Supporting Information

A High-Throughput Synthesis of 1,2,4-oxadiazoles and 1,2,4-triazoles Libraries in Continuous Flow Reactor

Andrew R Bogdan and Ying Wang

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General Information.

All starting materials were commercially available and used without purification unless noted. 4-fluorobenzohydrazonamide hydroiodide was synthesized from 4-fluorobenzothioamide.

General Purification Procedure.

Samples were purified by preparative HPLC on a Phenomenex Luna C8(2) 5 um 100Å AXIA column (50mm × 21.2mm). A gradient of acetonitrile (A) and 0.1% trifluoroacetic acid in water (B) was used, at a flow rate of 30mL/min (0-0.5 min 5% A, 0.5-6.5 min linear gradient 5-100% A, 6.5-8.5 min 100% A, 8.5-9.0 min linear gradient 100-5% A, 9.0-10 min 5% A). A sample volume of 1.0mL was injected directly from the flow reactor stream to the HPLC system. A custom purification system was used, consisting of the following modules: Gilson 305 and 306 pumps; Gilson 806 Manometric module; Gilson UV/Vis 155 detector; Gilson 506C interface box; Gilson FC204 fraction collector; Agilent G1968D Active Splitter; Thermo MSQ Plus mass spectrometer. The system was controlled through a combination of Thermo Xcalibur 2.0.7 software and a custom application written in-house using Microsoft Visual Basic 6.0.

General Procedure for Oxadiazole Formation.

A stock solution of carboxylic and DIPEA (0.60 M and 1.8 in DMA, respecitvely, 166.7 μL, 0.10 mmol carboxylic acid (1.0 eq) and 0.3 mmol DIPEA (3.0 eq)) and HATU (0.50 M in DMA, 200 μL, 0.10 mmol, 1.0 eq) were aspirated from their respective source vials, mixed through a PFA mixing tube (0.2 mm inner diameter), and loaded into an incubation chamber held at 30 °C for 5 minutes. The reaction segment was mixed with a stock solution of hydroxyamidine (0.60 M, 166.7 μL, 0.10 mmol, 1.0 eq), loaded into an injection loop for one minute, followed by injection into the flow reactor (Hastelloy coil, 0.75 mm inner diameter, 1.8 mL internal volume) set at 175 °C, and passed through the reactor at 163 μL min^{-1} (11 minute residence time) pressurized to 1000 psi using a back-pressure regulator. Upon exiting the reactor, the reaction was loaded directly into an injection loop and purified using prep LC to yield the final compound.

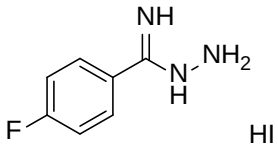
General Procedure for Monocyclic Triazole Formation.

A stock solution of carboxylic and DIPEA (0.60 M and 1.8 in DMA, respecitvely, 166.7 μL, 0.10 mmol carboxylic acid (1.0 eq) and 0.3 mmol DIPEA (3.0 eq)) and HATU (0.50 M in DMA, 200 μL, 0.10 mmol, 1.0 eq) were aspirated from their respective source vials, mixed through a PFA mixing tube (0.2 mm inner diameter), and loaded into an incubation chamber held at 30 °C for 5 minutes. The reaction segment was mixed with a stock solution of hydrazonamide (0.60 M, 166.7 μL, 0.10 mmol, 1.0 eq), loaded into an injection loop for one minute, followed by injection into the flow reactor (Hastelloy coil, 0.75 mm inner diameter, 1.8 mL internal volume) set at 175 °C, and passed through the reactor at 163 μL min^{-1} (11 minute residence time) pressurized to 1000 psi using a back-pressure

regulator. Upon exiting the reactor, the reaction was loaded directly into an injection loop and purified using prep LC to yield the final compound.

General Procedure for Bicyclic Triazole Formation.

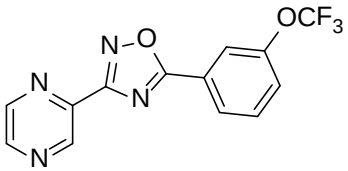
A stock solution of carboxylic and DIPEA (0.60 M and 1.8 in DMA, respecitvely, 166.7 µL, 0.10 mmol carboxylic acid (1.0 eq) and 0.3 mmol DIPEA (3.0 eq)) and HATU (0.50 M in DMA, 200 µL, 0.10 mmol, 1.0 eq) were aspirated from their respective source vials, mixed through a PFA mixing tube (0.2 mm inner diameter), and loaded into an incubation chamber held at 30 °C for 5 minutes. The reaction segment was mixed with a stock solution of hydrazinopyridine (0.60 M, 166.7 µL, 0.10 mmol, 1.0 eq), loaded into an injection loop for one minute, followed by injection into the flow reactor (Hastelloy coil, 0.75 mm inner diameter, 1.8 mL internal volume) set at 250 °C, and passed through the reactor at 90 µL min^{-1} (20 minute residence time) pressurized to 1000 psi using a back-pressure regulator. Upon exiting the reactor, the reaction was collected in a fraction collector. Samples were purified using prep LC to yield the final compound.



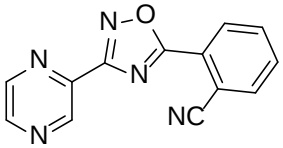
4-fluorobenzohydrazonamide hydroiodide. In a 20 mL vial was 4-fluorobenzothioamide (810 mg, 5.22 mmol) in Acetone (10 ml) to give a yellow solution. iodomethane (0.424 ml, 6.79 mmol) was added and the reaction was heated to 60 °C. After 2 hours, a solid precipitated out and starting material was fully consumed. Solvent was removed in vacuo.

In a 20 mL vial was hydrazine monohydrate (0.357 ml, 6.26 mmol) in Methanol (5 ml) to give a colorless solution. The solution was cooled to 0 °C. A solution of the thiobenzimidic acid methyl ester in THF (5 mL) was added dropwise over the course of 5 minutes. After addition, the reaction mixture was removed from the ice bath and warmed to room temperature and stirred for 1 hour until complete by LC. Solvent was removed in vacuo. The result solid was washed with 1:1 THF/diethyl ether and dried to yield (E)-4-fluorobenzohydrazonamide hydroiodide as a white solid (1.1 g, 75% yield). 1H NMR (501 MHz, DMSO:D_2O-d_6) δ 7.84 - 7.74 (m, 2H), 7.50 - 7.39 (m, 2H). 13C NMR (101 MHz, DMSO-d_6) δ 166.32, 163.82, 161.54, 131.05 (d, J = 9.3 Hz), 124.28 (d, J = 3.0 Hz), 116.63 (d, J = 22.3 Hz).

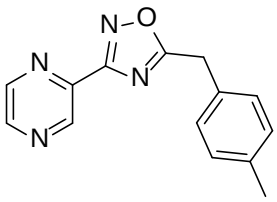
NMR Data.



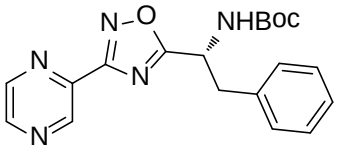
^{1}H NMR (400 MHz, DMSO-d_6) δ 9.31 (d, J = 1.4 Hz, 1H), 8.93 – 8.83 (m, 2H), 8.26 – 8.17 (m, 1H), 8.10 – 7.98 (m, 1H), 7.81 (t, J = 8.0 Hz, 1H), 7.76 – 7.70 (m, 1H). ^{13}C NMR (101 MHz, DMSO-d_6) δ 175.20, 167.15, 149.16, 147.67, 145.68, 144.27, 141.73, 132.54, 127.57, 126.49, 125.39, 124.25, 121.69, 120.61, 119.13, 116.57. MS (APCI+) m/z 309.0 $(M+H)^+$.



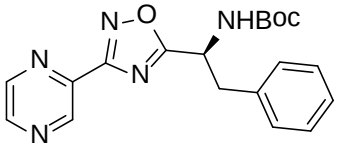
^{1}H NMR (400 MHz, DMSO-d_6) δ 9.35 (d, J = 1.1 Hz, 1H), 8.91 (s, 2H), 8.43 (dd, J = 7.9, 1.3 Hz, 1H), 8.17 (dd, J = 7.7, 1.4 Hz, 1H), 8.01 (td, J = 7.8, 1.4 Hz, 1H), 7.93 (td, J = 7.7, 1.4 Hz, 1H). ^{13}C NMR (101 MHz, DMSO-d_6) δ 167.12, 147.83, 145.83, 144.39, 141.76, 136.00, 134.60, 134.25, 131.06, 125.13, 117.41, 110.99, 110.79. MS (APCI+) m/z 250.0 $(M+H)^+$.



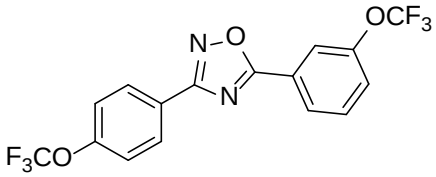
^{1}H NMR (400 MHz, DMSO-d_6) δ 9.20 (d, J = 1.4 Hz, 1H), 8.89 – 8.80 (m, 2H), 7.27 (d, J = 8.0 Hz, 2H), 7.17 (d, J = 7.8 Hz, 2H), 4.23 (s, 2H), 2.42 (s, 0H), 2.27 (s, 3H). ^{13}C NMR (101 MHz, DMSO-d_6) δ 180.35, 166.56, 147.45, 145.63, 144.10, 141.96, 137.21, 131.08, 129.83, 129.41, 32.08, 21.04. MS (APCI+) m/z 253.1 $(M+H)^+$.



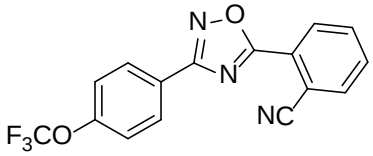
^{1}H NMR (400 MHz, DMSO-d_6) δ 9.24 (d, J = 1.5 Hz, 1H), 8.93 – 8.82 (m, 2H), 7.38 – 7.20 (m, 6H), 5.14 (dd, J = 9.7, 5.9 Hz, 1H), 3.32 (dd, J = 13.8, 6.0 Hz, 1H), 3.19 (dd, J = 13.7, 9.8 Hz, 1H), 1.38 – 1.11 (m, 9H). ^{13}C NMR (101 MHz, DMSO-d_6) δ 181.33, 166.51, 147.40, 145.61, 144.13, 136.96, 129.58, 128.74, 127.19, 79.74, 50.26, 38.42, 28.47. MS (APCI+) m/z 368.0 $(M+H)^+$.



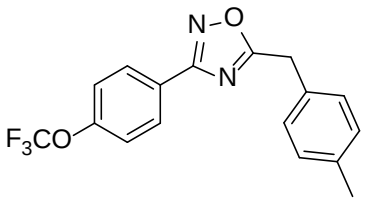
^{1}H NMR (400 MHz, DMSO-d_6) δ 9.22 (d, J = 1.1 Hz, 1H), 8.83 (s, 2H), 7.37 – 7.06 (m, 5H), 5.18 (dd, J = 9.1, 6.2 Hz, 1H), 3.42 – 3.20 (m, 2H), 1.33 (s, 9H). ^{13}C NMR (101 MHz, DMSO-d_6) δ 181.33, 166.51, 147.39, 145.59, 144.12, 142.11, 136.95, 129.58, 128.74, 127.19, 79.75, 50.26, 38.43, 28.47. MS (APCI+) m/z 368.0 $(M+H)^+$.



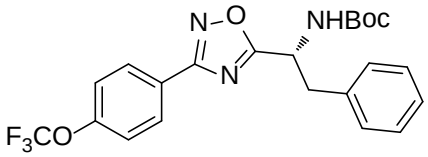
^{1}H NMR (400 MHz, DMSO-d_6) δ 8.30 – 8.20 (m, 3H), 8.11 (s, 1H), 7.85 (t, J = 8.0 Hz, 1H), 7.81 – 7.72 (m, 1H), 7.62 (d, J = 8.4 Hz, 2H). ^{13}C NMR (101 MHz, Chloroform-d) δ 174.58 , 168.11 , 151.44 , 151.42 , 149.69 , 130.85 , 129.30 , 126.41 , 125.92 , 125.22 , 125.20 , 121.10 , 120.95 (q, J = 256.8 Hz), 120.79 (q, J = 256.8 Hz), 120.65. MS (APCI+) m/z 391.0 $(M+H)^+$.



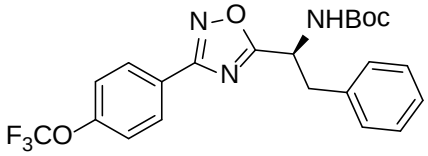
^{1}H NMR (400 MHz, DMSO-d_6) δ 8.36 (d, J = 7.8 Hz, 1H), 8.20 (d, J = 8.4 Hz, 2H), 8.13 (d, J = 7.6 Hz, 1H), 7.98 (t, J = 7.7 Hz, 1H), 7.91 (t, J = 7.6 Hz, 1H), 7.60 (d, J = 8.3 Hz, 2H). ^{13}C NMR (101 MHz, DMSO-d_6) δ 173.63, 167.79, 151.13, 135.93, 134.49, 134.07, 130.81, 129.87, 125.25, 125.16, 122.16, 120.39 (q, J = 257.6 Hz), 117.35, 110.75. MS (APCI+) m/z 332.0 $(M+H)^+$.



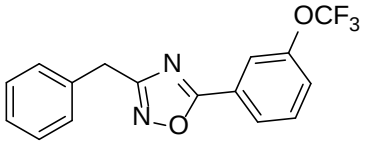
^{1}H NMR (400 MHz, DMSO-d_6) δ 8.16 – 8.06 (m, 2H), 7.60 – 7.51 (m, 2H), 7.26 (d, J = 8.0 Hz, 2H), 7.17 (d, J = 7.8 Hz, 2H), 4.36 (s, 2H), 2.27 (s, 3H). ^{13}C NMR (101 MHz, DMSO-d_6) δ 179.86, 167.22, 150.87, 137.17, 131.22, 129.83, 129.70, 129.34, 125.65, 124.23, 122.04, 121.66, 119.11, 32.04, 21.02. MS (APCI+) m/z 335.0 $(M+H)^+$.



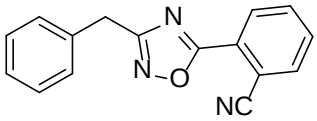
^{1}H NMR (400 MHz, DMSO-d_6) δ 8.17 – 8.06 (m, 2H), 7.49 (d, J = 8.2 Hz, 2H), 7.38 – 7.17 (m, 5H), 5.14 (dd, J = 9.0, 6.2 Hz, 1H), 3.40 – 3.19 (m, 2H), 1.32 (d, J = 2.9 Hz, 9H). ^{13}C NMR (101 MHz, DMSO-d_6) δ 180.75, 167.19, 155.35, 151.13, 151.11, 136.96, 129.67, 129.53, 128.67, 127.12, 125.77, 121.76, 119.20, 79.65, 50.24, 38.50, 28.40. MS (APCI+) m/z 449.8 $(M+H)^+$.



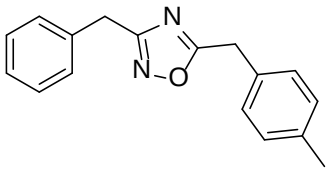
^{1}H NMR (400 MHz, DMSO-d_6) δ 8.11 (dt, J = 8.7, 2.0 Hz, 2H), 7.49 (t, J = 7.3 Hz, 2H), 7.45 – 7.19 (m, 5H), 5.14 (t, J = 7.6 Hz, 1H), 3.50 – 3.19 (m, 2H), 1.32 (d, J = 2.5 Hz, 9H). ^{13}C NMR (101 MHz, DMSO-d_6) δ 180.76, 167.19, 155.35, 151.13, 136.97, 129.66, 129.53, 128.68, 127.12, 125.76, 121.74, 79.65, 50.23, 38.49, 28.41. MS (APCI+) m/z 449.7 $(M+H)^+$.



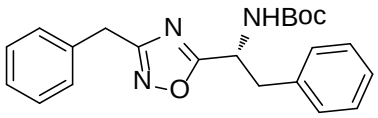
^{1}H NMR (400 MHz, DMSO-d_6) δ 8.03 – 7.94 (m, 1H), 7.89 – 7.83 (m, 1H), 7.69 (t, J = 8.0 Hz, 1H), 7.62 – 7.42 (m, 1H), 7.42 – 7.21 (m, 5H), 4.13 (s, 2H). ^{13}C NMR (101 MHz, DMSO-d_6) δ 174.16, 170.52, 149.06, 135.89, 132.31, 129.28, 129.02, 127.40, 127.20, 125.97, 125.66, 120.54 (q, J = 256.2 Hz), 120.22, 31.78. MS (APCI+) m/z 321.0 $(M+H)^+$.



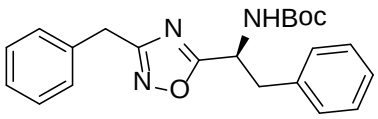
^{1}H NMR (400 MHz, DMSO-d_6) δ 8.24 (dd, J = 7.8, 1.3 Hz, 1H), 8.08 (dd, J = 7.7, 1.4 Hz, 1H), 7.92 (td, J = 7.7, 1.4 Hz, 1H), 7.85 (td, J = 7.6, 1.4 Hz, 1H), 7.45 – 7.13 (m, 5H), 4.21 (s, 2H). ^{13}C NMR (101 MHz, DMSO-d_6) δ 173.12, 170.55, 135.86, 135.84, 134.45, 133.85, 130.74, 129.40, 129.10, 127.50, 125.37, 117.35, 110.57, 31.80. MS (APCI+) m/z 262.1 $(M+H)^+$.



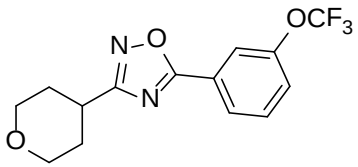
^{1}H NMR (400 MHz, DMSO-d_6) δ 7.38 – 7.21 (m, 5H), 7.18 (d, J = 8.2 Hz, 2H), 7.14 (d, J = 7.9 Hz, 2H), 4.03 (s, 2H), 3.76 (s, 2H), 2.26 (s, 3H). ^{13}C NMR (101 MHz, DMSO-d_6) δ 179.05, 169.80, 137.08, 136.10, 131.35, 129.78, 129.31, 129.29, 129.05, 127.38, 31.96, 31.78, 21.02. MS (APCI+) m/z 265.1 $(M+H)^+$.



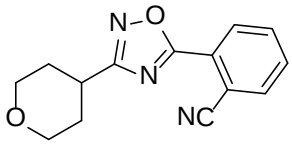
^{1}H NMR (400 MHz, DMSO-d_6) δ 7.41 – 7.16 (m, 10H), 5.02 (dd, J = 8.7, 6.6 Hz, 1H), 4.06 (s, 2H), 3.27 – 3.09 (m, 2H), 1.30 (s, 9H). ^{13}C NMR (101 MHz, DMSO-d_6) δ 180.01, 169.52, 136.94, 136.12, 129.51, 129.15, 128.90, 128.66, 127.25, 127.10, 79.59, 50.15, 38.56, 31.85, 28.44. MS (APCI+) m/z 380.1 $(M+H)^+$.



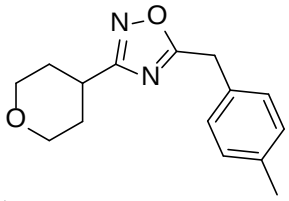
^{1}H NMR (400 MHz, DMSO-d_6) δ 7.40 – 7.14 (m, 10H), 5.01 (dd, J = 8.7, 6.6 Hz, 1H), 4.06 (s, 2H), 3.26 – 3.07 (m, 2H), 1.30 (s, 9H). ^{13}C NMR (101 MHz, DMSO-d_6) δ 180.01, 169.52, 136.93, 136.12, 129.51, 129.15, 128.91, 128.66, 127.26, 127.10, 79.59, 50.16, 38.56, 31.84, 28.44. MS (APCI+) m/z 380.1 $(M+H)^+$.



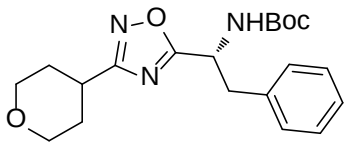
^{1}H NMR (400 MHz, DMSO-d_6) δ 8.05 (d, J = 7.7, 1.3 Hz, 1H), 7.92 – 7.86 (m, 1H), 7.73 (t, J = 8.0 Hz, 1H), 7.66 – 7.59 (m, 1H), 3.94 – 3.85 (m, 2H), 3.47 (td, J = 11.5, 2.3 Hz, 2H), 3.19 – 3.05 (m, 1H), 1.97 – 1.84 (m, 2H), 1.80 – 1.67 (m, 2H). ^{13}C NMR (101 MHz, DMSO-d_6) δ 173.90, 173.80, 149.11, 132.34, 127.17, 125.92, 125.78, 120.37 (q, J = 257.4 Hz), 120.17, 66.61, 32.69, 30.18. MS (APCI+) m/z 315.0 $(M+H)^+$.



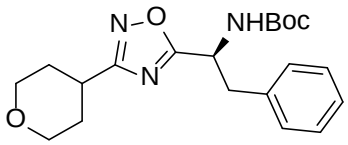
^{1}H NMR (400 MHz, DMSO-d_6) δ 8.32 – 8.24 (m, 1H), 8.09 (dd, J = 7.8, 1.3 Hz, 1H), 7.94 (td, J = 7.7, 1.4 Hz, 1H), 7.87 (td, J = 7.6, 1.3 Hz, 1H), 4.02 – 3.89 (m, 2H), 3.51 (td, J = 11.5, 2.4 Hz, 2H), 3.30 – 3.00 (m, 1H), 2.04 – 1.92 (m, 2H), 1.90 – 1.73 (m, 2H). ^{13}C NMR (101 MHz, DMSO-d_6) δ 173.85, 172.83, 135.85, 134.45, 133.80, 130.66, 125.48, 117.33, 110.61, 66.58, 32.62, 30.21. MS (APCI+) m/z 256.1 $(M+H)^+$.



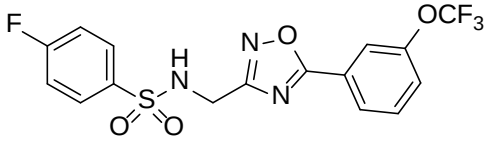
^{1}H NMR (400 MHz, DMSO-d_6) δ 7.21 (d, J = 8.1 Hz, 2H), 7.16 (d, J = 7.9 Hz, 2H), 4.24 (s, 2H), 3.87 (ddd, J = 11.5, 4.2, 2.5 Hz, 2H), 3.44 (td, J = 11.5, 2.3 Hz, 2H), 3.02 (tt, J = 11.3, 4.0 Hz, 1H), 2.27 (s, 3H), 1.91 – 1.79 (m, 2H), 1.78 – 1.59 (m, 2H). ^{13}C NMR (101 MHz, DMSO-d_6) δ 178.77, 173.11, 137.07, 131.42, 129.78, 129.28, 66.65, 32.61, 31.98, 30.24, 21.02. MS (APCI+) m/z 259.1 $(M+H)^+$.



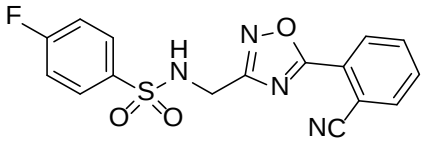
^{1}H NMR (400 MHz, DMSO-d_6) δ 7.36 – 7.12 (m, 5H), 5.11 – 4.94 (m, 1H), 3.88 (dt, J = 11.5, 3.7 Hz, 2H), 3.57 – 3.42 (m, 2H), 3.29 – 3.13 (m, 2H), 3.13 – 2.99 (m, 1H), 1.94 – 1.81 (m, 2H), 1.81 – 1.65 (m, 2H), 1.32 (s, 9H). ^{13}C NMR (101 MHz, DMSO-d_6) δ 179.67, 172.95, 137.00, 129.51, 128.65, 127.10, 79.59, 66.58, 50.19, 38.62, 32.64, 30.31, 28.44. MS (APCI+) m/z 374.1 $(M+H)^+$.



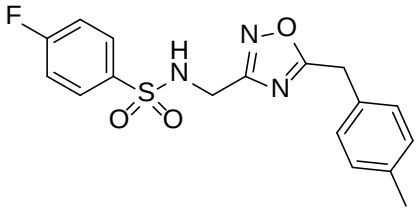
^{1}H NMR (400 MHz, DMSO-d_6) δ 7.35 – 7.10 (m, 5H), 5.02 (dd, J = 8.8, 6.5 Hz, 1H), 3.88 (dt, J = 11.5, 3.7 Hz, 2H), 3.55 – 3.41 (m, 2H), 3.27 – 3.12 (m, 2H), 3.12 – 2.99 (m, 1H), 1.92 – 1.81 (m, 2H), 1.81 – 1.63 (m, 2H), 1.32 (s, 9H). ^{13}C NMR (101 MHz, DMSO-d_6) δ 179.67, 172.95, 155.30, 137.00, 129.51, 128.65, 127.09, 79.58, 66.58, 50.19, 48.97, 38.62, 32.65, 30.31, 28.44. MS (APCI+) m/z 374.1 $(M+H)^+$.



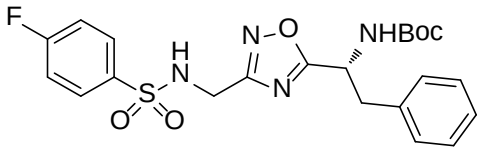
^{1}H NMR (400 MHz, DMSO-d_6) δ 7.99 (dt, J = 7.7, 1.3 Hz, 1H), 7.85 – 7.72 (m, 4H), 7.72 – 7.65 (m, 1H), 7.31 – 7.23 (m, 2H), 4.30 (s, 2H). ^{13}C NMR (101 MHz, DMSO-d_6) δ 174.21, 167.99, 165.82, 163.32, 149.11, 137.11, 137.08, 132.46, 130.17, 130.07, 127.20, 126.27, 125.30, 120.39 (q, J = 257.4 Hz), 120.22, 116.50, 116.28, 37.98. MS (APCI+) m/z 418.0 $(M+H)^+$.



