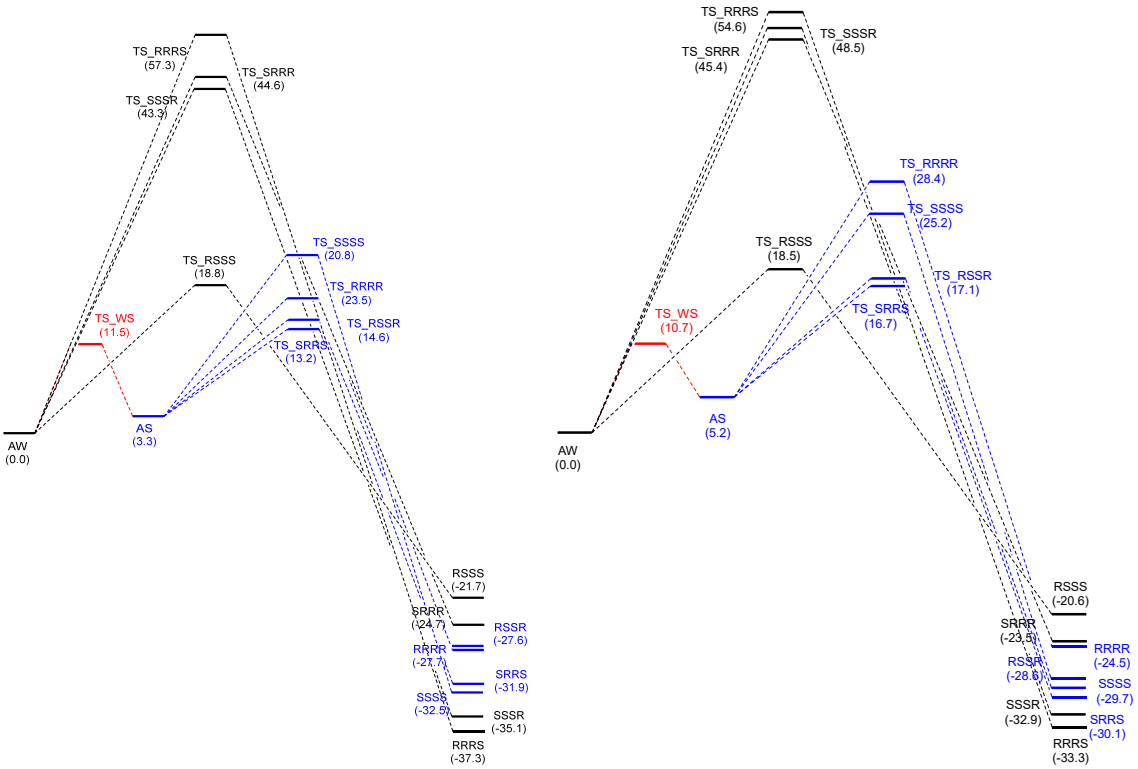

Figure S2 Energy profile for the intramolecular cycloaddition of the azomethine ylide derived from 3a and IV (left) and the azomethine ylide derived from 7 and IV (right).

Transition Structures

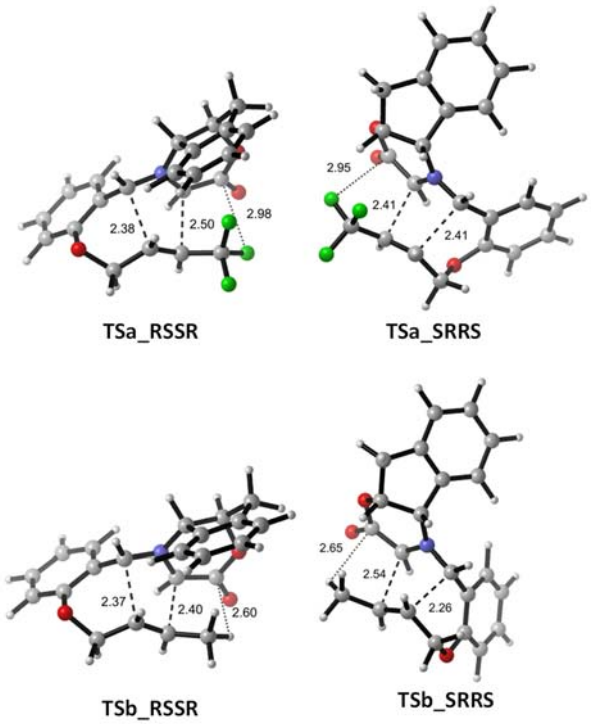

Figure S3 Optimized (b3lyp-3dbj/def2svp) for the intramolecular cycloaddition of the azomethine ylide derived from 3a and IV (top) and the azomethine ylide derived from 7 and IV (bottom).

NCI Analyses

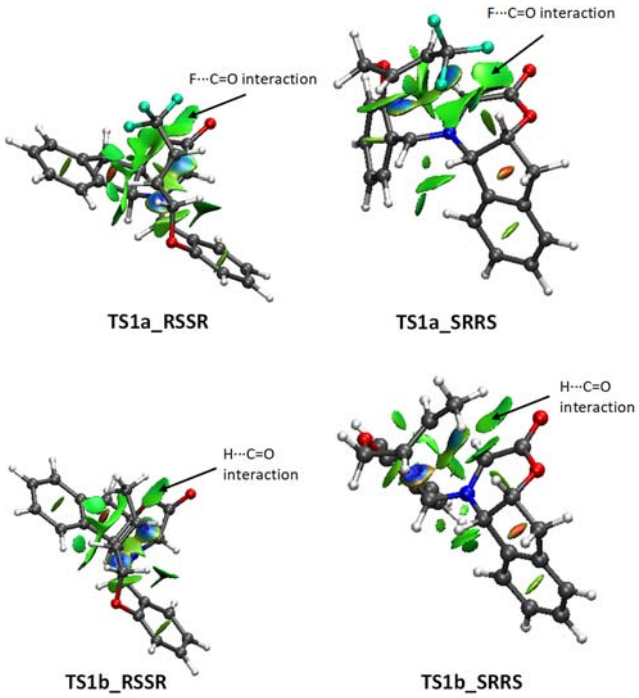

Figure S4 NCI analyses corresponding to the transition structures corresponding to the intramolecular cycloaddition of the azomethine ylide derived from 3a and IV (top) and the azomethine ylide derived from 7 and IV (bottom).

Cartesian Coordinates

ASa

0 1

H	0	2.1603620793	2.6827367134	-1.6308733832
C	0	1.1660300210	-2.0030560969	-0.7996290581
C	0	0.8093809805	0.3595625607	-0.7165713136
C	0	2.6538292344	1.8317148234	-1.1299742234
H	0	3.7287700784	1.8707128254	-1.3553493144
C	0	2.3354196009	1.8188127253	0.3497391321
C	0	2.9169873181	2.5235666555	1.4010821754
C	0	2.4522202762	2.3039317792	2.7045768699
C	0	1.4273707203	1.3834697064	2.9535996168
C	0	0.8339393485	0.6811007844	1.8963798651
C	0	1.2903452003	0.9206337066	0.6043639570
H	0	3.7339100958	3.2256467803	1.2174767079
H	0	2.9065981654	2.8441283001	3.5383590477
H	0	1.0949751150	1.2053159789	3.9788083913
H	0	0.0450126840	-0.0520451785	2.0815750857
O	0	2.9954252054	-0.5138500360	-1.3514372774
C	0	2.5633396335	-1.7963116175	-1.1066487156
O	0	3.3685072891	-2.6987667066	-1.1517998207
C	0	2.0435460749	0.5051576108	-1.6146835569
H	0	1.7849417476	0.5005300135	-2.6866224811
H	0	0.0113758081	1.0003476668	-1.1185130793
N	0	0.2646666244	-1.0096406724	-0.6402337113
C	0	-1.0366965190	-1.0464615161	-0.3201207212
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H	0	-1.2967503324	2.1107532454	1.5257978987
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C	0	-1.8742441265	-2.1285509368	0.1200633874
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H	0	-4.4342499174	0.5522728200	1.7517238674
H	0	-2.7041892471	0.1309072184	1.8696681312
H	0	0.8481600592	-3.0326532614	-0.7125369962
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C	0	-2.4065223593	-4.4138976673	0.8328098322
H	0	-2.0692243125	-5.4369757953	1.0128968271
C	0	-3.7388646591	-4.0652973829	1.0592236801
H	0	-4.4565602781	-4.8098952823	1.4097767589
C	0	-4.1491247480	-2.7467983268	0.8322550196
H	0	-0.4644422254	-3.7854272656	0.2142980670
H	0	-5.1831896242	-2.4368422796	0.9955534237
F	0	-2.5569785266	4.1024990109	-0.8176510645
F	0	-1.3193502984	4.6734398739	0.8690492159
F	0	-0.5000717450	3.4229772770	-0.6972522401

ASb

0 1

H	2.3590728680	2.4894335953	-1.9954156552
C	1.1791799133	-2.1002490928	-0.8647687766
C	0.8824292908	0.2816171905	-0.9169928943
C	2.7867889207	1.6676779432	-1.3940971301
H	3.8710725372	1.6427325150	-1.5726585534
C	2.4098801723	1.8003981121	0.0664123671
C	2.9702062275	2.5887109040	1.0694781607
C	2.4500690832	2.5040570724	2.3680681988
C	1.3903123283	1.6370663393	2.6592936414
C	0.8170716401	0.8531156102	1.6503418349
C	1.3312705044	0.9549341726	0.3623023928
H	3.8135531108	3.2495537390	0.8543492830
H	2.8874244349	3.1093215437	3.1656006255
H	1.0106106827	1.5685943953	3.6813213807
H	-0.0081435818	0.1722293101	1.8671785326
O	3.0622048341	-0.6906638889	-1.4204316756
C	2.5829804228	-1.9571207501	-1.1568849562
O	3.3621086990	-2.8837798371	-1.1685824632
C	2.1464573900	0.3255744078	-1.7883130321
H	1.9137756570	0.2440091749	-2.8635449586
H	0.1020910764	0.8893565304	-1.4012354278
N	0.3107291161	-1.0668401771	-0.7425719347
C	-0.9835281573	-1.0607750075	-0.4042622433
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H	-2.0042377078	1.8722983524	2.2013308907
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C	-1.8159717399	-2.1056423688	0.1279457667
C	-3.1929952107	-1.7661992310	0.3122369464
O	-3.6280013221	-0.5460236805	-0.1272304800
C	-3.9077155807	0.4658457009	0.8584838055
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C	-2.3088665640	-4.2724157894	1.1611451035
H	-1.9551086232	-5.2505860327	1.4942470673
C	-3.6482845470	-3.9159464633	1.3307813472
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H	-0.3697828309	-3.6945080194	0.4793876538
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H	-0.4151070563	3.3626526773	0.8583466471
H	-1.7971128205	3.9429030269	-0.1218420573

AWa

0 1

H	0	3.2153126898	2.5186816612	-2.0092274790
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C	0	1.7008262504	0.3463220669	-0.9504041563
C	0	3.6243084054	1.7254751679	-1.3585547133
H	0	4.7165318703	1.7129124519	-1.4792709536
C	0	3.1673785946	1.8982934569	0.0735075809
C	0	3.6838975202	2.7012872965	1.0872689420
C	0	3.0948890118	2.6520116280	2.3577472477
C	0	2.0077537460	1.8080933810	2.6102600582
C	0	1.4803745148	1.0056122323	1.5907072777
C	0	2.0667946881	1.0668937239	0.3301357475
H	0	4.5464809022	3.3461471559	0.9025137879
H	0	3.4977154592	3.2693536916	3.1641216973
H	0	1.5701892447	1.7702868246	3.6103043826
H	0	0.6362513313	0.3403840231	1.7840292777
O	0	3.9309026980	-0.6219662740	-1.2692896980
C	0	3.4508919809	-1.8728253114	-0.9447857096
O	0	4.2412823751	-2.7800082324	-0.8096287973
C	0	3.0259153271	0.3601309414	-1.7359964184
H	0	2.8612096384	0.2297424400	-2.8191161481
H	0	0.9696772526	0.9270945295	-1.5305887497
N	0	1.1318742374	-0.9988591918	-0.7843032846
C	0	-0.1868142768	-1.1897302253	-0.6474543328
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C	0	-4.4832197246	-2.8205434757	0.6250988858
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H	0	-4.2529584601	-2.0909016951	2.6103548908
C	0	-6.3834198091	-2.2985014716	2.1528426232
C	0	-1.2902613373	-0.2597082129	-0.6216932736
C	0	-2.5913723203	-0.8377806331	-0.7676901137
O	0	-2.6968742725	-2.2034044198	-0.9133838438
C	0	-3.0309269224	-2.9320029633	0.2696964854
H	0	-2.7882344499	-3.9818491604	0.0380455185
H	0	-2.3969266059	-2.6095216701	1.1147400280
H	0	1.6489202213	-3.0195093772	-0.5921131883
C	0	-1.2508463922	1.1492310042	-0.4506862678
C	0	-2.4077566843	1.9246560292	-0.4765798392
H	0	-2.3249004085	3.0047836400	-0.3366652995
C	0	-3.6590914090	1.3353210961	-0.6659594275
H	0	-4.5650358057	1.9438508562	-0.6951060013
C	0	-3.7406012739	-0.0525755143	-0.8034958524
H	0	-0.3130333427	1.6570424194	-0.2478560796
H	0	-4.7028005212	-0.5439370109	-0.9499753998
F	0	-7.1826411908	-2.6707771164	1.1404050325
F	0	-6.6871004017	-3.0671358230	3.2148467303
F	0	-6.7071566480	-1.0329697258	2.4797761184

AWb

0 1

H	3.2202735592	2.5300597916	-1.9397728148
C	2.0003027903	-2.0298310404	-0.8333496607
C	1.6784972720	0.3397585400	-0.9584523348

C	3.6132723638	1.7223736763	-1.2970226178
H	4.7078515809	1.7092074285	-1.3942658231
C	3.1258072689	1.8674002925	0.1280371342
C	3.6218185711	2.6485798405	1.1687543864
C	3.0047761846	2.5757245456	2.4247222138
C	1.9100631836	1.7302652549	2.6360746326
C	1.4032794161	0.9497937171	1.5893423152
C	2.0178986453	1.0340887928	0.3436571062
H	4.4898749103	3.2945039704	1.0158982990
H	3.3912555100	3.1756734091	3.2520127383
H	1.4501527846	1.6740106484	3.6252058259
H	0.5529275492	0.2838536110	1.7499342131
O	3.9126131394	-0.6269906003	-1.2512427978
C	3.4220607245	-1.8861121378	-0.9704202485
O	4.2093649464	-2.7980329709	-0.8450149026
C	3.0200202043	0.3666294430	-1.7154081235
H	2.8770247201	0.2601563482	-2.8043349886
H	0.9611365394	0.9342069612	-1.5419978474
N	1.1033588548	-1.0063784839	-0.8319037745
C	-0.2168405311	-1.1956811336	-0.7185222017
H	-0.4938815643	-2.2479499026	-0.7192481691
C	-4.4404347212	-2.8056542092	0.6472108594
H	-5.2131115356	-3.1504949665	-0.0513674300
C	-4.7909904944	-2.2770788794	1.8250181712
H	-3.9930375241	-1.9269259063	2.4937431238
C	-6.1927836869	-2.1096112502	2.3224720691
H	-6.3450774126	-2.6486891655	3.2736253348
H	-6.4114427031	-1.0472292663	2.5281756600
H	-6.9314728215	-2.4796063104	1.5954469142
C	-1.3202558698	-0.2653714293	-0.6886077743
C	-2.6193933952	-0.8469713883	-0.8489405326
O	-2.7256862623	-2.2055996526	-1.0051958825
C	-3.0235326053	-2.9559880322	0.1877608299
H	-2.8134229374	-4.0005563066	-0.0912836485
H	-2.3259206916	-2.6675654675	0.9947741147
H	1.6104490860	-3.0335335126	-0.6791439707
C	-1.2820744012	1.1419933752	-0.5055379529
C	-2.4390508207	1.9171747600	-0.5346732166
H	-2.3580861568	2.9964590572	-0.3866993569
C	-3.6879659757	1.3273950091	-0.7395769399
H	-4.5935966768	1.9366591363	-0.7731829424
C	-3.7680230291	-0.0594010313	-0.8864152397
H	-0.3462139534	1.6493625937	-0.2927430374
H	-4.7262336651	-0.5552330389	-1.0414491828

PRa-RRRR

0 1

H	0	3.7115495256	0.8717558034	-2.2431335853
C	0	0.3989418707	-2.1387742203	-0.4961467445
C	0	1.2095826522	0.1505209722	-1.0233156586
C	0	3.6162801500	0.3410737187	-1.2794769717
H	0	4.5738500524	-0.1550569205	-1.0673449051
C	0	3.1472868673	1.2731841225	-0.1863843479

C	0	3.8974790354	2.1728432141	0.5654406997
C	0	3.2504062623	2.9644849301	1.5216852837
C	0	1.8691472401	2.8579948093	1.7030428605
C	0	1.1124038946	1.9585291361	0.9400358049
C	0	1.7587438565	1.1501652208	0.0031533414
H	0	4.9772343353	2.2547428421	0.4168918102
H	0	3.8269819448	3.6677022967	2.1272116049
H	0	1.3682235112	3.4833221092	2.4456259450
H	0	0.0342156537	1.9203548952	1.0821134309
O	0	2.7439686434	-1.6257406883	-0.3058890018
C	0	1.7315964176	-2.3372852933	0.2211567049
O	0	1.9089426675	-3.0605105200	1.1628571914
C	0	2.4761540911	-0.6731983675	-1.3510631031
H	0	2.4025124868	-1.2045701852	-2.3126350224
H	0	0.9869134482	0.7297573580	-1.9423003602
N	0	0.0790000770	-0.7178326043	-0.7334220317
C	0	-1.0092277085	-0.3425212174	0.1571273484
H	0	-0.6338574575	-0.1466509933	1.1864368185
C	0	-1.8419420132	-1.6211799407	0.2147717775
H	0	-2.3538344059	-1.7211043516	-0.7554517877
C	0	-0.7777712163	-2.7098502729	0.3193570252
H	0	-0.4491525435	-2.8566626487	1.3592233658
C	0	-1.2421308298	-4.0628768425	-0.1734587629
C	0	-1.9434392860	0.7800542651	-0.2207823705
C	0	-3.2366236935	0.7111245816	0.3473235751
O	0	-3.6574438526	-0.3099586187	1.1455289921
C	0	-2.8724873321	-1.4930879242	1.3141596368
H	0	-2.3775415661	-1.4559096805	2.3017738121
H	0	-3.5747867143	-2.3383815161	1.3184377578
H	0	0.4904626084	-2.6624455183	-1.4670567372
C	0	-1.6400942546	1.8555419036	-1.0624277280
C	0	-2.5740372353	2.8609451188	-1.3212737446
H	0	-2.3116774639	3.6927342474	-1.9778774662
C	0	-3.8396801944	2.7934430552	-0.7321772988
H	0	-4.5778883891	3.5759477965	-0.9230653499
C	0	-4.1734852083	1.7209482223	0.0925714169
H	0	-0.6542466781	1.9174207032	-1.5203459690
H	0	-5.1614660106	1.6334628507	0.5478290668
F	0	-0.2617912926	-4.9742810725	-0.1326142356
F	0	-2.2610102437	-4.5201408892	0.5802065150
F	0	-1.6832902826	-4.0090667366	-1.4467437130

PRa-RRRS

0 1

H	0	3.6493943244	-1.8415739050	-1.9739279341
C	0	-0.8278366227	-1.6519498337	-0.3458162928
C	0	1.2680582664	-0.5015599777	-0.8847204388
C	0	3.2316615505	-1.9602065024	-0.9587700279
H	0	3.6191951022	-2.9025876780	-0.5452613779
C	0	3.5160807698	-0.7499450938	-0.0996343359
C	0	4.6857763432	-0.4180226529	0.5814919732
C	0	4.7153669561	0.7560588254	1.3428212148
C	0	3.5847228845	1.5766478176	1.4217688337

C	0	2.4108905431	1.2440161552	0.7353655332
C	0	2.3874093355	0.0796509535	-0.0307451956
H	0	5.5614772435	-1.0705844949	0.5353436612
H	0	5.6224322749	1.0265014493	1.8887794286
H	0	3.6135377973	2.4845996554	2.0287335066
H	0	1.5335499384	1.8841387727	0.8087109165
O	0	1.2425551578	-2.7627145856	0.0965860829
C	0	-0.0521805299	-2.6706933963	0.4678594425
O	0	-0.4920151700	-3.3237906780	1.3720666948
C	0	1.7029311808	-1.9864693308	-1.0267159235
H	0	1.3194017449	-2.4503197072	-1.9485343164
H	0	1.3204720446	-0.0573675323	-1.9013325875
N	0	-0.0762565610	-0.4030976277	-0.3494957505
C	0	-1.0257119941	0.6188421852	-0.7969050903
H	0	-1.2979289900	0.4541364281	-1.8621476811
C	0	-2.2344518744	0.2845366391	0.0982940067
H	0	-3.1708043595	0.6571579744	-0.3395305819
C	0	-2.2042076202	-1.2588842028	0.2127743837
H	0	-2.2861673521	-1.5999375574	1.2553030262
C	0	-3.3382712396	-1.9192887812	-0.5383966097
C	0	-0.5681689714	2.0442325033	-0.6384789655
C	0	-1.0021880860	2.8072723362	0.4623721795
O	0	-1.8624877211	2.3268706240	1.3957523691
C	0	-2.0171918758	0.9182166178	1.4687479748
H	0	-1.1170525391	0.4749174162	1.9294718775
H	0	-2.8786933926	0.7380818134	2.1265533547
H	0	-0.9539757341	-2.0612647184	-1.3739170875
C	0	0.2721939789	2.6497930742	-1.5826203447
C	0	0.7103619089	3.9635434169	-1.4316018218
H	0	1.3757803153	4.4105305820	-2.1724661112
C	0	0.2817697109	4.7041770694	-0.3230076130
H	0	0.6145632395	5.7364697314	-0.1913843541
C	0	-0.5761582192	4.1353268257	0.6143761242
H	0	0.5862680699	2.0706843301	-2.4547477628
H	0	-0.9342290463	4.6960625556	1.4794492410
F	0	-3.2281360519	-3.2556606555	-0.5276760639
F	0	-4.5269472187	-1.5992048718	-0.0012491078
F	0	-3.3700625118	-1.5336469685	-1.8337504493

PRa-RSSR

0 1

H	0	2.7409423989	1.3486503618	-2.7273148516
C	0	-0.0087764139	-1.9882177676	-0.4389290798
C	0	0.8346440456	0.3386557981	-0.8168829350
C	0	2.9419548184	0.5413649888	-2.0011318444
H	0	3.8133588283	-0.0269680476	-2.3562732979
C	0	3.0946814211	1.0863573360	-0.5982932914
C	0	4.2140636476	1.6627983265	-0.0041137322
C	0	4.1318270447	2.0896349484	1.3270127505
C	0	2.9420558861	1.9356229109	2.0441734928
C	0	1.8150453506	1.3590035739	1.4434281478
C	0	1.8955505683	0.9327984784	0.1177637009
H	0	5.1478568716	1.7685246801	-0.5624779190

H	0	5.0043503181	2.5353693285	1.8104177500
H	0	2.8894008572	2.2609948886	3.0857245191
H	0	0.9017089084	1.2417360503	2.0249176997
O	0	2.1988092052	-1.6229345858	-1.3800603384
C	0	1.4180011425	-2.4638705590	-0.6747195525
O	0	1.8180623742	-3.5494265927	-0.3589248610
C	0	1.7124850907	-0.3590451335	-1.8715934024
H	0	1.1791040280	-0.5350672962	-2.8188057761
H	0	0.3421321644	1.1891450336	-1.3311040670
N	0	-0.1764336647	-0.5523840181	-0.3312003009
C	0	-1.1841347408	-0.1753407733	0.6579901172
H	0	-0.7161986594	0.1669597971	1.5981964736
C	0	-1.8969919653	-1.5102227070	0.9247553727
H	0	-2.3462892723	-1.5271732675	1.9250587372
C	0	-0.7706725482	-2.5540191948	0.7780527830
H	0	-1.1610970477	-3.5613409586	0.5767016829
C	0	0.0720223426	-2.6778185008	2.0549280692
C	0	-2.1346678270	0.9067516406	0.1935797226
C	0	-3.4585032971	0.5921925694	-0.1619321379
O	0	-3.9487328973	-0.6772615508	-0.1028797348
C	0	-2.9985443070	-1.7262439283	-0.1121753517
H	0	-3.5589892727	-2.6475064531	0.0995394612
H	0	-2.5666343537	-1.8102533498	-1.1259994659
H	0	-0.5303880514	-2.3854365408	-1.3410870086
C	0	-1.7364243659	2.2516611655	0.1566505668
C	0	-2.6136124389	3.2587017688	-0.2448760668
H	0	-2.2808253011	4.2982899372	-0.2700404886
C	0	-3.9269416326	2.9256423698	-0.5975567532
H	0	-4.6273808257	3.7055432640	-0.9056836983
C	0	-4.3513417912	1.6001707145	-0.5513915770
H	0	-0.7219277855	2.5113780205	0.4693727504
H	0	-5.3727451067	1.3149952193	-0.8096674495
F	0	1.0311269603	-1.7326766678	2.1237451223
F	0	-0.6937951596	-2.5325065851	3.1585139009
F	0	0.6609964129	-3.8693119722	2.1534462813

PRa-RSSS

0 1

H	0	3.9435277656	-1.3331125127	-1.8615065836
C	0	-0.8760566515	-1.6164361355	-0.6100007693
C	0	1.2694859287	-0.4037614637	-1.0925821534
C	0	3.2776968607	-1.7938870853	-1.1105169074
H	0	3.6076219433	-2.8314853217	-0.9588309885
C	0	3.2456903344	-0.9560585740	0.1457405602
C	0	4.2080584333	-0.8745168314	1.1507400059
C	0	4.0429327332	0.0624812049	2.1758825963
C	0	2.9455711032	0.9293075250	2.1638027255
C	0	1.9823389630	0.8460945540	1.1520146303
C	0	2.1072378500	-0.1343330260	0.1657692575
H	0	5.0832113959	-1.5292453533	1.1336662368
H	0	4.7828311471	0.1308938901	2.9768489594
H	0	2.8394699081	1.6848814065	2.9456387382
H	0	1.1670878283	1.5673452151	1.1342189132

O	0	1.1858510083	-2.8895283179	-0.9964052893
C	0	-0.0849204622	-2.9121392131	-0.5758021077
O	0	-0.5885288952	-3.9410890936	-0.2167540844
C	0	1.8290460941	-1.7502881015	-1.5956327541
H	0	1.7171710082	-1.8523210433	-2.6852278674
H	0	1.5859097469	0.3485103906	-1.8347065365
N	0	-0.1814856248	-0.4439988715	-1.1340971229
C	0	-1.0268688503	0.6546129149	-0.6855154742
H	0	-1.9774235591	0.5453919047	-1.2501742591
C	0	-1.3415800940	0.3172469969	0.7770958651
H	0	-0.4252426979	0.4829930787	1.3565649992
C	0	-1.5971133725	-1.1920858240	0.7467308521
H	0	-2.6690588001	-1.4257105731	0.6717449390
C	0	-1.1124642563	-1.8533552939	2.0297220718
C	0	-0.5988623228	2.0874742481	-0.8120689644
C	0	-1.0526063468	2.9822752077	0.1839968104
O	0	-1.8274470751	2.6134988198	1.2437798861
C	0	-2.3696654329	1.2907157620	1.3033951813
H	0	-2.6156500634	1.1138120135	2.3578568465
H	0	-3.3037754430	1.2459460557	0.7114208638
H	0	-1.7058554831	-1.8470819748	-1.3002640684
C	0	0.1552104475	2.5910810684	-1.8786258988
C	0	0.5115023356	3.9381996369	-1.9415602692
H	0	1.1088515632	4.3093115779	-2.7765723274
C	0	0.0917261406	4.8064427290	-0.9279844017
H	0	0.3662897516	5.8633491823	-0.9619649599
C	0	-0.6910790431	4.3354375659	0.1237039135
H	0	0.4592596911	1.9096369197	-2.6753853659
H	0	-1.0444516069	4.9981097434	0.9155643505
F	0	-1.4919527782	-1.1166654927	3.1019263942
F	0	-1.6125223440	-3.0756821902	2.2092582526
F	0	0.2306949117	-1.9358316181	2.0708546946

PRa-SRRR

0 1

H	0	3.6164470604	-1.3149994905	-2.5030974240
C	0	-0.2626272828	-1.3032104927	0.5304114474
C	0	1.4291087915	-0.2452956166	-0.8655134206
C	0	3.1499472977	-1.7996972378	-1.6271991696
H	0	3.3809019698	-2.8734207718	-1.6761634278
C	0	3.5937792372	-1.1266034799	-0.3470557212
C	0	4.7847806762	-1.2769907568	0.3610450880
C	0	4.9889186118	-0.5121426122	1.5162344856
C	0	4.0173442629	0.3974263372	1.9483406354
C	0	2.8221607184	0.5520306700	1.2344892436
C	0	2.6142335075	-0.2235228086	0.0931656936
H	0	5.5473290747	-1.9842145287	0.0248647357
H	0	5.9144543160	-0.6265700366	2.0854417166
H	0	4.1915592330	0.9908466623	2.8488803468
H	0	2.0743576192	1.2722975297	1.5708778711
O	0	1.0227828669	-2.7035116641	-1.0111321043
C	0	0.1266212089	-2.6688169004	-0.0082655693
O	0	-0.2648831187	-3.6909348956	0.4826634937

C	0	1.6327205469	-1.5638660435	-1.6444826505
H	0	1.2043868473	-1.5062479649	-2.6547911598
H	0	1.5347666206	0.5632647961	-1.6047558573
N	0	0.0871456273	-0.1978831223	-0.3487957441
C	0	-0.5278603746	0.9491666122	0.3105281749
H	0	-0.1266773379	1.0447473906	1.3477759725
C	0	-1.9545588413	0.4118553827	0.4144689260
H	0	-2.3309363609	0.3710067836	-0.6190427728
C	0	-1.7630854034	-1.0362204194	0.9035160684
H	0	-1.8936972336	-1.1189319112	1.9917922967
C	0	-2.8054846342	-1.9585932087	0.2830492733
C	0	-0.5410901890	2.3283537759	-0.2963527046
C	0	-1.7330209422	3.0792612404	-0.1548229569
O	0	-2.8591455408	2.6219204180	0.4620284819
C	0	-2.8242671886	1.3842394260	1.1724555182
H	0	-2.4401897653	1.5534743905	2.1966662329
H	0	-3.8649006836	1.0435719333	1.2420277142
H	0	0.3029542282	-1.2352464856	1.4875130248
C	0	0.5686230905	2.9529767544	-0.8842054966
C	0	0.4954174594	4.2523205753	-1.3867373260
H	0	1.3734439750	4.7098844237	-1.8467061390
C	0	-0.7053465003	4.9617466603	-1.2859552447
H	0	-0.7788121695	5.9789606731	-1.6777448510
C	0	-1.8092514619	4.3824868173	-0.6667612724
H	0	1.5194395376	2.4231940420	-0.9356099892
H	0	-2.7510027218	4.9221778626	-0.5531737806
F	0	-2.9216892821	-3.1227085929	0.9198248115
F	0	-4.0242170985	-1.3672280949	0.3328201590
F	0	-2.5446092539	-2.2055030214	-1.0127126296

PRa-SRRS

0 1

H	0	3.7024893794	0.1376032553	-2.0878557583
C	0	-0.0106587440	-1.6866117306	0.7154400285
C	0	1.0430144633	-0.1089459961	-0.8992037936
C	0	3.4781651307	-0.1622100121	-1.0486021557
H	0	4.3615961894	-0.6823603984	-0.6506181113
C	0	3.0377738565	1.0275787833	-0.2207243078
C	0	3.8048429284	2.0112441687	0.4016221703
C	0	3.1535604610	3.0191379378	1.1244031122
C	0	1.7567544723	3.0389530850	1.2232856970
C	0	0.9856998713	2.0514502075	0.5981456565
C	0	1.6407661346	1.0557007760	-0.1215670993
H	0	4.8960781784	1.9926171435	0.3393600269
H	0	3.7422030742	3.7920276382	1.6247313033
H	0	1.2648209957	3.8275789649	1.7977103803
H	0	-0.1026104549	2.0561679013	0.6761569775
O	0	2.3796175190	-1.9177434300	0.1363494804
C	0	1.3914592409	-2.2204099756	0.9940447593
O	0	1.6144493516	-2.8810762868	1.9716657978
C	0	2.2442324078	-1.0744672708	-1.0271346749
H	0	2.1573150841	-1.7384700602	-1.8982819087
H	0	0.7943529808	0.2360859175	-1.9191454270

N	0	-0.1149559049	-0.7437176191	-0.3635427564
C	0	-1.4216470632	-0.7186703614	-1.0016969891
H	0	-1.3241946711	-0.9203597886	-2.0838876312
C	0	-2.1833860297	-1.8813866880	-0.2928020843
H	0	-2.7495111667	-2.4711826144	-1.0260269313
C	0	-1.0682397112	-2.7479547170	0.3370869995
H	0	-1.4162440987	-3.3026086573	1.2194343099
C	0	-0.5790425786	-3.8039162860	-0.6454299614
C	0	-2.0706259120	0.6349960359	-0.7968023524
C	0	-2.6298364955	0.8987225605	0.4642416774
O	0	-2.7711066325	-0.1294095057	1.3557163698
C	0	-3.1901113732	-1.3403591058	0.7329141681
H	0	-3.3546111982	-2.0616910151	1.5451842448
H	0	-4.1572457827	-1.1588050078	0.2314466243
H	0	-0.3267522685	-1.2603406276	1.6879718083
C	0	-1.9551854611	1.6812270176	-1.7137853895
C	0	-2.3566383517	2.9769846572	-1.3714702651
H	0	-2.2532597394	3.7905661996	-2.0923108890
C	0	-2.8778272822	3.2275394597	-0.0987465683
H	0	-3.1837378860	4.2393860899	0.1771008427
C	0	-3.0291771711	2.1860954043	0.8228872505
H	0	-1.5212502231	1.4826441115	-2.6980289786
H	0	-3.4544863999	2.3516840246	1.8142676875
F	0	0.3585786151	-4.5964920886	-0.1147296010
F	0	-0.0553946409	-3.2659567568	-1.7705512534
F	0	-1.5989166835	-4.5955798999	-1.0316164253

PRa-SSSR

0 1

H	0	3.5937954016	-0.7320654675	-2.5234348734
C	0	-0.1445729267	-1.1521011615	0.6354519528
C	0	1.5656915954	0.0840820291	-0.5504434880
C	0	3.0791572930	-1.3814224725	-1.7932912171
H	0	3.1734379771	-2.4190507276	-2.1447589098
C	0	3.6151589082	-1.1512794675	-0.3976948011
C	0	4.7796083215	-1.6446879566	0.1888563946
C	0	5.0776973463	-1.2906014285	1.5100464343
C	0	4.2200713597	-0.4522099675	2.2310114660
C	0	3.0531809043	0.0470575393	1.6394449087
C	0	2.7565863027	-0.3076377312	0.3227640104
H	0	5.4461677083	-2.3071817475	-0.3693452562
H	0	5.9824849843	-1.6775133569	1.9847750951
H	0	4.4597980582	-0.1886147847	3.2637593577
H	0	2.3884342415	0.6964269794	2.2119907132
O	0	0.8477097869	-2.1559194155	-1.3626321983
C	0	-0.0958972328	-2.2653233929	-0.4037923586
O	0	-0.8095009743	-3.2292903986	-0.3763266957
C	0	1.6062015589	-0.9703974003	-1.6772888253
H	0	1.1817785164	-0.5778629347	-2.6122984135
H	0	1.7465481912	1.0681535967	-1.0139158058
N	0	0.2554490045	0.1014421127	0.0376625587
C	0	-0.2316999859	1.2447866199	0.8093989953
H	0	0.5010523179	1.5775457028	1.5691229202

C	0	-1.4983732813	0.6763615196	1.5187819695
H	0	-1.3813984893	0.8003719760	2.6039757793
C	0	-1.5427532757	-0.8366191026	1.1767441284
H	0	-2.2859490156	-1.0310700738	0.3907573799
C	0	-1.9486080291	-1.6501430550	2.3910371681
C	0	-0.5250927162	2.3944116404	-0.1276444627
C	0	-1.7895937108	2.4601928741	-0.7379189465
O	0	-2.7949162713	1.6402694795	-0.3145345667
C	0	-2.7619741890	1.4149766361	1.0916399808
H	0	-2.8247690305	2.3885112876	1.6110228682
H	0	-3.6564263767	0.8292188924	1.3394065577
H	0	0.5226659440	-1.4658742465	1.4696377908
C	0	0.4583373211	3.3099562996	-0.5167922652
C	0	0.2108841235	4.2414434167	-1.5291376817
H	0	0.9879736789	4.9488951518	-1.8257820399
C	0	-1.0376723867	4.2594226025	-2.1595112480
H	0	-1.2377889690	4.9803698181	-2.9557144514
C	0	-2.0457881131	3.3806962141	-1.7573777889
H	0	1.4336324167	3.2849285688	-0.0217904065
H	0	-3.0396884122	3.4010313499	-2.2079225403
F	0	-3.1516451895	-1.2349172815	2.8486530674
F	0	-2.0392356931	-2.9561239216	2.1536011926
F	0	-1.0689513031	-1.4850531148	3.4055819411

PRa-SSSS

0 1

H	0	2.8761928487	1.6618487942	-2.5859811276
C	0	0.5072227068	-1.5309736844	0.3221165122
C	0	0.9831513548	0.6659789276	-0.5682027388
C	0	2.9486736231	0.7161092708	-2.0202622189
H	0	3.6292761309	0.0502423971	-2.5708814111
C	0	3.3567733632	0.9735348650	-0.5859991165
C	0	4.6176754715	1.2226334048	-0.0453954614
C	0	4.7323769158	1.4309008245	1.3350631416
C	0	3.6028281273	1.3891551440	2.1624113628
C	0	2.3361115013	1.1428320599	1.6196447259
C	0	2.2313564598	0.9410903987	0.2459701513
H	0	5.5052497835	1.2441107997	-0.6828167130
H	0	5.7157786370	1.6175860925	1.7731525499
H	0	3.7134382489	1.5428628374	3.2383806779
H	0	1.4446833483	1.0897260302	2.2492259579
O	0	1.7279860673	-1.3475015578	-1.8266306629
C	0	1.2142613770	-2.1593724116	-0.8884945786
O	0	1.3494695027	-3.3497685025	-0.9924503073
C	0	1.5549632200	0.0821920699	-1.8827452156
H	0	0.9085594160	0.2746530252	-2.7514976362
H	0	0.4982332276	1.6188546713	-0.8286349420
N	0	0.0201378237	-0.1619688207	0.1227636793
C	0	-1.3213077531	-0.2959650994	-0.4196085013
H	0	-1.2935701932	-0.6685622321	-1.4725380195
C	0	-1.9163944655	-1.4043214917	0.4532463800
H	0	-2.1738765052	-0.9327507288	1.4133196596
C	0	-0.7466207634	-2.3709793326	0.6803630308

H	0	-0.7917481914	-3.2537518051	0.0279225581
C	0	-0.7107419324	-2.9044426246	2.0963255616
C	0	-2.2947371451	0.8494256410	-0.3652947864
C	0	-3.6434203356	0.4528342689	-0.5141600920
O	0	-4.0071685536	-0.8514936193	-0.6781940108
C	0	-3.1736796370	-1.9236869426	-0.2114530404
H	0	-3.7738125496	-2.5343096455	0.4807795860
H	0	-2.9179529625	-2.5479829013	-1.0847724864
H	0	1.2555731117	-1.5470449510	1.1314778145
C	0	-2.0110968842	2.1958351691	-0.1248290342
C	0	-3.0312718519	3.1520211089	-0.1086752154
H	0	-2.7909124486	4.2015621486	0.0723924000
C	0	-4.3545736898	2.7554338810	-0.3184852583
H	0	-5.1569736404	3.4969299462	-0.3137759465
C	0	-4.6652541778	1.4080189706	-0.5061236467
H	0	-0.9844839432	2.5072009924	0.0689133410
H	0	-5.6947594887	1.0687575048	-0.6327772836
F	0	-0.5837204409	-1.9181820842	3.0055660928
F	0	-1.8503908304	-3.5648671697	2.3812869965
F	0	0.3100563367	-3.7511949992	2.2835847517

PRb-RRRR

0 1

H	0.2800386977	1.1780417901	-1.1121021166
C	-3.0167633757	-2.2127204770	-0.0455907932
C	-2.2558721346	0.1661379468	-0.1806472401
C	0.1514697907	0.4822805054	-0.2642412698
H	1.1145568478	-0.0159266131	-0.0839138658
C	-0.4122204134	1.1966951643	0.9423797113
C	0.2564500554	1.9822583160	1.8772841032
C	-0.4768165175	2.5860319733	2.9058178094
C	-1.8617216724	2.4127879680	2.9771727685
C	-2.5356381512	1.6280267134	2.0317214313
C	-1.8023624675	1.0010131366	1.0225975233
H	1.3386844565	2.1217319552	1.8128824763
H	0.0348549103	3.1970991438	3.6531790548
H	-2.4295007667	2.8956580469	3.7759388519
H	-3.6186993320	1.5356348346	2.0920681188
O	-0.6748713061	-1.6668112142	0.2639471071
C	-1.6628577202	-2.5273579898	0.5735777325
O	-1.4392581776	-3.4857800665	1.2643656890
C	-0.9414349433	-0.5377226767	-0.5839479923
H	-0.9490017255	-0.8755200929	-1.6322179316
H	-2.4630231378	0.8836975535	-1.0012214934
N	-3.3505779022	-0.7774064498	-0.0893134148
C	-4.5469073653	-0.5539328562	0.7104549685
H	-4.2895548290	-0.4541362013	1.7884263642
C	-5.2889360228	-1.8785023805	0.5565227962
H	-5.6792859096	-1.9240157913	-0.4757390334
C	-4.1724893160	-2.9067312328	0.7089715561
H	-3.8855506165	-2.9624411736	1.7723998981
C	-4.4818716161	-4.3123015699	0.2122371467
H	-3.6004894992	-4.9593321101	0.3276764947

H	-5.3087578963	-4.7628494023	0.7832658072
H	-4.7717815711	-4.3004000443	-0.8517204414
C	-5.5000775133	0.5646272875	0.3626741445
C	-6.8534509797	0.3570418850	0.7206018720
O	-7.3212392039	-0.7864781964	1.2960782877
C	-6.4551038146	-1.9026421798	1.5155306236
H	-6.0954798684	-1.8814582431	2.5612213312
H	-7.0791688978	-2.7999448980	1.3907142381
H	-2.9608089720	-2.6141678825	-1.0807409397
C	-5.1540034642	1.7754114230	-0.2484780939
C	-6.1059575975	2.7667762503	-0.4965400155
H	-5.8070295610	3.7025668115	-0.9729927127
C	-7.4363725993	2.5510279748	-0.1276602106
H	-8.1912559539	3.3189121544	-0.3130461612
C	-7.8098255031	1.3509907587	0.4738182603
H	-4.1188030103	1.9559105586	-0.5324918170
H	-8.8438905937	1.1510320504	0.7601102564

PRb-RRRS

0 1

H	0	2.2646188381	-3.3081580552	-2.1243028385
C	0	-1.5000483366	-1.0513507936	-0.1989597247
C	0	0.8554653051	-1.0277539341	-0.8984025578
C	0	1.8959340895	-3.2355885828	-1.0859923474
H	0	1.8150353776	-4.2574462263	-0.6876033562
C	0	2.7659629796	-2.3201857111	-0.2556750517
C	0	3.9927981238	-2.5892449326	0.3487439739
C	0	4.6153223371	-1.5810367607	1.0938730080
C	0	4.0099208677	-0.3269209222	1.2331007850
C	0	2.7785787446	-0.0568115090	0.6244577955
C	0	2.1661832012	-1.0597032121	-0.1252717884
H	0	4.4556547301	-3.5751928323	0.2557784936
H	0	5.5739129454	-1.7784900955	1.5799036590
H	0	4.4988234649	0.4492841570	1.8265878824
H	0	2.3083949288	0.9184004035	0.7426061845
O	0	-0.1863906178	-3.0426735355	0.0734746616
C	0	-1.2780743793	-2.3730484698	0.5068551528
O	0	-1.9739811576	-2.8228570932	1.3755410082
C	0	0.5329233108	-2.5373644851	-1.0655900412
H	0	-0.0667776490	-2.7378624348	-1.9671682282
H	0	1.0494072197	-0.6341770676	-1.9185628044
N	0	-0.2433020210	-0.3193934126	-0.2735753539
C	0	-0.6314592918	1.0280067317	-0.6957744865
H	0	-1.0181807744	1.0007363573	-1.7401739024
C	0	-1.7953057711	1.3023207643	0.2774921498
H	0	-2.4863463072	2.0522805837	-0.1362258052
C	0	-2.4777960534	-0.0775112779	0.4819665153
H	0	-2.5005717378	-0.3261512518	1.5543346402
C	0	-3.8976042546	-0.1744067711	-0.0636629211
C	0	0.4491653928	2.0764121144	-0.6291948936
C	0	0.4860610703	2.9878747293	0.4442464030
O	0	-0.4373920450	2.9893807012	1.4368629445
C	0	-1.2105019328	1.8066584986	1.5920545826

H	0	-0.5746141699	1.0135398544	2.0231377932
H	0	-2.0032927275	2.0537580570	2.3118565700
H	0	-1.8914713489	-1.2898742847	-1.2190864426
C	0	1.4151075390	2.1966503900	-1.6381649603
C	0	2.4190689907	3.1607096094	-1.5784093910
H	0	3.1681611817	3.2251194692	-2.3698472701
C	0	2.4502652280	4.0490537804	-0.4963211820
H	0	3.2293744627	4.8127090077	-0.4355186119
C	0	1.4859702129	3.9709520151	0.5044874598
H	0	1.3716494106	1.5149488985	-2.4912856164
H	0	1.4807088809	4.6593502491	1.3513838570
H	0	-3.9307383775	0.0708463058	-1.1383279755
H	0	-4.5717329168	0.5195581259	0.4620810166
H	0	-4.2918346938	-1.1937620119	0.0689235043

PRb-RSSR

0 1

H	0	-0.5036064895	1.4468648152	-1.4270455990
C	0	-3.4217099069	-2.0589288389	0.2151281846
C	0	-2.6703256725	0.3196613306	0.1446930572
C	0	-0.3949846184	0.6805115046	-0.6395995317
H	0	0.5679695645	0.1723777254	-0.7923811981
C	0	-0.5600893091	1.2789114866	0.7402441769
C	0	0.3702415075	1.9566241089	1.5244795993
C	0	-0.0082620729	2.3940192786	2.8004444107
C	0	-1.2976208179	2.1448289591	3.2814770771
C	0	-2.2329642230	1.4639802554	2.4904023488
C	0	-1.8586686808	1.0420053237	1.2157727434
H	0	1.3858239851	2.1311552382	1.1596380224
H	0	0.7131316990	2.9205662287	3.4298214040
H	0	-1.5762802411	2.4762707754	4.2845776203
H	0	-3.2313201777	1.2612263079	2.8807115393
O	0	-1.0866377128	-1.5411886540	-0.1313955106
C	0	-1.9639166692	-2.4766646692	0.2982689968
O	0	-1.5719951553	-3.5545876685	0.6545306733
C	0	-1.5574498583	-0.3145166114	-0.7179293175
H	0	-1.8901524396	-0.5248435035	-1.7466611185
H	0	-3.1597616194	1.0890449855	-0.4896600599
N	0	-3.6140769266	-0.6690580849	0.5663969486
C	0	-4.9355595926	-0.4041696769	1.1369725717
H	0	-4.8360572505	-0.0925739581	2.1947289092
C	0	-5.6063162541	-1.7947614158	1.0891962889
H	0	-6.2798381961	-1.9274141411	1.9492593892
C	0	-4.4219980403	-2.7863646054	1.1320154237
H	0	-4.7042269301	-3.7575710168	0.6956439528
C	0	-3.9009239097	-2.9975957631	2.5540990544
H	0	-4.7084559973	-3.3650200986	3.2060115644
H	0	-3.0803357955	-3.7256128115	2.5641256228
H	0	-3.5219300778	-2.0538923920	2.9769840429
C	0	-5.7543791189	0.6680147115	0.4395334237
C	0	-6.9284772380	0.3416520073	-0.2641302825
O	0	-7.3793974536	-0.9356672419	-0.3774694397
C	0	-6.4132697966	-1.9555479609	-0.1964731888

H	0	-6.9691803064	-2.9032602069	-0.1870287928
H	0	-5.7399491703	-1.9655919079	-1.0735623782
H	0	-3.6903693480	-2.2764543978	-0.8487337441
C	0	-5.4084526691	2.0250900771	0.5492285994
C	0	-6.1775771011	3.0269499048	-0.0406966253
H	0	-5.8815310007	4.0734592686	0.0564672252
C	0	-7.3394717478	2.6796661910	-0.7405861820
H	0	-7.9571355153	3.4546819470	-1.2007499052
C	0	-7.7171381641	1.3446059905	-0.8473695180
H	0	-4.5253823936	2.3016632128	1.1293138075
H	0	-8.6236683175	1.0443234205	-1.3759820864

PRb-RSSS

0 1

H	0	1.5950349481	3.8361607313	-1.4564286516
C	0	1.1392132624	-1.1259158333	-1.4636736747
C	0	0.3153833145	1.2281980167	-1.1650948518
C	0	2.0413072574	2.9437737394	-0.9829381074
H	0	3.1320649575	3.0795776088	-0.9657427612
C	0	1.4186274047	2.7022677170	0.3720823679
C	0	1.6776157512	3.3652795507	1.5703867820
C	0	0.9003518403	3.0668232928	2.6947407366
C	0	-0.1445799373	2.1423787434	2.5996501132
C	0	-0.4035458624	1.4792622715	1.3939007976
C	0	0.4119224030	1.7253265121	0.2870489329
H	0	2.4722252794	4.1137542328	1.6285444035
H	0	1.0973681138	3.5714070771	3.6436424585
H	0	-0.7735130149	1.9397190993	3.4697079680
H	0	-1.2560613842	0.8057566788	1.3289808104
O	0	2.7241202304	0.7505186573	-1.5243243876
C	0	2.5492058313	-0.5772507210	-1.4361577107
O	0	3.5067943841	-1.3011890657	-1.3550766368
C	0	1.6593883002	1.6877123236	-1.7644831281
H	0	1.5892513065	1.8366714352	-2.8522438189
H	0	-0.4567188242	1.8550500827	-1.6435495675
N	0	0.0571978431	-0.1409350416	-1.5637086120
C	0	-1.1064285047	-0.8996514451	-1.1175667955
H	0	-1.2856043940	-1.6564869135	-1.9111699528
C	0	-0.6114363693	-1.6652933383	0.1133542413
H	0	-0.4981456570	-0.9416006846	0.9314573719
C	0	0.7955603111	-2.1301812394	-0.2757510590
H	0	0.7557593626	-3.1448967489	-0.7048078959
C	0	1.7567554502	-2.1285467751	0.9099127045
C	0	-2.4234974242	-0.2372700449	-0.8346189716
C	0	-3.2237461735	-0.8140205693	0.1792489175
O	0	-2.8622453146	-1.9102305671	0.9046426791
C	0	-1.6798729207	-2.6380919083	0.5486660047
H	0	-1.4028721027	-3.2080668044	1.4466942302
H	0	-1.9201112062	-3.3582697029	-0.2564869064
H	0	1.1208518044	-1.7334491747	-2.3862900583
C	0	-2.9246206103	0.8600459264	-1.5447471166
C	0	-4.1617182388	1.4242375359	-1.2318033780
H	0	-4.5292097774	2.2864030240	-1.7918029224

C	0	-4.9254467430	0.8709347657	-0.1986694924
H	0	-5.8944602724	1.3039850618	0.0606335699
C	0	-4.4649730952	-0.2447259190	0.4973788030
H	0	-2.3308607828	1.2707776701	-2.3634966805
H	0	-5.0522167410	-0.7040322950	1.2945037525
H	0	1.8719720414	-1.1105260531	1.3166025701
H	0	1.3632586134	-2.7677448184	1.7167761710
H	0	2.7508860198	-2.4943626606	0.6248776117

PRb-SRRR

0 1

H	0	-3.7797401458	0.6309234512	2.4971403017
C	0	-0.3146481125	-1.3024843318	-0.4083511209
C	0	-1.3348472561	0.5100939773	0.8532744746
C	0	-3.5605243031	-0.0786030662	1.6796040799
H	0	-4.2274439583	-0.9442309259	1.8013059270
C	0	-3.6731849365	0.6085189544	0.3369303638
C	0	-4.8158713589	0.9284501956	-0.3946348730
C	0	-4.6755648435	1.6113318051	-1.6089359360
C	0	-3.4083717180	1.9778488109	-2.0760021132
C	0	-2.2606176639	1.6599109181	-1.3391021430
C	0	-2.4015999783	0.9629482980	-0.1380733332
H	0	-5.8074043331	0.6480951448	-0.0298168900
H	0	-5.5623606689	1.8609345221	-2.1963985495
H	0	-3.3132217071	2.5154932790	-3.0223026186
H	0	-1.2769252541	1.9601485523	-1.7038346010
O	0	-2.0176749864	-1.8637269619	1.2566106414
C	0	-1.2099611257	-2.3133783745	0.2751673770
O	0	-1.2795094196	-3.4645124569	-0.0656440774
C	0	-2.0874756998	-0.5097184147	1.7401720014
H	0	-1.6789458857	-0.5304400487	2.7602302501
H	0	-1.0678143540	1.3473924090	1.5157839628
N	0	-0.1163399604	-0.0857456445	0.3718580436
C	0	0.9254063640	0.6133517071	-0.3770050406
H	0	0.5728683172	0.8041541936	-1.4184858160
C	0	1.9558391684	-0.5126107907	-0.4412751139
H	0	2.3248644764	-0.6405638662	0.5897540936
C	0	1.1337970369	-1.7639372247	-0.8029351017
H	0	1.1522685323	-1.9228376026	-1.8931397082
C	0	1.6535933790	-3.0201543825	-0.1100651056
C	0	1.5739214627	1.8812693026	0.1173391536
C	0	2.9687572757	2.0097052721	-0.0941016187
O	0	3.7465528562	1.0589894442	-0.6844733110
C	0	3.1311477879	-0.0842563958	-1.2827053700
H	0	2.8188305233	0.1624004211	-2.3154036923
H	0	3.9158659152	-0.8521518338	-1.3374657844
H	0	-0.8547533628	-1.0730341670	-1.3555186987
C	0	0.8869190663	2.9737888090	0.6660291494
C	0	1.5521455147	4.1343209010	1.0634225818
H	0	0.9902749067	4.9651107388	1.4948674777
C	0	2.9369748739	4.2245127168	0.8942567068
H	0	3.4726615873	5.1253329837	1.2030487925
C	0	3.6389500621	3.1727137068	0.3119989954

H	0	-0.1967920822	2.9293486451	0.7701357318
H	0	4.7164571774	3.2258010719	0.1464782329
H	0	1.5771050024	-2.9192398194	0.9845289591
H	0	1.0838125434	-3.9090842438	-0.4066399000
H	0	2.7154681555	-3.1764586002	-0.3597041312

PRb-SRRS

0 1

H	0	0.3398748830	0.8190585905	-0.9718766800
C	0	-3.3426110613	-1.7810481714	1.0712153937
C	0	-2.3654695833	-0.0068811574	-0.2819136850
C	0	0.0532349186	0.2568913503	-0.0648862056
H	0	0.9564984425	-0.2295029920	0.3308667115
C	0	-0.6507228143	1.1487639380	0.9331070131
C	0	-0.0949717767	2.0172061985	1.8705846704
C	0	-0.9460702658	2.7309021030	2.7226188631
C	0	-2.3323743371	2.5669376608	2.6349559894
C	0	-2.8909452180	1.6983431599	1.6893862273
C	0	-2.0434938978	0.9953265899	0.8340242020
H	0	0.9895926009	2.1284555609	1.9503898322
H	0	-0.5244184611	3.4087098903	3.4688831416
H	0	-2.9899465805	3.1163897072	3.3127748837
H	0	-3.9696452625	1.5747295025	1.6394222446
O	0	-0.9301382069	-1.8375513091	0.5534830414
C	0	-1.9338153338	-2.2892420489	1.3368138174
O	0	-1.6978164343	-3.0869141500	2.2049381535
C	0	-1.0288879645	-0.7698647404	-0.4123209634
H	0	-0.9115315592	-1.2297842596	-1.4040954748
H	0	-2.5364923817	0.5388034018	-1.2261442183
N	0	-3.4138321980	-0.9673378668	-0.1135322110
C	0	-4.7848333308	-0.8326132156	-0.5940705129
H	0	-4.7719414693	-0.8186596968	-1.6976294732
C	0	-5.4590040012	-2.1382619399	-0.0523116372
H	0	-5.7664789588	-2.7672914835	-0.9011354952
C	0	-4.3724719419	-2.8920024751	0.7695592882
H	0	-4.7952693896	-3.2705395302	1.7112668339
C	0	-3.7748900092	-4.0571061787	-0.0200674111
H	0	-3.0405294288	-4.6093809498	0.5822711956
H	0	-4.5631231051	-4.7610061776	-0.3300091951
H	0	-3.2720522071	-3.6868513514	-0.9280662958
C	0	-5.4755543456	0.4357103676	-0.1158110752
C	0	-6.2224297320	0.4197292391	1.0749694475
O	0	-6.5119656575	-0.7655165402	1.6841638394
C	0	-6.7170466479	-1.8208110041	0.7469517725
H	0	-7.0411422407	-2.6930149179	1.3313434502
H	0	-7.5395915979	-1.5321435351	0.0663599218
H	0	-3.6463027449	-1.2439489718	1.9953192638
C	0	-5.2759465621	1.6624979430	-0.7592764435
C	0	-5.7520108030	2.8535288188	-0.2078825391
H	0	-5.5759943127	3.8030850607	-0.7171466555
C	0	-6.4460820109	2.8226578821	1.0068286581
H	0	-6.8132653681	3.7504994451	1.4515812652
C	0	-6.6971872590	1.6060924901	1.6439118781

H	0	-4.7170250145	1.6831703836	-1.6991648388
H	0	-7.2669876696	1.5497324894	2.5730836716

PRb-SSSR

0 1

H	0	3.0939761917	2.5770245237	-1.9895962142
C	0	0.3107845094	-1.1283591780	-0.3156922128
C	0	1.0801701420	1.1764429589	-0.3724194283
C	0	3.0554143383	1.4935759714	-1.7784994818
H	0	3.6646616884	0.9825757300	-2.5379533123
C	0	3.4780393607	1.2088113346	-0.3539891694
C	0	4.7618333149	1.1224291225	0.1824614302
C	0	4.9109480137	0.8502371897	1.5477293473
C	0	3.7875695510	0.6690695046	2.3623157738
C	0	2.4981819794	0.7596740150	1.8232813811
C	0	2.3512325296	1.0293846170	0.4622880550
H	0	5.6409418895	1.2550230365	-0.4535575852
H	0	5.9116087687	0.7717827632	1.9794326183
H	0	3.9172678379	0.4516705366	3.4251896253
H	0	1.6270159548	0.6137812215	2.4646658988
O	0	1.6186052974	-0.3688243215	-2.2502153994
C	0	1.0110603106	-1.4033604086	-1.6336923331
O	0	1.0747404751	-2.5021003012	-2.1200493507
C	0	1.6006406160	1.0068040149	-1.8169112670
H	0	0.9716409939	1.5465004752	-2.5387106106
H	0	0.6949597777	2.2062265296	-0.2852463264
N	0	-0.0059156113	0.2687314017	-0.1519937341
C	0	-0.9887960797	0.4453681300	0.9195111675
H	0	-0.5048460596	0.6270496885	1.8991603053
C	0	-1.7191575061	-0.9358539649	0.9421711121
H	0	-1.5456904224	-1.4173160931	1.9179602186
C	0	-1.0604920718	-1.7958129847	-0.1632383528
H	0	-1.6096142901	-1.6196916674	-1.1024692070
C	0	-1.0263460907	-3.2862319185	0.1406970714
C	0	-1.8966785346	1.6133925374	0.6048564491
C	0	-3.0894102189	1.3837220567	-0.1029447030
O	0	-3.5294585832	0.1114347760	-0.3190173779
C	0	-3.2211328790	-0.7772205015	0.7522211054
H	0	-3.6922106799	-0.3960750842	1.6772392725
H	0	-3.6887584156	-1.7386293544	0.4964610729
H	0	0.9974315365	-1.5156965877	0.4749650823
C	0	-1.5314078478	2.9342719097	0.8902046466
C	0	-2.2988044673	4.0091875200	0.4339172172
H	0	-1.9982523171	5.0340780892	0.6614720292
C	0	-3.4541938806	3.7617357474	-0.3150182183
H	0	-4.0584302268	4.5953421768	-0.6809197176
C	0	-3.8608176531	2.4515165781	-0.5721698260
H	0	-0.6271532236	3.1194038825	1.4774395970
H	0	-4.7789160120	2.2317546382	-1.1200695104
H	0	-2.0445240975	-3.6894862352	0.2629309184
H	0	-0.4705264989	-3.4846262217	1.0726902024
H	0	-0.5312194497	-3.8294791347	-0.6754173493

PRb-SSSS

0 1

H	0	-0.2587460463	1.1369983545	-1.5341535412
C	0	-3.2292370217	-1.5006707028	1.4668621924
C	0	-2.4957112690	0.4826286963	0.2013738980
C	0	-0.2212094131	0.4522517564	-0.6680651770
H	0	0.6647444865	-0.1890932525	-0.7828742531
C	0	-0.2636460679	1.2209448170	0.6364918663
C	0	0.7576960429	1.8668174907	1.3303403270
C	0	0.4540931414	2.5048795430	2.5407333750
C	0	-0.8503640407	2.4928389063	3.0496498857
C	0	-1.8772178095	1.8446932646	2.3516203779
C	0	-1.5679876805	1.2199521082	1.1476194629
H	0	1.7815539605	1.8671586049	0.9476239256
H	0	1.2471861014	3.0072662903	3.0998574968
H	0	-1.0649175249	2.9851585779	4.0011733530
H	0	-2.8985170601	1.8095191179	2.7380053020
O	0	-1.1798831725	-1.6053199160	0.0818727821
C	0	-1.8669522687	-2.0880941662	1.1345626466
O	0	-1.4285146485	-3.0243289975	1.7514438800
C	0	-1.5078909025	-0.3866884783	-0.6102801315
H	0	-1.8938441421	-0.6697631781	-1.6010271070
H	0	-2.9315110409	1.2095915901	-0.5043607314
N	0	-3.5828575017	-0.2240330884	0.8274258433
C	0	-4.8058883124	-0.3918937732	0.0605680411
H	0	-4.5782824752	-0.6996737286	-0.9873557319
C	0	-5.4960087669	-1.5655740849	0.7437280733
H	0	-5.8944542004	-1.2013981011	1.7072146461
C	0	-4.3362472522	-2.5153955596	1.0325612662
H	0	-4.0229750919	-2.9708645540	0.0750481218
C	0	-4.5984631644	-3.6151934448	2.0499673841
H	0	-5.3603376507	-4.3213330691	1.6842153994
H	0	-3.6744583398	-4.1732980936	2.2563885101
H	0	-4.9574491140	-3.1861032521	2.9998299759
C	0	-5.7893324293	0.7463383180	-0.0010475138
C	0	-7.1188234787	0.3727351271	-0.2951546389
O	0	-7.5070610965	-0.9229911346	-0.4766664965
C	0	-6.6494174655	-2.0172274429	-0.1245323559
H	0	-7.2853945293	-2.7583034094	0.3835301070
H	0	-6.2706335205	-2.4771725523	-1.0556103647
H	0	-3.2451572889	-1.4056846810	2.5670158785
C	0	-5.4985271443	2.0919749447	0.2351492789
C	0	-6.4921405223	3.0699080116	0.1337038040
H	0	-6.2481974882	4.1184771789	0.3161260511
C	0	-7.7972151772	2.6937305392	-0.1973841110
H	0	-8.5812070212	3.4500037726	-0.2831404081
C	0	-8.1153892925	1.3505382097	-0.4005437524
H	0	-4.4835551332	2.3781056539	0.5155170776
H	0	-9.1337785266	1.0315918570	-0.6296089353

TSa-RRRR

0 1

H	0	-2.8480033611	1.0866798230	0.1460134139
C	0	-0.0734869050	1.3776275306	-0.8517048471
C	0	-1.2400786861	-0.5491520358	-1.8161932891
C	0	-3.2043116525	0.3526670733	-0.5937383719
H	0	-4.2754241213	0.5473662895	-0.7517972728
C	0	-2.9180278384	-1.0633371216	-0.1721674942
C	0	-3.5821154435	-1.8447446029	0.7744624542
C	0	-3.1652147698	-3.1636483976	0.9849100460
C	0	-2.1133123011	-3.7059882235	0.2369404399
C	0	-1.4487509679	-2.9258431816	-0.7152659002
C	0	-1.8379618785	-1.5964717747	-0.8954248496
H	0	-4.4221570083	-1.4341616928	1.3398370739
H	0	-3.6771513511	-3.7820728515	1.7258609807
H	0	-1.8151875793	-4.7454260732	0.3899933083
H	0	-0.6441725206	-3.3621993476	-1.3115501615
O	0	-2.0180472435	1.8047568862	-2.2091677251
C	0	-0.9846846753	2.3387927209	-1.4927412036
O	0	-0.8385518841	3.5311442873	-1.4390927388
C	0	-2.4013880129	0.4802363695	-1.9080343867
H	0	-3.0377969387	0.1629475370	-2.7456629235
N	0	0.0014430229	0.0829394357	-1.2812661850
C	0	0.9608887945	-0.7184938613	-0.7505177030
H	0	0.6758874409	-1.7699152902	-0.7119901985
C	0	0.8945679101	-0.0539900485	1.3433652765
H	0	1.7859131846	0.5823490253	1.3992400498
C	0	-0.2947269875	0.6682541611	1.3756526035
H	0	-1.2454335893	0.1330428459	1.4446289408
C	0	-0.3621282297	2.0377017571	1.9638451778
C	0	2.4104021510	-0.5339482498	-0.7443928822
C	0	3.0570404645	-1.3166997954	0.2443531798
O	0	2.3018637479	-2.0640359390	1.1030008654
C	0	1.1809270818	-1.4485731780	1.8015550544
H	0	1.4668227524	-1.4416020066	2.8684234622
H	0	0.3105564134	-2.1122263813	1.6831506915
H	0	0.8622479229	1.8343738367	-0.5389165023
C	0	3.1741865559	0.2774553597	-1.5907918834
C	0	4.5682845888	0.2682432174	-1.4921142189
H	0	5.1630825143	0.8912636775	-2.1634764269
C	0	5.2015223892	-0.5449464461	-0.5457247205
H	0	6.2917003294	-0.5545216151	-0.4772171988
C	0	4.4482673236	-1.3305934876	0.3336387554
H	0	2.6748879474	0.8966726904	-2.3397273882
H	0	4.9210480490	-1.9452463832	1.1017815822
F	0	0.7182749661	2.7884095365	1.6797441298
F	0	-0.4530062537	1.9925131917	3.3156697977
F	0	-1.4554306123	2.7112416263	1.5442776241
H	0	-0.9806657390	-0.9539948939	-2.8051284361

TSa-RRRS

0 1

H	0	3.0840936326	-2.3331561652	-2.3627335224
C	0	-0.7460816988	-1.5320200569	0.3916525722

C	0	1.3319768747	-0.6993350025	-0.7703961338
C	0	2.9464964524	-2.4379457244	-1.2719302090
H	0	3.2891857227	-3.4400332131	-0.9785532644
C	0	3.6216478474	-1.3217814811	-0.5137020742
C	0	4.9498198054	-1.2208411417	-0.1084093915
C	0	5.3422864167	-0.1285549839	0.6739083983
C	0	4.4057812568	0.8348125571	1.0582811890
C	0	3.0711809889	0.7389200502	0.6435607546
C	0	2.6881095192	-0.3309020685	-0.1646053659
H	0	5.6694828688	-1.9990382468	-0.3742227352
H	0	6.3791429757	-0.0423757583	1.0071074917
H	0	4.7105529395	1.6673902936	1.6961941740
H	0	2.3565325710	1.4893090655	0.9772553043
O	0	1.2665423245	-2.8553264724	0.3623264096
C	0	0.0260762795	-2.6634261188	0.9846103674
O	0	-0.2900272817	-3.4171439391	1.8572019894
C	0	1.4742727888	-2.2389834755	-0.9045593954
H	0	0.7809812867	-2.6602006441	-1.6496437887
H	0	1.2098353258	-0.2461171237	-1.7731004436
N	0	0.1616475398	-0.4107398975	0.0664018669
C	0	-0.2279866872	0.7612401522	0.4874518703
H	0	-0.9371340844	0.6945243485	1.3013295955
C	0	-2.9677926236	0.7692704774	0.1009765813
H	0	-2.9737128101	0.9303215999	-0.9806031305
C	0	-2.9577318349	-0.5240995651	0.5650027779
H	0	-3.0535723619	-0.7353566312	1.6325695930
C	0	-3.5125498932	-1.6257866220	-0.2950397510
C	0	-0.0021310248	2.0994731999	0.0003085353
C	0	-0.9507712188	3.0407283052	0.5072426676
O	0	-1.8549560613	2.6561174943	1.4261320301
C	0	-3.1034044624	1.9647603213	0.9741676635
H	0	-3.5736134490	1.7186902522	1.9346609165
H	0	-3.7050215031	2.7380674690	0.4701947970
H	0	-1.0451357643	-1.9097290974	-0.6015301544
C	0	0.9227192869	2.5281030647	-0.9795666720
C	0	0.9251612767	3.8436634572	-1.4221112012
H	0	1.6540322983	4.1625415745	-2.1695746700
C	0	-0.0012943904	4.7631588594	-0.9046935151
H	0	0.0103839963	5.7995113741	-1.2505668924
C	0	-0.9390149331	4.3627150810	0.0430992597
H	0	1.6612484193	1.8363267009	-1.3788182748
H	0	-1.6746070981	5.0589905916	0.4493092153
F	0	-3.2100606165	-2.8562775201	0.1353059060
F	0	-4.8621198343	-1.5515103588	-0.3172461748
F	0	-3.1052330624	-1.5308319812	-1.5828111661

TSa-RSSR

0 1

H	0	-3.4106541950	-2.8778434804	1.6189426315
C	0	0.3958244046	-1.1639219115	-0.9848324730
C	0	-0.9646073219	-1.3116605628	1.0560091355
C	0	-3.2167335566	-2.1949415081	0.7735552804
H	0	-3.9282644367	-2.4408021036	-0.0275300357

C	0	-3.2709883719	-0.7575110433	1.2306014793
C	0	-4.3914349578	0.0180254640	1.5258196468
C	0	-4.2110873634	1.3152360341	2.0154675633
C	0	-2.9226252080	1.8169714791	2.2306008173
C	0	-1.7992857195	1.0375592628	1.9380242590
C	0	-1.9810125115	-0.2385461298	1.4066458720
H	0	-5.3970188664	-0.3823005583	1.3751407714
H	0	-5.0803530995	1.9378154104	2.2394283218
H	0	-2.7909135722	2.8255097884	2.6287179375
H	0	-0.8028487406	1.4382556239	2.1215597454
O	0	-1.8023191044	-2.1163531778	-1.1323368332
C	0	-0.6279582297	-1.8344583031	-1.7722401676
O	0	-0.5050814993	-2.0858543056	-2.9445548658
C	0	-1.7796523313	-2.3632745552	0.2672569855
H	0	-1.3787922370	-3.3769757213	0.4344094277
H	0	-0.6293290598	-1.7929217809	1.9897040350
N	0	0.2841423390	-0.9457489167	0.3509833212
C	0	1.2209733701	-0.2376699510	1.0169315880
H	0	0.9425177399	0.0597118462	2.0300069688
C	0	0.9234671265	1.7497843844	-0.2547069150
H	0	0.1333748681	2.0865584528	0.4180622622
C	0	0.5509970857	1.2783451881	-1.4927465320
H	0	1.2948995380	1.1617371297	-2.2849122676
C	0	-0.8399812451	1.4459811104	-2.0156896550
C	0	2.6604613289	-0.4252680898	0.7717308710
C	0	3.5280949127	0.6684483469	0.9487782294
O	0	3.0015490145	1.9137503815	1.1280398117
C	0	2.2778205676	2.3647098763	-0.0317137308
H	0	2.1567675677	3.4482732252	0.1211528650
H	0	2.9121264509	2.2175477285	-0.9231772211
H	0	1.3897204177	-1.1319199043	-1.4154014027
C	0	3.2212136111	-1.6872848633	0.5005265361
C	0	4.6032561147	-1.8551177875	0.4391157778
H	0	5.0211657647	-2.8441149744	0.2390049928
C	0	5.4525449413	-0.7623214252	0.6529388254
H	0	6.5362280425	-0.8942765969	0.6141167553
C	0	4.9150643388	0.5016047670	0.8974440156
H	0	2.5621130242	-2.5471859622	0.3606561629
H	0	5.5496451664	1.3783037002	1.0392624539
F	0	-1.7893553056	1.0635462474	-1.1366349163
F	0	-1.0387272262	0.7681707556	-3.1540409021
F	0	-1.0973925763	2.7488464102	-2.2961444285

TSa-RSSS

0 1

H	0	3.9774339373	-1.8758525793	-1.5377268889
C	0	-0.8888171140	-1.6440695658	-0.8945302401
C	0	1.3407024301	-0.6631134386	-1.1942524016
C	0	3.2219786687	-2.1337774590	-0.7747801736
H	0	3.4581188146	-3.1361593847	-0.3904911237
C	0	3.1487526427	-1.0649192524	0.2891432604
C	0	4.0078098803	-0.8450736977	1.3643704993
C	0	3.7757970859	0.2473832372	2.2066284917

C	0	2.7071258802	1.1162503567	1.9610136897
C	0	1.8485364510	0.9005568820	0.8785688914
C	0	2.0626359424	-0.2074973696	0.0604907068
H	0	4.8466551746	-1.5202616473	1.5504043284
H	0	4.4341800568	0.4244140371	3.0603135614
H	0	2.5387551641	1.9712889853	2.6195049393
H	0	1.0280618674	1.5881606325	0.6880748911
O	0	1.0407922141	-3.0577685563	-0.6577243487
C	0	-0.3270609310	-2.9690556490	-0.7116284915
O	0	-0.9945747821	-3.9598932562	-0.5422751399
C	0	1.8170038359	-2.1213698473	-1.3872957625
H	0	1.8029501697	-2.4040973362	-2.4535287008
H	0	1.7126948028	-0.0925394945	-2.0570127814
N	0	-0.1317336647	-0.5594773204	-1.2623793656
C	0	-0.7526384036	0.5843008219	-1.5472960455
H	0	-1.8299507229	0.4695917078	-1.6414365677
C	0	-1.7574415312	0.6577616871	1.0297048320
C	0	-1.9314295428	-0.6921343863	1.0914536625
C	0	-0.3084305705	1.9598626027	-1.5184799629
C	0	-1.3033819321	2.8505075347	-1.0145357390
O	0	-2.5346518448	2.3673577155	-0.6909201736
H	0	-1.9278897400	-1.6199382679	-1.2066996637
C	0	0.9372216122	2.5019052520	-1.8933800082
C	0	1.1885103568	3.8665289457	-1.7708590710
H	0	2.1602022133	4.2632536529	-2.0723475965
C	0	0.2038960772	4.7265370920	-1.2714475935
H	0	0.4043276098	5.7962189445	-1.1792541545
C	0	-1.0391576158	4.2157400659	-0.8918074915
H	0	1.7182464240	1.8578128241	-2.2958621308
H	0	-1.8261850037	4.8625934030	-0.4996116462
C	0	-1.1663147935	-1.5092385981	2.0980152528
F	0	0.1683281849	-1.3652084691	1.9951005180
F	0	-1.4499251380	-2.8124229780	2.0054325404
F	0	-1.4890618112	-1.1314206125	3.3582607161
H	0	-2.8824161241	-1.1471584352	0.8043699475
C	0	-2.7763375266	1.6459594228	0.5555782724
H	0	-2.9133539070	2.4102810886	1.3413590869
H	0	-3.7453148208	1.1563476334	0.3858461661
H	0	-0.8494155163	1.0728255259	1.4744976287

TSa-SRRR

0 1

H	0	-3.2071846809	-1.6962794248	-1.8623318815
C	0	-0.9661291068	0.6345437403	-0.7367516633
C	0	-0.3902592045	-1.6647389064	-0.2001245904
C	0	-2.5351714485	-2.3626808880	-1.2985861301
H	0	-2.7684769746	-3.3899990743	-1.6222889311
C	0	-2.6938734269	-2.2022850535	0.1924786905
C	0	-3.8425391273	-2.3805397166	0.9676840138
C	0	-3.7770347760	-2.1591683132	2.3467663771
C	0	-2.5762616566	-1.7666143240	2.9535692269
C	0	-1.4244152705	-1.5928093314	2.1814345302
C	0	-1.4973719916	-1.8132707254	0.8052176260