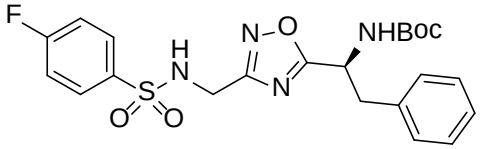
^{1}H NMR (400 MHz, DMSO-d_6) δ 8.15 (dd, J = 8.0, 1.3 Hz, 1H), 8.11 (dd, J = 7.8, 1.4 Hz, 1H), 7.95 (td, J = 7.8, 1.5 Hz, 1H), 7.89 (td, J = 7.7, 1.4 Hz, 1H), 7.86 – 7.79 (m, 2H), 7.38 – 7.26 (m, 2H), 4.33 (s, 2H). ^{13}C NMR (101 MHz, DMSO-d_6) δ 173.23, 168.07, 164.60 (d, J = 251.3 Hz), 136.91, 135.93, 134.52, 134.05, 130.78, 130.20, 130.11, 124.99, 117.24, 116.67, 116.44, 110.39, 38.06. MS (APCI+) m/z 358.9 $(M+H)^+$.



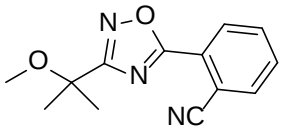
^{1}H NMR (400 MHz, DMSO-d_6) δ 7.88 – 7.74 (m, 2H), 7.40 – 7.27 (m, 2H), 7.19 – 7.09 (m, 4H), 4.18 (s, 2H), 4.15 (s, 2H), 2.28 (s, 3H). ^{13}C NMR (101 MHz, DMSO-d_6) δ 179.28, 167.35, 165.88, 163.38, 137.16, 136.93, 131.09, 130.07, 129.98, 129.76, 129.30, 116.71, 116.49, 37.98, 31.83, 21.04. MS (APCI+) m/z 361.9 $(M+H)^+$.



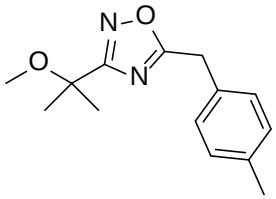
^{1}H NMR (400 MHz, DMSO-d_6) δ 7.95 – 7.81 (m, 2H), 7.41 – 7.18 (m, 7H), 5.05 – 4.93 (m, 1H), 4.22 (s, 2H), 3.21 – 3.02 (m, 2H), 1.31 (s, 9H). ^{13}C NMR (101 MHz, DMSO-d_6) δ 180.27, 167.47, 166.03, 163.53, 155.28, 137.39, 136.95, 130.10, 130.00, 129.50, 128.70, 127.14, 116.63, 116.40, 79.66, 49.96, 38.48, 38.19, 28.45. MS (APCI+) m/z 477.0 $(M+H)^+$.



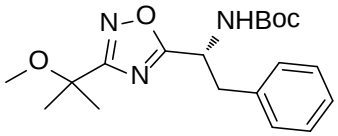
^{1}H NMR (400 MHz, DMSO-d_6) δ 7.95 – 7.81 (m, 2H), 7.46 – 7.18 (m, 7H), 5.05 – 4.93 (m, 1H), 4.22 (s, 2H), 3.19 – 3.04 (m, 2H), 1.31 (s, 9H). ^{13}C NMR (101 MHz, DMSO-d_6) δ 180.27, 167.47, 137.42, 137.39, 136.95, 130.10, 130.00, 129.50, 128.70, 127.14, 116.63, 116.40, 79.66, 49.96, 38.48, 38.19, 28.45. MS (APCI+) m/z 477.0 $(M+H)^+$.



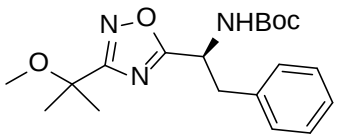
^{1}H NMR (400 MHz, DMSO-d_6) δ 8.29 (dd, J = 7.8, 1.3 Hz, 1H), 8.11 (dd, J = 7.8, 1.3 Hz, 1H), 7.96 (td, J = 7.7, 1.4 Hz, 1H), 7.89 (td, J = 7.6, 1.3 Hz, 1H), 3.14 (s, 3H), 1.60 (s, 6H). ^{13}C NMR (101 MHz, DMSO-d_6) δ 173.80, 173.25, 135.85, 134.48, 133.91, 130.81, 125.47, 117.31, 110.71, 73.19, 51.36, 25.25. MS (APCI+) m/z 244.1 $(M+H)^+$.



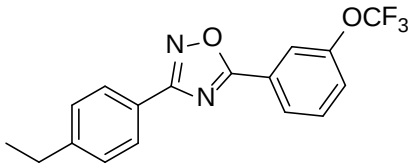
^{1}H NMR (400 MHz, DMSO-d_6) δ 7.21 (d, J = 8.2 Hz, 2H), 7.16 (d, J = 8.0 Hz, 2H), 4.28 (s, 2H), 2.27 (s, 3H), 1.49 (s, 6H). ^{13}C NMR (101 MHz, DMSO-d_6) δ 179.14, 173.01, 137.09, 131.39, 129.81, 129.22, 72.97, 51.12, 31.97, 25.15, 21.02. MS (APCI+) m/z 247.1 $(M+H)^+$.



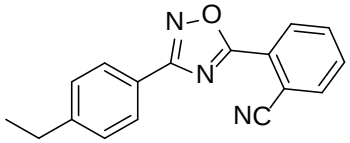
^{1}H NMR (400 MHz, DMSO-d_6) δ 7.34 – 7.16 (m, 5H), 5.10 – 4.97 (m, 1H), 3.28 – 3.14 (m, 2H), 3.06 (s, 3H), 1.51 (s, 6H), 1.33 (s, 9H). ^{13}C NMR (101 MHz, DMSO-d_6) δ 180.00, 173.09, 155.33, 136.89, 129.52, 128.67, 127.13, 79.62, 73.11, 51.06, 50.27, 38.62, 28.44, 25.26. MS (APCI+) m/z 362.1 $(M+H)^+$.



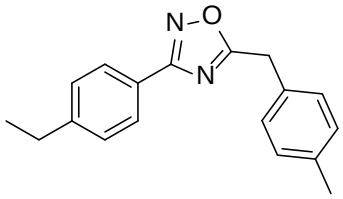
^{1}H NMR (400 MHz, DMSO-d_6) δ 7.34 – 7.16 (m, 5H), 5.09 – 4.95 (m, 1H), 3.26 – 3.12 (m, 2H), 3.06 (s, 3H), 1.51 (s, 6H), 1.33 (s, 9H). ^{13}C NMR (101 MHz, DMSO-d_6) δ 180.00, 173.08, 155.30, 136.89, 129.52, 128.67, 127.13, 79.62, 73.11, 51.07, 50.26, 38.62, 28.44, 25.26. MS (APCI+) m/z 362.1 $(M+H)^+$.



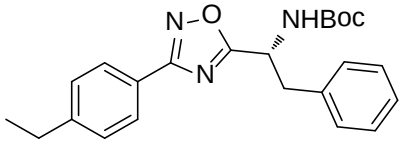
^{1}H NMR (400 MHz, DMSO-d_6) δ 8.20 (dt, J = 7.7, 1.3 Hz, 1H), 8.08 – 8.02 (m, 1H), 8.02 – 7.93 (m, 2H), 7.81 (t, J = 8.0 Hz, 1H), 7.77 – 7.69 (m, 1H), 7.43 (d, J = 8.2 Hz, 2H), 2.69 (q, J = 7.6 Hz, 2H), 1.22 (t, J = 7.6 Hz, 3H). ^{13}C NMR (101 MHz, DMSO-d_6) δ 174.42, 168.83, 149.18, 149.16, 148.52, 132.50, 129.15, 127.65, 127.48, 126.23, 125.77, 123.66, 120.53, 120.44 (q, J = 257.6 Hz), 28.59, 15.63. MS (APCI+) m/z 355.0 $(M+H)^+$.



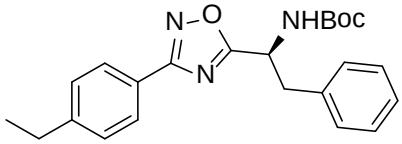
^{1}H NMR (400 MHz, DMSO-d_6) δ 8.33 (dd, J = 7.9, 1.3 Hz, 1H), 8.11 (dd, J = 7.7, 1.3 Hz, 1H), 8.04 – 7.92 (m, 3H), 7.89 (td, J = 7.7, 1.3 Hz, 1H), 7.48 – 7.40 (m, 2H), 2.68 (q, J = 7.6 Hz, 2H), 1.21 (t, J = 7.6 Hz, 3H). ^{13}C NMR (101 MHz, DMSO-d_6) δ 173.18, 168.74, 148.62, 135.89, 134.44, 133.90, 130.71, 129.16, 127.64, 125.33, 123.53, 117.39, 110.71, 28.60, 15.62. MS (APCI+) m/z 276.1 $(M+H)^+$.



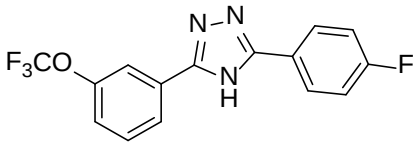
^{1}H NMR (400 MHz, DMSO-d_6) δ 7.91 – 7.84 (m, 2H), 7.38 – 7.30 (m, 2H), 7.27 – 7.18 (m, 2H), 7.14 (d, J = 7.9 Hz, 2H), 4.31 (s, 2H), 2.62 (q, J = 7.6 Hz, 2H), 2.24 (s, 3H), 1.16 (d, J = 7.7 Hz, 2H). ^{13}C NMR (101 MHz, DMSO-d_6) δ 179.25, 168.16, 148.13, 137.08, 131.33, 129.78, 129.28, 128.99, 127.46, 123.97, 32.06, 28.54, 21.00, 15.57. MS (APCI+) m/z 279.1 $(M+H)^+$.



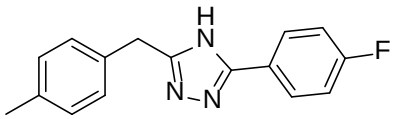
^{1}H NMR (400 MHz, DMSO-d_6) δ 7.96 – 7.86 (m, 2H), 7.37 (d, J = 8.0 Hz, 2H), 7.33 – 7.20 (m, 5H), 5.12 (dd, J = 9.0, 6.3 Hz, 1H), 3.38 – 3.12 (m, 2H), 2.68 (q, J = 7.6 Hz, 2H), 1.33 (s, 9H), 1.22 (t, J = 7.6 Hz, 3H). ^{13}C NMR (101 MHz, DMSO-d_6) δ 180.21, 168.17, 155.36, 148.21, 137.04, 129.54, 128.89, 128.68, 127.55, 127.11, 124.17, 79.62, 50.23, 38.58, 28.52, 28.45, 15.25. MS (APCI+) m/z 394.1 $(M+H)^+$.



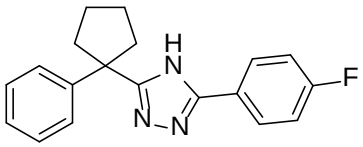
^{1}H NMR (400 MHz, DMSO-d_6) δ 7.90 (d, J = 8.2 Hz, 2H), 7.38 (d, J = 8.0 Hz, 2H), 7.32 – 7.15 (m, 5H), 5.11 (dd, J = 9.0, 6.3 Hz, 1H), 3.39 – 3.17 (m, 2H), 2.69 (q, J = 7.6 Hz, 2H), 1.33 (s, 9H), 1.23 (t, J = 7.6 Hz, 3H). ^{13}C NMR (101 MHz, DMSO-d_6) δ 180.23, 168.17, 155.36, 148.24, 137.05, 129.55, 128.92, 128.69, 127.55, 127.13, 124.15, 79.64, 50.23, 48.98, 38.55, 28.52, 28.46, 15.27. MS (APCI+) m/z 394.1 $(M+H)^+$.



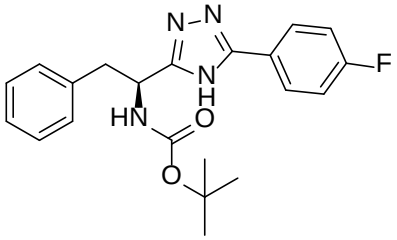
^{1}H NMR (400 MHz, DMSO-d_6) δ 8.13 – 8.02 (m, 3H), 7.94 (s, 1H), 7.61 (t, J = 8.1 Hz, 1H), 7.38 (d, J = 7.2 Hz, 1H), 7.35 – 7.22 (m, 2H). ^{13}C NMR (101 MHz, DMSO-d_6) δ 164.73, 162.26, 149.19, 131.45, 128.87, 125.26, 124.33, 121.78, 119.23, 118.47, 116.67, 116.48, 116.25. MS (APCI+) m/z 324.0 $(M+H)^+$.



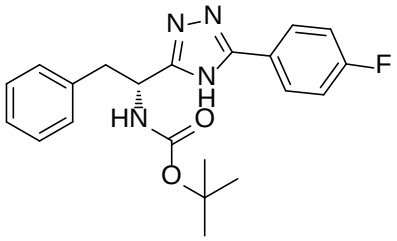
^{1}H NMR (400 MHz, DMSO-d_6) δ 8.07 – 7.98 (m, 2H), 7.32 – 7.23 (m, 2H), 7.20 (d, J = 7.9 Hz, 2H), 7.10 (d, J = 7.8 Hz, 2H), 4.08 (s, 2H), 2.23 (s, 3H). ^{13}C NMR (101 MHz, DMSO-d_6) δ 164.53, 162.08, 158.29, 158.21, 136.38, 134.07, 129.59, 128.94, 128.81, 128.70, 128.61, 126.36, 126.32, 116.36, 116.14, 32.12, 20.93. MS (APCI+) m/z 268.1 $(M+H)^+$.



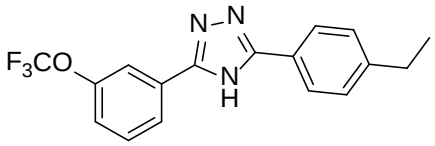
^{1}H NMR (400 MHz, DMSO-d_6) δ 8.11 – 7.95 (m, 2H), 7.34 (d, J = 7.4 Hz, 2H), 7.31 – 7.21 (m, 4H), 7.16 (t, J = 7.3 Hz, 1H), 2.84 – 2.69 (m, 2H), 2.22 – 1.96 (m, 2H), 1.78 – 1.63 (m, 2H), 1.63 – 1.42 (m, 2H). ^{13}C NMR (101 MHz, DMSO-d_6) δ 164.41, 161.95, 158.31, 145.69, 128.73, 128.68, 128.60, 126.86, 126.80, 116.23, 116.01, 52.07, 37.78, 23.28. MS (APCI+) m/z 308.1 $(M+H)^+$.



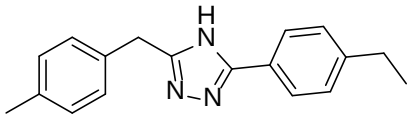
^{1}H NMR (400 MHz, DMSO-d_6) δ 8.09 – 7.94 (m, 2H), 7.32 – 7.09 (m, 7H), 5.00 (dd, J = 8.4, 6.2 Hz, 1H), 3.33 – 3.06 (m, 2H), 1.31 (s, 9H). ^{13}C NMR (101 MHz, DMSO-d_6) δ 164.47, 162.02, 160.79, 158.15, 155.58, 138.07, 129.60, 128.64, 128.58, 126.82, 126.67, 116.37, 116.16, 78.91, 49.80, 28.50. MS (APCI+) m/z 383.0 $(M+H)^+$.



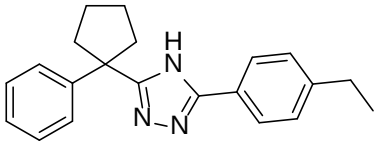
^{1}H NMR (400 MHz, DMSO-d_6) δ 8.11 – 7.97 (m, 2H), 7.33 – 7.12 (m, 7H), 5.00 (dd, J = 8.5, 6.2 Hz, 1H), 3.33 – 3.07 (m, 2H), 1.31 (s, 9H). ^{13}C NMR (101 MHz, DMSO-d_6) δ 164.49, 162.03, 160.75, 158.10, 155.59, 138.05, 129.60, 128.66, 128.58, 126.82, 126.61, 116.37, 116.15, 78.92, 49.79, 28.49. MS (APCI+) m/z 383.0 $(M+H)^+$.



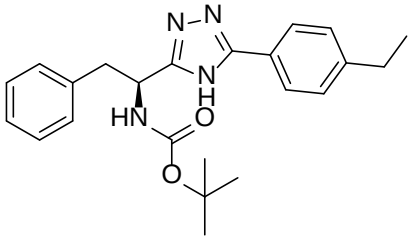
^{1}H NMR (400 MHz, DMSO-d_6) δ 8.09 (dt, J = 7.8, 1.2 Hz, 1H), 8.03 – 7.92 (m, 3H), 7.65 (t, J = 8.0 Hz, 1H), 7.46 – 7.33 (m, 3H), 2.70 (q, J = 7.6 Hz, 2H), 1.24 (t, J = 7.6 Hz, 3H). ^{13}C NMR (101 MHz, DMSO-d_6) δ 158.78, 157.54, 149.22, 146.73, 132.58, 131.57, 128.87, 126.69, 125.66, 125.33, 122.26, 120.55 (q, J = 256.7 Hz), 118.48, 28.48, 15.70. MS (APCI+) m/z 334.0 $(M+H)^+$.



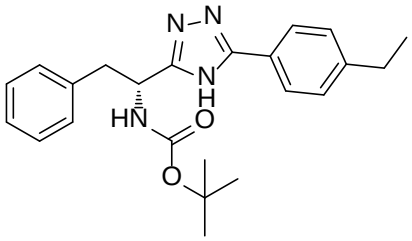
^{1}H NMR (400 MHz, DMSO-d_6) δ 7.92 – 7.81 (m, 2H), 7.35 – 7.25 (m, 2H), 7.20 (d, J = 8.1 Hz, 2H), 7.11 (d, J = 7.8 Hz, 2H), 4.05 (s, 2H), 2.65 (q, J = 7.6 Hz, 2H), 2.26 (s, 3H), 1.21 (t, J = 7.6 Hz, 3H). ^{13}C NMR (101 MHz, DMSO-d_6) δ 158.18, 157.75, 146.58, 136.41, 133.95, 129.60, 128.99, 128.78, 126.61, 125.99, 32.11, 28.47, 20.97, 15.69. MS (APCI+) m/z 278.1 $(M+H)^+$.



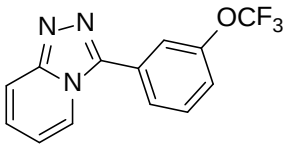
^{1}H NMR (400 MHz, DMSO-d_6) δ 7.90 – 7.82 (m, 2H), 7.39 – 7.31 (m, 2H), 7.31 – 7.23 (m, 4H), 7.21 – 7.12 (m, 1H), 2.84 – 2.70 (m, 2H), 2.65 (q, J = 7.5 Hz, 2H), 2.23 – 2.06 (m, 2H), 1.83 – 1.70 (m, 2H), 1.70 – 1.56 (m, 2H), 1.20 (t, J = 7.6 Hz, 3H). ^{13}C NMR (101 MHz, DMSO-d_6) δ 164.25, 157.82, 146.42, 145.55, 128.76, 128.68, 126.91, 126.86, 126.71, 126.27, 52.11, 37.80, 28.47, 23.33, 15.74. MS (APCI+) m/z 318.1 $(M+H)^+$.



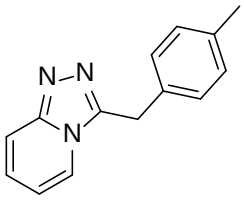
^{1}H NMR (400 MHz, DMSO-d_6) δ 7.88 (d, J = 8.3 Hz, 2H), 7.32 (d, J = 8.2 Hz, 2H), 7.28 – 7.08 (m, 5H), 4.96 (dd, J = 8.5, 6.2 Hz, 1H), 3.28 – 3.02 (m, 2H), 2.67 (q, J = 7.6 Hz, 2H), 1.31 (s, 9H), 1.22 (t, J = 7.6 Hz, 3H). ^{13}C NMR (101 MHz, DMSO-d_6) δ 160.92, 157.62, 155.57, 146.43, 138.09, 129.63, 128.80, 128.58, 126.82, 126.58, 126.30, 78.88, 49.89, 28.52, 28.48, 15.74. MS (APCI+) m/z 393.1 $(M+H)^+$.



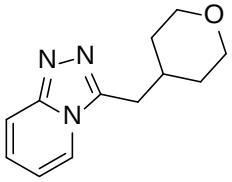
^{1}H NMR (400 MHz, DMSO-d_6) δ 7.88 (d, J = 8.2 Hz, 2H), 7.32 (d, J = 7.9 Hz, 2H), 7.28 – 7.11 (m, 5H), 4.95 (t, J = 7.3 Hz, 1H), 3.25 – 3.02 (m, 2H), 2.67 (q, J = 7.6 Hz, 2H), 1.31 (s, 9H), 1.22 (t, J = 7.6 Hz, 3H). ^{13}C NMR (101 MHz, DMSO-d_6) δ 161.29, 158.09, 155.57, 146.05, 138.23, 129.63, 128.72, 128.56, 127.00, 126.77, 126.46, 78.79, 49.99, 28.54, 28.48, 15.78. MS (APCI+) m/z 393.1 $(M+H)^+$.



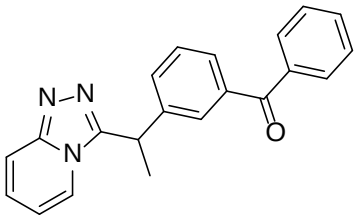
^{1}H NMR (400 MHz, DMSO-d_6) δ 8.59 (dt, J = 7.0, 1.1 Hz, 1H), 7.95 (dt, J = 7.7, 1.3 Hz, 1H), 7.92 – 7.83 (m, 2H), 7.79 (t, J = 8.1 Hz, 1H), 7.69 – 7.59 (m, 1H), 7.56 (dd, J = 9.3, 6.7 Hz, 1H), 7.14 (td, J = 6.9, 1.1 Hz, 1H). ^{13}C NMR (101 MHz, DMSO-d_6) δ 149.23, 149.22, 149.03, 145.23, 132.05, 131.65, 127.88, 127.73, 124.90, 123.46, 121.36, 119.94 (d, J = 258.3 Hz), 116.46, 114.63. MS (APCI+) m/z 280.0 $(M+H)^+$.



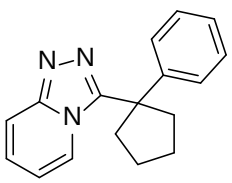
^{1}H NMR (400 MHz, DMSO-d_6) δ 8.65 – 8.55 (m, 1H), 8.02 – 7.91 (m, 1H), 7.90 – 7.77 (m, 1H), 7.35 (td, J = 6.8, 2.2 Hz, 1H), 7.24 (d, J = 8.0 Hz, 2H), 7.15 (d, J = 7.8 Hz, 2H), 4.57 (s, 2H), 2.26 (s, 3H). ^{13}C NMR (101 MHz, DMSO-d_6) δ 147.22, 146.47, 137.02, 134.13, 131.42, 129.80, 129.23, 125.30, 116.80, 113.11, 29.64, 20.99. MS (APCI+) m/z 224.1 $(M+H)^+$.



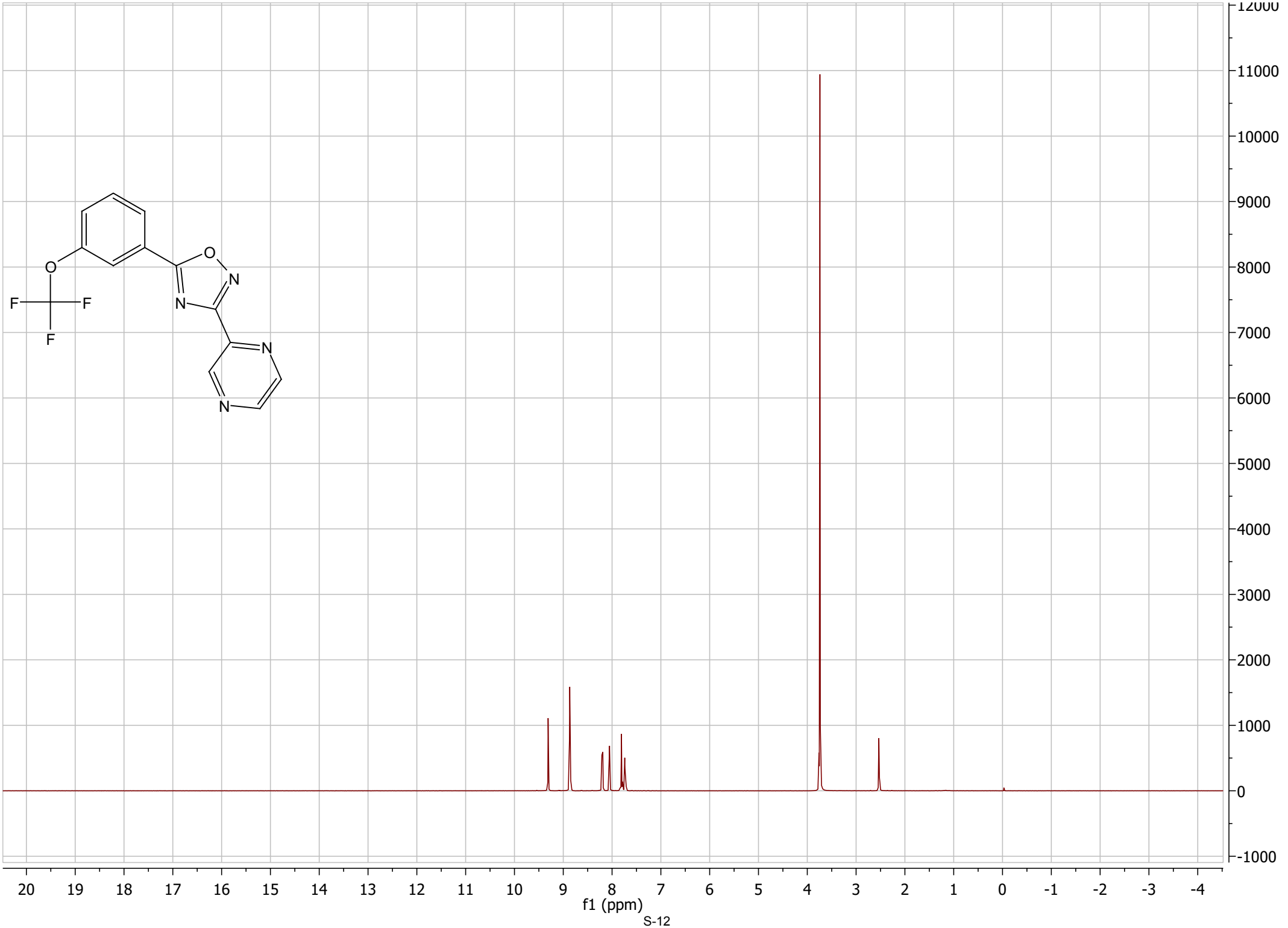
^{1}H NMR (400 MHz, DMSO-d_6) δ 8.87 (d, J = 6.9 Hz, 1H), 8.11 – 7.98 (m, 2H), 7.50 (td, J = 6.6, 1.6 Hz, 1H), 3.82 (ddd, J = 11.7, 4.5, 1.8 Hz, 2H), 3.28 (td, J = 11.8, 2.0 Hz, 2H), 3.18 (d, J = 7.1 Hz, 2H), 2.27 – 1.97 (m, 1H), 1.76 – 1.55 (m, 2H), 1.47 – 1.18 (m, 2H). ^{13}C NMR (101 MHz, DMSO-d_6) δ 159.39, 146.82, 145.12, 136.20, 126.04, 117.65, 112.00, 67.14, 32.74, 32.39, 30.35. MS (APCI+) m/z 218.1 $(M+H)^+$.



^{1}H NMR (400 MHz, DMSO-d_6) δ 8.38 (dt, J = 7.0, 1.1 Hz, 1H), 7.88 (dt, J = 9.3, 1.1 Hz, 1H), 7.75 – 7.58 (m, 7H), 7.58 – 7.48 (m, 3H), 7.17 (td, J = 6.9, 1.0 Hz, 1H), 4.99 (q, J = 7.0 Hz, 1H), 1.82 (d, J = 7.0 Hz, 3H). ^{13}C NMR (101 MHz, DMSO-d_6) δ 196.07, 149.65, 146.63, 141.18, 137.92, 137.09, 134.31, 133.31, 132.17, 130.03, 129.74, 129.28, 128.98, 128.91, 125.12, 116.96, 113.20, 35.34, 20.80. MS (APCI+) m/z 328.0 $(M+H)^+$.