H	0	-4.7844490562	-2.6804285807	0.5019688728
H	0	-4.6724711572	-2.2916386049	2.9585822223
H	0	-2.5417544870	-1.5976506876	4.0321235842
H	0	-0.4833441625	-1.2871502931	2.6464411103
O	0	-0.9339015656	-0.9355710581	-2.5437055303
C	0	-1.4028943310	0.3453356840	-2.1046529961
O	0	-2.1223840708	0.9707793308	-2.8311311600
C	0	-1.0586517435	-1.9985792570	-1.6106803179
H	0	-0.5246951935	-2.8413536173	-2.0709349412
N	0	0.0609025505	-0.2850363240	-0.3803024771
C	0	1.2896643461	0.0528094267	-0.6652795473
H	0	1.3972453576	1.0777969031	-1.0180460406
C	0	1.2634820076	2.3838184933	0.8252466776
C	0	-0.0901051258	2.3502577856	0.7553139455
C	0	2.4948246614	-0.7265531498	-0.4042979923
C	0	3.4647646259	-0.1376799590	0.4473453524
O	0	3.3345729735	1.0786145519	1.0322146517
H	0	-1.8186037278	0.5905481354	-0.0534620430
C	0	2.7601727646	-1.9780617302	-0.9917676983
C	0	3.9588167119	-2.6424048753	-0.7514554667
H	0	4.1570464024	-3.6036271655	-1.2291981036
C	0	4.9118279160	-2.0580186643	0.0924301084
H	0	5.8566733824	-2.5704385155	0.2877514981
C	0	4.6642915631	-0.8249477751	0.6895310577
H	0	2.0291137313	-2.4018081019	-1.6829978687
H	0	5.3917193922	-0.3562501009	1.3543012706
C	0	-0.8433748836	3.4700961764	0.0933352732
F	0	-0.2998089050	3.8152387690	-1.0837654562
F	0	-2.1364915827	3.1790260933	-0.1048705627
F	0	-0.8225756174	4.5805248914	0.8711861579
H	0	-0.6770342554	1.7654518249	1.4638534674
C	0	2.1200442905	1.5162280189	1.6929136160
H	0	2.5029445350	2.0848161377	2.5572932626
H	0	1.5618981813	0.6487152528	2.0859732698
H	0	1.8115548268	3.1034582203	0.2077320702
H	0	0.4652003090	-2.3130292180	0.0271204655

TSa-SRRS

0 1

H	0	3.8391226331	-1.6438960895	-1.2714690967
C	0	-0.3067787181	-0.4799740883	1.0144253364
C	0	1.3822124564	-0.2275713870	-0.6915205741
C	0	3.5535312742	-1.2200190861	-0.2927040796
H	0	4.1564725484	-1.7178922237	0.4800071353
C	0	3.6728128729	0.2854426294	-0.2883741839
C	0	4.7987521090	1.0858129665	-0.1077026774
C	0	4.6495404681	2.4781030435	-0.1112902452
C	0	3.3879296373	3.0571374633	-0.2857309375
C	0	2.2569659094	2.2533150961	-0.4745422611
C	0	2.4135241243	0.8703474546	-0.4841000542
H	0	5.7812287290	0.6350363742	0.0529832887
H	0	5.5226675613	3.1171691187	0.0400696505
H	0	3.2810691543	4.1440589074	-0.2645997836

H	0	1.2727629493	2.7066839214	-0.5832178455
O	0	1.8759348440	-1.4489552377	1.3794330984
C	0	0.6655438990	-1.1256781012	1.9049724483
O	0	0.4237629298	-1.3650333169	3.0609800129
C	0	2.0589524593	-1.4505145264	-0.0370009848
H	0	1.6926839407	-2.3999300442	-0.4393341606
H	0	1.2554047139	-0.4411099130	-1.7656404181
N	0	0.0473851238	0.0775363574	-0.1574962462
C	0	-0.8453519599	0.7168625822	-0.9674902792
H	0	-0.4227653815	0.9259352625	-1.9538148776
C	0	-2.3135506922	-1.1919626638	-1.0206227364
H	0	-2.0477060013	-1.3486469267	-2.0672940743
C	0	-1.8120121460	-2.0350624820	-0.0548887062
H	0	-2.3123446751	-2.1477501538	0.9078968343
C	0	-0.9796195446	-3.2034978292	-0.4464154202
C	0	-1.7410616752	1.7857124790	-0.4509402944
C	0	-2.8977626002	1.5768961704	0.3306332827
O	0	-3.4507254101	0.3440552469	0.4917003347
C	0	-3.5582482979	-0.4089136647	-0.7257230990
H	0	-4.4148931888	-1.0834956817	-0.5649007856
H	0	-3.8110996872	0.2709455356	-1.5557894229
H	0	-1.2098917220	-0.1156452897	1.4944072145
C	0	-1.3848393531	3.1230995741	-0.7279237358
C	0	-2.0639211564	4.2003767413	-0.1662195200
H	0	-1.7463132935	5.2213972872	-0.3875248824
C	0	-3.1444377077	3.9622187916	0.6914948782
H	0	-3.6770426398	4.7965615732	1.1535735301
C	0	-3.5696405269	2.6572478636	0.9195310922
H	0	-0.5360962184	3.3107446668	-1.3895841841
H	0	-4.4483140925	2.4381048984	1.5285739318
F	0	-0.1310625182	-3.6069605564	0.5222509205
F	0	-0.2268482834	-2.9435252809	-1.5494169749
F	0	-1.7316248477	-4.2821384625	-0.7526224480

TSa-SSSR

0 1

H	0	-3.2362439096	1.7749796580	2.1034467791
C	0	-0.7525044550	-0.5928103552	1.0348539233
C	0	-0.7717172185	1.5346338459	-0.0769553047
C	0	-2.7661675715	2.2831164582	1.2467817321
H	0	-3.0632352488	3.3431134665	1.3079753349
C	0	-3.1662131311	1.6753499112	-0.0747534947
C	0	-4.4513139427	1.5013807495	-0.5941010412
C	0	-4.6042252505	0.8946496424	-1.8444063352
C	0	-3.4869225927	0.4642822815	-2.5725751184
C	0	-2.2003584652	0.6410332152	-2.0576942292
C	0	-2.0551271847	1.2491511908	-0.8105338399
H	0	-5.3273198292	1.8259626569	-0.0270999589
H	0	-5.6058748362	0.7485587977	-2.2557490330
H	0	-3.6231860663	-0.0168360110	-3.5436127070
H	0	-1.3263694333	0.2897202599	-2.6093810845
O	0	-0.8159158181	1.3324650618	2.4379706541
C	0	-1.0184674692	-0.0693205915	2.3805011656

O	0	-1.4142355148	-0.6365680951	3.3603368237
C	0	-1.2258631570	2.1317396688	1.3324561679
H	0	-0.7301983686	3.0977799041	1.4961701397
N	0	0.0006366923	0.3513847698	0.2873353141
C	0	1.3044213007	0.3276343257	0.5114535638
H	0	1.5819603228	-0.3900120141	1.2730530972
C	0	1.7624297988	-1.9795788096	-0.3513700567
H	0	1.6664144068	-1.6393157049	-1.3858308325
C	0	0.6600543163	-2.5298733833	0.2483954982
H	0	0.7191292218	-3.0079084970	1.2288013130
C	0	-0.4850841324	-3.0072568230	-0.5944480625
C	0	2.4259091999	1.0684815744	-0.0137670183
C	0	3.6603632574	0.3689089689	0.1557244639
O	0	3.6901882563	-0.8075473155	0.8242926650
C	0	3.1449800909	-2.0299799749	0.2218595971
H	0	3.2033760017	-2.7518767372	1.0465220041
H	0	3.8546928346	-2.3393927003	-0.5637910874
H	0	-1.6766924364	-0.8859876051	0.5318008372
C	0	2.4539645814	2.3146487029	-0.6759422508
C	0	3.6507435766	2.8500472667	-1.1402533608
H	0	3.6505712240	3.8225888305	-1.6364979122
C	0	4.8522971507	2.1502378047	-0.9658040337
H	0	5.7902397386	2.5751029330	-1.3305831420
C	0	4.8550047625	0.9114844810	-0.3268339836
H	0	1.5401998748	2.8909861641	-0.8085986134
H	0	5.7761986231	0.3456797006	-0.1779947608
F	0	-1.6017707150	-3.2507523311	0.1058778984
F	0	-0.1643408624	-4.1699421840	-1.2084415539
F	0	-0.7972566352	-2.1351823784	-1.5795684808
H	0	-0.1496179877	2.2435462204	-0.6331026765

TSa-SSSS

0 1

H	0	3.8263193567	-1.3998191479	-2.1543667257
C	0	-0.0180270474	-0.8754647261	0.7742183907
C	0	1.6027483103	-0.0872949639	-0.8381471269
C	0	3.6614548135	-1.3383262286	-1.0642595553
H	0	4.2549194414	-2.1310880599	-0.5870827971
C	0	3.9573077490	0.0517273256	-0.5441866165
C	0	5.1767350112	0.6459148952	-0.2255894494
C	0	5.1833608861	1.9632710793	0.2507480739
C	0	3.9878433948	2.6750566257	0.4062939658
C	0	2.7616122760	2.0817439947	0.0818872538
C	0	2.7657960484	0.7730596565	-0.3916661434
H	0	6.1126537900	0.0918000744	-0.3314327775
H	0	6.1318088555	2.4377129661	0.5134098350
H	0	4.0112479803	3.6980518638	0.7884886444
H	0	1.8245533234	2.6290626241	0.2095810522
O	0	2.0972812803	-2.0208105420	0.5891017567
C	0	0.9604239343	-1.8301434457	1.3161356929
O	0	0.7946349742	-2.4344381438	2.3429382215
C	0	2.1701712635	-1.5184369600	-0.7419141381
H	0	1.6533837125	-2.2202270531	-1.4156507141

H	0	1.3722802293	0.1182884593	-1.8980691002
N	0	0.3628947564	0.1117611803	-0.0830942538
C	0	-0.5486380481	0.9763143097	-0.5940486913
H	0	-0.2665544534	1.3638868338	-1.5784816942
C	0	-2.2300019179	-0.4881162384	-0.9390466251
H	0	-2.8971293106	-0.2695631313	-0.0967095363
C	0	-1.5543310812	-1.6920749919	-0.7994016919
H	0	-0.9368233234	-2.0788206691	-1.6178588074
C	0	-2.0983995236	-2.7810614422	0.0697062130
C	0	-1.4997840555	1.8279427016	0.1110160919
C	0	-2.5996737056	2.2181212374	-0.6914528248
O	0	-2.7143362373	1.7114071868	-1.9543941608
C	0	-2.6163440047	0.2735455520	-2.1648934130
H	0	-3.6220822935	-0.0417917543	-2.4962660120
H	0	-1.9181982158	0.1065458535	-3.0000205934
H	0	-0.8476589740	-0.6612288635	1.4432825437
C	0	-1.4049713295	2.2944976028	1.4279724915
C	0	-2.3651293121	3.1816170588	1.9217417392
H	0	-2.2822289550	3.5554847204	2.9444606694
C	0	-3.4219465679	3.6008041815	1.1057997214
H	0	-4.1654568992	4.3008507717	1.4934893572
C	0	-3.5500125047	3.1111519963	-0.1987380975
H	0	-0.5667288218	1.9780951658	2.0533746451
H	0	-4.3859891941	3.3980183161	-0.8391733489
F	0	-2.6156335016	-2.3166895967	1.2238466200
F	0	-3.0970224661	-3.4522960011	-0.5541093692
F	0	-1.1634256432	-3.6988492740	0.3713152843

TSb-RRRR

0 1

H	0	2.8720194307	-0.9352764209	0.2431171551
C	0	0.0850907412	-1.3711440174	-0.8602291248
C	0	1.2594801353	0.5782508781	-1.8058933350
C	0	3.2244144448	-0.2212230146	-0.5182951676
H	0	4.3027283637	-0.3965611268	-0.6478360028
C	0	2.8950795519	1.2019139142	-0.1560833462
C	0	3.5263676979	2.0391316260	0.7646479866
C	0	3.0774589528	3.3564376492	0.9090627051
C	0	2.0269182318	3.8406958000	0.1206387192
C	0	1.3962252016	3.0042679475	-0.8064767211
C	0	1.8165597936	1.6770632986	-0.9202835940
H	0	4.3669491100	1.6739783884	1.3598294877
H	0	3.5632331402	4.0188460190	1.6294202149
H	0	1.7024833319	4.8784908702	0.2231541714
H	0	0.5912491523	3.3934466194	-1.4340067852
O	0	2.1168823191	-1.7674551183	-2.0967553776
C	0	1.0706400105	-2.3056971436	-1.3951755087
O	0	1.0131935326	-3.5015621952	-1.2346597460
C	0	2.4492567355	-0.4211525046	-1.8404713365
H	0	3.0937938022	-0.1133745378	-2.6758017503
N	0	0.0218845442	-0.0601556863	-1.2786861222
C	0	-0.9409854601	0.7303366027	-0.7467330837
H	0	-0.6506256447	1.7765087009	-0.6528397831

C	0	-0.9182336203	-0.0951273775	1.3699479310
H	0	-1.8441479678	-0.6850425459	1.4173503649
C	0	0.2330433244	-0.8843179785	1.3279441247
H	0	1.1920537706	-0.3547826552	1.3692442782
C	0	0.2475611397	-2.3004048222	1.8477178577
C	0	-2.3854160545	0.5469169946	-0.7269866266
C	0	-3.0172165943	1.2933716214	0.3010940508
O	0	-2.2450248381	1.9837318627	1.1879496820
C	0	-1.1336759603	1.2982387928	1.8571406011
H	0	-1.4175506186	1.2991472545	2.9251328670
H	0	-0.2368041939	1.9266060152	1.7408129442
H	0	-0.8726453735	-1.8442421800	-0.6538477774
C	0	-3.1653509794	-0.2263919629	-1.5956246032
C	0	-4.5584066525	-0.2124111848	-1.4807883222
H	0	-5.1650533139	-0.8033677390	-2.1706352622
C	0	-5.1763507403	0.5677872971	-0.4971134799
H	0	-6.2658226537	0.5832016539	-0.4175702092
C	0	-4.4073428132	1.3118290362	0.4054161423
H	0	-2.6781892210	-0.8151951497	-2.3765840072
H	0	-4.8676897519	1.8955574205	1.2048266984
H	0	1.0172597239	0.9400070695	-2.8162263055
H	0	0.4546724767	-2.3135279941	2.9330675160
H	0	1.0041604338	-2.9263492727	1.3517591742
H	0	-0.7306374308	-2.7841296346	1.6974357157

TSb-RRRS

0 1

H	0	3.2565390000	-0.5788710000	2.5543640000
C	0	0.0607460000	1.9975750000	-0.0588510000
C	0	1.0989020000	-0.0571780000	0.7488630000
C	0	3.3160760000	0.0904550000	1.6779010000
H	0	4.1741460000	0.7629520000	1.8174770000
C	0	3.3583390000	-0.6935290000	0.3855630000
C	0	4.4402070000	-1.2829880000	-0.2632530000
C	0	4.2301970000	-1.9180880000	-1.4942840000
C	0	2.9554900000	-1.9532570000	-2.0690010000
C	0	1.8640320000	-1.3685210000	-1.4138150000
C	0	2.0767890000	-0.7522280000	-0.1835300000
H	0	5.4423190000	-1.2342050000	0.1699330000
H	0	5.0726100000	-2.3762470000	-2.0178740000
H	0	2.8092940000	-2.4345740000	-3.0386020000
H	0	0.8711980000	-1.3860880000	-1.8677250000
O	0	2.3320540000	2.0387440000	0.7518170000
C	0	1.2483640000	2.7429940000	0.2577840000
O	0	1.3547030000	3.9470880000	0.1213980000
C	0	2.0187190000	0.8963090000	1.5310730000
H	0	1.5758090000	1.2074890000	2.4923720000
H	0	0.6481850000	-0.7801250000	1.4484290000
N	0	-0.0126570000	0.6367840000	0.0794290000
C	0	-1.0486980000	-0.0397950000	-0.4236820000
H	0	-1.5599630000	0.4918180000	-1.1985350000
C	0	-3.0756670000	1.8342180000	-0.2354360000
H	0	-3.5278290000	2.0911500000	0.7306140000

C	0	-2.1695050000	2.6801150000	-0.7641680000
H	0	-1.7418500000	2.4563120000	-1.7480310000
C	0	-2.0233330000	4.1204110000	-0.3232140000
C	0	-1.5973230000	-1.3229880000	0.0012200000
C	0	-3.0160560000	-1.4529360000	0.0991200000
O	0	-3.9365530000	-0.4817300000	-0.1286680000
C	0	-3.7393120000	0.6811290000	-0.9292610000
H	0	-3.2634970000	0.4233660000	-1.8916490000
H	0	-4.7696140000	0.9894400000	-1.1724940000
H	0	-0.8296600000	2.5554770000	0.0172410000
C	0	-0.8266890000	-2.4617090000	0.3473370000
C	0	-1.4010250000	-3.6479680000	0.7899560000
H	0	-0.7620420000	-4.4990300000	1.0338370000
C	0	-2.7916080000	-3.7456440000	0.8965110000
H	0	-3.2603840000	-4.6706170000	1.2397810000
C	0	-3.5821030000	-2.6572850000	0.5469560000
H	0	0.2518120000	-2.4331890000	0.2181760000
H	0	-4.6703020000	-2.6959110000	0.6196340000
H	0	-0.9799990000	4.4707970000	-0.3644500000
H	0	-2.6236620000	4.7538500000	-0.9971670000
H	0	-2.4054120000	4.2613400000	0.6995390000

TSb-RSSR

0 1

H	0	-3.6611359300	-1.7724460826	2.1994100802
C	0	0.2810326398	-1.3650258951	-0.6840700808
C	0	-1.1860512672	-0.6381348394	1.1401913466
C	0	-3.4337925770	-1.5612738463	1.1397435550
H	0	-4.1203304627	-2.1557575790	0.5206143730
C	0	-3.4846868635	-0.0757834571	0.8738459934
C	0	-4.5997027778	0.7411418870	0.6936205398
C	0	-4.4153191498	2.1190755206	0.5359409945
C	0	-3.1305118626	2.6707764123	0.5850919714
C	0	-2.0115829044	1.8507771480	0.7686391329
C	0	-2.1927560084	0.4725960298	0.8785553845
H	0	-5.6042586813	0.3112470151	0.6757859954
H	0	-5.2799013744	2.7692749856	0.3834046510
H	0	-2.9969078059	3.7497036719	0.4794975918
H	0	-1.0181617476	2.2937536257	0.8176723061
O	0	-1.9452903135	-2.2489683465	-0.5629597238
C	0	-0.7456957586	-2.2248102593	-1.2258662119
O	0	-0.6375508685	-2.8308566003	-2.2672956872
C	0	-1.9802659668	-1.9238021867	0.8207362164
H	0	-1.6033808815	-2.7835459050	1.3992145754
H	0	-0.9553920709	-0.6506236488	2.2189857009
N	0	0.1182028539	-0.6314226870	0.4587148995
C	0	1.0365920068	0.3058723251	0.7827902892
H	0	0.7256266934	1.0145249764	1.5548361607
C	0	0.8359203384	1.4969812882	-1.2613374321
H	0	0.1219272021	2.1947439269	-0.8191484616
C	0	0.3417772947	0.5456429137	-2.1384354812
H	0	1.0628828700	0.0431409835	-2.7929937015
C	0	-1.0881650629	0.5130860030	-2.6089138635

H	0	-1.2406744247	1.2647420910	-3.4054484698
H	0	-1.3560606355	-0.4646275504	-3.0331513108
H	0	-1.7931348696	0.7507577294	-1.7995292829
C	0	2.4787920011	0.0003469705	0.7273202906
C	0	3.4003555872	1.0021090604	0.3674132725
O	0	2.9543833234	2.1859293084	-0.1336005049
C	0	2.2363929516	2.0204453909	-1.3769553721
H	0	2.2227272865	3.0326821310	-1.8112951357
H	0	2.8339865289	1.3747848676	-2.0450488066
H	0	1.2960021806	-1.5362782179	-1.0241507271
C	0	2.9783864167	-1.2462786401	1.1495088546
C	0	4.3493155496	-1.4753061693	1.2458604169
H	0	4.7159231230	-2.4458906241	1.5873176363
C	0	5.2517324071	-0.4538882376	0.9242076825
H	0	6.3274707798	-0.6250703762	1.0084065265
C	0	4.7776642503	0.7780407498	0.4747435754
H	0	2.2726803047	-2.0335293438	1.4251887931
H	0	5.4555606751	1.5828554807	0.1844744474

TSb-RSSS

0 1

H	0	-2.1344168844	3.4858710549	1.7441138954
C	0	-0.9474522180	-1.2522179265	1.5297225334
C	0	-0.5016353419	1.1358713485	1.3202076021
C	0	-2.4340655573	2.5848354407	1.1801951755
H	0	-3.5310255666	2.5739515677	1.1137225804
C	0	-1.7311674180	2.5315417291	-0.1557201177
C	0	-2.0403356817	3.2050345737	-1.3355996164
C	0	-1.2105457510	3.0383039055	-2.4504395703
C	0	-0.0764285805	2.2230947298	-2.3736611556
C	0	0.2393999418	1.5512038722	-1.1870637461
C	0	-0.6086295919	1.6904620527	-0.0896246142
H	0	-2.9207311052	3.8499889752	-1.3914915826
H	0	-1.4475791141	3.5519964672	-3.3851171596
H	0	0.5723508180	2.1092117452	-3.2449781894
H	0	1.1337083036	0.9363394618	-1.1277589979
O	0	-2.8027453468	0.2723020251	1.4934348028
C	0	-2.3669308927	-1.0287181819	1.5637158127
O	0	-3.1893959397	-1.9196585997	1.5565533744
C	0	-1.9288491431	1.3200761881	1.8825289515
H	0	-1.9216336731	1.3956111545	2.9828531160
H	0	0.1648751009	1.7754673889	1.9165420301
N	0	-0.0202105256	-0.2423173162	1.5167339498
C	0	1.2719404543	-0.5660124912	1.5106447714
H	0	1.4431083472	-1.6160119299	1.7336871989
C	0	0.9052111736	-1.9304735891	-0.8683709330
C	0	-0.3733139837	-2.3106213990	-0.5886495388
C	0	2.4373456928	0.1245383688	1.0115198604
C	0	3.3698212268	-0.7536755483	0.3776068993
O	0	3.1324516337	-2.0920168636	0.3597746004
H	0	-0.5983631369	-2.2239849383	1.8583112109
C	0	2.7422496454	1.5001896849	1.0499500789
C	0	3.9186794068	1.9887686949	0.4856791163

H	0	4.1343382113	3.0583438173	0.5331235462
C	0	4.8233233839	1.1169105324	-0.1306687689
H	0	5.7464527365	1.5026738777	-0.5689746217
C	0	4.5443662245	-0.2506042815	-0.1857728201
H	0	2.0628512483	2.1993965286	1.5369348693
H	0	5.2298572638	-0.9536385201	-0.6628863565
C	0	-1.5637250808	-1.7749841084	-1.3413526676
H	0	-0.5266330777	-3.2658700117	-0.0738462461
C	0	2.1465771727	-2.6948611984	-0.5470973997
H	0	2.6938777183	-2.9072967974	-1.4831901431
H	0	1.9069741208	-3.6563138531	-0.0703612891
H	0	1.0446976399	-1.0495098330	-1.5015381540
H	0	-1.4598436155	-0.7000296148	-1.5510320404
H	0	-1.6512560048	-2.2944741857	-2.3125210383
H	0	-2.5024115640	-1.9439947478	-0.7986279687

TSb-SRRR

0 1

H	0	-3.4969470000	-0.7730280000	-1.8734780000
C	0	-0.8927520000	1.2851530000	-0.7667290000
C	0	-0.7098140000	-1.0689030000	-0.1652560000
C	0	-2.9248750000	-1.4904330000	-1.2642850000
H	0	-3.2880480000	-2.4956930000	-1.5339740000
C	0	-3.0720480000	-1.2307480000	0.2138220000
C	0	-4.2417760000	-1.1951480000	0.9771950000
C	0	-4.1567310000	-0.9203660000	2.3456260000
C	0	-2.9159170000	-0.6857330000	2.9533980000
C	0	-1.7438020000	-0.7257260000	2.1931810000
C	0	-1.8361050000	-0.9981550000	0.8276340000
H	0	-5.2137890000	-1.3709510000	0.5098090000
H	0	-5.0677360000	-0.8862520000	2.9479380000
H	0	-2.8660540000	-0.4720640000	4.0234690000
H	0	-0.7717490000	-0.5418580000	2.6584280000
O	0	-1.1390560000	-0.3203830000	-2.5224360000
C	0	-1.4458700000	1.0101530000	-2.0789200000
O	0	-2.1565980000	1.6964460000	-2.7683010000
C	0	-1.4110500000	-1.3397930000	-1.5739790000
H	0	-0.9957050000	-2.2570450000	-2.0144000000
N	0	-0.0339090000	0.2105210000	-0.3793550000
C	0	1.2312780000	0.3277100000	-0.6705690000
H	0	1.5113340000	1.3134710000	-1.0364980000
C	0	1.6117650000	2.7203760000	0.6659710000
C	0	0.2735940000	2.9399870000	0.5891890000
C	0	2.2922900000	-0.6320000000	-0.3918980000
C	0	3.3608520000	-0.1663600000	0.4177050000
O	0	3.4340820000	1.0783700000	0.9418820000
H	0	-1.6888830000	1.4674160000	-0.0408270000
C	0	2.3403350000	-1.9362500000	-0.9194020000
C	0	3.4217750000	-2.7726710000	-0.6614670000
H	0	3.4538960000	-3.7747320000	-1.0931610000
C	0	4.4730420000	-2.3101500000	0.1409440000
H	0	5.3269960000	-2.9588120000	0.3498600000
C	0	4.4390670000	-1.0270000000	0.6795720000

H	0	1.5375210000	-2.2692070000	-1.5797870000
H	0	5.2451170000	-0.6514710000	1.3121000000
C	0	-0.3155350000	4.1333620000	-0.1111290000
H	0	-0.3693570000	2.4330640000	1.3133320000
C	0	2.3051670000	1.7518400000	1.5715640000
H	0	2.7862040000	2.2723490000	2.4168790000
H	0	1.6067510000	1.0083300000	1.9941270000
H	0	2.2874420000	3.3182410000	0.0412270000
H	0	0.0222600000	-1.8436470000	0.0965260000
H	0	0.3433820000	4.4734840000	-0.9245640000
H	0	-0.4331870000	4.9739160000	0.5967560000
H	0	-1.2968470000	3.9104940000	-0.5504350000

TSb-SRRS

0 1

H	0	3.9062470726	-1.4965601139	-1.6365457334
C	0	-0.1597956019	-0.7155646020	0.9852894379
C	0	1.3733663367	-0.2903341325	-0.8518126285
C	0	3.6326550486	-1.1427727452	-0.6268396260
H	0	4.3049821738	-1.6274999711	0.0952716101
C	0	3.6430952166	0.3676930073	-0.5620913203
C	0	4.7169484845	1.2456655631	-0.4253909098
C	0	4.4682501343	2.6236636317	-0.4053954577
C	0	3.1633426051	3.1157019553	-0.5268883854
C	0	2.0844969978	2.2347828155	-0.6693740650
C	0	2.3386073083	0.8660275118	-0.6785748932
H	0	5.7370629506	0.8667650714	-0.3247940775
H	0	5.3003937691	3.3220010208	-0.2889231162
H	0	2.9851352058	4.1932553689	-0.5072790977
H	0	1.0658374295	2.6155615258	-0.7678159748
O	0	2.0704717806	-1.6205032459	1.0977481082
C	0	0.8677140288	-1.4116261312	1.7259903450
O	0	0.7128379223	-1.8448012860	2.8445893353
C	0	2.1708125111	-1.4968130704	-0.3140841333
H	0	1.8428339043	-2.4400467373	-0.7779390800
H	0	1.1834127769	-0.4596692435	-1.9252352757
N	0	0.0707750662	-0.1154951204	-0.2124697280
C	0	-0.9675323845	0.3046138719	-0.9706262653
H	0	-0.6832595036	0.6686002050	-1.9626004980
C	0	-1.7920063691	-1.7652821474	-1.3440139506
H	0	-1.0735762090	-2.0453089333	-2.1254778326
C	0	-1.6942450408	-2.4074062765	-0.1259987314
H	0	-2.5182309635	-2.2593559145	0.5809339025
C	0	-0.8133941608	-3.5971471072	0.1418703609
H	0	-0.4630782703	-3.6404589394	1.1841832667
H	0	-1.3716146439	-4.5337748756	-0.0476984024
H	0	0.0653316346	-3.6144057011	-0.5218515855
C	0	-2.1093957085	0.9747356269	-0.2781666293
C	0	-3.4458783144	0.5233552031	-0.2809646586
O	0	-3.8977153707	-0.5776865860	-0.9247766752
C	0	-3.0764760980	-1.1989168968	-1.8974093452
H	0	-3.7077612189	-2.0009344622	-2.3149545725
H	0	-2.8701330408	-0.4865712712	-2.7179874646

H	0	-1.0496593654	-0.4270422392	1.5335584113
C	0	-1.8116001329	2.1272703880	0.4817954566
C	0	-2.7801277441	2.8168851628	1.2012220107
H	0	-2.5084621886	3.7041485769	1.7763988092
C	0	-4.1015159333	2.3522257501	1.1832498907
H	0	-4.8794914261	2.8758916604	1.7437282383
C	0	-4.4259659969	1.2185811597	0.4510969800
H	0	-0.7738219471	2.4654768020	0.5158545244
H	0	-5.4449157248	0.8289458715	0.4210194260

TSb-SSSR

0 1

H	0	3.1970574960	-1.7382023021	2.1379295931
C	0	0.7137172822	0.5455199335	1.1183909683
C	0	0.8078244332	-1.5195220153	-0.1068639907
C	0	2.7841790381	-2.2515478053	1.2549838880
H	0	3.1315002589	-3.2964422949	1.3083006901
C	0	3.2057985302	-1.5962930274	-0.0371046179
C	0	4.4997580441	-1.3646568388	-0.5111620499
C	0	4.6717479808	-0.7166334035	-1.7382539401
C	0	3.5638572986	-0.3022092225	-2.4900412144
C	0	2.2688002621	-0.5362770471	-2.0194605898
C	0	2.1044108724	-1.1851345659	-0.7952356882
H	0	5.3685268945	-1.6771347327	0.0736480418
H	0	5.6803815543	-0.5277623516	-2.1136614256
H	0	3.7144736734	0.2056838700	-3.4454275008
H	0	1.3982521421	-0.2105057618	-2.5945821400
O	0	0.7406799767	-1.4570831439	2.4071325272
C	0	0.9574823645	-0.0552776676	2.4281100634
O	0	1.3541242239	0.4542064586	3.4423140933
C	0	1.2345109163	-2.1747083300	1.2824621998
H	0	0.7826289998	-3.1715921872	1.3714927730
N	0	0.0113884079	-0.3554895204	0.2660875738
C	0	-1.3084578262	-0.3624386231	0.4511471909
H	0	-1.6181720142	0.2130780074	1.3146444166
C	0	-1.7910601554	1.9104810457	-0.1789413942
H	0	-1.7409086075	1.6745898937	-1.2474442845
C	0	-0.6732290781	2.4698813069	0.4092518066
H	0	-0.7593862329	2.8518625591	1.4310805814
C	0	0.4615922986	3.0084009182	-0.4192502711
C	0	-2.3943030873	-1.0691330633	-0.1860294795
C	0	-3.6589083836	-0.4508820190	0.0624566213
O	0	-3.7401995228	0.6347774599	0.8605087013
C	0	-3.1521672661	1.9219115353	0.4377831830
H	0	-3.1621576538	2.5076746002	1.3662599063
H	0	-3.8786602050	2.3666871769	-0.2631887590
H	0	1.6351575585	0.9231688224	0.6680671841
C	0	-2.3648038704	-2.1999083580	-1.0309503576
C	0	-3.5360550449	-2.7209818411	-1.5707687552
H	0	-3.4894525839	-3.6070012806	-2.2072753964
C	0	-4.7703950945	-2.1161582613	-1.2969308278
H	0	-5.6884457146	-2.5305843073	-1.7199432489
C	0	-4.8286751191	-0.9785516137	-0.4943493245

H	0	-1.4240741611	-2.6975988487	-1.2584484495
H	0	-5.7735204393	-0.4775489700	-0.2770313882
H	0	0.2135078120	-2.2176180576	-0.7049526829
H	0	0.7270577911	2.3141188260	-1.2329439675
H	0	1.3615227320	3.1964553760	0.1812799358
H	0	0.1649889285	3.9633055315	-0.8906627151

TSb-SSSS

0 1

H	0	3.8229419635	0.9990567687	2.1561384653
C	0	0.0054994368	1.2134325310	-0.8841298884
C	0	1.3813289113	0.1696560822	0.8238109421
C	0	3.6589459853	0.9575417864	1.0648665075
H	0	4.4117423705	1.5991751757	0.5850242721
C	0	3.6585733060	-0.4714472035	0.5667009700
C	0	4.7270538292	-1.3168489506	0.2740891068
C	0	4.4580994909	-2.6129769013	-0.1843693972
C	0	3.1399142338	-3.0558578972	-0.3478402529
C	0	2.0650827667	-2.2092049738	-0.0498844034
C	0	2.3426183737	-0.9241285846	0.4062384097
H	0	5.7584587779	-0.9734597515	0.3866994814
H	0	5.2864850302	-3.2830609915	-0.4263237451
H	0	2.9490060370	-4.0667342324	-0.7152729987
H	0	1.0335001894	-2.5441806837	-0.1827933018
O	0	2.2916933643	1.9446377644	-0.6111212069
C	0	1.1526245504	1.9773281847	-1.3640037906
O	0	1.1172274490	2.6729813936	-2.3518438101
C	0	2.2425919233	1.4445747958	0.7215753967
H	0	1.8796603140	2.2448784886	1.3866675421
H	0	1.1038851197	0.0315075718	1.8833319483
N	0	0.1401536377	0.2215829043	0.0545581482
C	0	-0.9579502969	-0.3617996948	0.5926441655
H	0	-0.8037720797	-0.7081519483	1.6201019402
C	0	-2.2810773269	1.5301302032	0.6669919521
H	0	-2.9936433516	1.3764813436	-0.1552121913
C	0	-1.3270646111	2.5079357513	0.3864023094
H	0	-0.6243712092	2.7736513801	1.1892207690
C	0	-1.5853665713	3.5921262918	-0.6308071159
H	0	-2.1010421235	4.4468538372	-0.1575713073
H	0	-0.6641982247	3.9703344100	-1.0973229613
H	0	-2.2405421068	3.2232191928	-1.4359471076
C	0	-2.0777069149	-1.0089962267	-0.0731639113
C	0	-3.2559307067	-1.0322875821	0.7149233427
O	0	-3.2630262688	-0.3761488536	1.9098058349
C	0	-2.8226800349	1.0217885737	1.9597221192
H	0	-3.7316214671	1.5818725572	2.2457320479
H	0	-2.0980633990	1.1121353783	2.7842731087
H	0	-0.7893033520	1.0928549641	-1.6169014902
C	0	-2.0811724695	-1.6101052757	-1.3386374829
C	0	-3.2246315384	-2.2754530706	-1.7896084230
H	0	-3.2201273105	-2.7575821401	-2.7696982027
C	0	-4.3663649182	-2.3396377094	-0.9828523209
H	0	-5.2539601883	-2.8701825309	-1.3351538510

C	0	-4.3904482552	-1.7063747527	0.2653112018
H	0	-1.1783160002	-1.5758622699	-1.9533756794
H	0	-5.2840543351	-1.7102851059	0.8922828585

TS-WSa

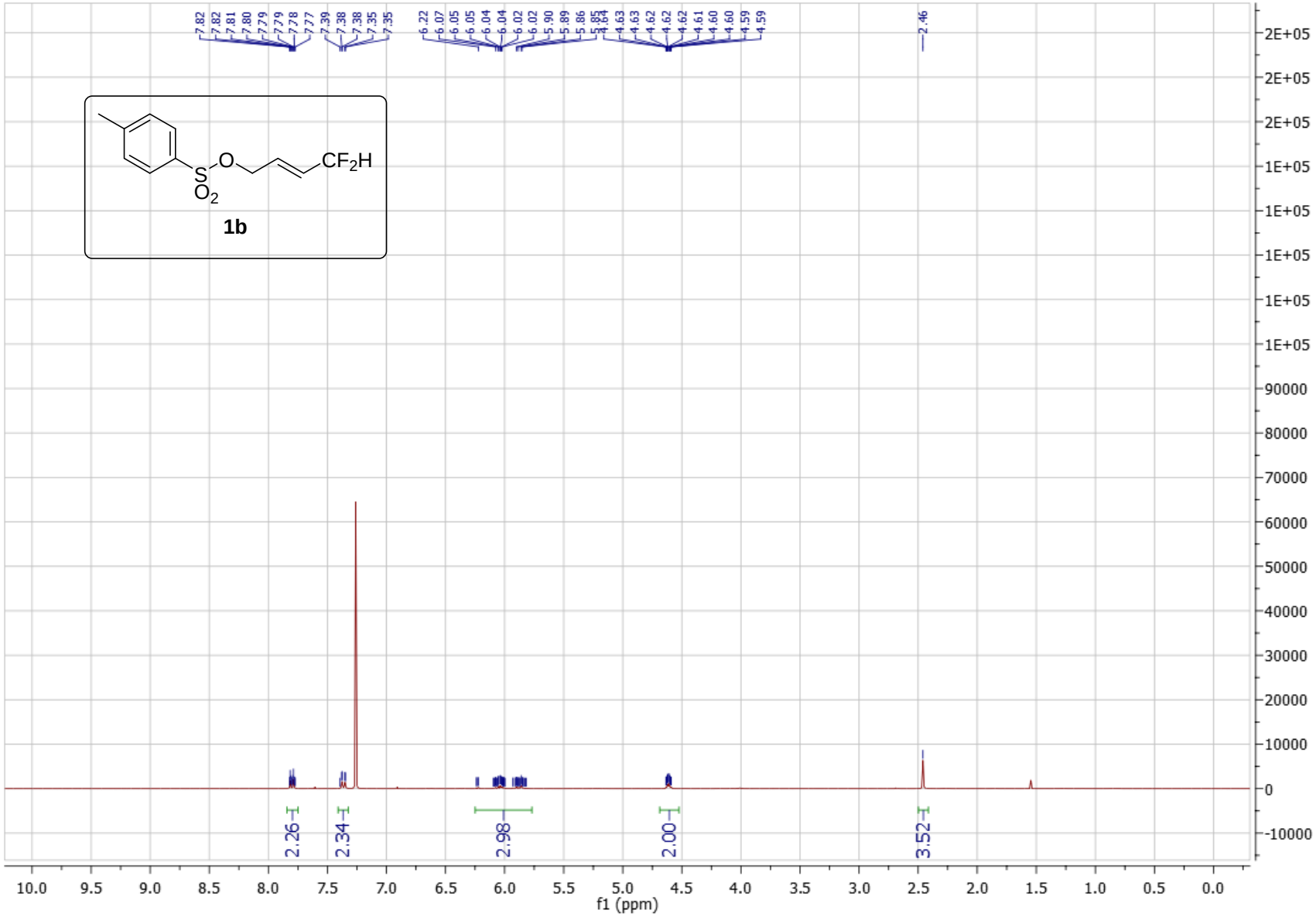
0 1

H	0	4.5959028520	0.4757693262	-1.5772801172
C	0	1.3684418096	-2.5355454331	0.4250518814
C	0	2.0667990191	-0.4208975967	-0.4933389398
C	0	4.4402015885	0.0295314905	-0.5792430777
H	0	5.4106927746	-0.3379979044	-0.2165490796
C	0	3.7635286045	1.0071810448	0.3560180008
C	0	4.3103253033	2.0568803375	1.0911582399
C	0	3.4672348945	2.8281630198	1.9008387454
C	0	2.0967744618	2.5525250307	1.9710179508
C	0	1.5417762841	1.5039598923	1.2272460924
C	0	2.3885578635	0.7406920111	0.4263973721
H	0	5.3816754176	2.2682891004	1.0482789747
H	0	3.8849189279	3.6476331311	2.4905843804
H	0	1.4538267949	3.1563827955	2.6154028763
H	0	0.4751285220	1.2837118440	1.2874614589
O	0	3.7015816729	-1.9866010118	0.4330517401
C	0	2.7240753695	-2.8786914251	0.7999980731
O	0	3.0262190793	-3.8892649053	1.3915374377
C	0	3.4294081661	-1.1223869892	-0.6626451932
H	0	3.4855921464	-1.6965101181	-1.6022732093
H	0	1.7272324010	-0.0466417581	-1.4739385486
N	0	0.9980130640	-1.3104405889	-0.0007861648
C	0	-0.2764598639	-0.9072262573	-0.2526979089
H	0	-0.3238550125	-0.1502819300	-1.0379824099
C	0	-4.7660505794	0.6593213412	-1.5416377180
H	0	-5.1248937676	-0.0548214394	-0.7943241942
C	0	-5.4486590352	0.8188075270	-2.6754884787
H	0	-5.1270883234	1.5098950656	-3.4609829290
C	0	-6.7137652062	0.0806105912	-2.9861256909
C	0	-1.2834929519	-0.7348983761	0.7714850514
C	0	-2.4145070719	0.0816362078	0.4719876629
O	0	-2.4623925274	0.5620879656	-0.8048340972
C	0	-3.5134071643	1.4189698162	-1.2125812699
H	0	-3.7147297512	2.1794596573	-0.4351814805
H	0	-3.1414137261	1.9486147397	-2.1013753897
H	0	0.5819694550	-3.2583570496	0.6315100382
C	0	-1.1908598707	-1.2661240784	2.0759868929
C	0	-2.1321166156	-0.9628570921	3.0574047012
H	0	-2.0213196618	-1.3797229712	4.0605229524
C	0	-3.2213147840	-0.1464946575	2.7488770680
H	0	-3.9768030736	0.0811121772	3.5037065643
C	0	-3.3618368960	0.3729252753	1.4559833667
H	0	-0.3500895288	-1.9158273622	2.3243283059
H	0	-4.2243991166	0.9987098833	1.2292830985
F	0	-7.0716119107	-0.7676667301	-2.0098100167
F	0	-7.7359350603	0.9372059471	-3.1748498354
F	0	-6.5881999932	-0.6329223739	-4.1201167971

TS-WSb

0 1

H	0	4.6329653323	-0.3986915372	3.1528842675
C	0	2.3276427690	2.2960599703	-0.1509057212
C	0	2.6106703288	0.3314264164	1.2155683816
C	0	4.8165827705	-0.0991036943	2.1059355958
H	0	5.8669033466	0.2143423028	2.0215414946
C	0	4.4241016438	-1.2008803916	1.1465296669
C	0	5.1267890511	-2.3437200815	0.7704356773
C	0	4.5458858079	-3.2232721719	-0.1516857173
C	0	3.2793243010	-2.9619539935	-0.6870546906
C	0	2.5661437622	-1.8189357873	-0.3053738392
C	0	3.1529404468	-0.9487334289	0.6107822955
H	0	6.1208954236	-2.5455701495	1.1771605369
H	0	5.0906073831	-4.1178183208	-0.4630495944
H	0	2.8438438432	-3.6520575626	-1.4132871255
H	0	1.5822722406	-1.6105341819	-0.7278668058
O	0	4.5195870718	1.7515065910	0.6495506768
C	0	3.7438082873	2.5859358178	-0.1203862989
O	0	4.2611659054	3.5075724574	-0.7093757752
C	0	3.8816271779	1.0517546468	1.7091812061
H	0	3.6659616721	1.7532018468	2.5322459497
H	0	1.9660121964	0.0991381994	2.0801458313
N	0	1.7897060985	1.1395582175	0.2949014455
C	0	0.4852294081	0.7743503026	0.1849375715
H	0	0.1610480456	0.1356503040	1.0091398738
C	0	-4.2664276019	-0.6212721927	0.2221412840
H	0	-4.4266902425	-0.1452448668	-0.7522288065
C	0	-5.1879195549	-0.4872824638	1.1824088957
H	0	-5.0003295879	-0.9622513069	2.1553350933
C	0	-6.4777600586	0.2615390746	1.0505728666
C	0	-0.1639874509	0.4604245631	-1.0690382720
C	0	-1.3690307379	-0.3047310450	-1.0253564131
O	0	-1.8296177577	-0.5939723454	0.2199538899
C	0	-2.9945244793	-1.3973787337	0.3963085837
H	0	-2.9510009559	-2.2642597452	-0.2883489926
H	0	-2.9262164986	-1.7846400382	1.4231869201
H	0	1.6762891132	2.9801309849	-0.6905565760
C	0	0.3526453766	0.7999879213	-2.3377668315
C	0	-0.2496497040	0.3577538897	-3.5135370906
H	0	0.1846614329	0.6255445422	-4.4789711602
C	0	-1.4156511198	-0.4076504588	-3.4508964466
H	0	-1.9084594695	-0.7432987635	-4.3659546383
C	0	-1.9739425811	-0.7355602922	-2.2097100635
H	0	1.2574054397	1.4075089326	-2.3952629036
H	0	-2.8914241478	-1.3219960322	-2.1789827777
H	0	-6.5464800456	1.0643249217	1.8050641237
H	0	-6.5863061727	0.7153139365	0.0539331079
H	0	-7.3424882293	-0.4027948543	1.2230060645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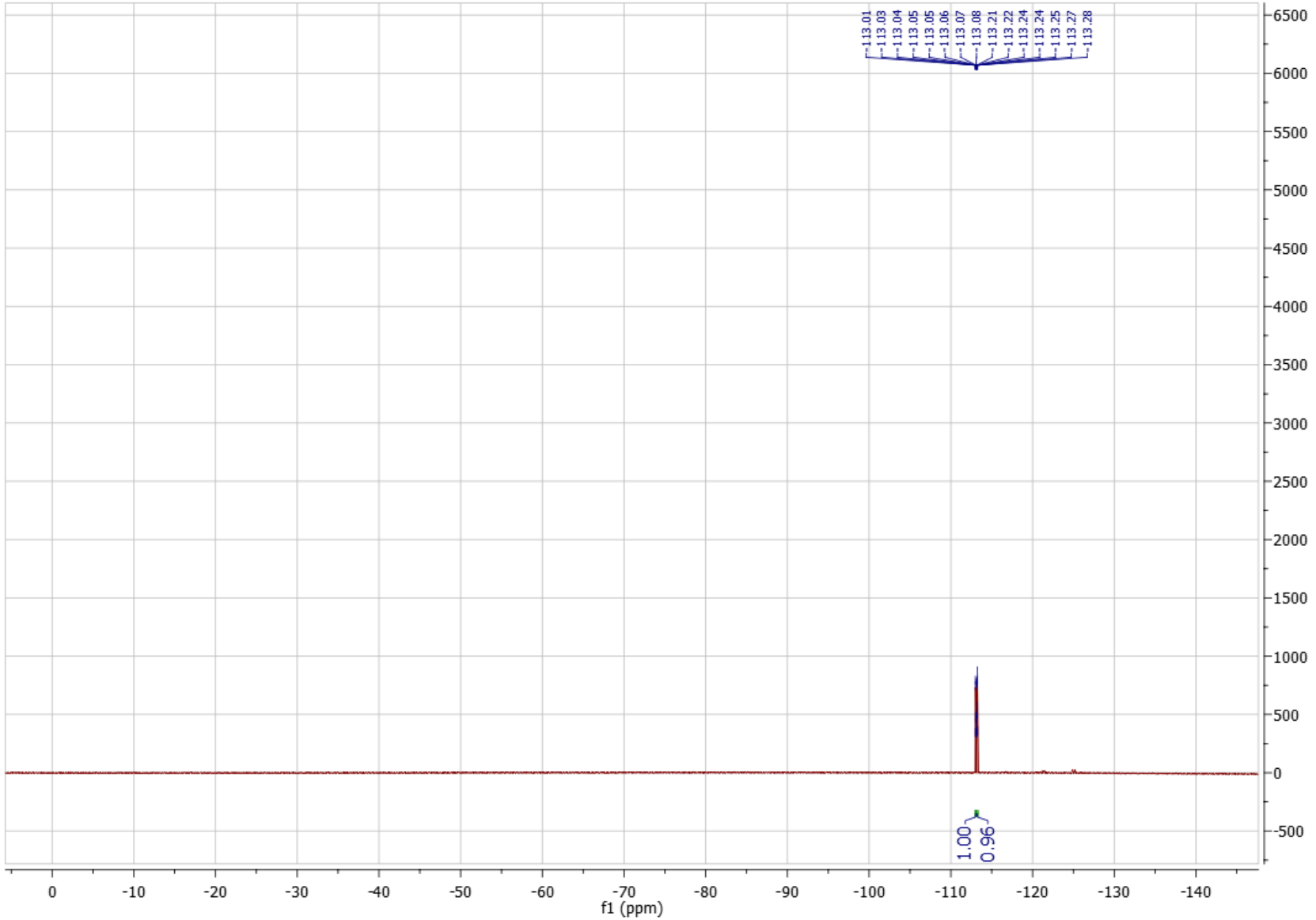
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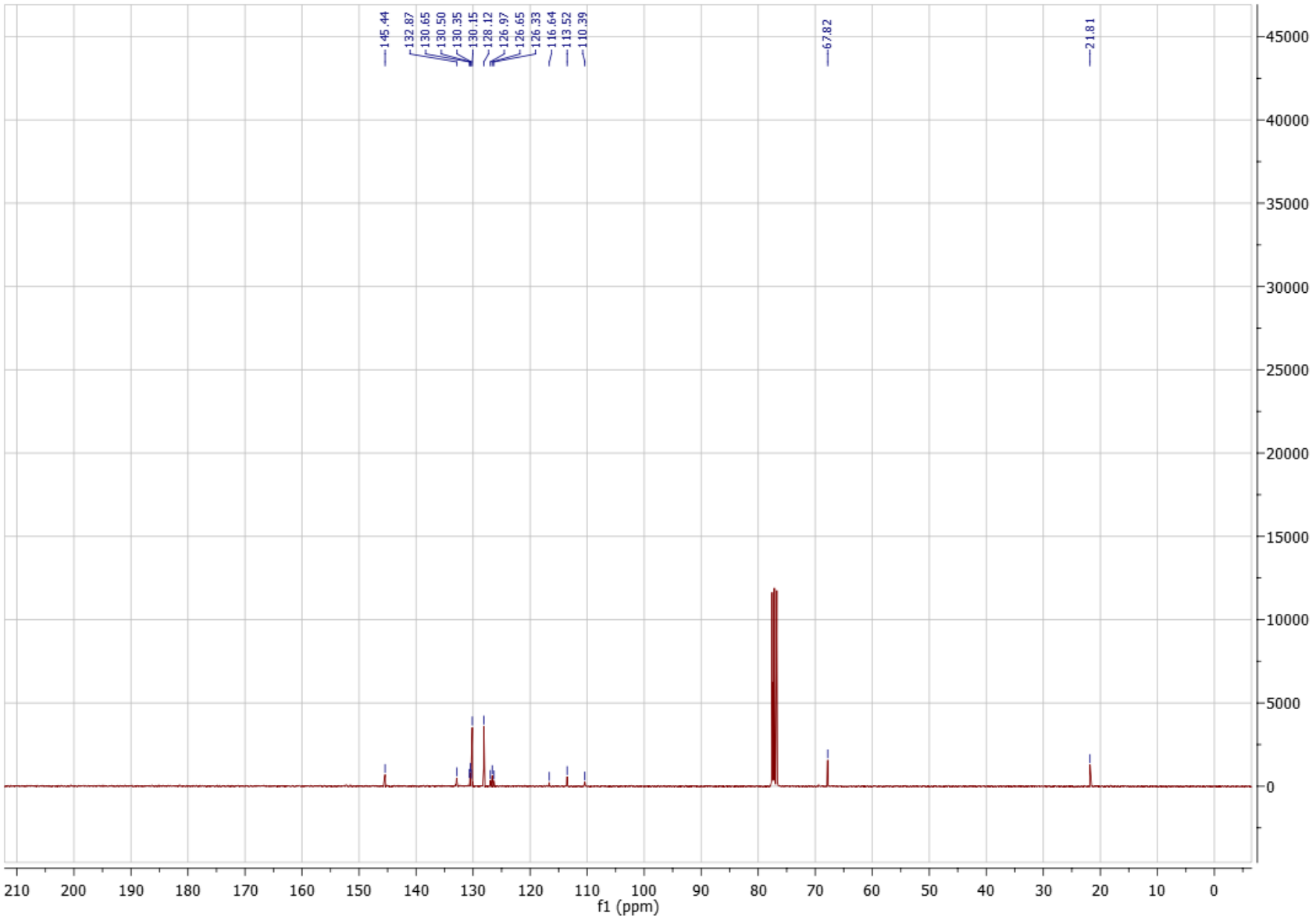
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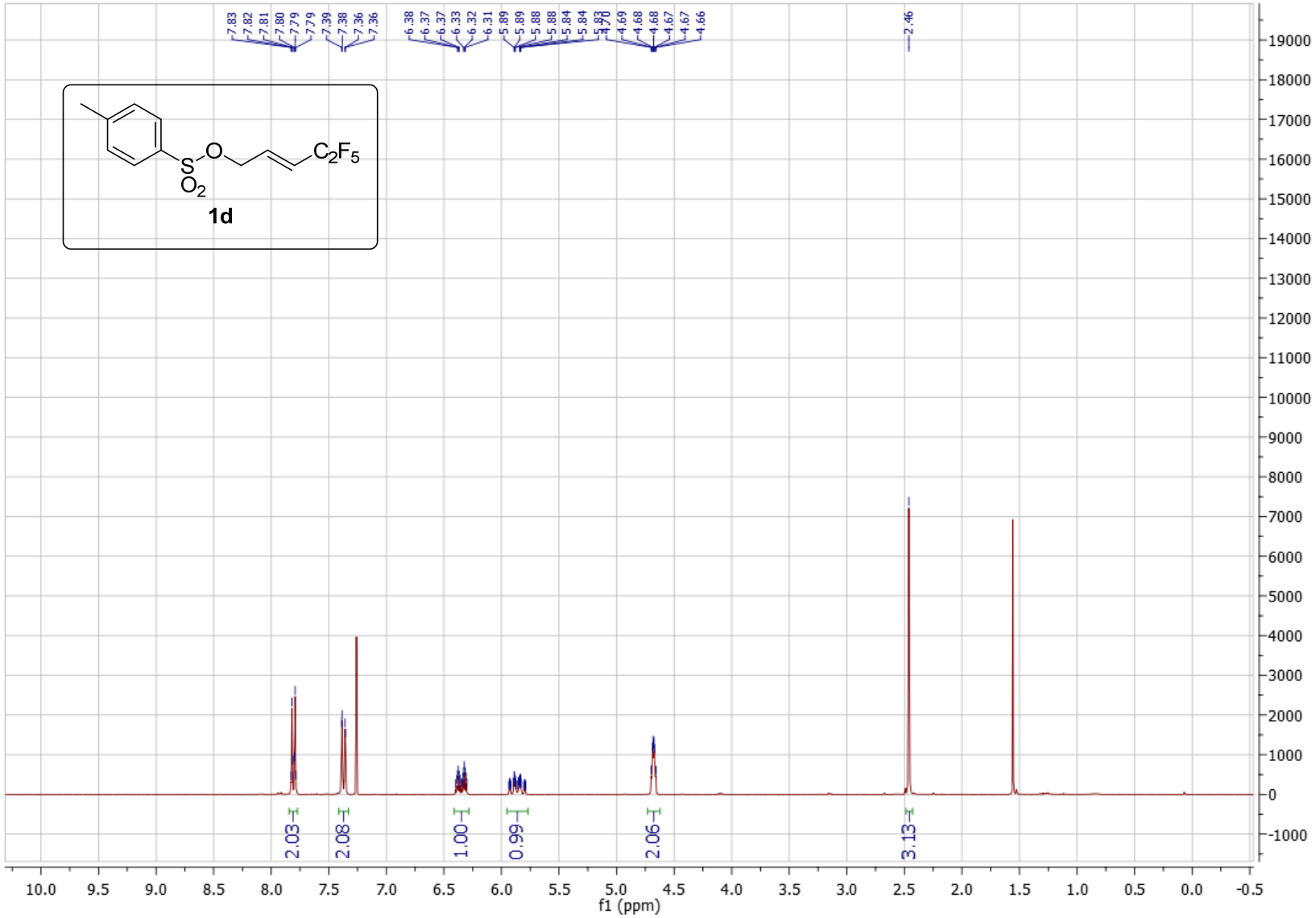
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4.69
4.68
4.68
4.67
4.67
4.66
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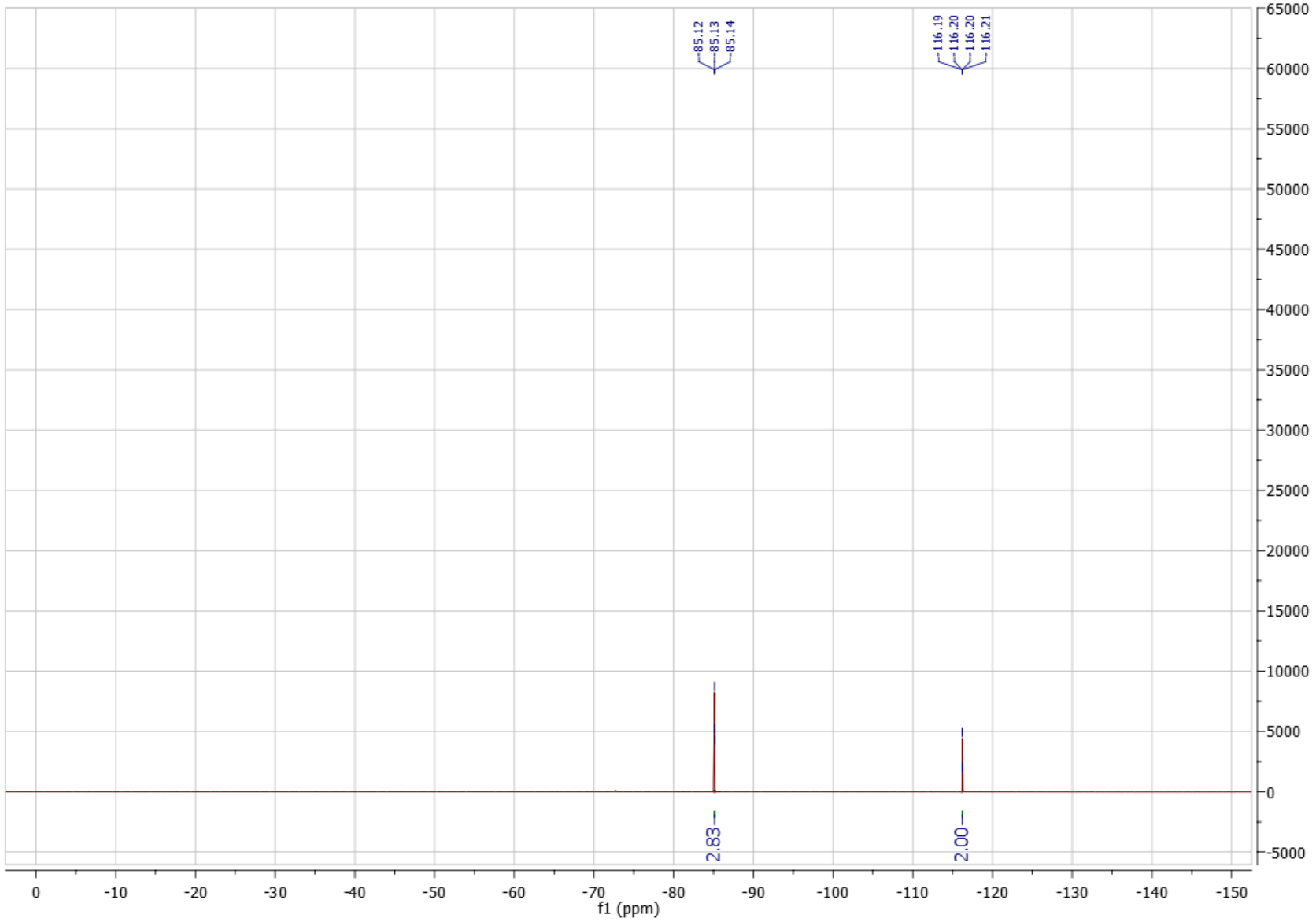
f1 (ppm)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40000
35000
30000
25000
20000
15000
10000
5000
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-5000
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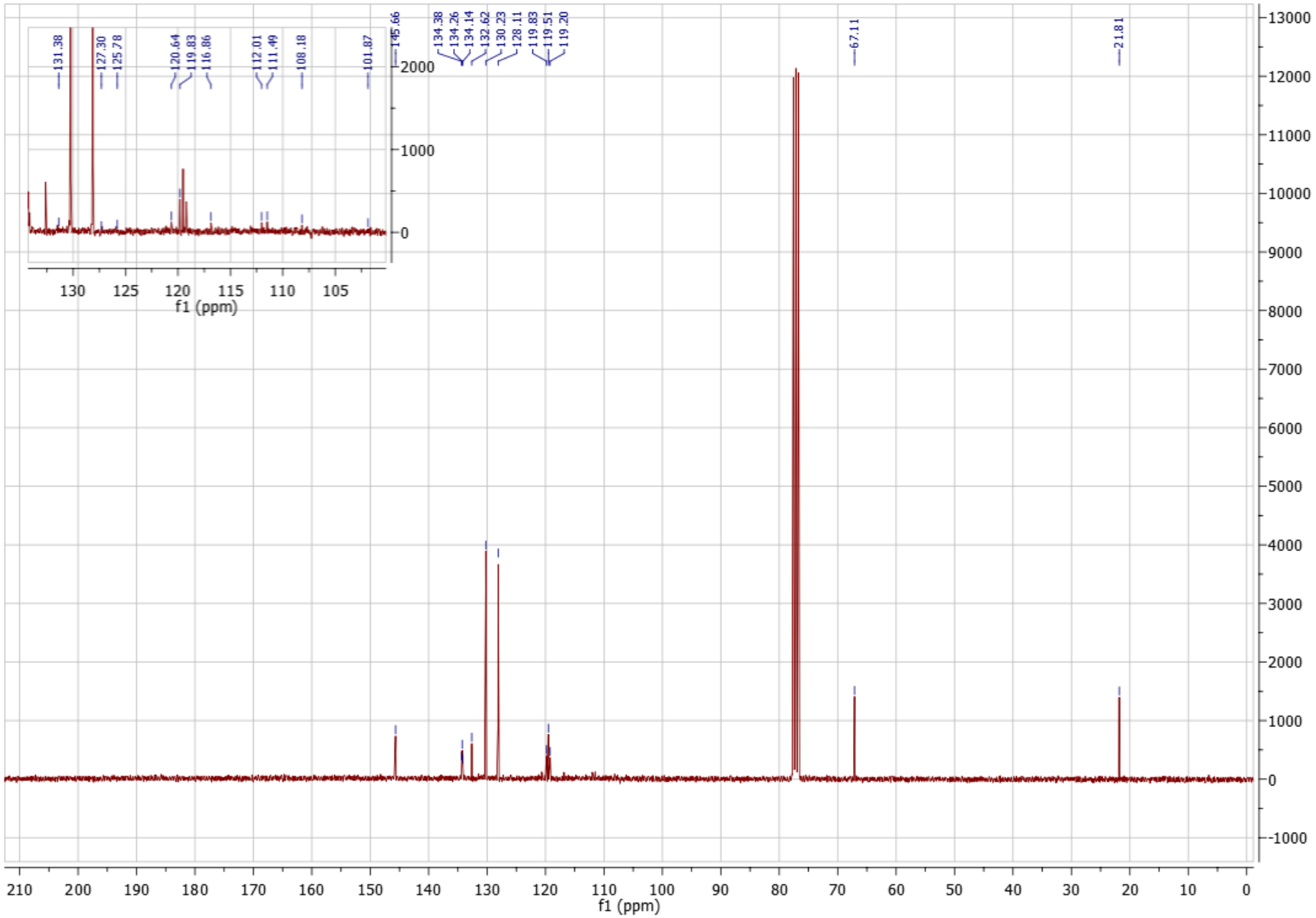
-150
f1 (ppm)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111.49
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145.66
134.38
134.26
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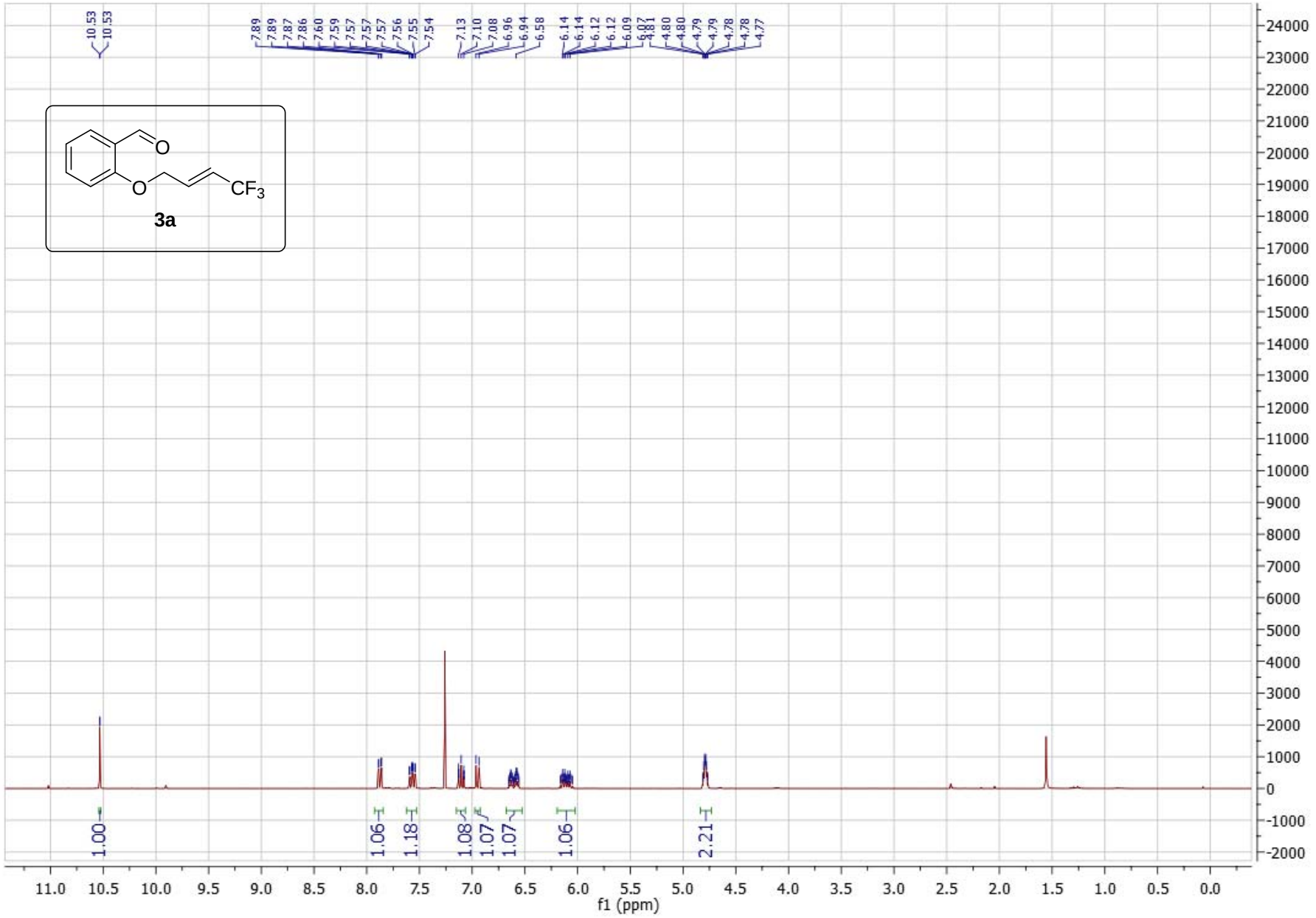
119.51
119.20
67.11
21.81
f1 (ppm)
f1 (ppm)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7.54
7.13
7.10
7.08
6.96
6.94
6.58
6.14
6.14
6.12
6.12
6.09
4.81
4.80
4.80
4.79
4.79
4.78
4.78
4.77
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1.08
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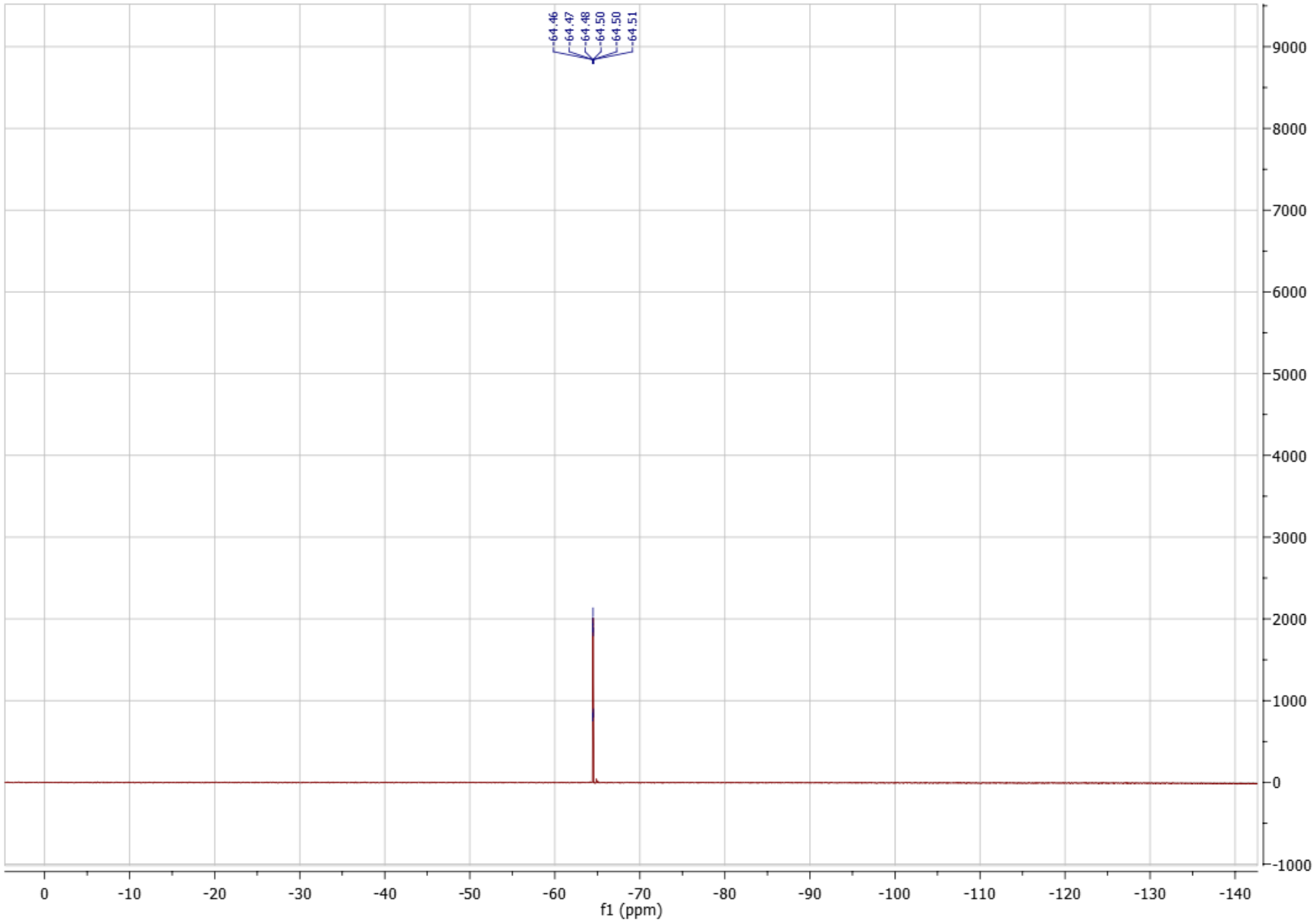
1.07
1.06
2.21
f1 (ppm)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1000
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0
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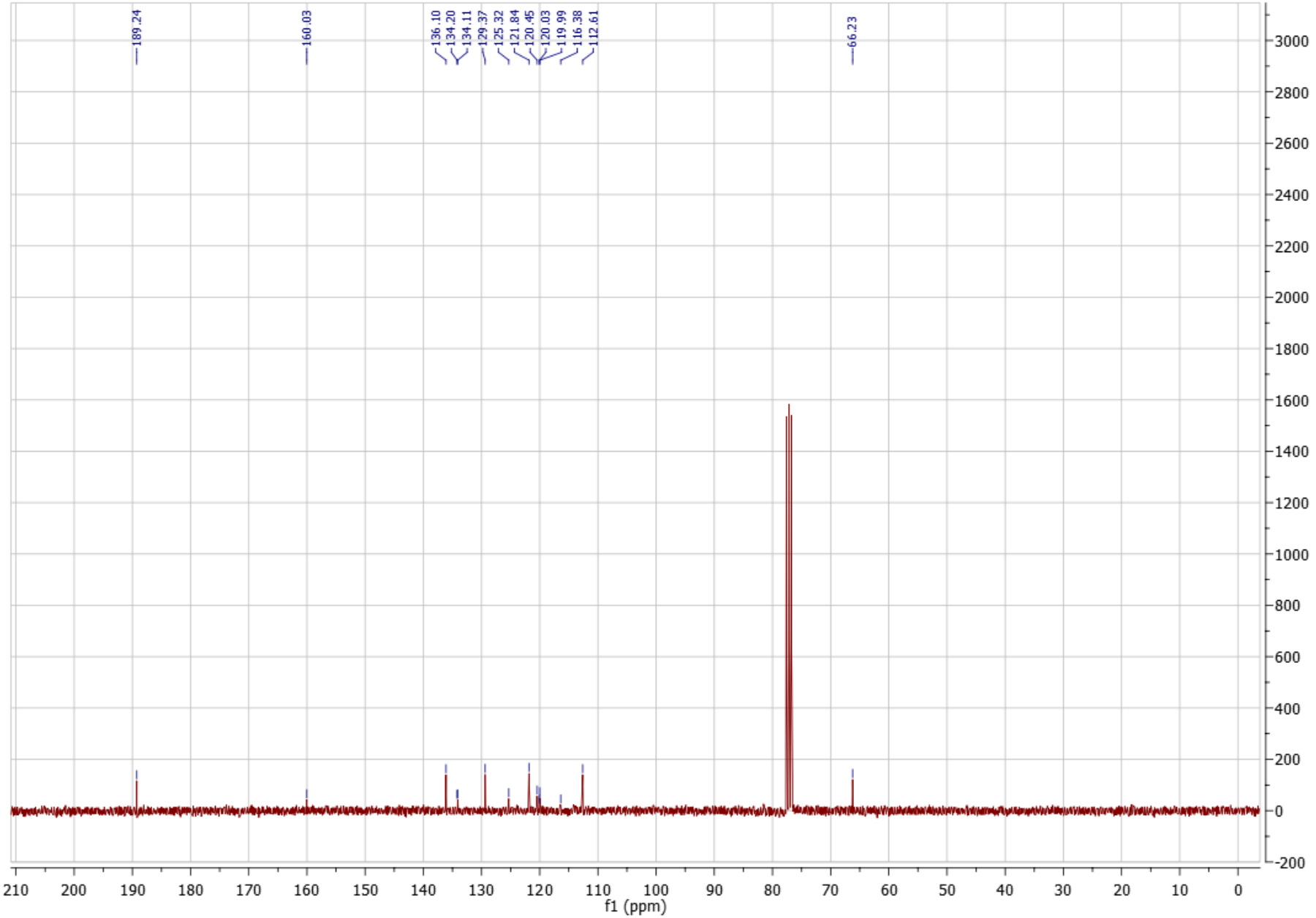
-130
-140
f1 (ppm)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120.03
119.99
116.38
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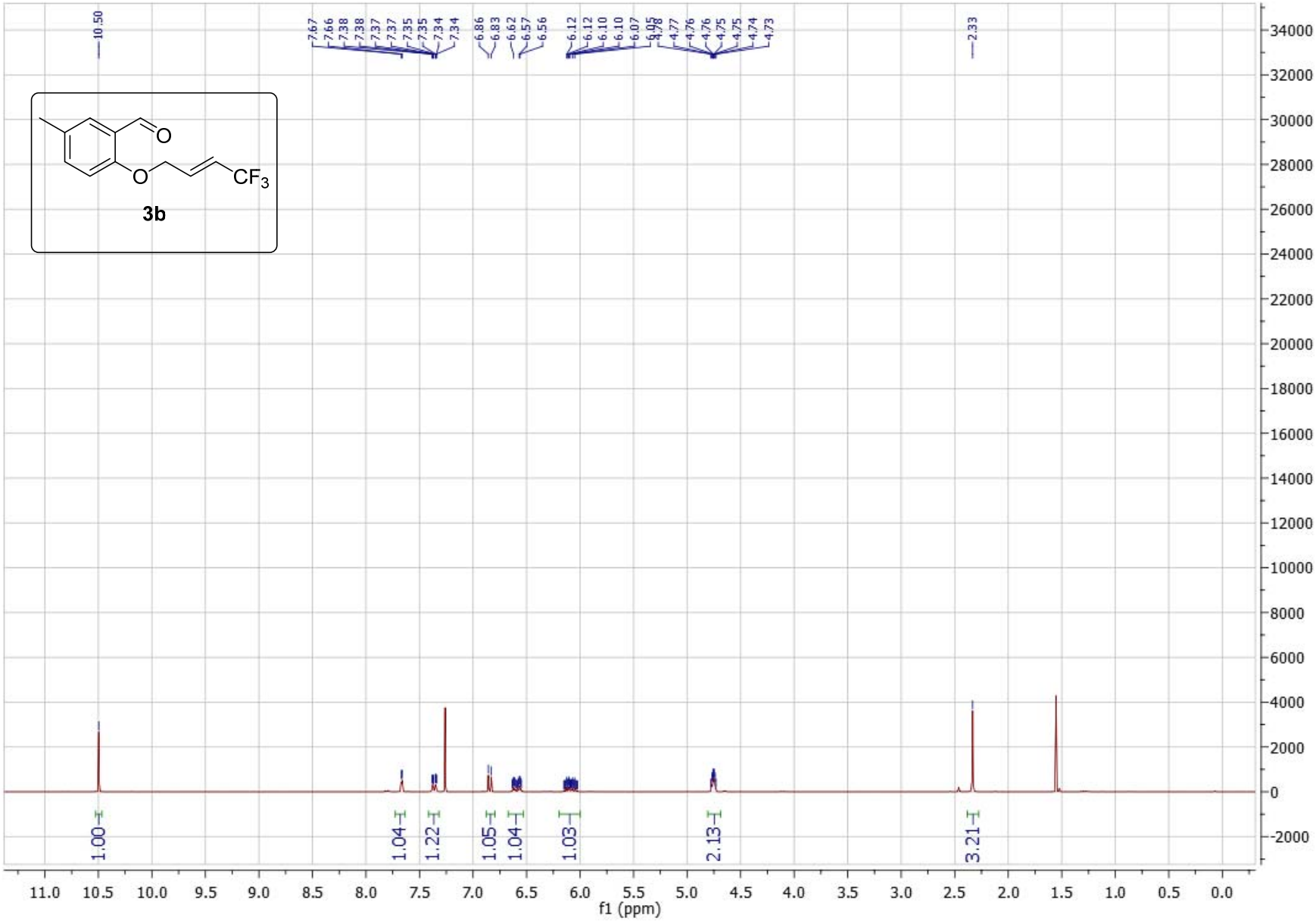
66.23
f1 (ppm)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6.62
6.57
6.56
6.12
6.12
6.10
6.10
6.07
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4.77
4.76
4.76
4.75
4.75
4.74
4.73
2.33
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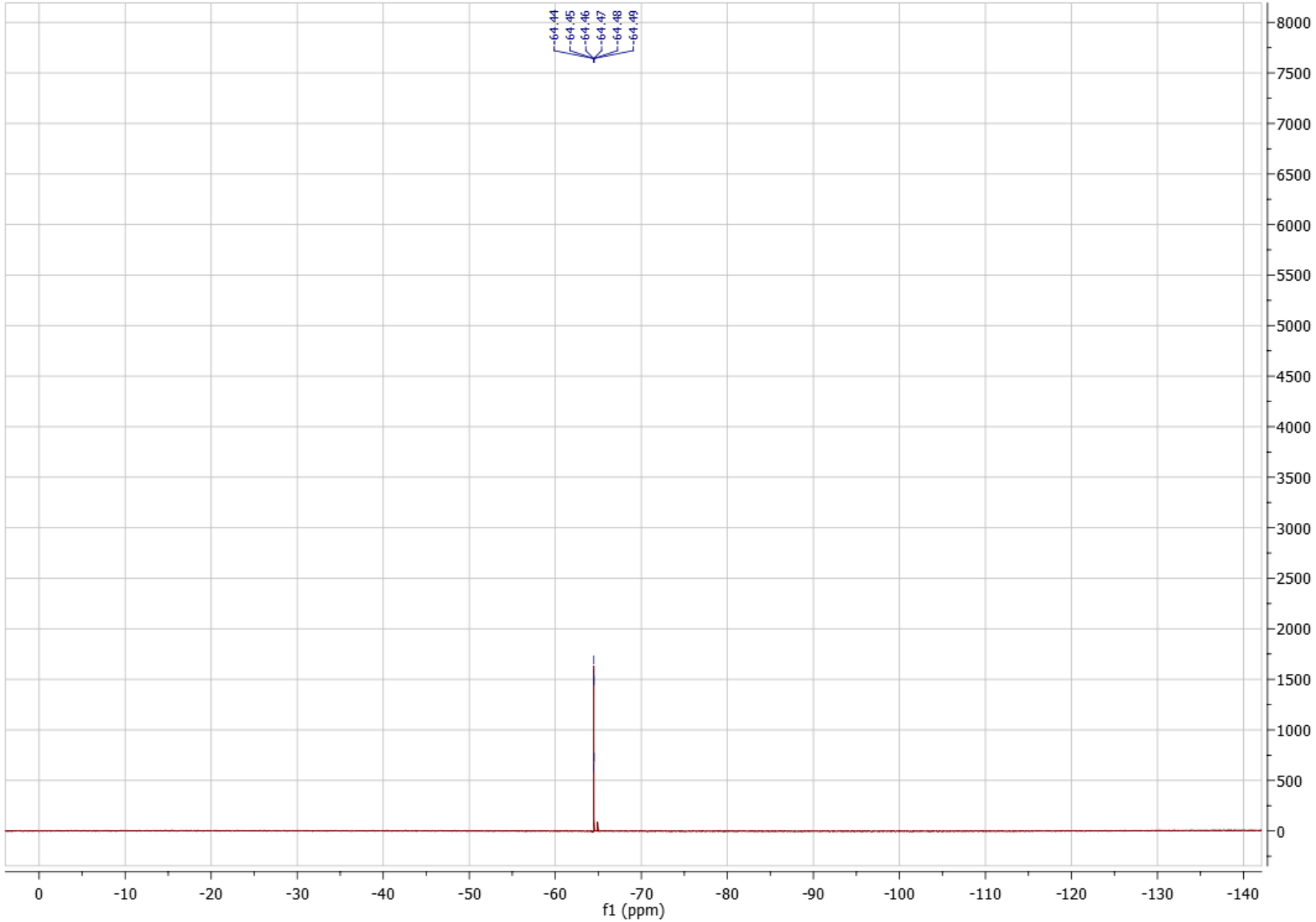
1.05
1.04
1.03
2.13
3.21
f1 (ppm)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3000
2500
2000
1500
1000
500
0
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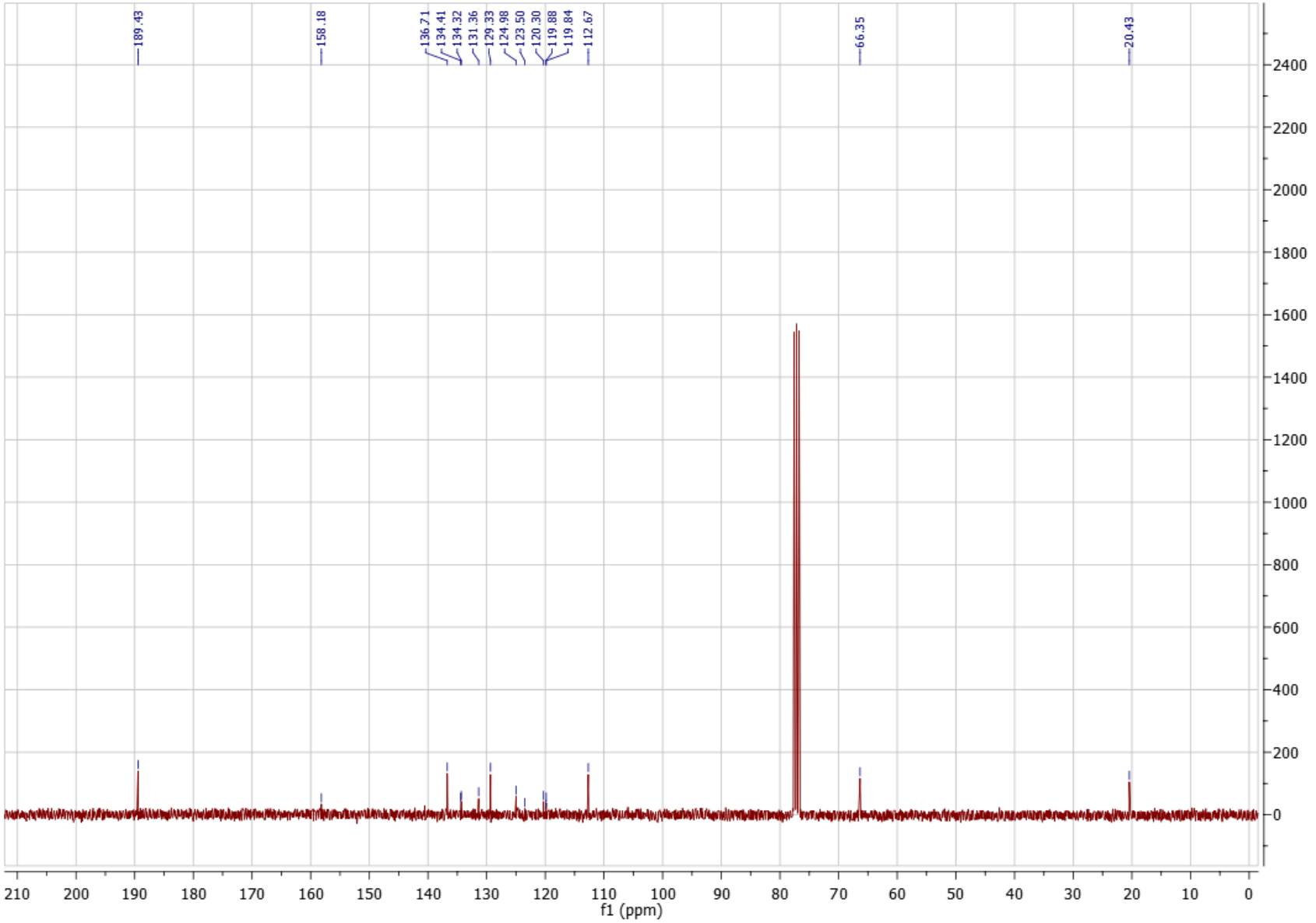
f1 (ppm)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120.30
119.88
119.84
112.67
66.35
20.43
2400
2200
2000
1800
1600
1400
1200
1000
800
600
400
200
0
210
200
190
180
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160
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130
120
110
100
90
80
70
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50
40
30
20
10
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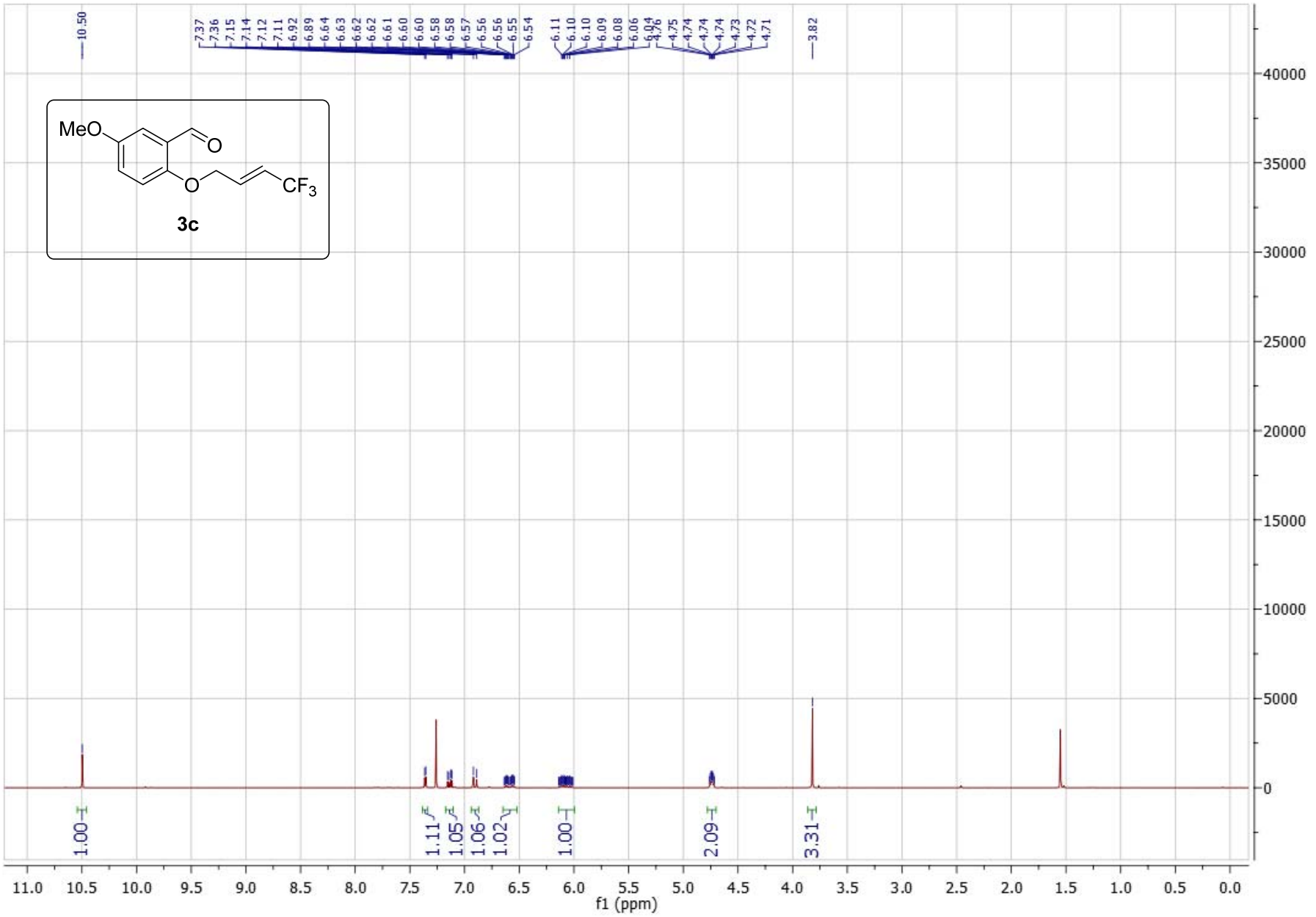
f1 (ppm)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6.63
6.62
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6.61
6.60
6.60
6.58
6.58
6.57
6.56
6.56
6.55
6.54
6.11
6.10
6.10
6.09
6.08
6.06
4.76
4.75
4.74
4.74
4.74
4.73
4.72
4.71
3.82
MeO
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O
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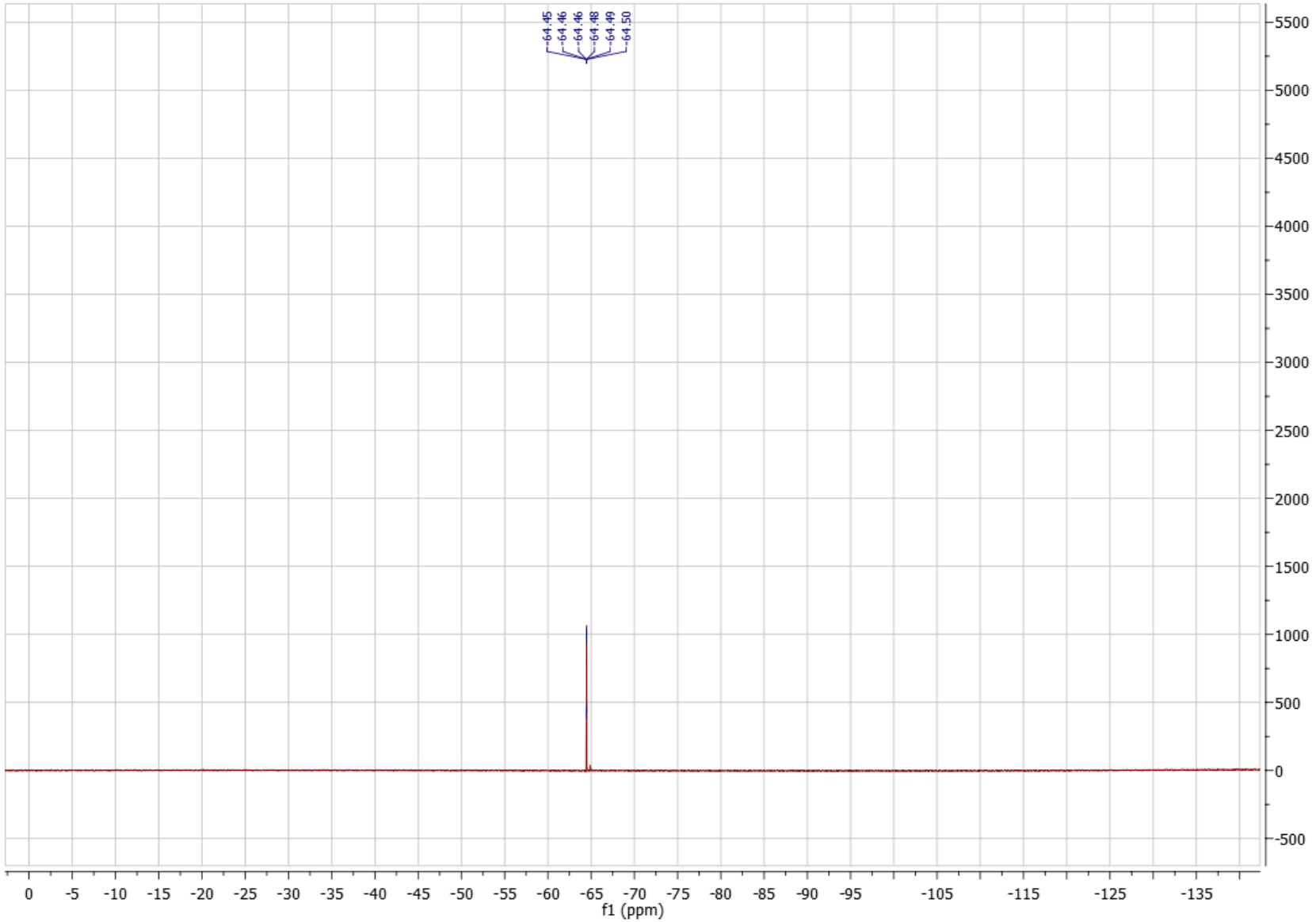
1.05
1.06
1.02
1.00
2.09
3.31
f1 (ppm)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3500
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2500
2000
1500
1000
500
0
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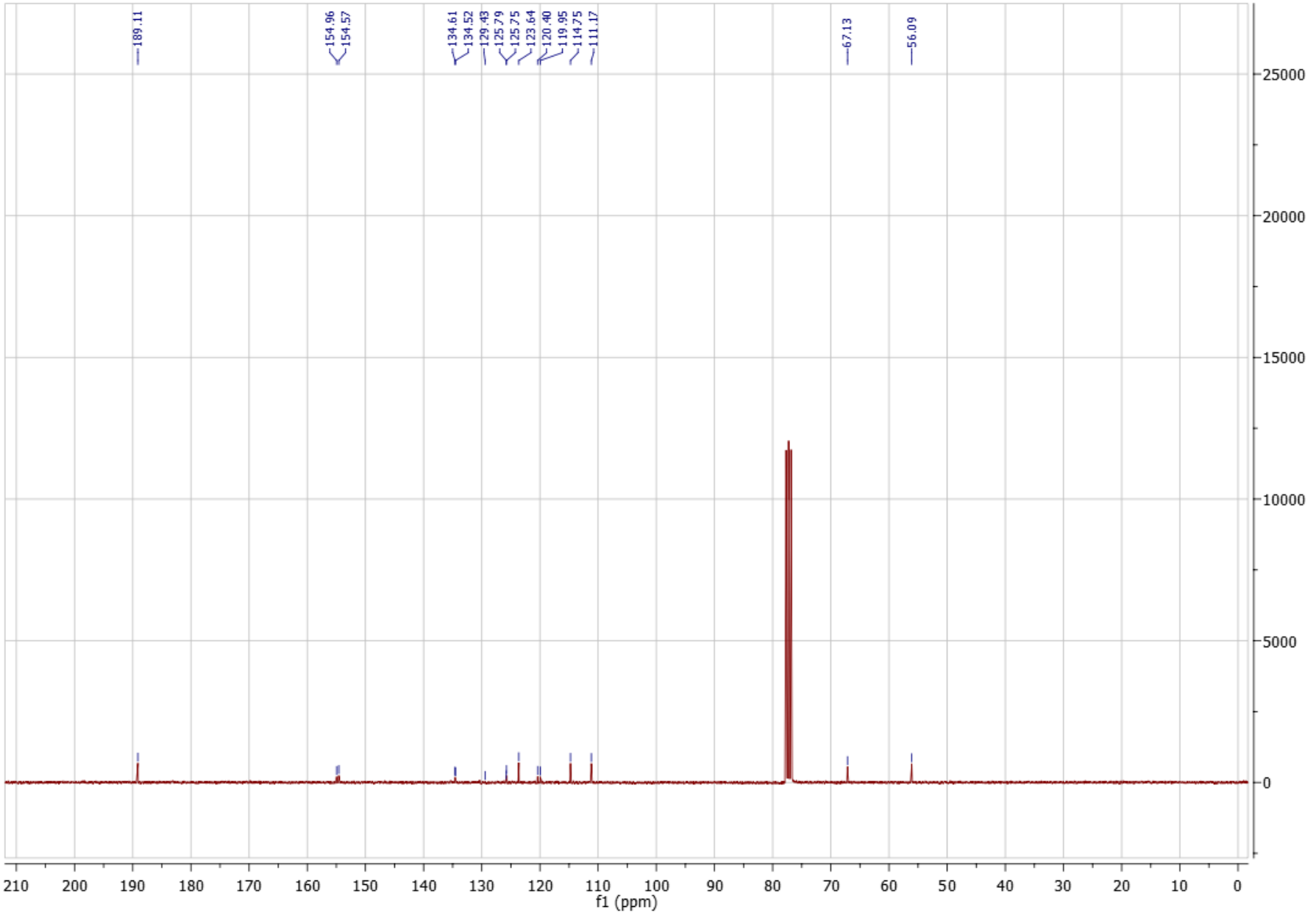
0 -5 -10 -15 -20 -25 -30 -35 -40 -45 -50 -55 -60 -65 -70 -75 -80 -85 -90 -95 -105 -115 -125 -135
f1 (ppm)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134.52
129.43
125.79
125.75
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120.40
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114.75
111.17
67.13
56.09
25000
20000
15000
10000
5000
0
210
200
190
180
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150
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130
120
110
100
90
80
70
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50
40
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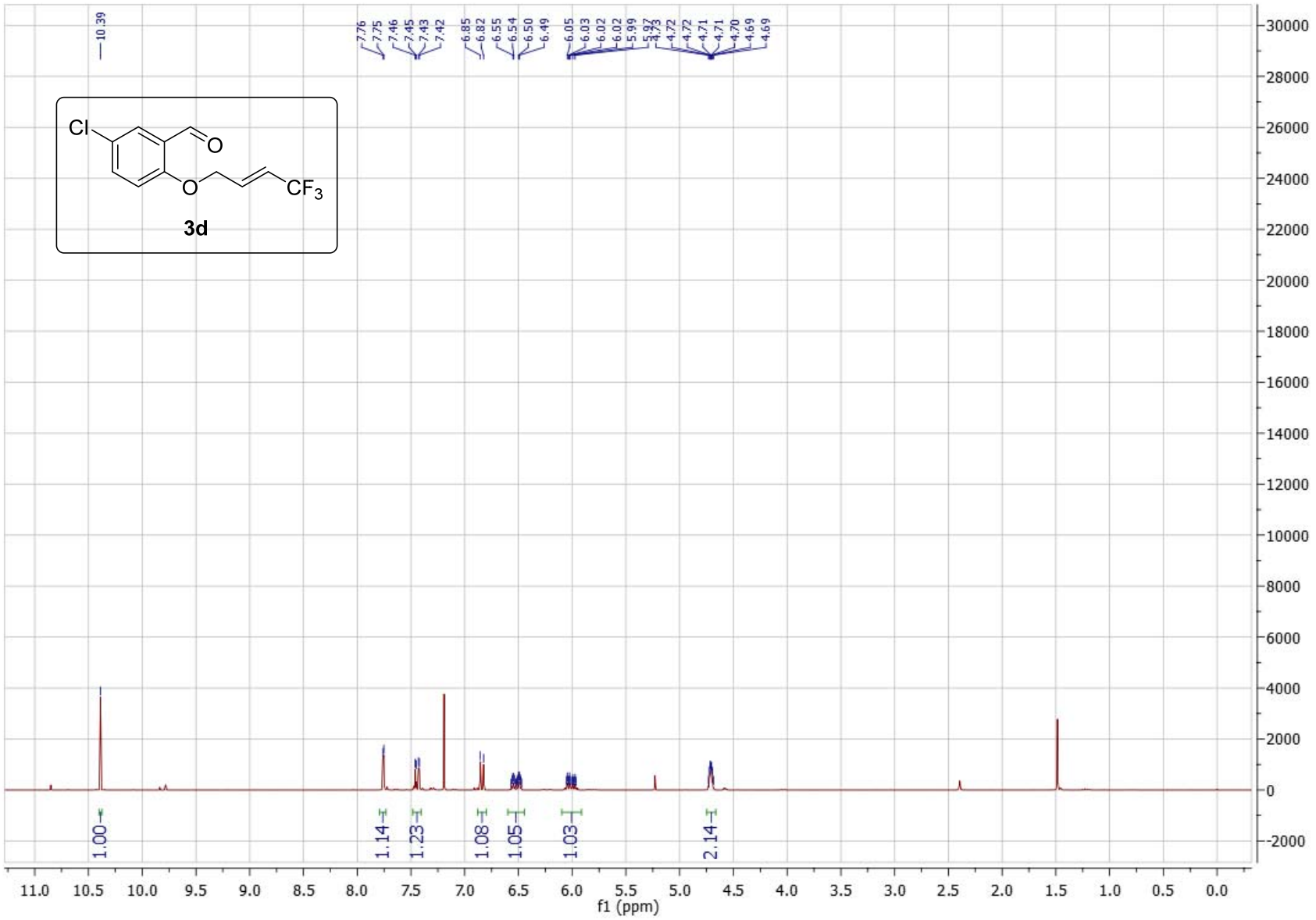
20
10
0
f1 (ppm)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6.49
6.05
6.03
6.02
6.02
5.99
4.72
4.72
4.71
4.71
4.70
4.69
4.69
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CF3
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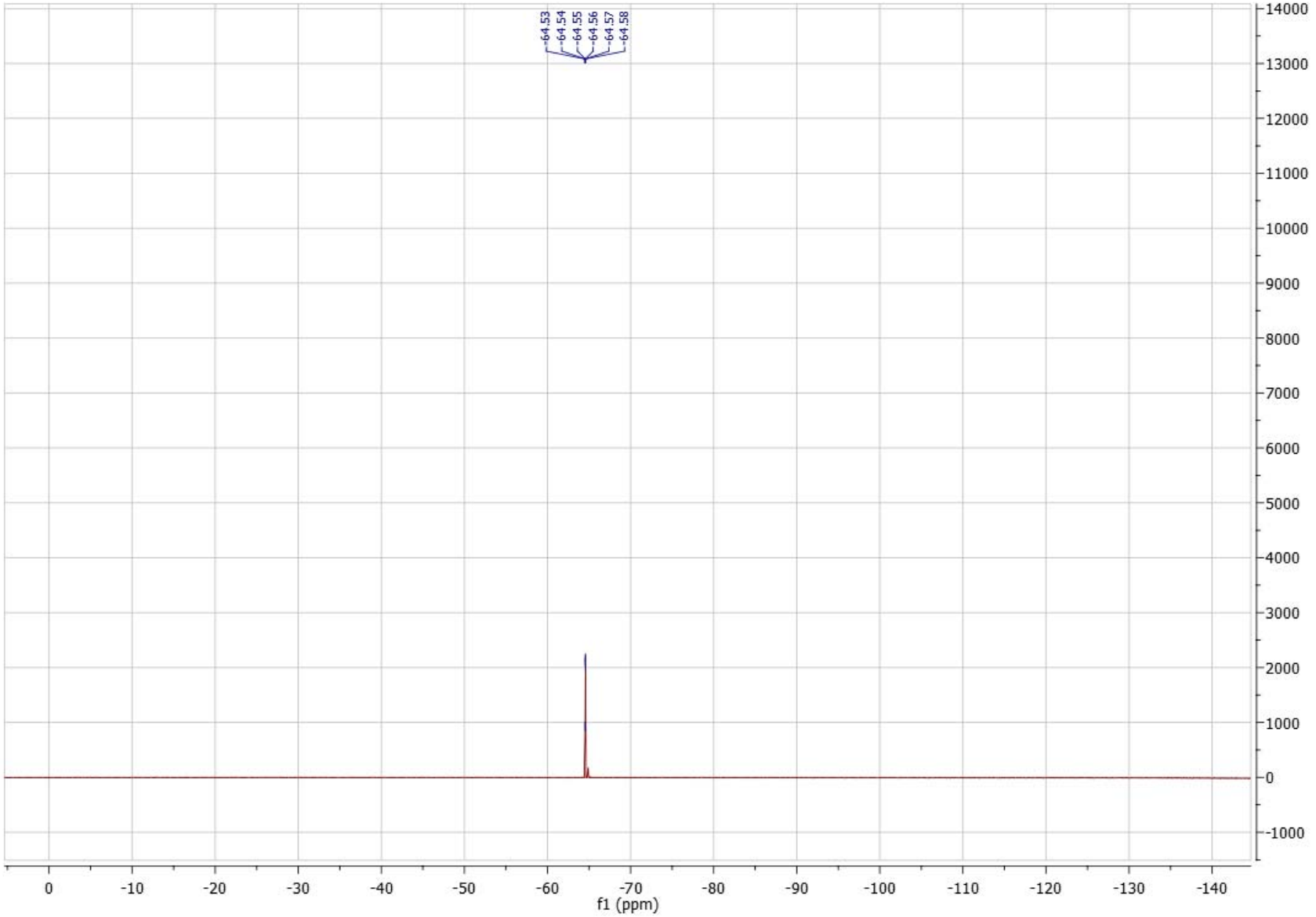
1.05
1.03
2.14
f1 (ppm)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12000
11000
10000
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8000
7000
6000
5000
4000
3000
2000
1000
0
-1000
0
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-60
-70
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-90
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-110
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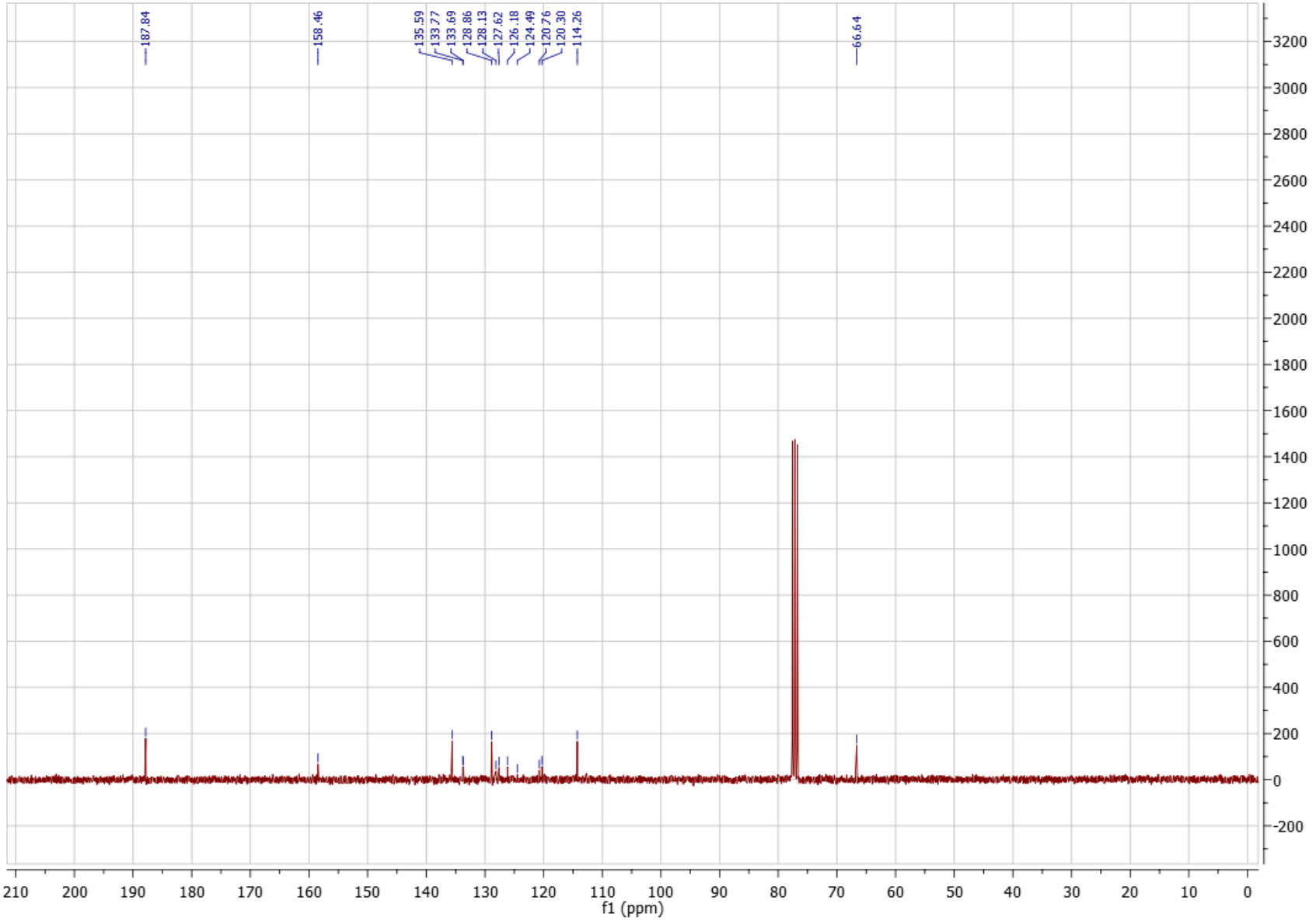
-130
-140
f1 (ppm)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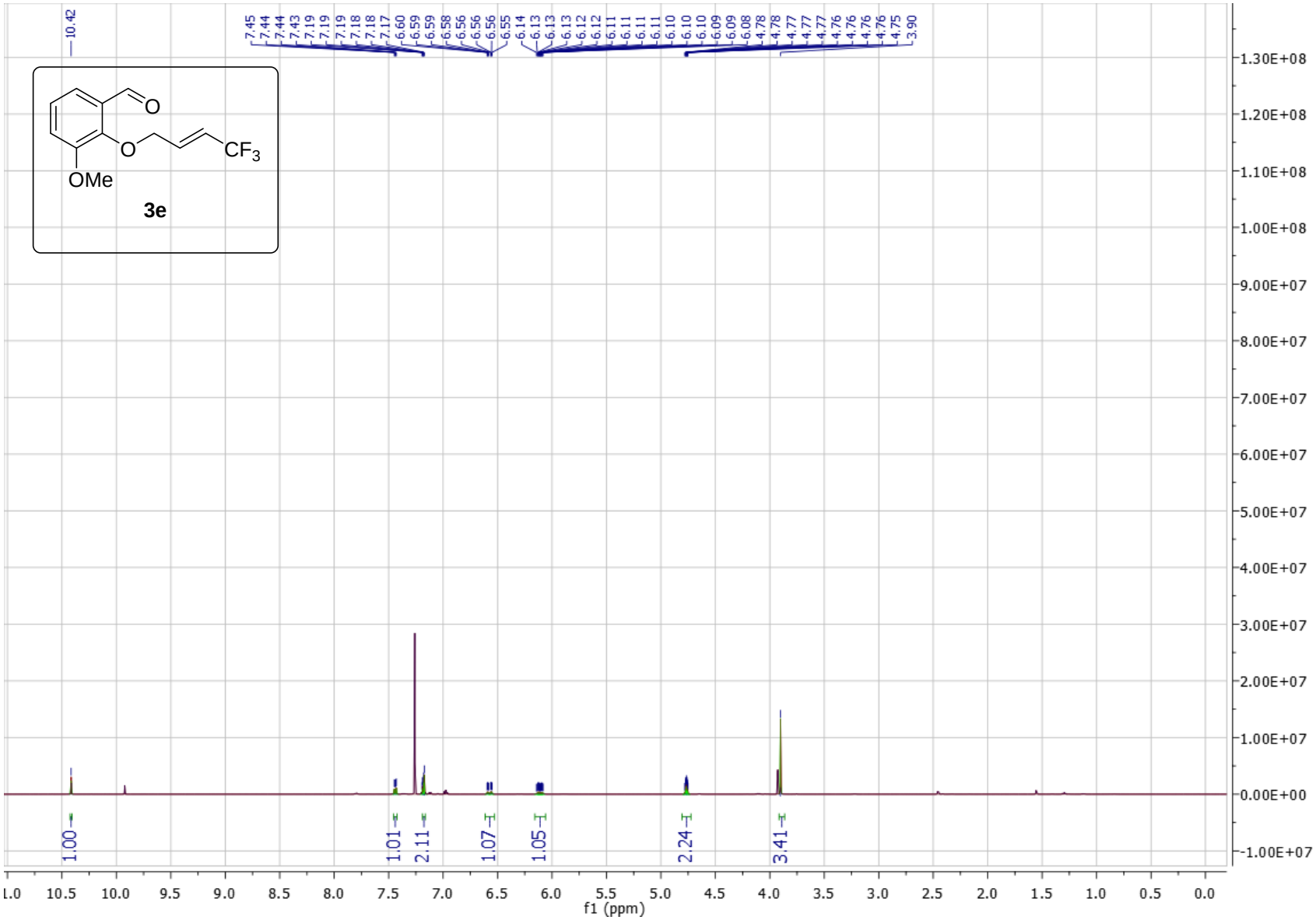
126.18
124.49
120.76
120.30
114.26
66.64
f1 (ppm)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6.13
6.13
6.12
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6.11
6.11
6.11
6.10
6.10
6.10
6.09
6.09
6.08
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4.78
4.77
4.77
4.77
4.76
4.76
4.76
4.76
4.75
3.90
O
O
CF3
OMe
3e
1.30E+08
1.20E+08
1.10E+08
1.00E+08
9.00E+07
8.00E+07
7.00E+07
6.00E+07
5.00E+07
4.00E+07
3.00E+07
2.00E+07
1.00E+07
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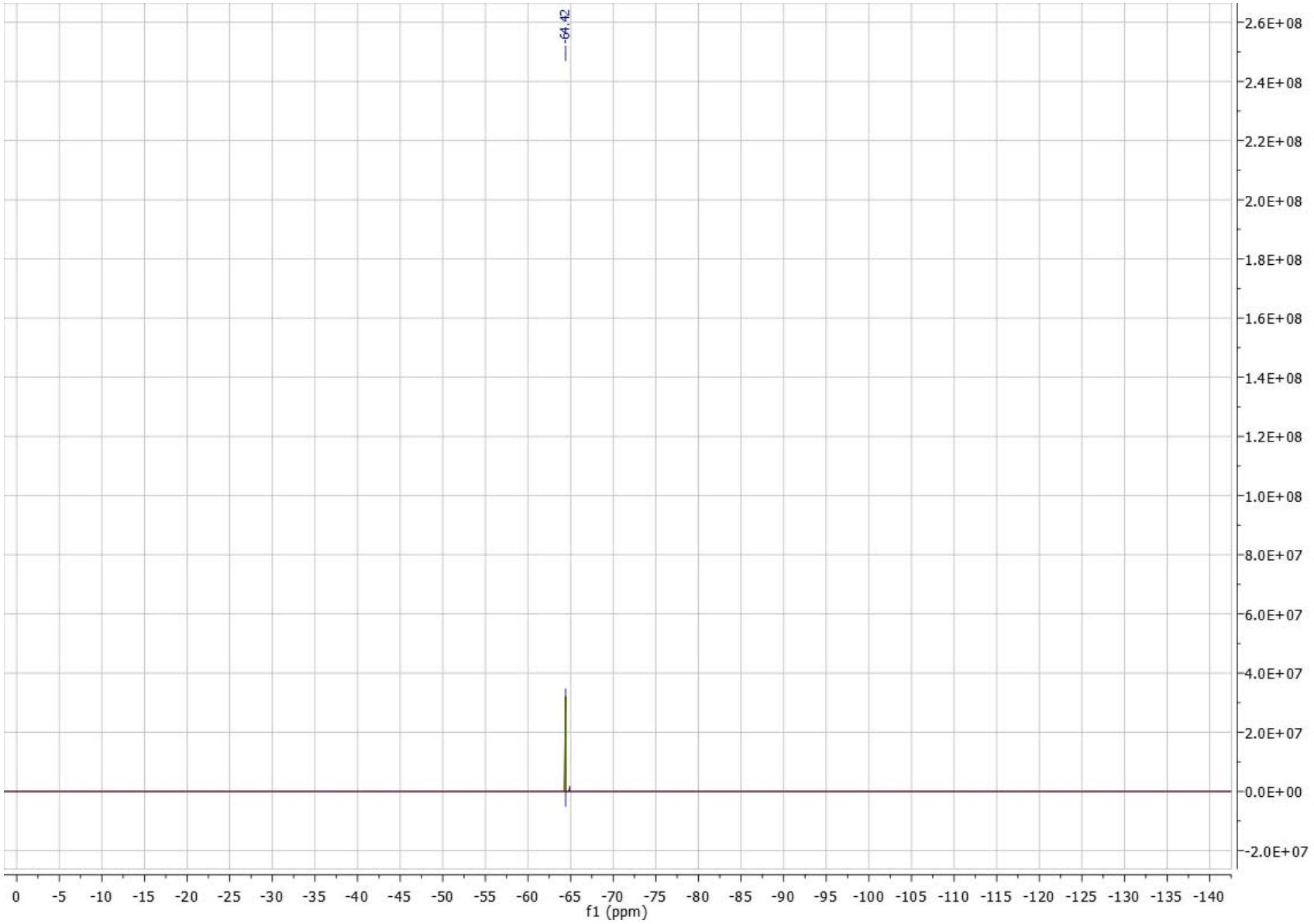
1.01
2.11
1.07
1.05
2.24
3.41
f1 (ppm)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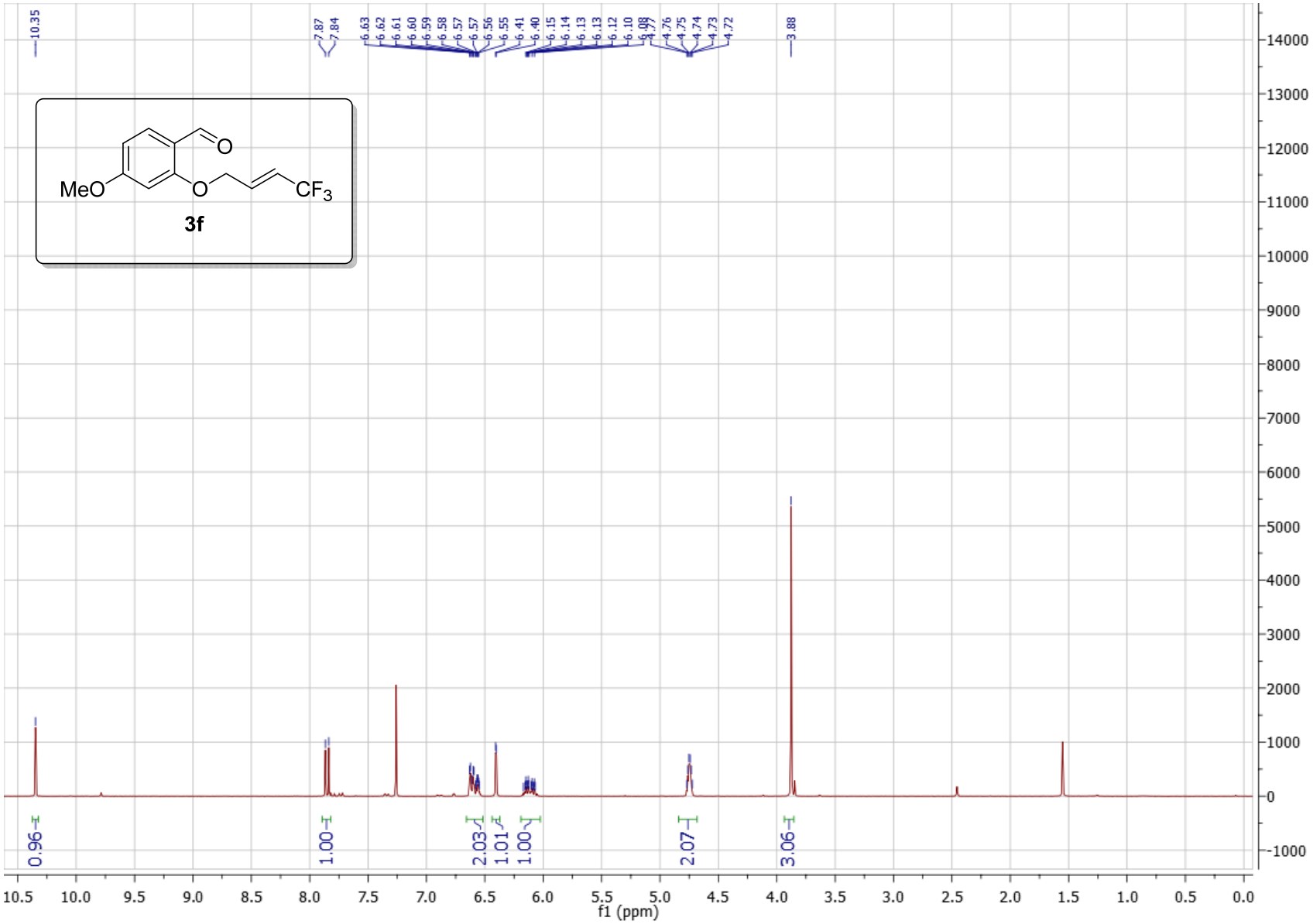
2.4E+08
2.2E+08
2.0E+08
1.8E+08
1.6E+08
1.4E+08
1.2E+08
1.0E+08
8.0E+07
6.0E+07
4.0E+07
2.0E+07
0.0E+00
-2.0E+07
0 -5 -10 -15 -20 -25 -30 -35 -40 -45 -50 -55 -60 -65 -70 -75 -80 -85 -90 -95 -100 -105 -110 -115 -120 -125 -130 -135 -140
f1 (ppm)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6.41
6.40
6.15
6.14
6.13
6.13
6.12
6.10
6.08
4.76
4.75
4.74
4.73
4.72
3.88
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O
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1.01
1.00
2.07
3.06
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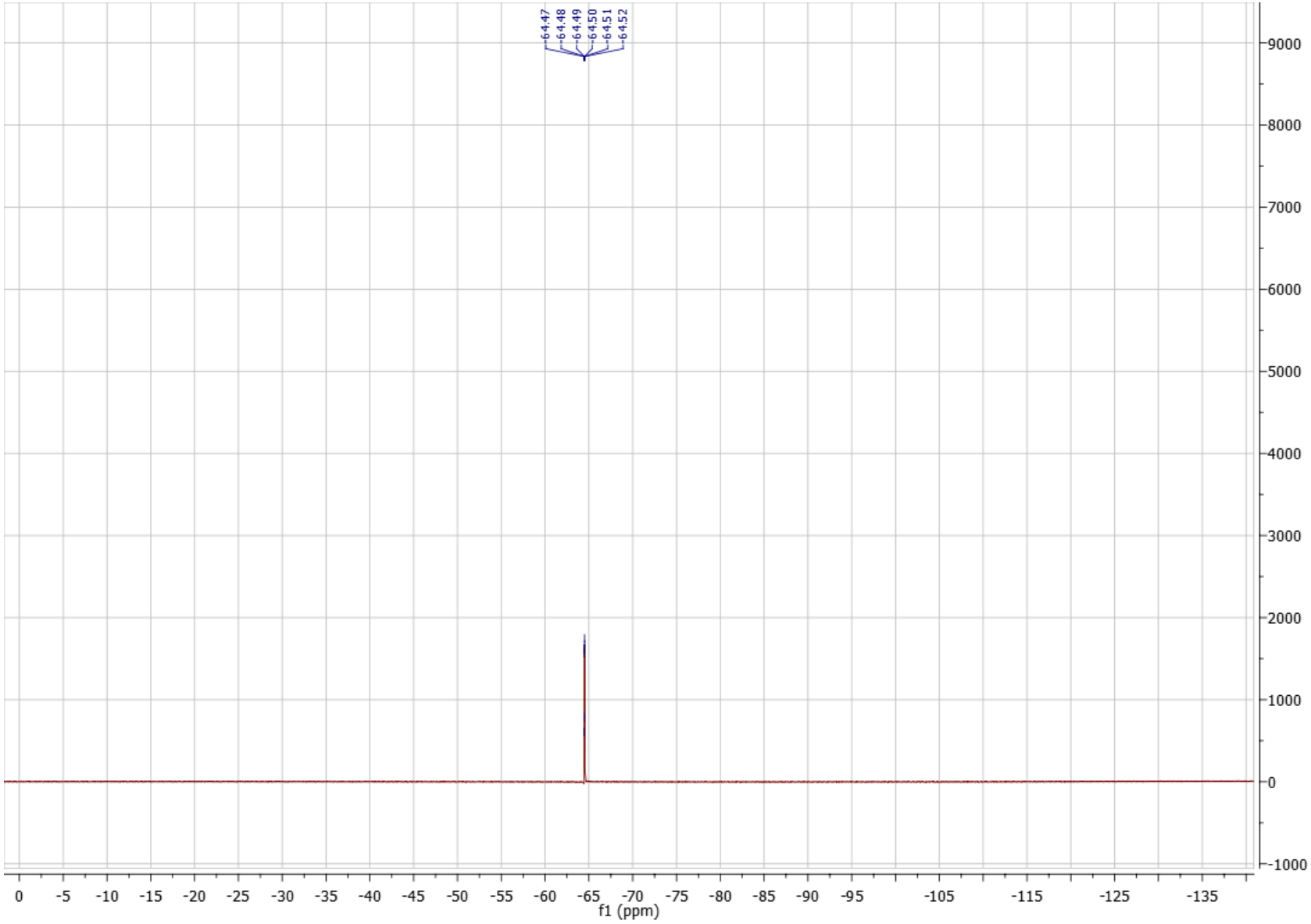
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1000
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0
-5
-10
-15
-20
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-30
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-40
-45
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-60
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-70
-75
-80
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-90
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-105
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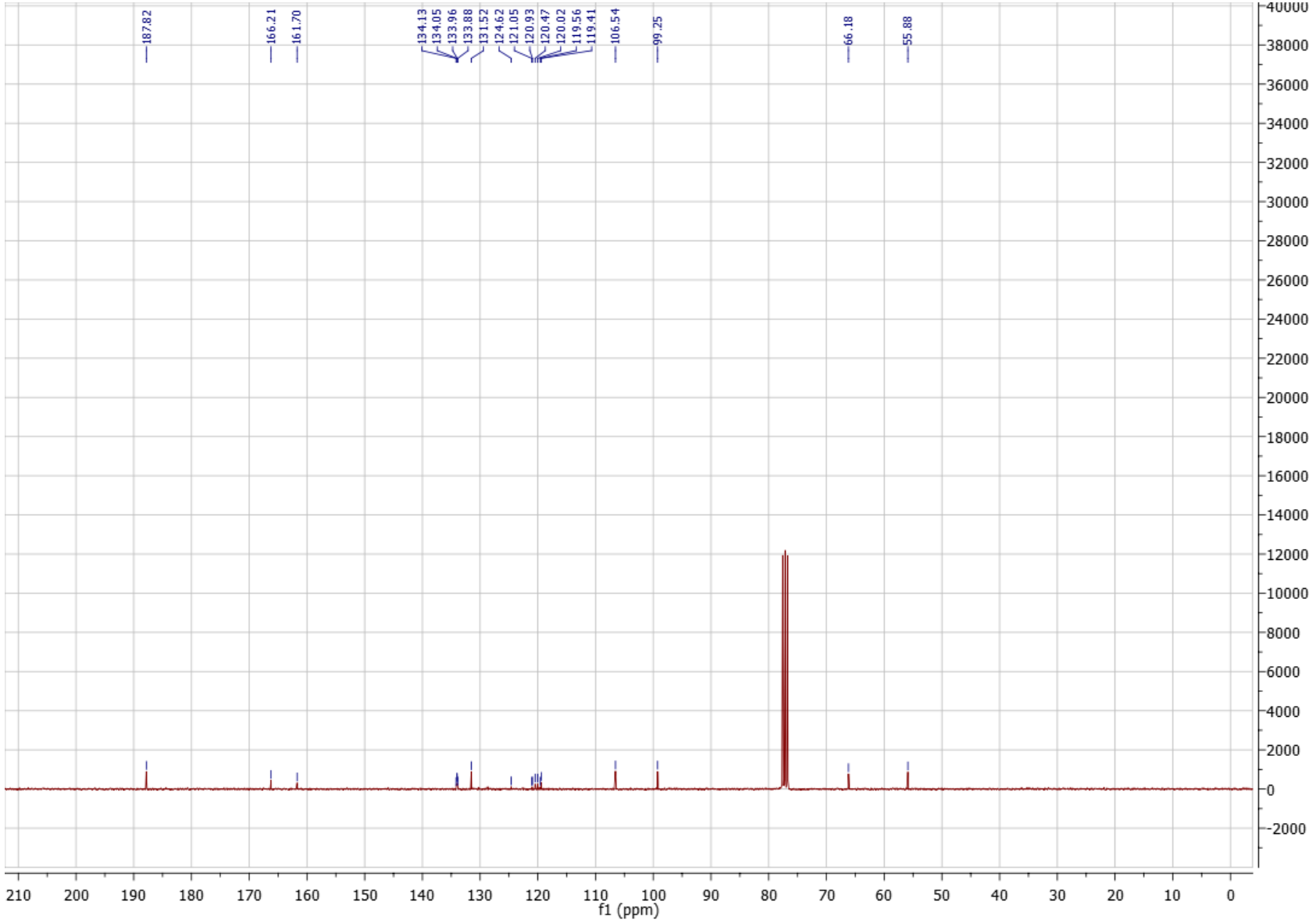
-125
-135
f1 (ppm)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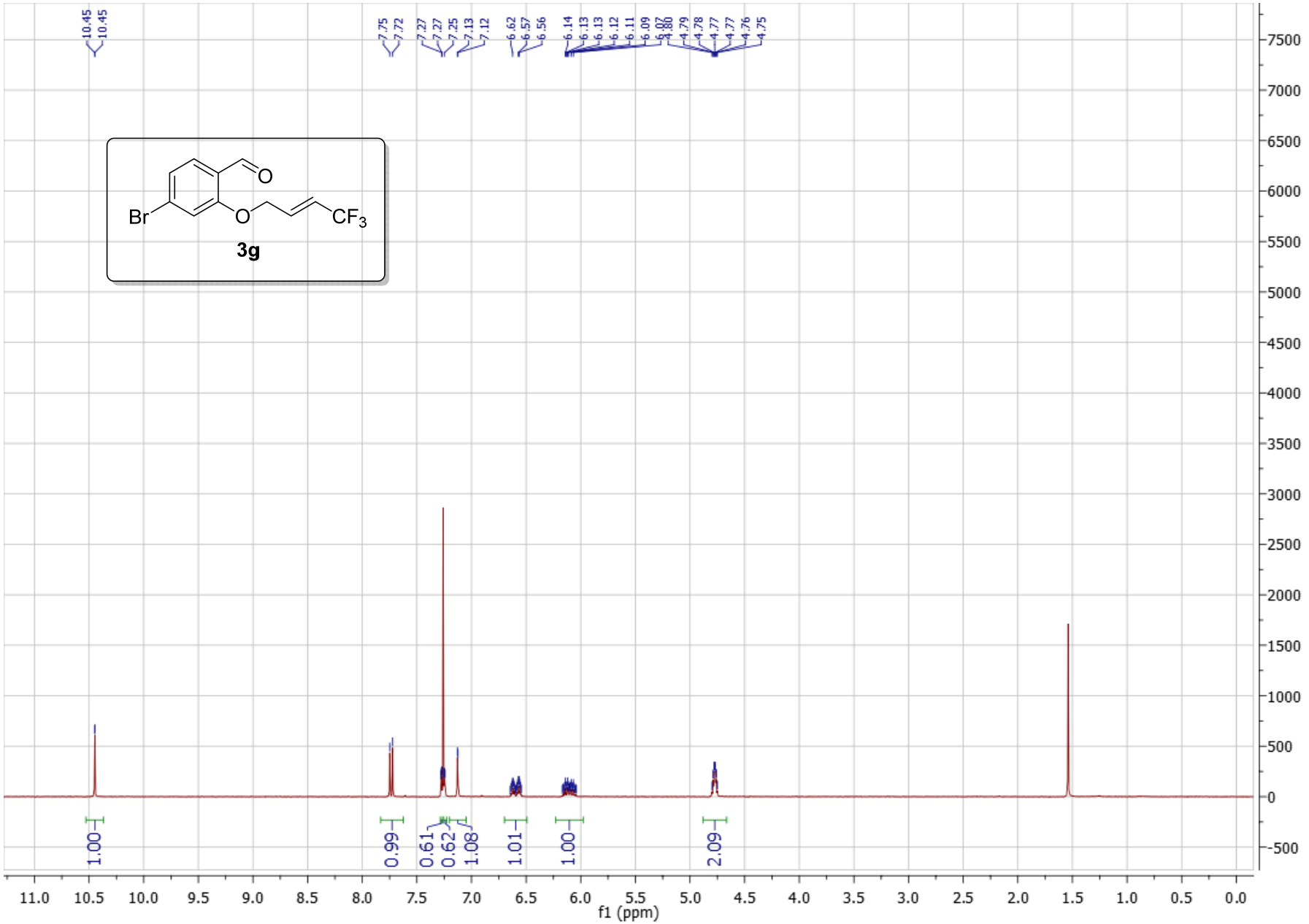
55.88
f1 (ppm)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6.13
6.13
6.12
6.11
6.09
4.79
4.78
4.77
4.77
4.76
4.75
Br
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0.62
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1.01
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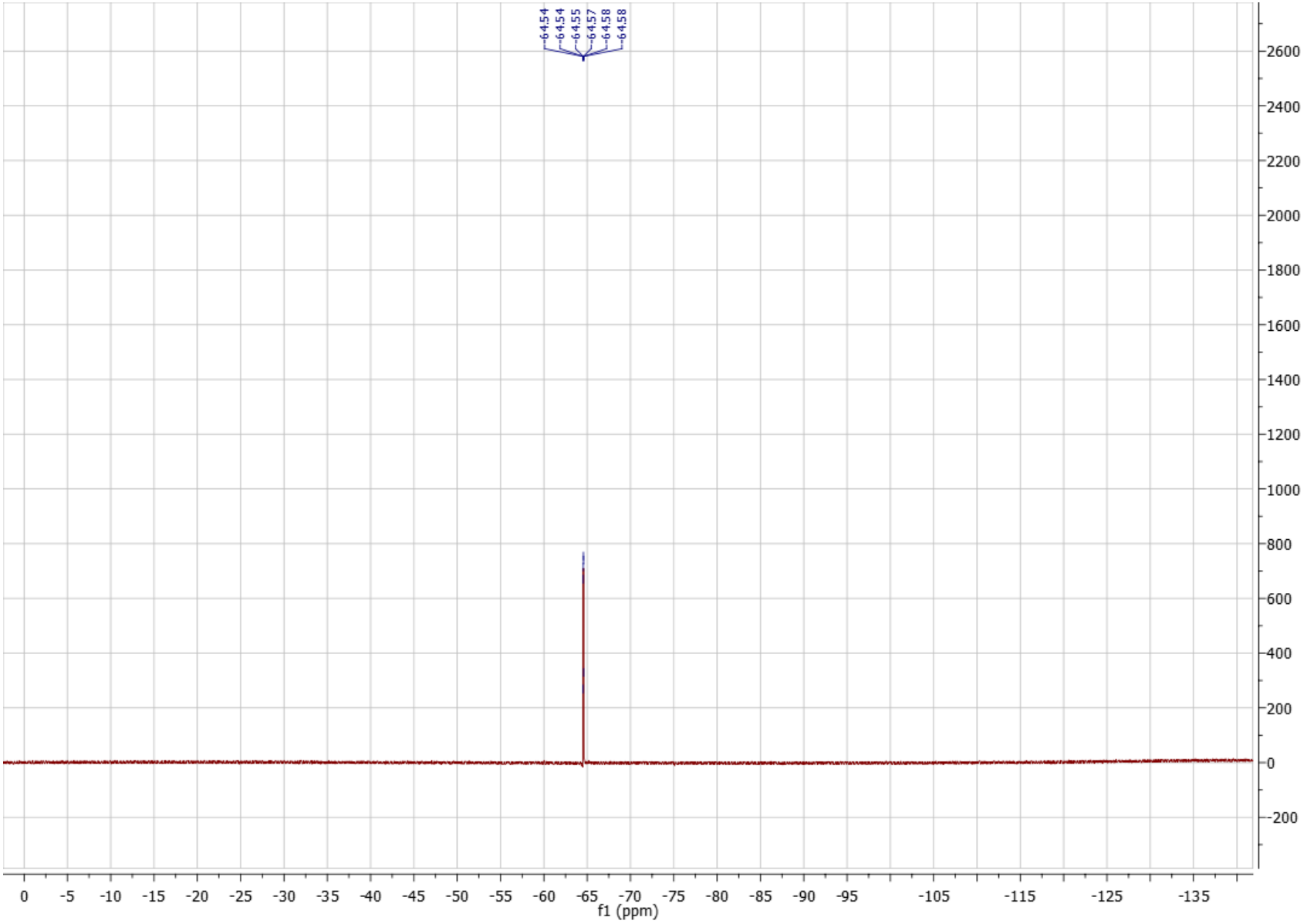
2.09
f1 (ppm)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1400
1200
1000
800
600
400
200
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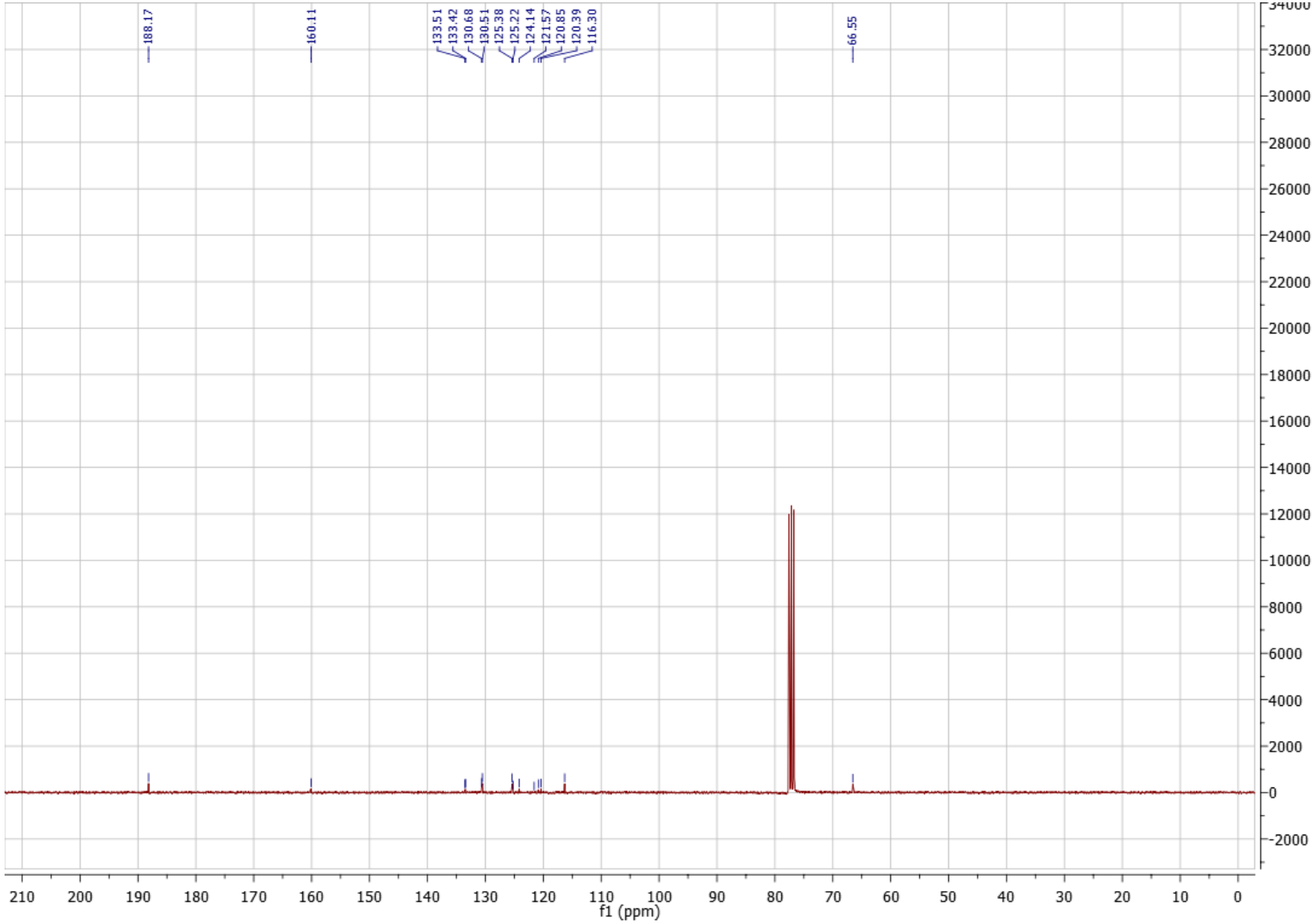
0 -5 -10 -15 -20 -25 -30 -35 -40 -45 -50 -55 -60 -65 -70 -75 -80 -85 -90 -95 -105 -115 -125 -135
f1 (ppm)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66.55
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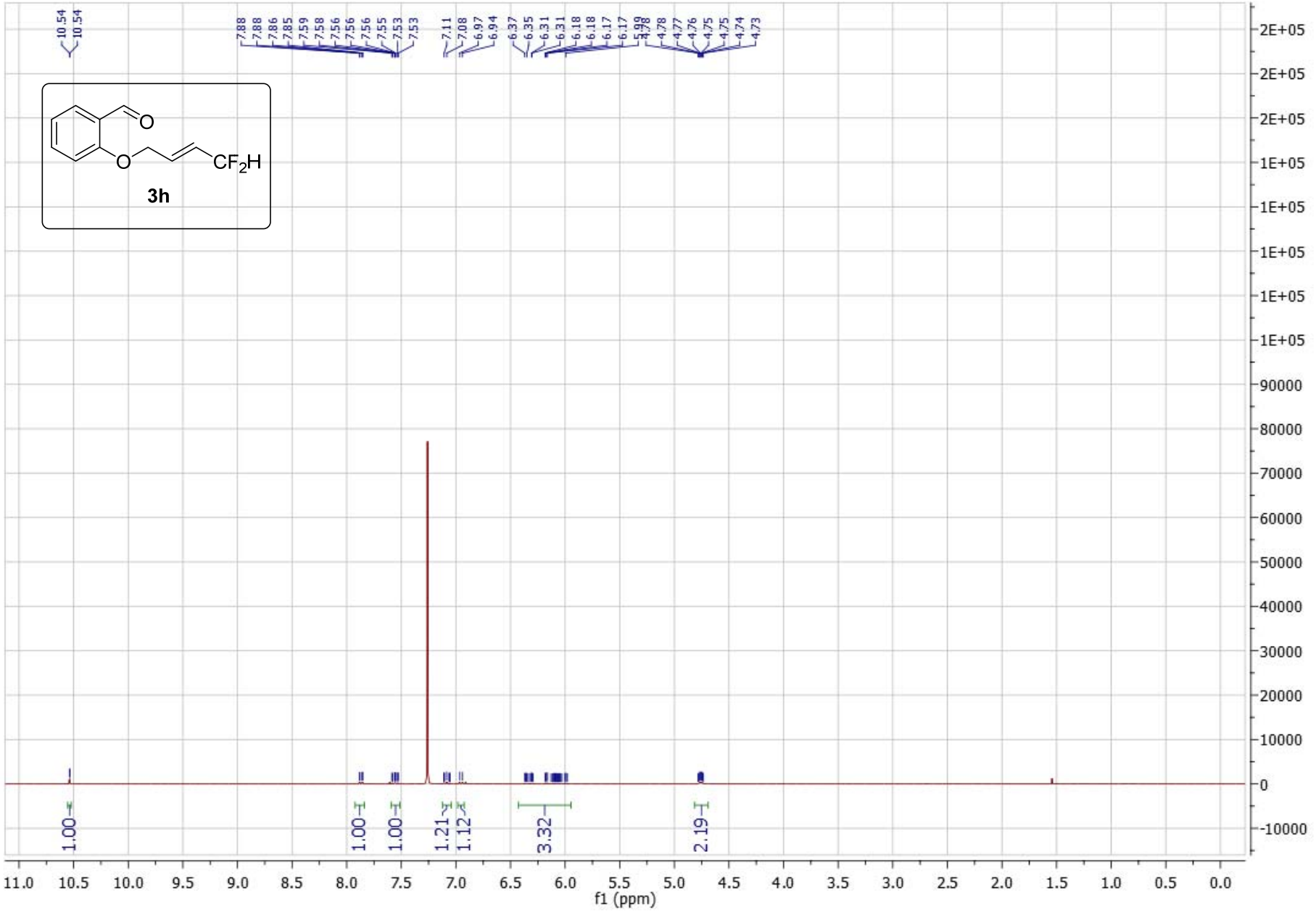
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7.08
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4.76
4.75
4.75
4.74
4.73
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2E+05
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70000
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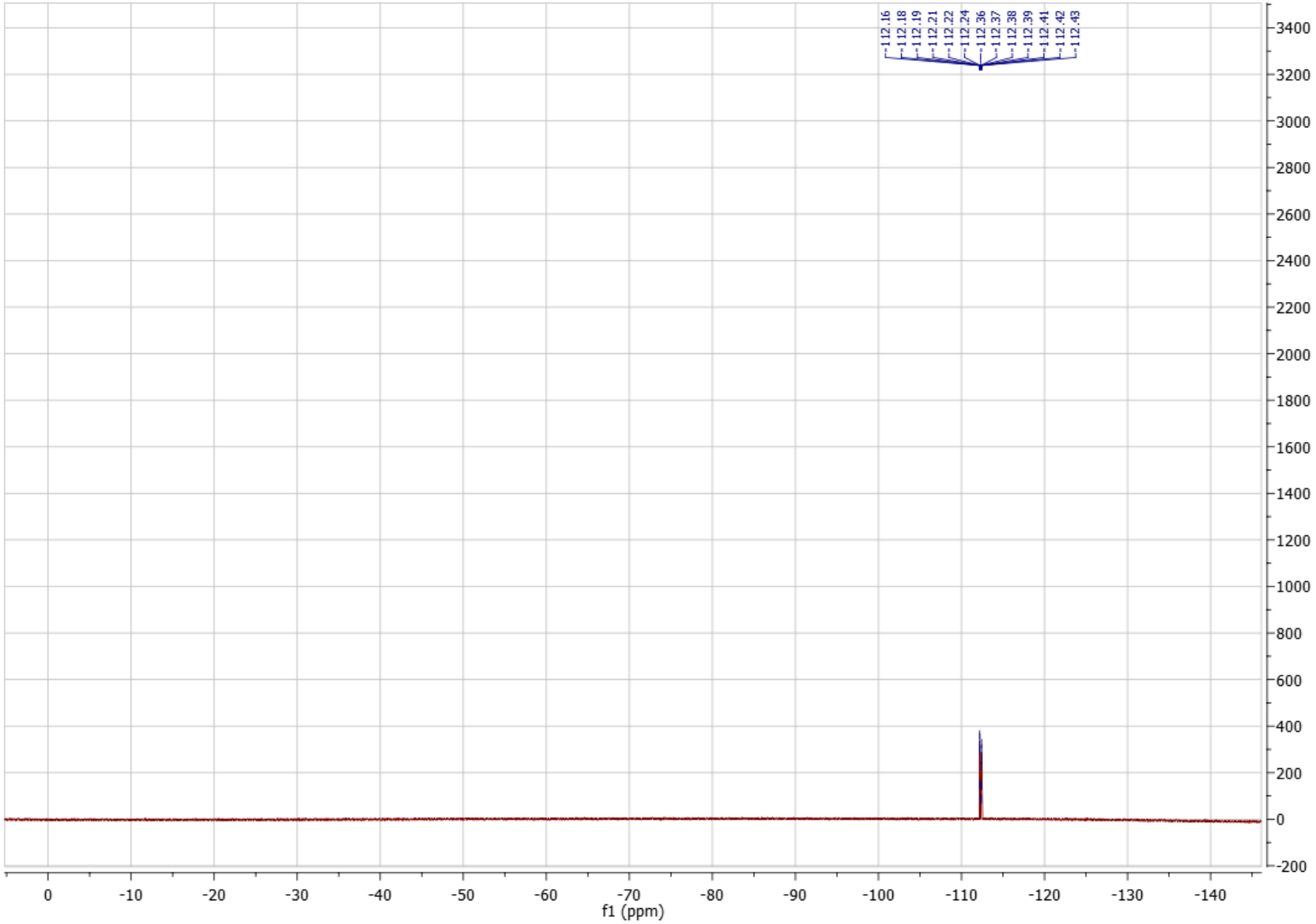
f1 (ppm)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3200
3000
2800
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2200
2000
1800
1600
1400
1200
1000
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600
400
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0
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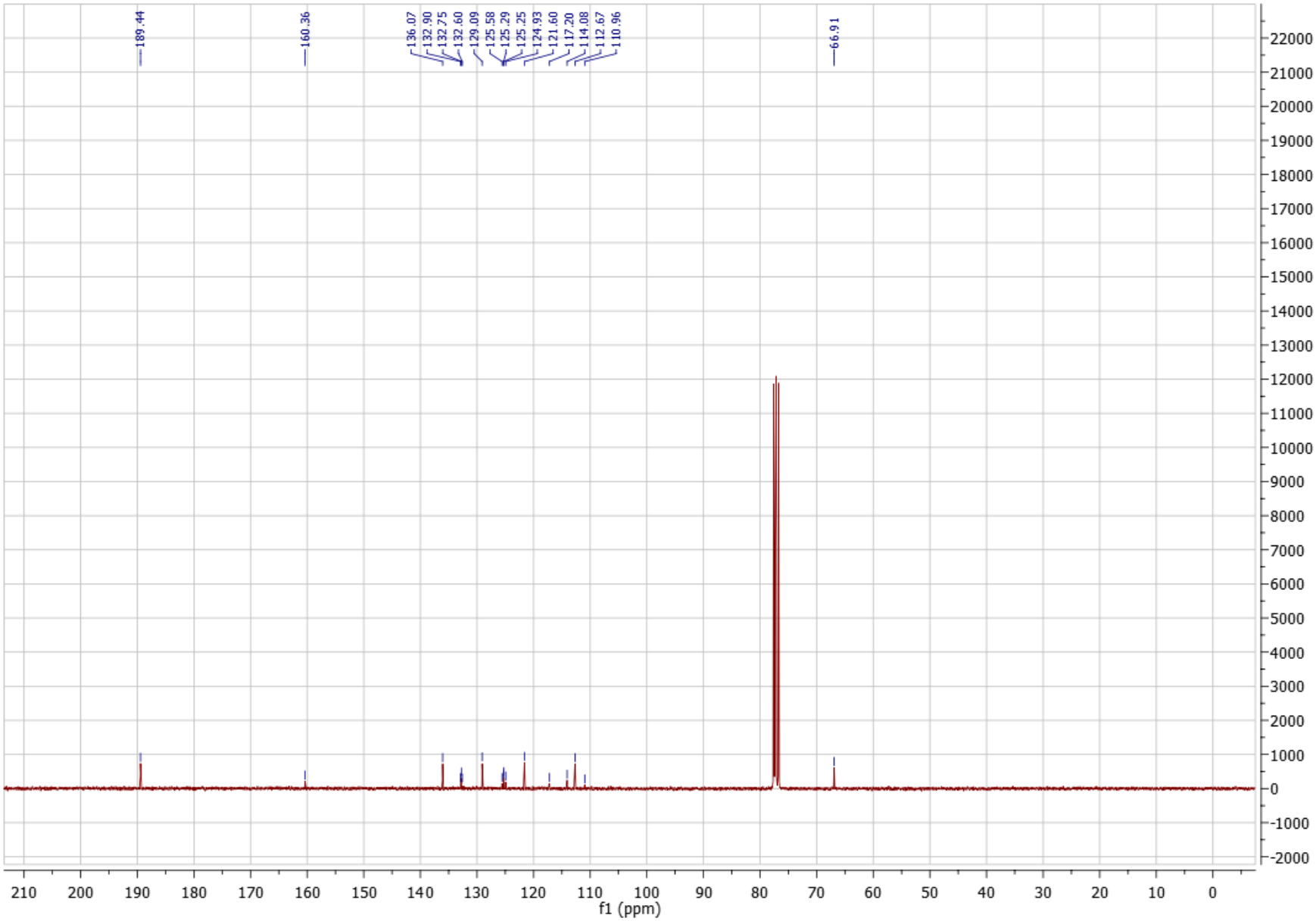
f1 (ppm)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117.20
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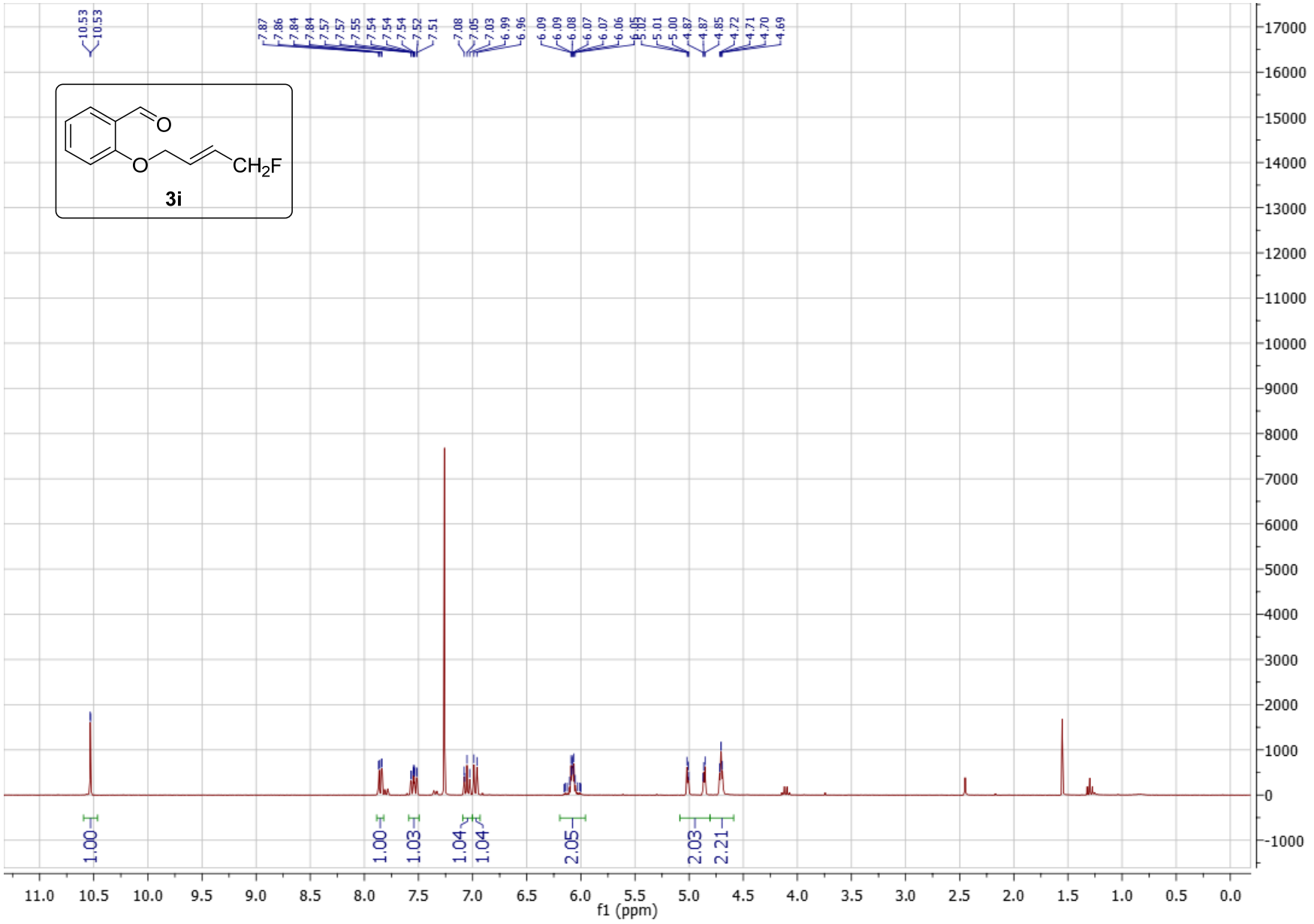
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4.72
4.71
4.70
4.69
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2.05
2.03
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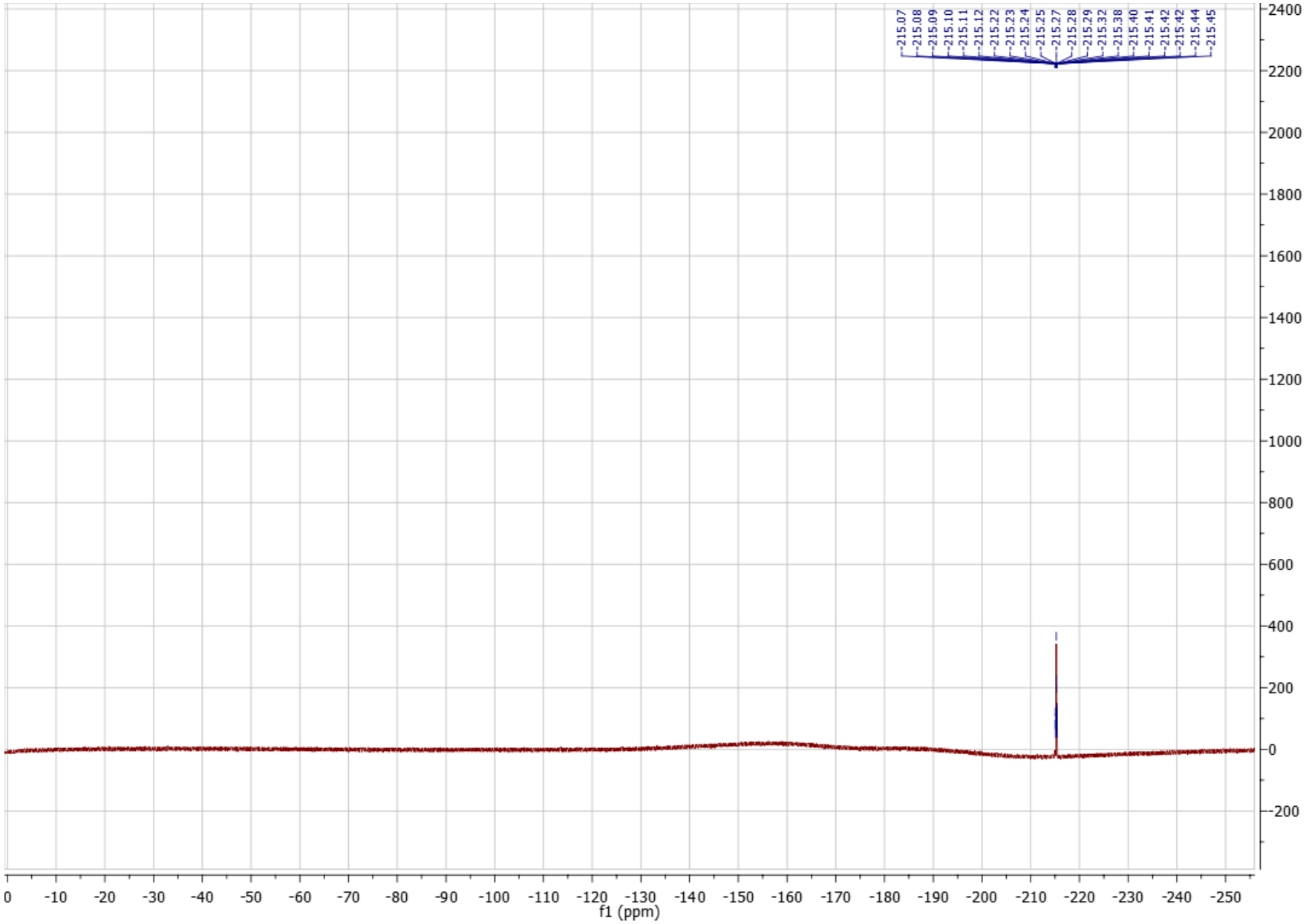
f1 (ppm)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215.32
215.38
215.40
215.41
215.42
215.42
215.44
215.45
2400
2200
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1800
1600
1400
1200
1000
800
600
400
200
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-200
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-10
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-100
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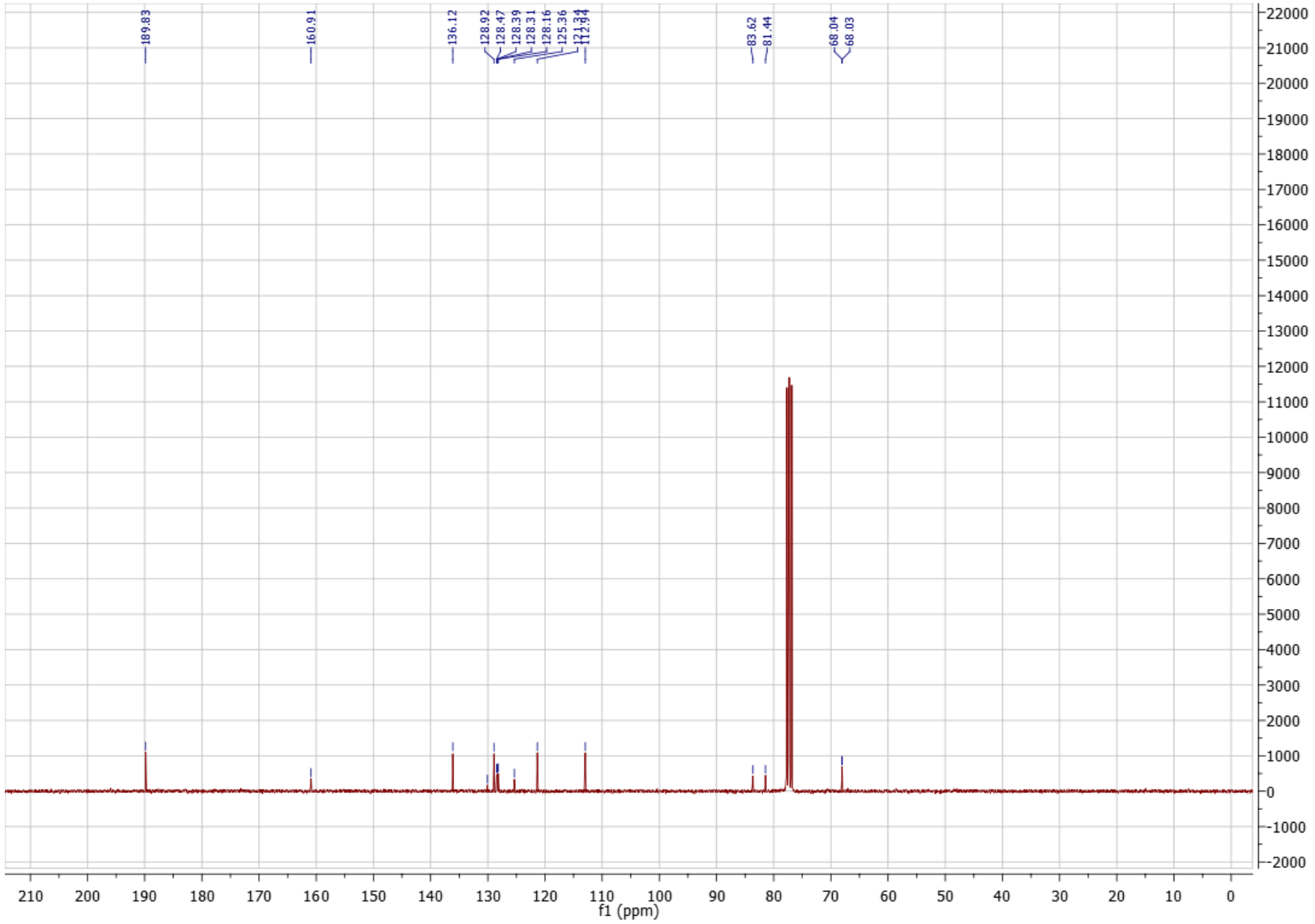
f1 (ppm)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112.94
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81.44
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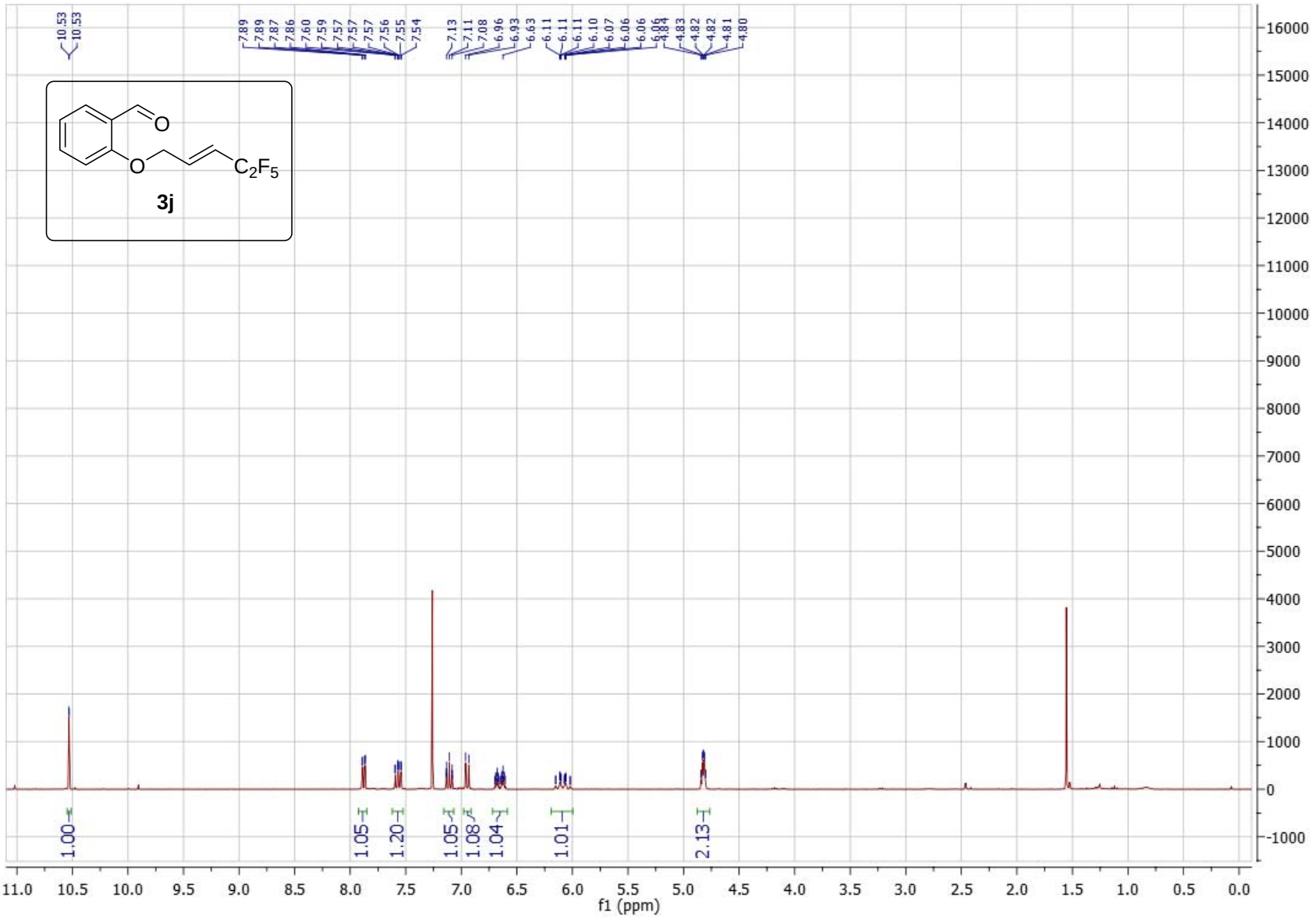
68.03
f1 (ppm)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7.55
7.54
7.13
7.11
7.08
6.96
6.93
6.63
6.11
6.11
6.11
6.10
6.07
6.06
6.06
4.84
4.83
4.82
4.82
4.81
4.80
O
O
C2F5
3j
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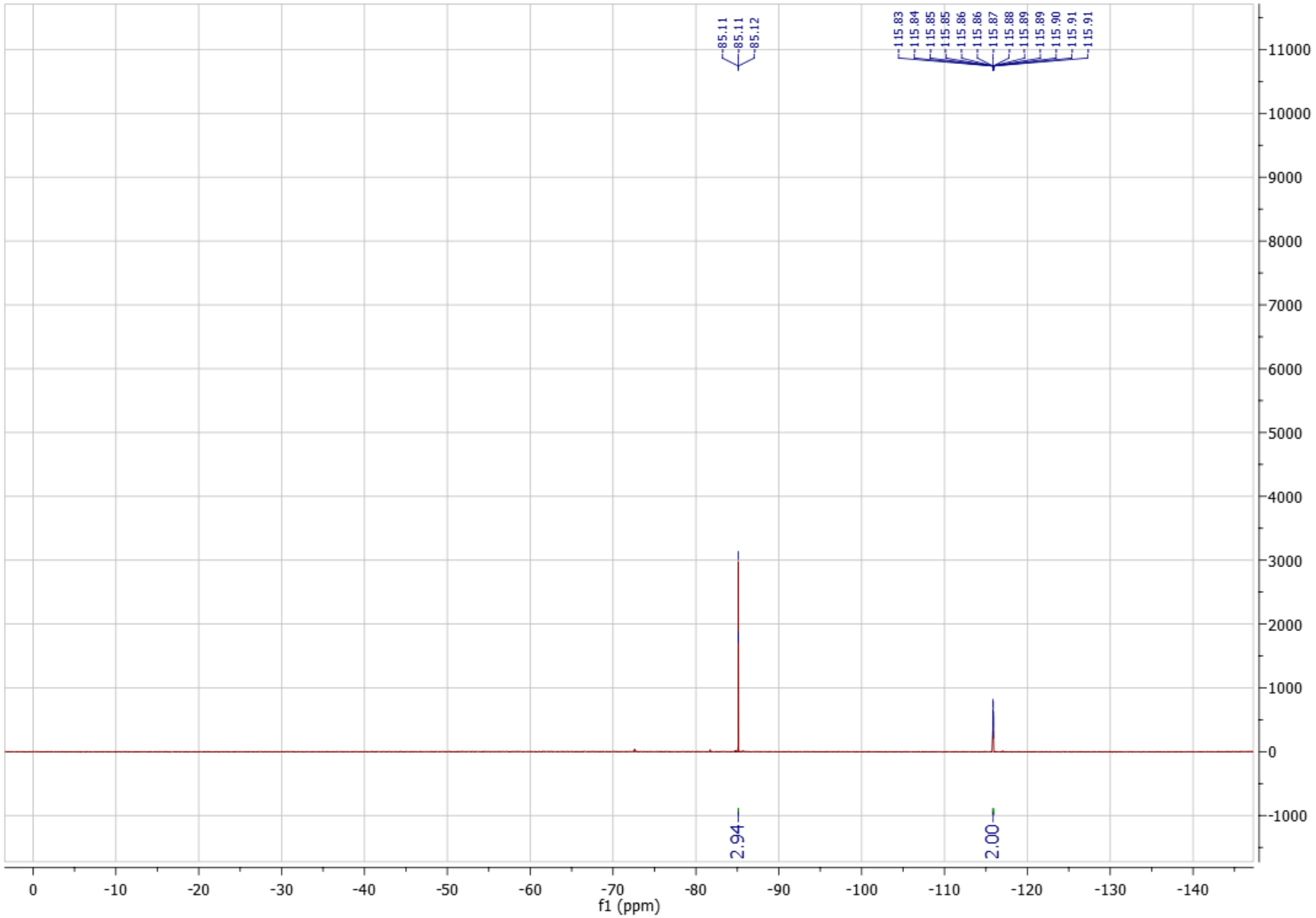
1.08
1.04
1.01
2.13
f1 (ppm)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115.86
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115.87
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115.89
115.89
115.90
115.91
115.91
11000
10000
9000
8000
7000
6000
5000
4000
3000
2000
1000
0
-1000
2.94
2.00
0
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-90
-100
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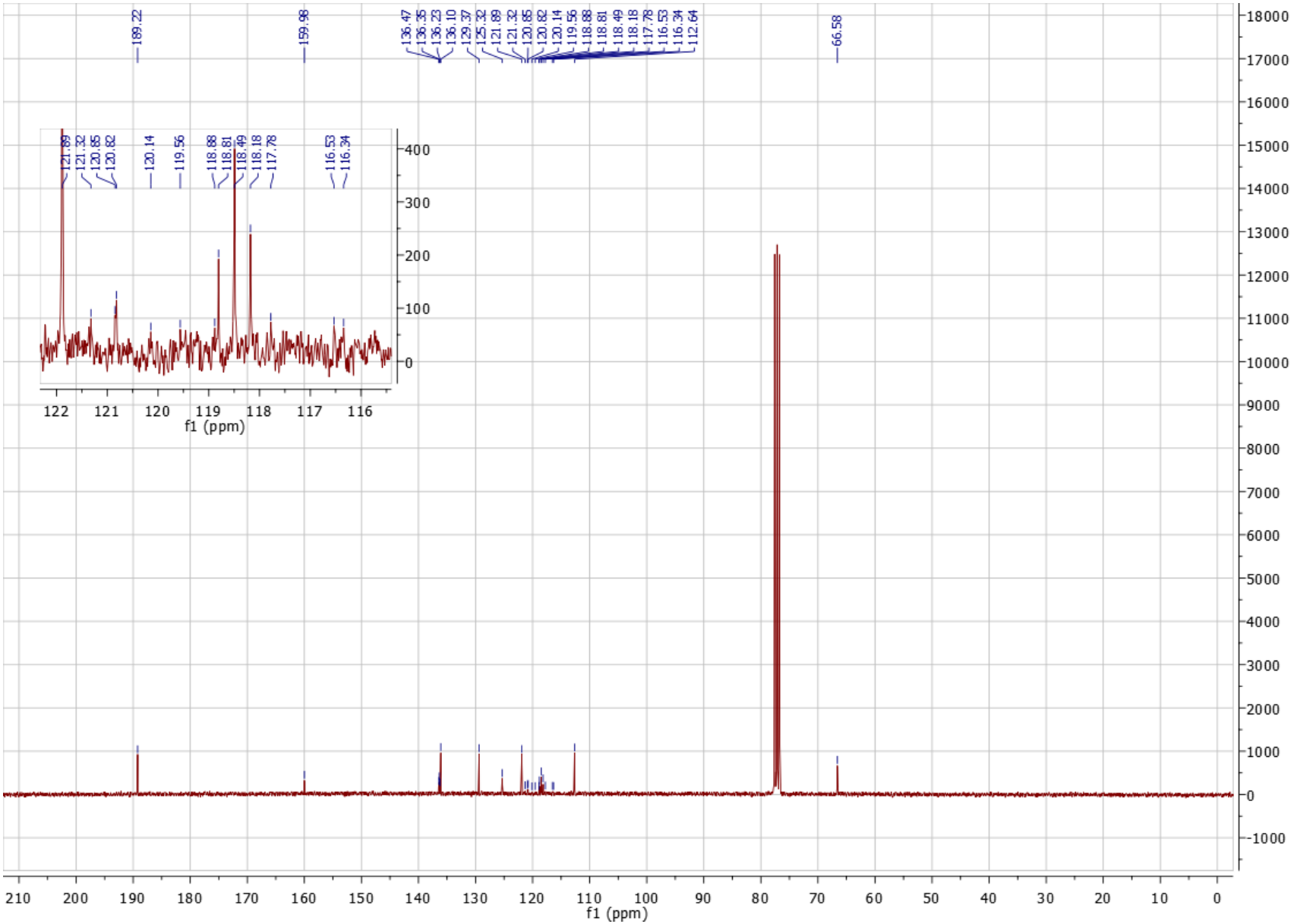
-130
-140
f1 (ppm)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121.32
120.85
120.82
120.14
119.56
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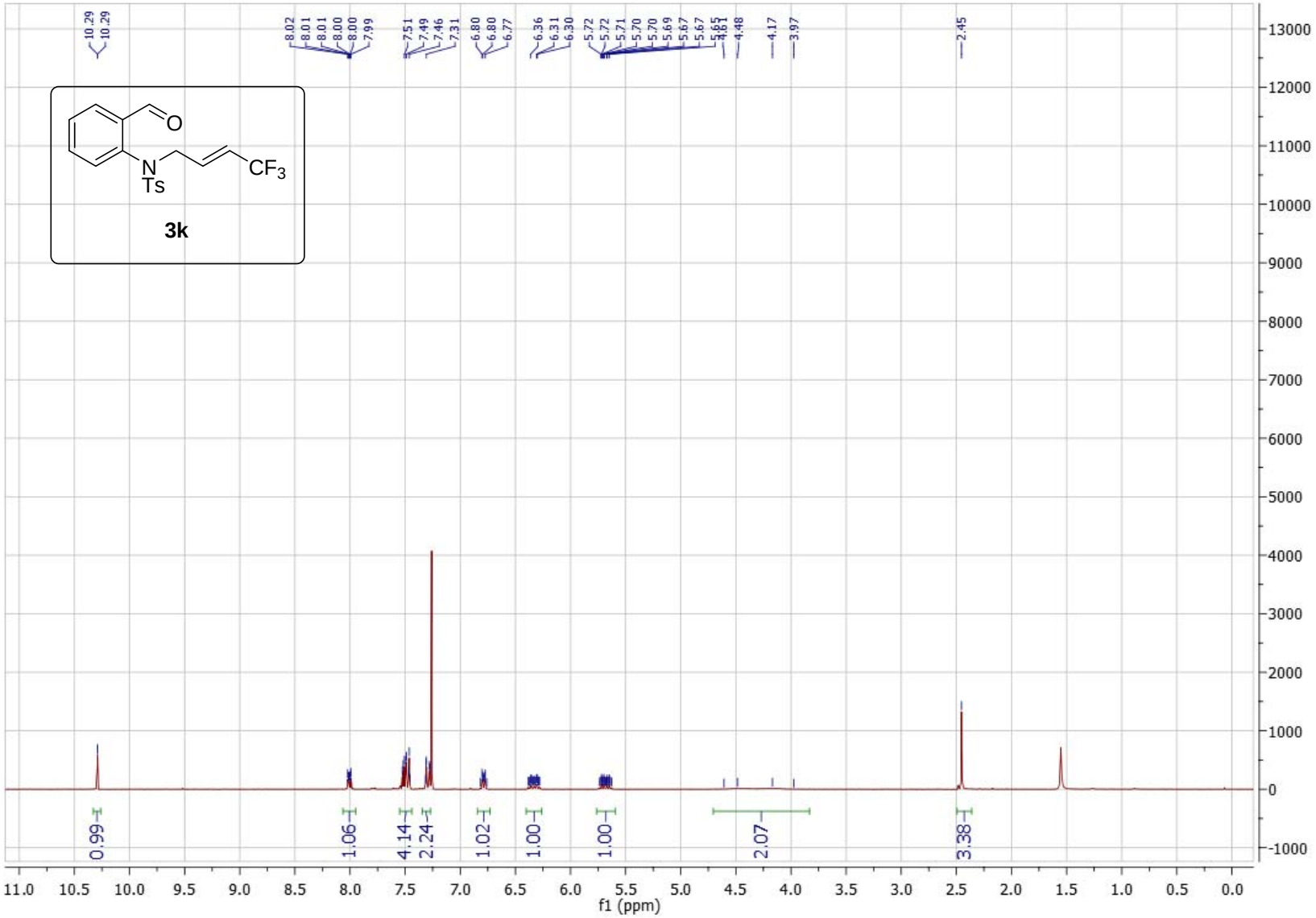
118.49
118.18
117.78
116.53
116.34
112.64
66.58
f1 (ppm)
f1 (ppm)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7.49
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6.80
6.77
6.36
6.31
6.30
5.72
5.72
5.71
5.70
5.70
5.69
5.67
5.67
5.65
4.61
4.48
4.17
3.97
2.45
O
N
Ts
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1.00
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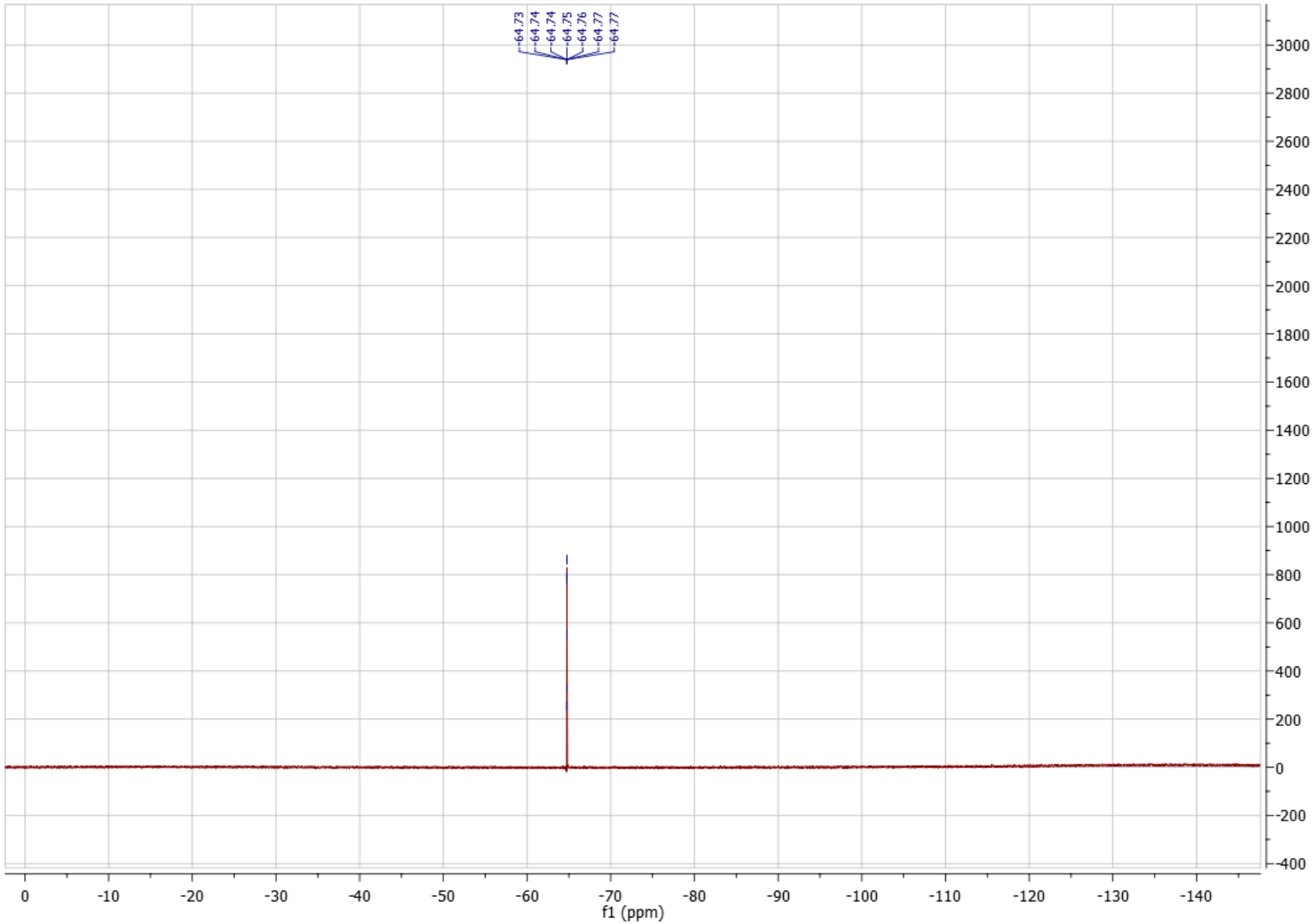
3.38
f1 (ppm)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-64.77
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2000
1800
1600
1400
1200
1000
800
600
400
200
0
-200
-400
0
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-90
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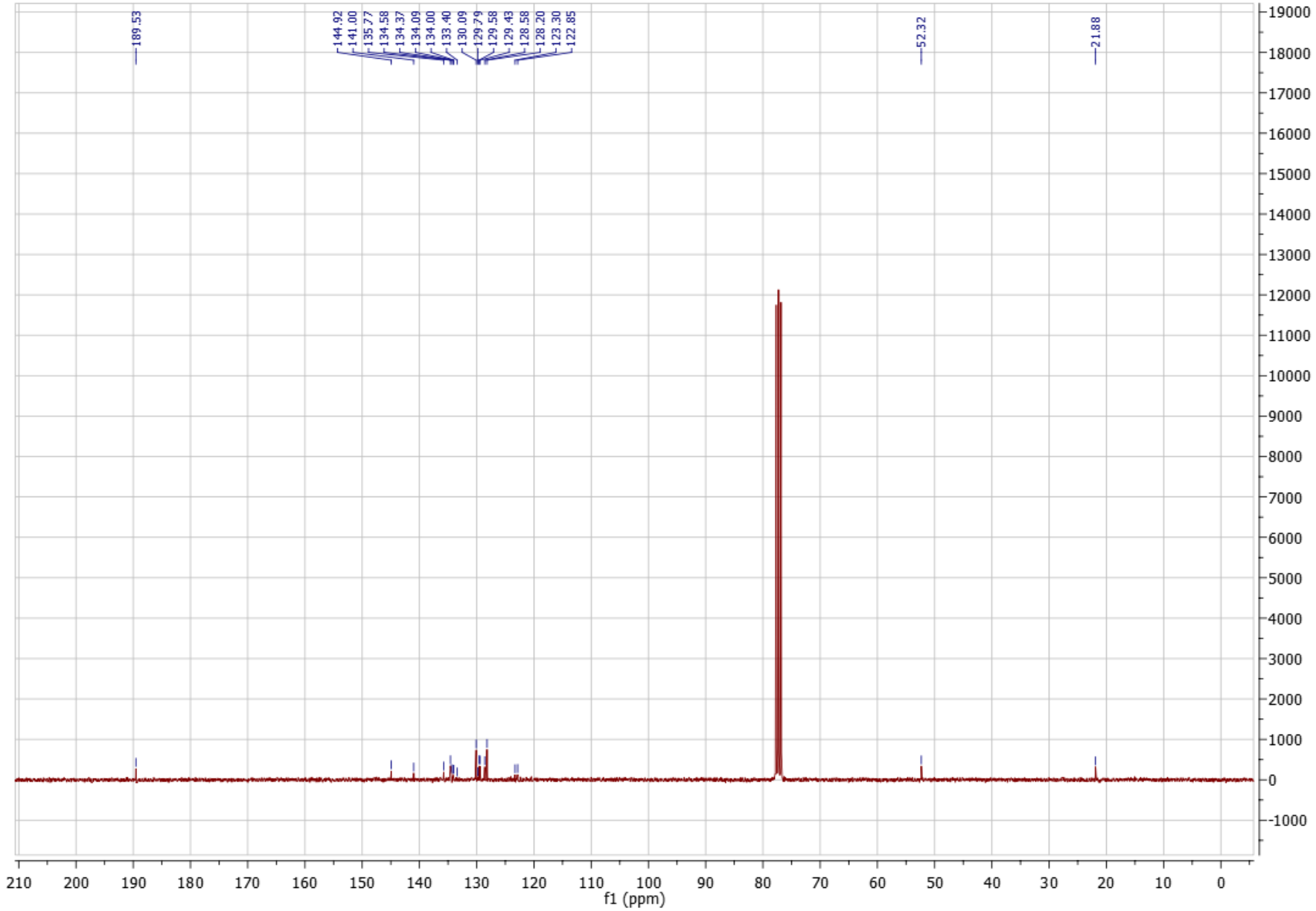
-110
-120
-130
-140
f1 (ppm)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134.58
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134.09
134.00
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130.09
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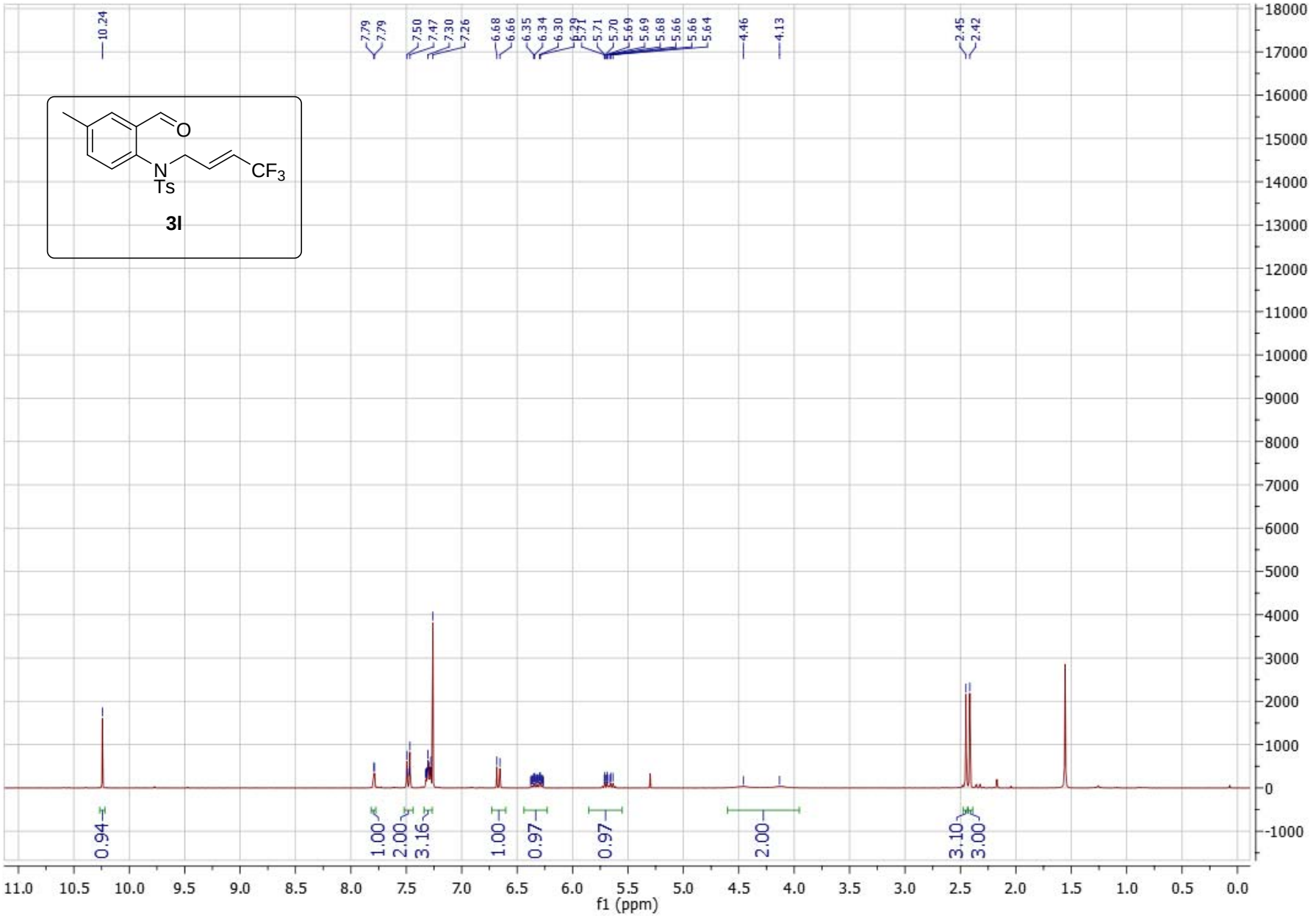
129.58
129.43
128.58
128.20
123.30
122.85
52.32
21.88
f1 (ppm)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6.66
6.35
6.34
6.30
6.29
5.71
5.70
5.69
5.69
5.68
5.66
5.66
5.64
4.46
4.13
2.45
2.42
O
N
Ts
CF3
3l
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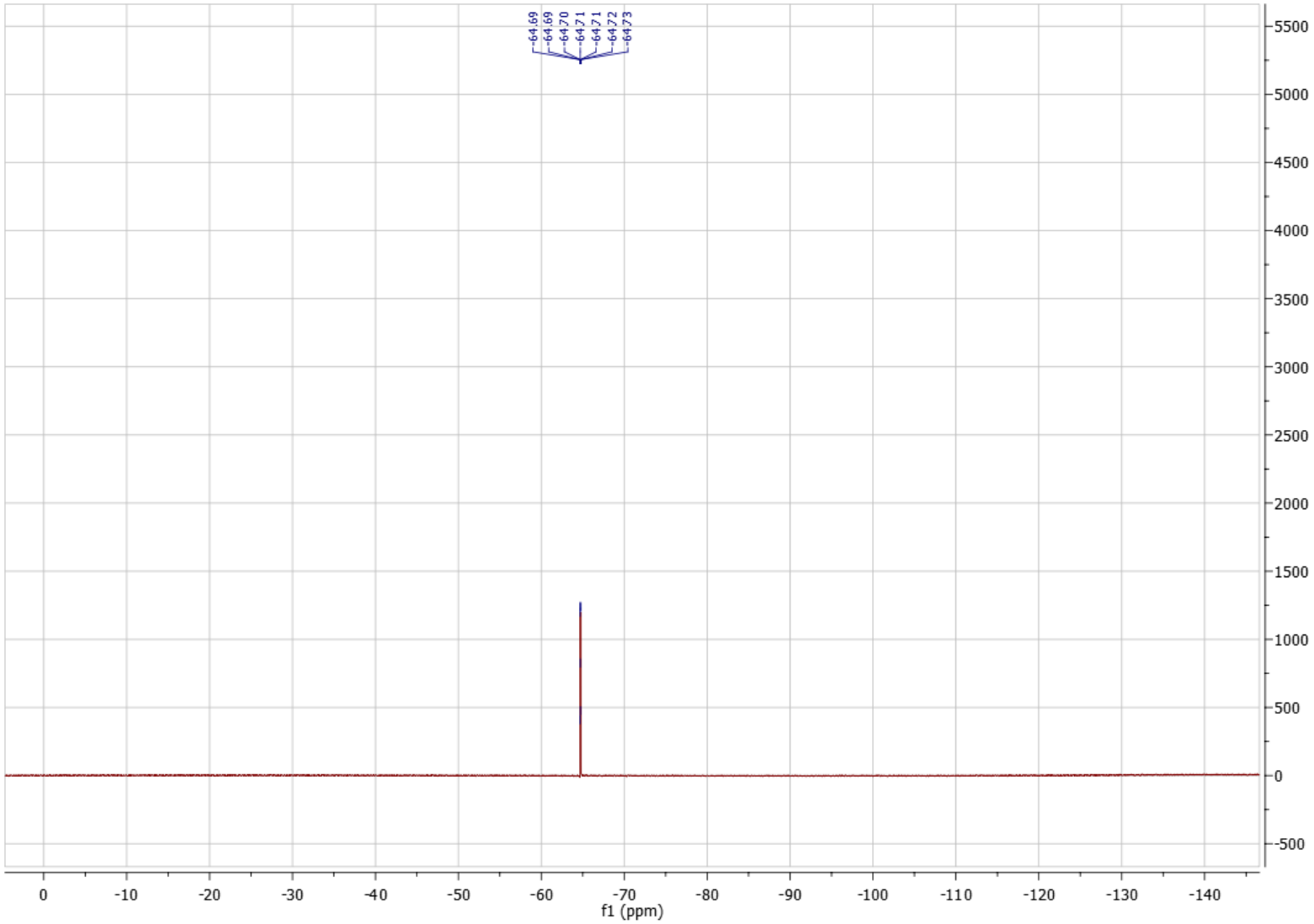
2.00
3.16
1.00
0.97
0.97
2.00
3.10
3.00
f1 (ppm)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-64.71
-64.71
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5000
4500
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3500
3000
2500
2000
1500
1000
500
0
-500
0
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-50
-60
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-80
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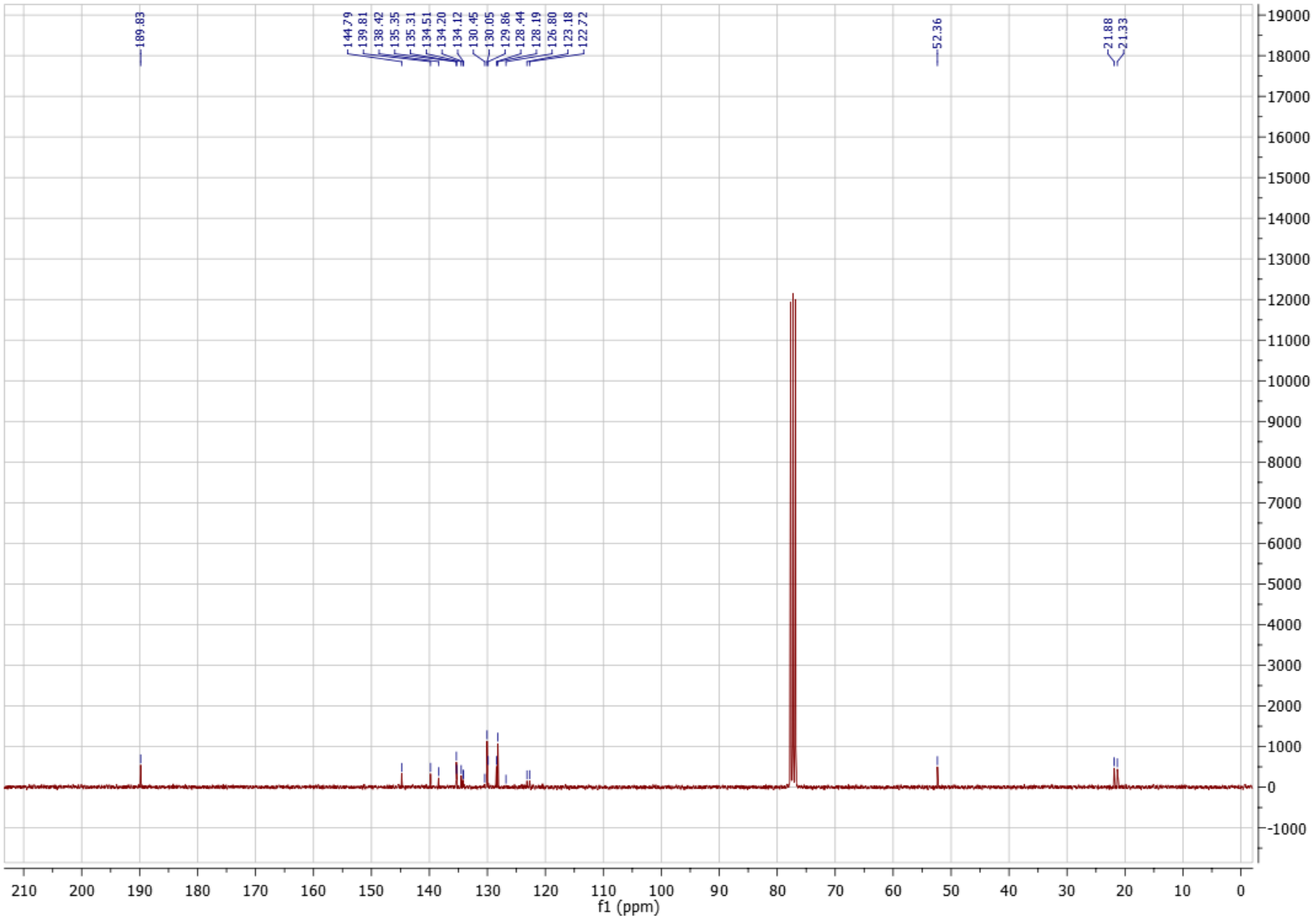
-100
-110
-120
-130
-140
f1 (ppm)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134.20
134.12
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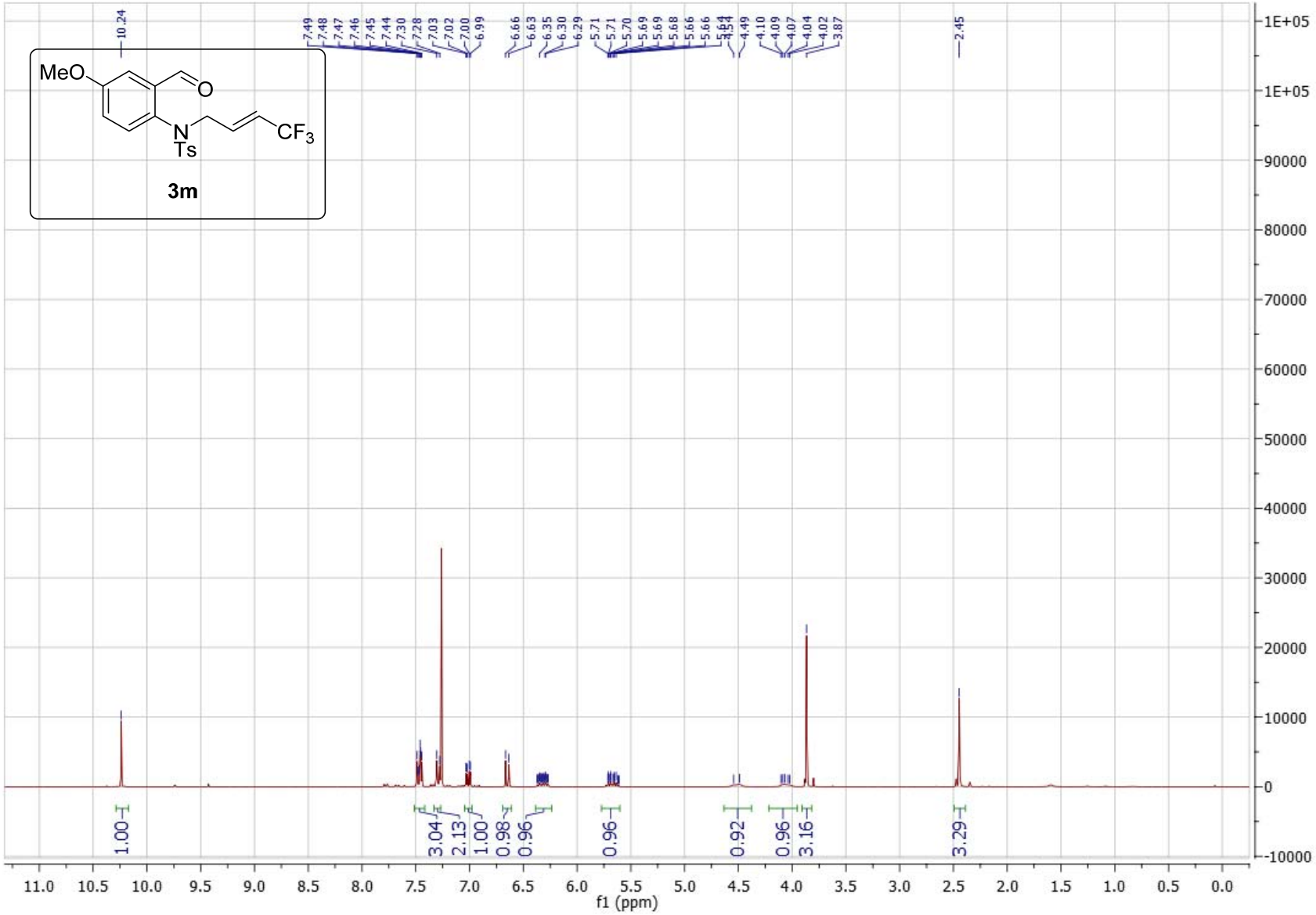
128.44
128.19
126.80
123.18
122.72
52.36
21.88
21.33
f1 (ppm)