^{1}H NMR (400 MHz, DMSO-d_6) δ 7.89 – 7.77 (m, 2H), 7.49 (dd, J = 9.3, 6.7 Hz, 1H), 7.41 – 7.27 (m, 2H), 7.27 – 7.17 (m, 3H), 6.92 (t, J = 7.0 Hz, 1H), 2.75 – 2.60 (m, 2H), 2.46 – 2.31 (m, 2H), 1.91 – 1.66 (m, 4H). ^{13}C NMR (101 MHz, DMSO-d_6) δ 151.42, 147.50, 142.24, 133.97, 129.49, 127.77, 126.59, 125.45, 116.83, 113.59, 51.37, 37.58, 24.11. MS (APCI+) m/z 264.1 $(M+H)^+$.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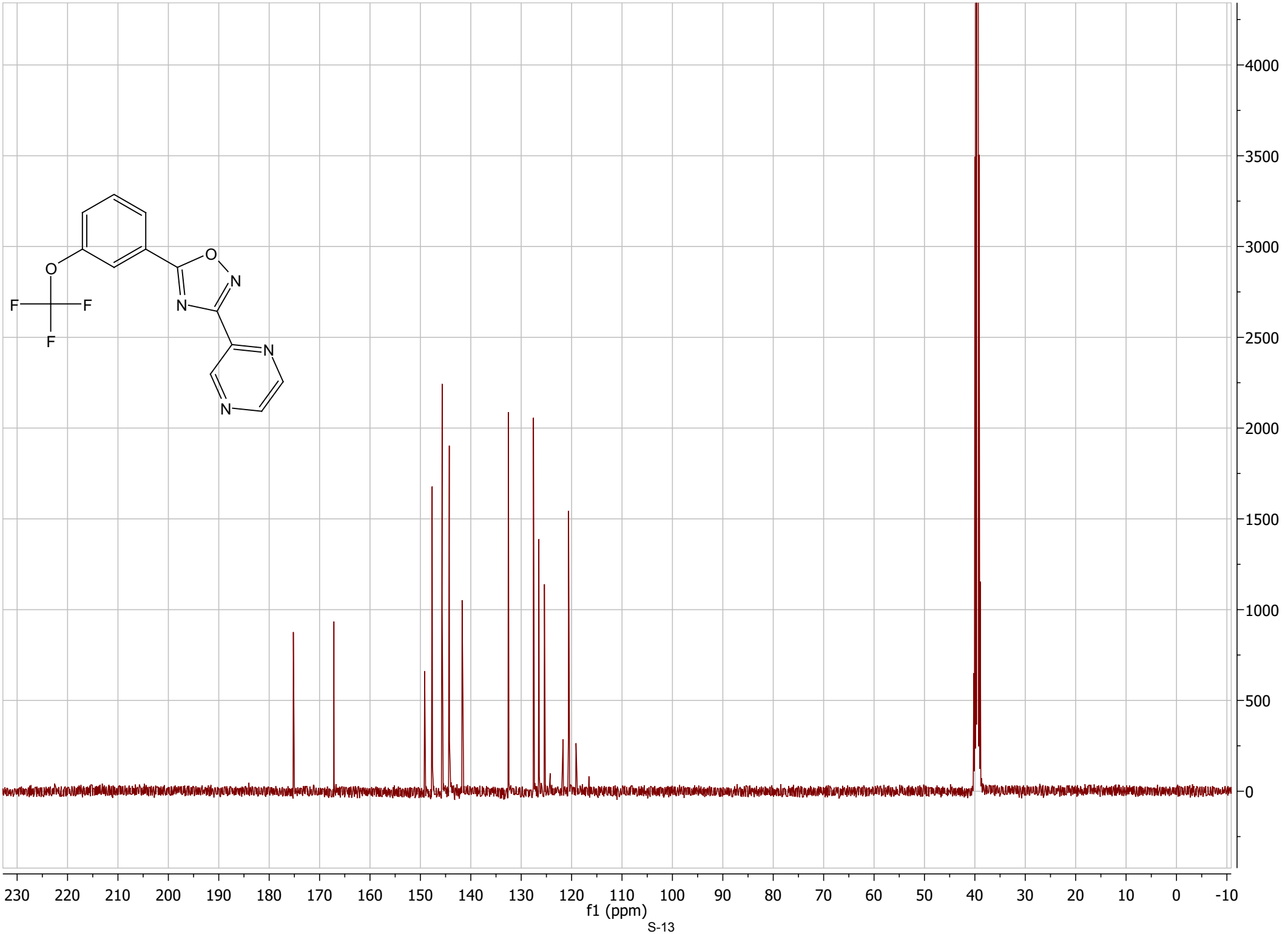
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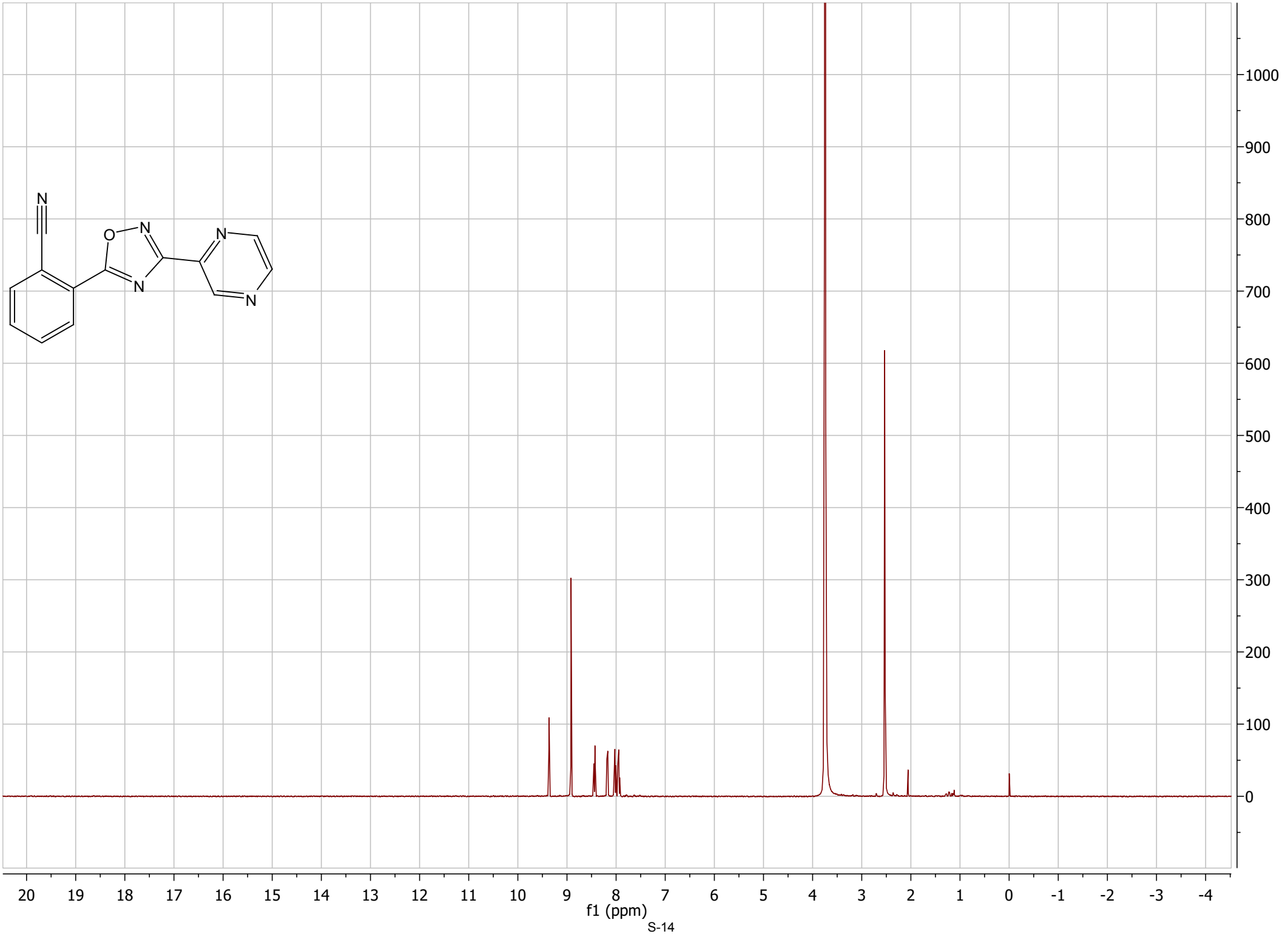
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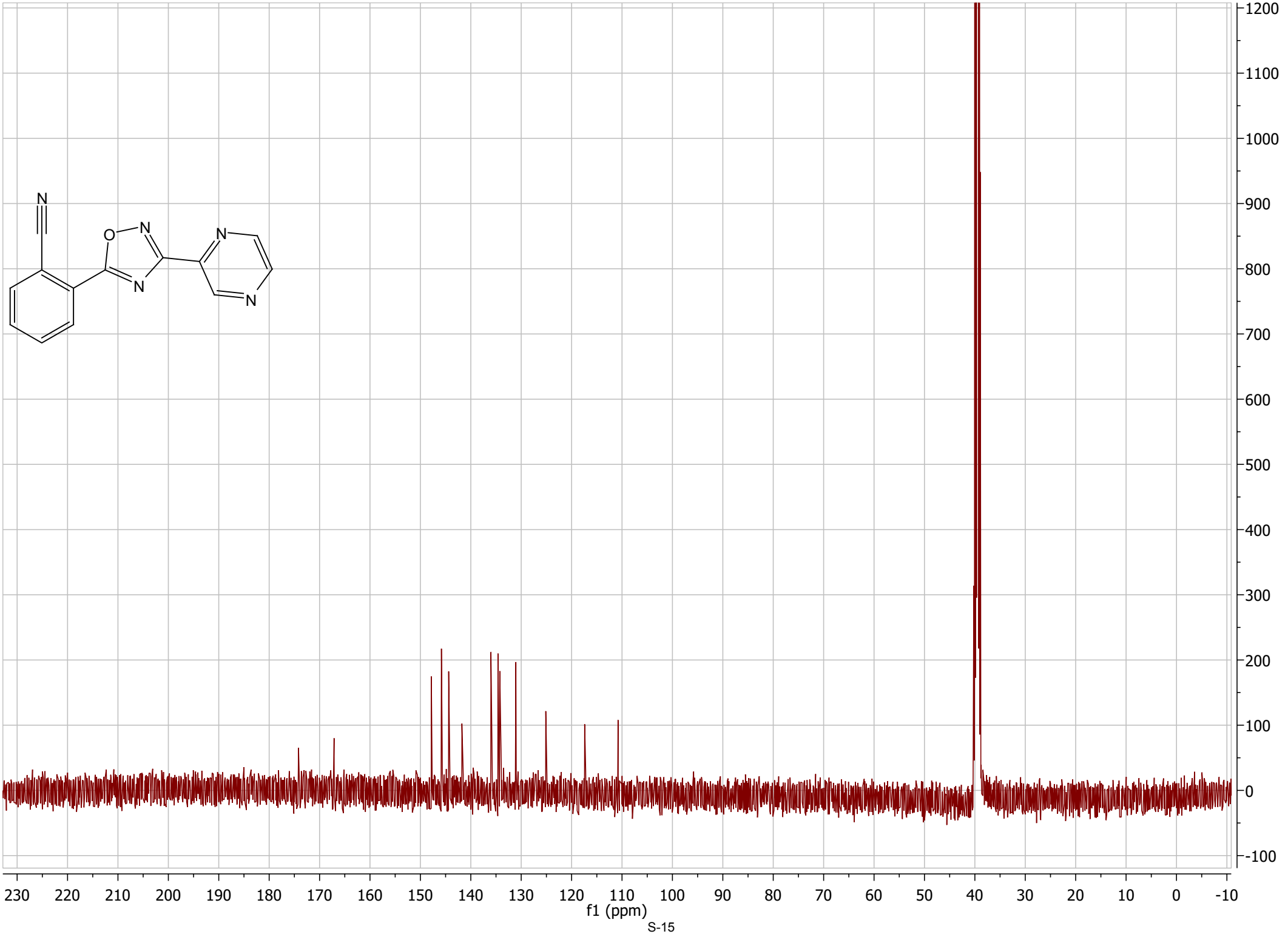
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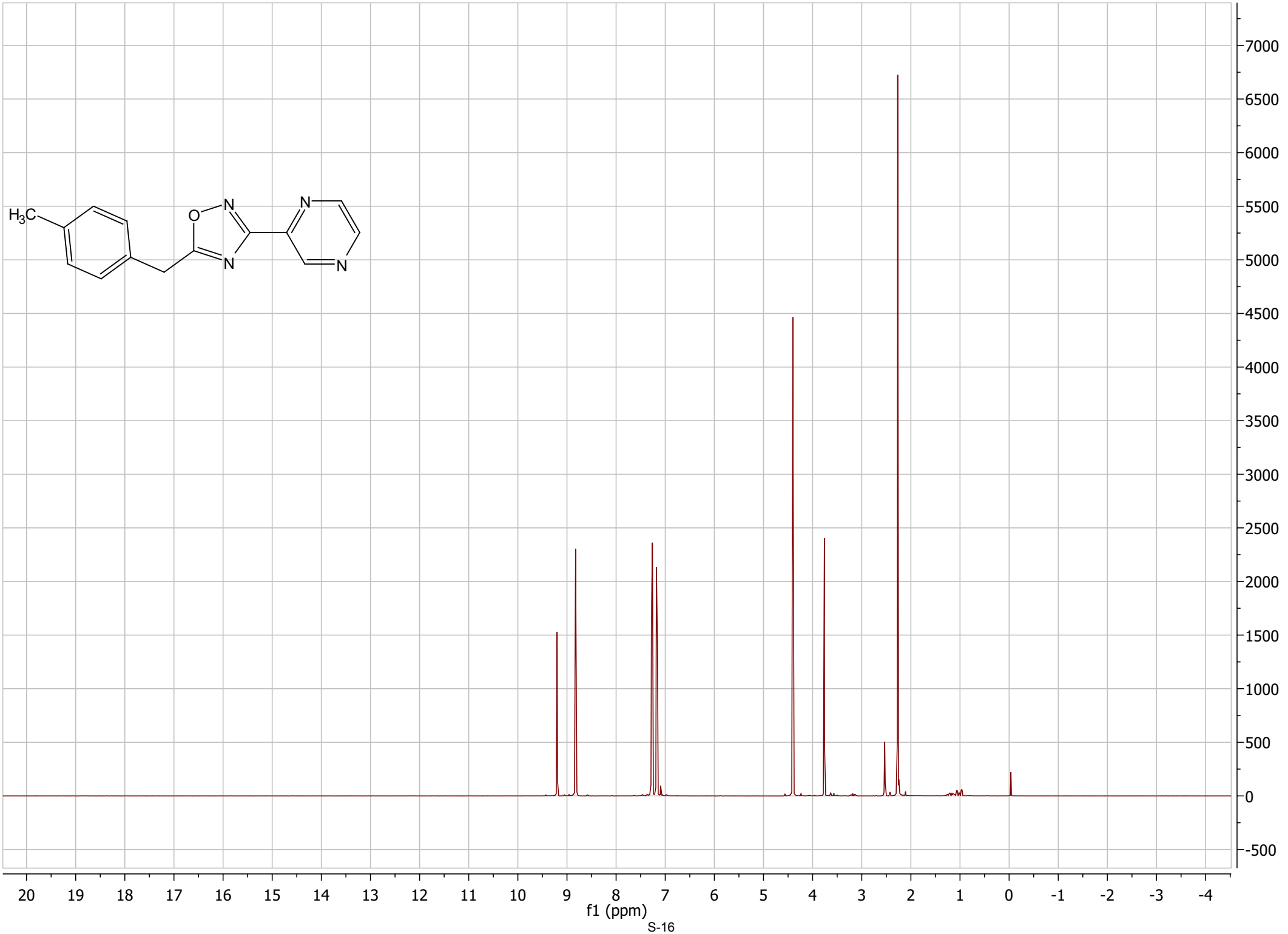
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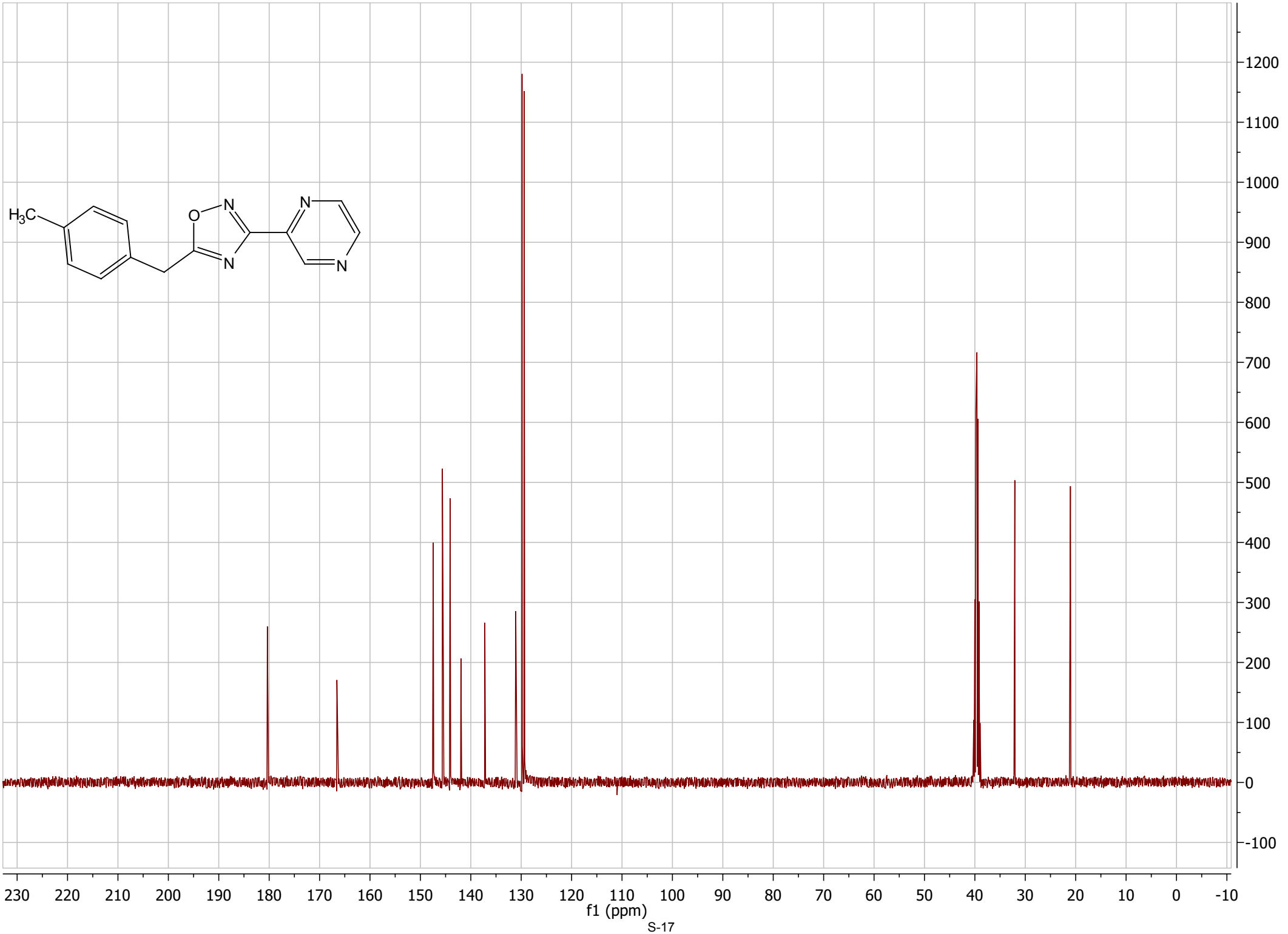
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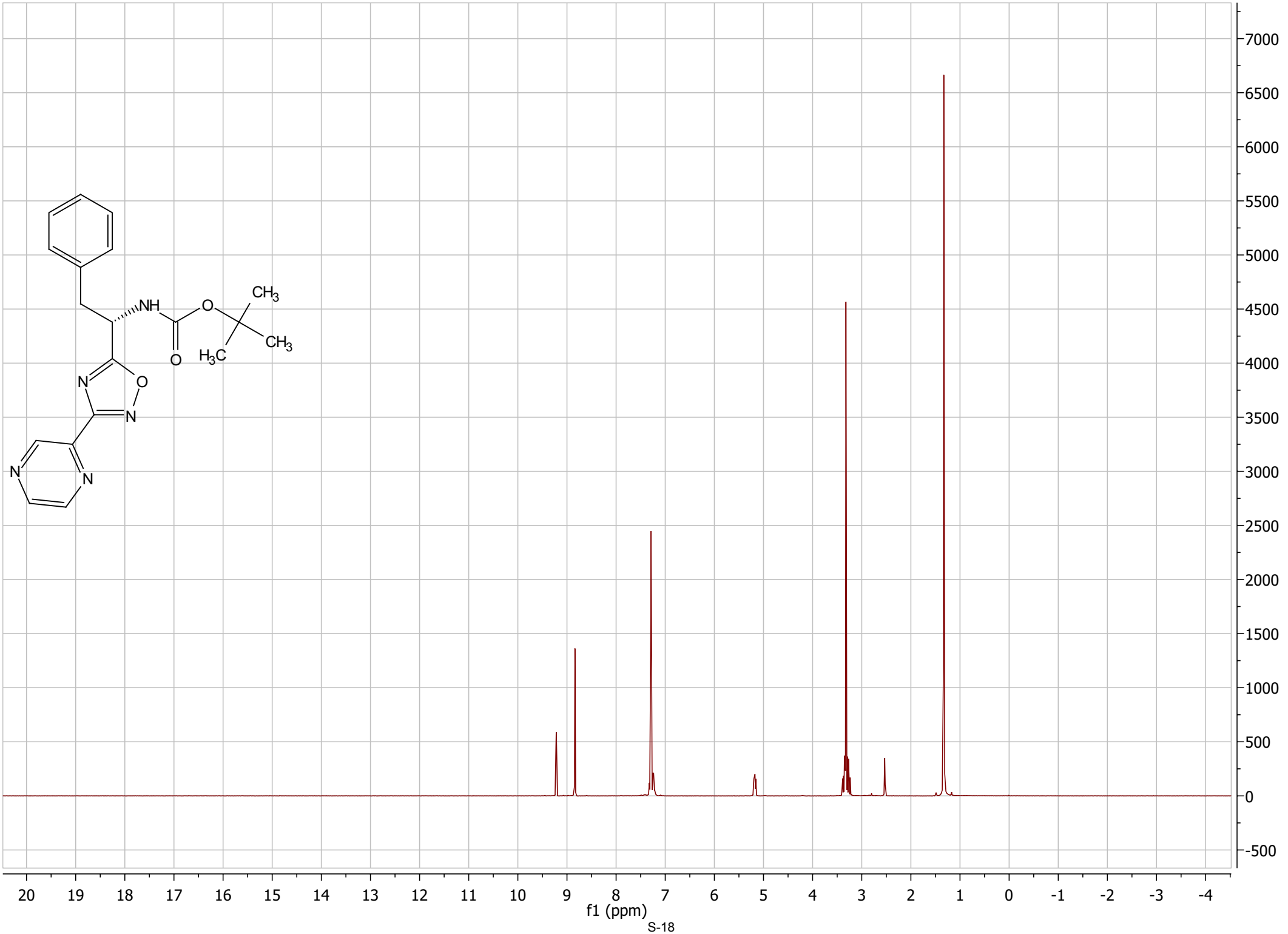
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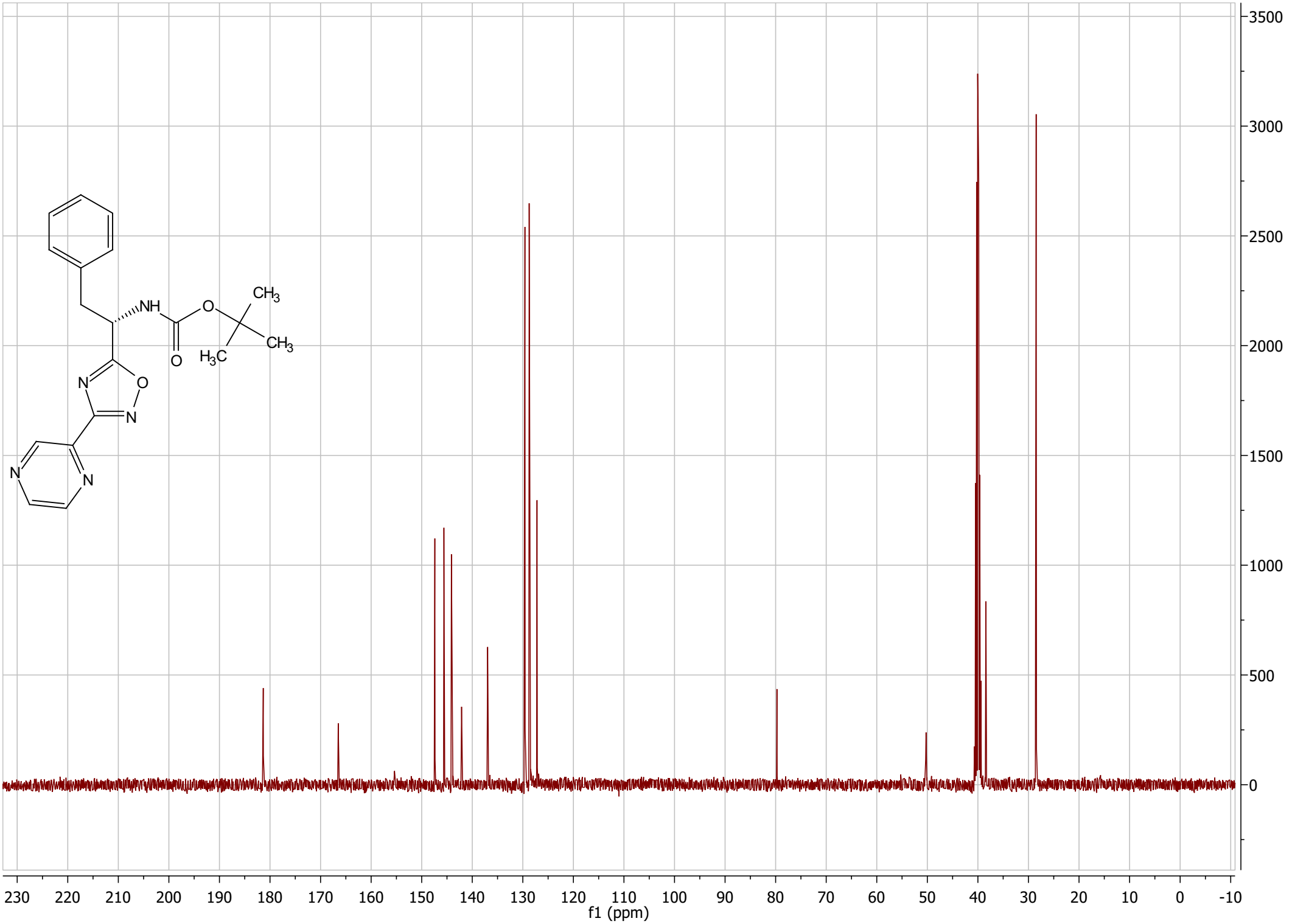
f1 (ppm)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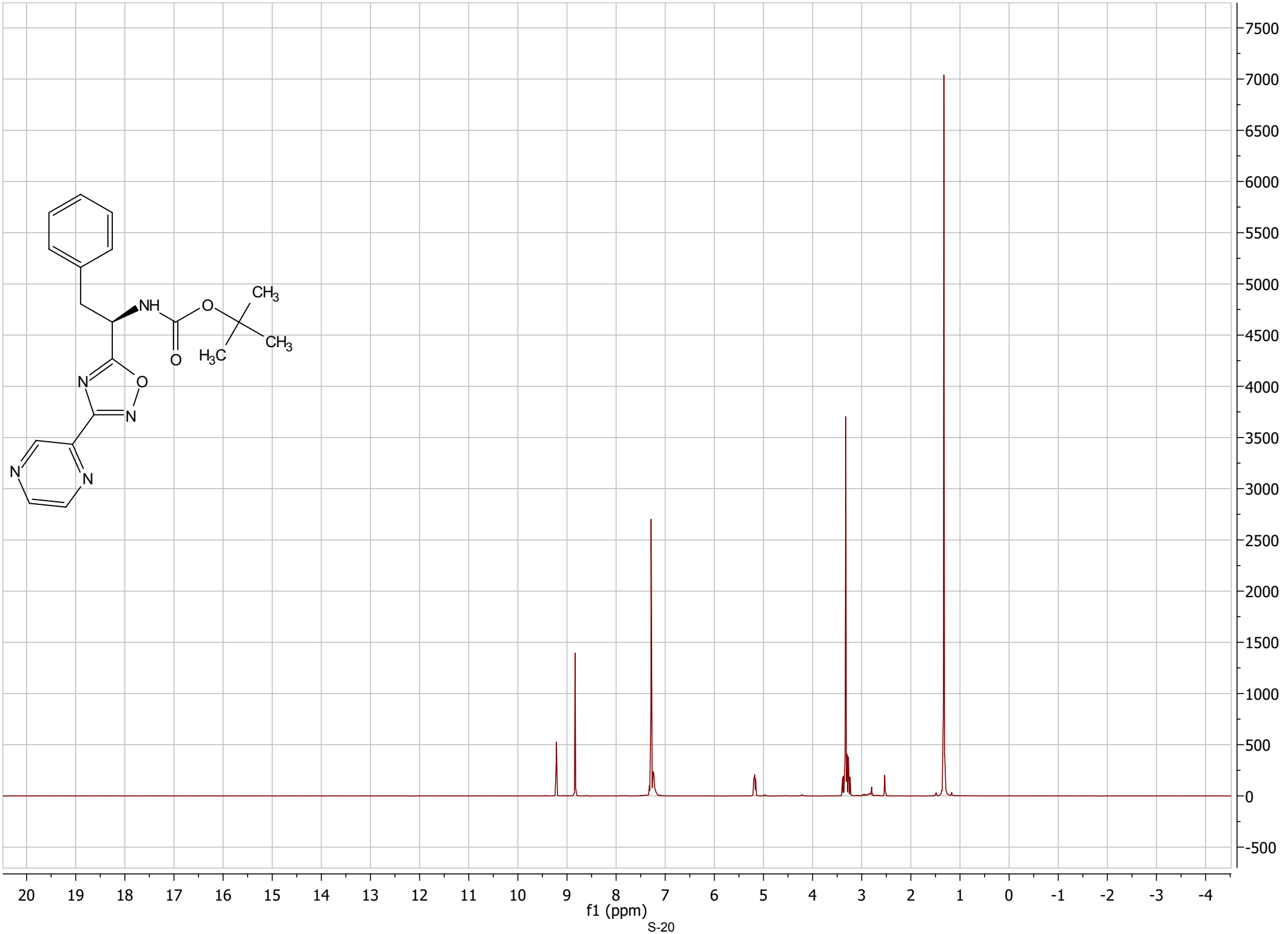
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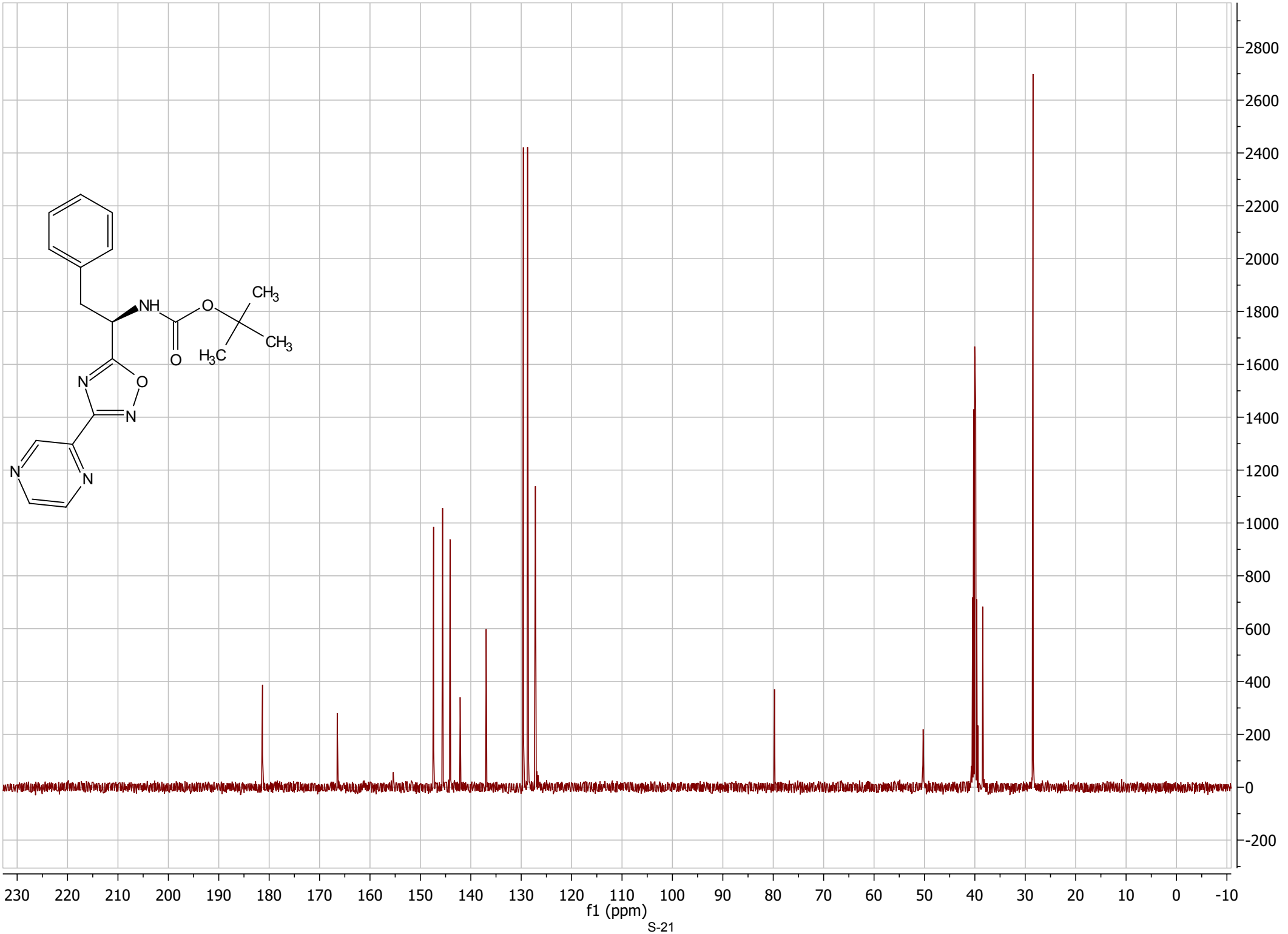
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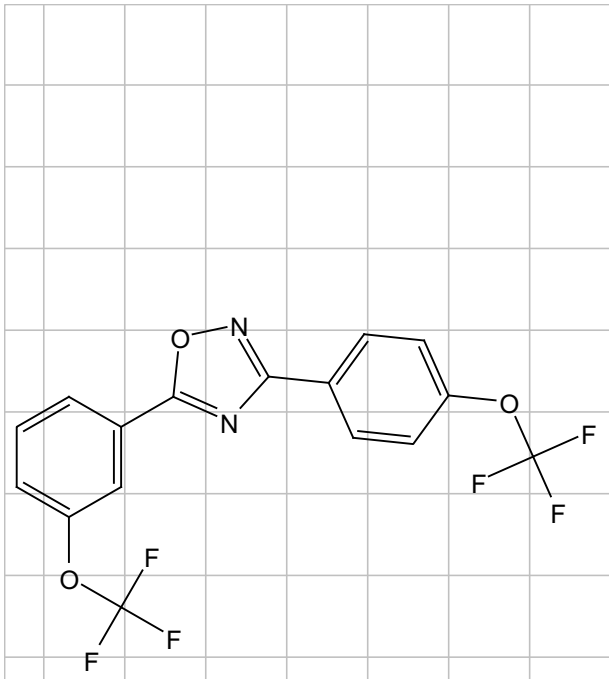
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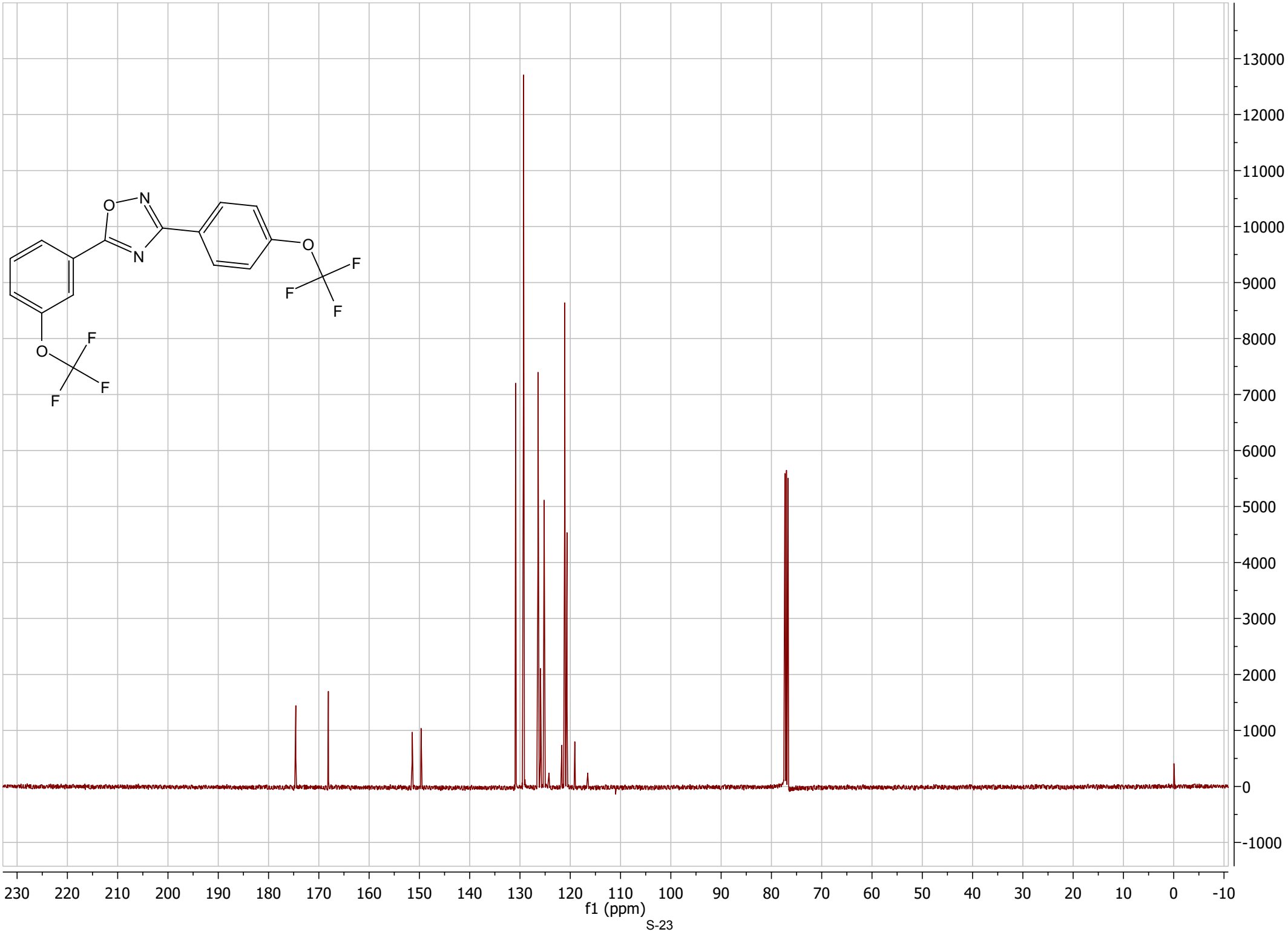
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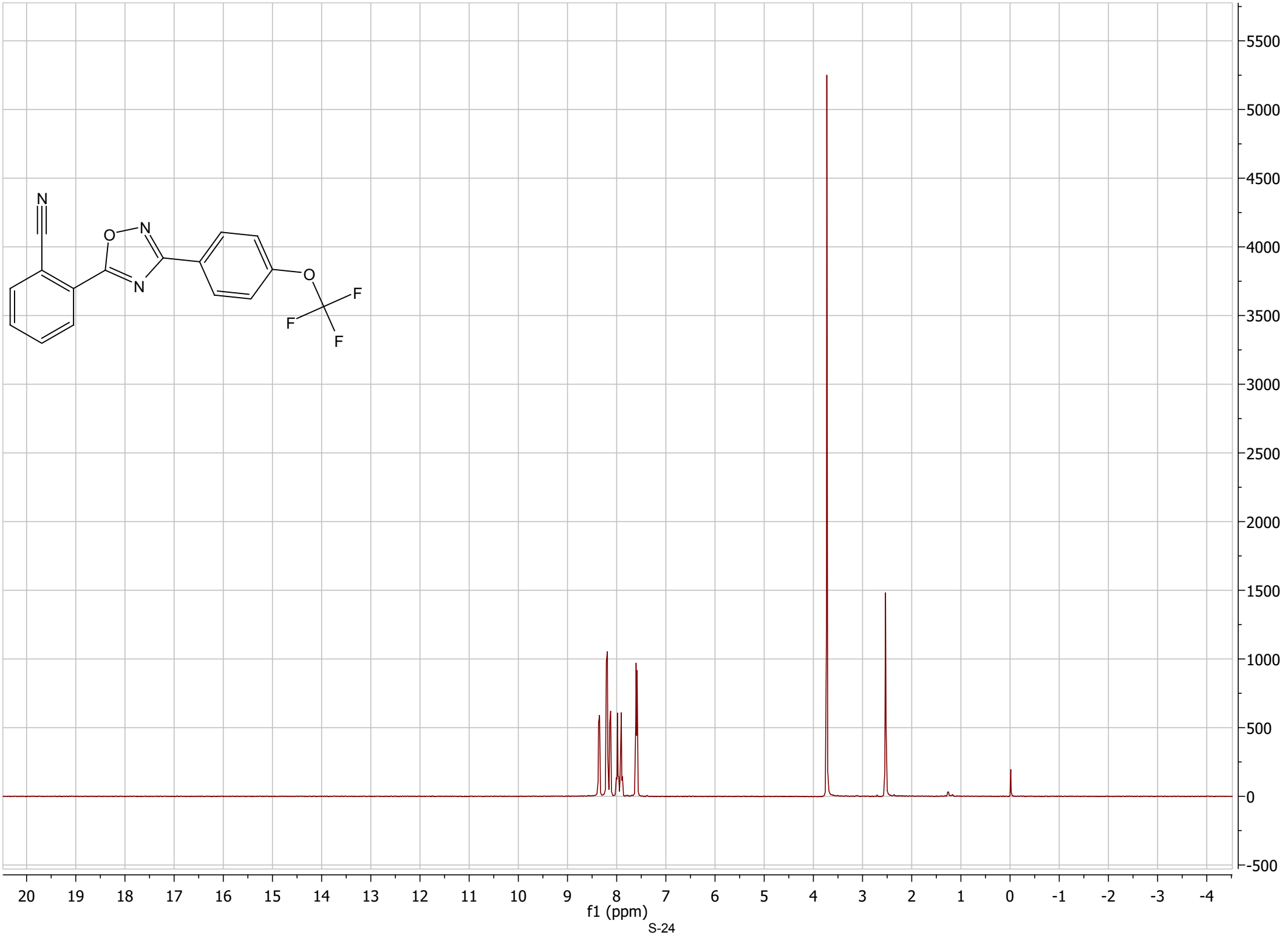
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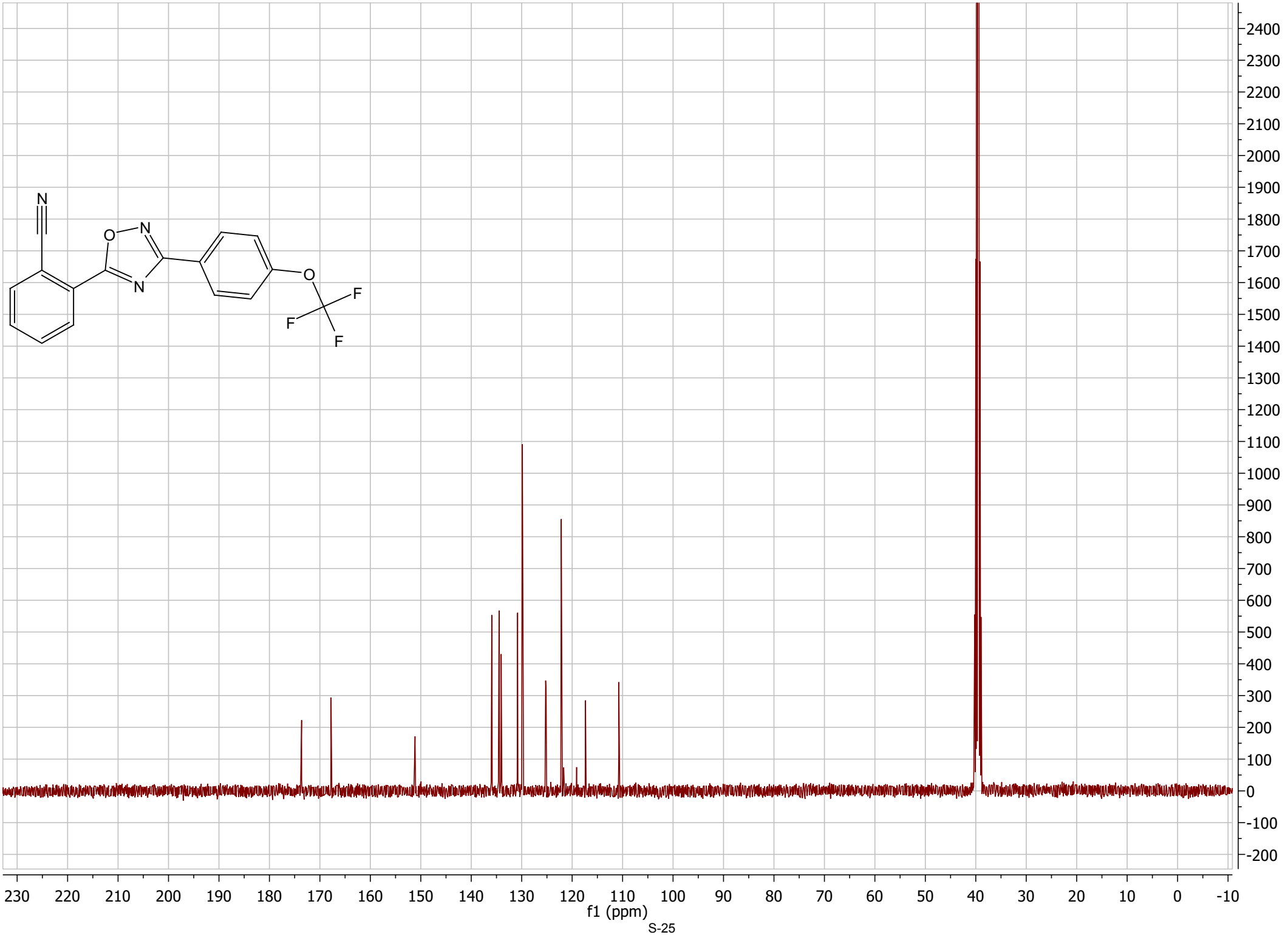
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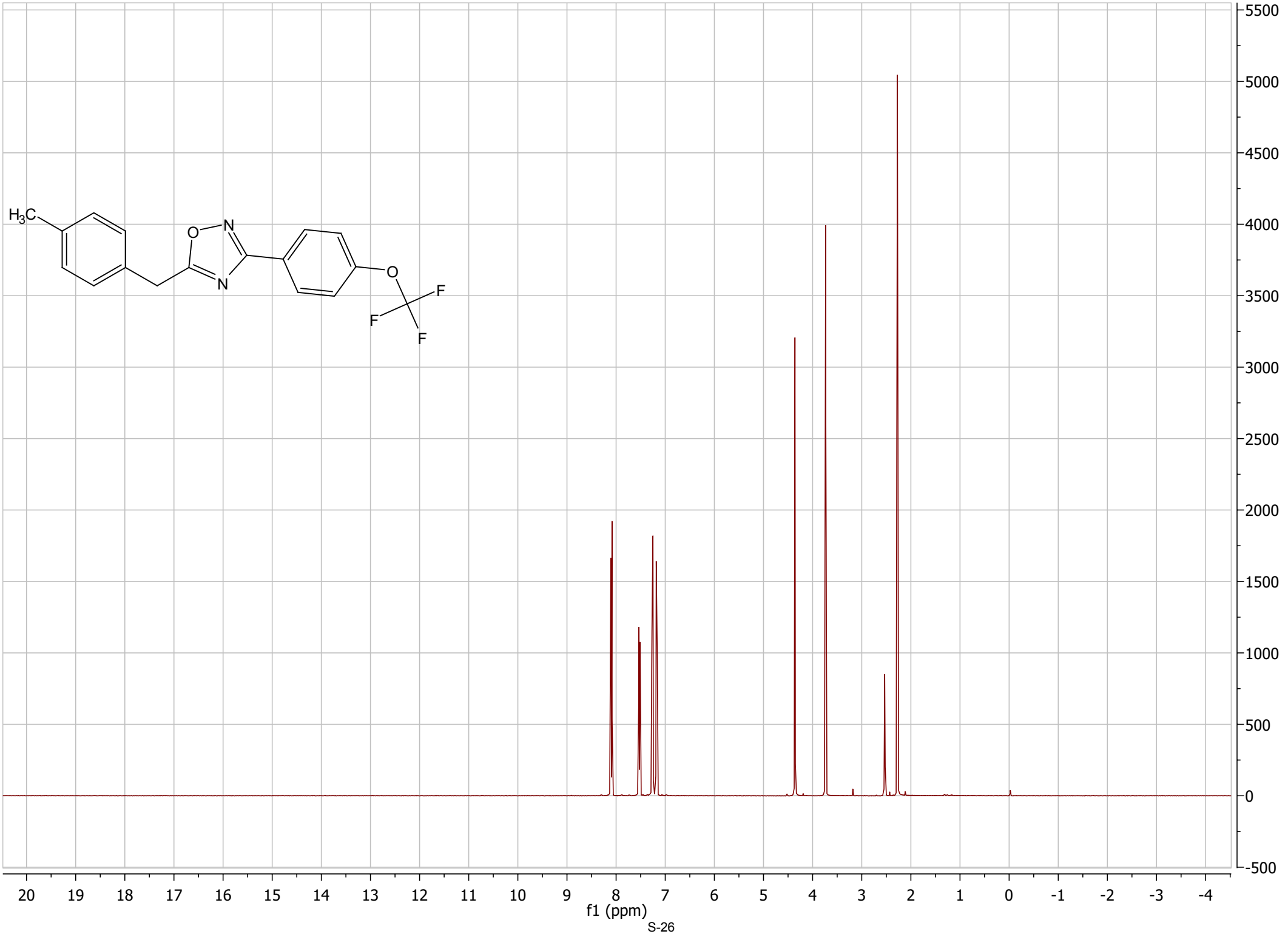
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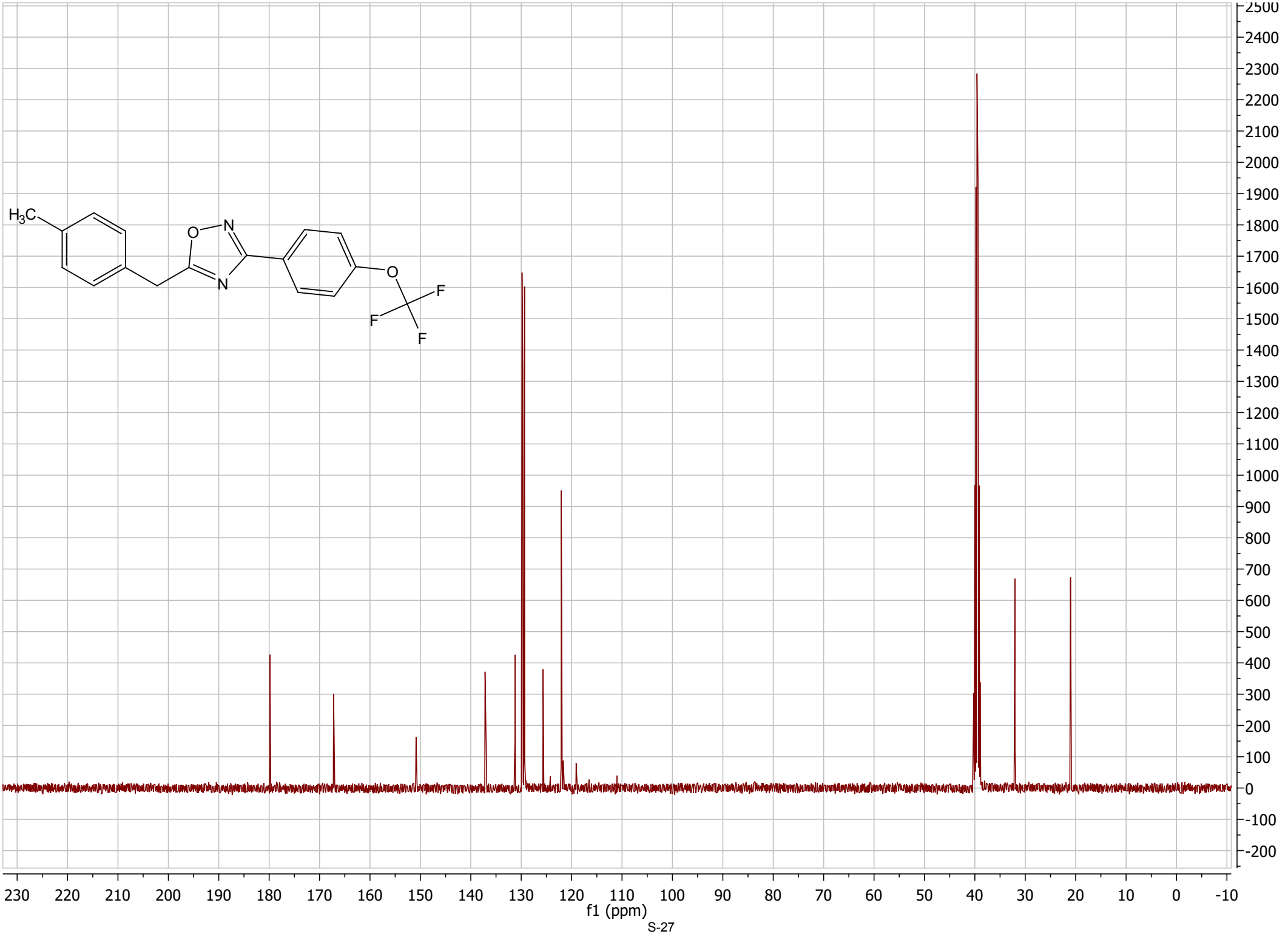
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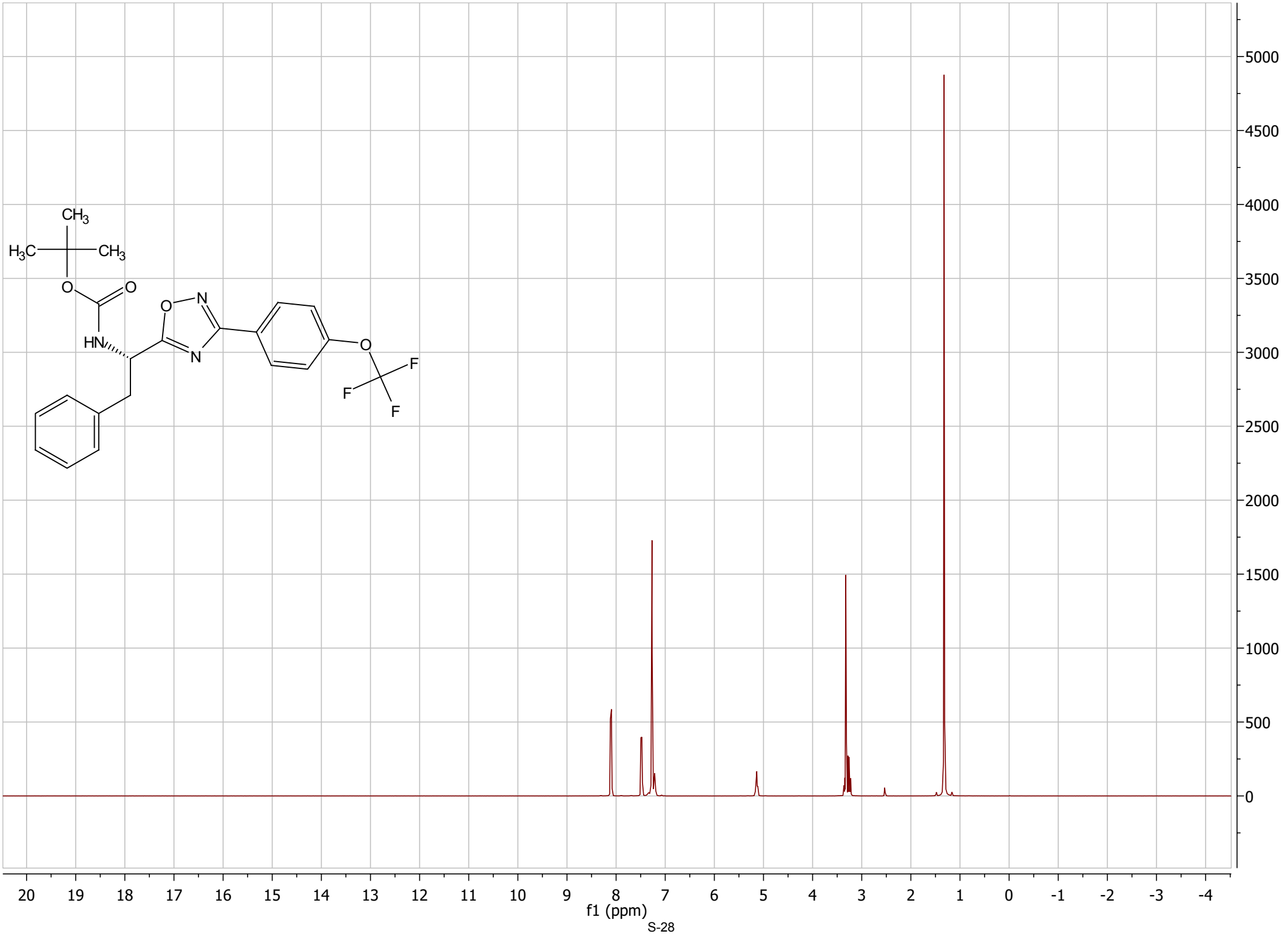
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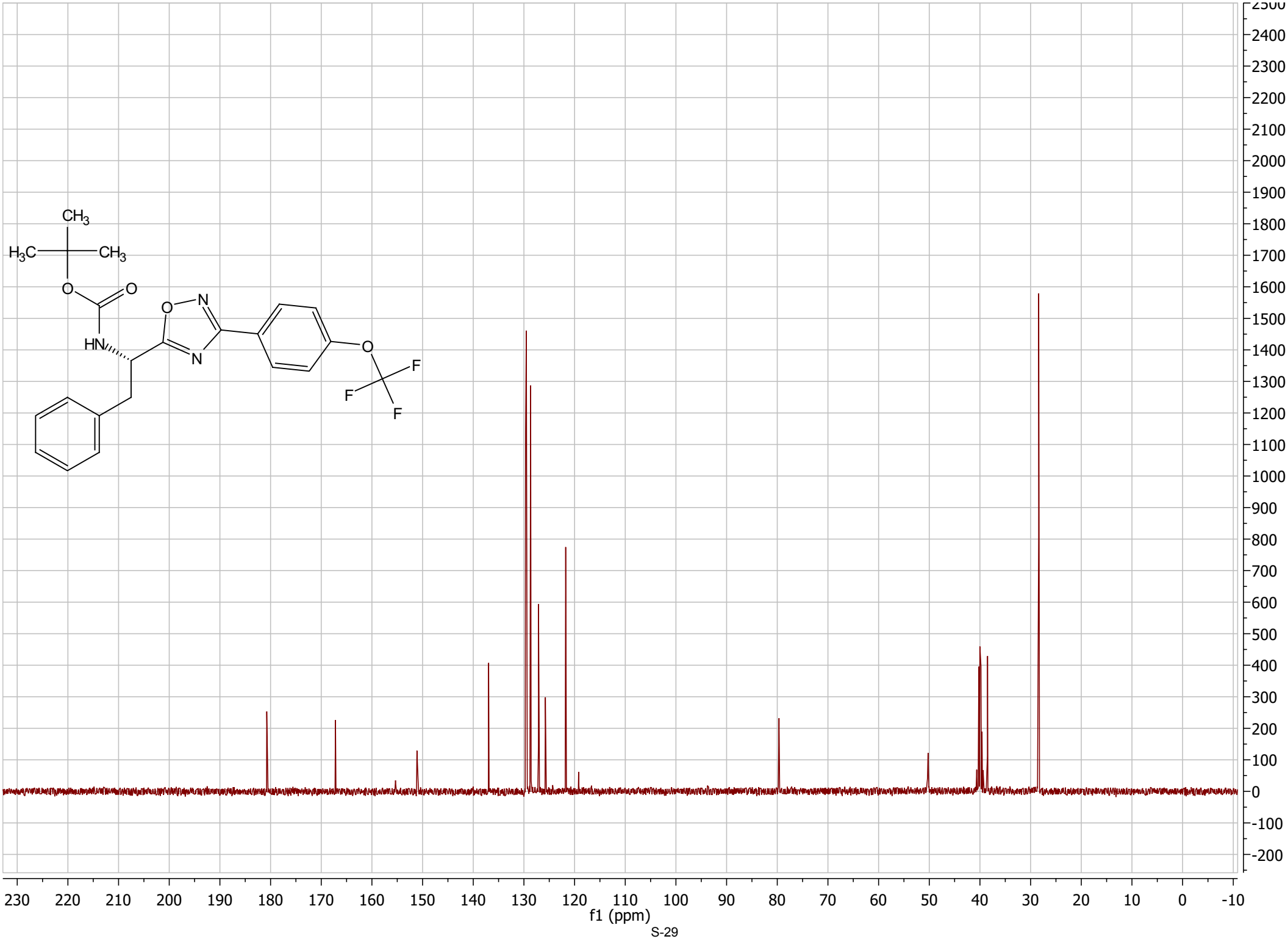
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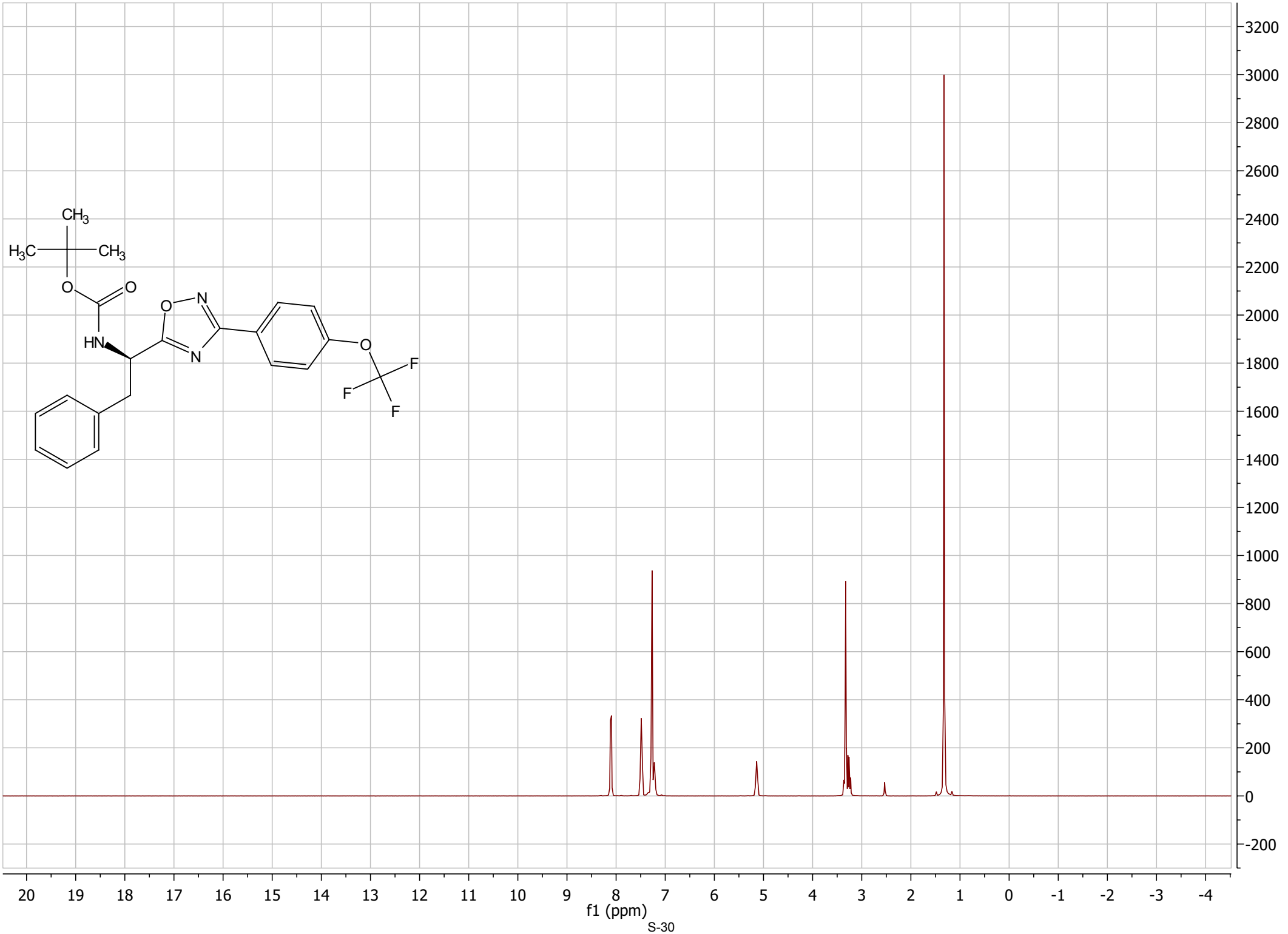
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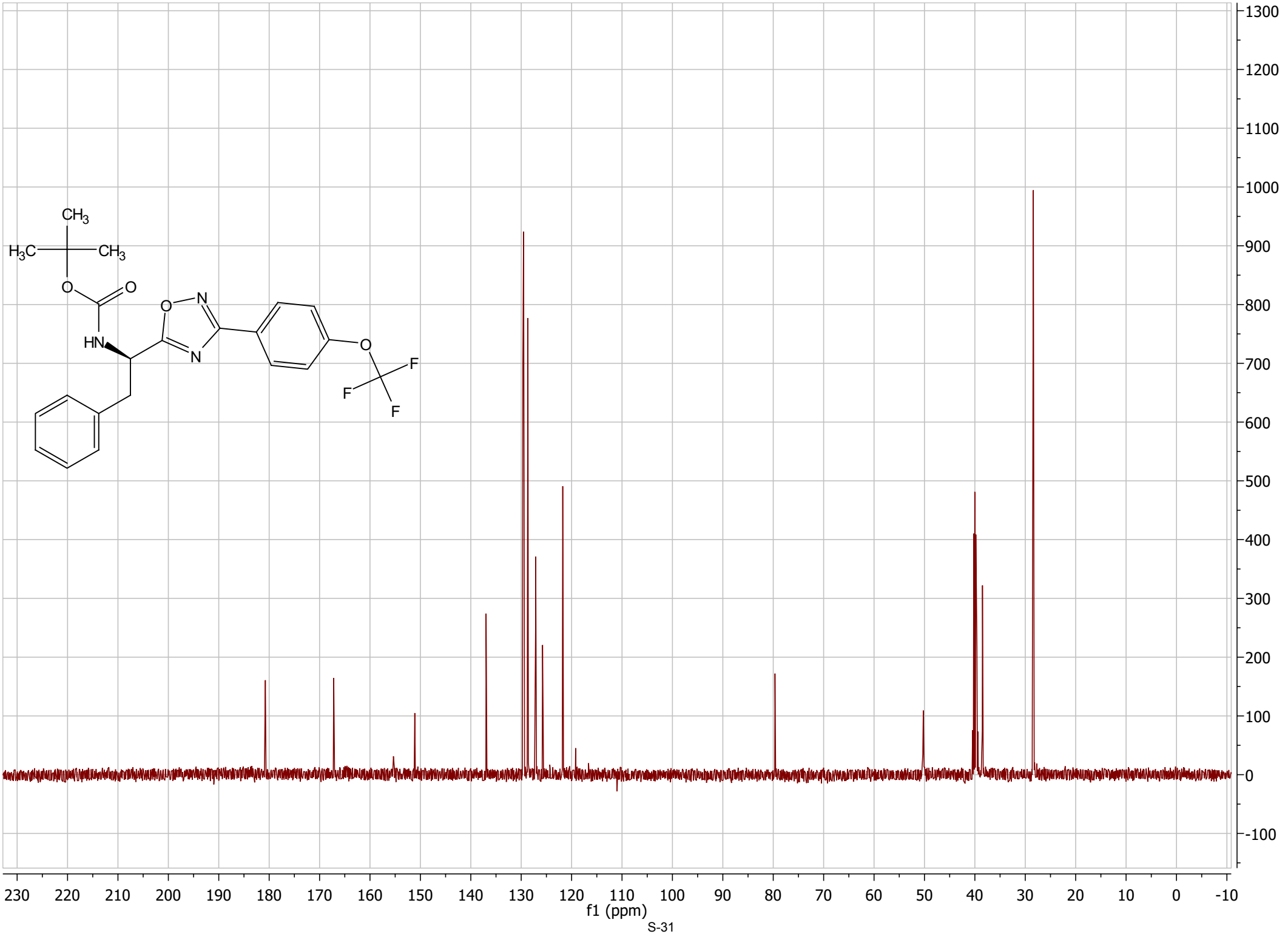
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-100
230
220
210
200
190
180
170
160
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140
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100
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80
70
60
50
40
30
20
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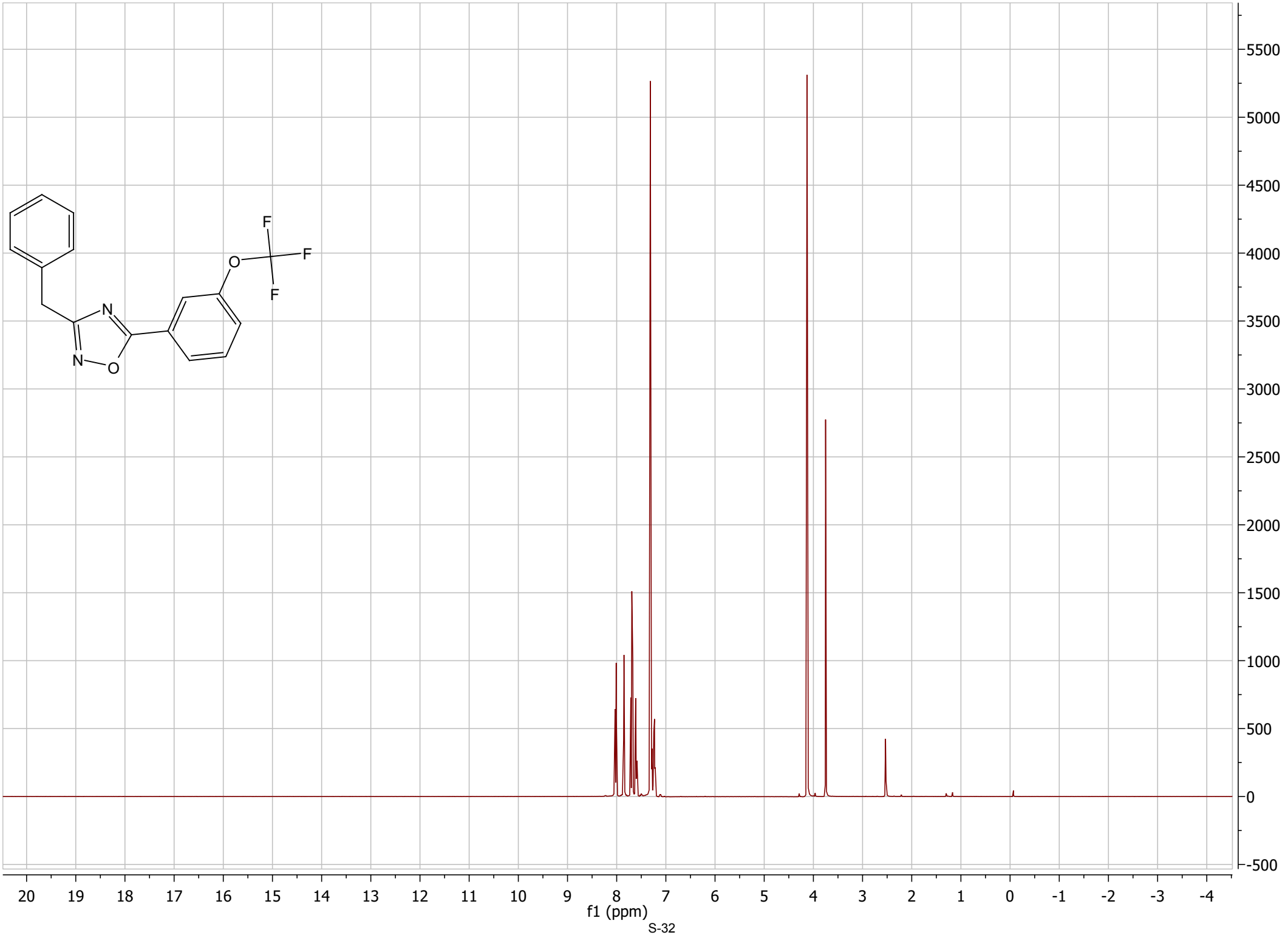
0
-10
f1 (ppm)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F
F
O
N
N
O
5500
5000
4500
4000
3500
3000
2500
2000
1500
1000
500
0
-500