MeO
O
N
Ts
CF3
3m
10.24
7.49
7.48
7.47
7.46
7.45
7.44
7.30
7.28
7.03
7.02
7.00
6.99
6.66
6.63
6.35
6.30
6.29
5.71
5.71
5.70
5.69
5.69
5.68
5.66
5.66
5.64
5.64
4.49
4.10
4.09
4.07
4.04
4.02
3.87
2.45
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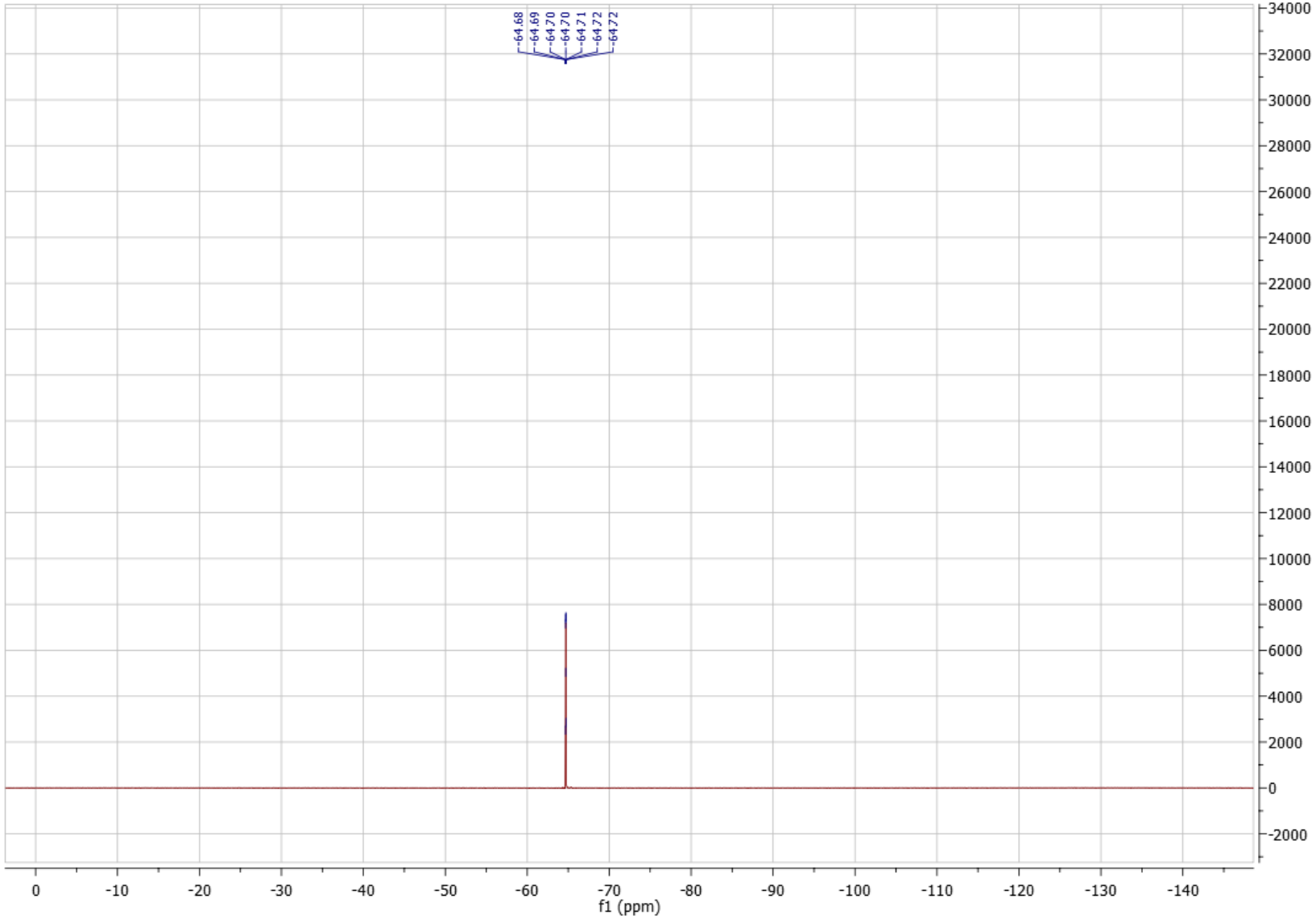
3.04
2.13
1.00
0.98
0.96
0.96
0.92
0.96
3.16
3.29
f1 (ppm)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-64.69
-64.70
-64.70
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-64.72
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32000
30000
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26000
24000
22000
20000
18000
16000
14000
12000
10000
8000
6000
4000
2000
0
-2000
0
-10
-20
-30
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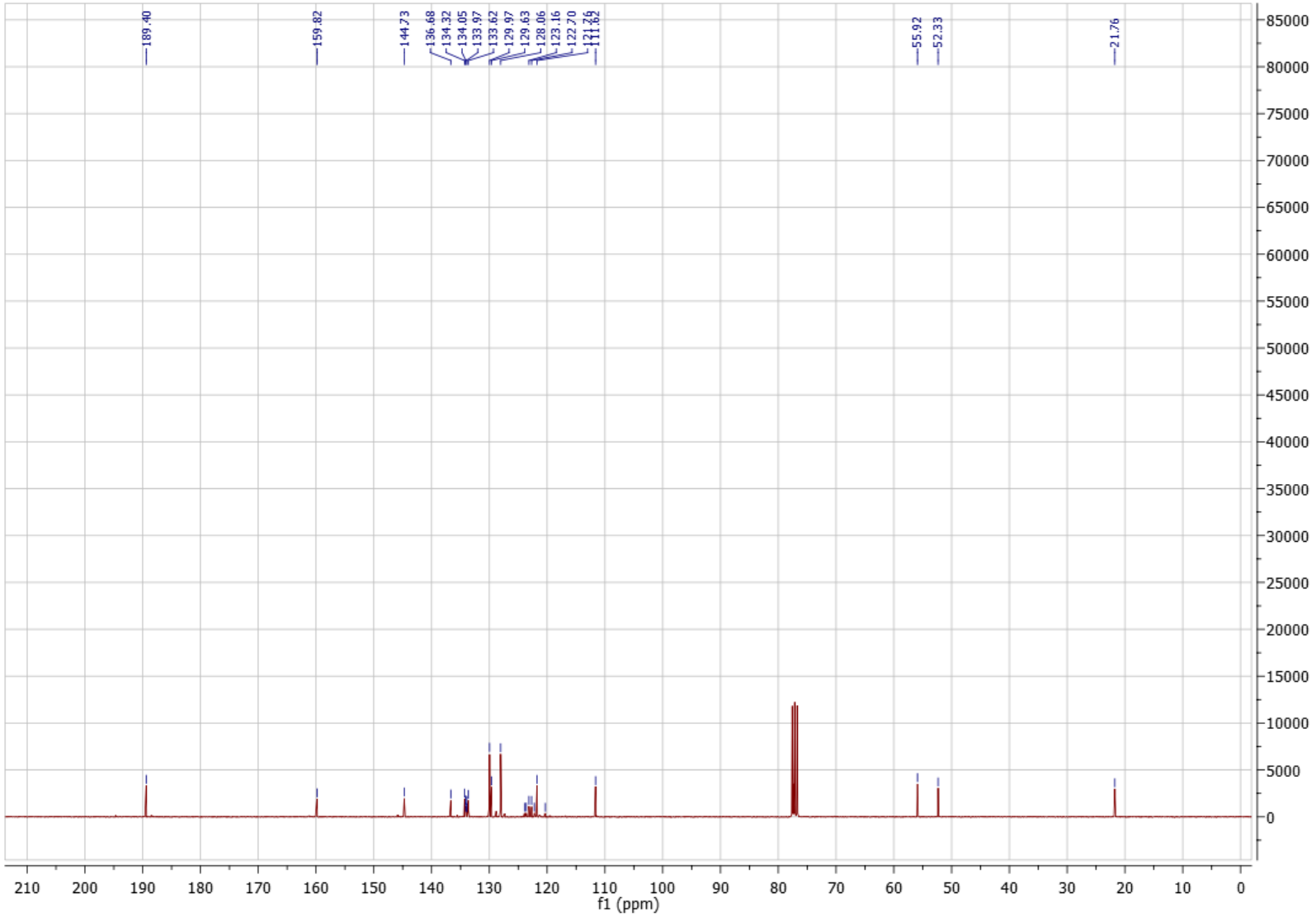
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
f1 (ppm)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133.62
129.97
129.63
128.06
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122.70
121.26
111.62
55.92
52.33
21.76
85000
80000
75000
70000
65000
60000
55000
50000
45000
40000
35000
30000
25000
20000
15000
10000
5000
0
210
200
190
180
170
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130
120
110
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90
80
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50
40
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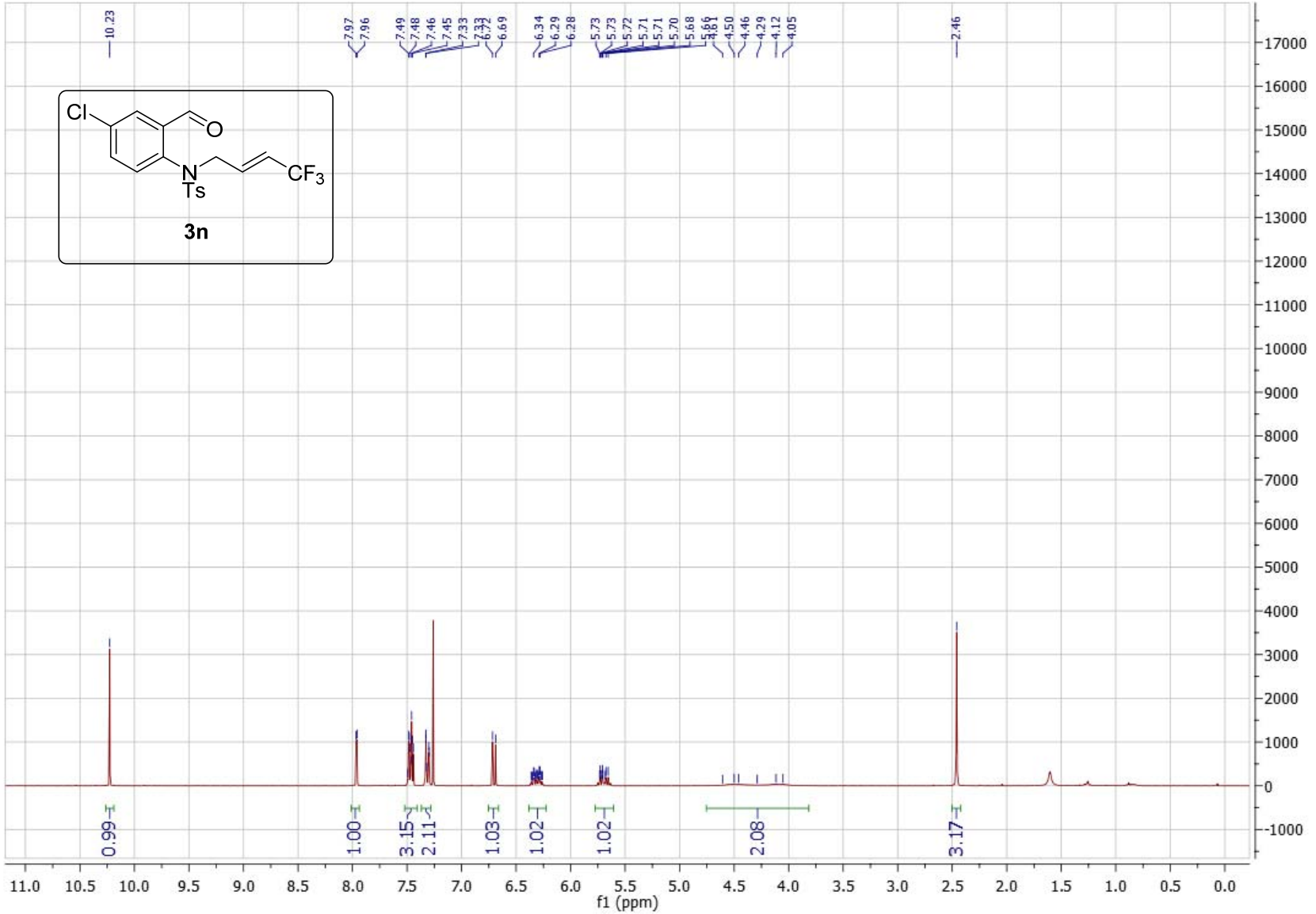
20
10
0
f1 (ppm)


Cl
O
N
Ts
CF3
3n
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7.46
7.45
7.33
7.32
6.69
6.34
6.29
6.28
5.73
5.73
5.72
5.71
5.71
5.70
5.68
4.61
4.50
4.46
4.29
4.12
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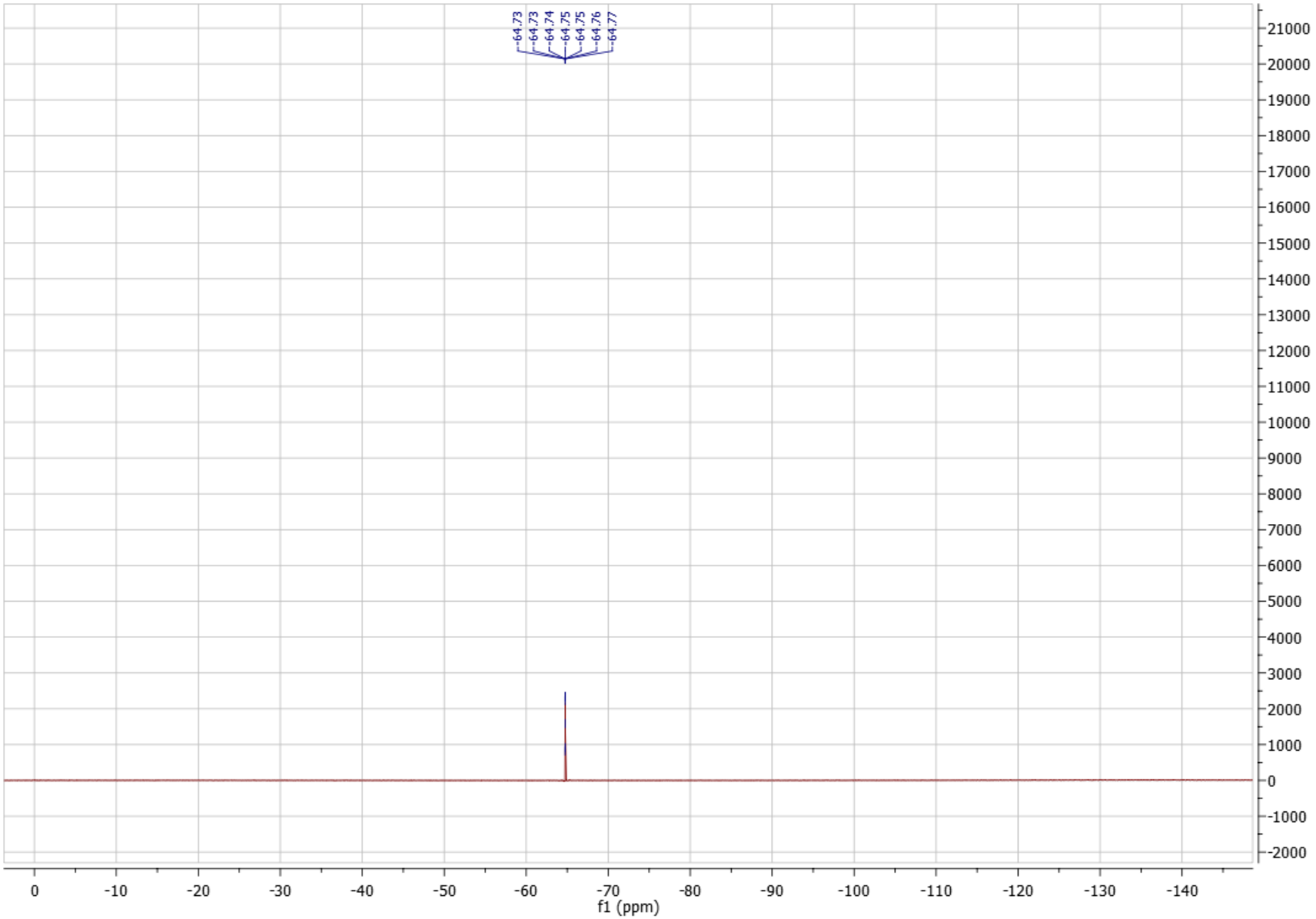
1.03
1.02
1.02
2.08
3.17
f1 (ppm)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-64.77
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20000
19000
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16000
15000
14000
13000
12000
11000
10000
9000
8000
7000
6000
5000
4000
3000
2000
1000
0
-1000
-2000
0
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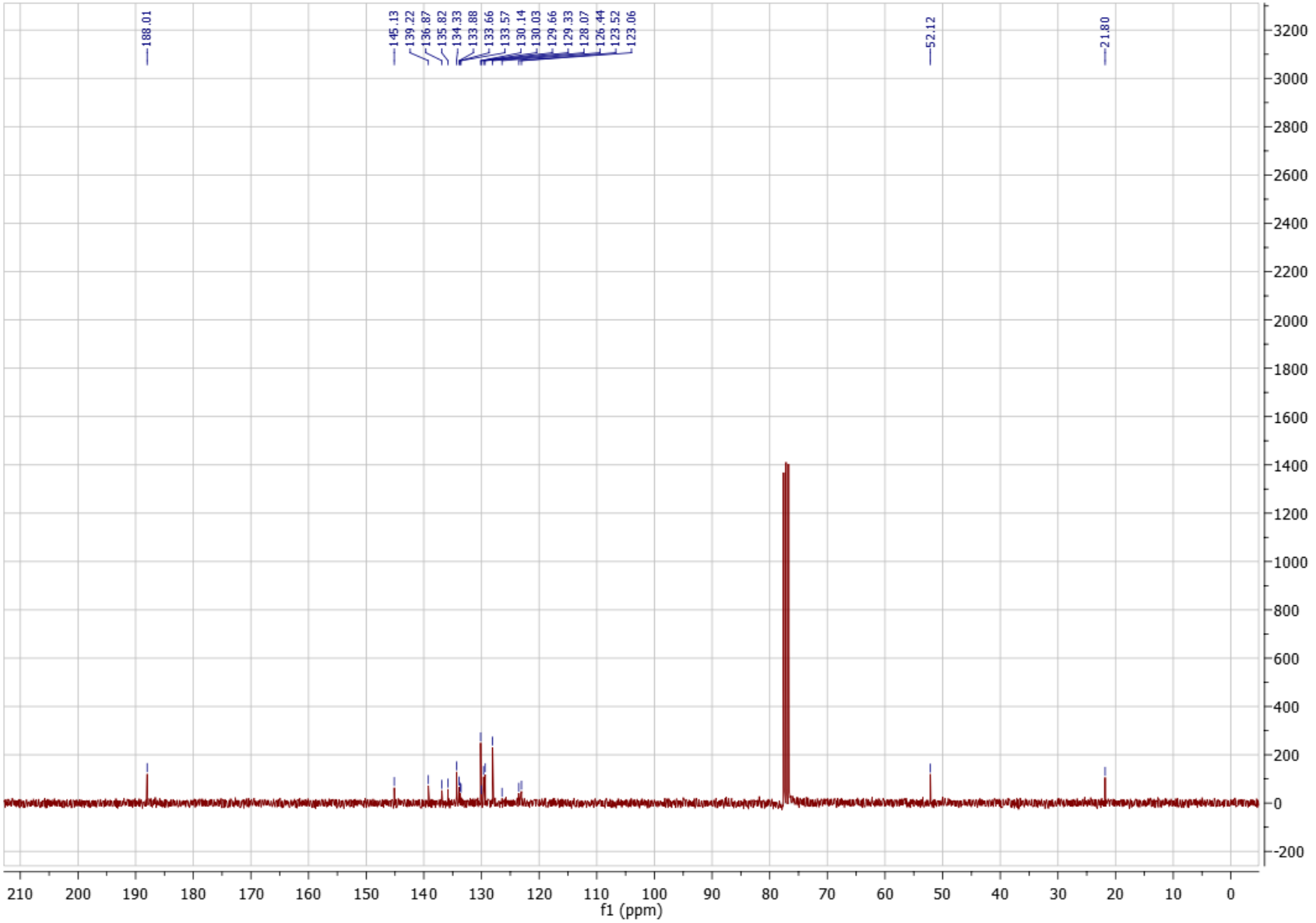
-60
-70
-80
-90
-100
-110
-120
-130
-140
f1 (ppm)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123.06
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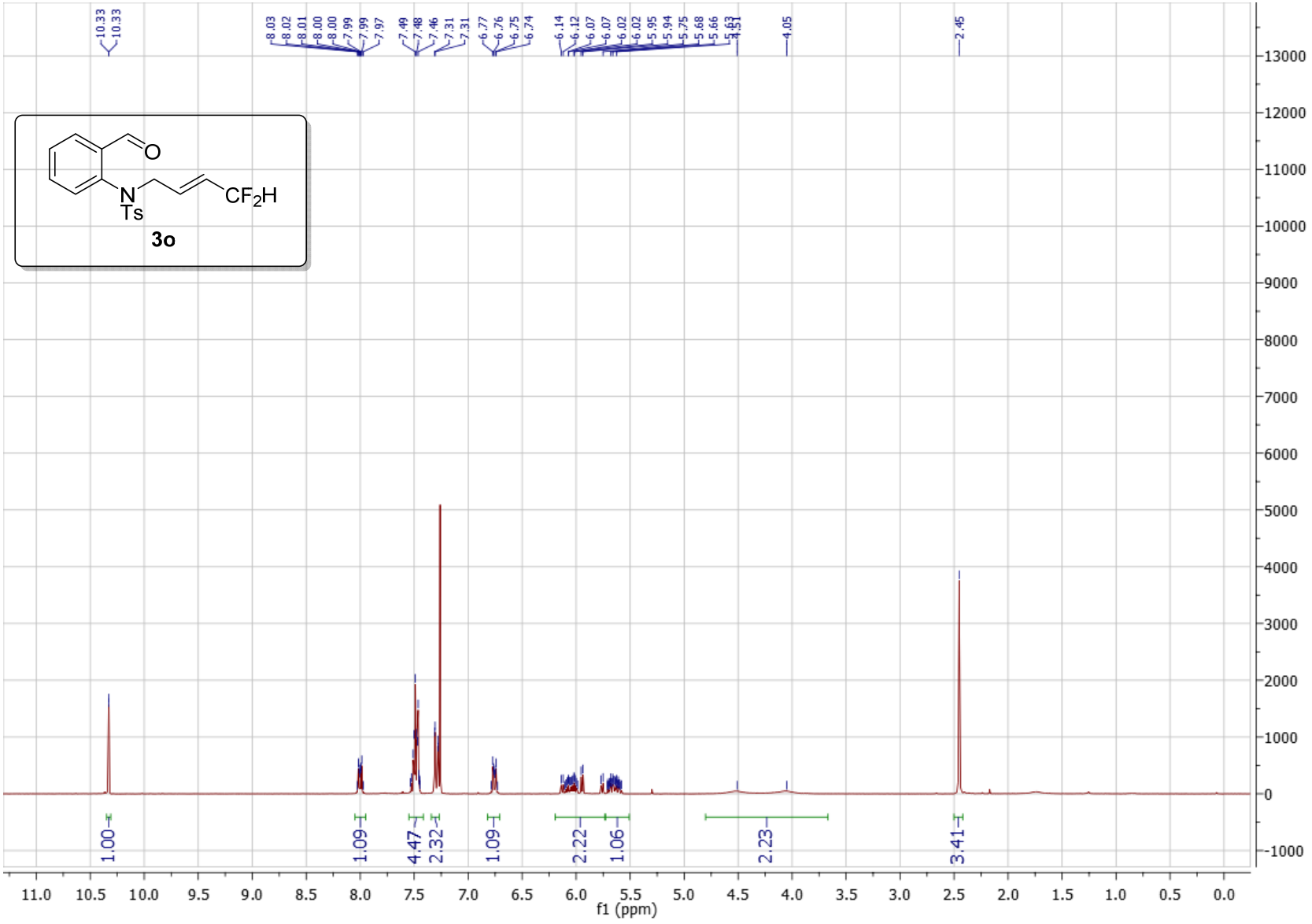
21.80
f1 (ppm)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8.01
8.00
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7.99
7.99
7.97
7.49
7.48
7.46
7.31
7.31
6.77
6.76
6.75
6.74
6.14
6.12
6.07
6.07
6.02
6.02
5.95
5.94
5.75
5.68
5.66
5.63
5.51
4.05
2.45
O
N
Ts
CF2H
3o
13000
12000
11000
10000
9000
8000
7000
6000
5000
4000
3000
2000
1000
0
-1000
1.00
1.09
4.47
2.32
1.09
2.22
1.06
2.23
3.41
11.0
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
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3.0
2.5
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1.5
1.0
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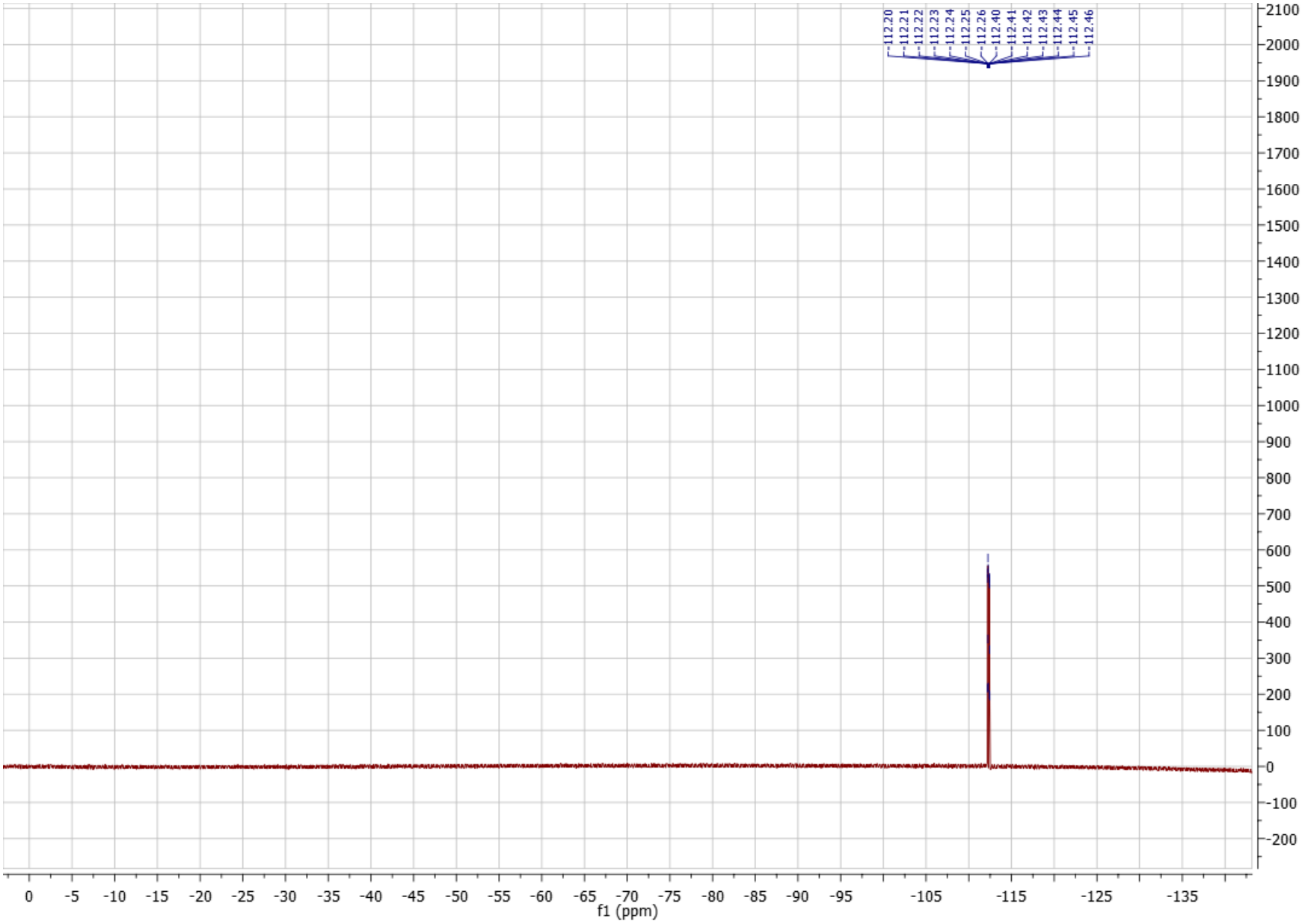
0.0
f1 (ppm)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112.41
112.42
112.43
112.44
112.45
112.46
2100
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1900
1800
1700
1600
1500
1400
1300
1200
1100
1000
900
800
700
600
500
400
300
200
100
0
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0
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-45
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-105
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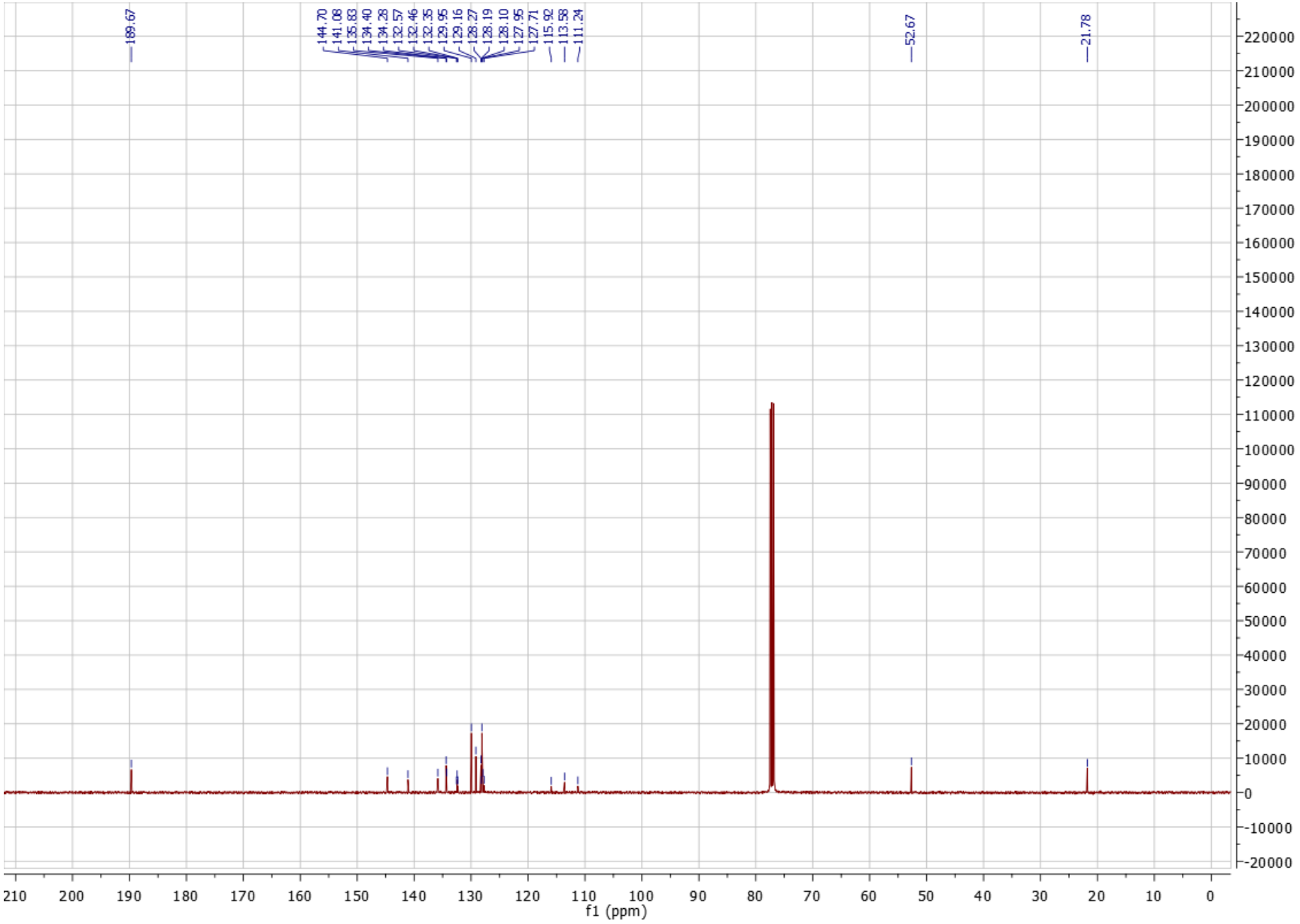
-125
-135
f1 (ppm)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132.35
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128.19
128.10
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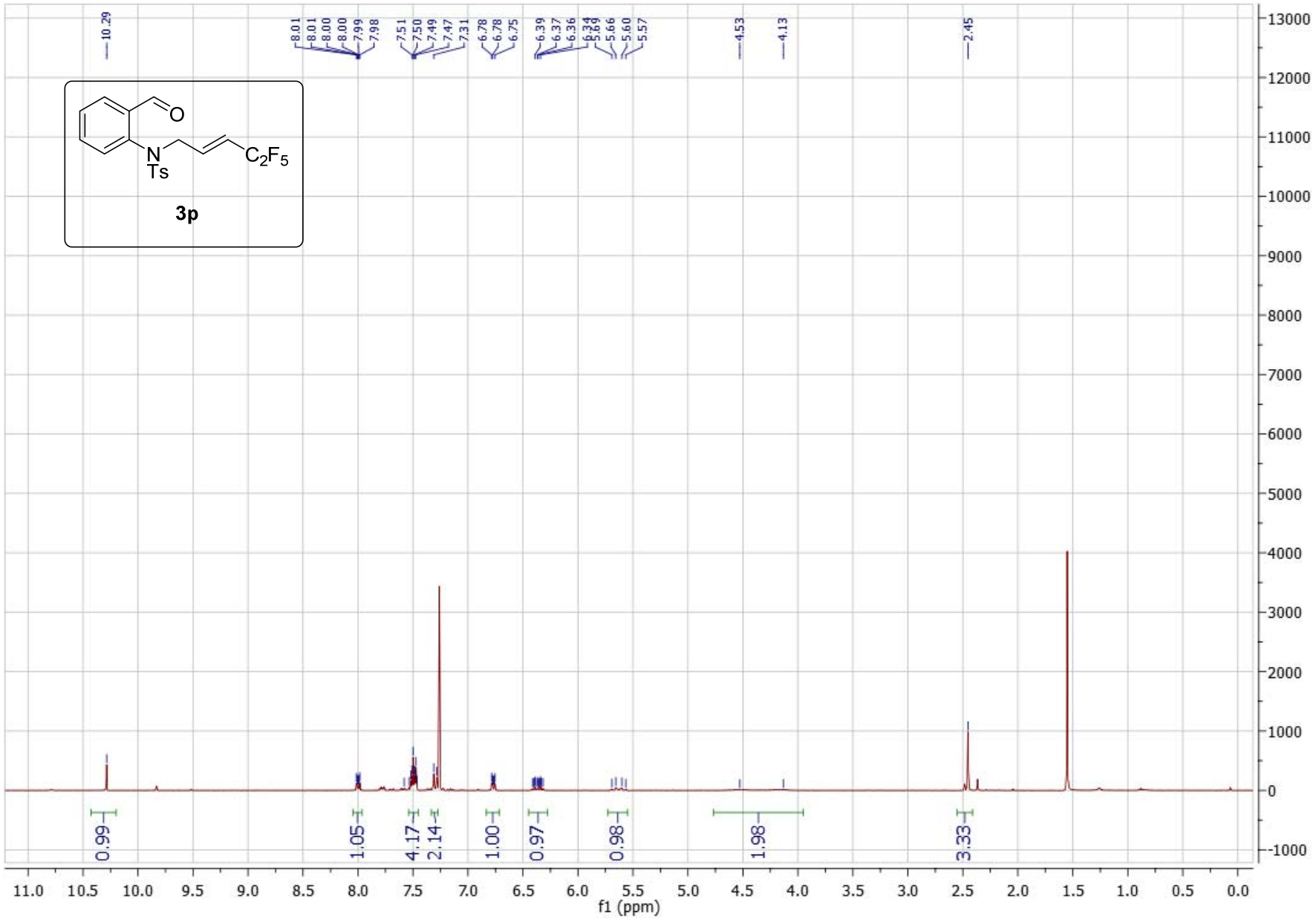
127.71
115.92
113.58
111.24
52.67
21.78
f1 (ppm)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7.51
7.50
7.49
7.47
7.31
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6.78
6.75
6.39
6.37
6.36
6.34
5.69
5.66
5.60
5.57
4.53
4.13
2.45
O
N
Ts
C2F5
3p
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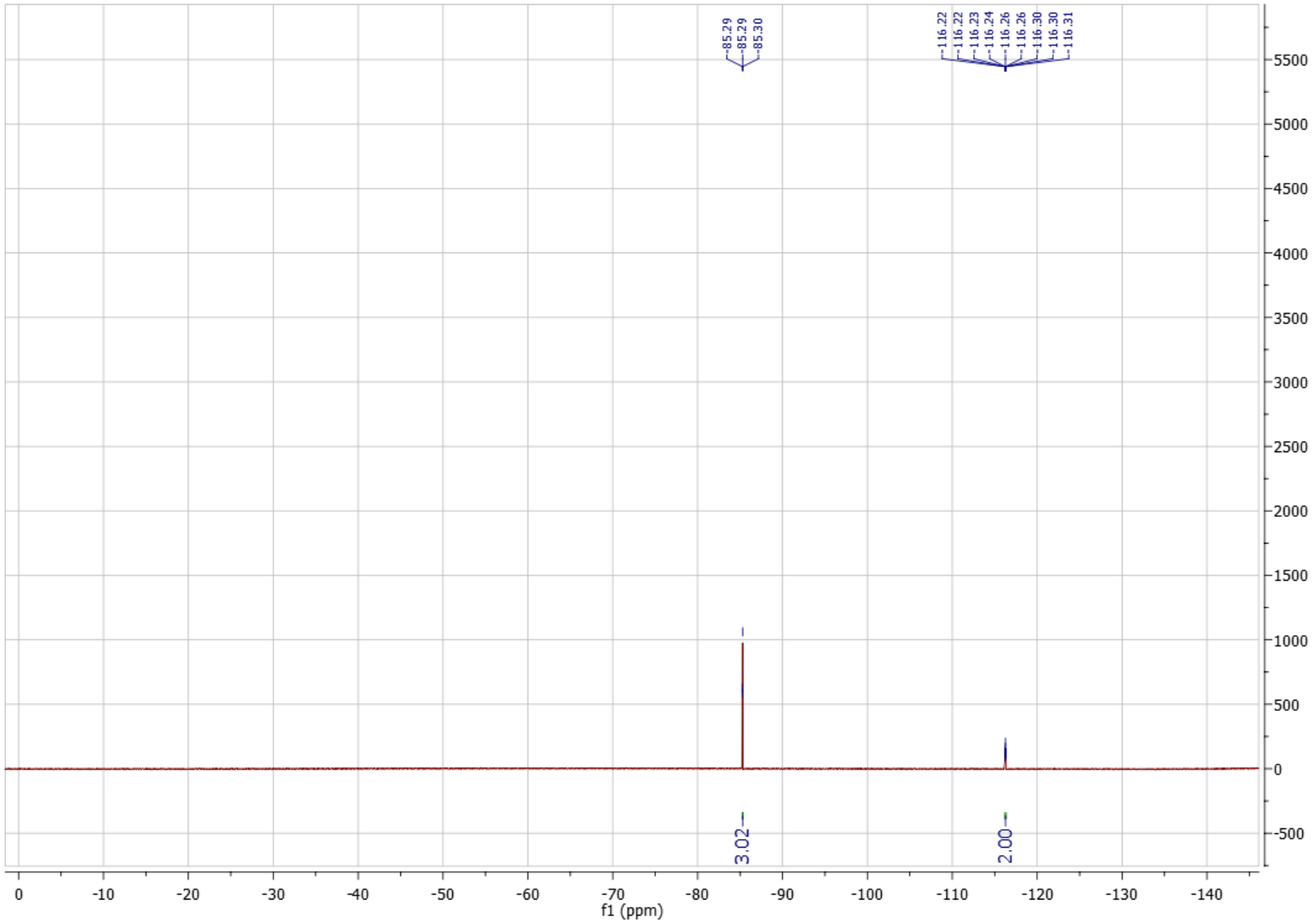
4.17
2.14
1.00
0.97
0.98
1.98
3.33
f1 (ppm)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-116.24
-116.26
-116.26
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-116.30
-116.31
5500
5000
4500
4000
3500
3000
2500
2000
1500
1000
500
0
-500
3.02
2.00
0
-10
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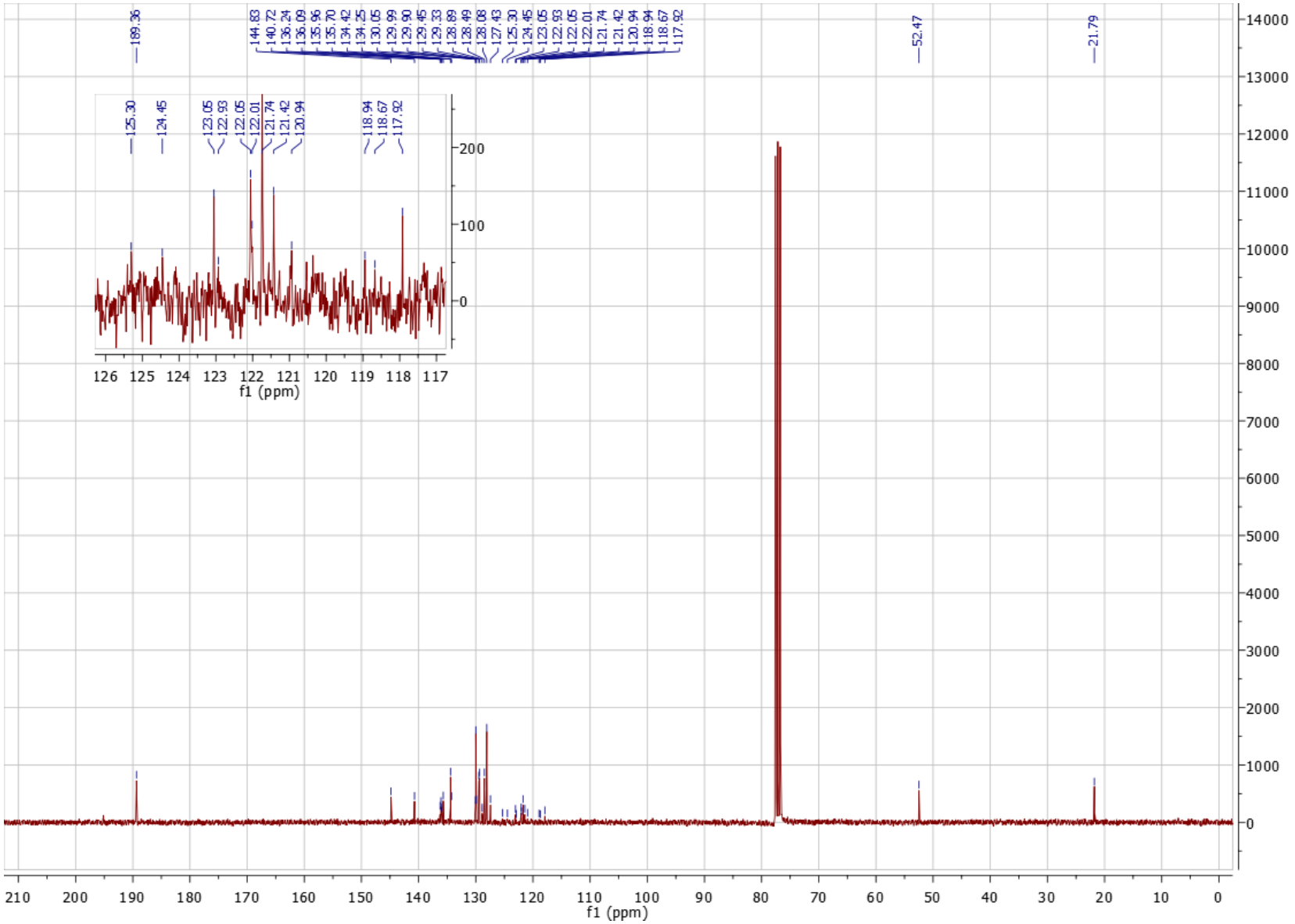
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
f1 (ppm)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130.05
129.99
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129.45
129.33
128.89
128.49
128.08
127.43
125.30
124.45
123.05
122.93
122.05
122.01
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121.42
120.94
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118.67
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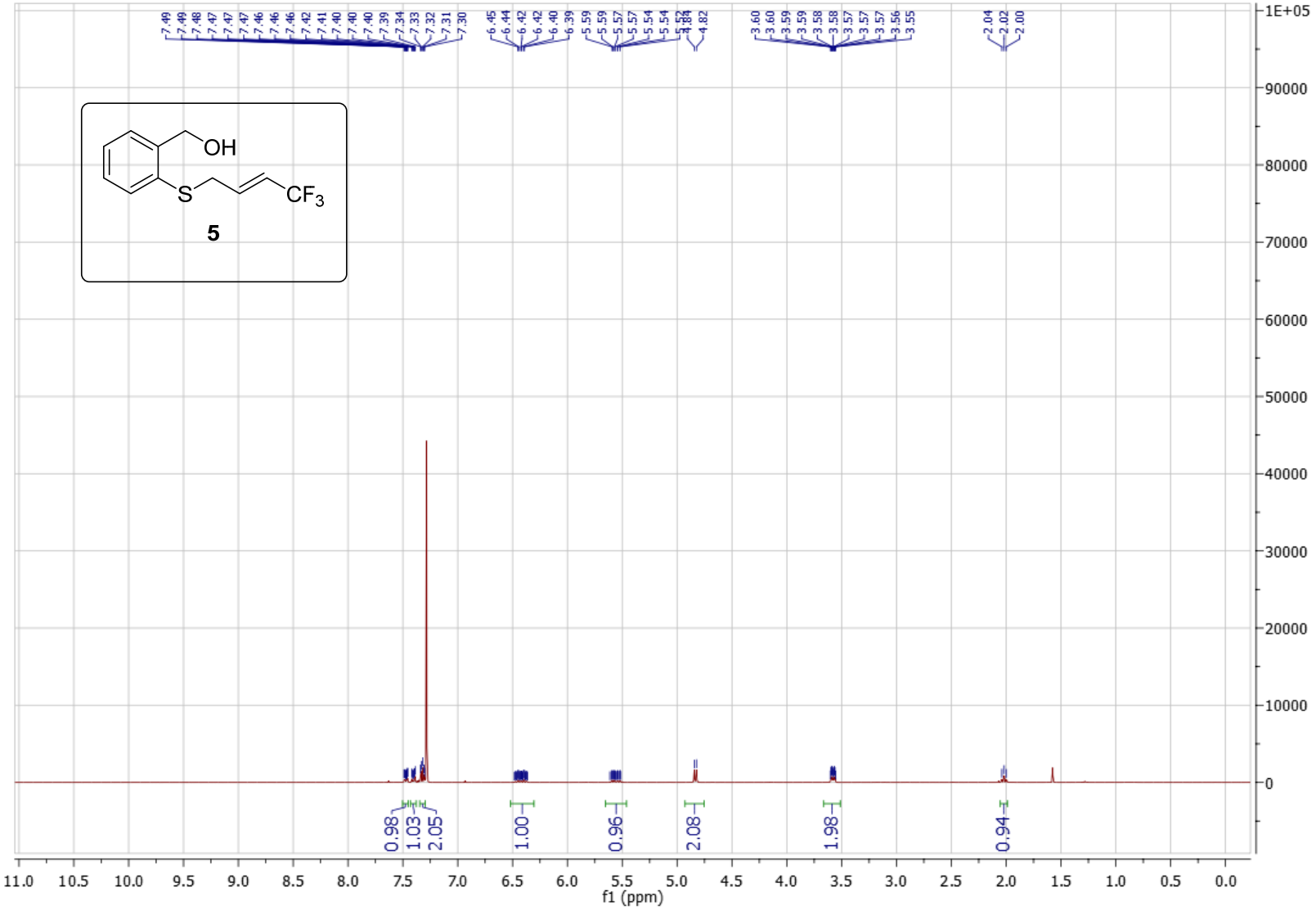
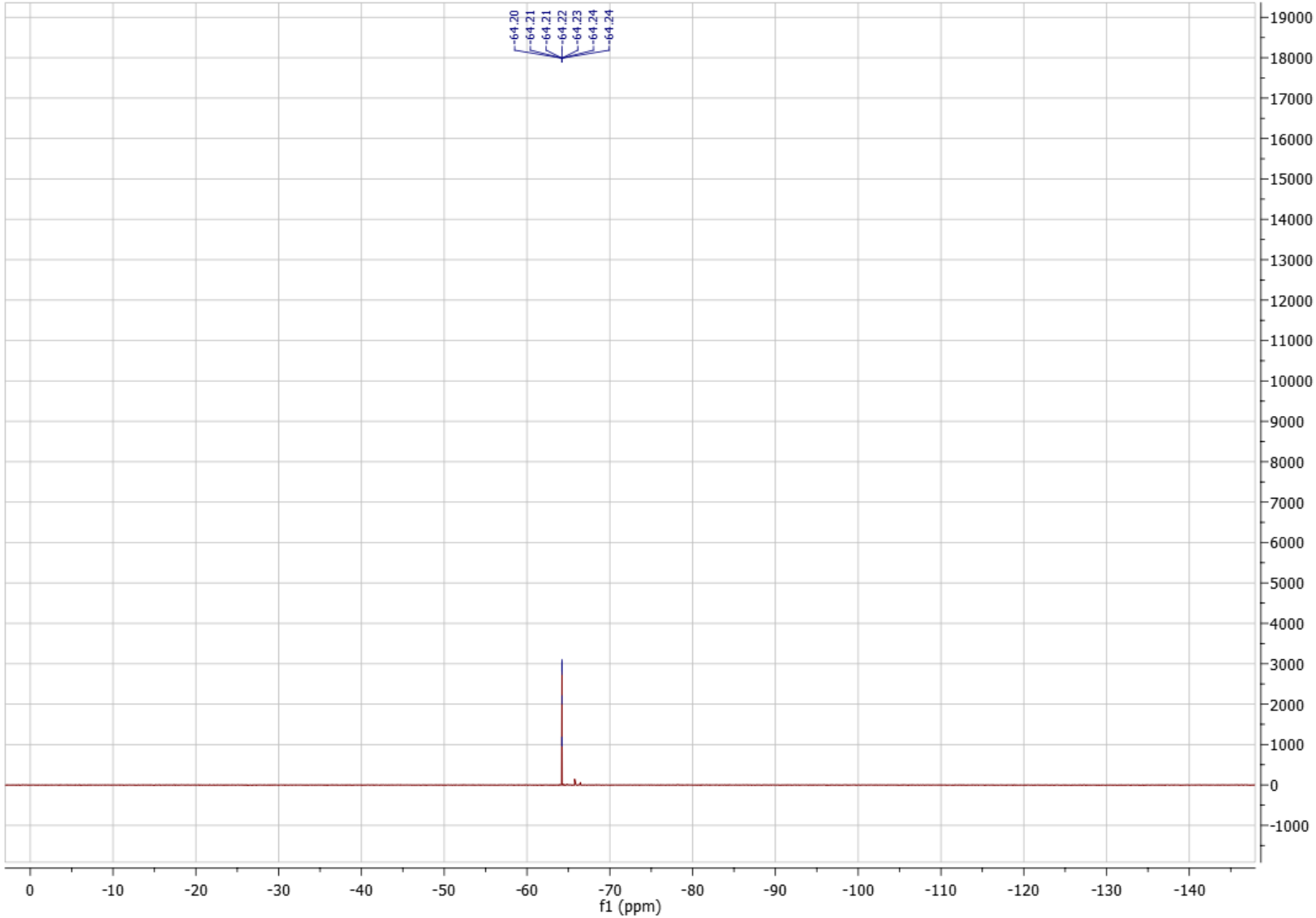
52.47
21.79
f1 (ppm)
f1 (ppm)


OH
S
CF3
5
f1 (ppm)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18000
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16000
15000
14000
13000
12000
11000
10000
9000
8000
7000
6000
5000
4000
3000
2000
1000
0
-1000
0
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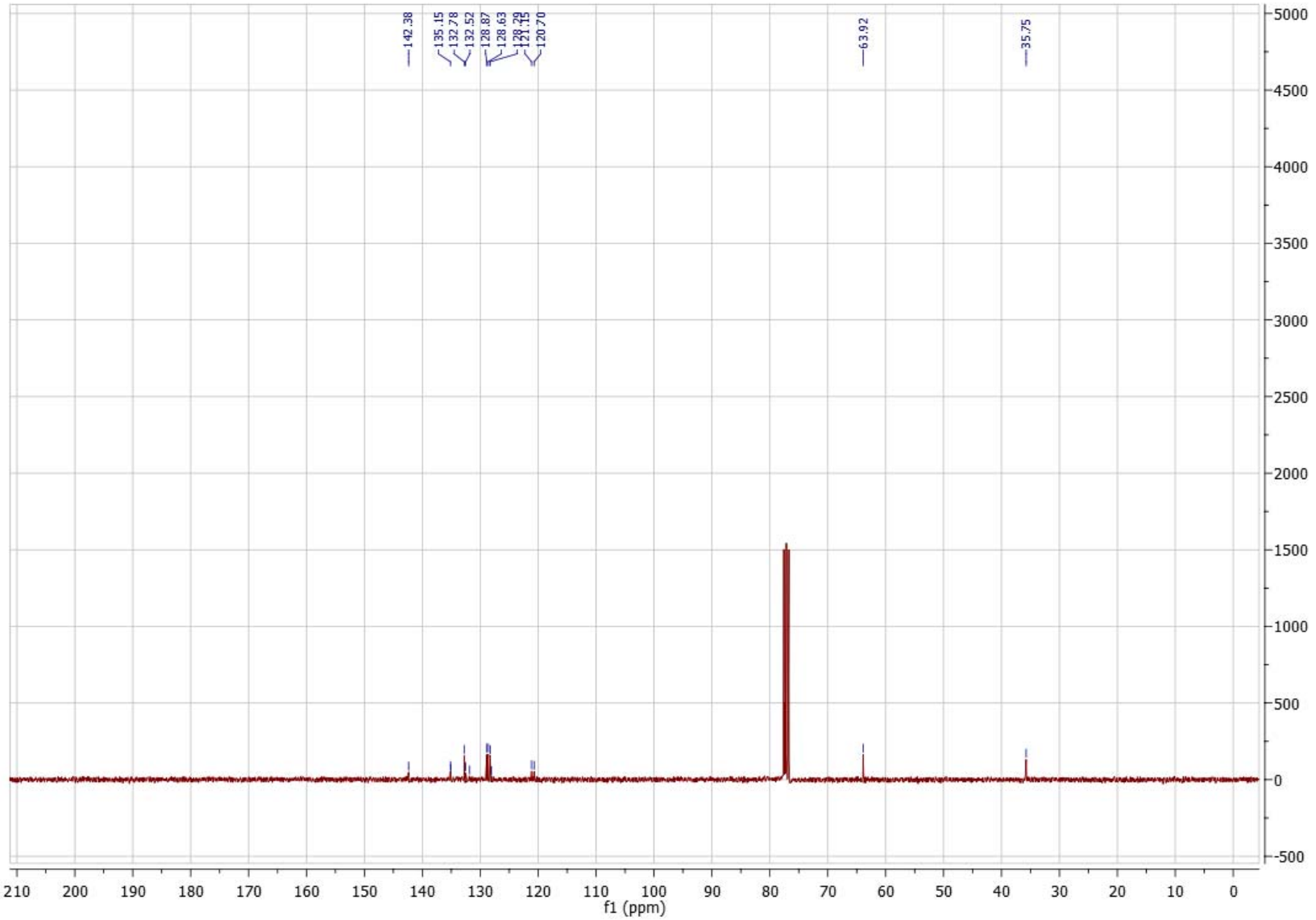
-60
-70
-80
-90
-100
-110
-120
-130
-140
f1 (ppm)


142.38
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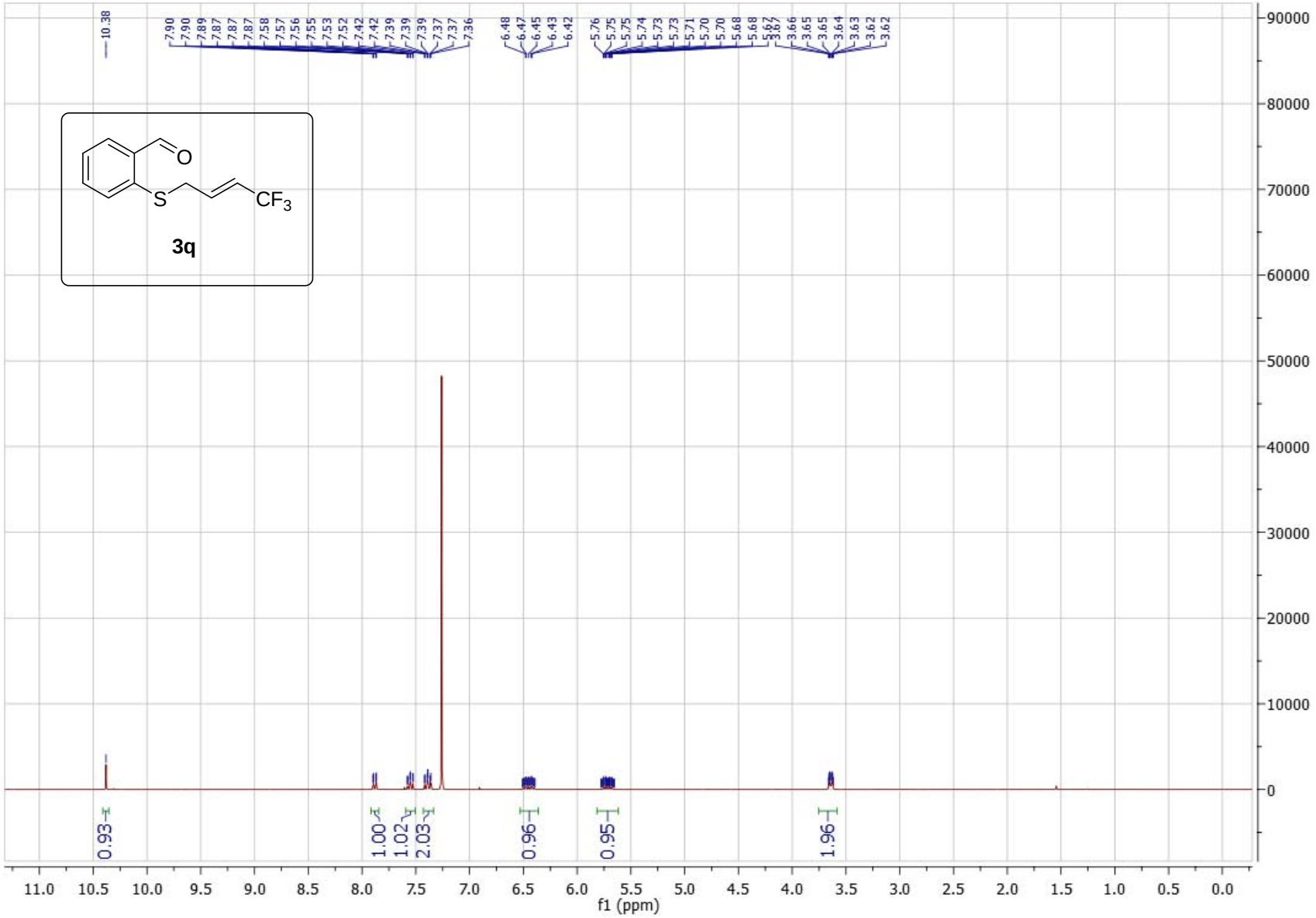
128.63
128.29
121.15
120.70
63.92
35.75
f1 (ppm)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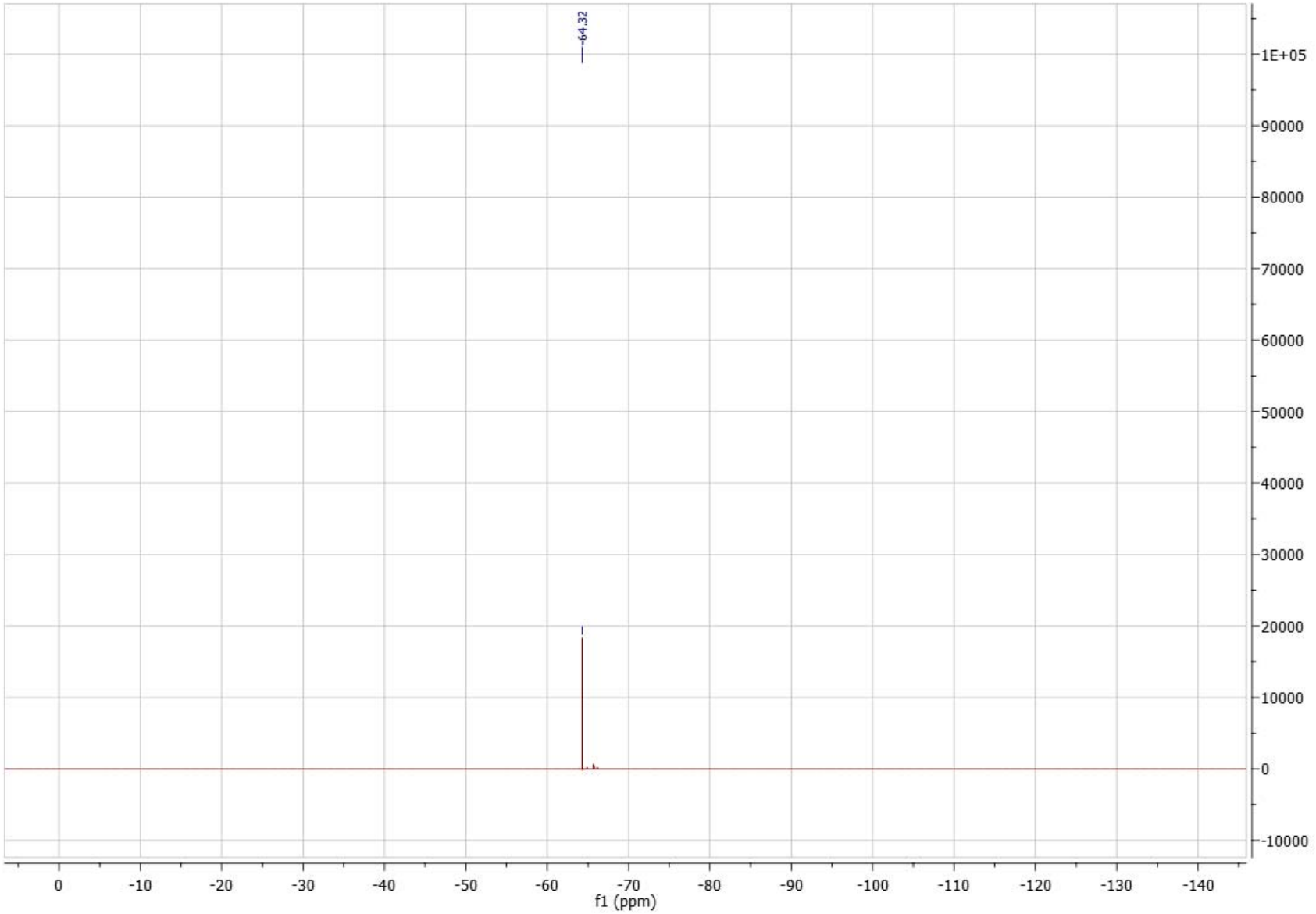
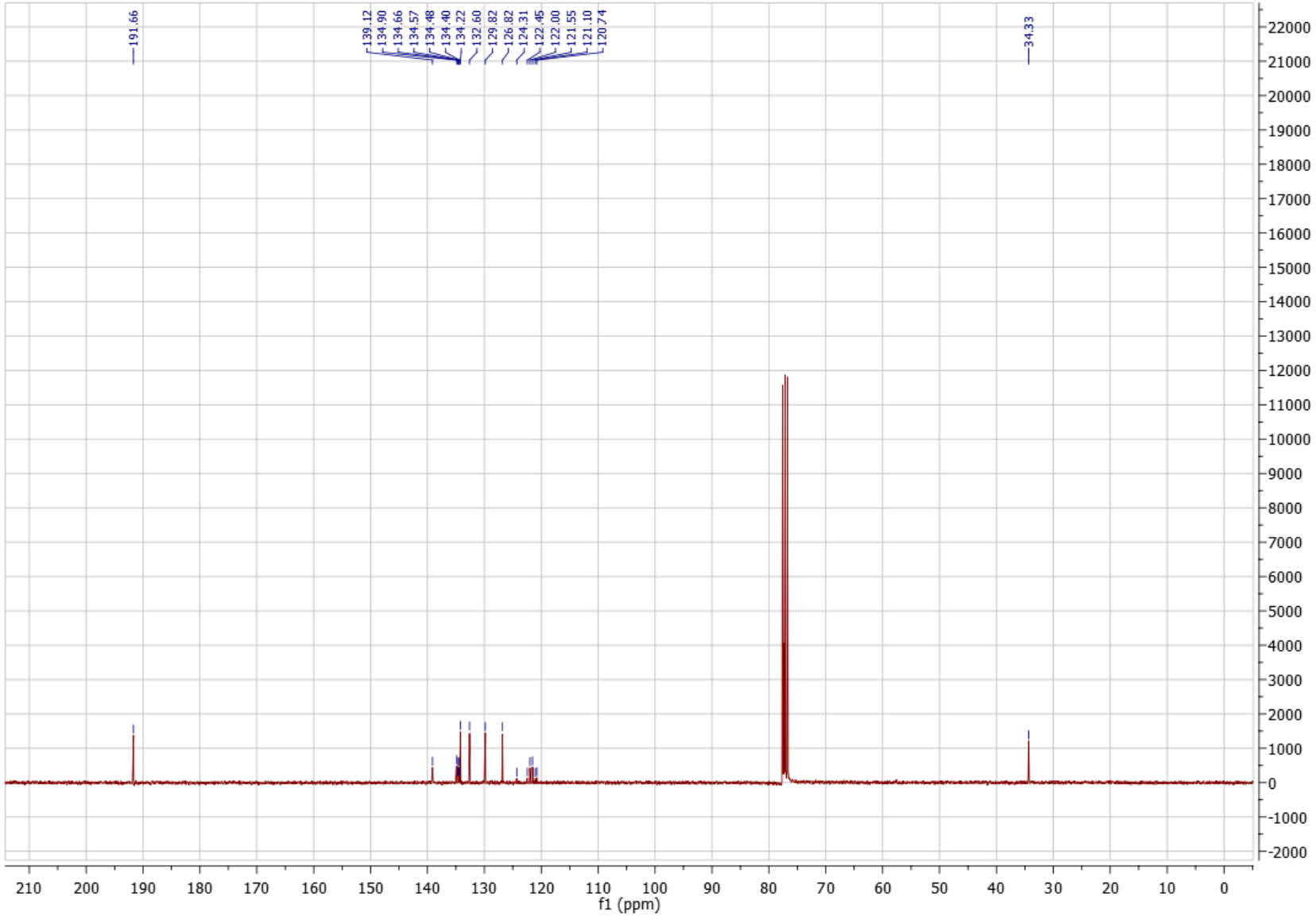
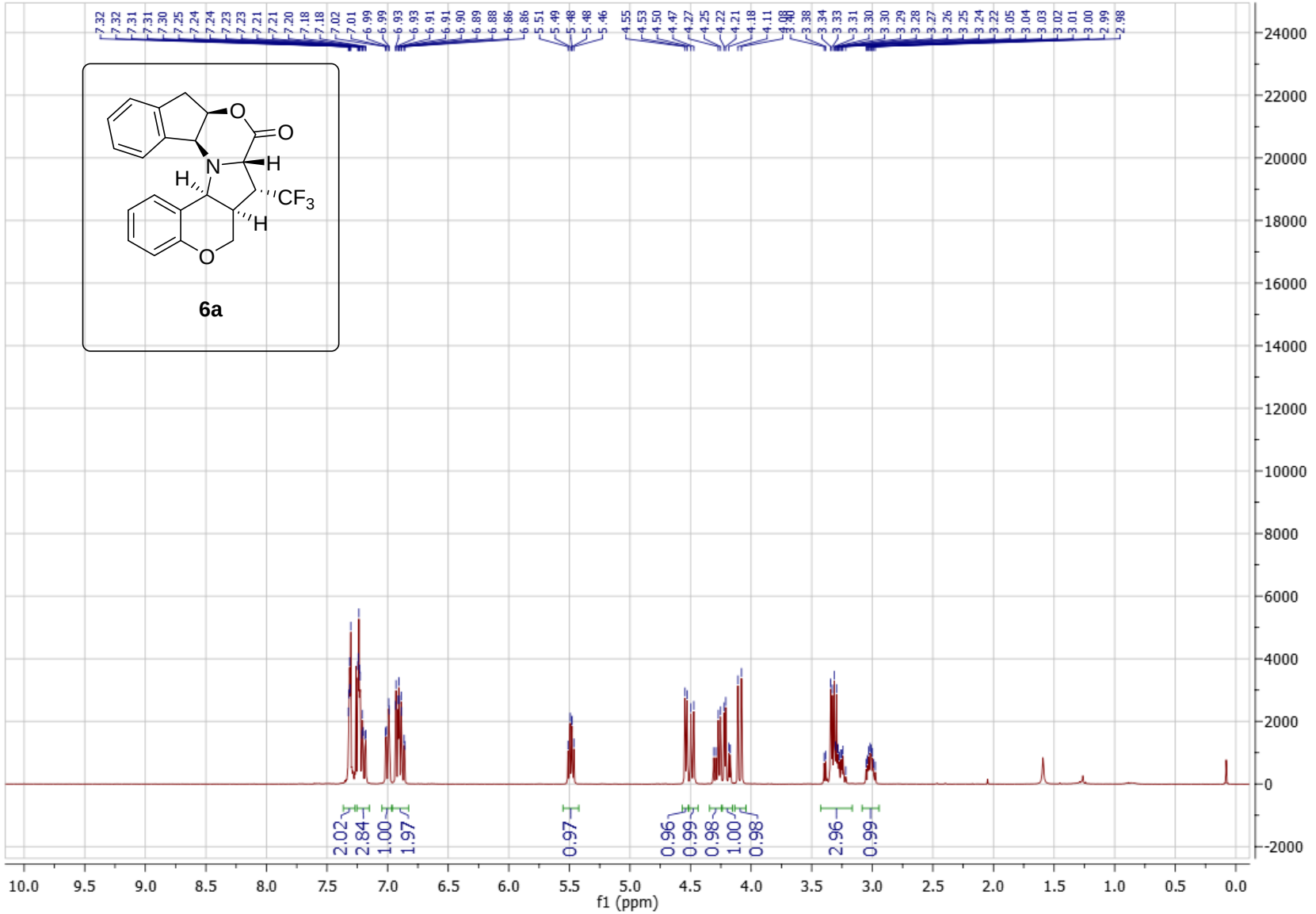
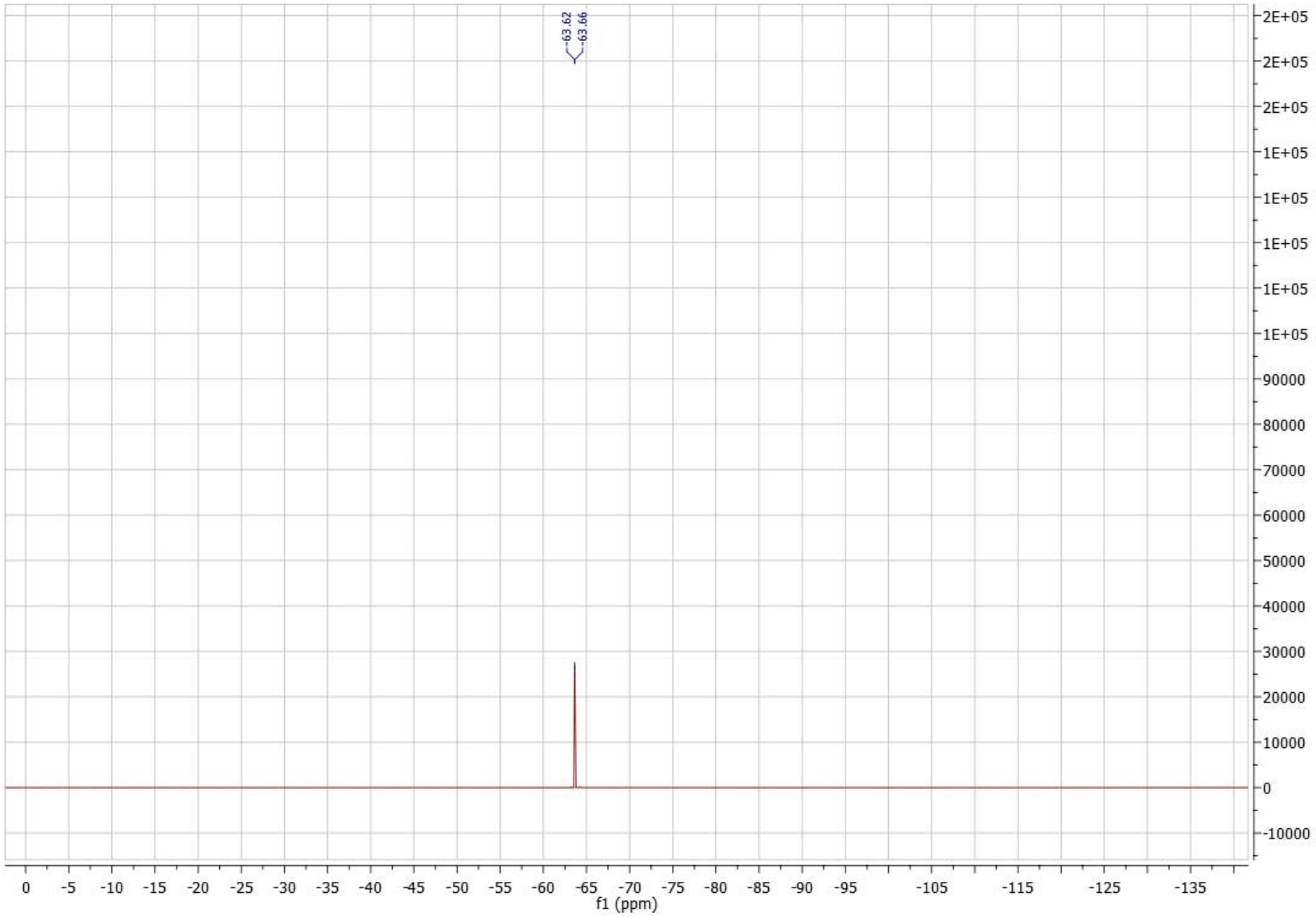
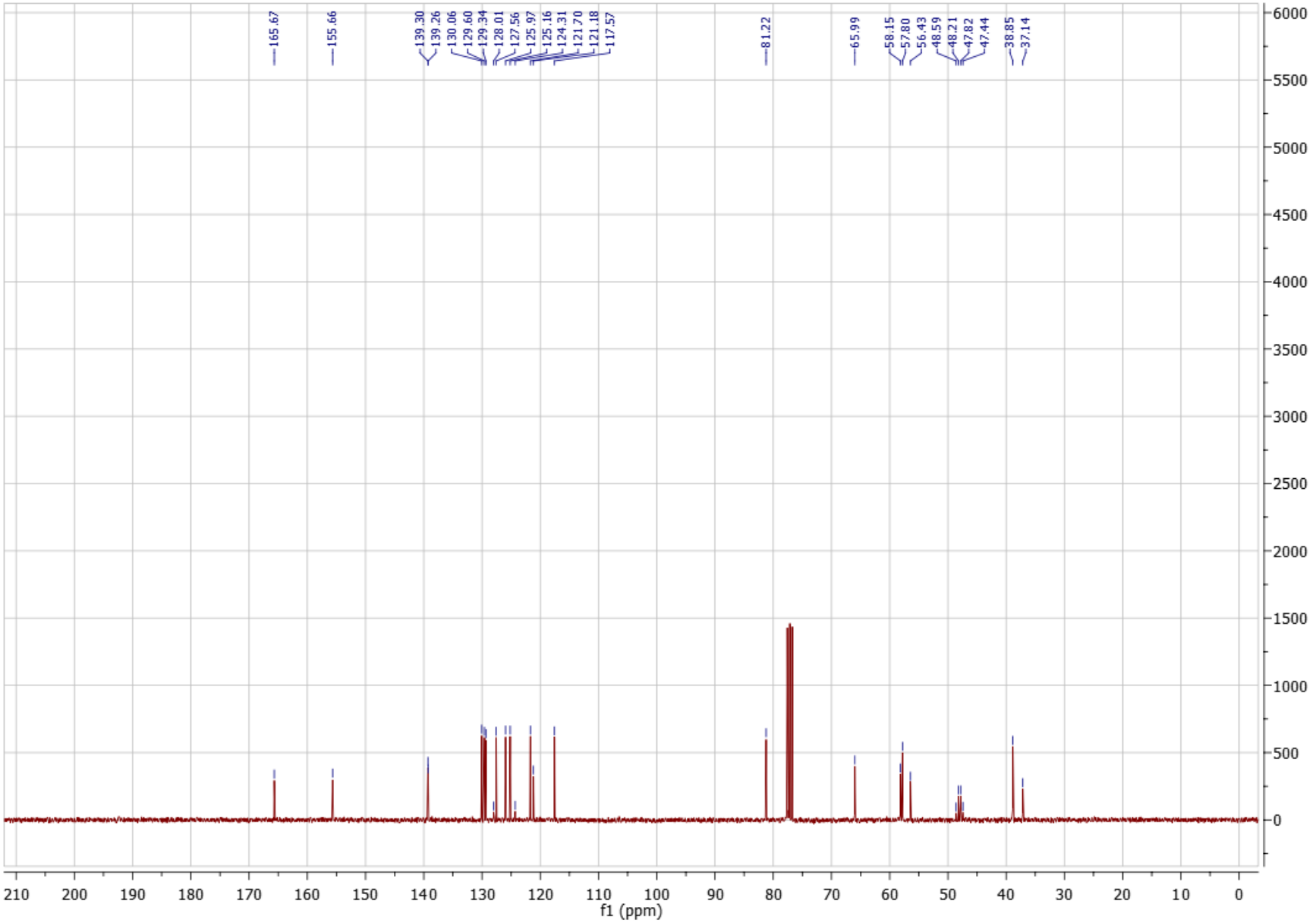
7.90
7.90
7.89
7.87
7.87
7.87
7.58
7.57
7.56
7.55
7.53
7.52
7.42
7.42
7.39
7.39
7.39
7.37
7.37
7.36
6.48
6.47
6.45
6.43
6.42
5.76
5.75
5.75
5.74
5.73
5.73
5.71
5.70
5.70
5.68
5.68
3.66
3.65
3.65
3.64
3.63
3.62
3.62
O
S
CF3
3q
0.93
1.00
1.02
2.03
0.96
0.95
1.96
f1 (ppm)


-64.32
1E+05
90000
80000
70000
60000
50000
40000
30000
20000
10000
0
-10000
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
f1 (ppm)


191.66
139.12
134.90
134.66
134.57
134.48
134.40
134.22
132.60
129.82
126.82
124.31
122.45
122.00
121.55
121.10
120.74
34.33
f1 (ppm)

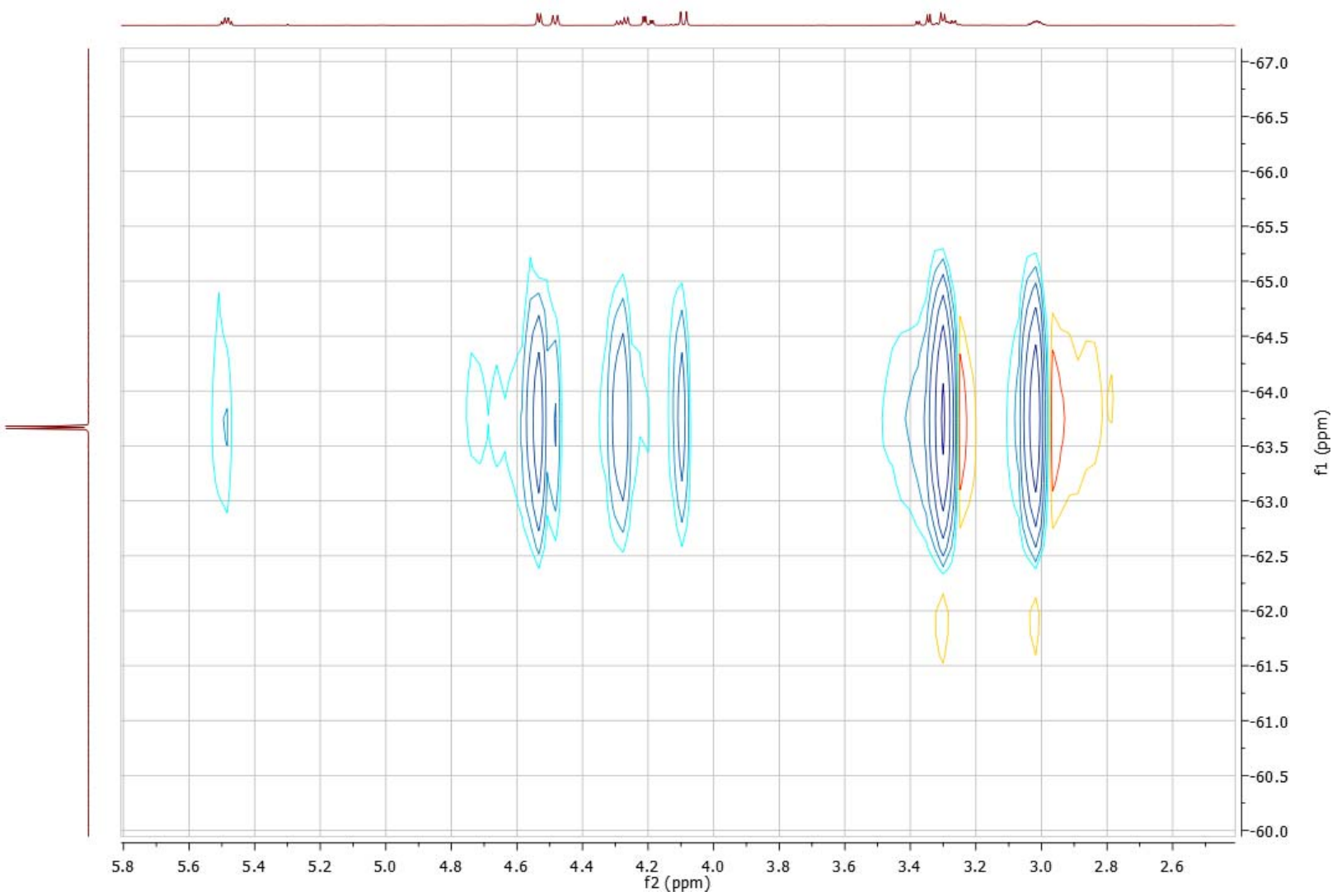

6a
f1 (ppm)


-63.62
-63.66
2E+05
2E+05
2E+05
1E+05
1E+05
1E+05
1E+05
1E+05
90000
80000
70000
60000
50000
40000
30000
20000
10000
0
-10000
0 -5 -10 -15 -20 -25 -30 -35 -40 -45 -50 -55 -60 -65 -70 -75 -80 -85 -90 -95 -105 -115 -125 -135
f1 (ppm)

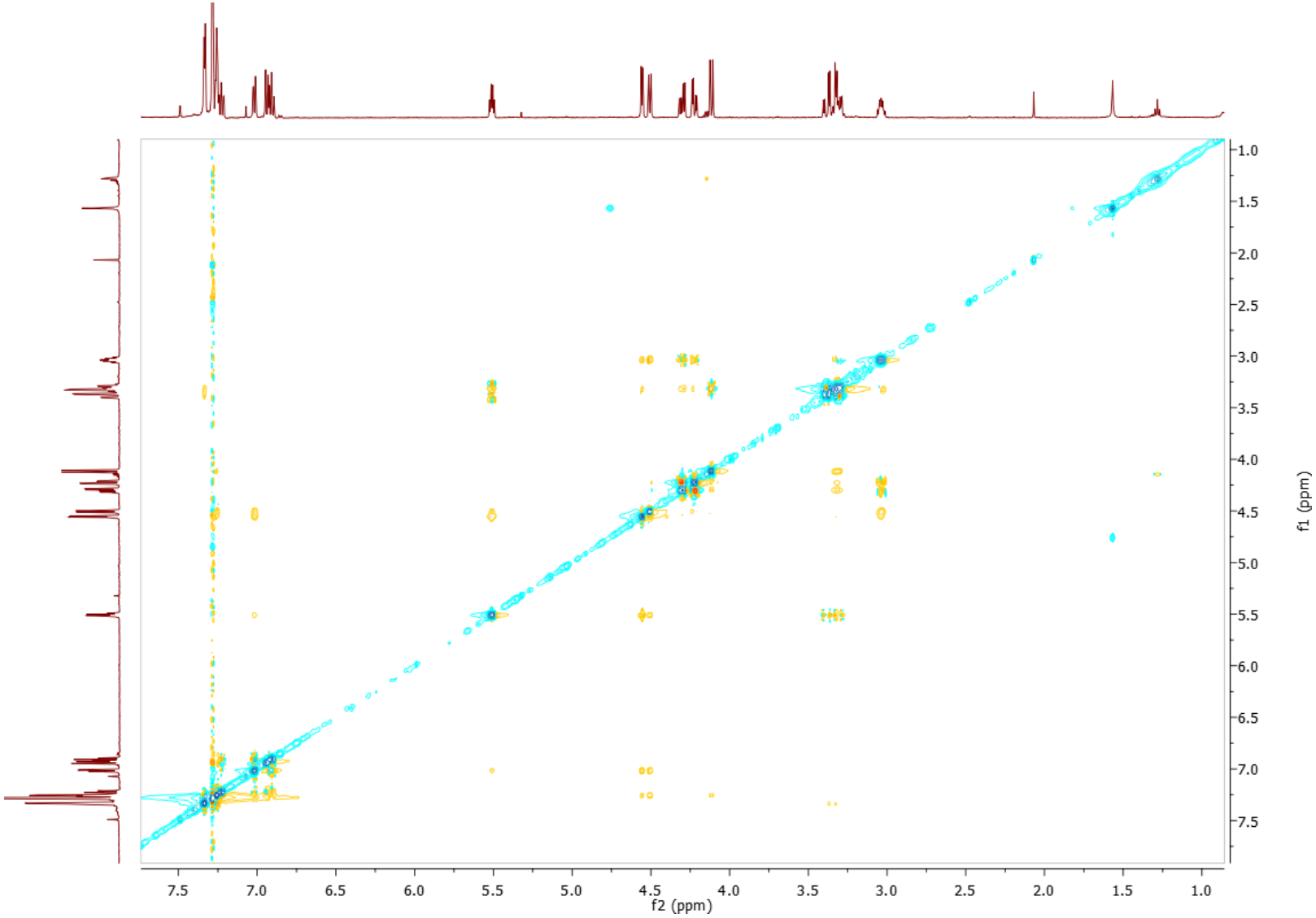

165.67
155.66
139.30
139.26
130.06
129.60
129.34
128.01
127.56
125.97
125.16
124.31
121.70
121.18
117.57
81.22
65.99
58.15
57.80
56.43
48.59
48.21
47.82
47.44
38.85
37.14
6000
5500
5000
4500
4000
3500
3000
2500
2000
1500
1000
500
0
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

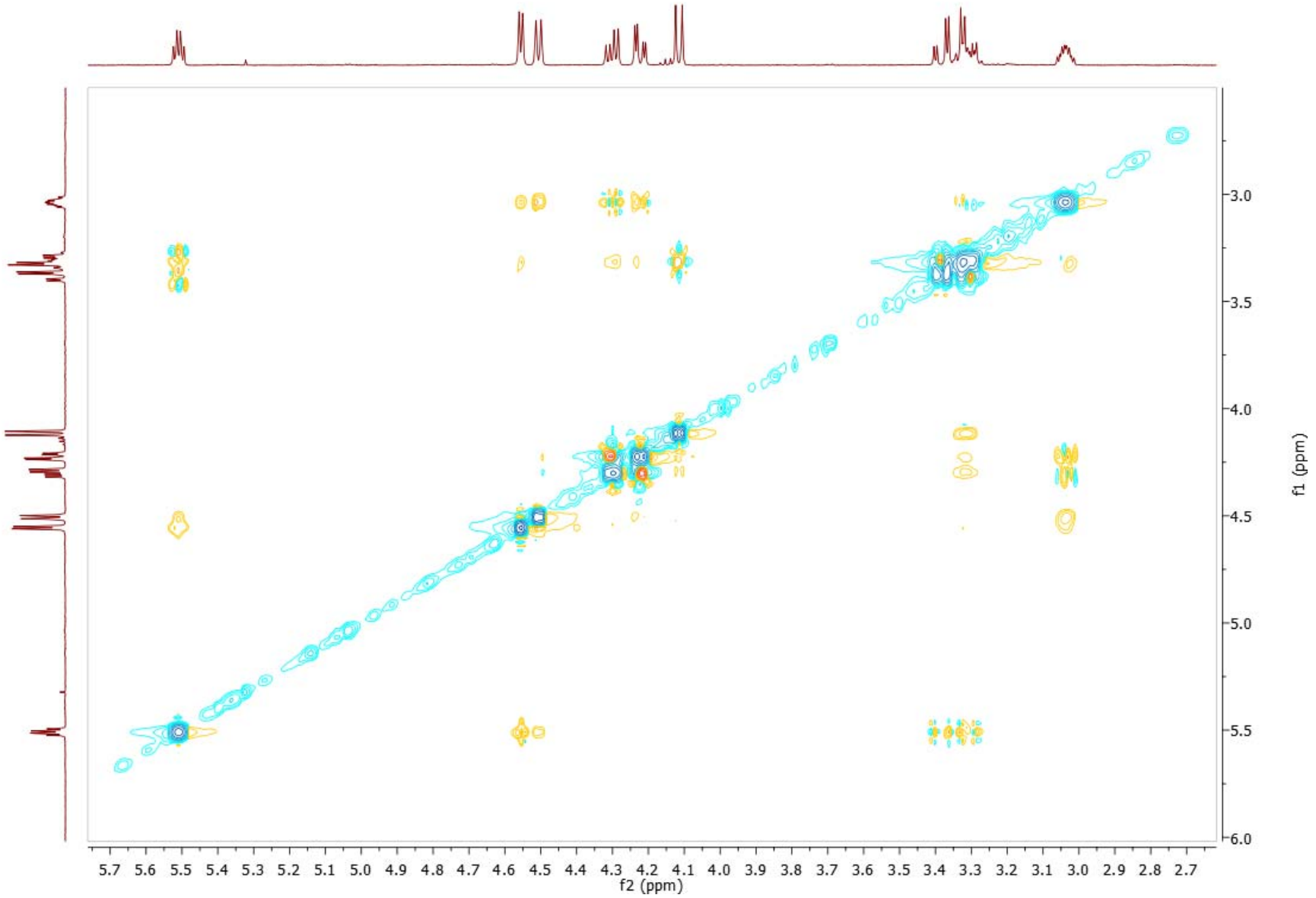
HOESY

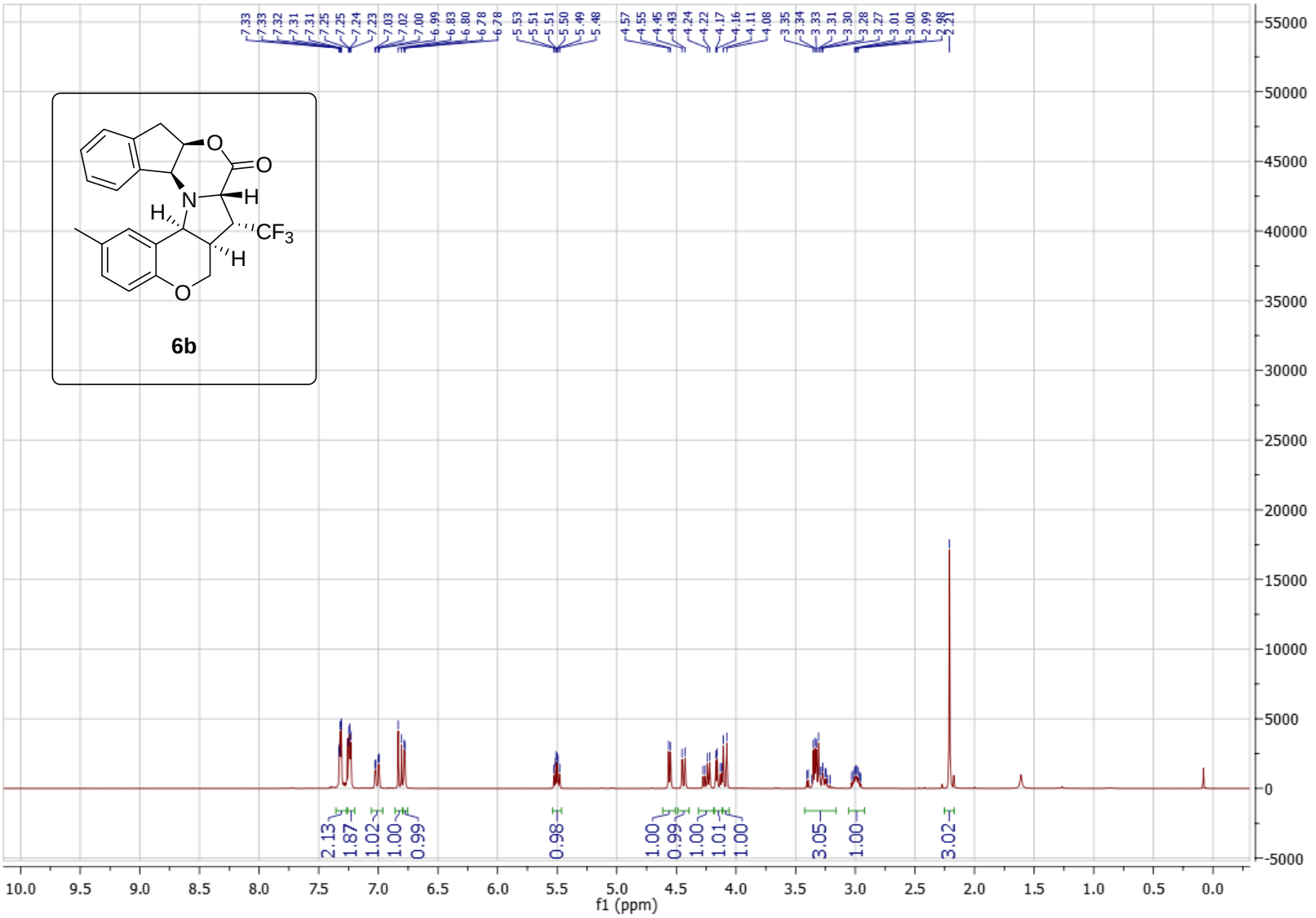

-66.0
-65.5
-65.0
-64.5
-64.0
-63.5
-63.0
-62.5
-62.0
-61.5
f1 (ppm)
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f2 (ppm)

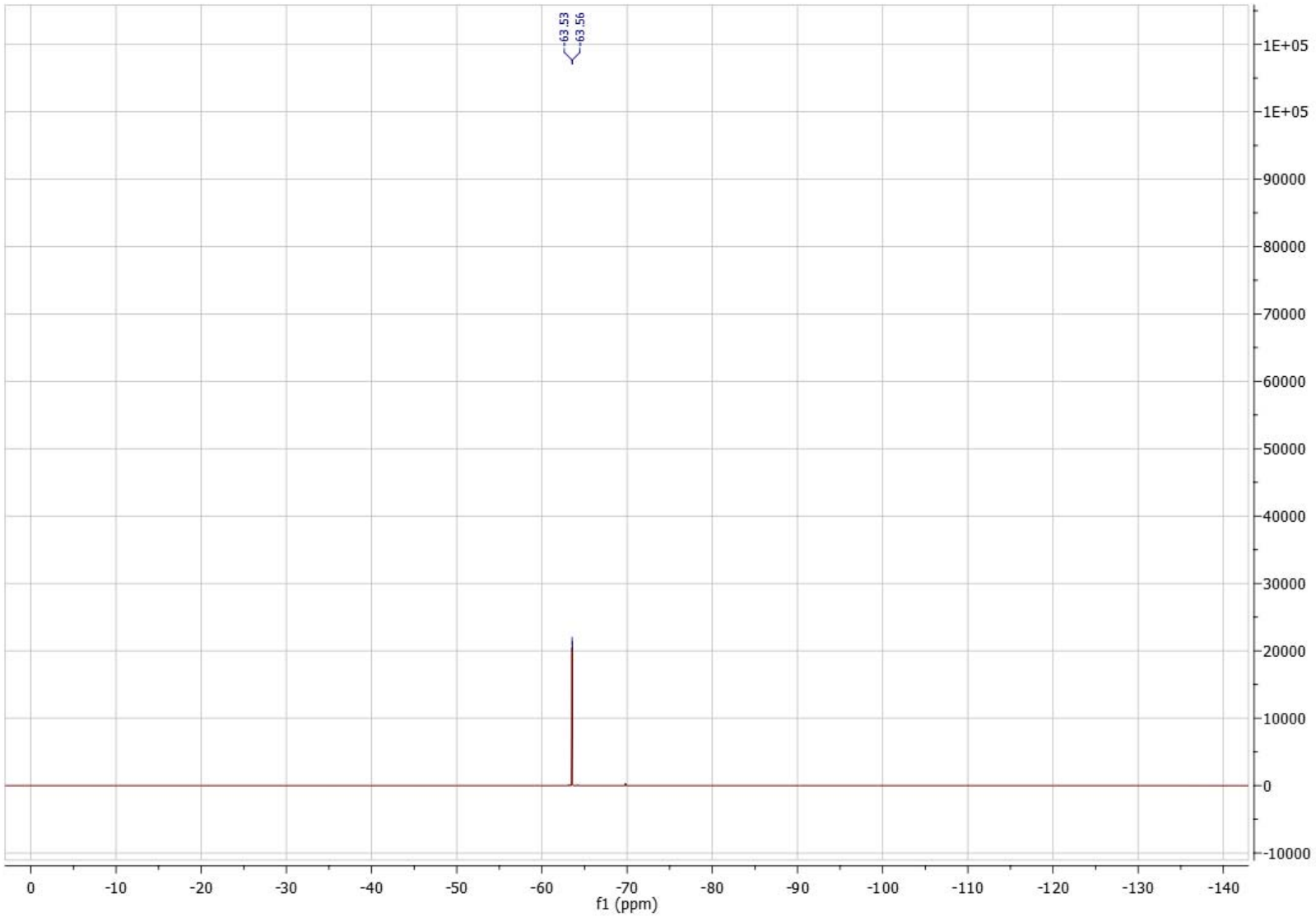

-67.0
-66.5
-66.0
-65.5
-65.0
-64.5
-64.0
-63.5
-63.0
-62.5
-62.0
-61.5
-61.0
-60.5
-60.0
f1 (ppm)
5.8
5.6
5.4
5.2
5.0
4.8
4.6
4.4
4.2
4.0
3.8
3.6
3.4
3.2
3.0
2.8
2.6
f2 (ppm)

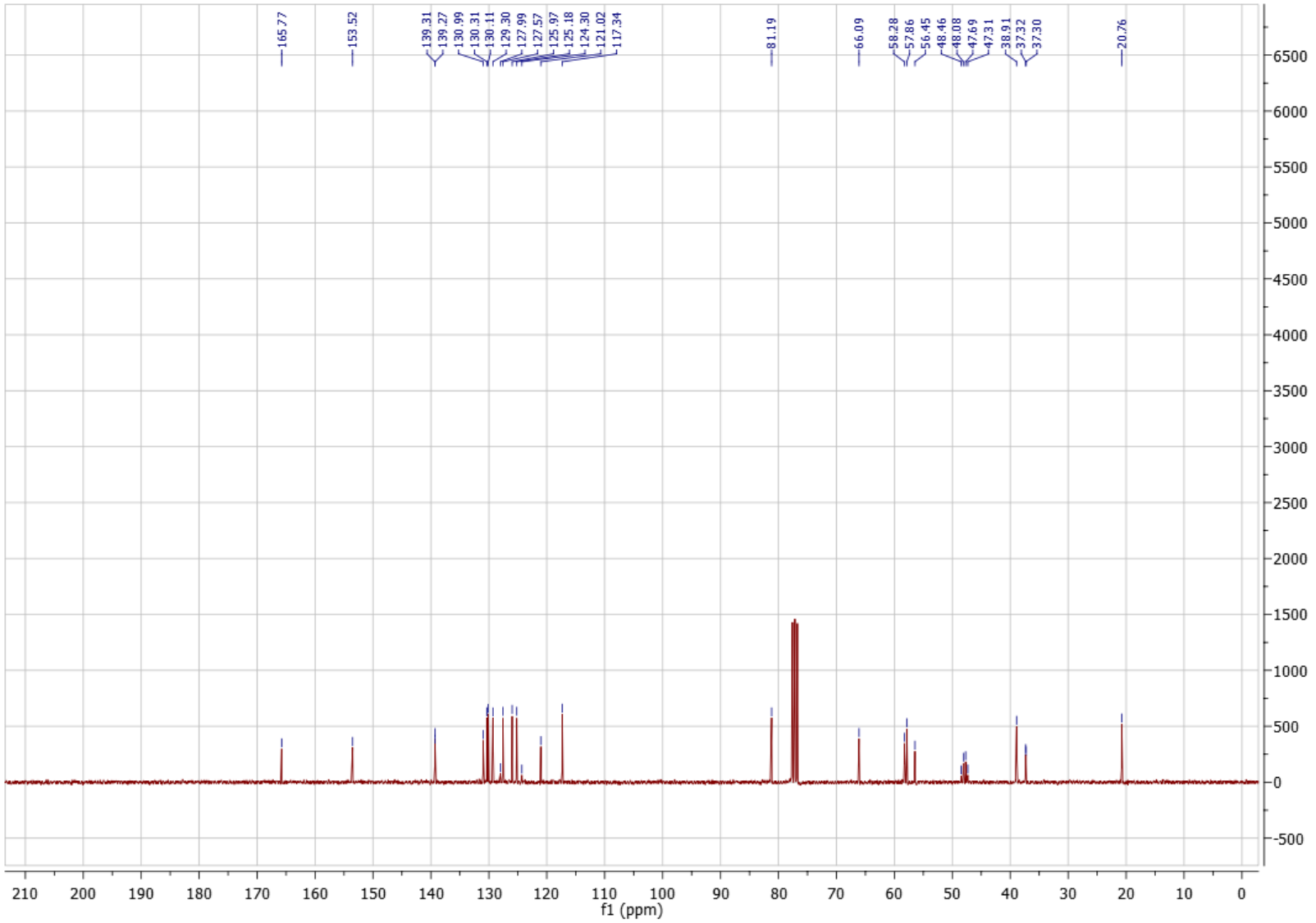
NOESY

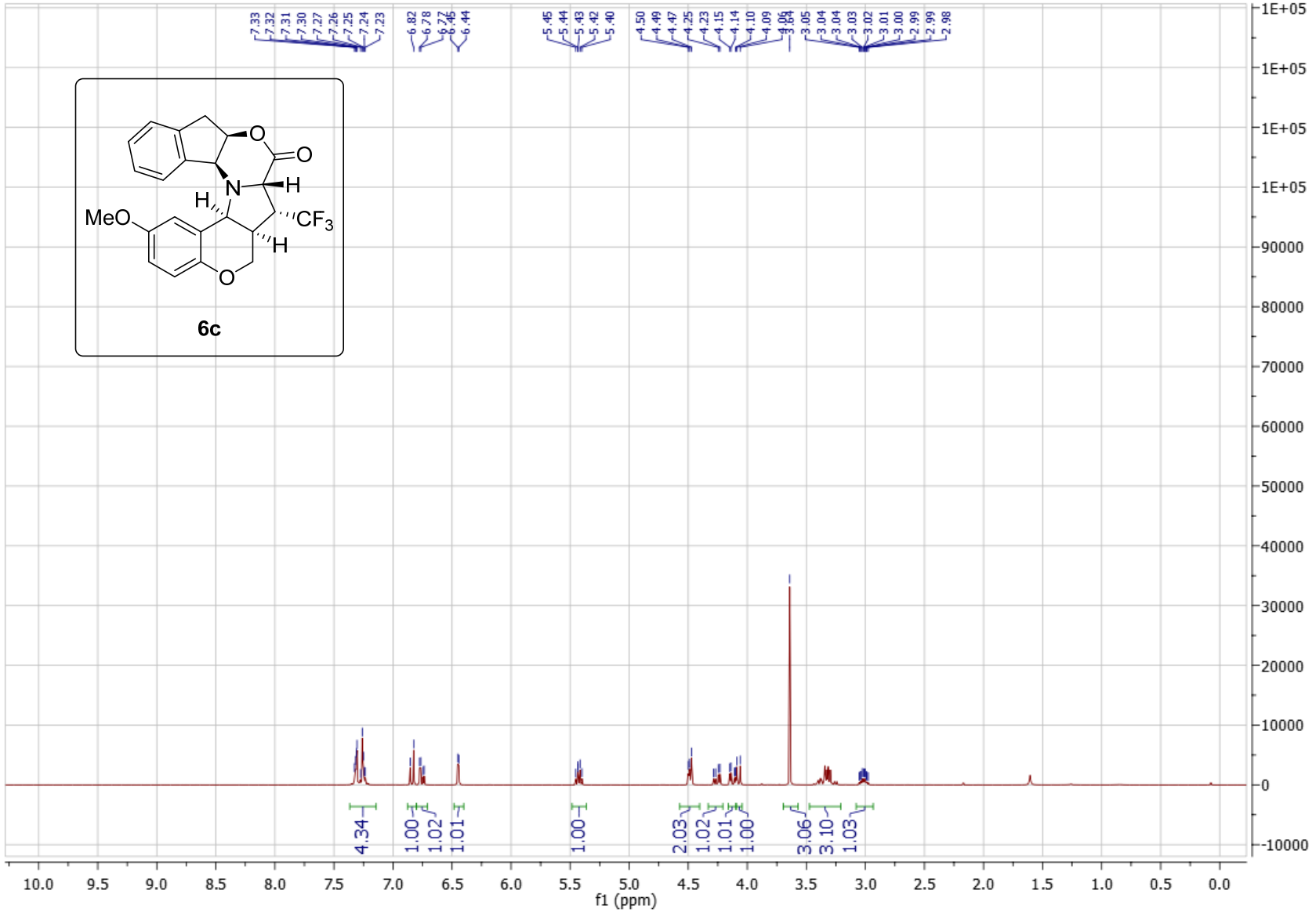

7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
f2 (ppm)
1.0
1.5
2.0
2.5
3.0
3.5
4.0
4.5
5.0
5.5
6.0
6.5
7.0
7.5
f1 (ppm)