20
19
18
17
16
15
14
13
12
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10
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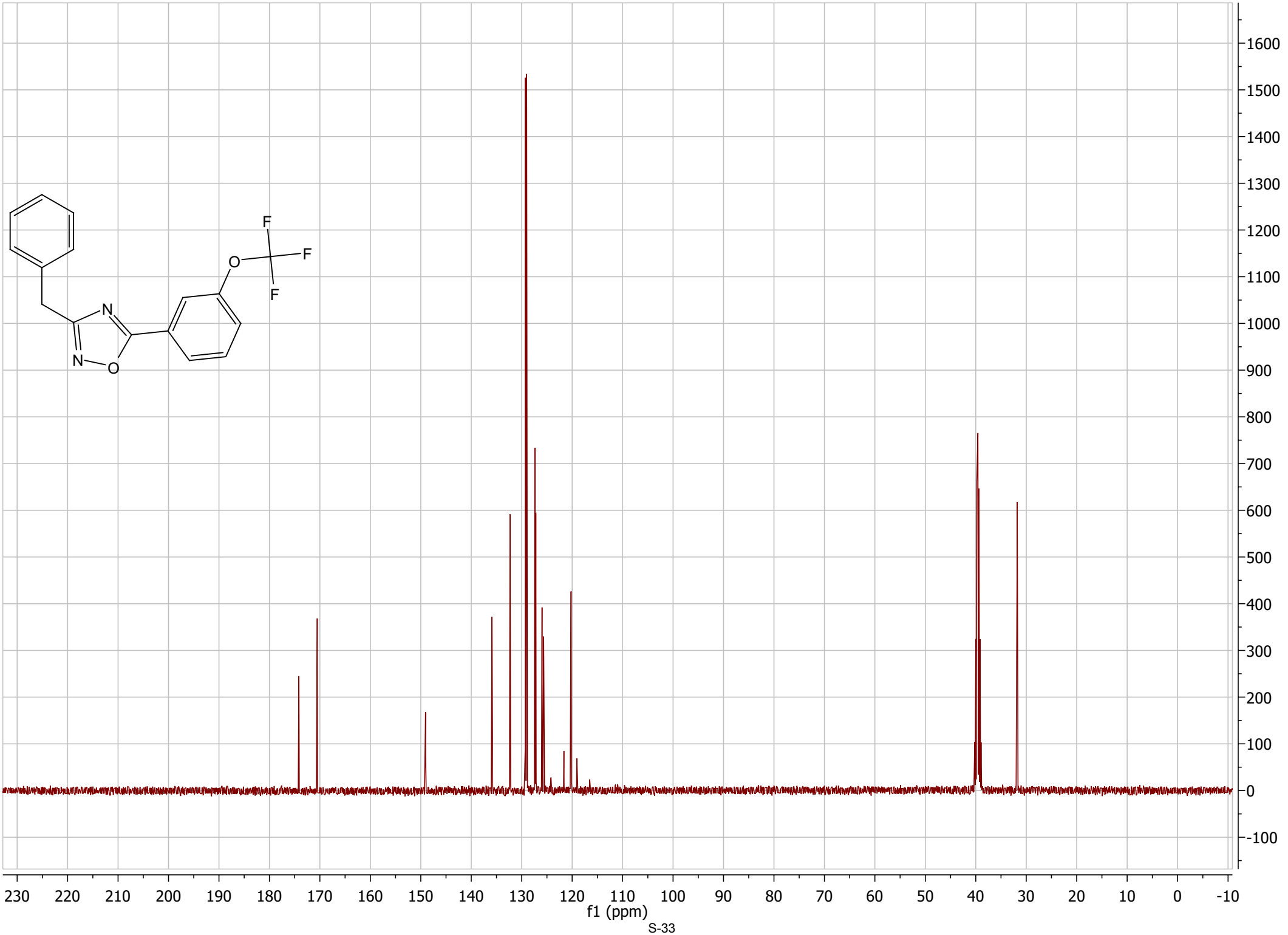
8
7
6
5
4
3
2
1
0
-1
-2
-3
-4
f1 (ppm)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F
F
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N
N
O
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1500
1400
1300
1200
1100
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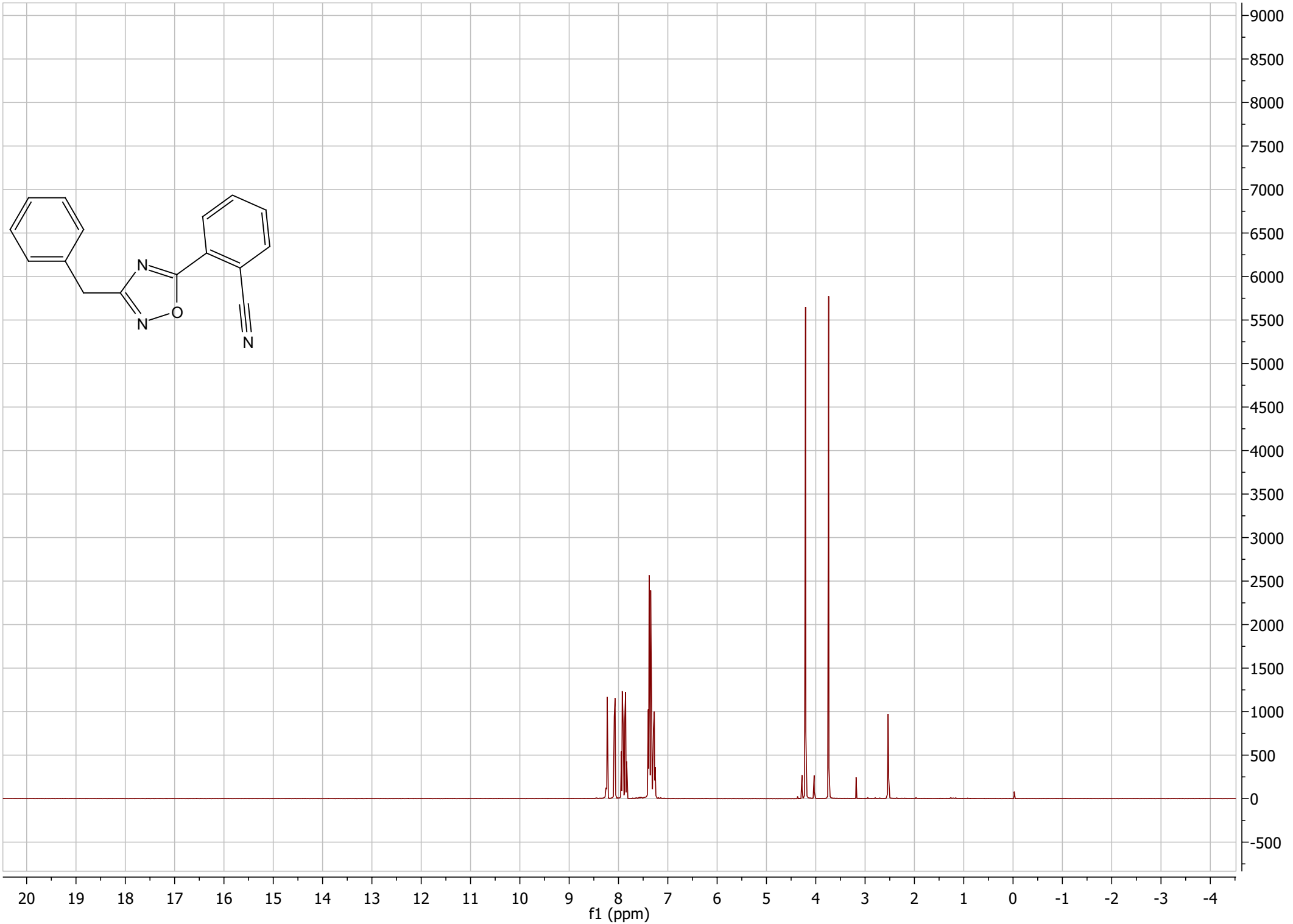
900
800
700
600
500
400
300
200
100
0
-100
230
220
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)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O
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N
9000
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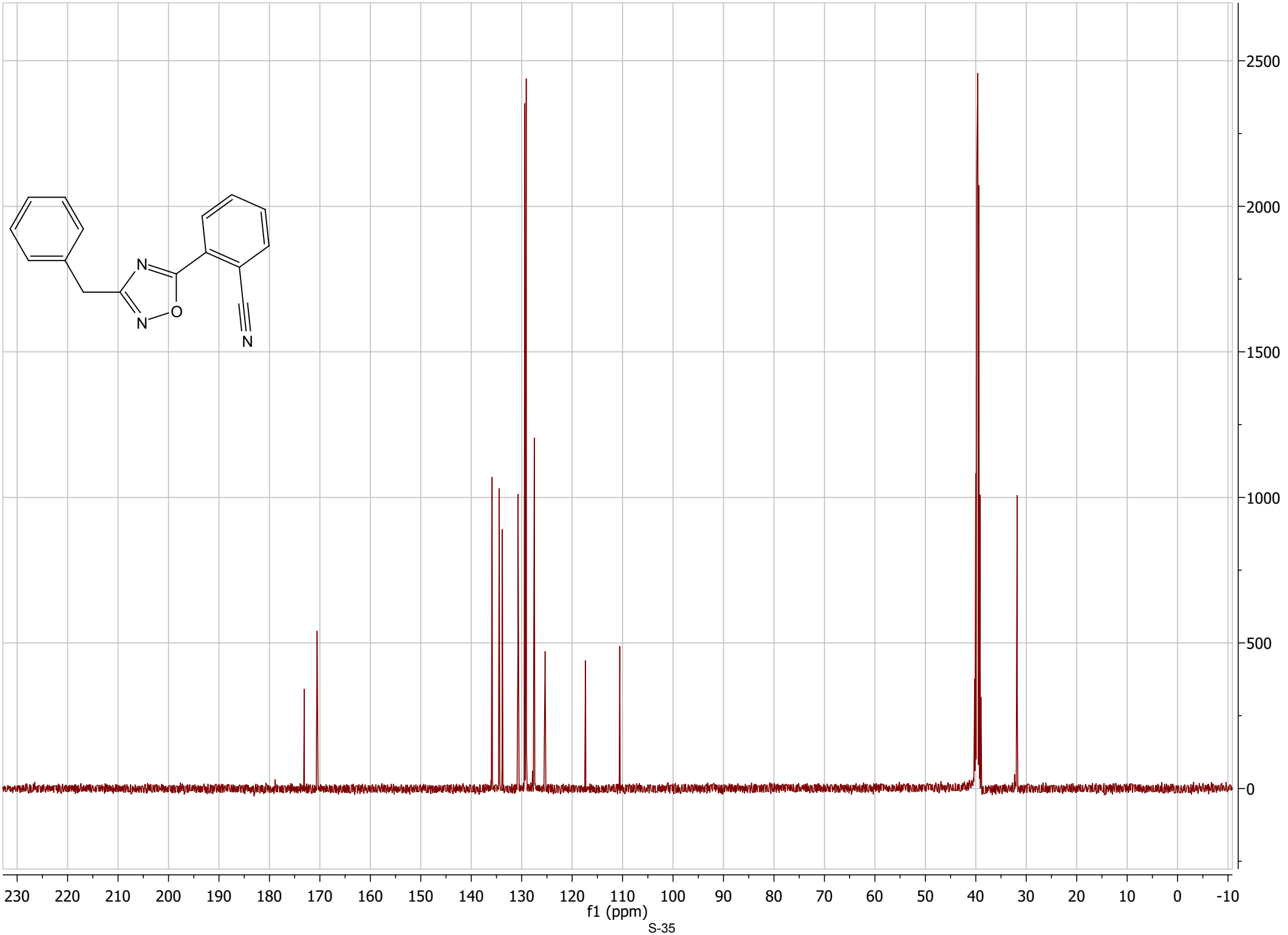
8000
7500
7000
6500
6000
5500
5000
4500
4000
3500
3000
2500
2000
1500
1000
500
0
-500
20 19 18 17 16 15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1 -2 -3 -4
f1 (ppm)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N
N
2500
2000
1500
1000
500
0
230
220
210
200
190
180
170
160
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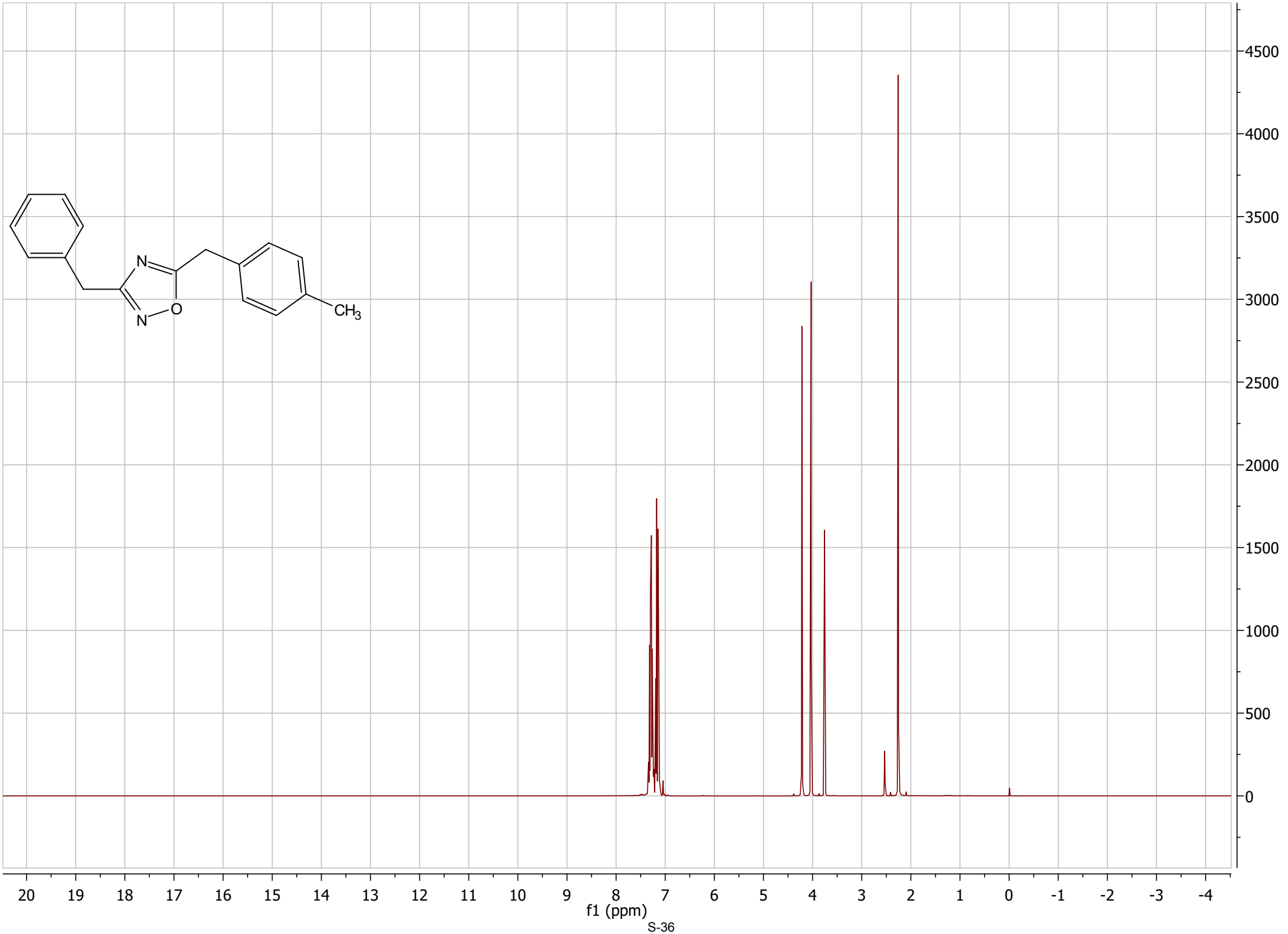
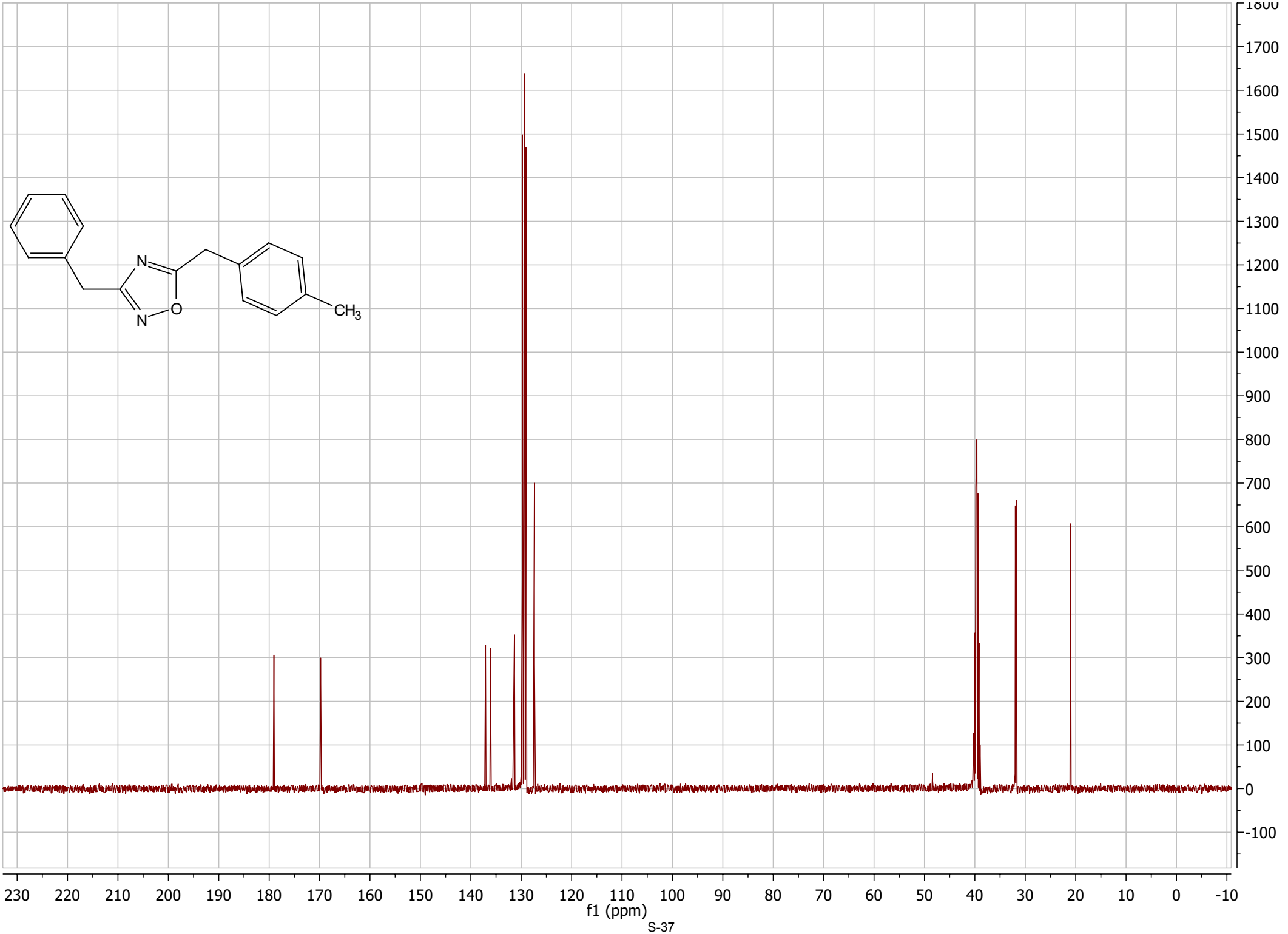
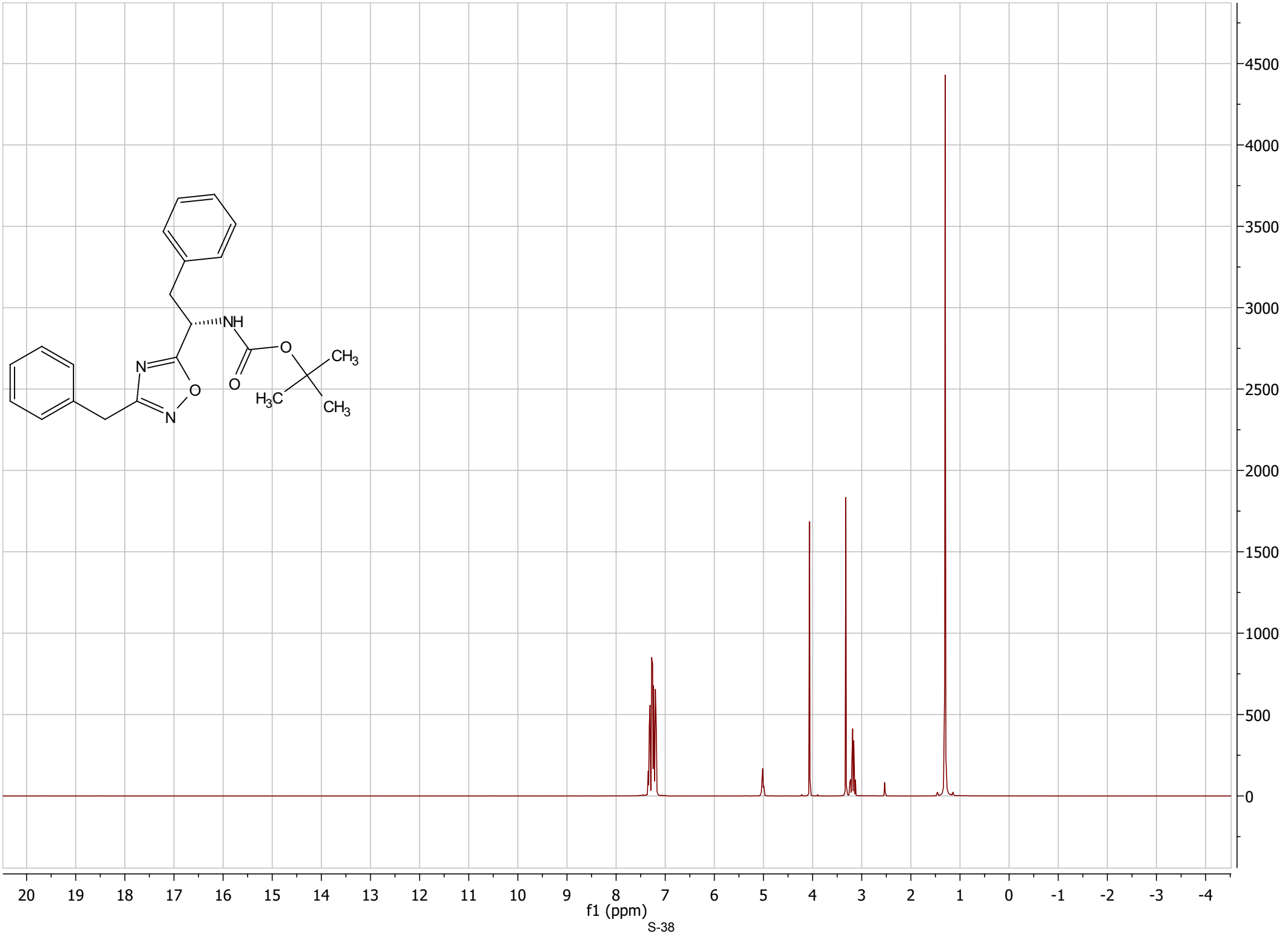
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)