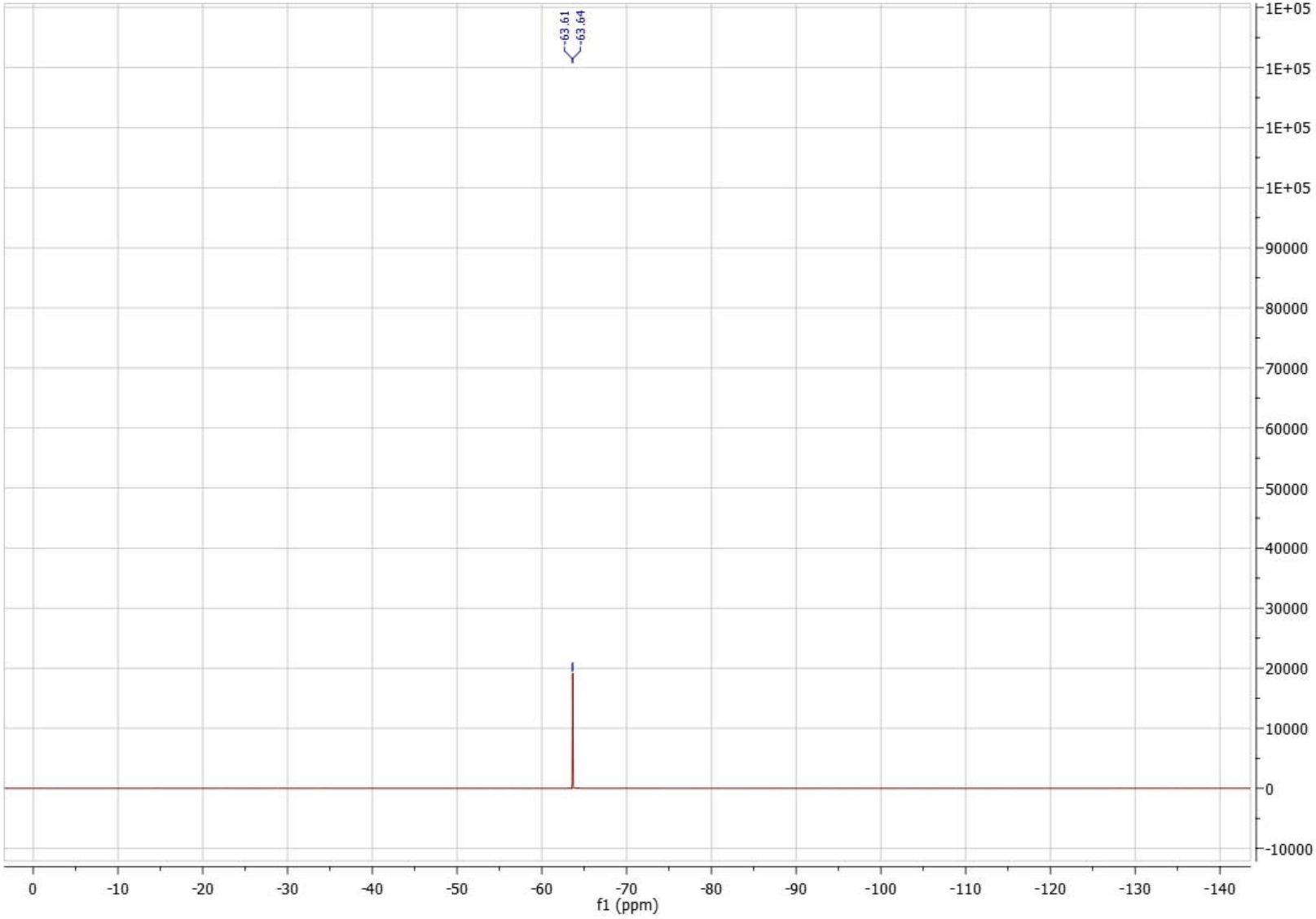

5.7 5.6 5.5 5.4 5.3 5.2 5.1 5.0 4.9 4.8 4.7 4.6 4.5 4.4 4.3 4.2 4.1 4.0 3.9 3.8 3.7 3.6 3.5 3.4 3.3 3.2 3.1 3.0 2.9 2.8 2.7
f2 (ppm)
3.0
3.5
4.0
4.5
5.0
5.5
6.0
f1 (ppm)


6b
f1 (ppm)


-63.53
-63.56
1E+05
1E+05
90000
80000
70000
60000
50000
40000
30000
20000
10000
0
-10000
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
f1 (ppm)


165.77
153.52
139.31
139.27
130.99
130.31
130.11
129.30
127.99
127.57
125.97
125.18
124.30
121.02
117.34
81.19
66.09
58.28
57.86
56.45
48.46
48.08
47.69
47.31
38.91
37.32
37.30
20.76
6500
6000
5500
5000
4500
4000
3500
3000
2500
2000
1500
1000
500
0
-500
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


7.33
7.32
7.31
7.30
7.27
7.26
7.25
7.24
7.23
6.82
6.78
6.77
6.45
6.44
5.45
5.44
5.43
5.42
5.40
4.50
4.49
4.47
4.25
4.23
4.15
4.14
4.10
4.09
3.05
3.04
3.04
3.03
3.02
3.01
3.00
2.99
2.99
2.98
MeO
CF3
O
O
N
H
H
H
O
6c
4.34
1.00
1.02
1.01
1.00
2.03
1.02
1.01
1.00
3.06
3.10
1.03
1E+05
90000
80000
70000
60000
50000
40000
30000
20000
10000
0
-10000
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)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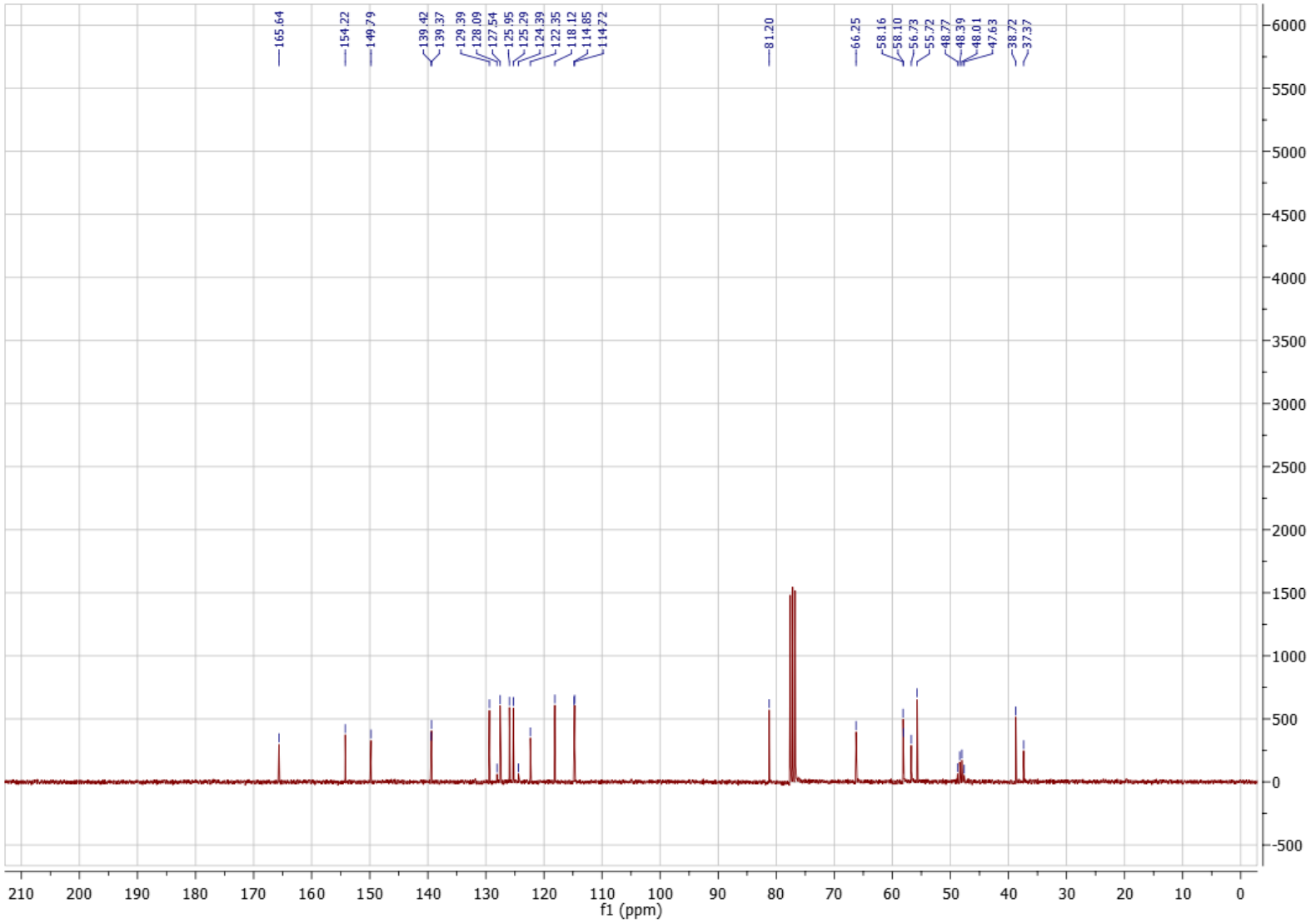
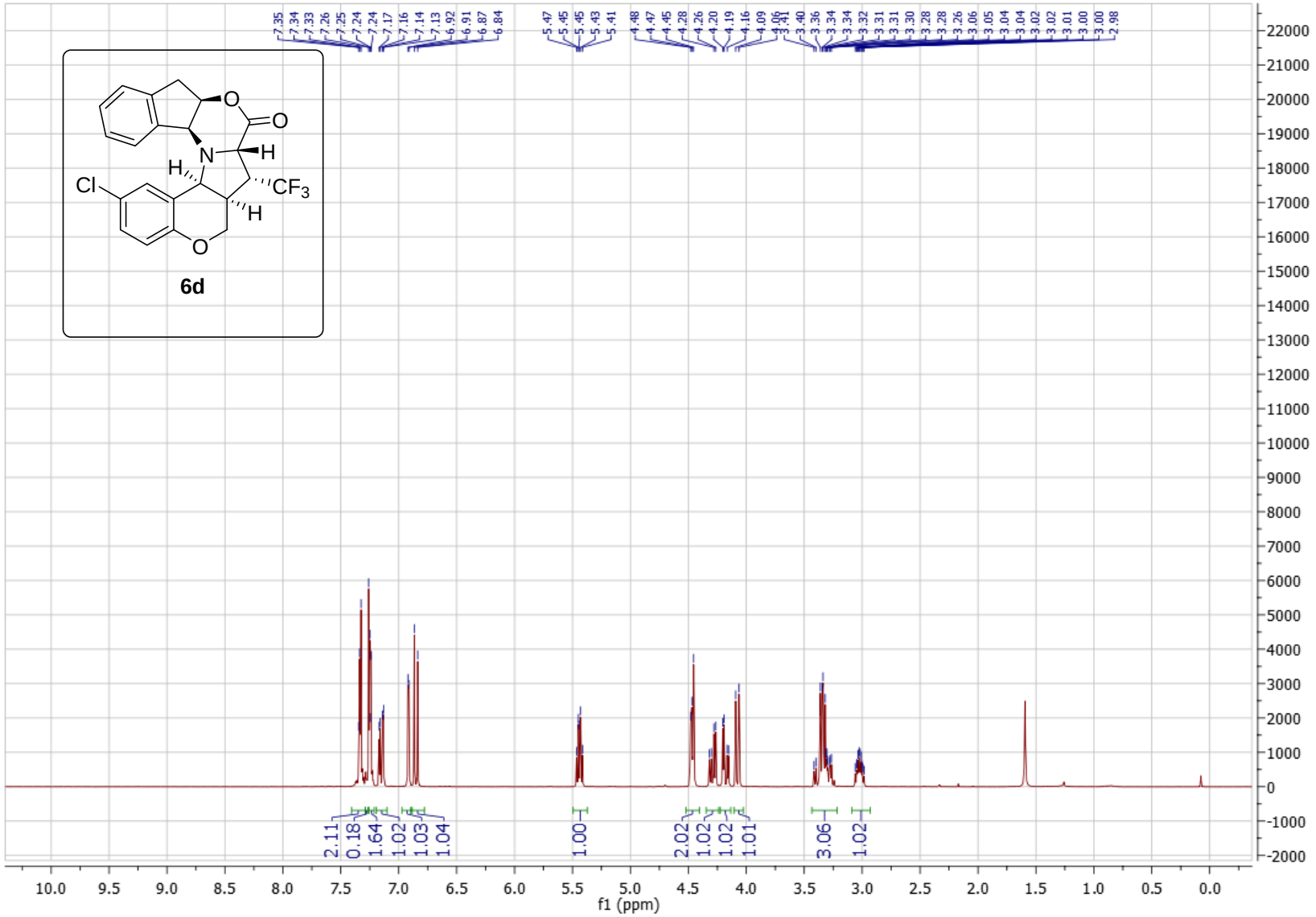
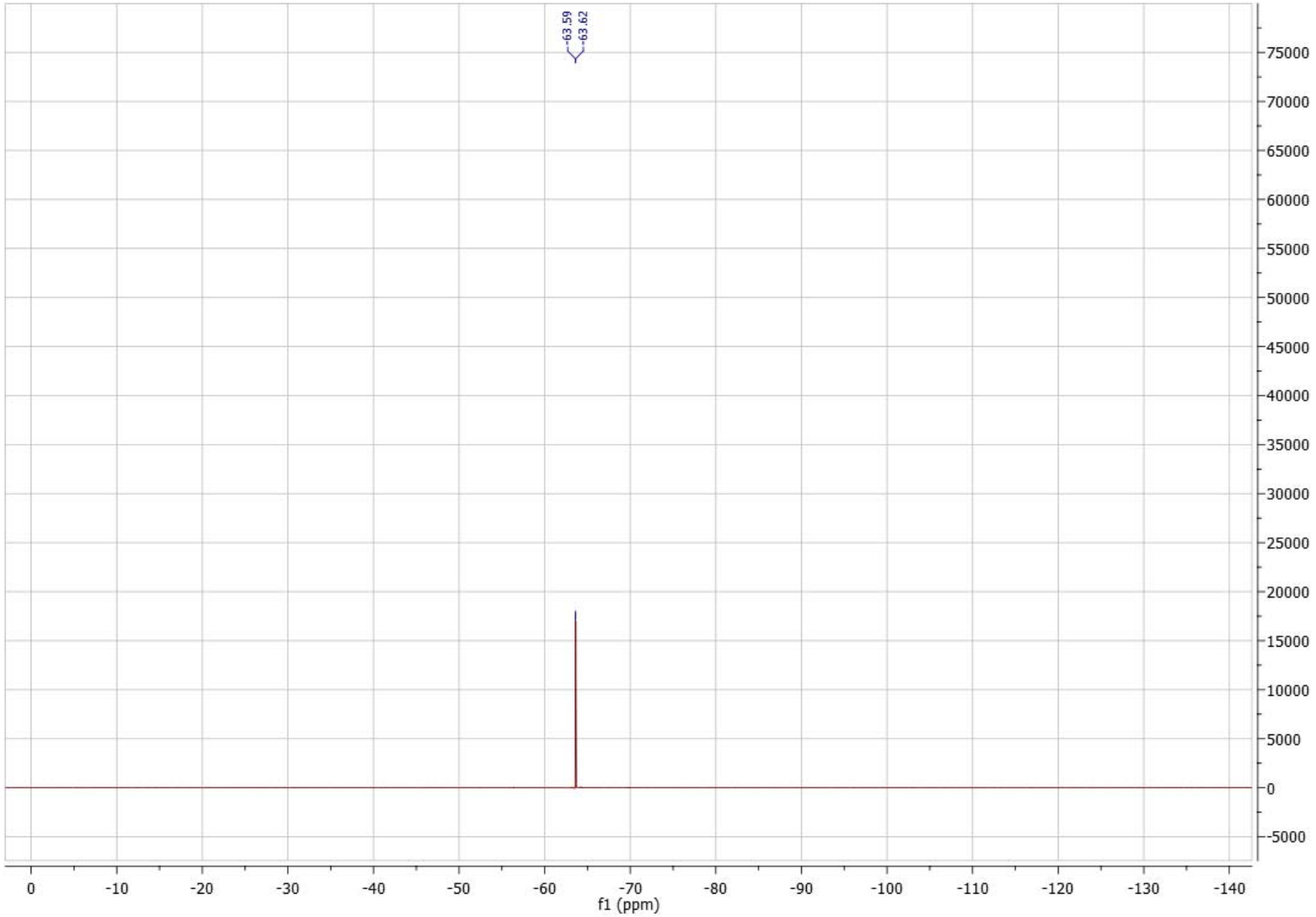
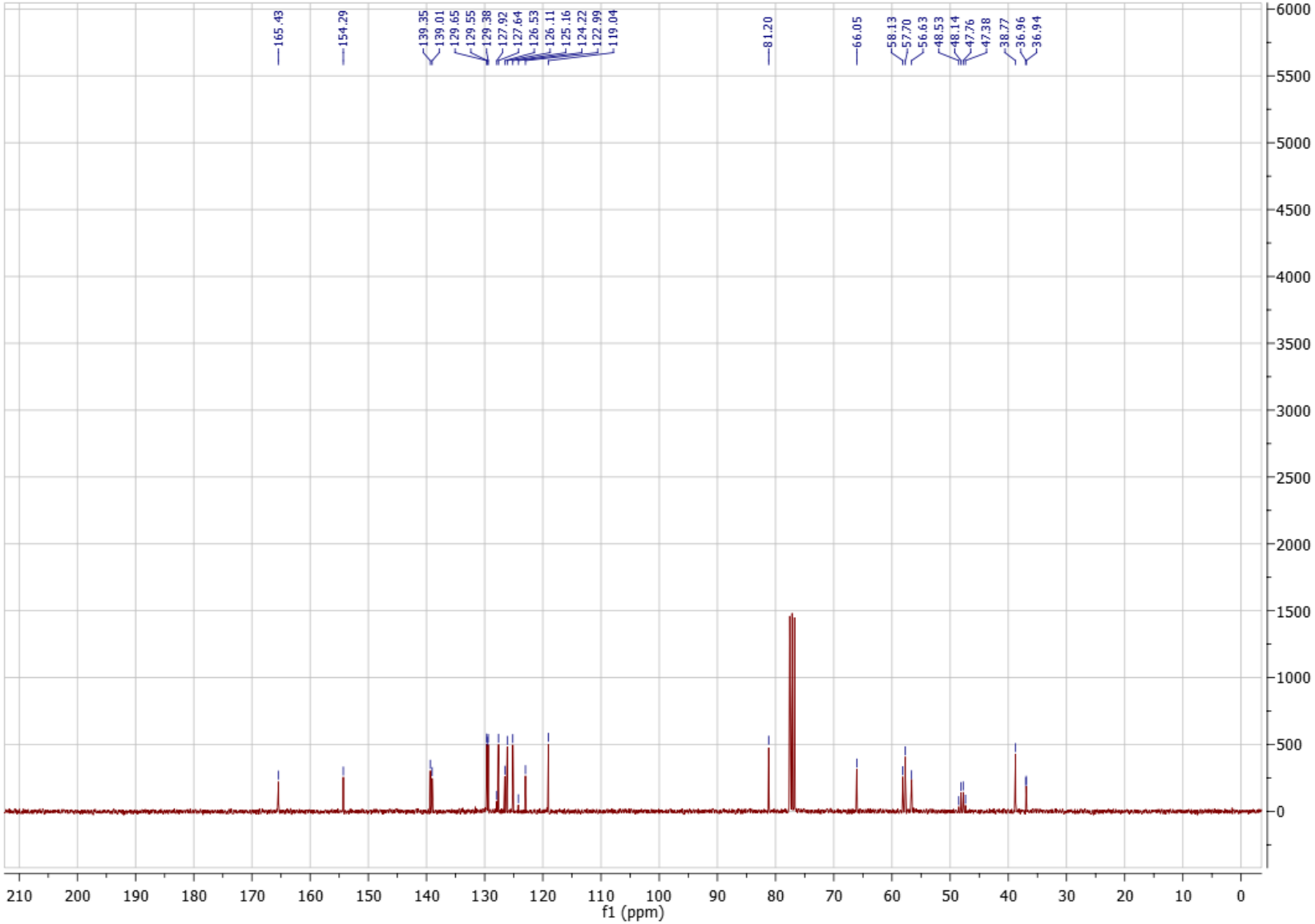
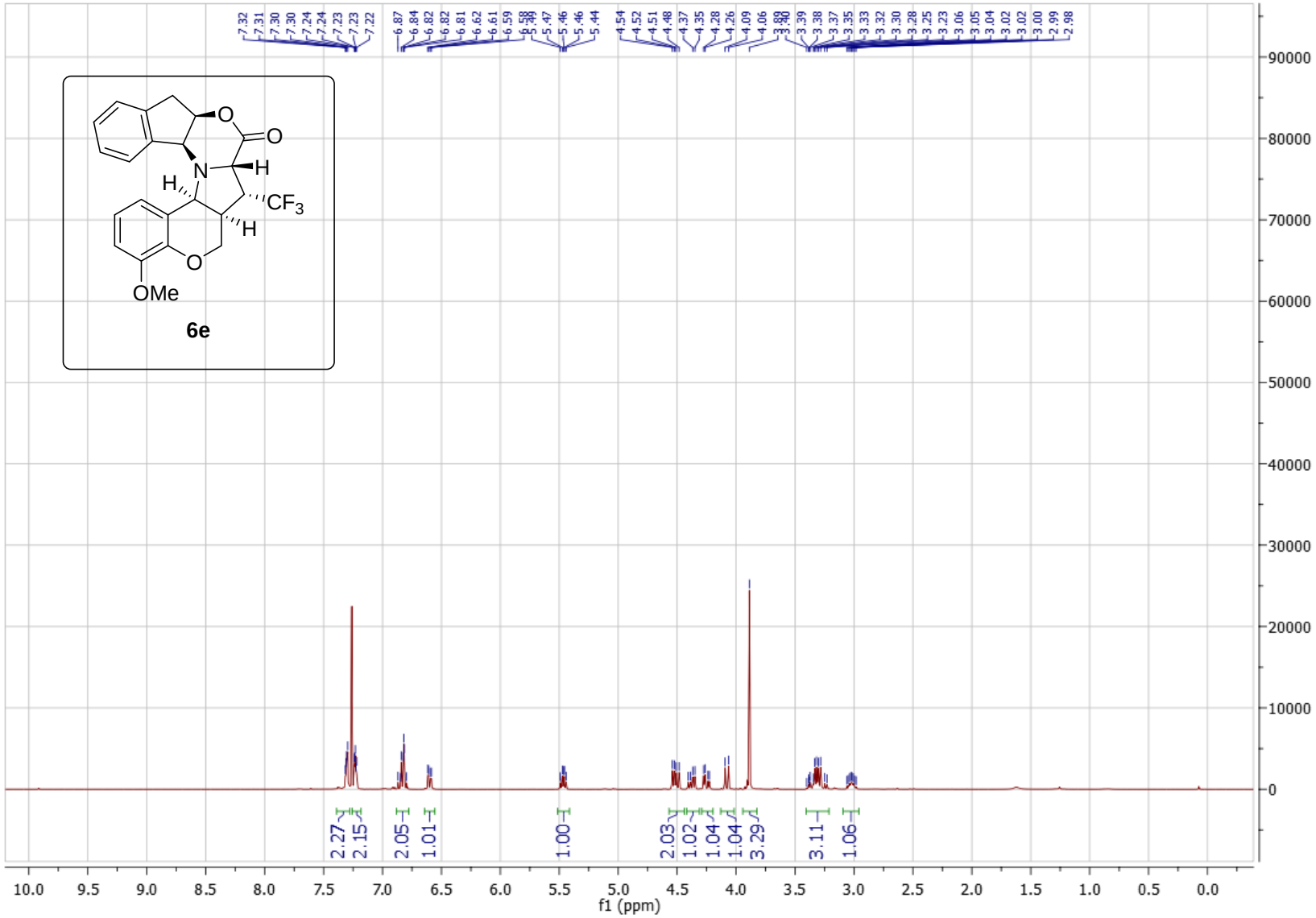
-63.64
1E+05
1E+05
1E+05
1E+05
90000
80000
70000
60000
50000
40000
30000
20000
10000
0
-10000
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
f1 (ppm)

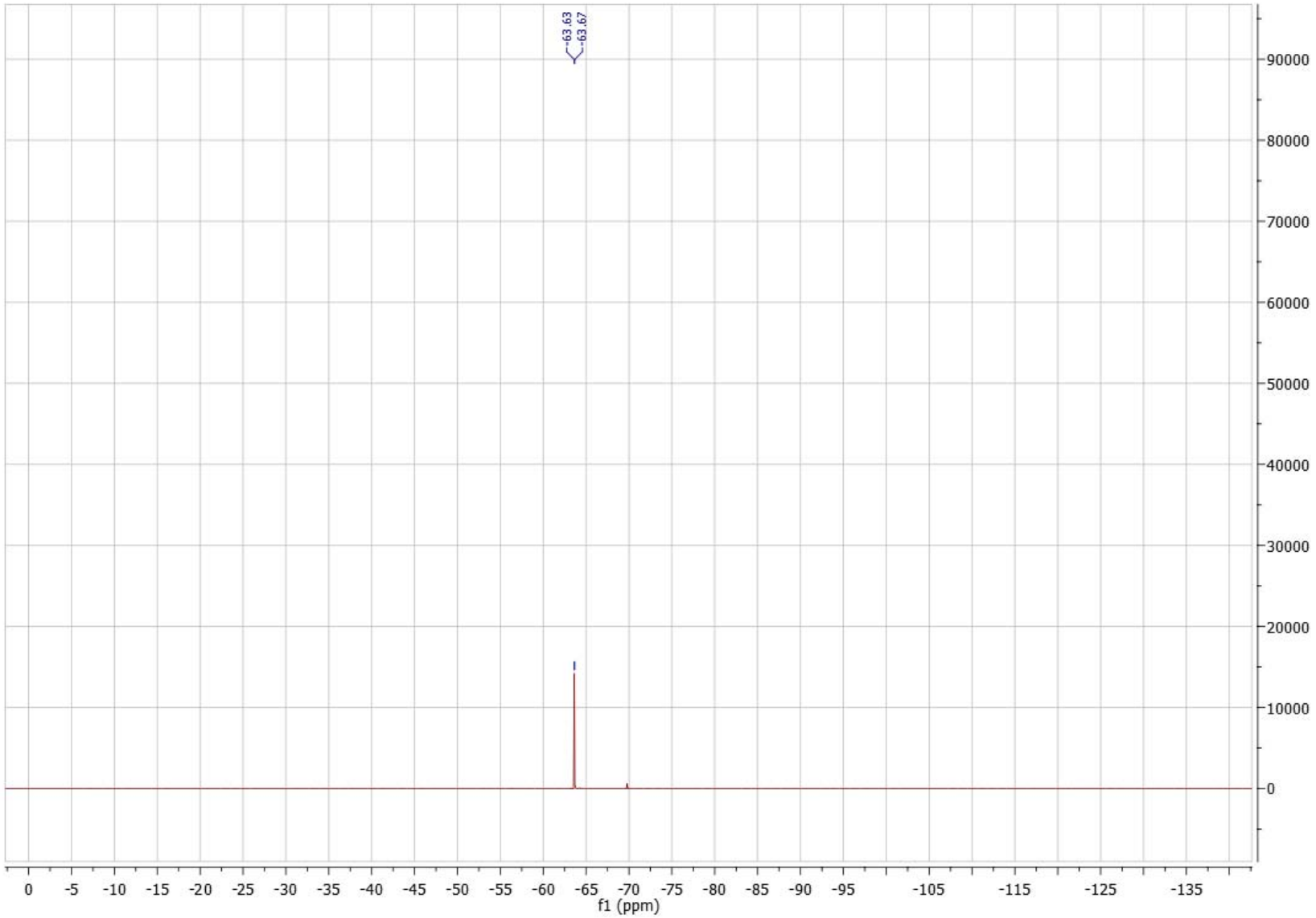

165.64
154.22
149.79
139.42
139.37
129.39
128.09
127.54
125.95
125.29
124.39
122.35
118.12
114.85
114.72
81.20
66.25
58.16
58.10
56.73
55.72
48.77
48.39
48.01
47.63
38.72
37.37
f1 (ppm)

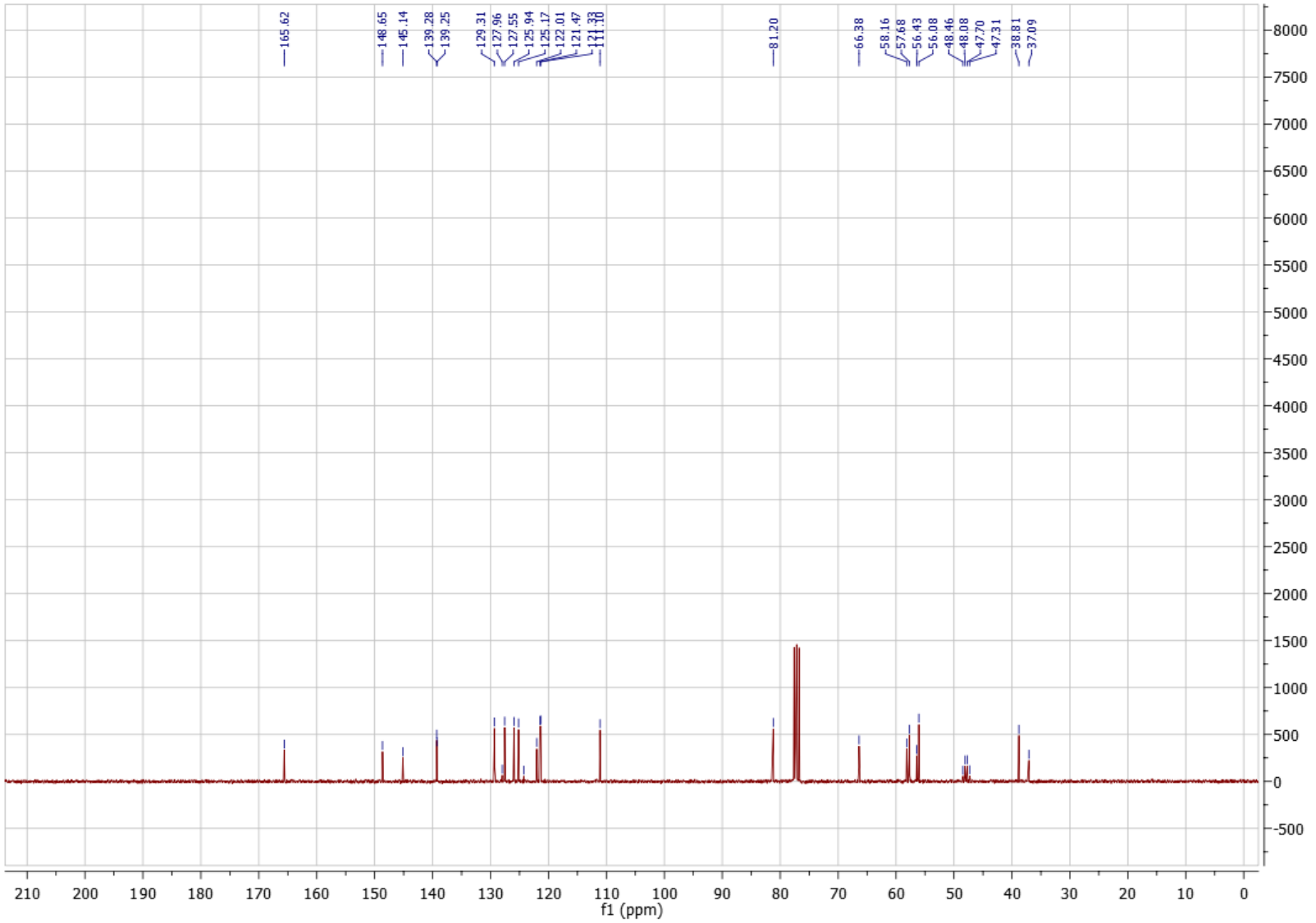

6d
f1 (ppm)


-63.59
-63.62
75000
70000
65000
60000
55000
50000
45000
40000
35000
30000
25000
20000
15000
10000
5000
0
-5000
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
f1 (ppm)


165.43
154.29
139.35
139.01
129.65
129.55
129.38
127.92
127.64
126.53
126.11
125.16
124.22
122.99
119.04
81.20
66.05
58.13
57.70
56.63
48.53
48.14
47.76
47.38
38.77
36.96
36.94
6000
5500
5000
4500
4000
3500
3000
2500
2000
1500
1000
500
0
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


6e
f1 (ppm)


-63.63
-63.67
90000
80000
70000
60000
50000
40000
30000
20000
10000
0
0 -5 -10 -15 -20 -25 -30 -35 -40 -45 -50 -55 -60 -65 -70 -75 -80 -85 -90 -95 -105 -115 -125 -135
f1 (ppm)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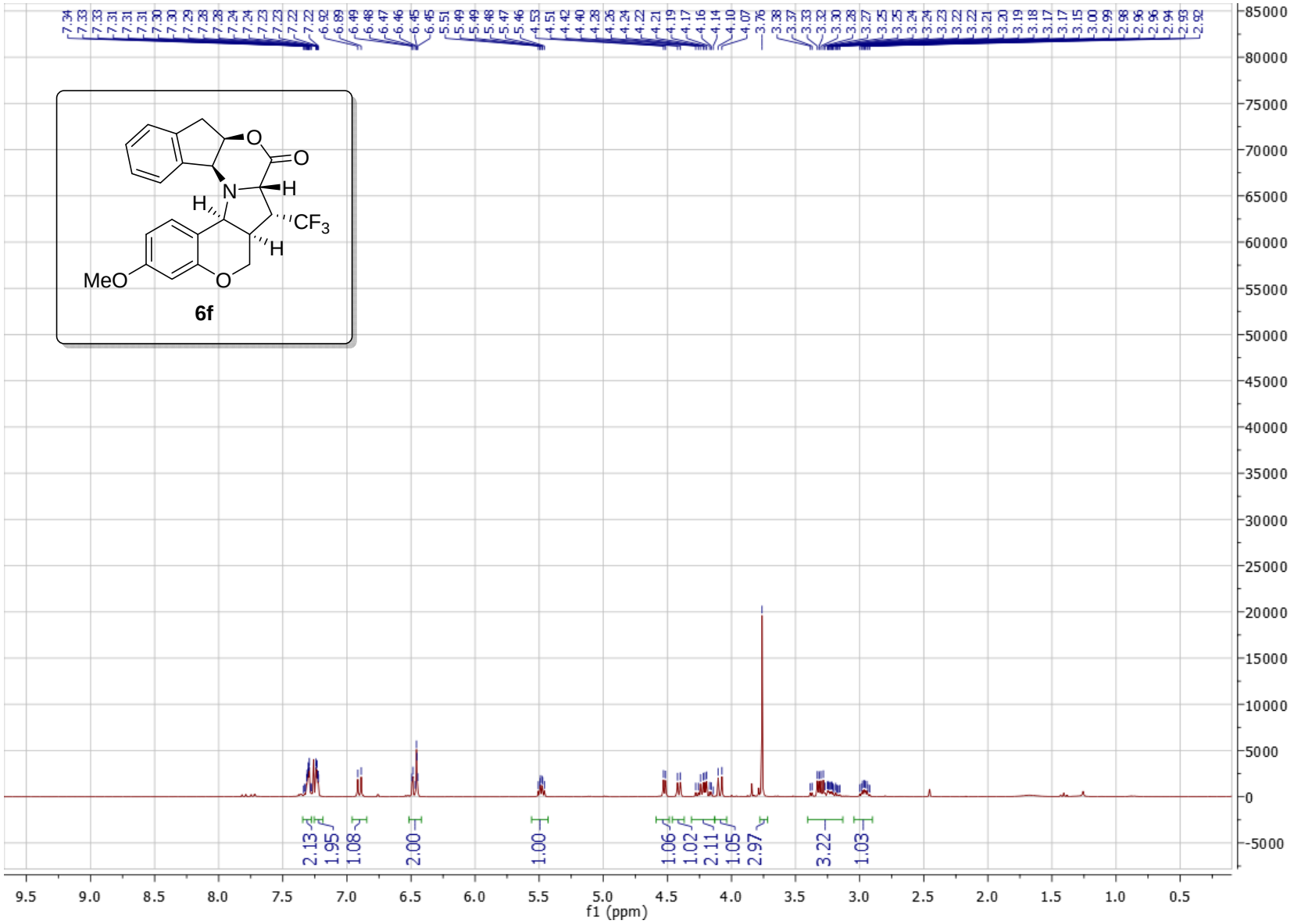
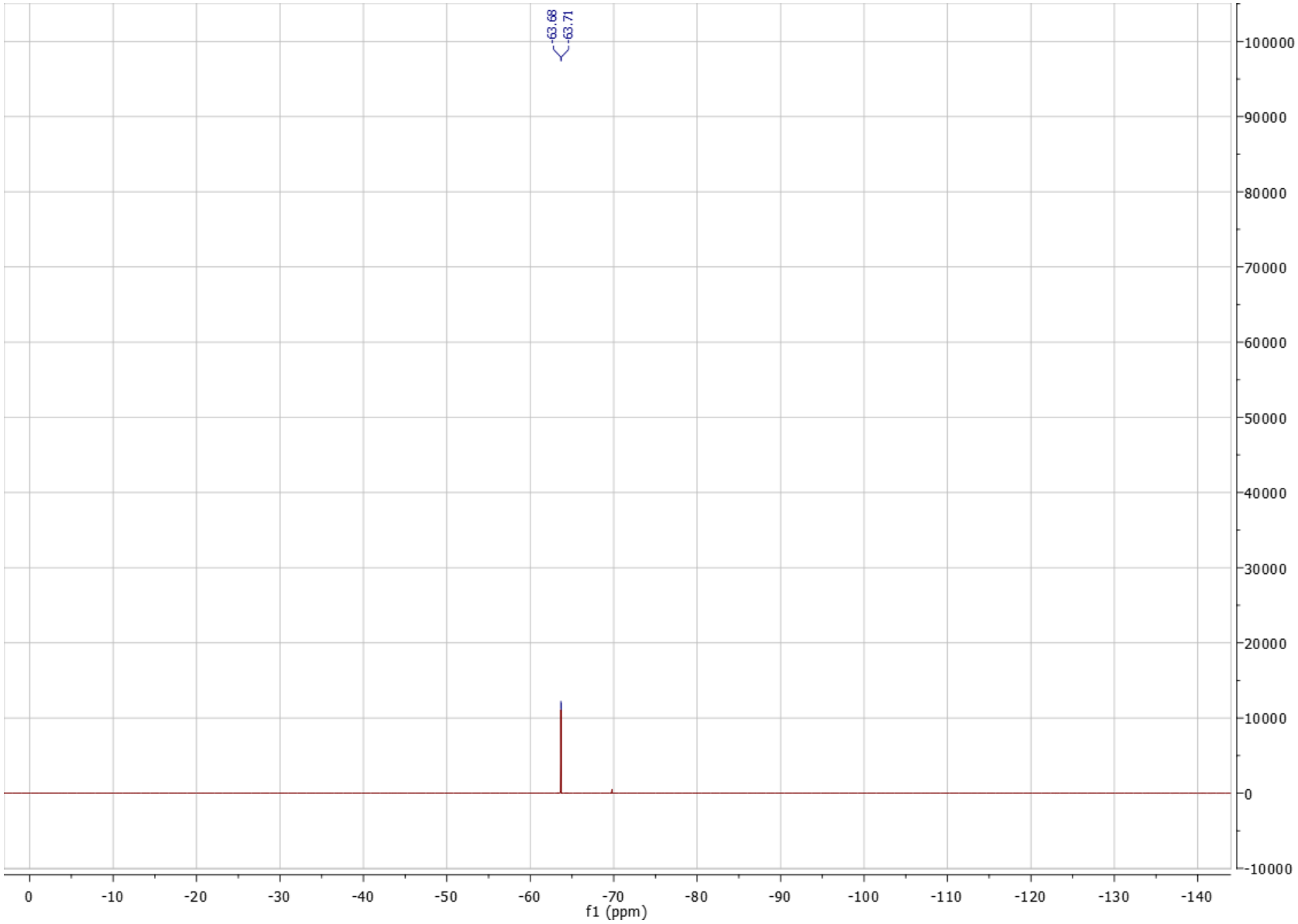
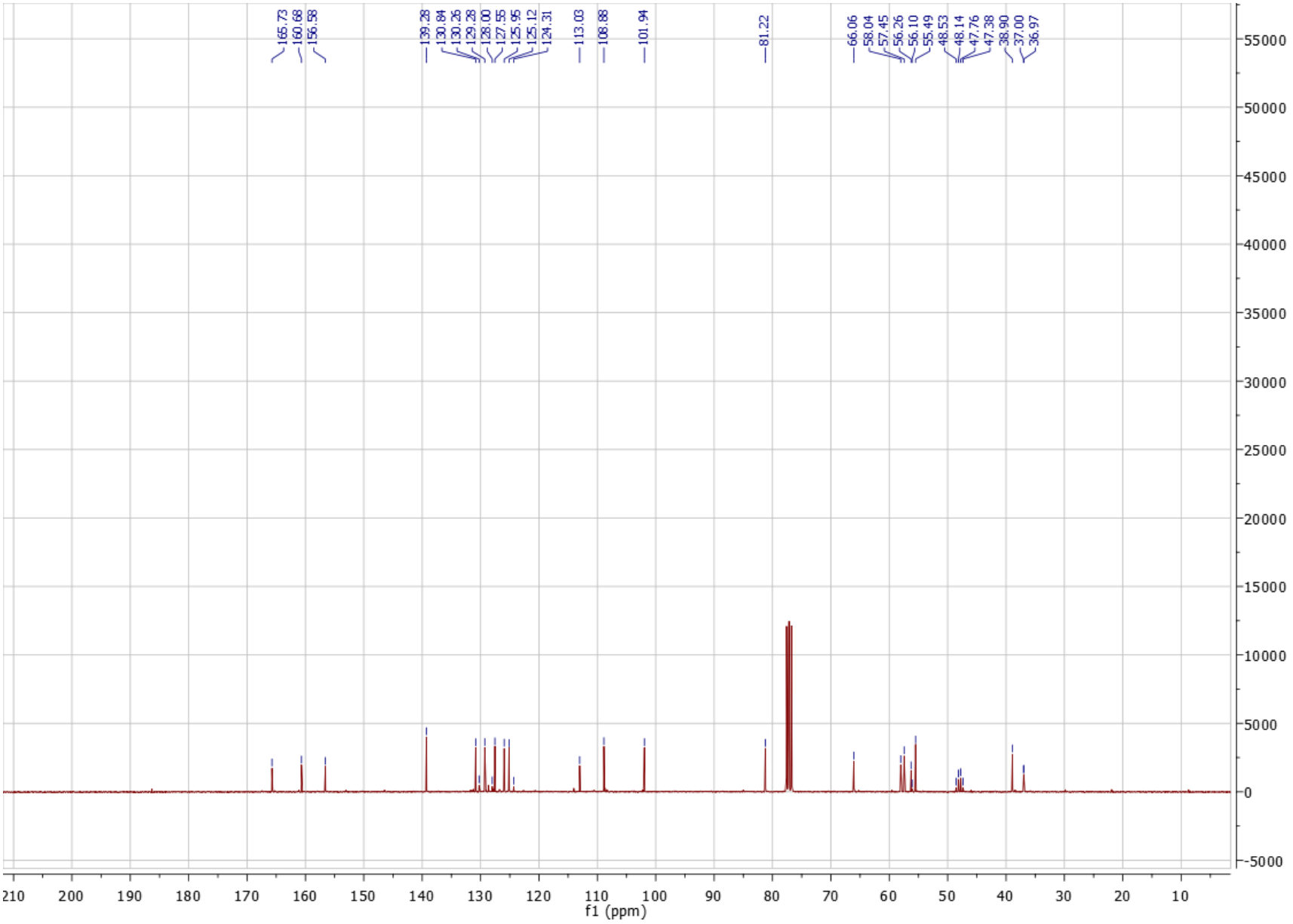
148.65
145.14
139.28
139.25
129.31
127.96
127.55
125.94
125.17
122.01
121.47
121.33
111.10
81.20
66.38
58.16
57.68
56.43
56.08
48.46
48.08
47.70
47.31
38.81
37.09
f1 (ppm)


6f
MeO
O
N
H
CF3
f1 (ppm)


-63.68
-63.71
100000
90000
80000
70000
60000
50000
40000
30000
20000
10000
0
-10000
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
f1 (ppm)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130.26
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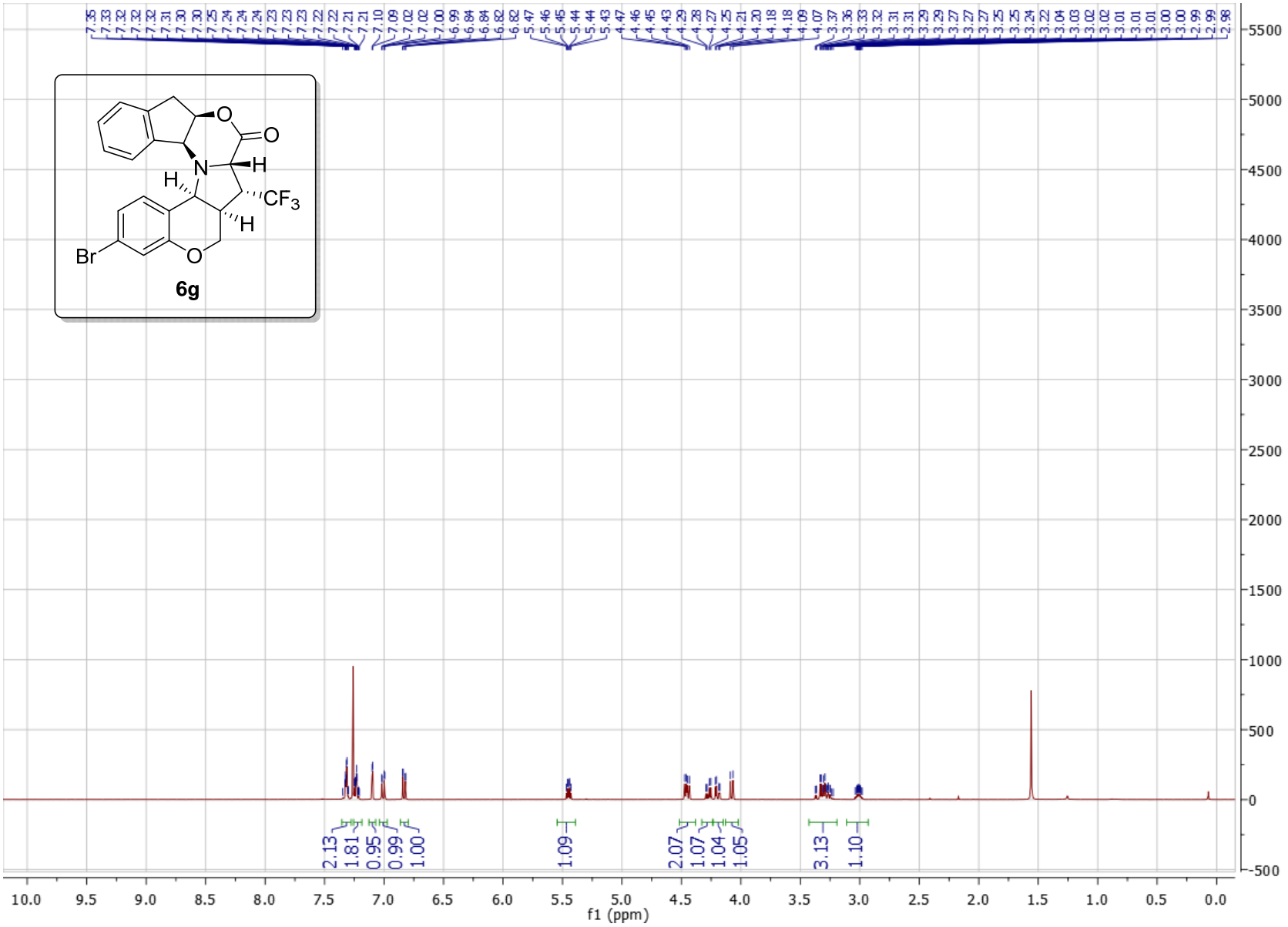
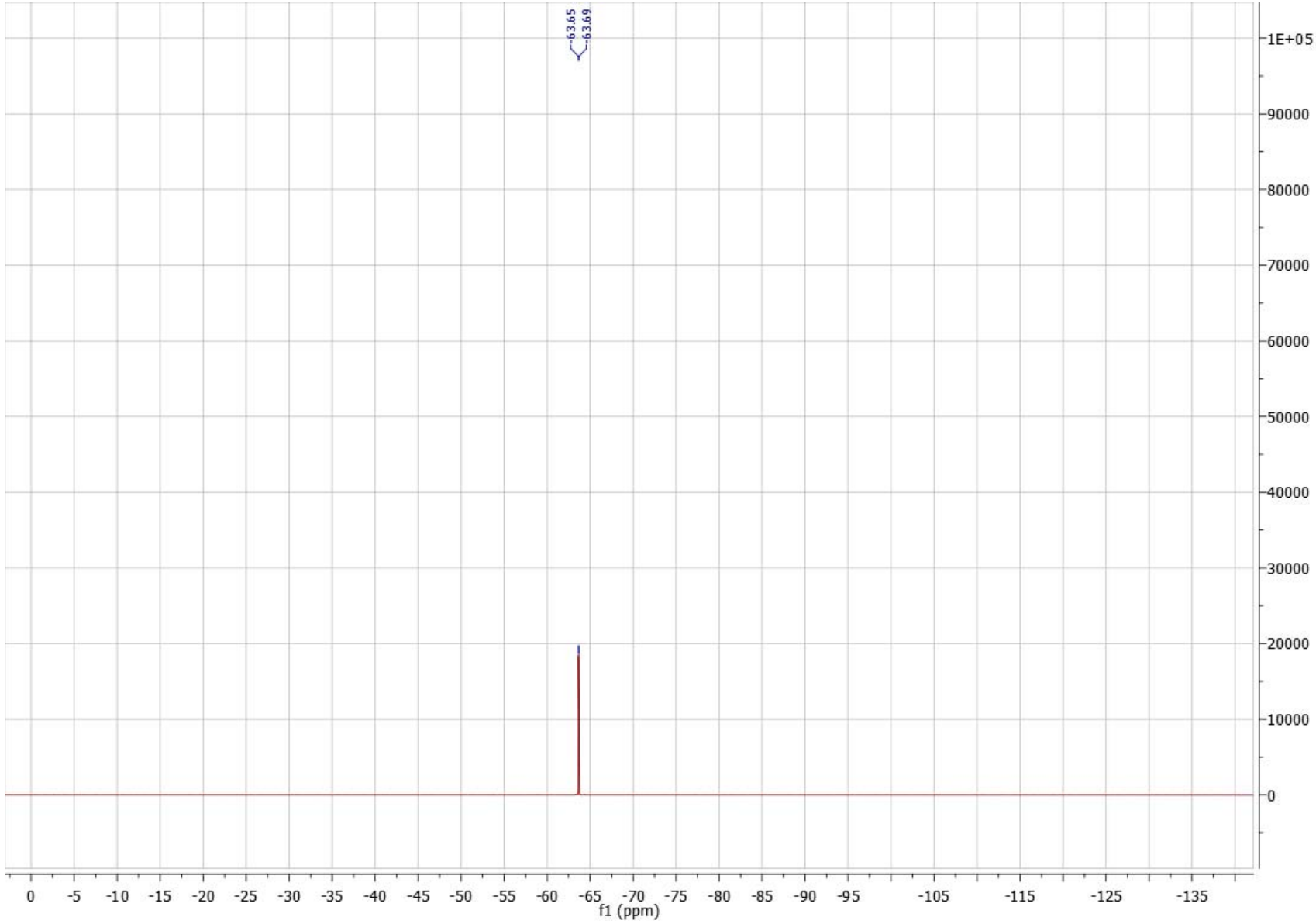
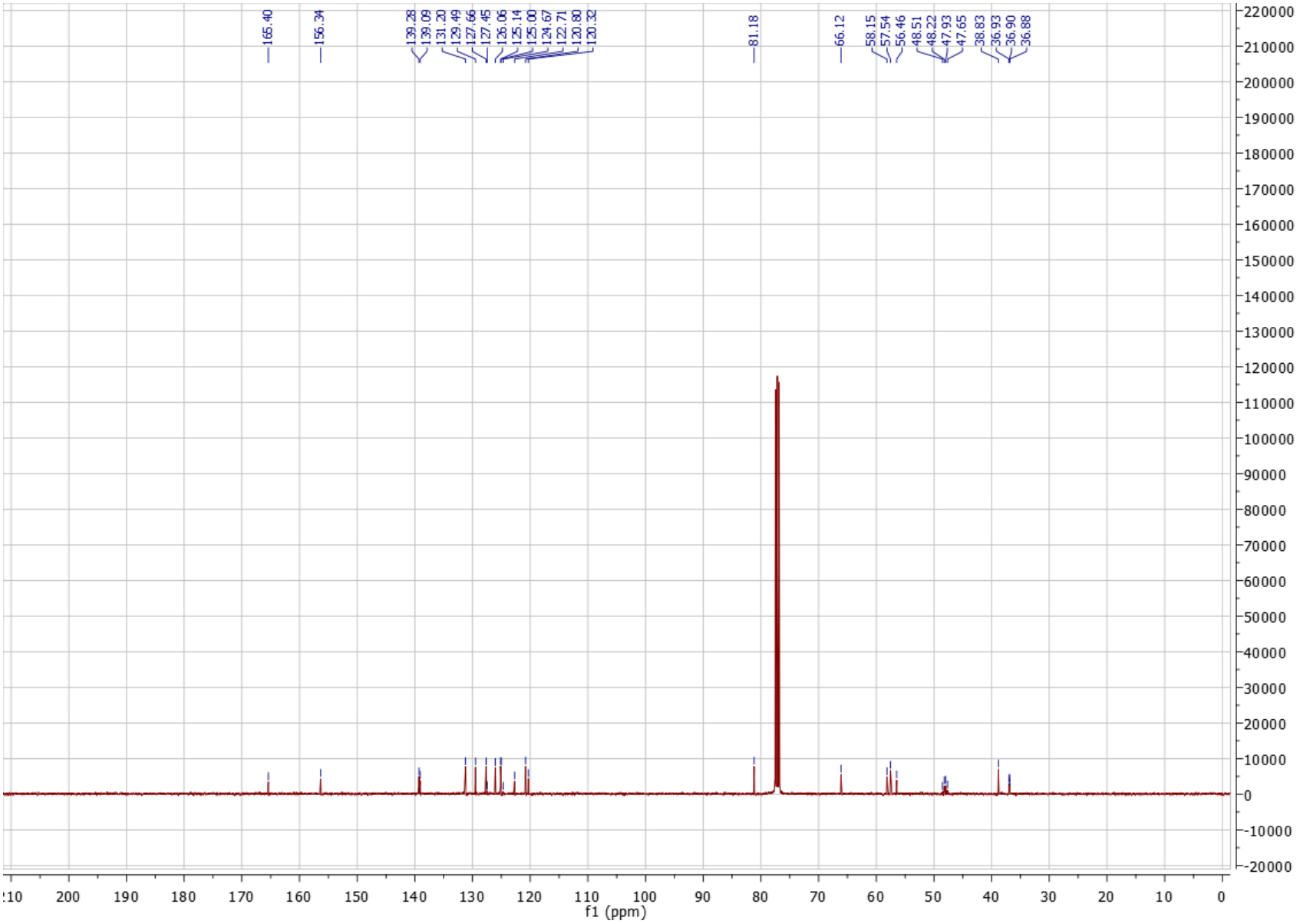
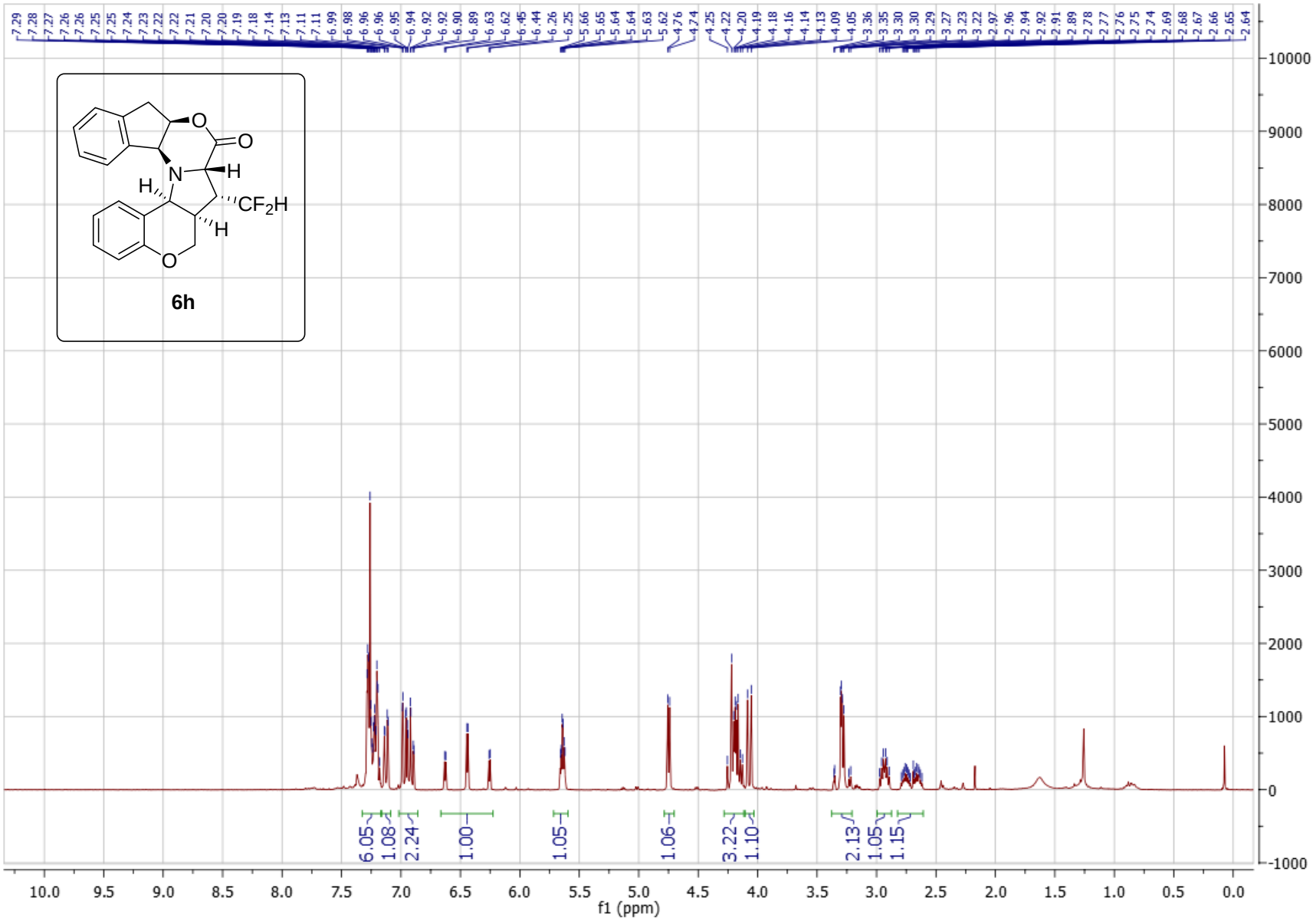
128.00
127.55
125.95
125.12
124.31
113.03
108.88
101.94
81.22
66.06
58.04
57.45
56.26
56.10
55.49
48.53
48.14
47.76
47.38
38.90
37.00
36.97
55000
50000
45000
40000
35000
30000
25000
20000
15000
10000
5000
0
-5000
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)

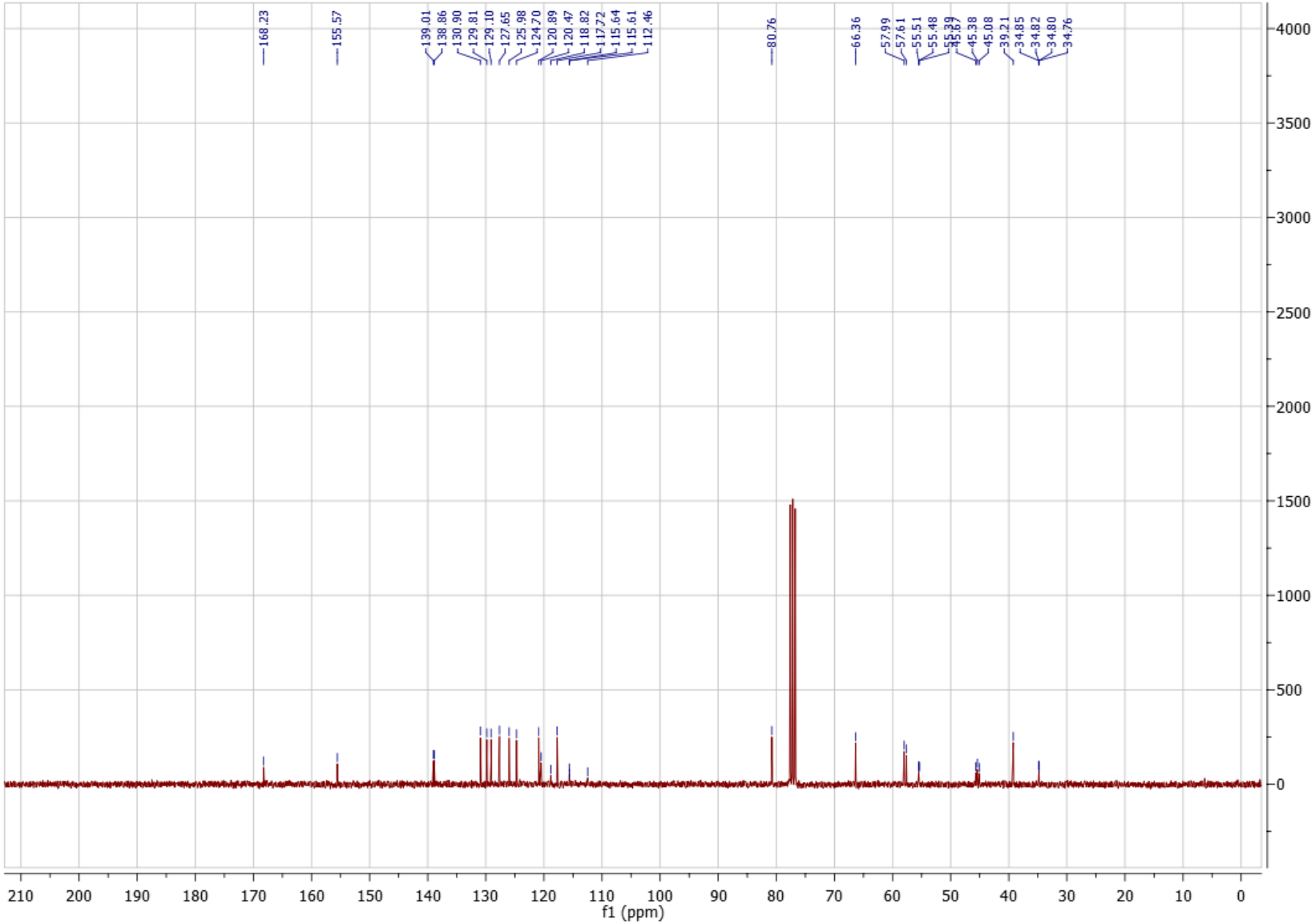

6g
f1 (ppm)


-63.65
-63.69
1E+05
90000
80000
70000
60000
50000
40000
30000
20000
10000
0
0 -5 -10 -15 -20 -25 -30 -35 -40 -45 -50 -55 -60 -65 -70 -75 -80 -85 -90 -95 -105 -115 -125 -135
f1 (ppm)


165.40
156.34
139.28
139.09
131.20
129.49
127.66
127.45
126.06
125.14
125.00
124.67
122.71
120.80
120.32
81.18
66.12
58.15
57.54
56.46
48.51
48.22
47.93
47.65
38.83
36.93
36.90
36.88
f1 (ppm)


6h
f1 (ppm)


118.03
118.05
118.23
118.25
119.04
119.07
119.24
119.26
124.47
124.57
124.66
124.77
125.48
125.58
125.68
125.78
10000
9000
8000
7000
6000
5000
4000
3000
2000
1000
0
-1000
1.00
0.88
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
f1 (ppm)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155.57
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129.81
129.10
127.65
125.98
124.70
120.89
120.47
118.82
117.72
115.64
115.61
112.46
80.76
66.36
57.99
57.61
55.51
55.48
45.38
45.08
39.21
34.85
34.82
34.80
34.76
4000
3500
3000
2500
2000
1500
1000
500
0
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
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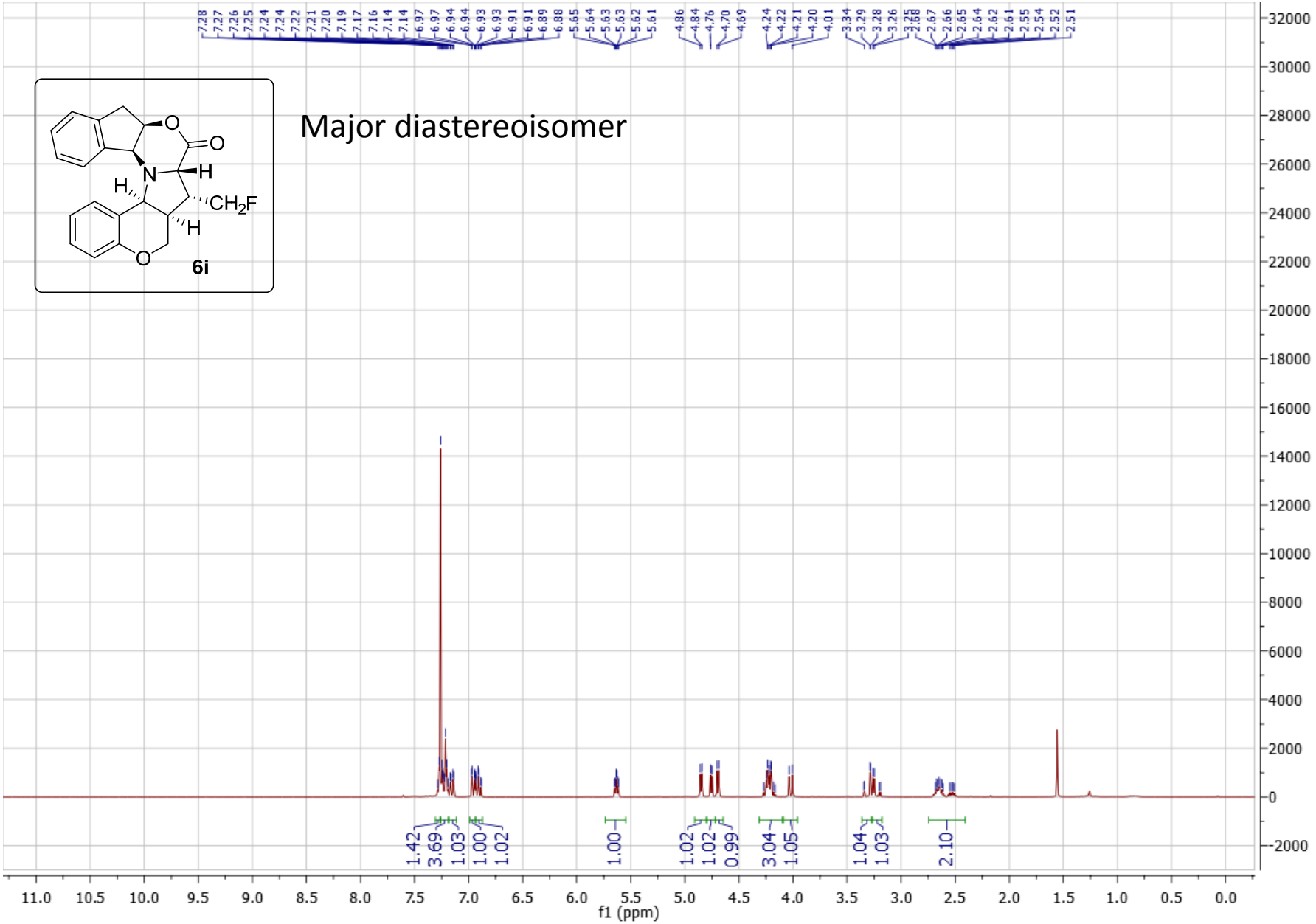
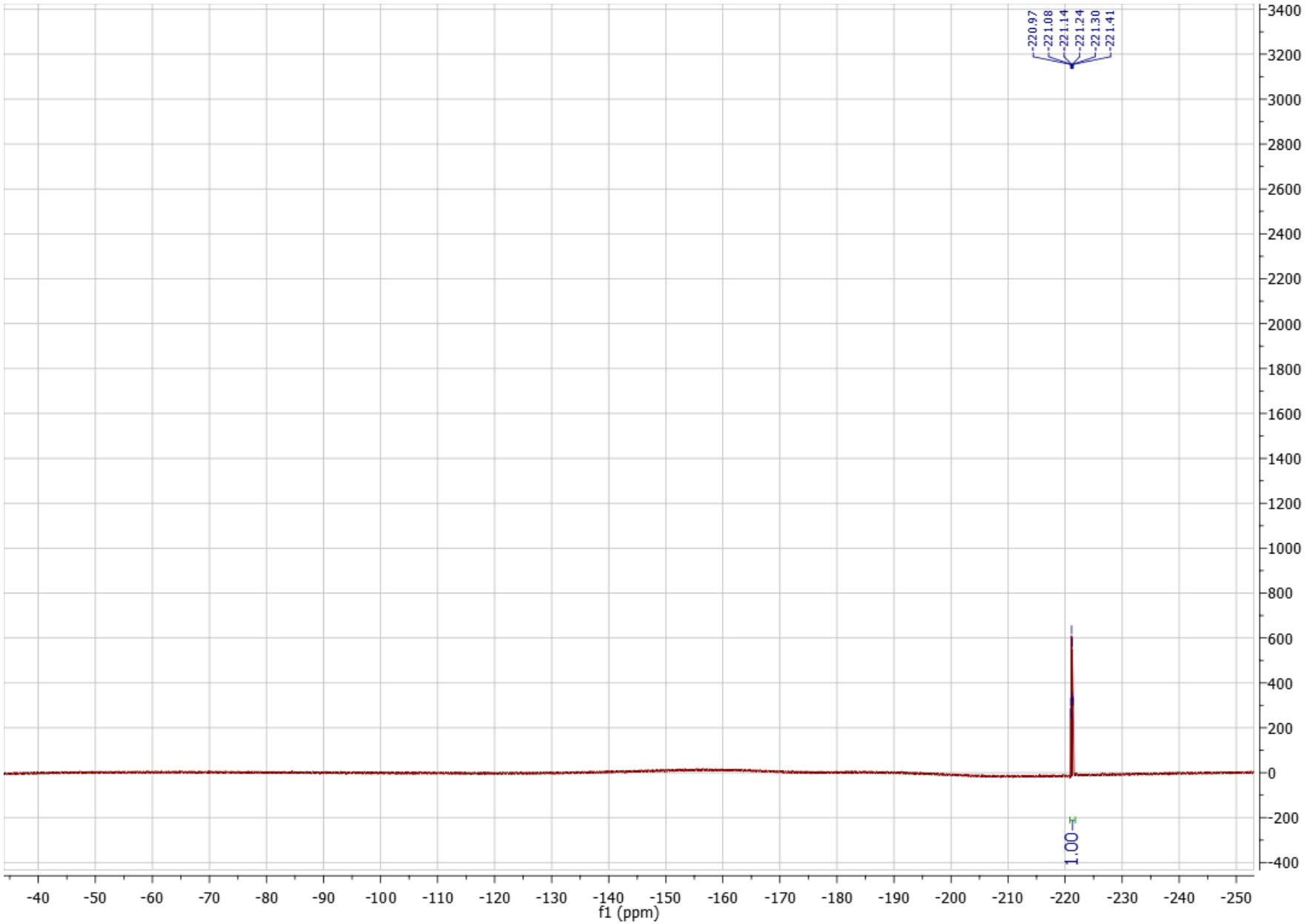
50
40
30
20
10
0
f1 (ppm)


Major diastereoisomer
6i
f1 (ppm)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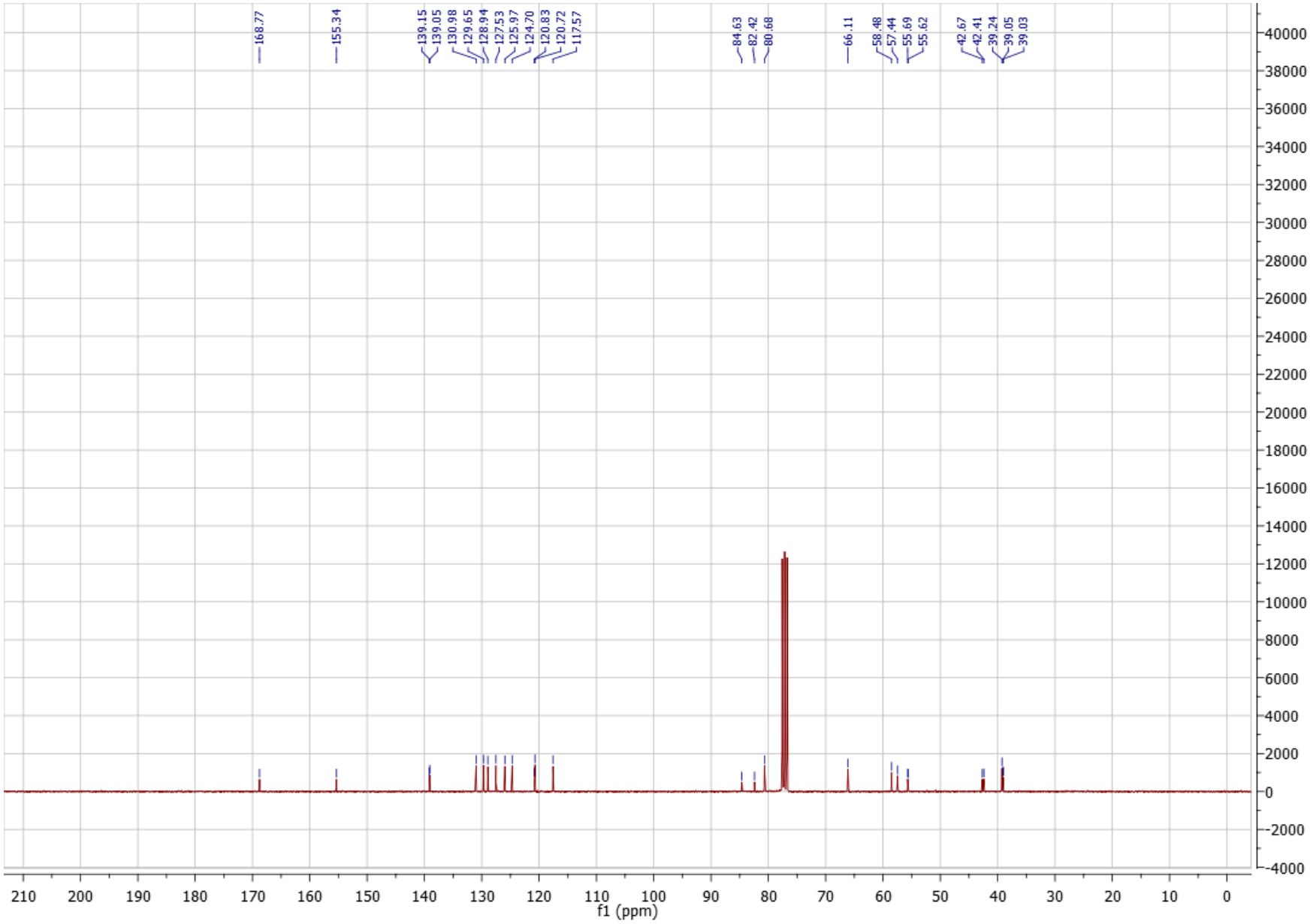
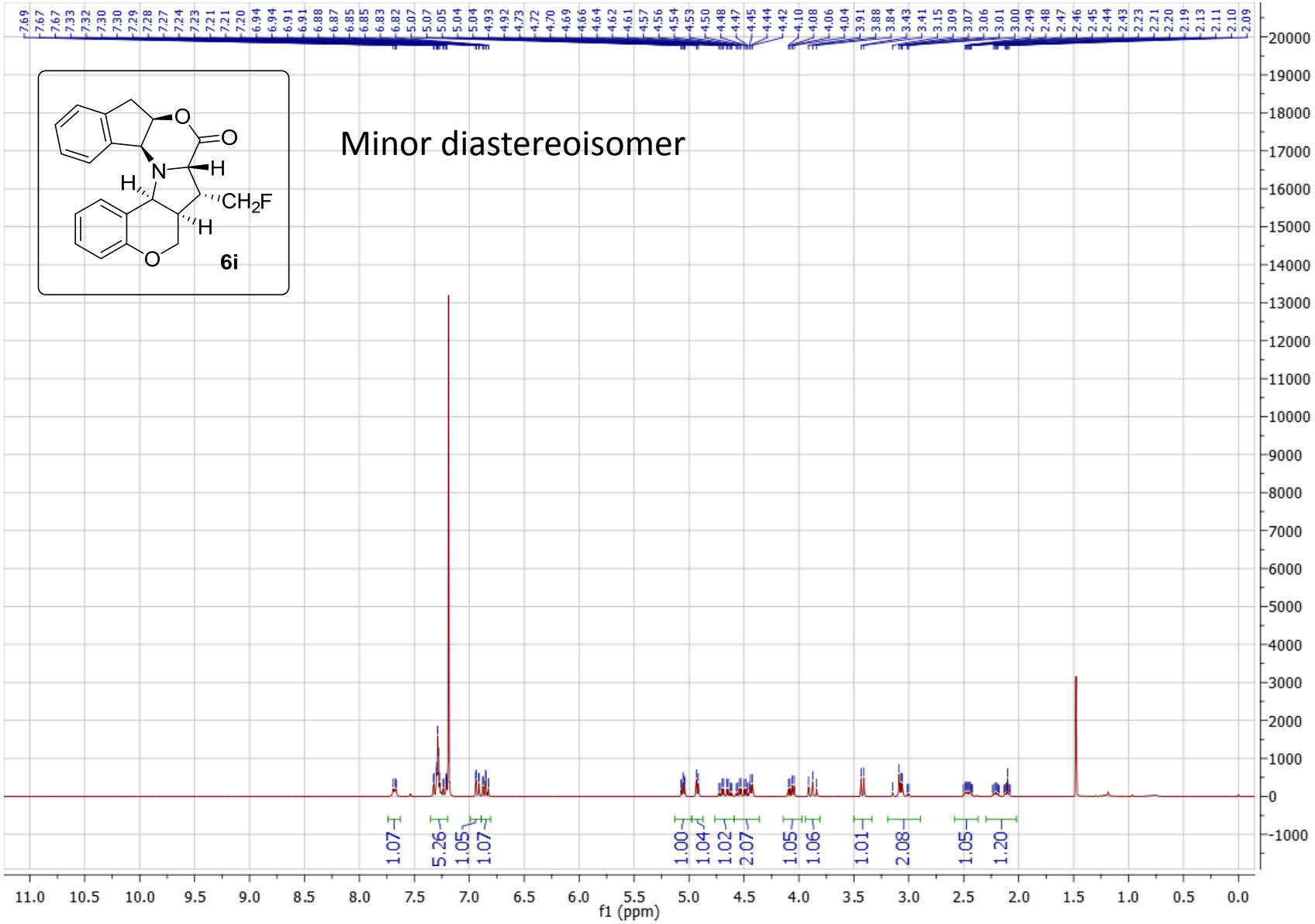
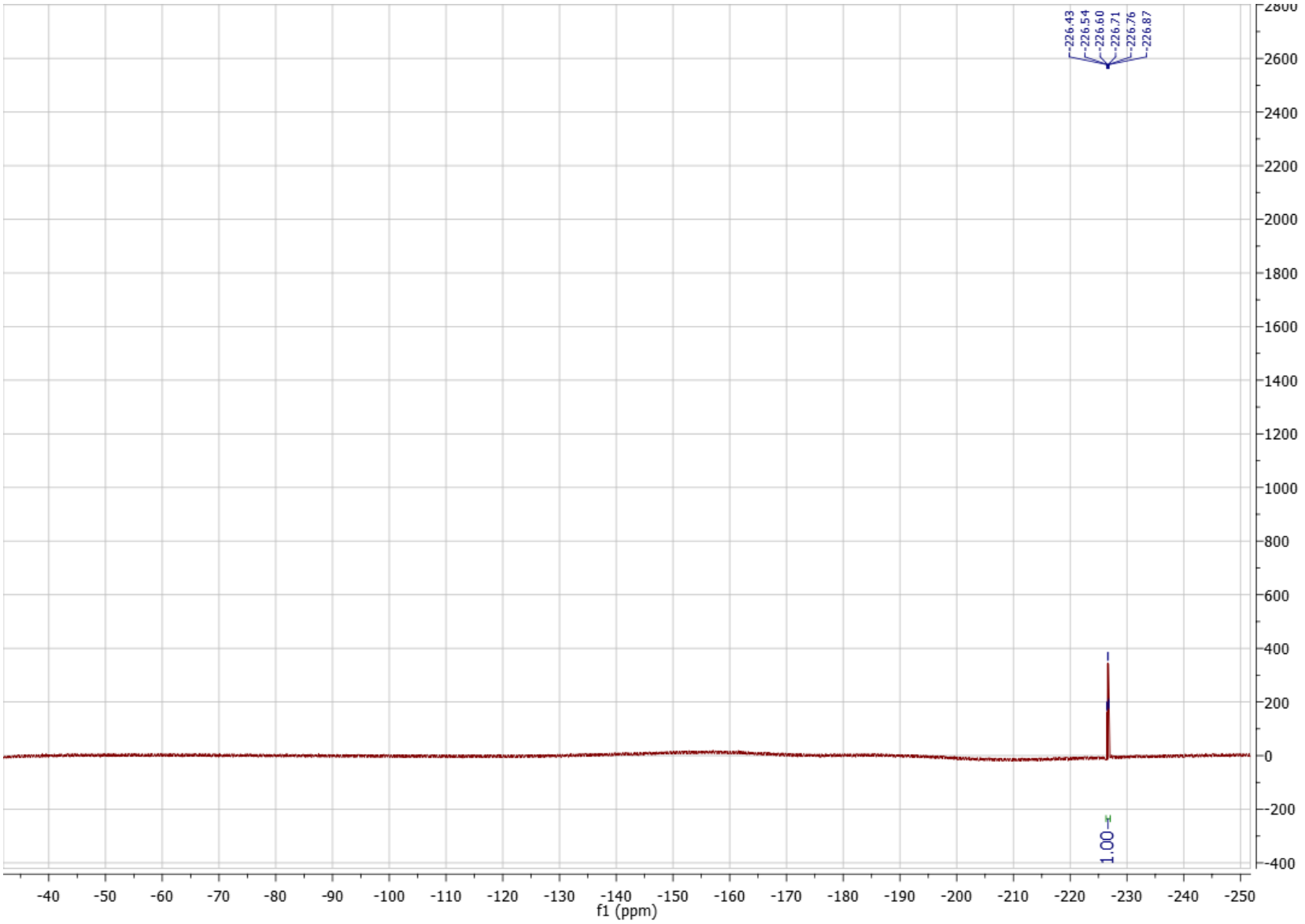
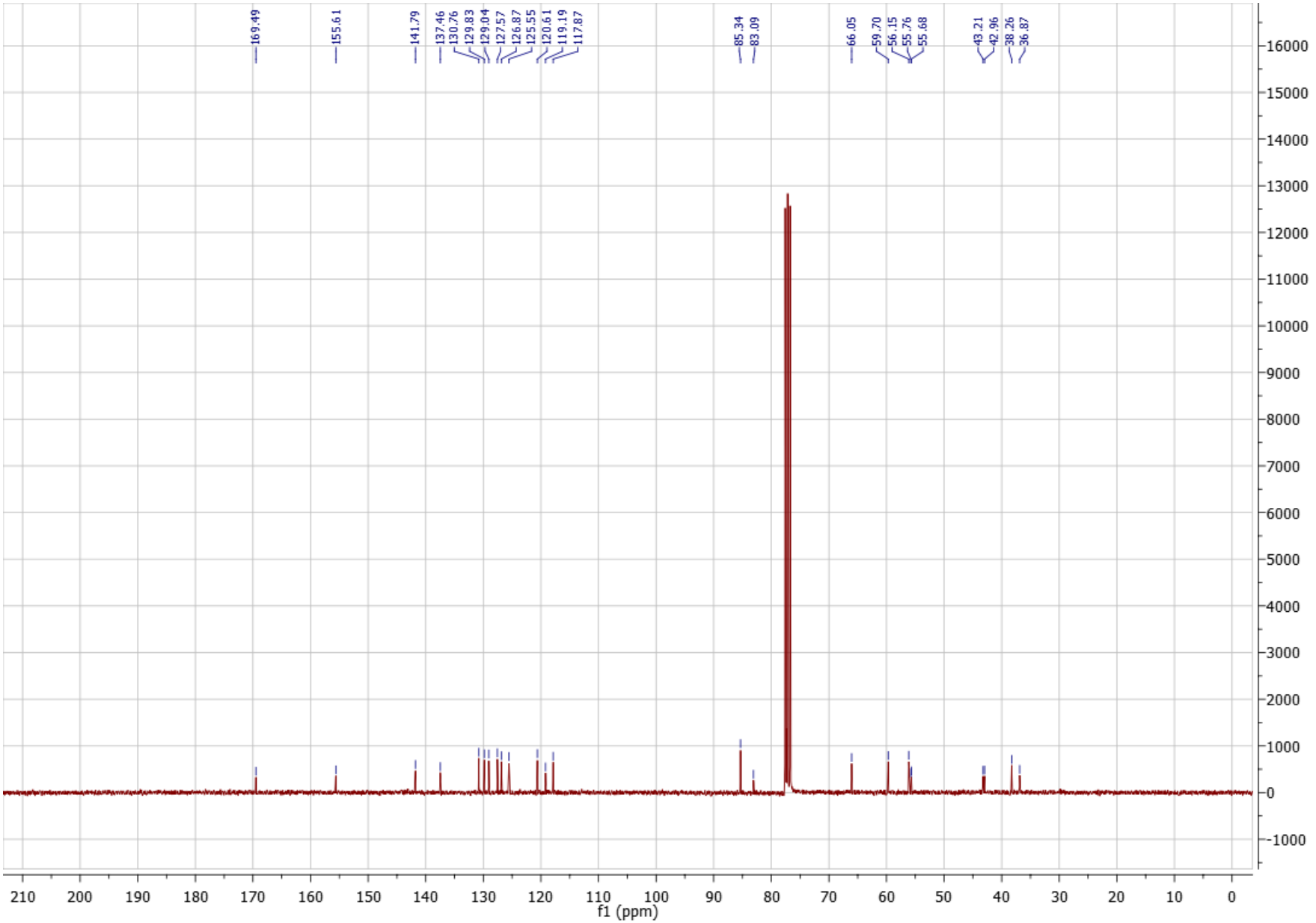
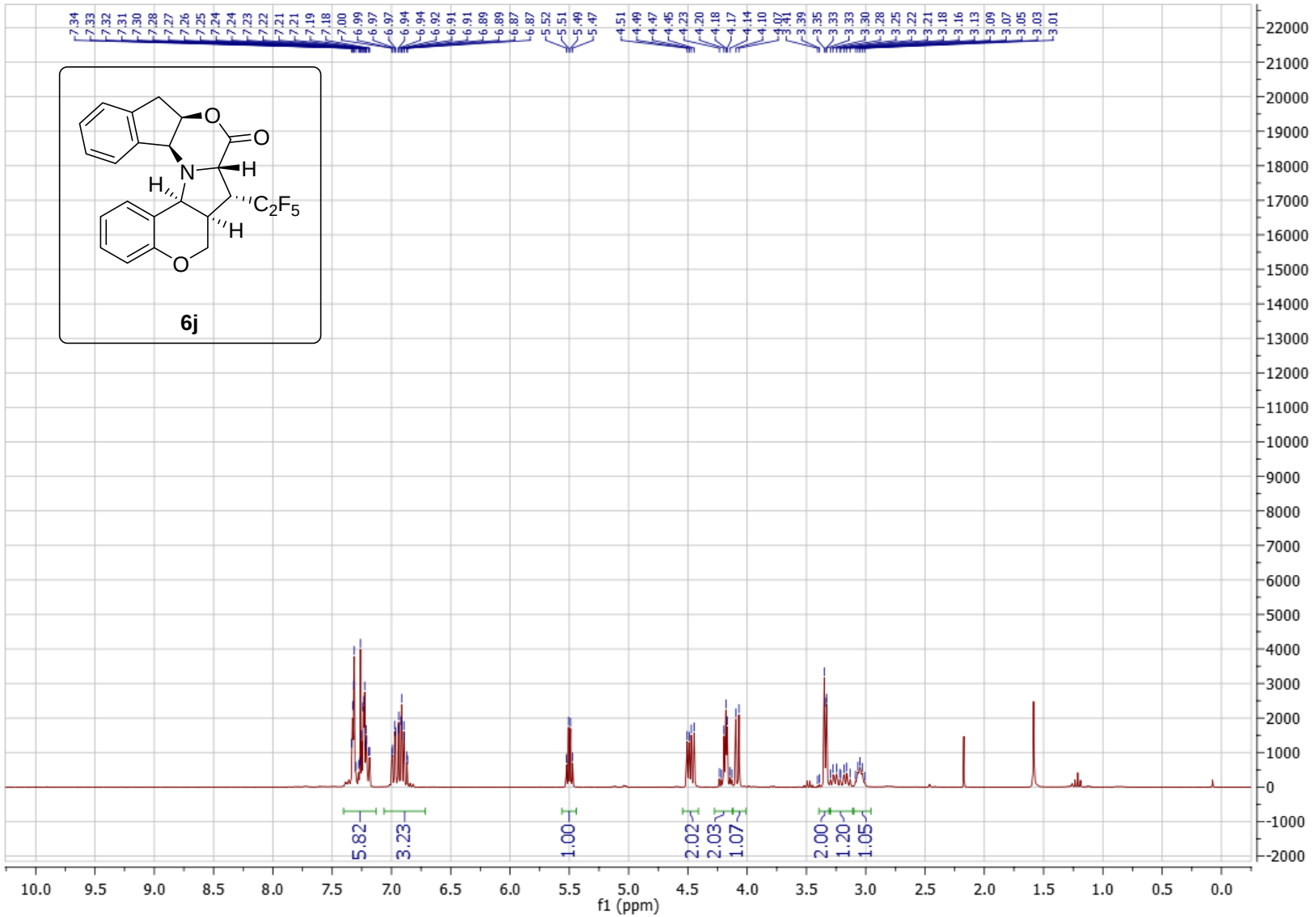
-221.08
-221.14
-221.24
-221.30
-221.41
1.00
f1 (ppm)

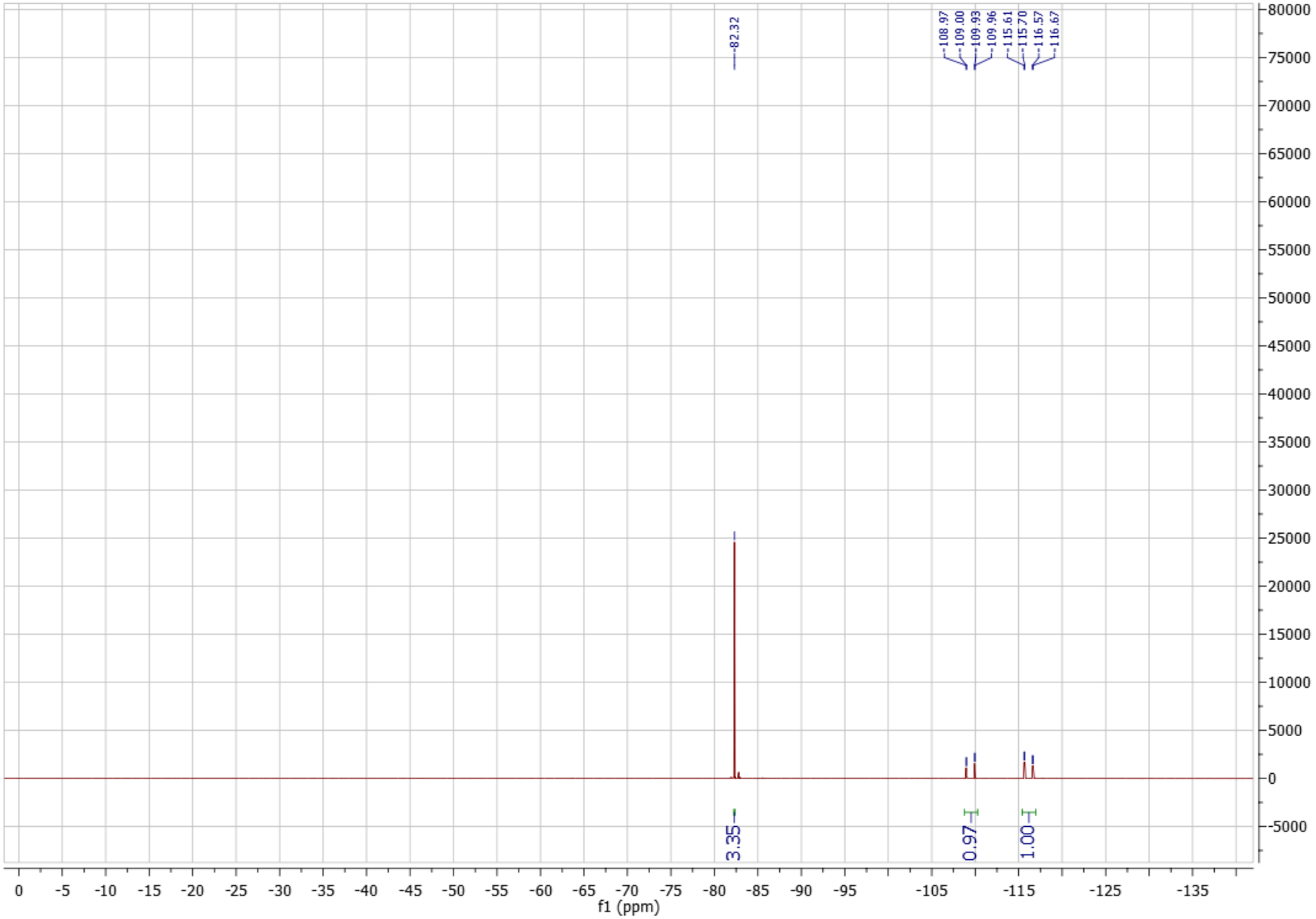

168.77
155.34
139.15
139.05
130.98
129.65
128.94
127.53
125.97
124.70
120.83
120.72
117.57
84.63
82.42
80.68
66.11
58.48
57.44
55.69
55.62
42.67
42.41
39.24
39.05
39.03
f1 (ppm)

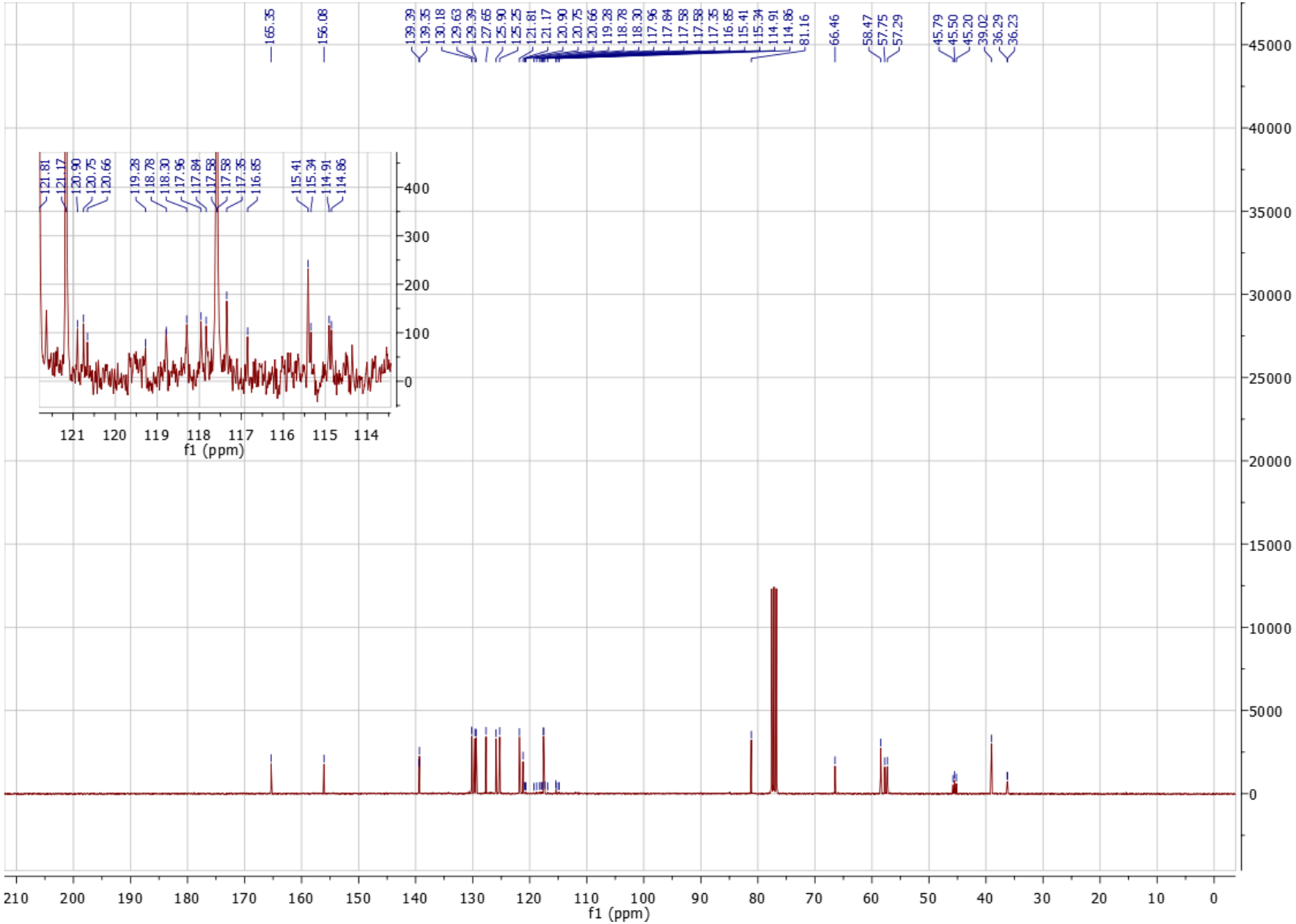

Minor diastereoisomer
6i
f1 (ppm)

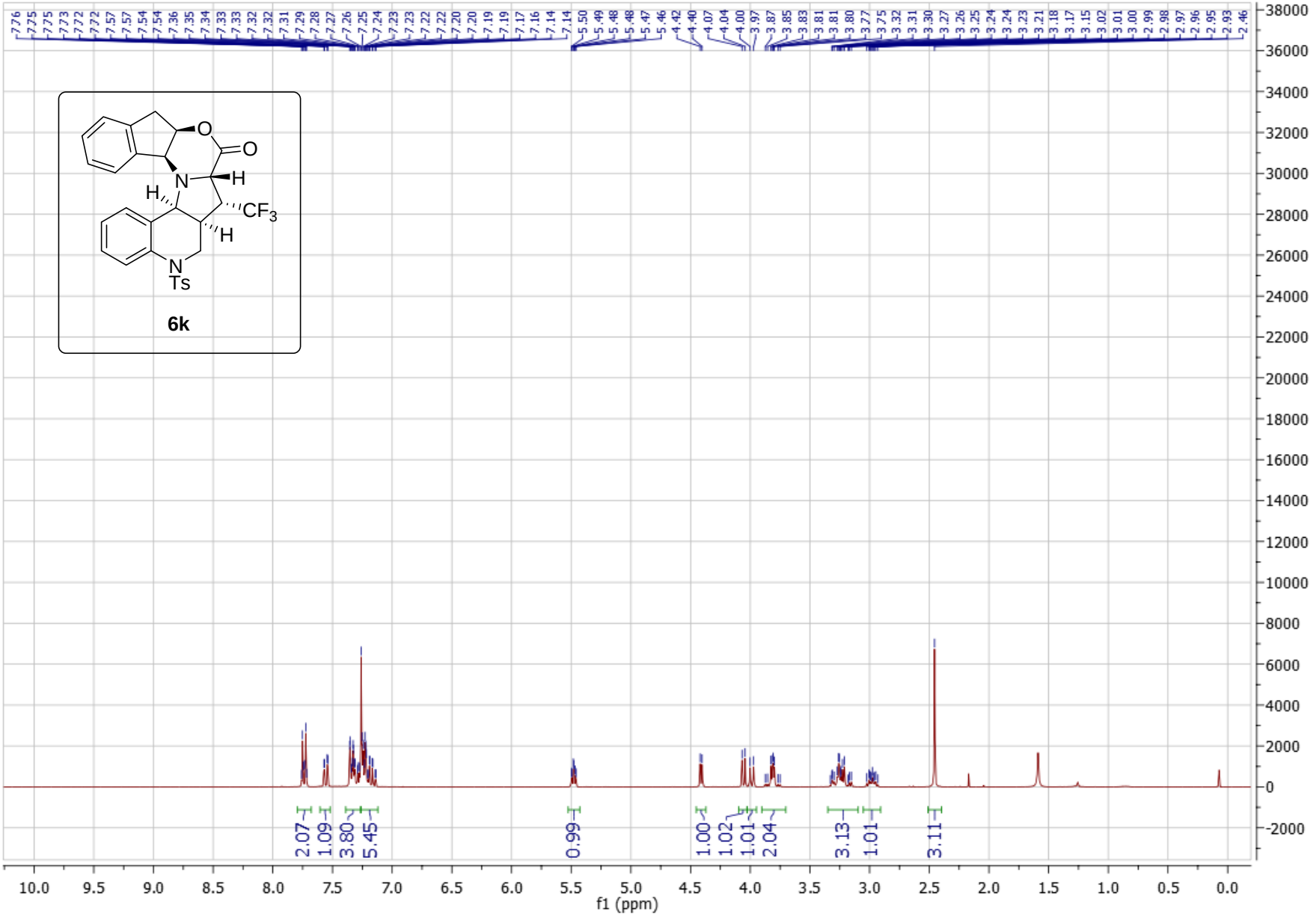

226.43
226.54
226.60
226.71
226.76
226.87
1.00
f1 (ppm)

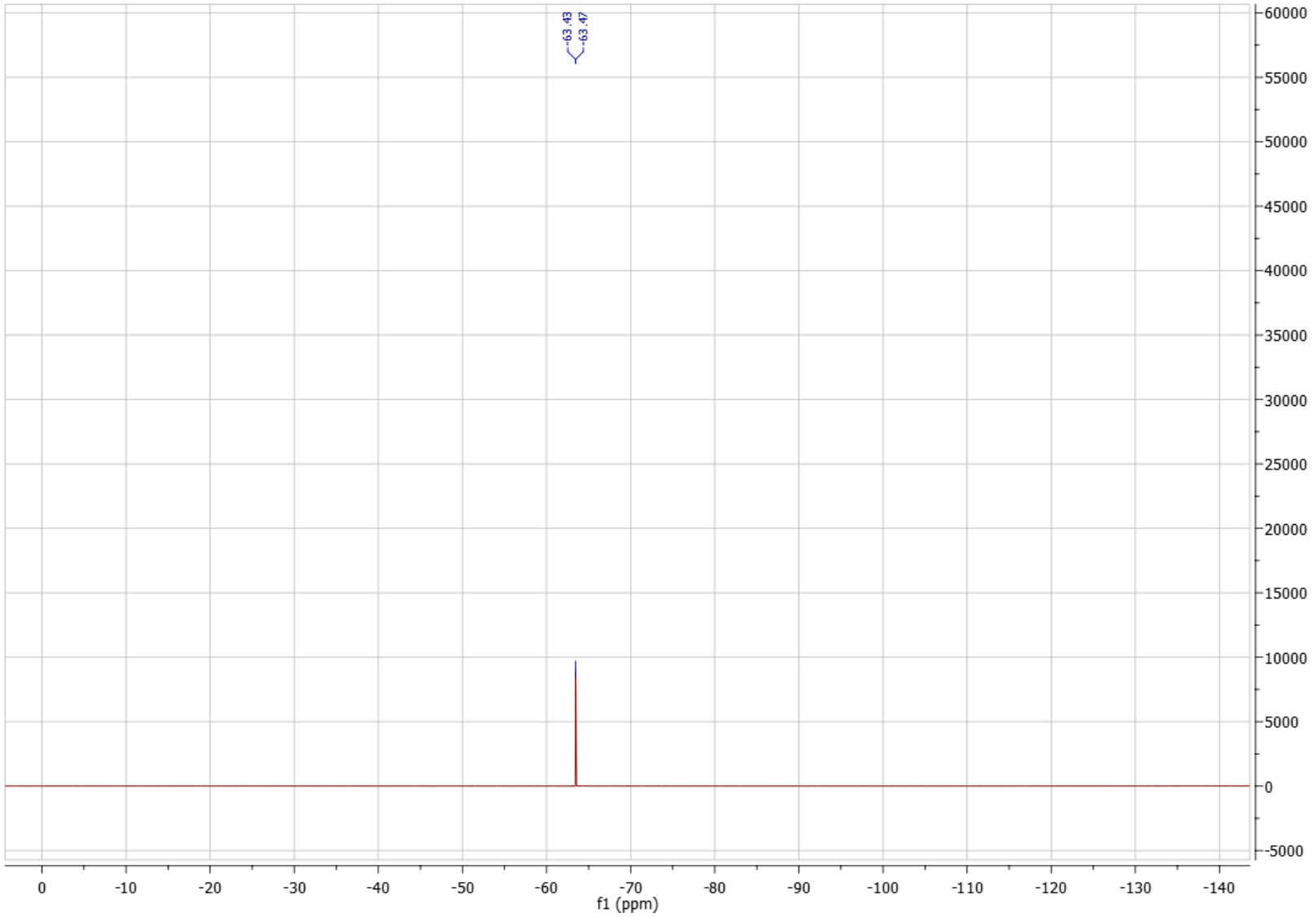

169.49
155.61
141.79
137.46
130.76
129.83
129.04
127.57
126.87
125.55
120.61
119.19
117.87
85.34
83.09
66.05
59.70
56.15
55.76
55.68
43.21
42.96
38.26
36.87
f1 (ppm)


6j
f1 (ppm)
5.82
3.23
1.00
2.02
2.03
1.07
2.00
1.20
1.05


-82.32
-108.97
-109.00
-109.93
-109.96
-115.61
-115.70
-116.57
-116.67
3.35
0.97
1.00
f1 (ppm)


165.35
156.08
139.39
139.35
130.18
129.63
129.39
127.65
125.90
125.25
121.81
121.17
120.90
120.75
120.66
119.28
118.78
118.30
117.96
117.84
117.58
117.58
117.35
116.85
115.41
115.34
114.91
114.86
81.16
66.46
58.47
57.75
57.29
45.79
45.50
45.20
39.02
36.29
36.23
f1 (ppm)


6k
f1 (ppm)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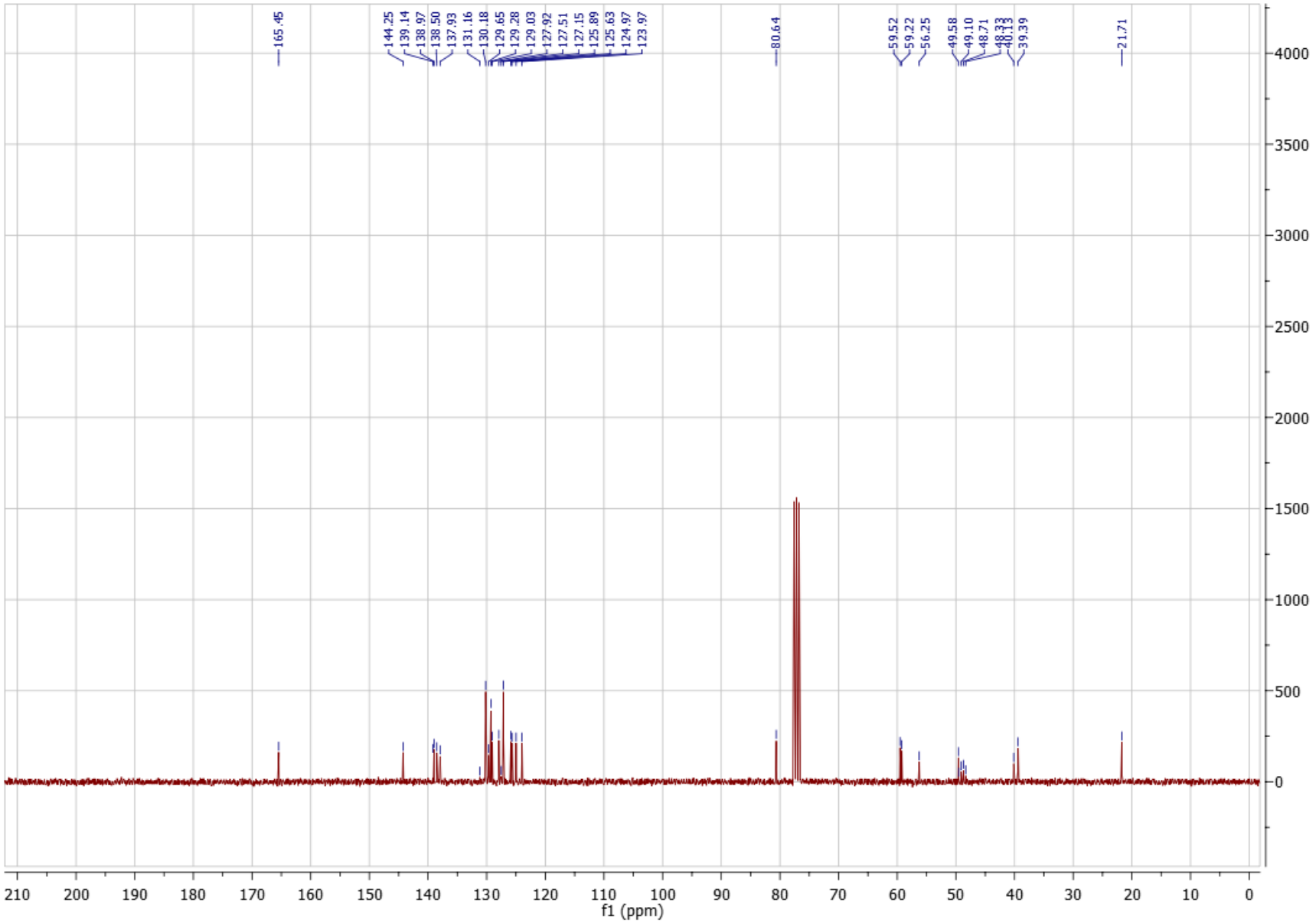
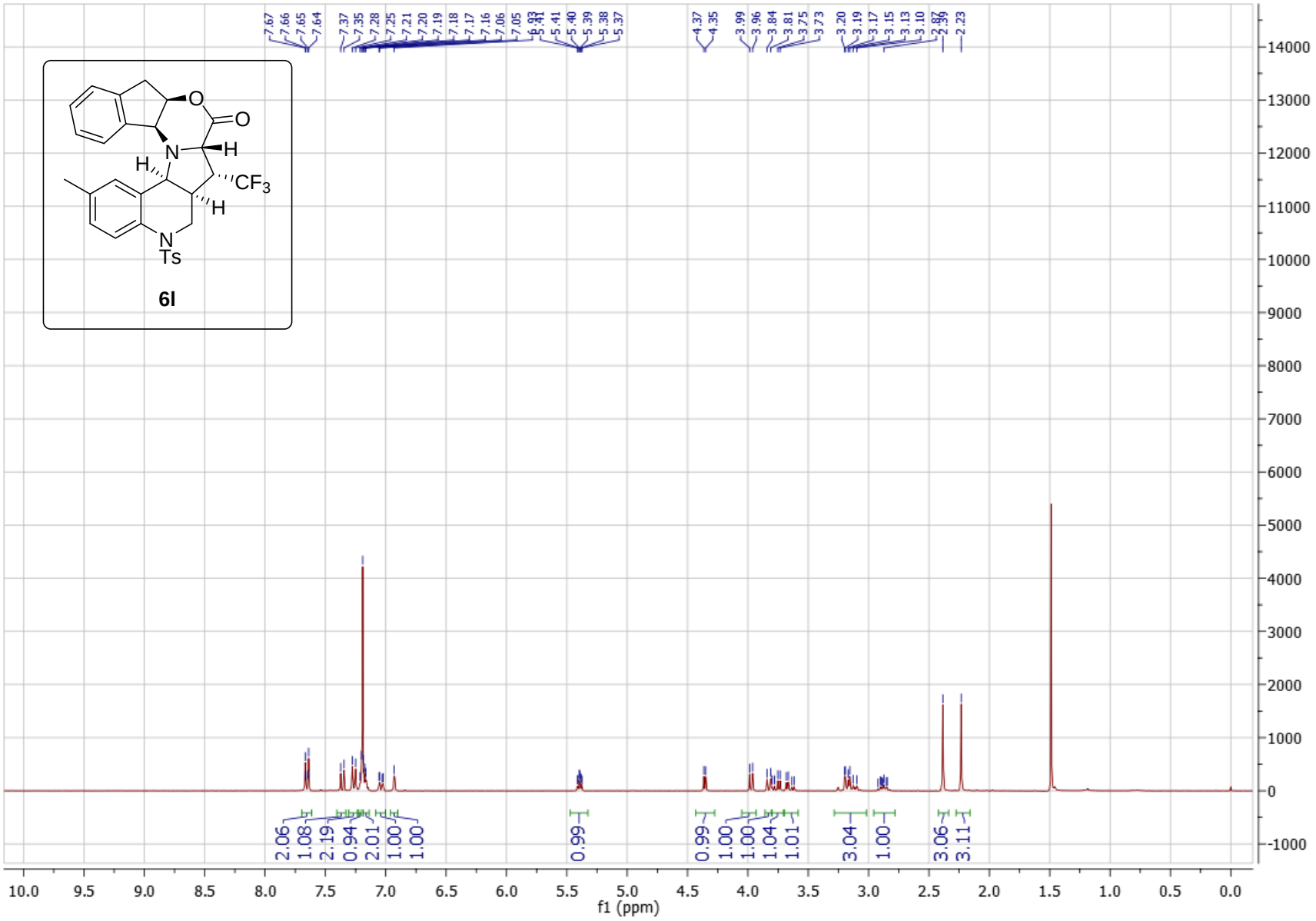
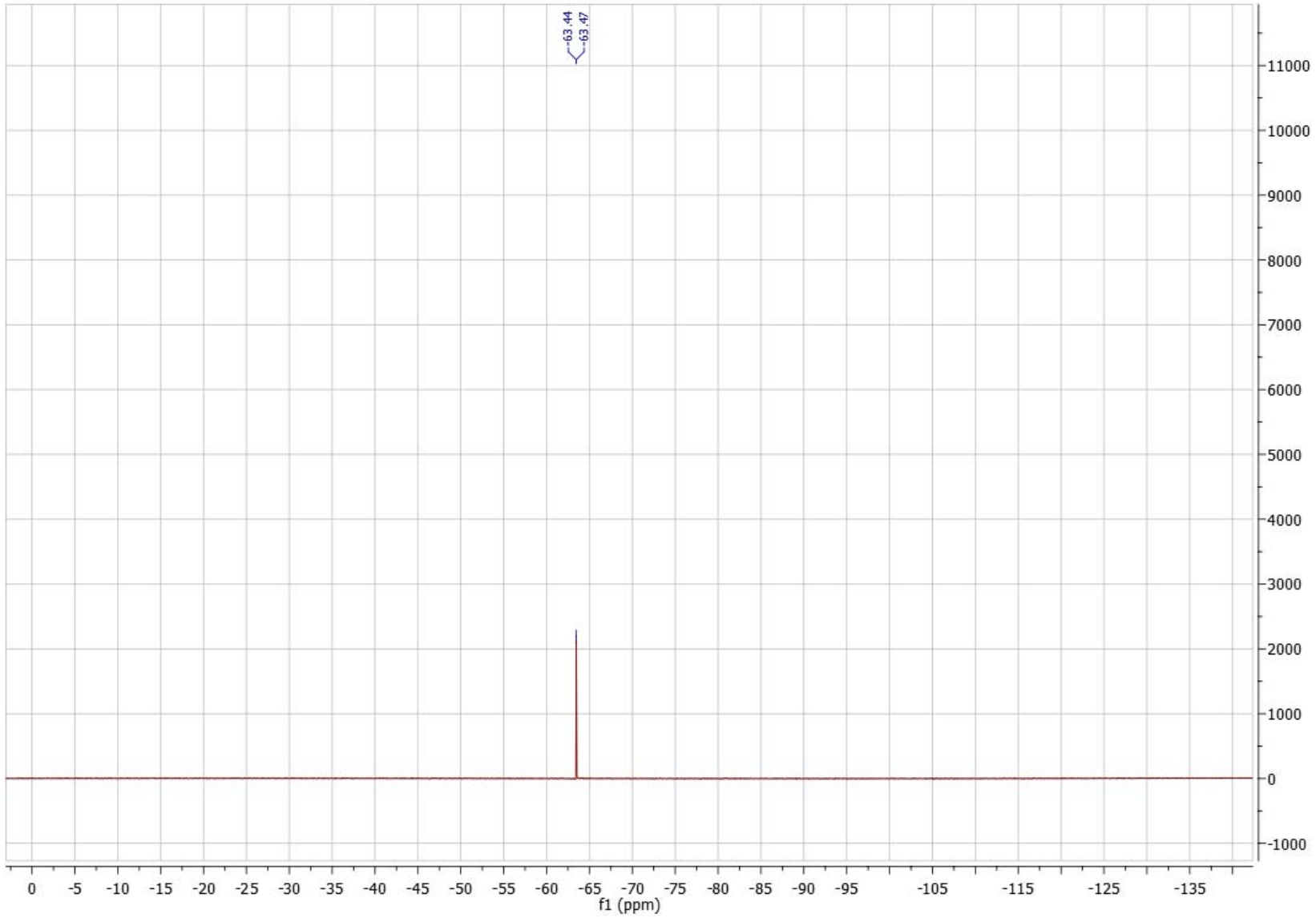
-63.47
60000
55000
50000
45000
40000
35000
30000
25000
20000
15000
10000
5000
0
-5000
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
f1 (ppm)


165.45
144.25
139.14
138.97
138.50
137.93
131.16
130.18
129.65
129.28
129.03
127.92
127.51
127.15
125.89
125.63
124.97
123.97
80.64
59.52
59.22
56.25
49.58
49.10
48.71
48.33
40.13
39.39
21.71
4000
3500
3000
2500
2000
1500
1000
500
0
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


6l
f1 (ppm)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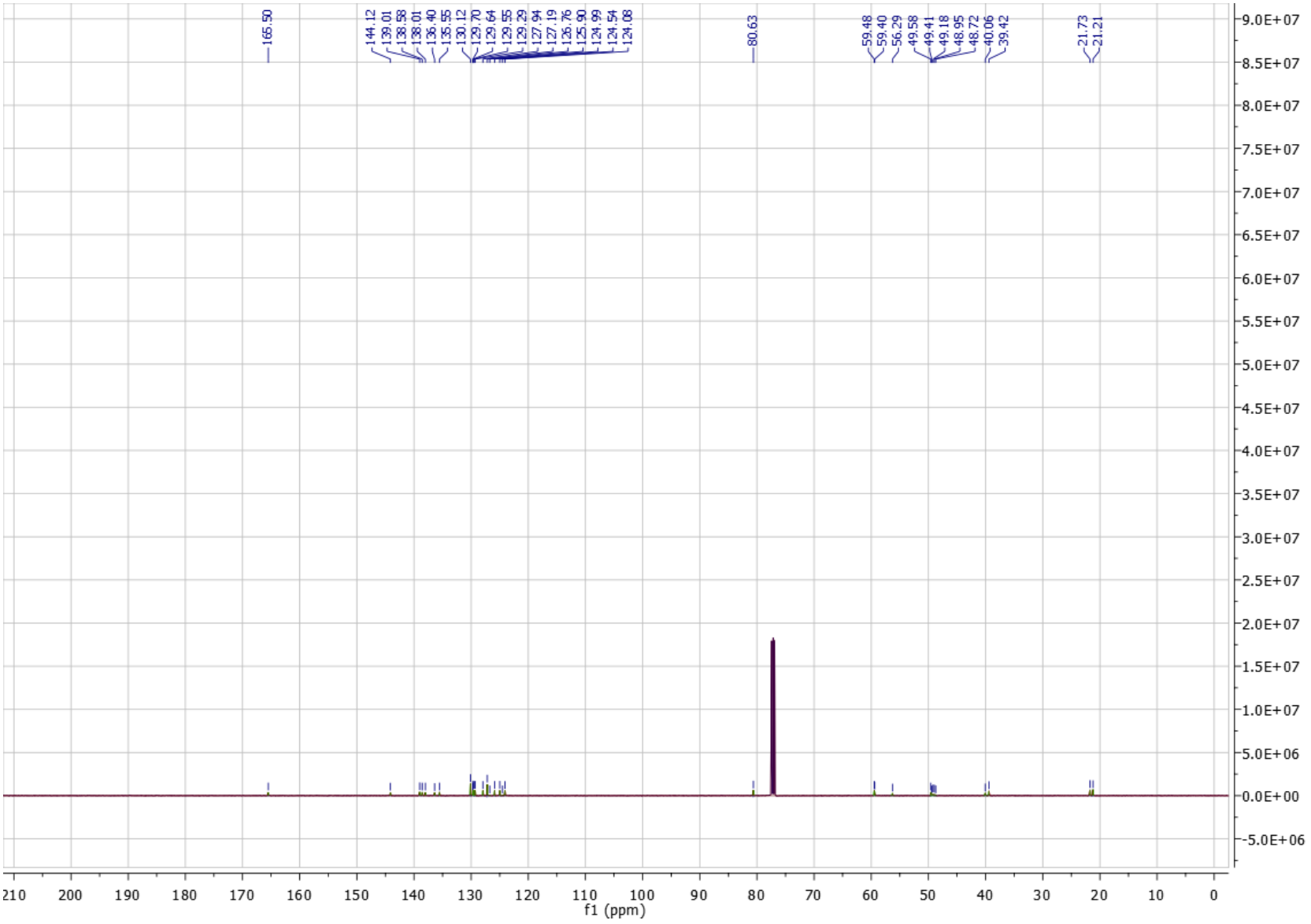
-63.47
11000
10000
9000
8000
7000
6000
5000
4000
3000
2000
1000
0
-1000
0 -5 -10 -15 -20 -25 -30 -35 -40 -45 -50 -55 -60 -65 -70 -75 -80 -85 -90 -95 -105 -115 -125 -135
f1 (ppm)


165.50
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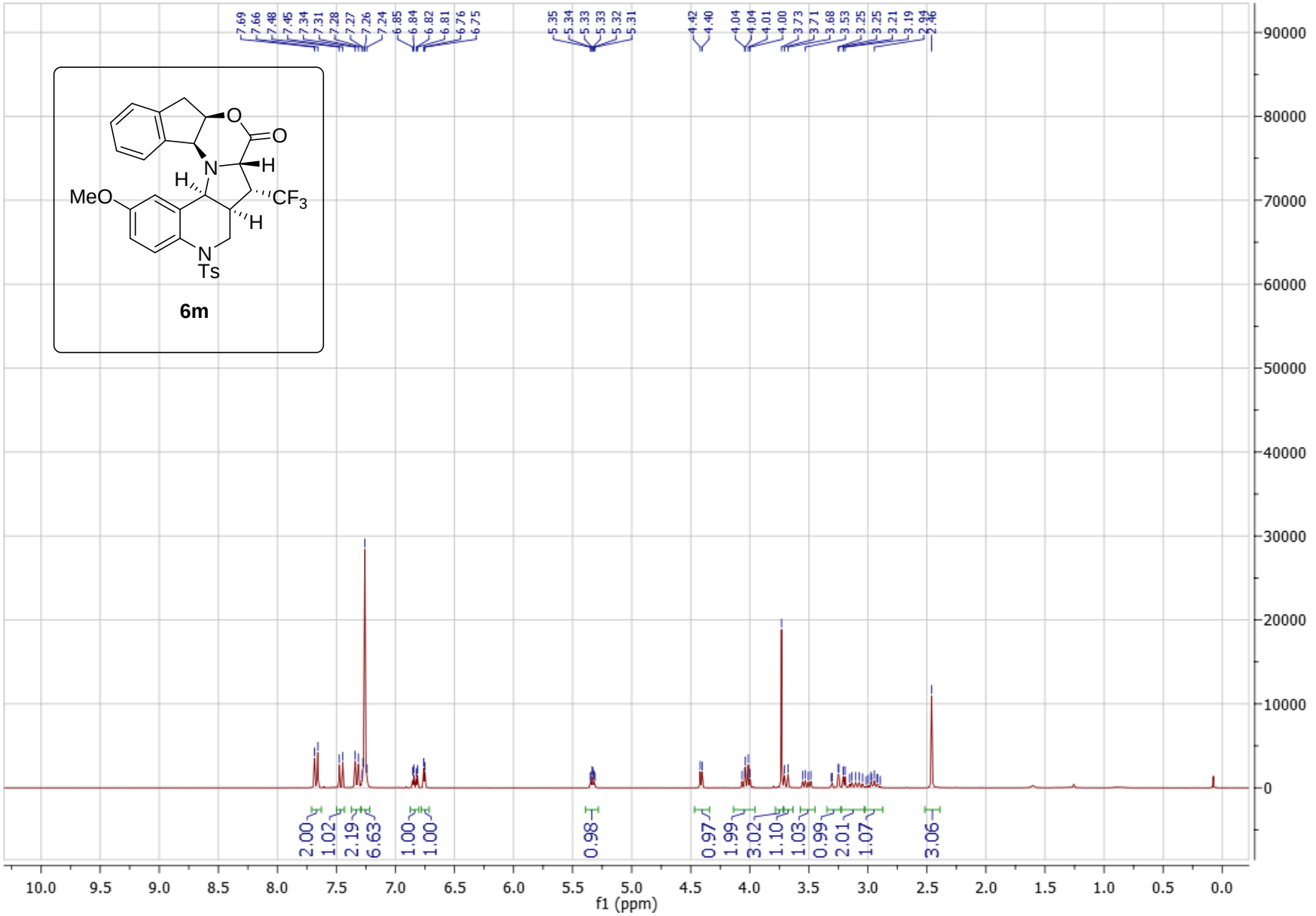
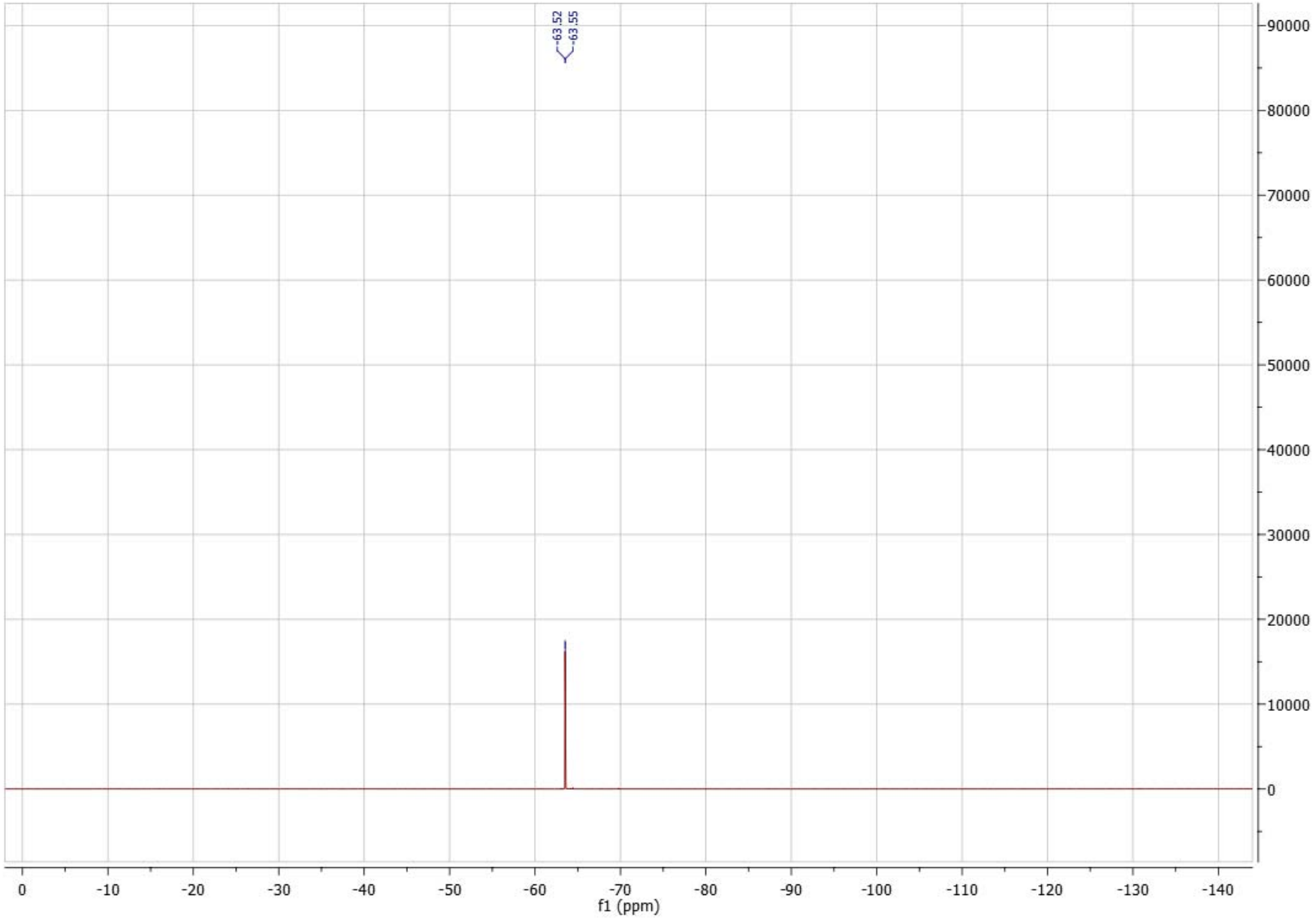
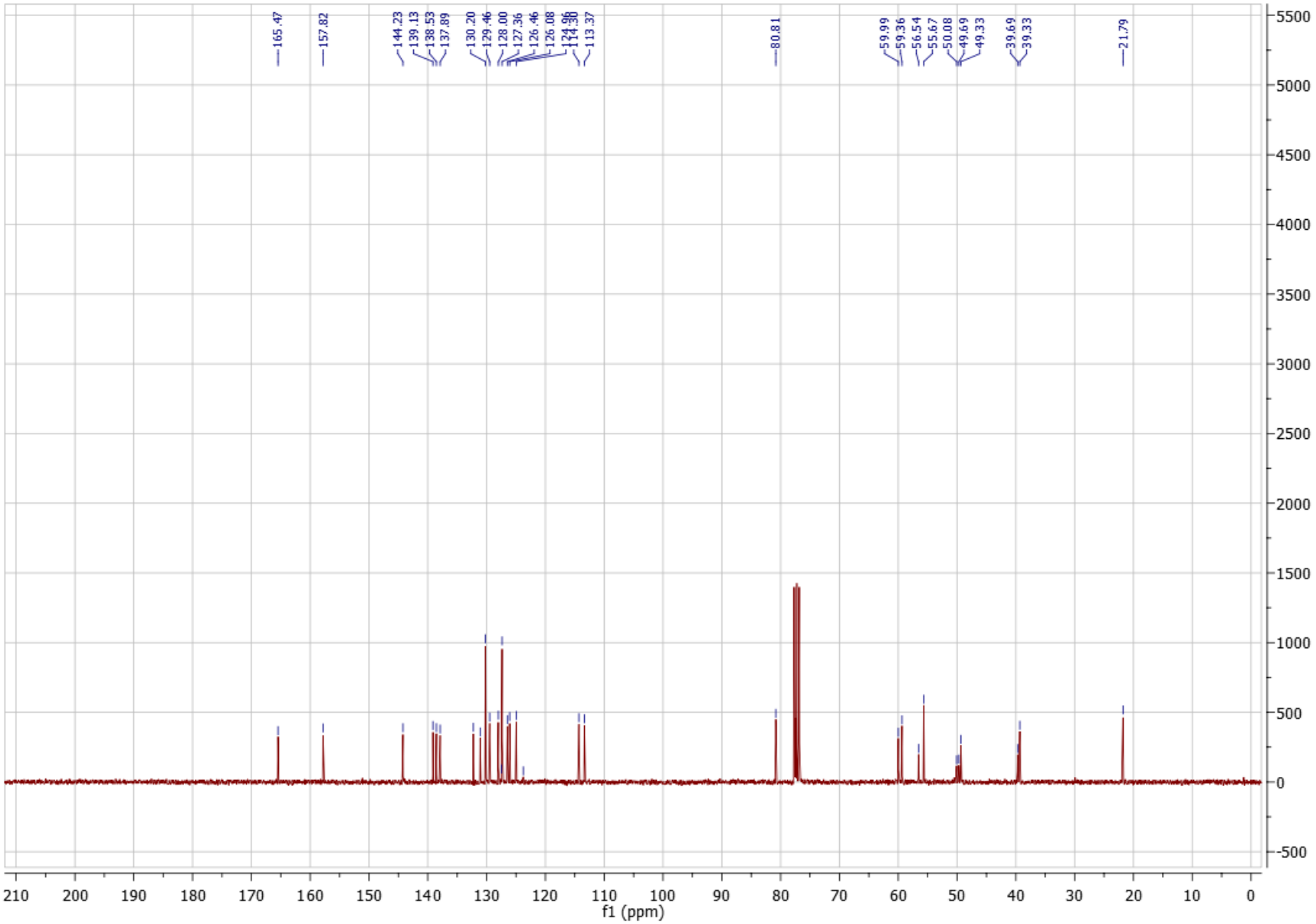
139.01
138.58
138.01
136.40
135.55
130.12
129.70
129.64
129.55
129.29
127.94
127.19
126.76
125.90
124.99
124.54
124.08
80.63
59.48
59.40
56.29
49.58
49.41
49.18
48.95
48.72
40.06
39.42
21.73
21.21
9.0E+07
8.5E+07
8.0E+07
7.5E+07
7.0E+07
6.5E+07
6.0E+07
5.5E+07
5.0E+07
4.5E+07
4.0E+07
3.5E+07
3.0E+07
2.5E+07
2.0E+07
1.5E+07
1.0E+07
5.0E+06
0.0E+00
-5.0E+06
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


MeO
O
O
N
H
H
CF3
H
N
Ts
6m
f1 (ppm)


-63.52
-63.55
90000
80000
70000
60000
50000
40000
30000
20000
10000
0
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
f1 (ppm)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157.82
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139.13
138.53
137.89
130.20
129.46
128.00
127.36
126.46
126.08
124.96
114.30
113.37
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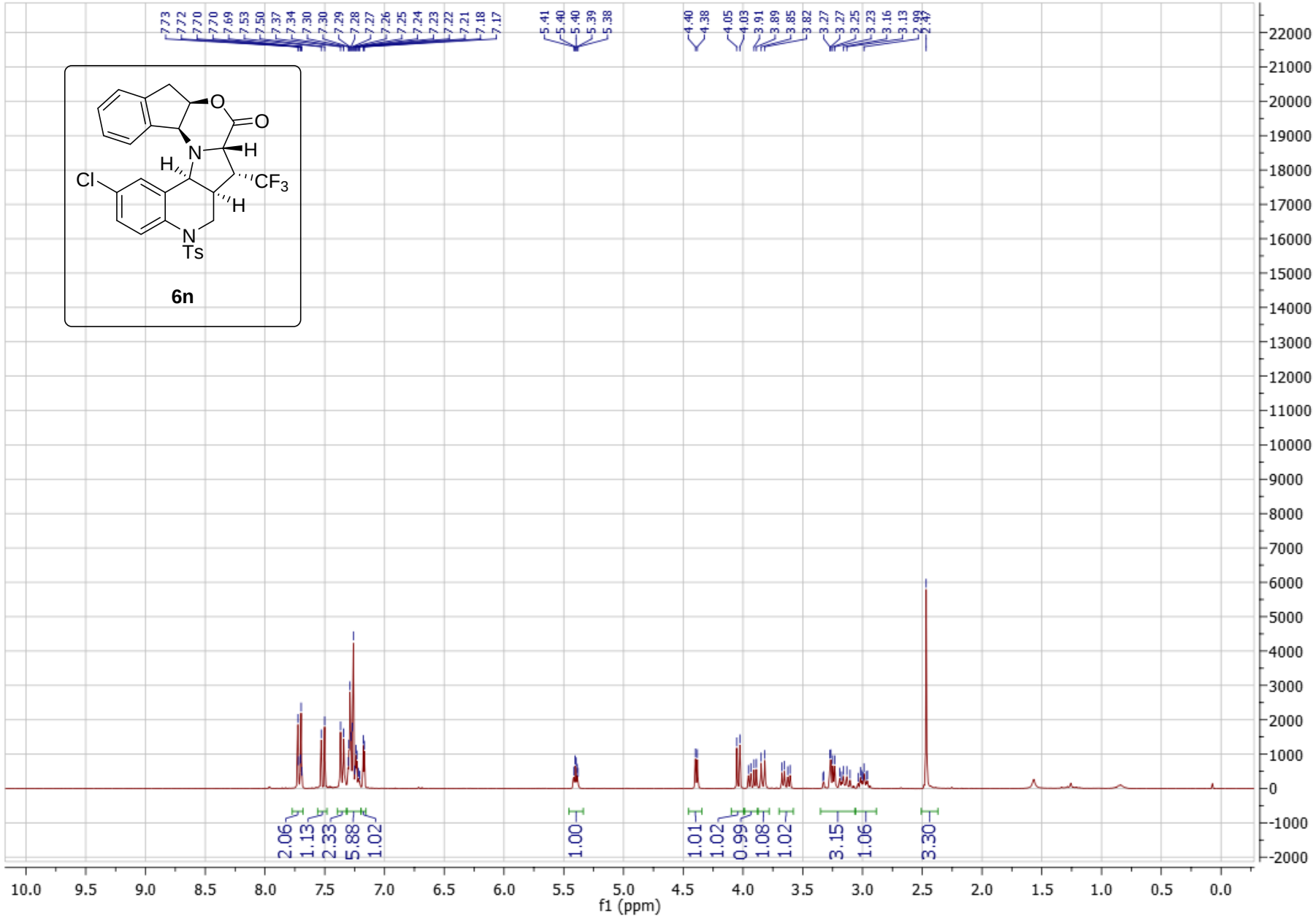
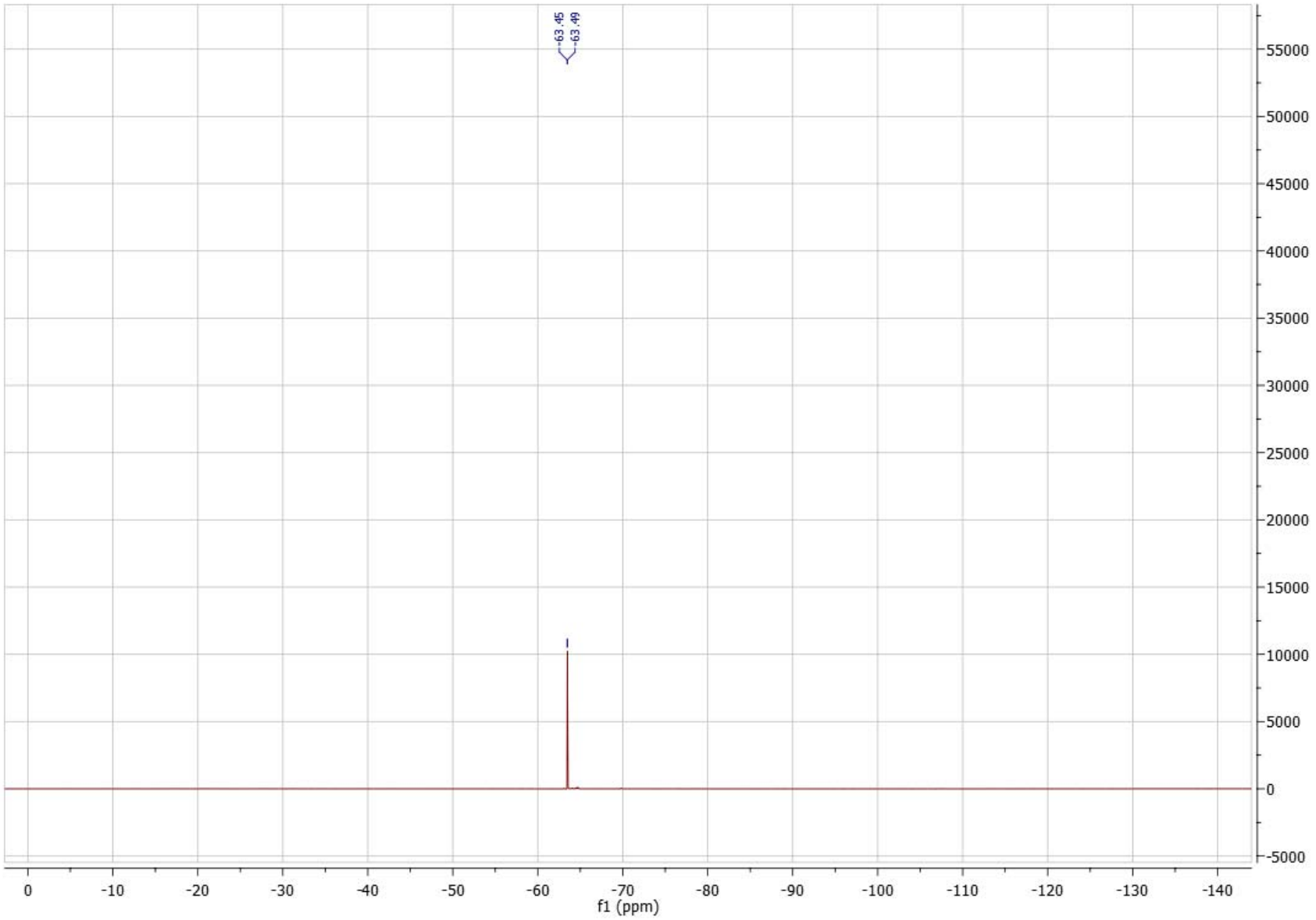
59.99
59.36
56.54
55.67
50.08
49.69
49.33
39.69
39.33
21.79
f1 (ppm)


7.73
7.72
7.70
7.70
7.69
7.53
7.50
7.37
7.34
7.30
7.30
7.29
7.28
7.27
7.26
7.25
7.24
7.23
7.22
7.21
7.18
7.17
5.41
5.40
5.40
5.39
5.38
4.40
4.38
4.05
4.03
3.91
3.89
3.85
3.82
3.27
3.27
3.25
3.23
3.16
3.13
2.99
2.97
O
O
N
H
H
Cl
CF3
H
N
Ts
6n
22000
21000
20000
19000
18000
17000
16000
15000
14000
13000
12000
11000
10000
9000
8000
7000
6000
5000
4000
3000
2000
1000
0
-1000
-2000
2.06
1.13
2.33
5.88
1.02
1.00
1.01
1.02
0.99
1.08
1.02
3.15
1.06
3.30
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)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-63.49
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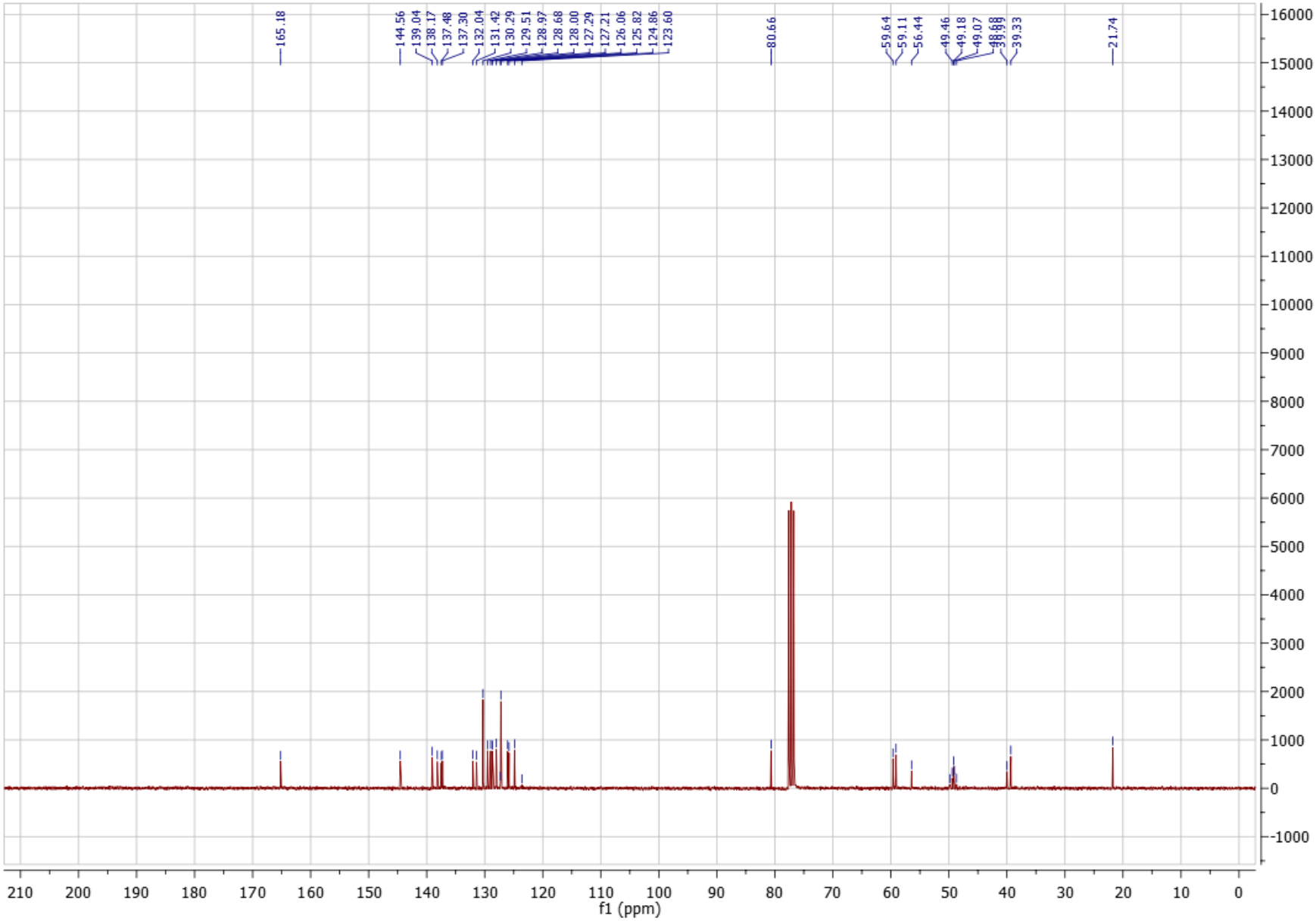
50000
45000
40000
35000
30000
25000
20000
15000
10000
5000
0
-5000
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
f1 (ppm)


165.18
144.56
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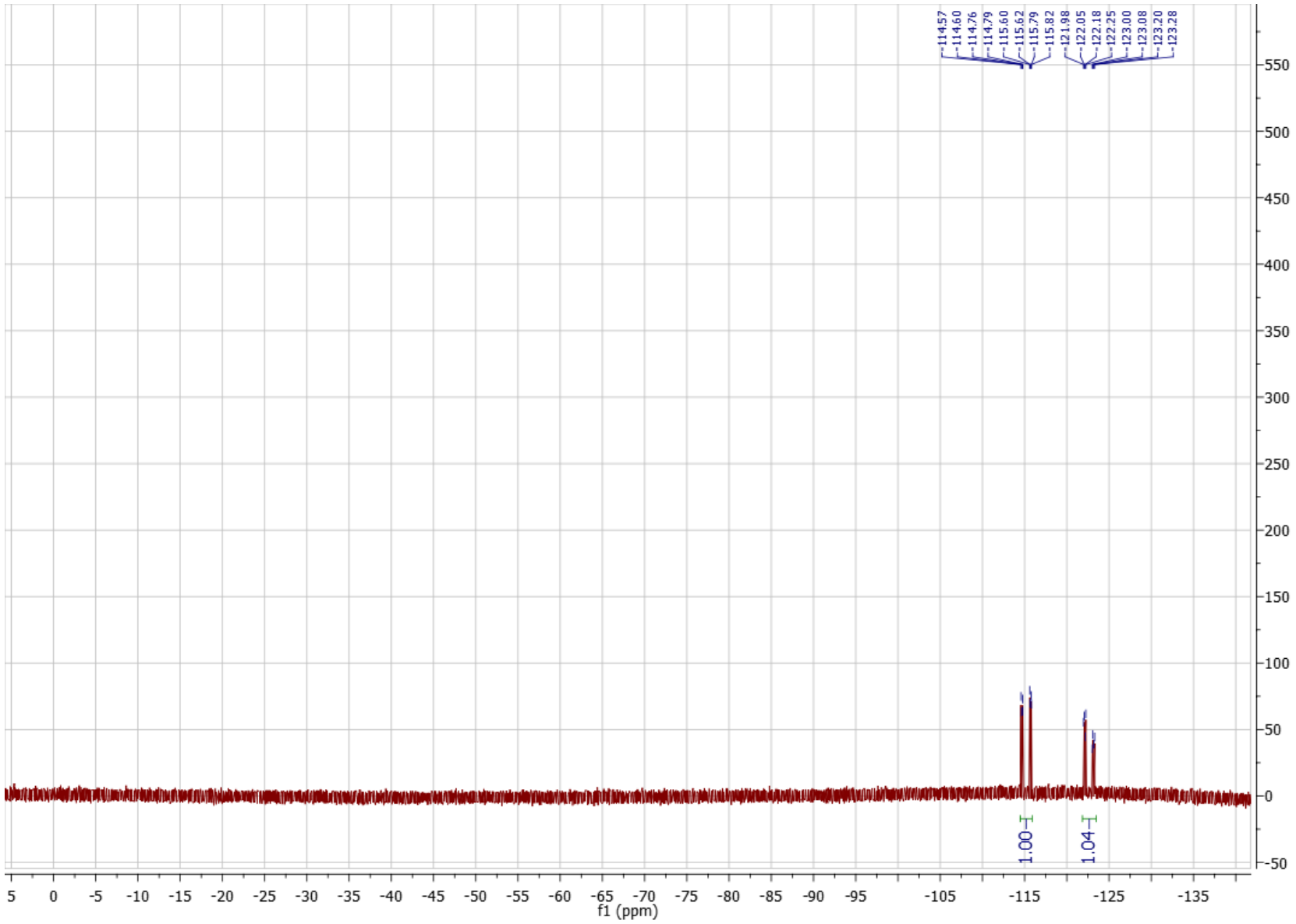
138.17
137.48
137.30
132.04
131.42
130.29
129.51
128.97
128.68
128.00
127.29
127.21
126.06
125.82
124.86
123.60
80.66
59.64
59.11
56.44
49.46
49.18
49.07
39.33
21.74
f1 (ppm)


6o
f1 (ppm)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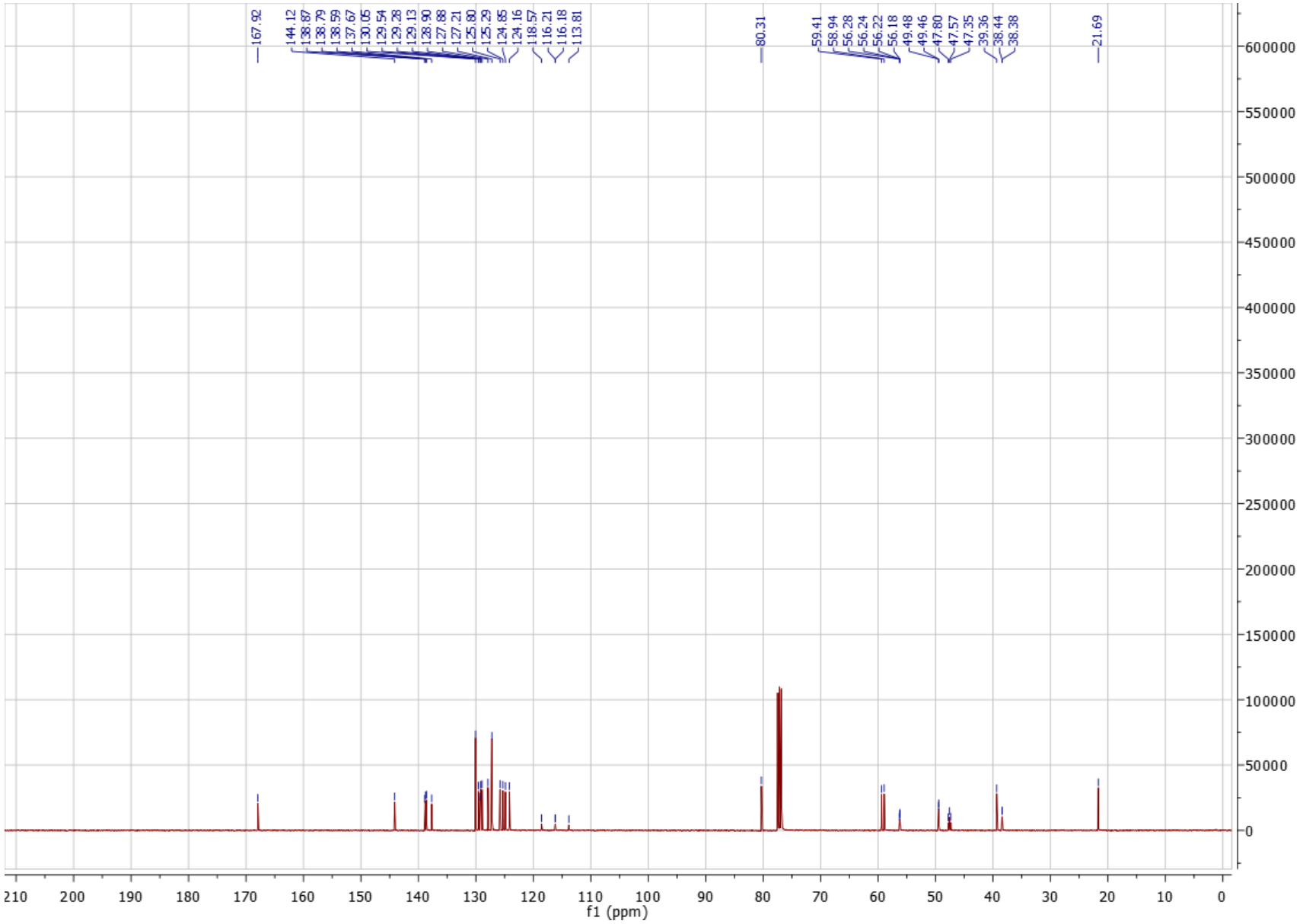
-114.60
-114.76
-114.79
-115.60
-115.62
-115.79
-115.82
-121.98
-122.05
-122.18
-122.25
-123.00
-123.08
-123.20
-123.28
1.00
1.04
f1 (ppm)