N
O
N
CH3
4500
4000
3500
3000
2500
2000
1500
1000
500
0
20 19 18 17 16 15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1 -2 -3 -4
f1 (ppm)


N
O
N
CH3
1800
1700
1600
1500
1400
1300
1200
1100
1000
900
800
700
600
500
400
300
200
100
0
-100
230
220
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)


NH
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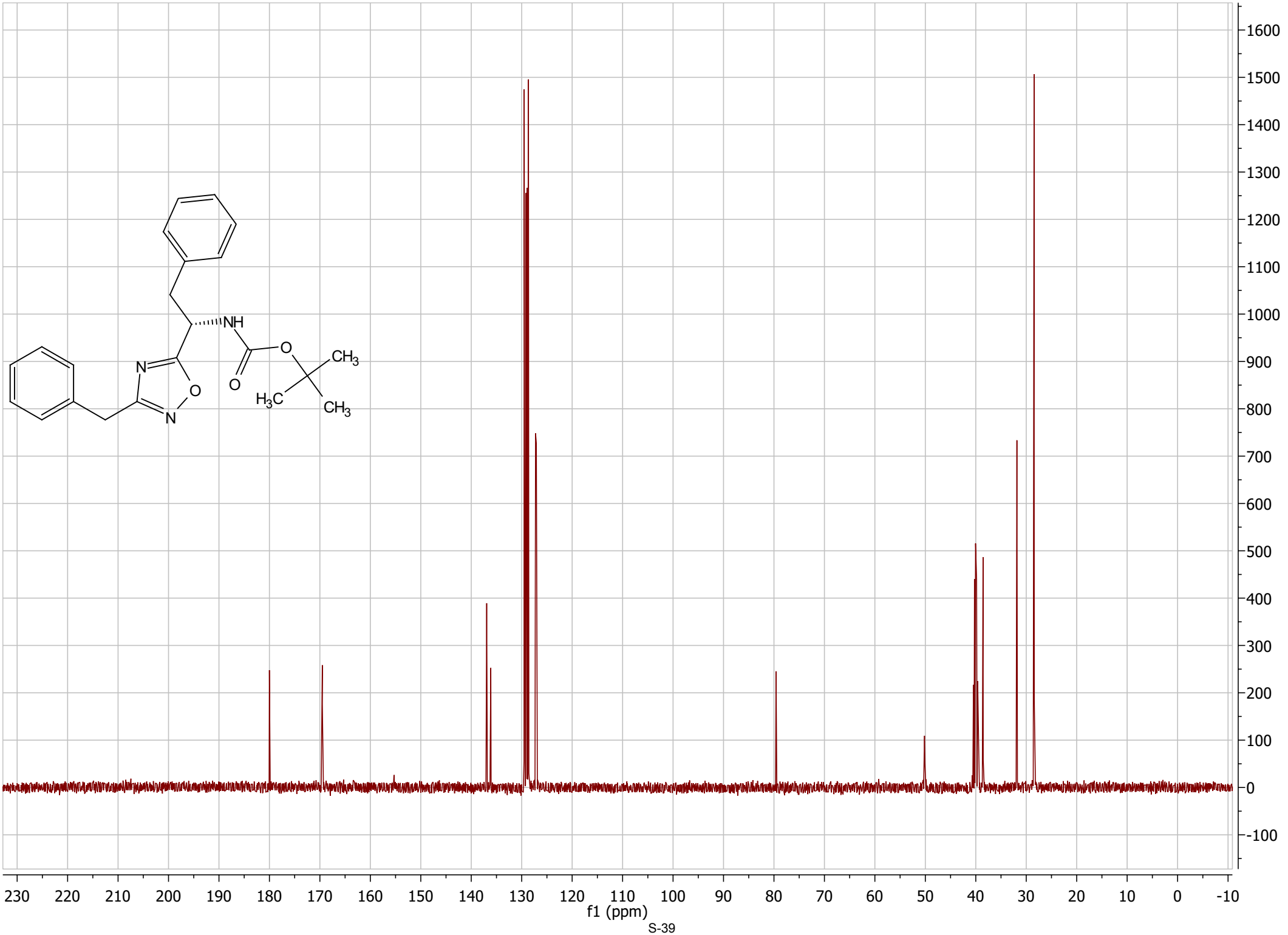
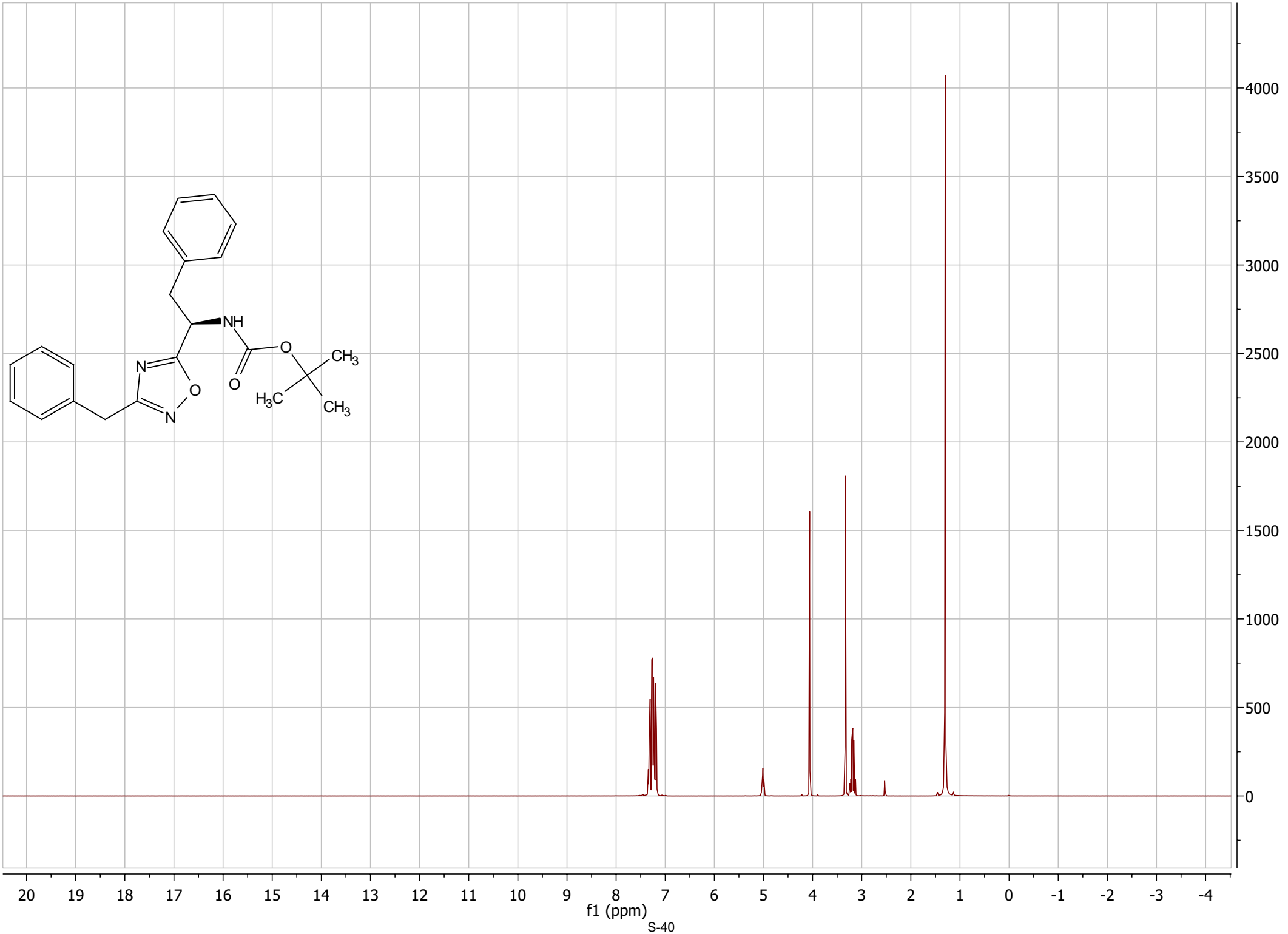
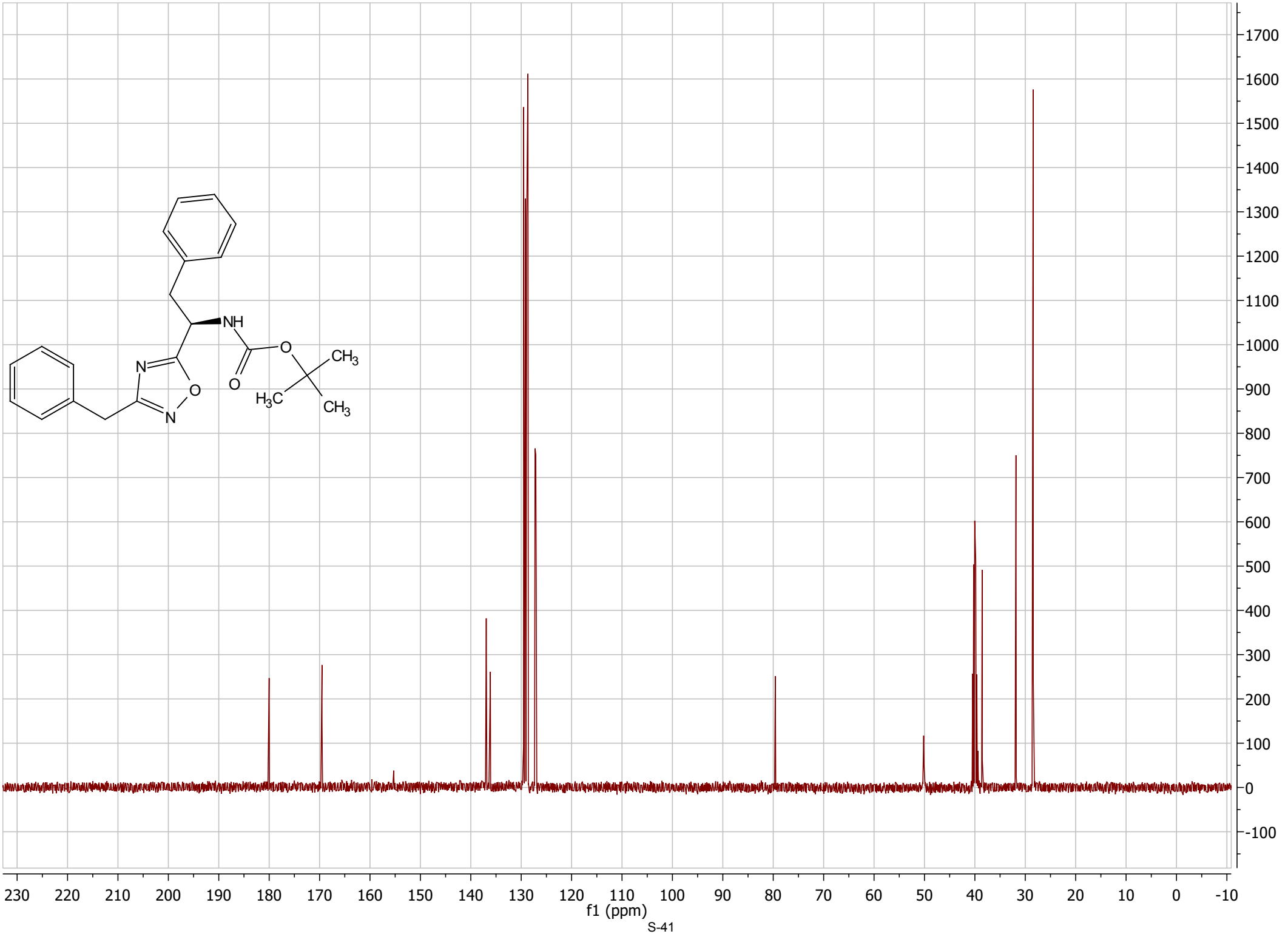
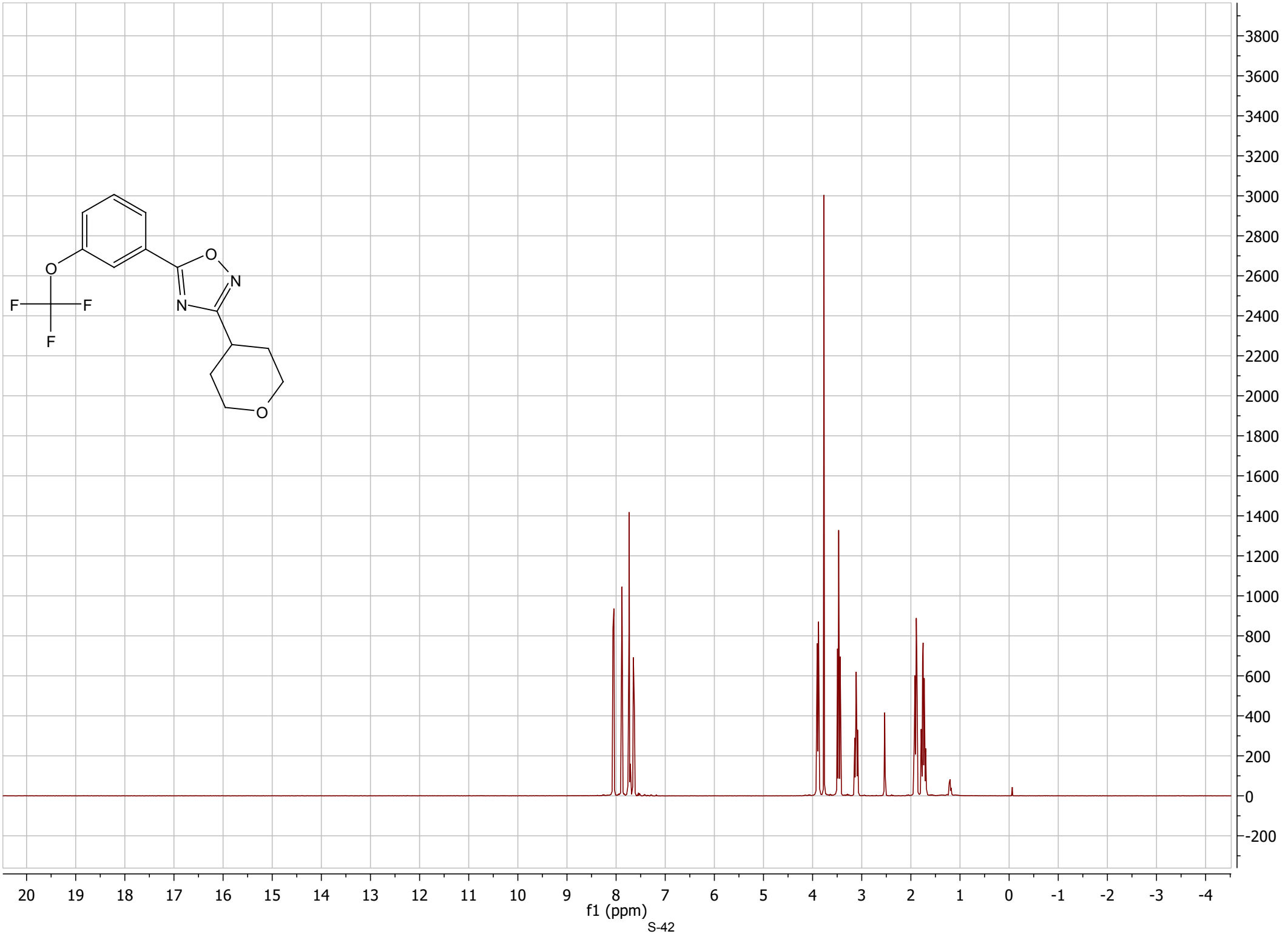
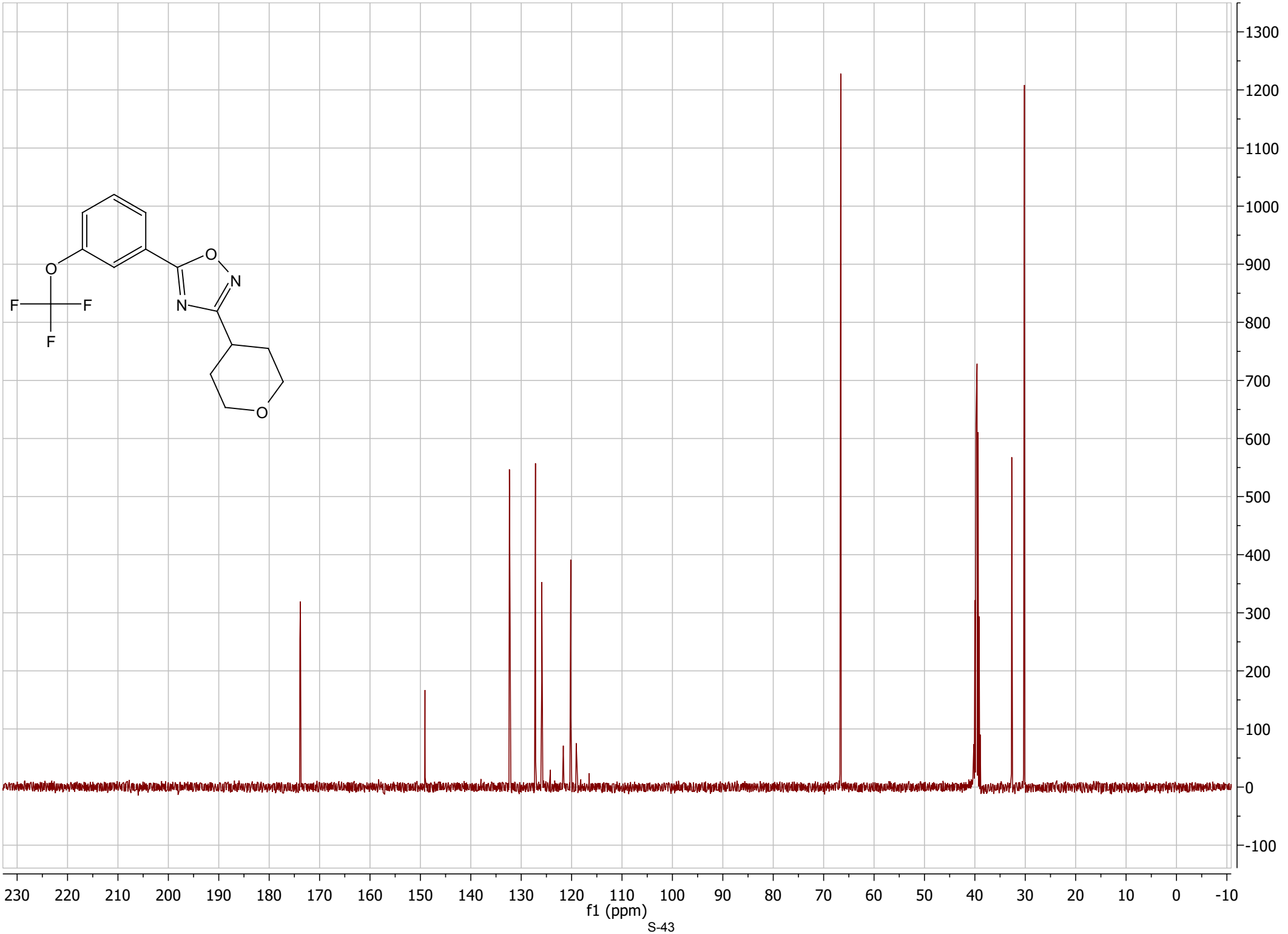
O
CH3
H3C
CH3
N
O
N
4500
4000
3500
3000
2500
2000
1500
1000
500
0
20
19
18
17
16
15
14
13
12
11
10
9
8
7
6
5
4
3
2
1
0
-1
-2
-3
-4
f1 (ppm)

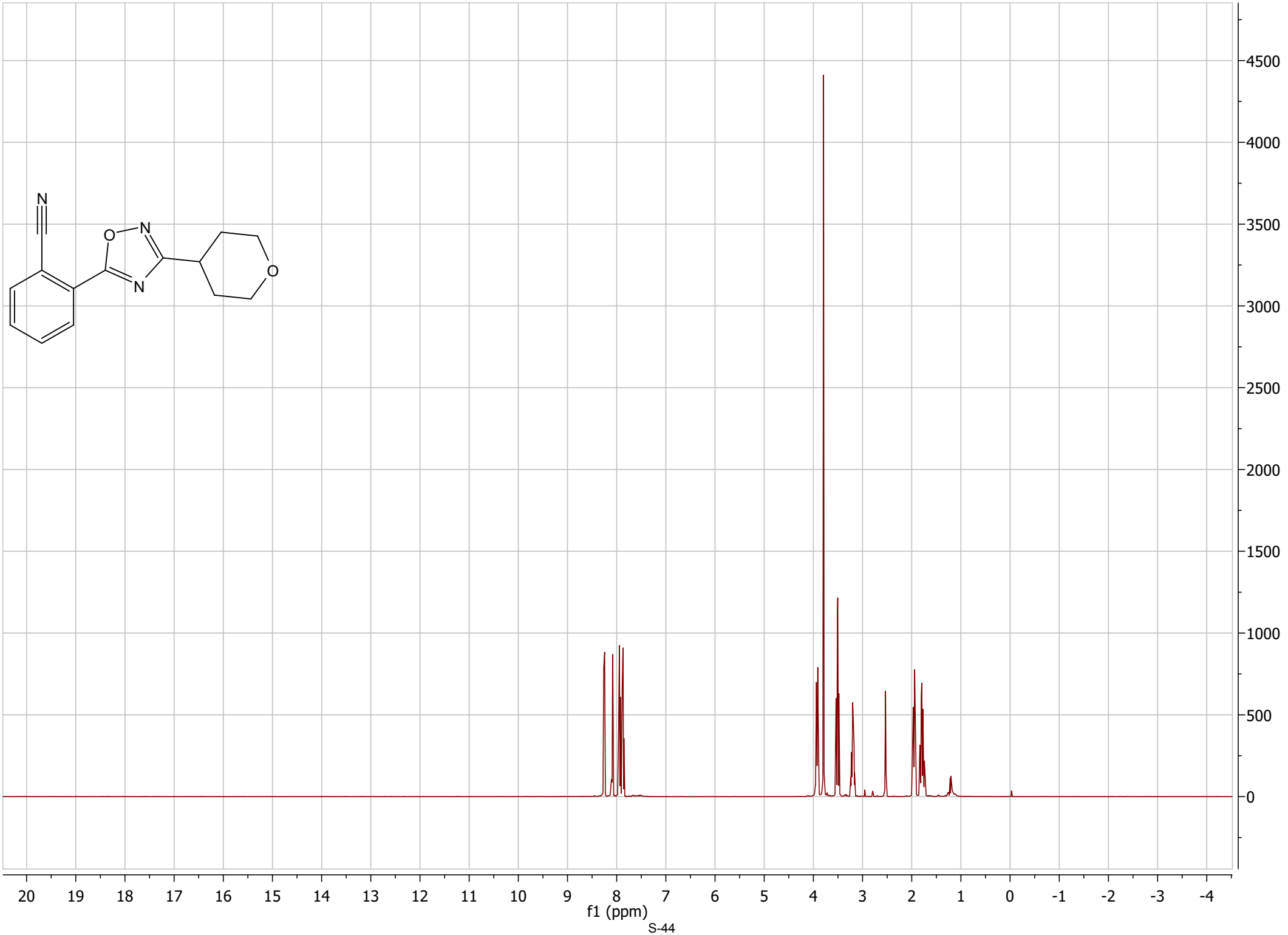

NH
O
O
CH3
H3C
CH3
N
O
N
1600
1500
1400
1300
1200
1100
1000
900
800
700
600
500
400
300
200
100
0
-100
230
220
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

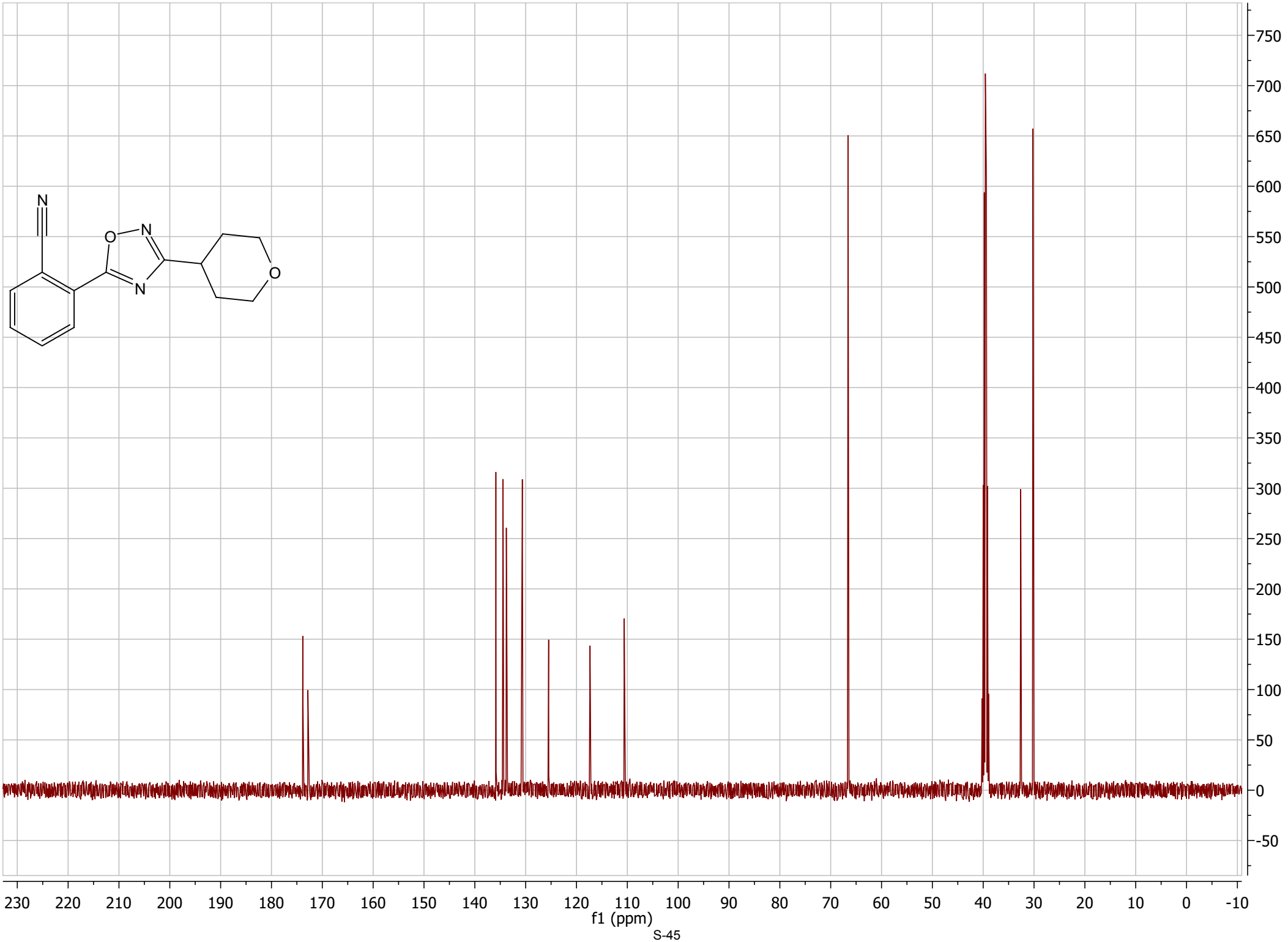

NH
O
O
CH3
H3C
CH3
N
O
N
4000
3500
3000
2500
2000
1500
1000
500
0
20 19 18 17 16 15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1 -2 -3 -4
f1 (ppm)