167.92
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138.87
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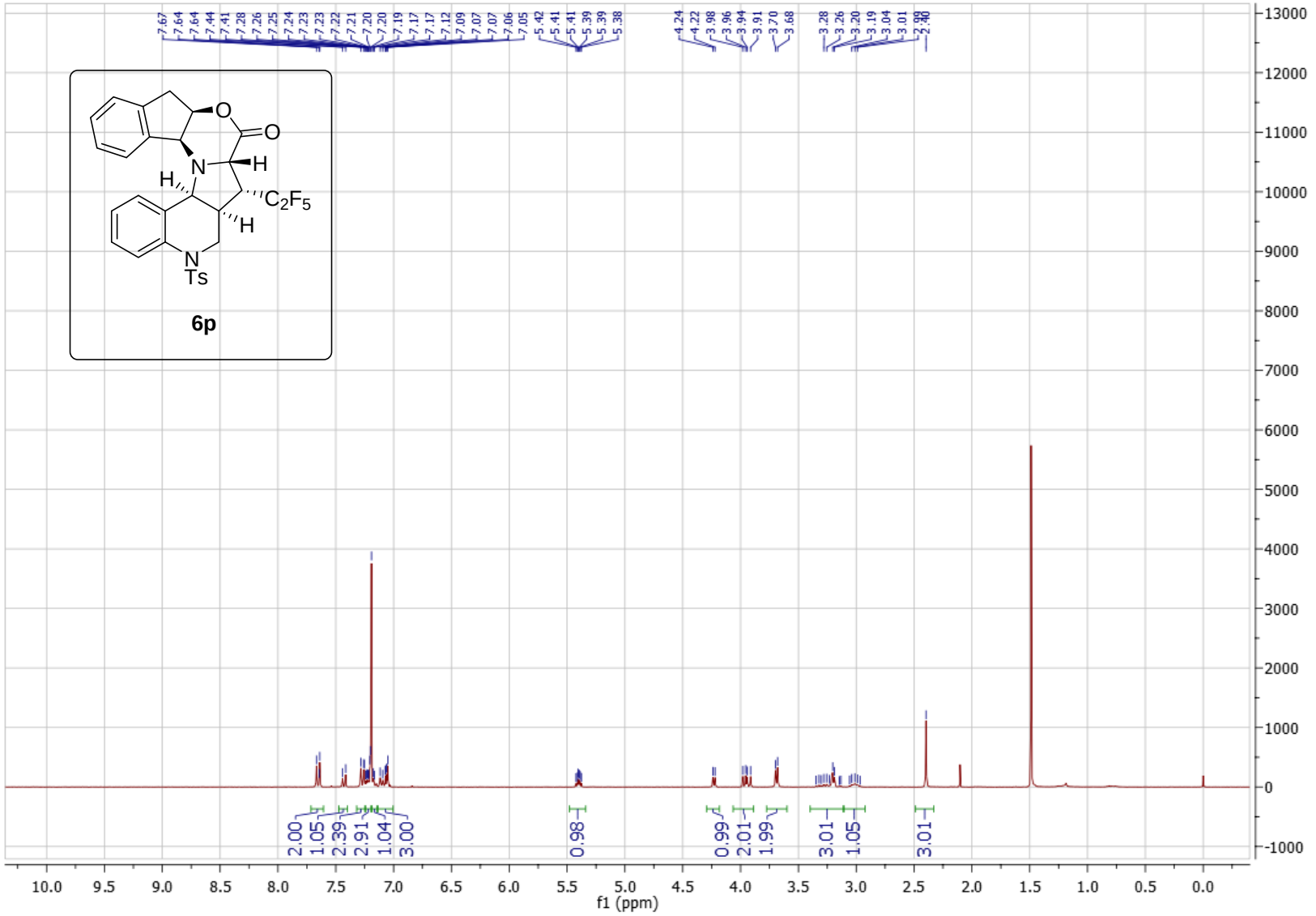
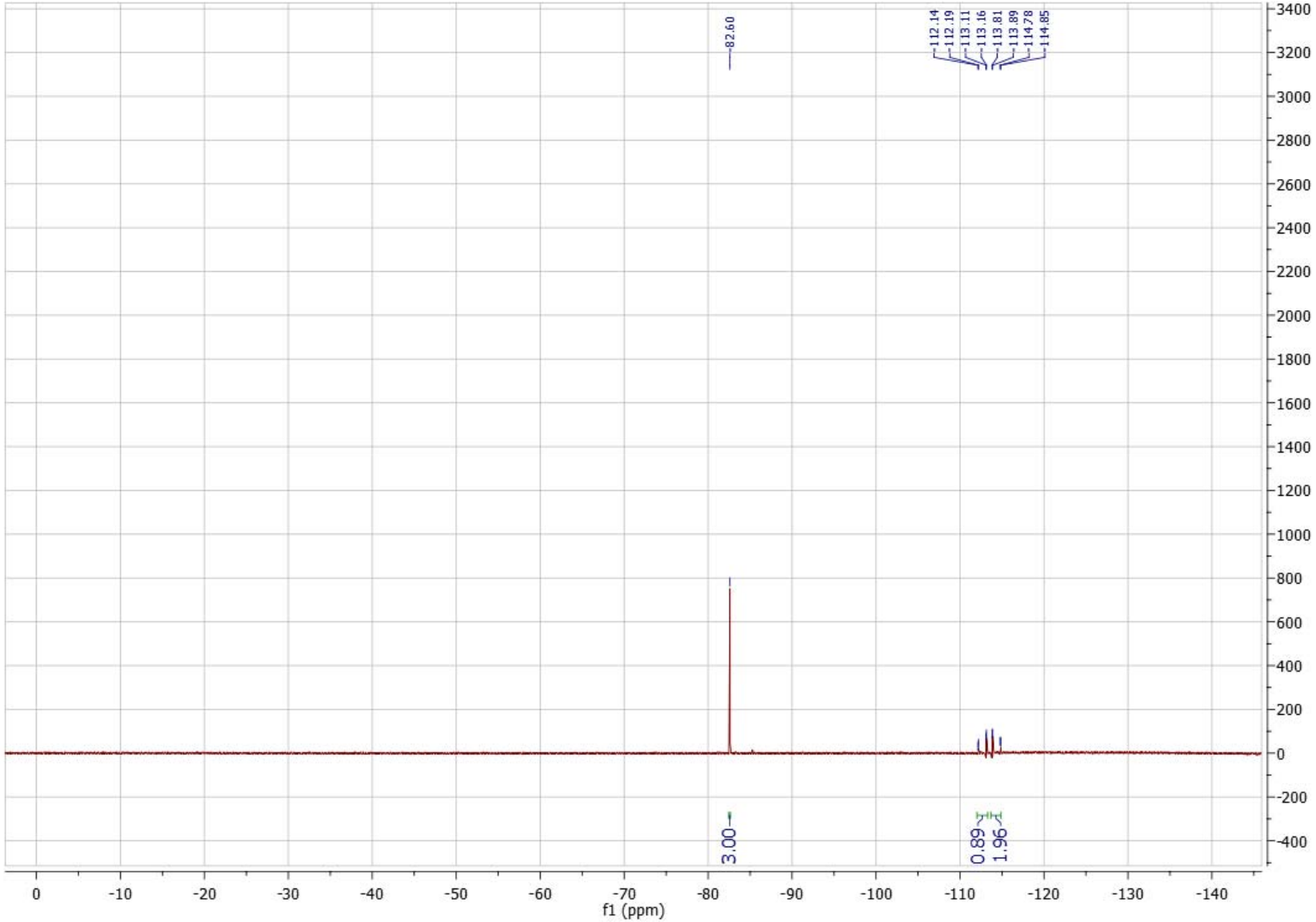
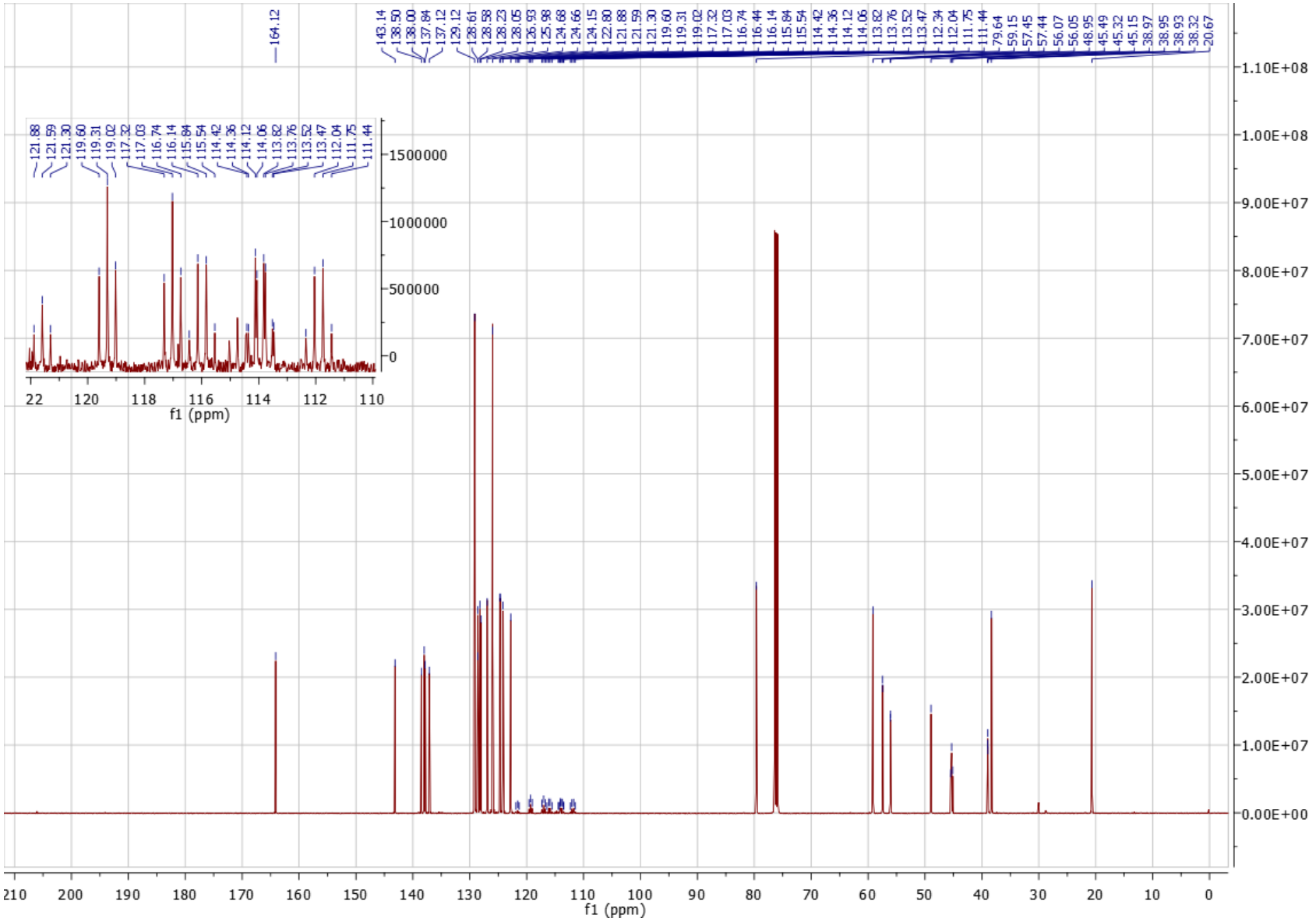
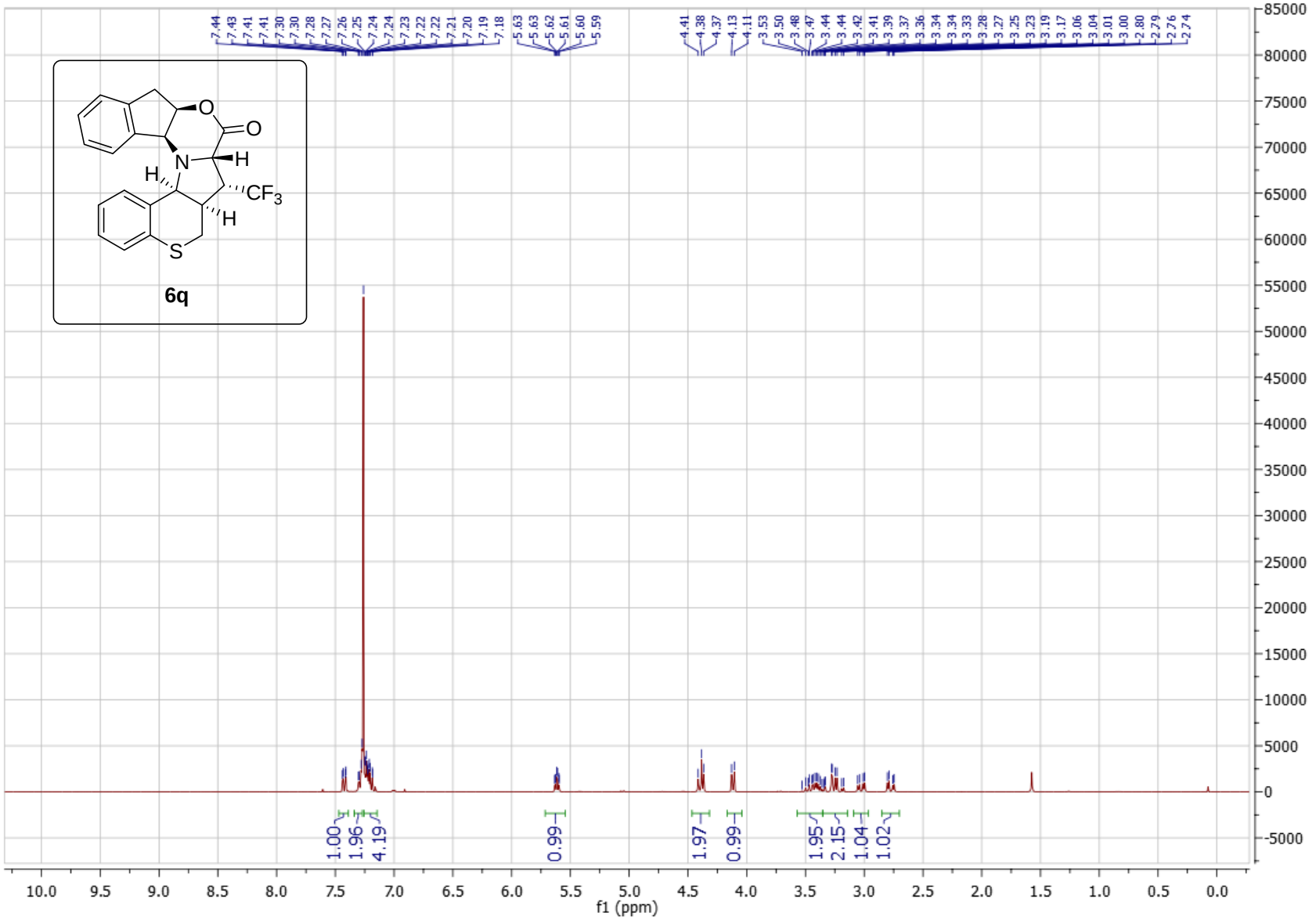
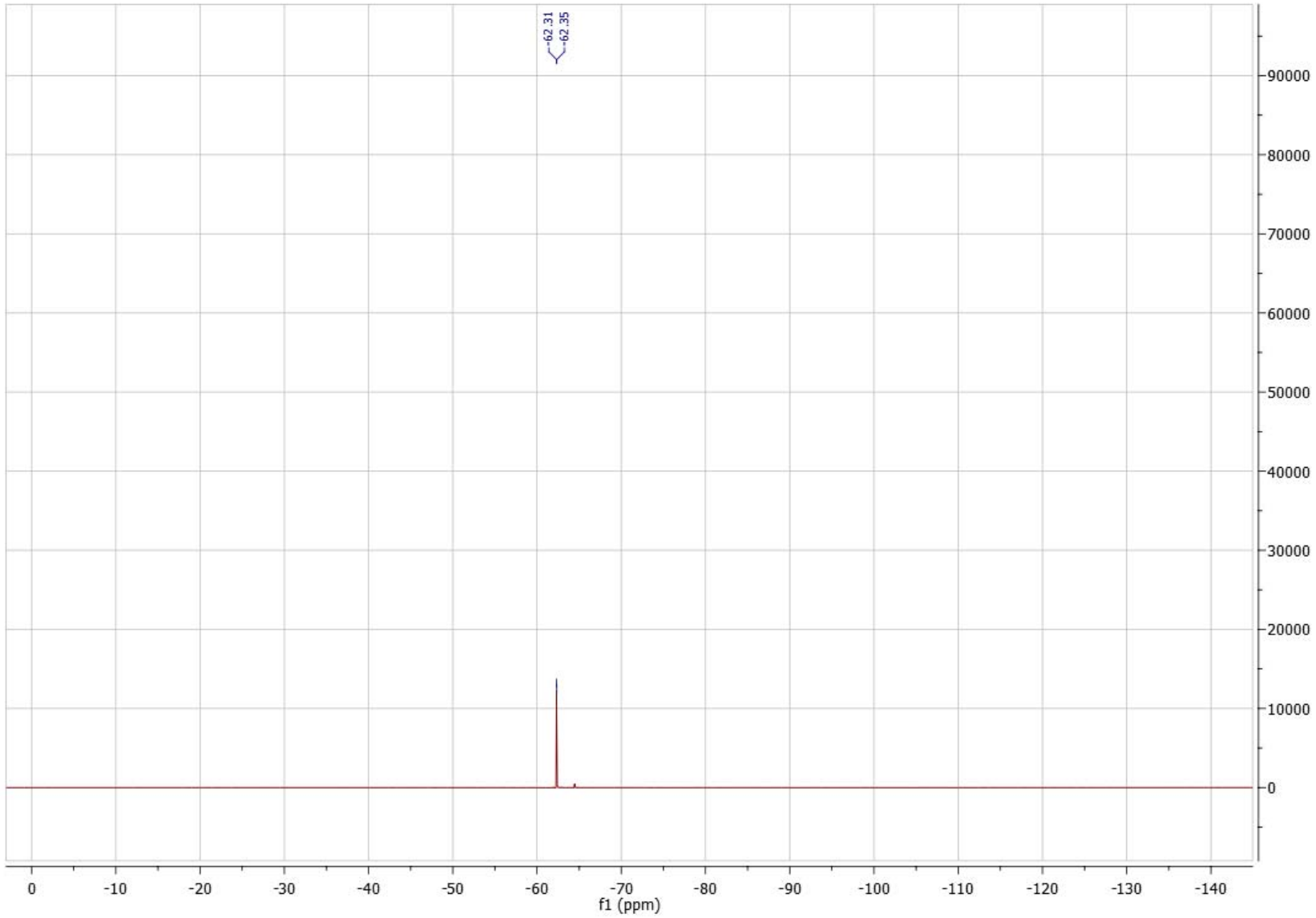
138.59
137.67
130.05
129.54
129.28
129.13
128.90
127.88
127.21
125.80
125.29
124.85
124.16
118.57
116.21
116.18
113.81
80.31
59.41
58.94
56.28
56.24
56.22
56.18
49.48
49.46
47.80
47.57
47.35
39.36
38.44
38.38
21.69
600000
550000
500000
450000
400000
350000
300000
250000
200000
150000
100000
50000
0
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


6p
f1 (ppm)


82.60
112.14
112.19
113.11
113.16
113.81
113.89
114.78
114.85
3.00
0.89
1.96
f1 (ppm)


164.12
143.14
138.50
138.00
137.84
137.12
129.12
128.61
128.58
128.23
128.05
126.93
125.98
124.68
124.66
124.15
122.80
121.88
121.59
121.30
119.60
119.31
119.02
117.32
117.03
116.74
116.44
116.14
115.84
115.54
114.42
114.36
114.12
114.06
113.82
113.76
113.52
113.47
112.34
112.04
111.75
111.44
79.64
59.15
57.45
57.44
56.07
56.05
48.95
45.49
45.32
45.15
38.97
38.95
38.93
38.32
20.67
1.10E+08
1.00E+08
9.00E+07
8.00E+07
7.00E+07
6.00E+07
5.00E+07
4.00E+07
3.00E+07
2.00E+07
1.00E+07
0.00E+00
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)
1500000
1000000
500000
0
22 120 118 116 114 112 110
f1 (ppm)


6q
f1 (ppm)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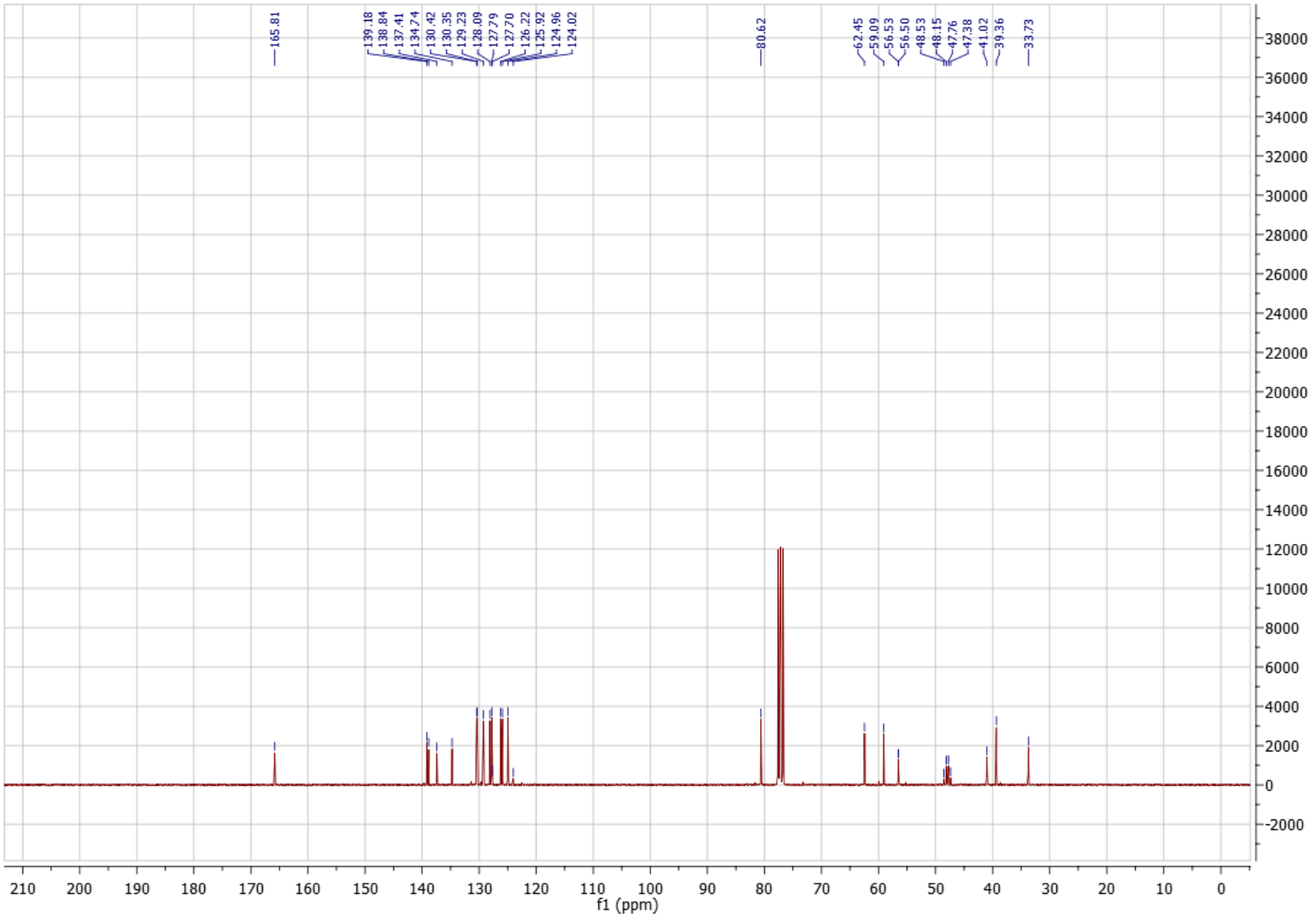
-62.35
90000
80000
70000
60000
50000
40000
30000
20000
10000
0
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
f1 (ppm)


165.81
139.18
138.84
137.41
134.74
130.42
130.35
129.23
128.09
127.79
127.70
126.22
125.92
124.96
124.02
80.62
62.45
59.09
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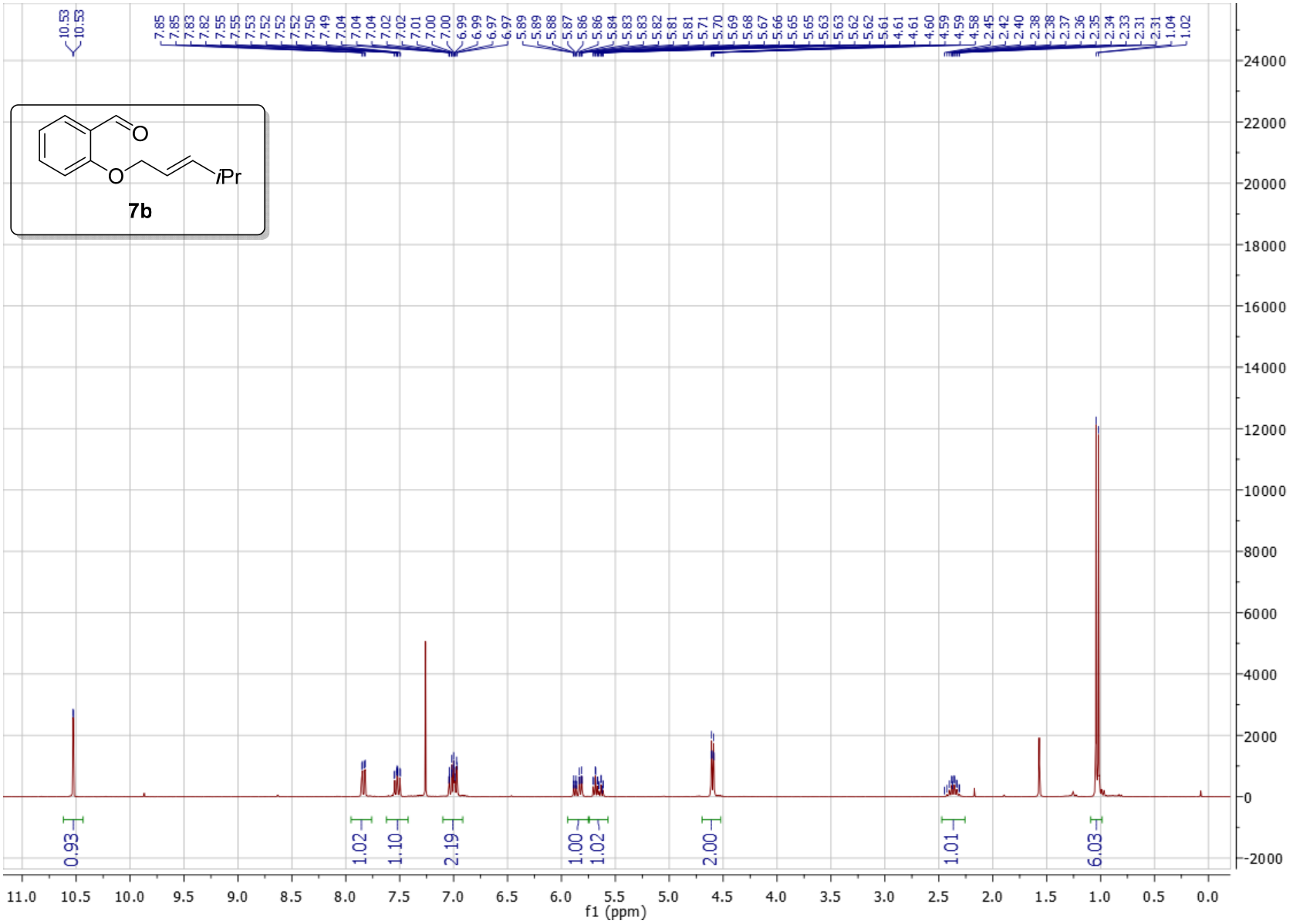
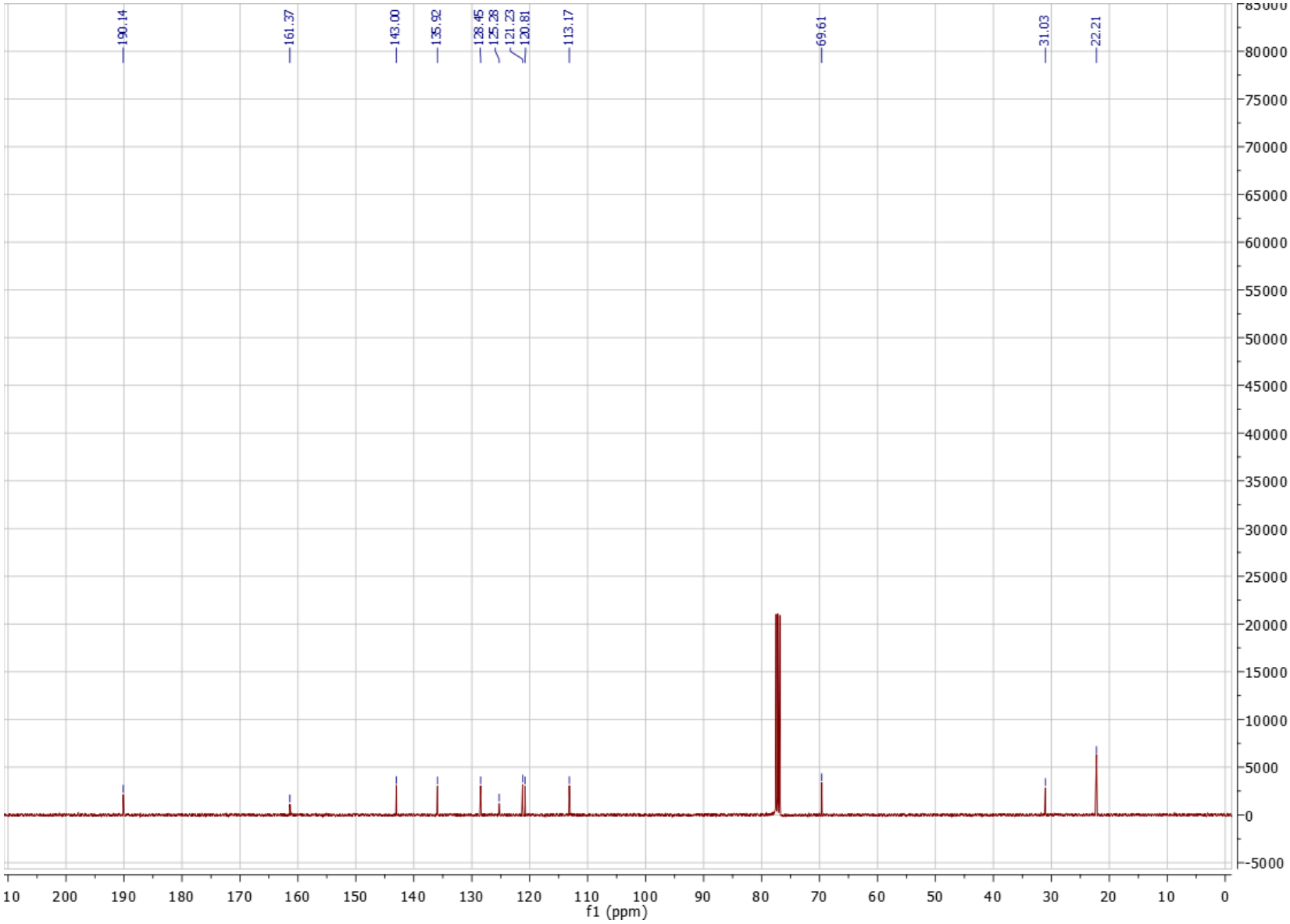
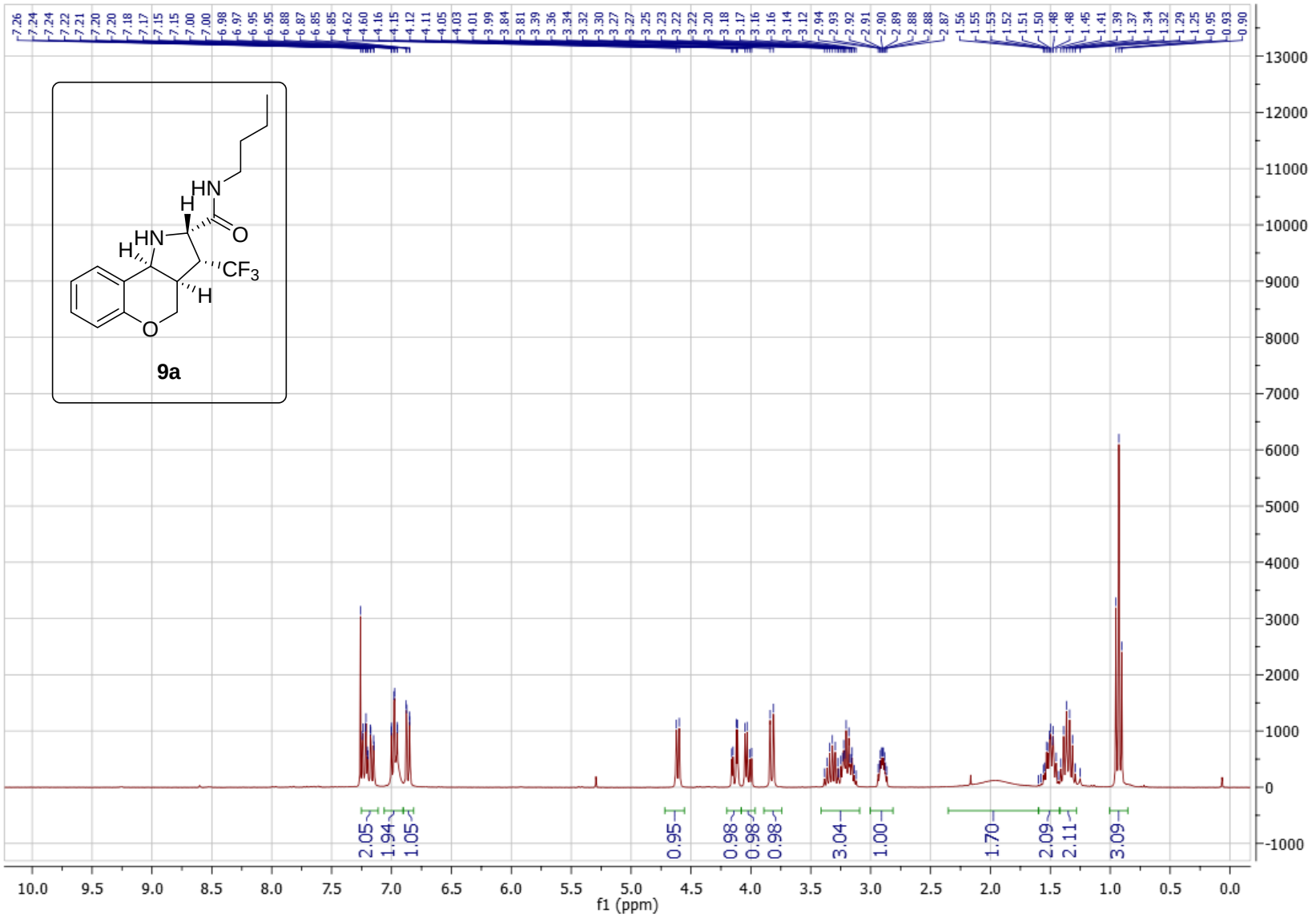
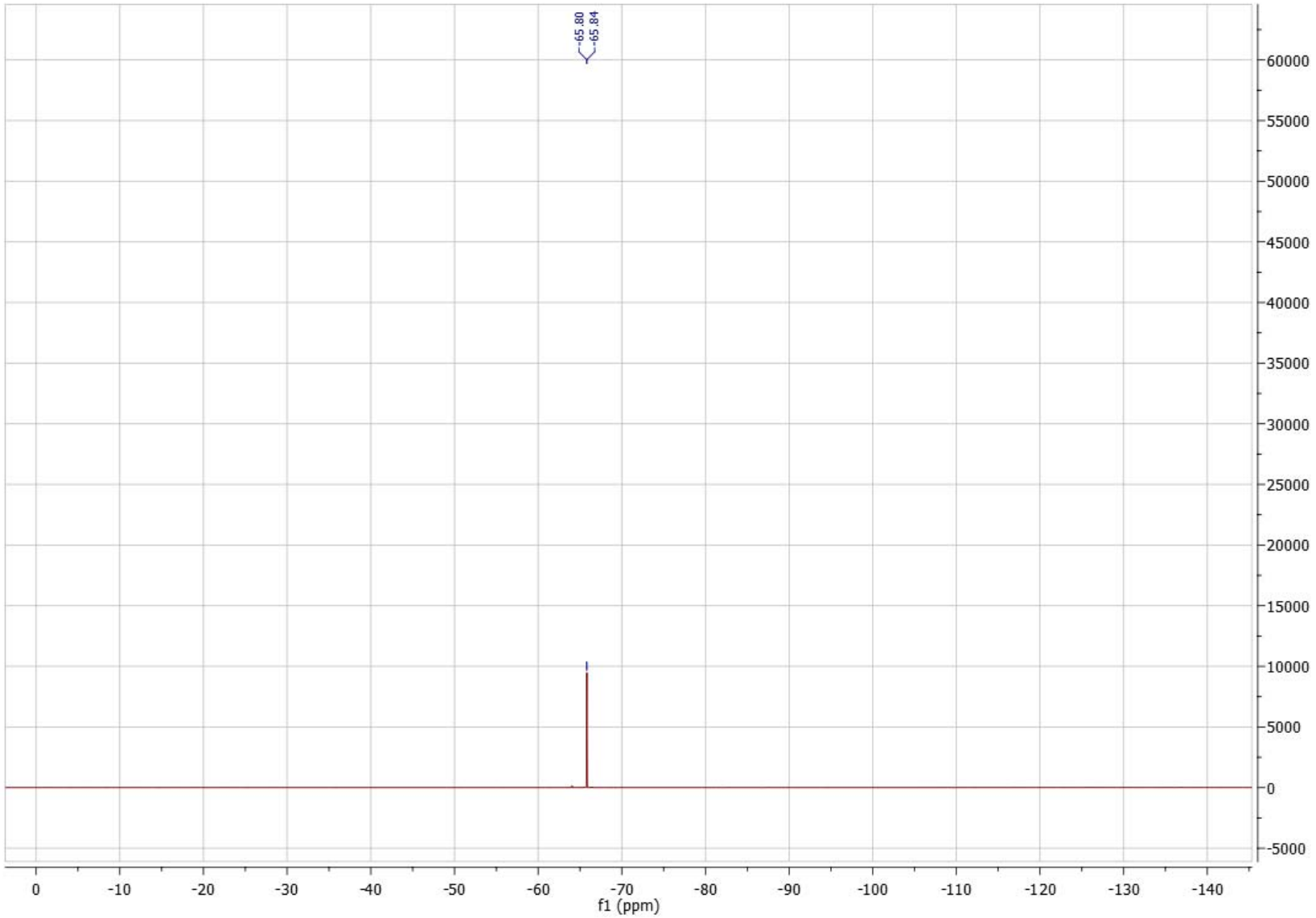
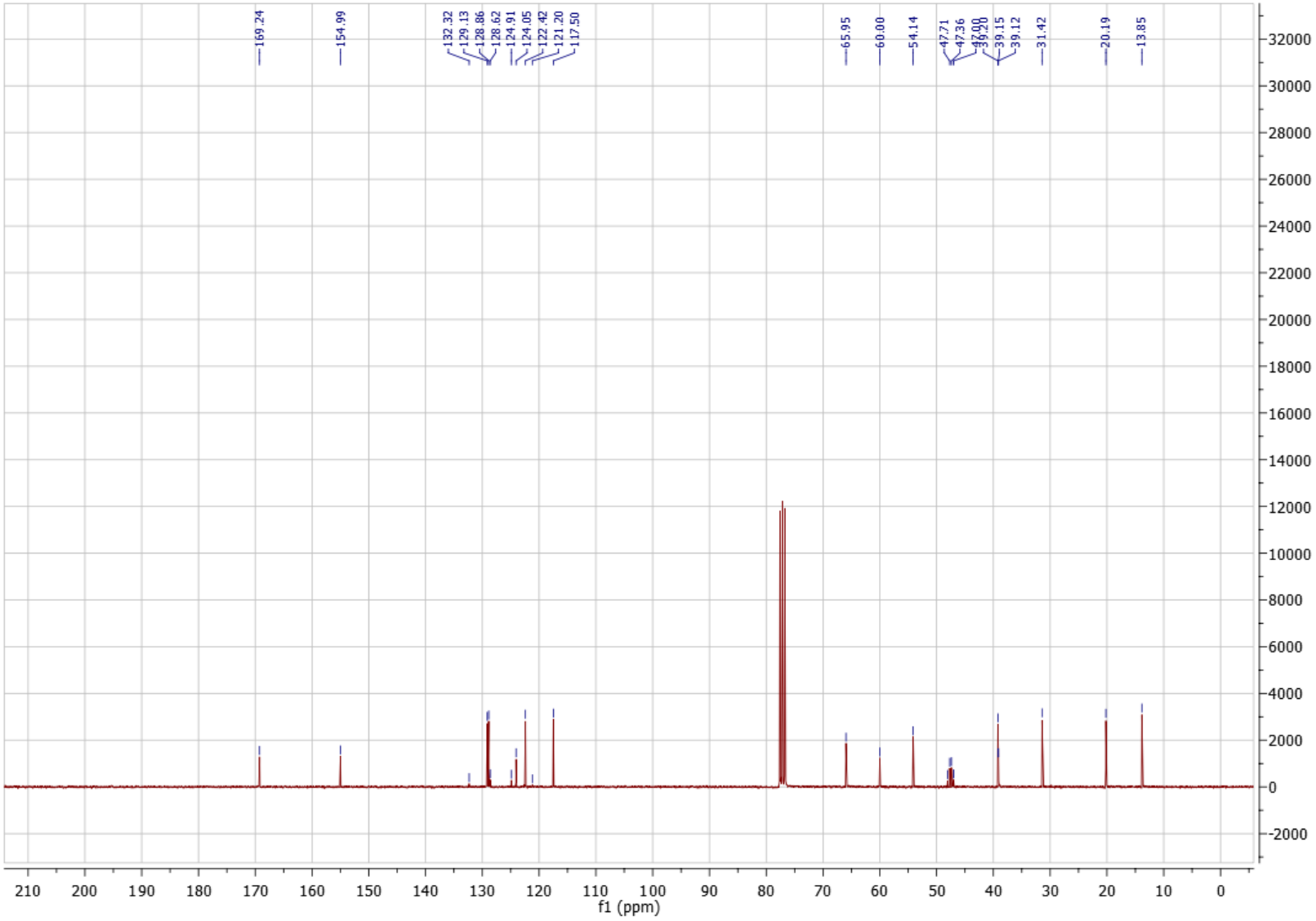
56.50
48.53
48.15
47.76
47.38
41.02
39.36
33.73
f1 (ppm)

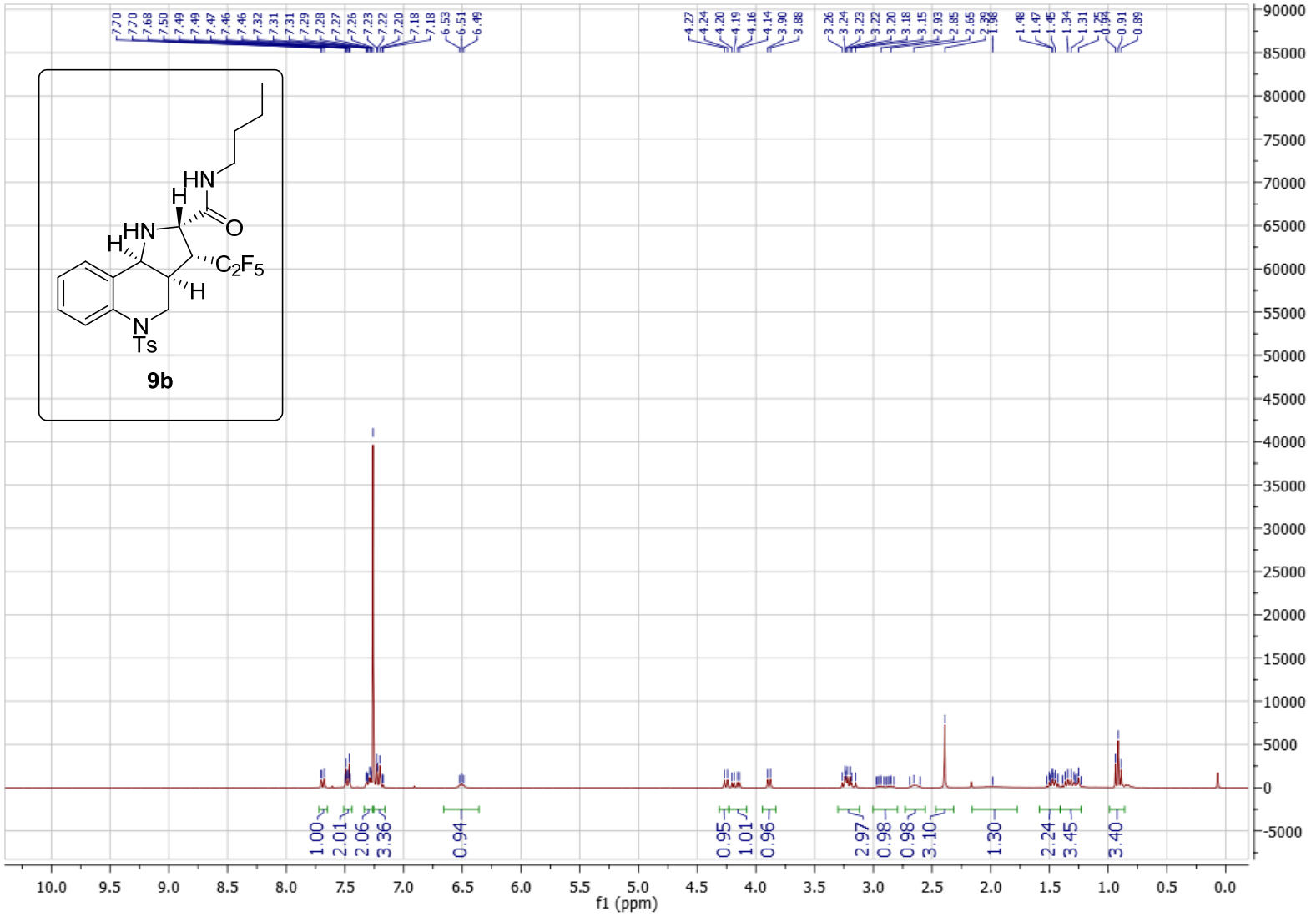

10.53
10.53
7.85
7.85
7.83
7.82
7.55
7.55
7.53
7.52
7.52
7.50
7.49
7.04
7.04
7.04
7.02
7.02
7.01
7.00
7.00
6.99
6.99
6.97
6.97
5.89
5.89
5.88
5.87
5.86
5.86
5.84
5.83
5.83
5.82
5.81
5.81
5.71
5.70
5.69
5.68
5.67
5.66
5.65
5.65
5.63
5.63
5.62
5.62
5.61
4.61
4.61
4.60
4.59
4.59
4.58
2.45
2.42
2.40
2.38
2.38
2.37
2.36
2.35
2.34
2.33
2.31
2.31
1.04
1.02
O
O
iPr
7b
24000
22000
20000
18000
16000
14000
12000
10000
8000
6000
4000
2000
0
-2000
0.93
1.02
1.10
2.19
1.00
1.02
2.00
1.01
6.03
11.0
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

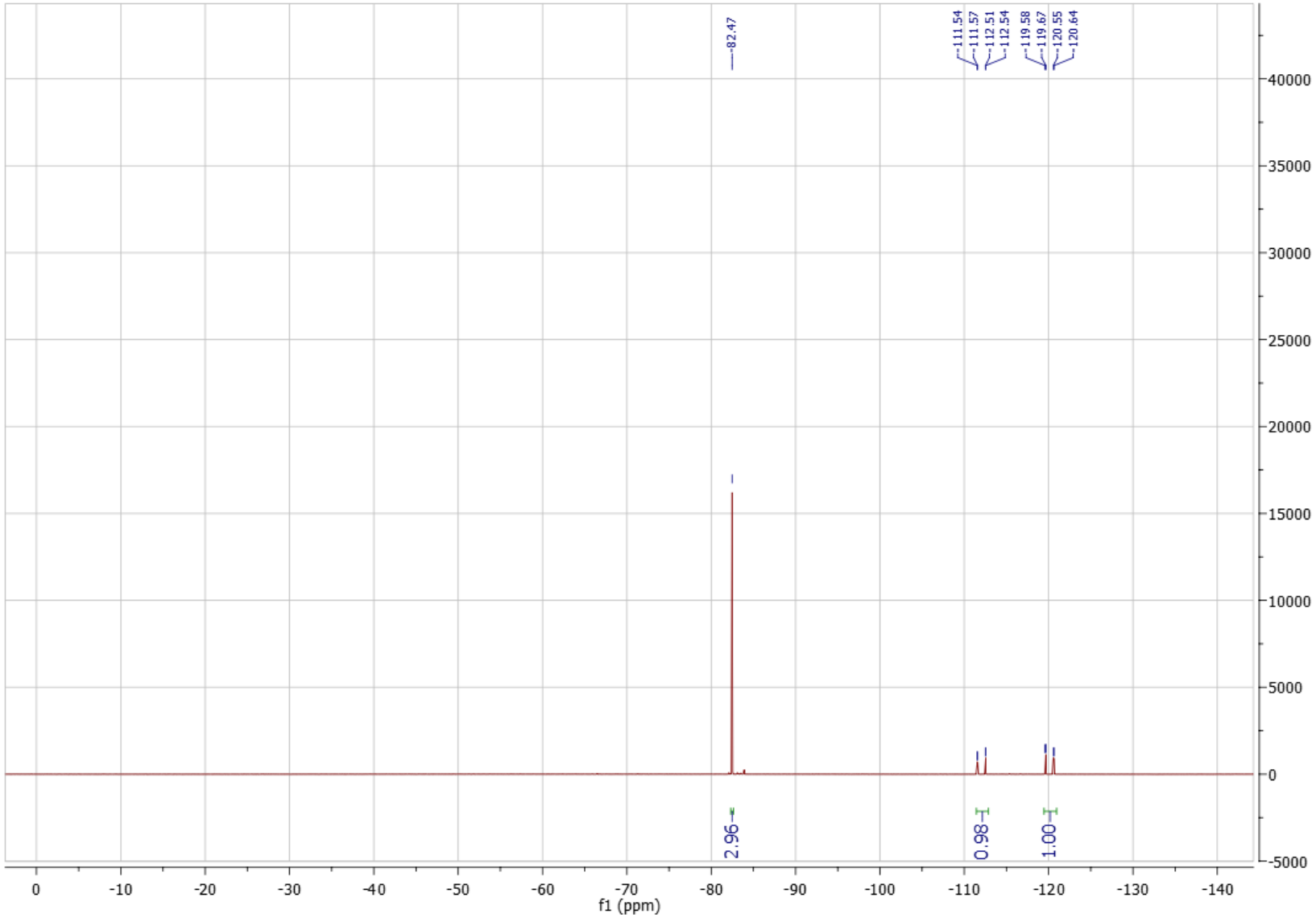

190.14
161.37
143.00
135.92
128.45
125.28
121.23
120.81
113.17
69.61
31.03
22.21
f1 (ppm)

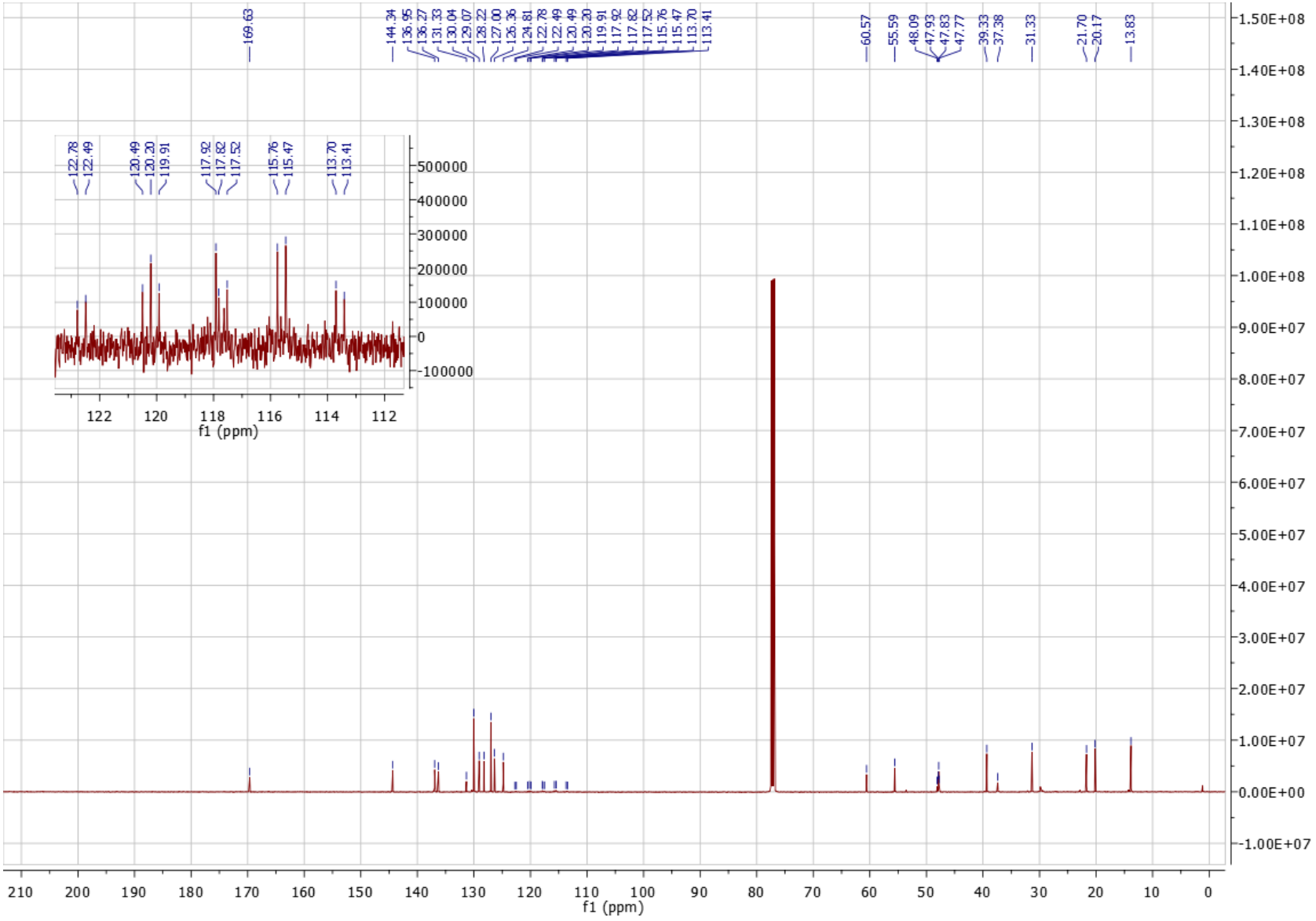

9a
f1 (ppm)

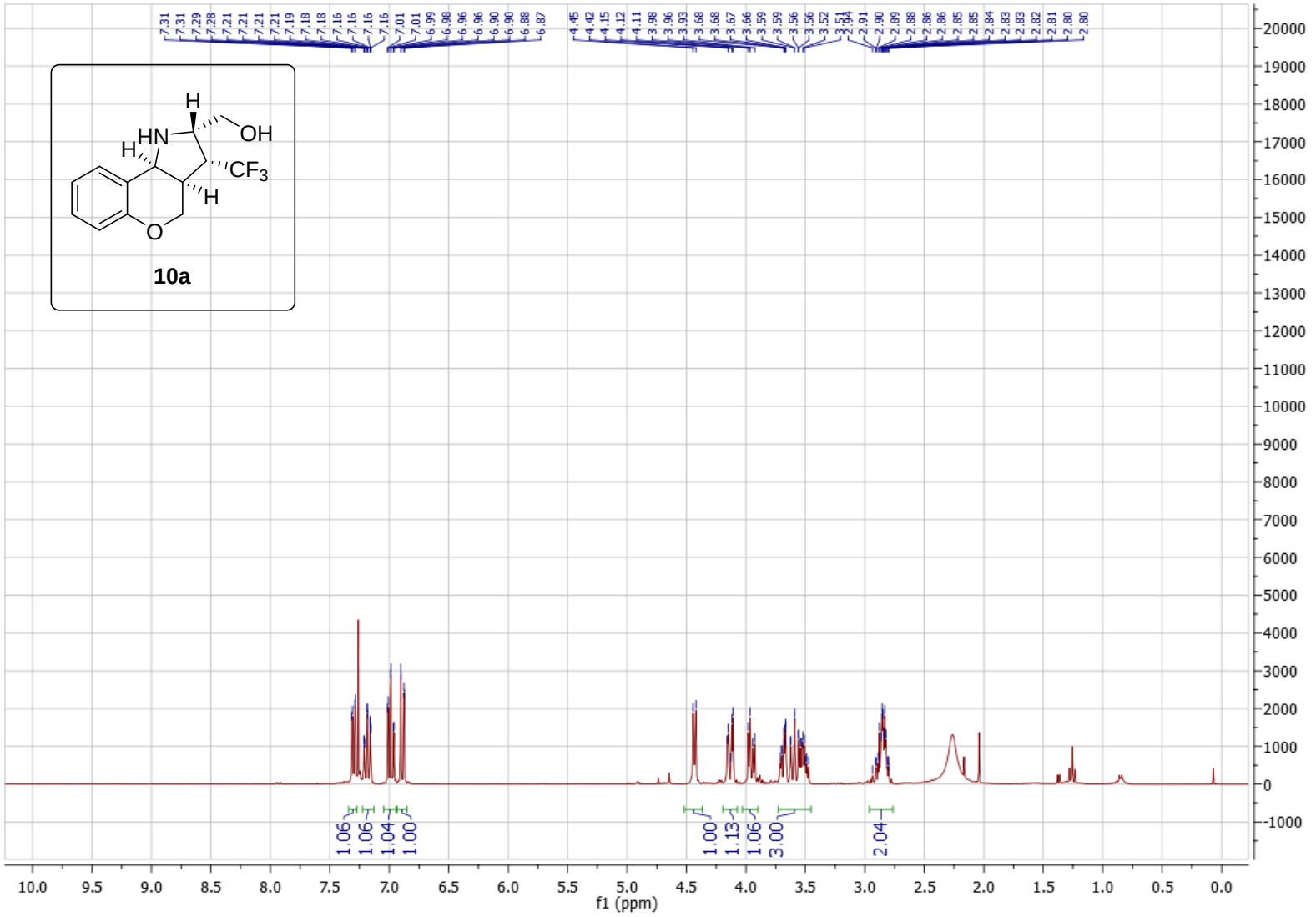

-65.80
-65.84
60000
55000
50000
45000
40000
35000
30000
25000
20000
15000
10000
5000
0
-5000
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
f1 (ppm)

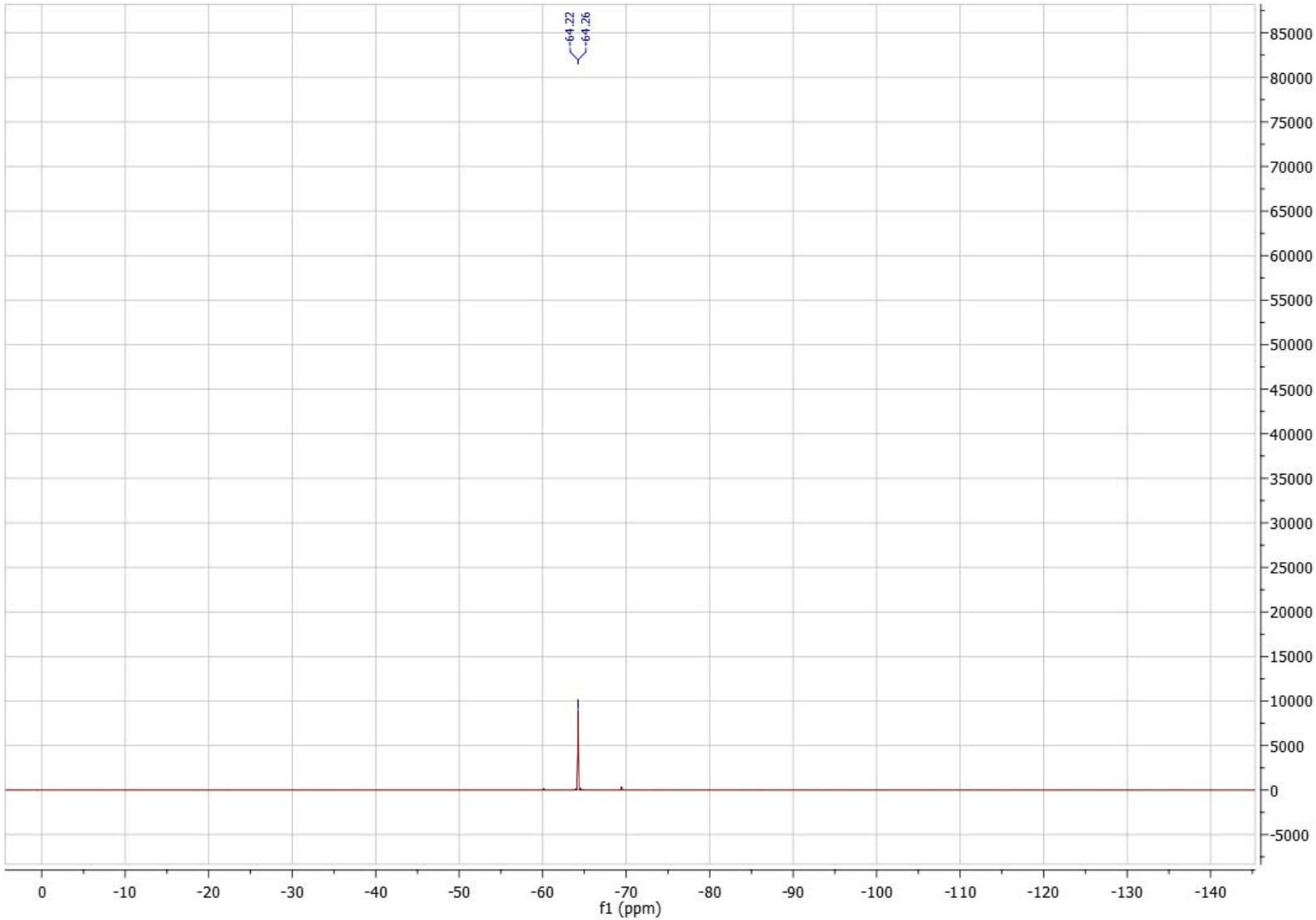

169.24
154.99
132.32
129.13
128.86
128.62
124.91
124.05
122.42
121.20
117.50
65.95
60.00
54.14
47.71
47.36
47.00
39.20
39.15
39.12
31.42
20.19
13.85
32000
30000
28000
26000
24000
22000
20000
18000
16000
14000
12000
10000
8000
6000
4000
2000
0
-2000
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

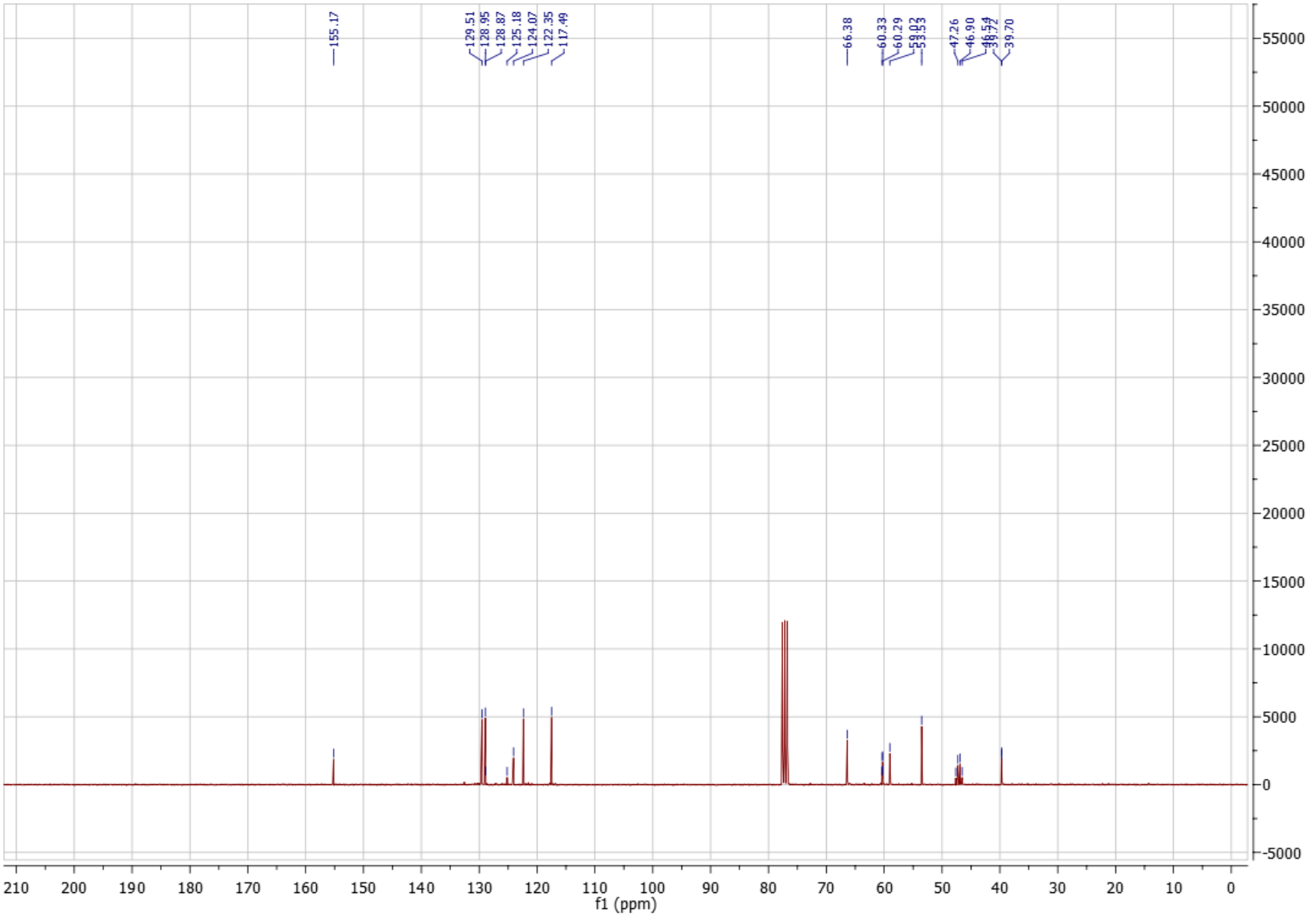

HN
H
HN
H
O
C2F5
H
N
Ts
9b
f1 (ppm)

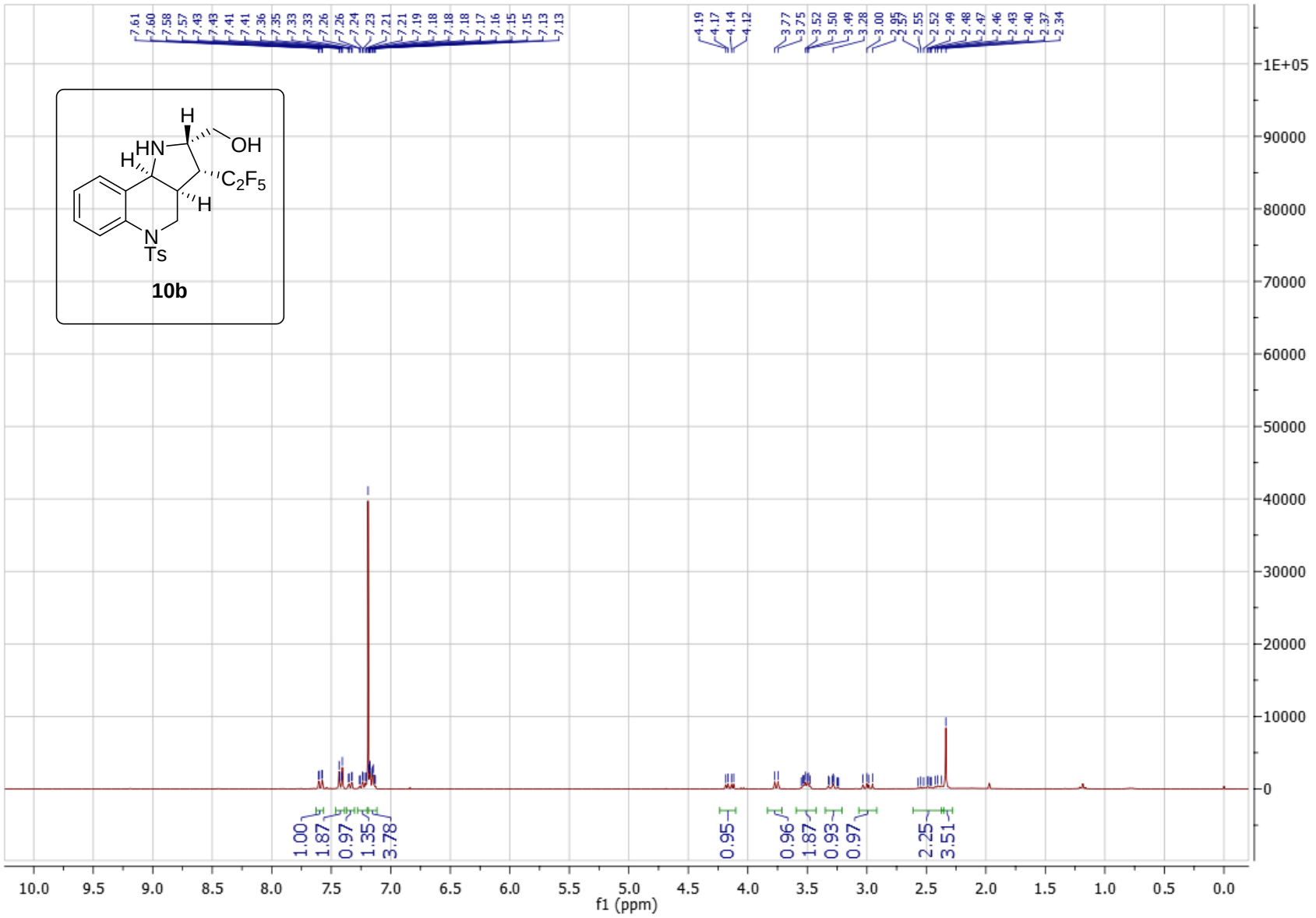

-82.47
111.54
111.57
112.51
112.54
119.58
119.67
120.55
120.64
40000
35000
30000
25000
20000
15000
10000
5000
0
-5000
2.96
0.98
1.00
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
f1 (ppm)

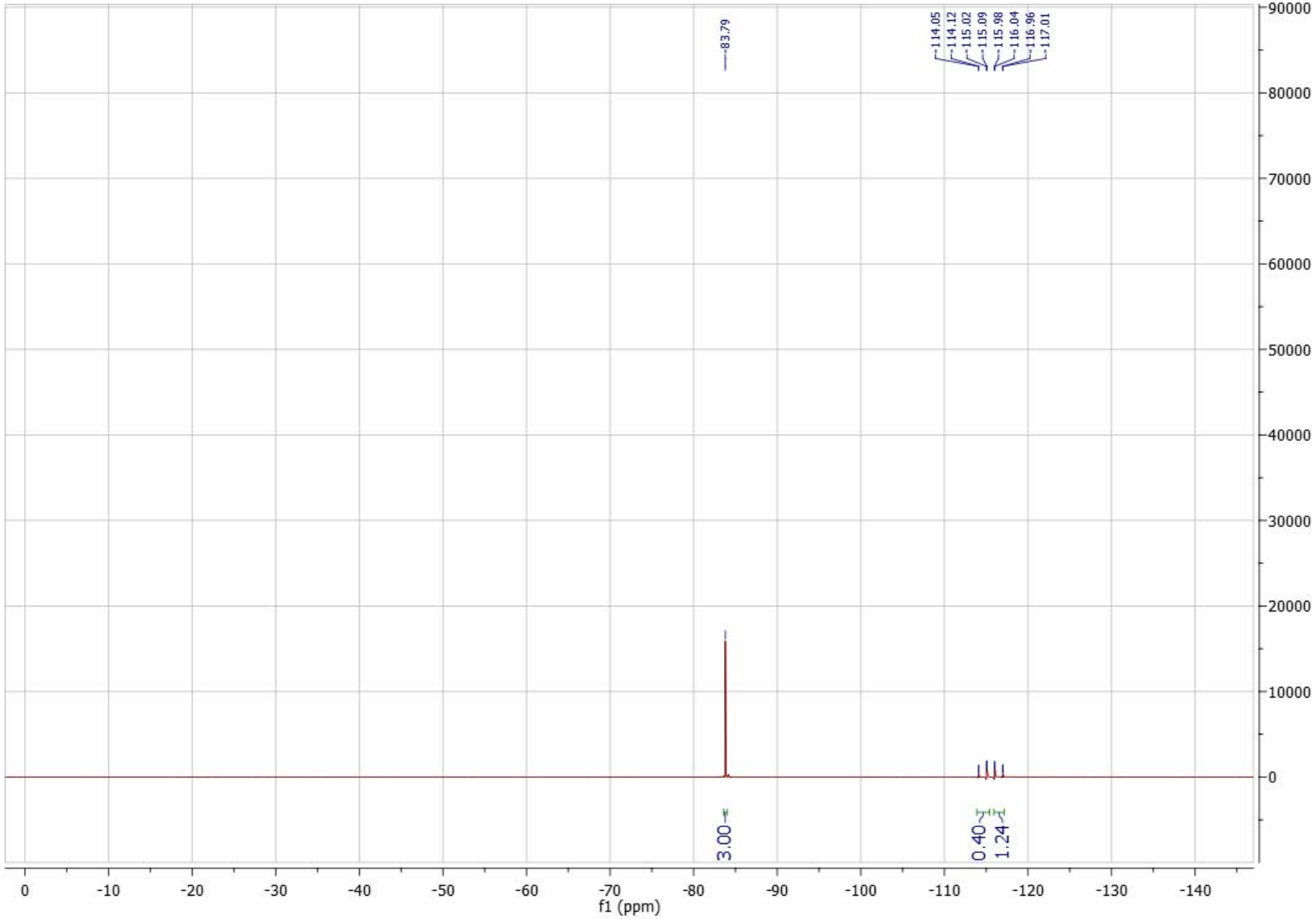

169.63
144.34
136.95
136.27
131.33
130.04
129.07
128.22
127.00
126.36
124.81
122.78
122.49
120.49
120.20
119.91
117.92
117.82
117.52
115.76
115.47
113.70
113.41
60.57
55.59
48.09
47.93
47.83
47.77
39.33
37.38
31.33
21.70
20.17
13.83
f1 (ppm)

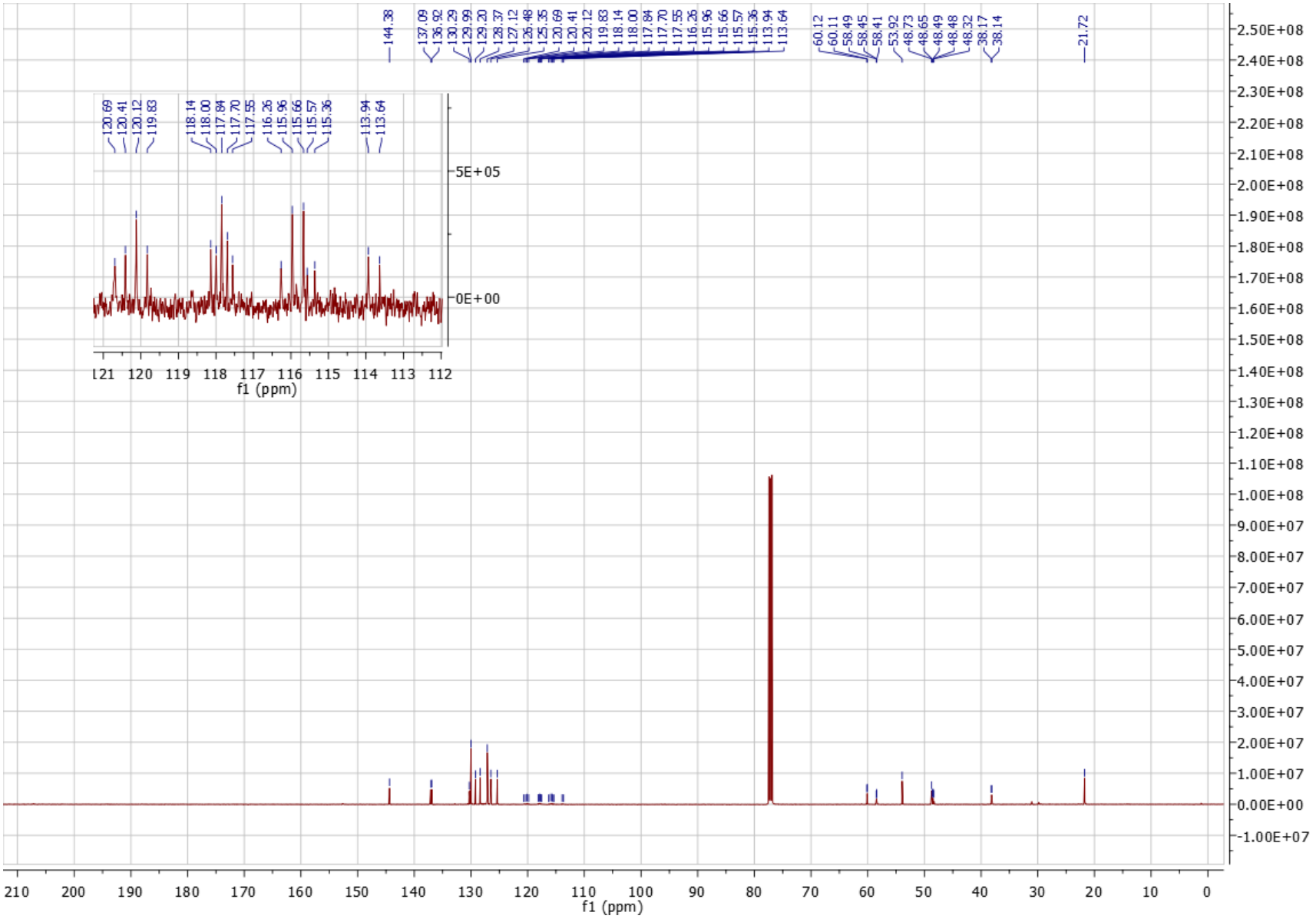

H
HN
H
OH
CF3
H
O
10a
f1 (ppm)


-64.22
-64.26
85000
80000
75000
70000
65000
60000
55000
50000
45000
40000
35000
30000
25000
20000
15000
10000
5000
0
-5000
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
f1 (ppm)


155.17
129.51
128.95
128.87
125.18
124.07
122.35
117.49
66.38
60.33
60.29
59.03
53.53
47.26
46.90
46.54
39.72
39.70
55000
50000
45000
40000
35000
30000
25000
20000
15000
10000
5000
0
-5000
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


10b
f1 (ppm)


-83.79
-114.05
-114.12
-115.02
-115.09
-115.98
-116.04
-116.96
-117.01
3.00
0.40
1.24
f1 (ppm)


144.38
137.09
136.92
130.29
129.99
129.20
128.37
127.12
126.48
125.35
120.69
120.41
120.12
119.83
118.14
118.00
117.84
117.70
117.55
116.26
115.96
115.66
115.57
115.36
113.94
113.64
60.12
60.11
58.49
58.45
58.41
53.92
48.73
48.65
48.49
48.48
48.32
38.17
38.14
21.72
5E+05
0E+00
f1 (ppm)
f1 (ppm)