NH
O
O
CH3
H3C
CH3
N
O
N
1700
1600
1500
1400
1300
1200
1100
1000
900
800
700
600
500
400
300
200
100
0
-100
230
220
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)


O
F
F
F
O
N
N
O
3800
3600
3400
3200
3000
2800
2600
2400
2200
2000
1800
1600
1400
1200
1000
800
600
400
200
0
-200
20 19 18 17 16 15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1 -2 -3 -4
f1 (ppm)


O
F
F
F
O
N
N
O
1300
1200
1100
1000
900
800
700
600
500
400
300
200
100
0
-100
230
220
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)


N
O
N
N
O
4500
4000
3500
3000
2500
2000
1500
1000
500
0
20 19 18 17 16 15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1 -2 -3 -4
f1 (ppm)


N
O
N
N
O
750
700
650
600
550
500
450
400
350
300
250
200
150
100
50
0
-50
230
220
210
200
190
180
170
160
150
140
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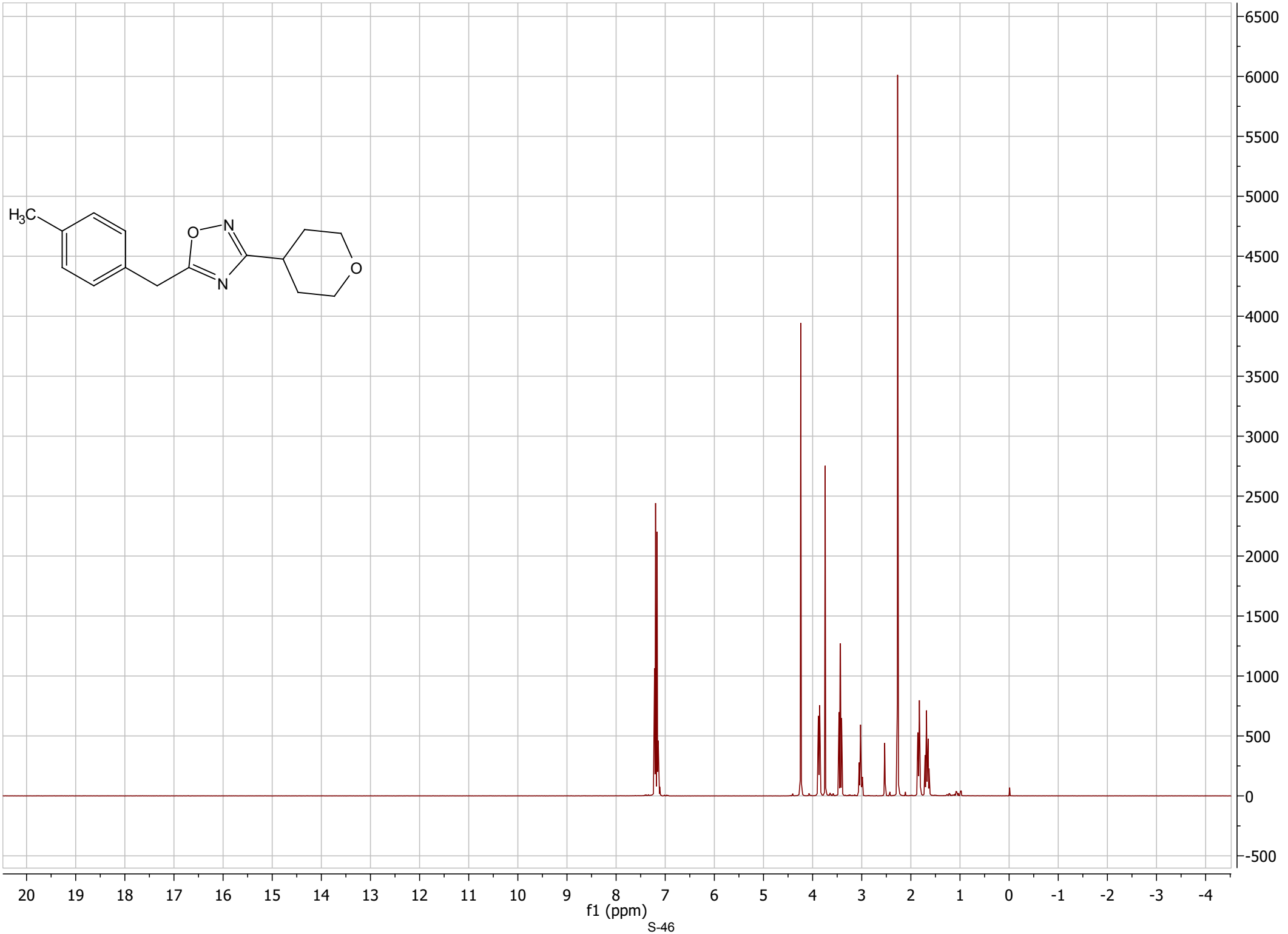
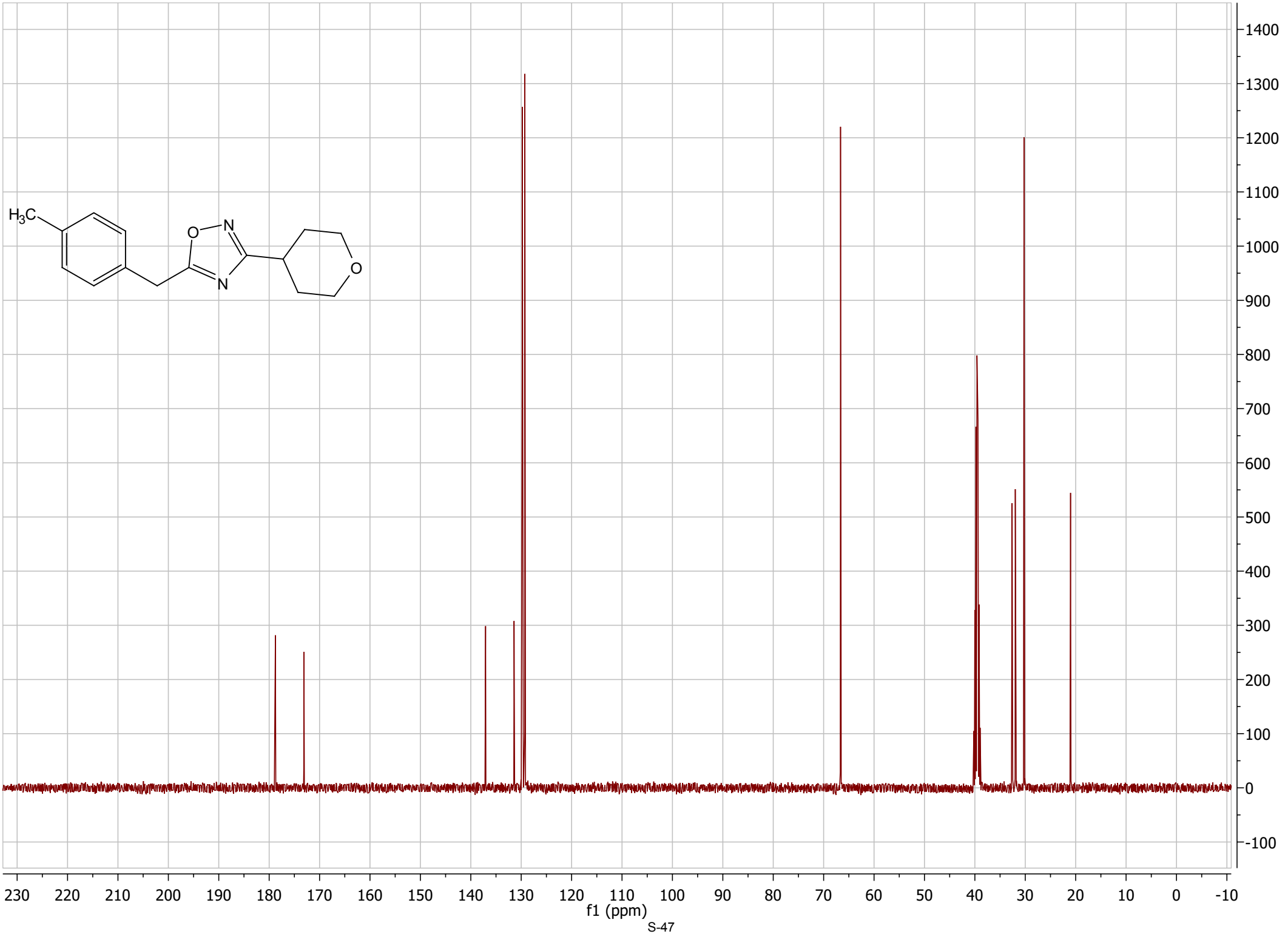
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)


H3C
O
N
N
O
6500
6000
5500
5000
4500
4000
3500
3000
2500
2000
1500
1000
500
0
-500
20 19 18 17 16 15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1 -2 -3 -4
f1 (ppm)


H3C
O
N
N
O
1400
1300
1200
1100
1000
900
800
700
600
500
400
300
200
100
0
-100
230
220
210
200
190
180
170
160
150
140
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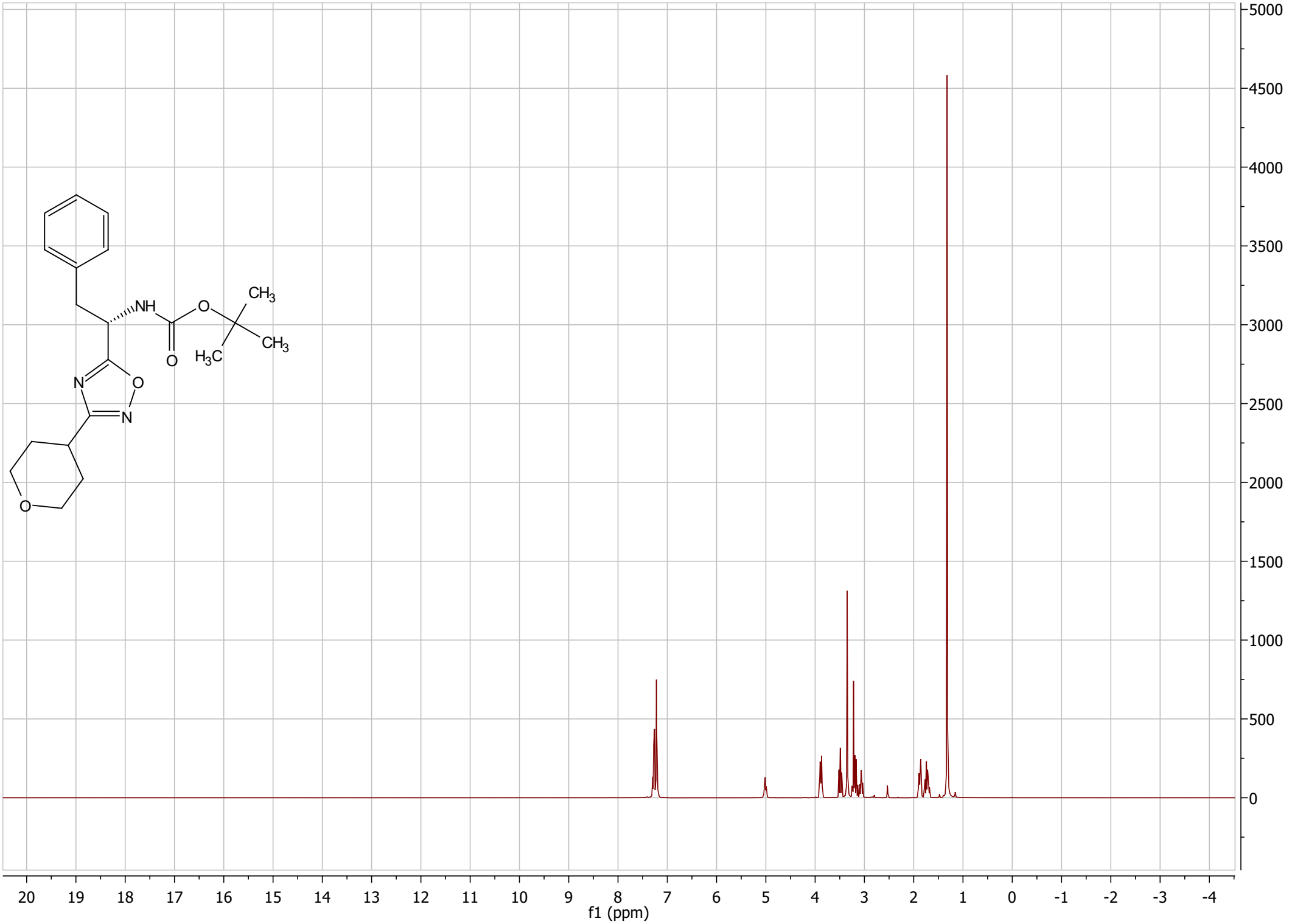
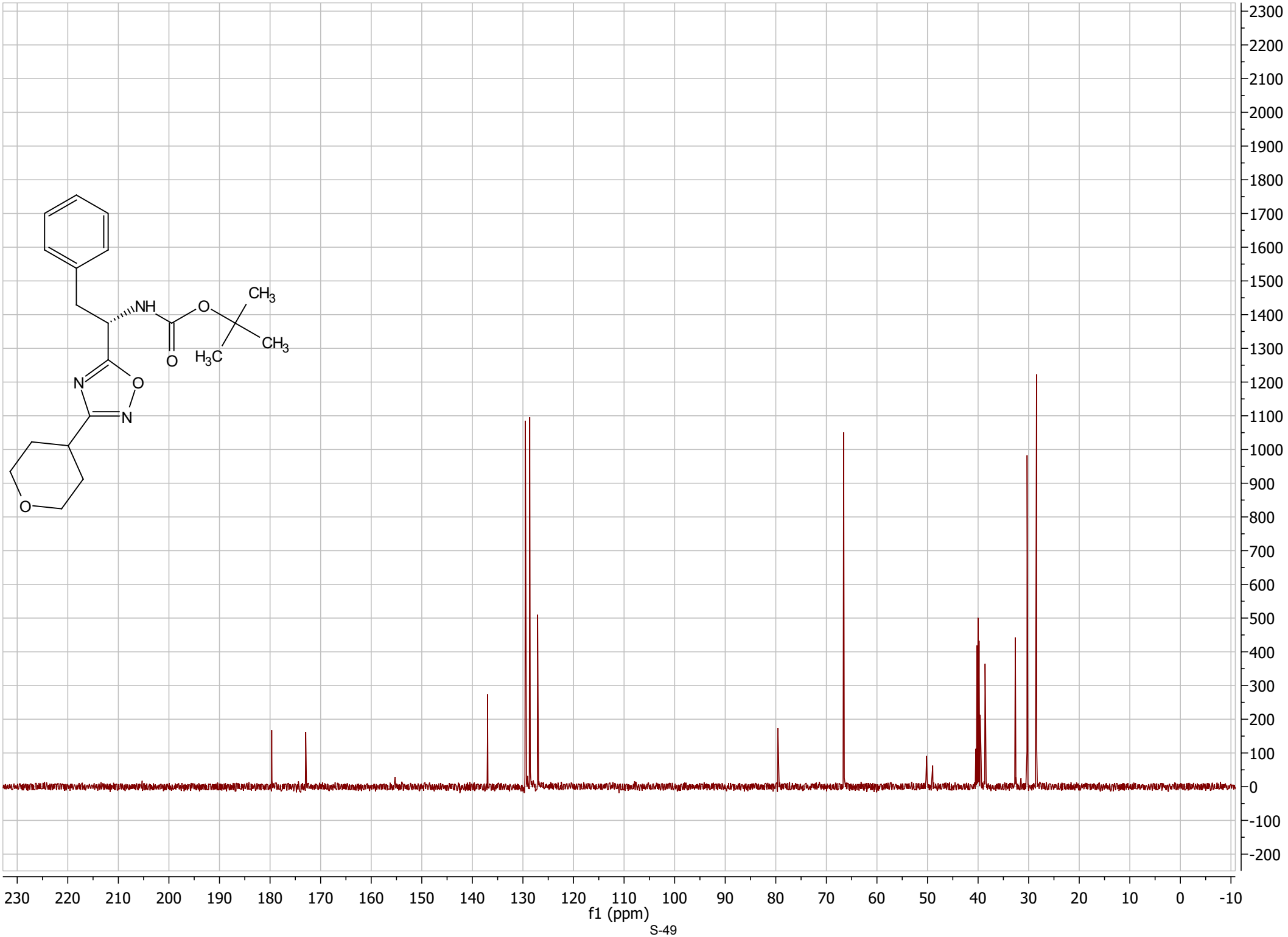
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)


NH
O
O
CH3
CH3
H3C
N
O
N
O
5000
4500
4000
3500
3000
2500
2000
1500
1000
500
0
20 19 18 17 16 15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1 -2 -3 -4
f1 (ppm)


NH
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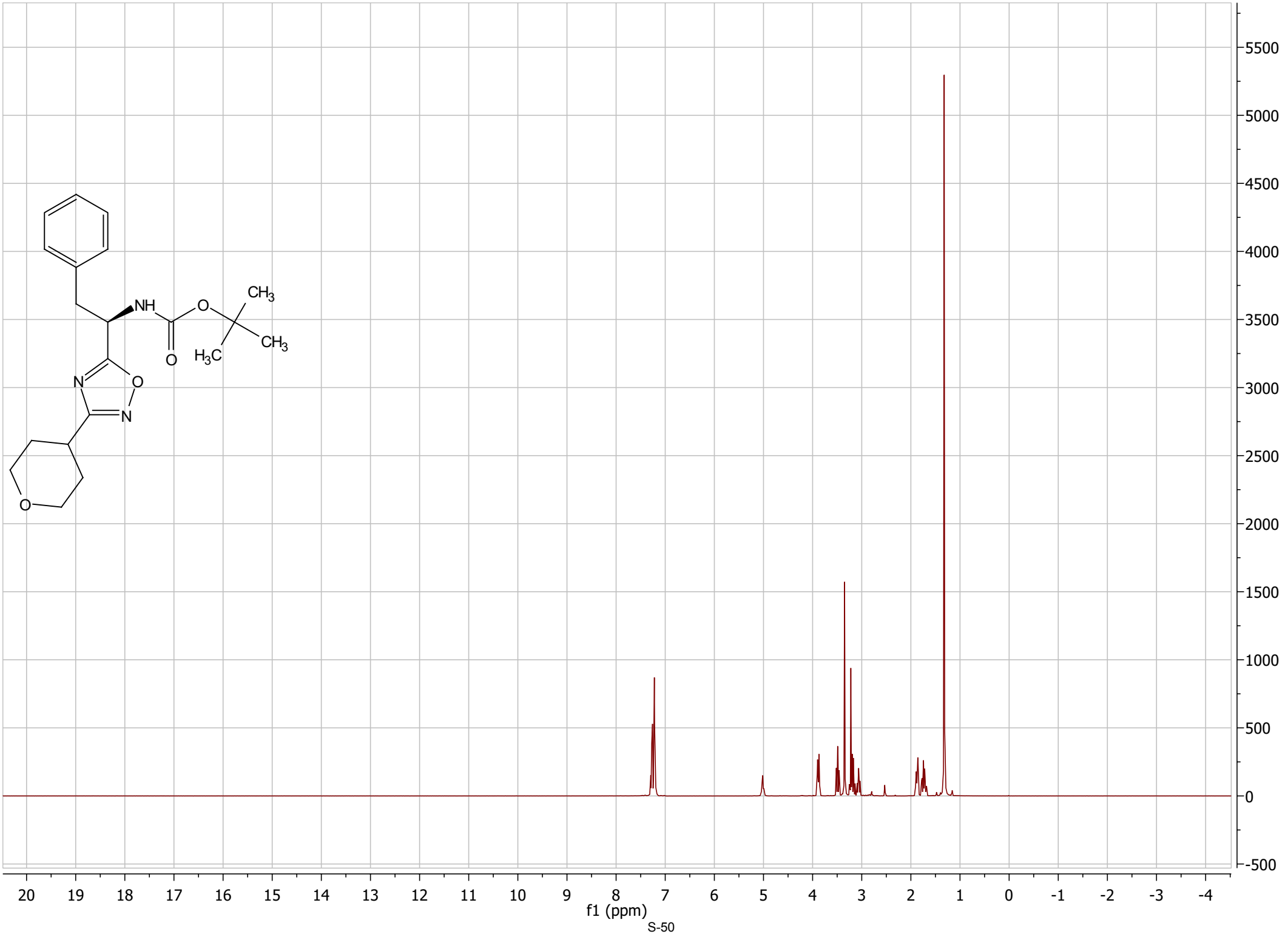
O
CH3
CH3
H3C
N
O
N
O
2300
2200
2100
2000
1900
1800
1700
1600
1500
1400
1300
1200
1100
1000
900
800
700
600
500
400
300
200
100
0
-100
-200
230
220
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)


NH
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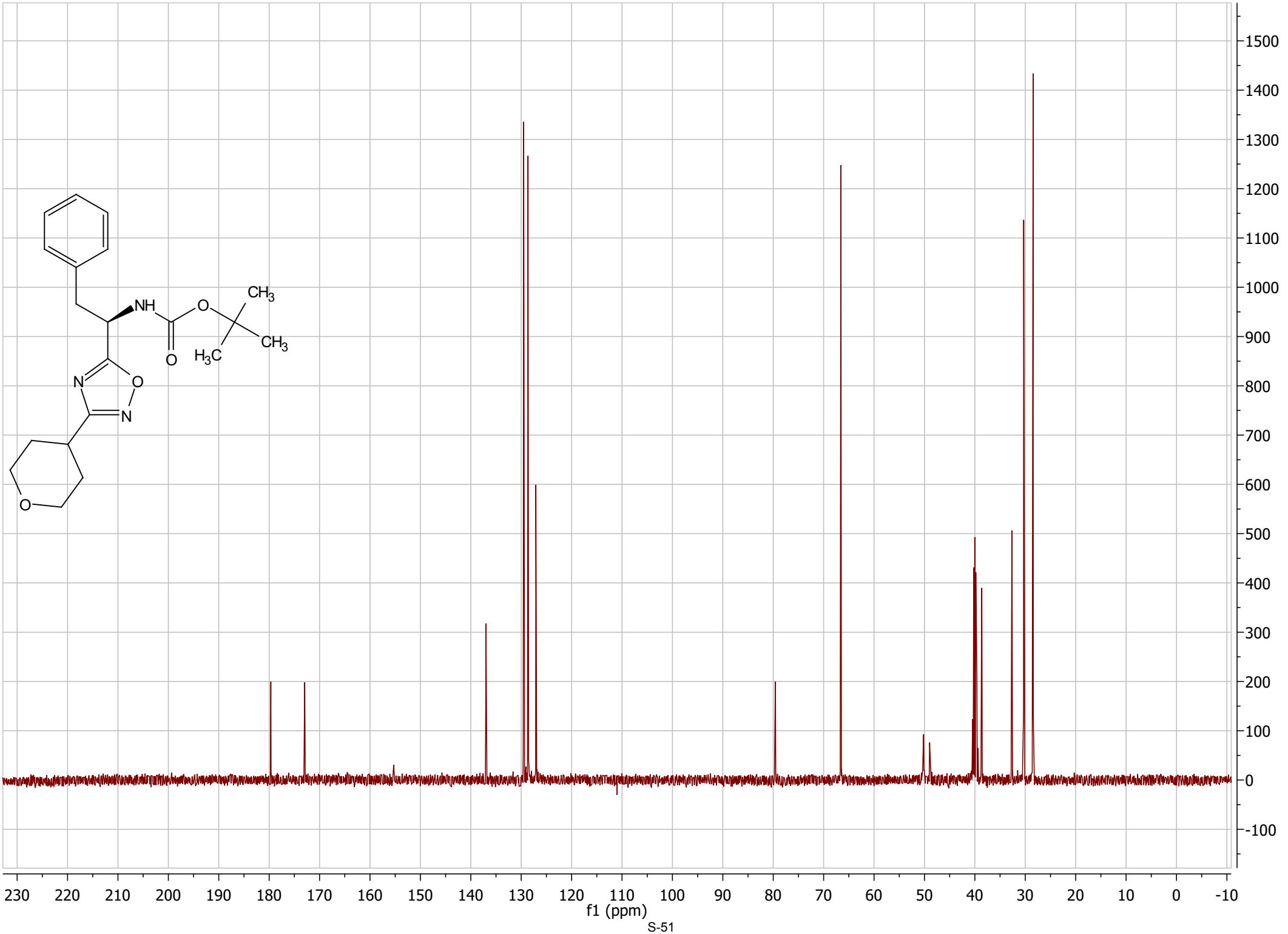
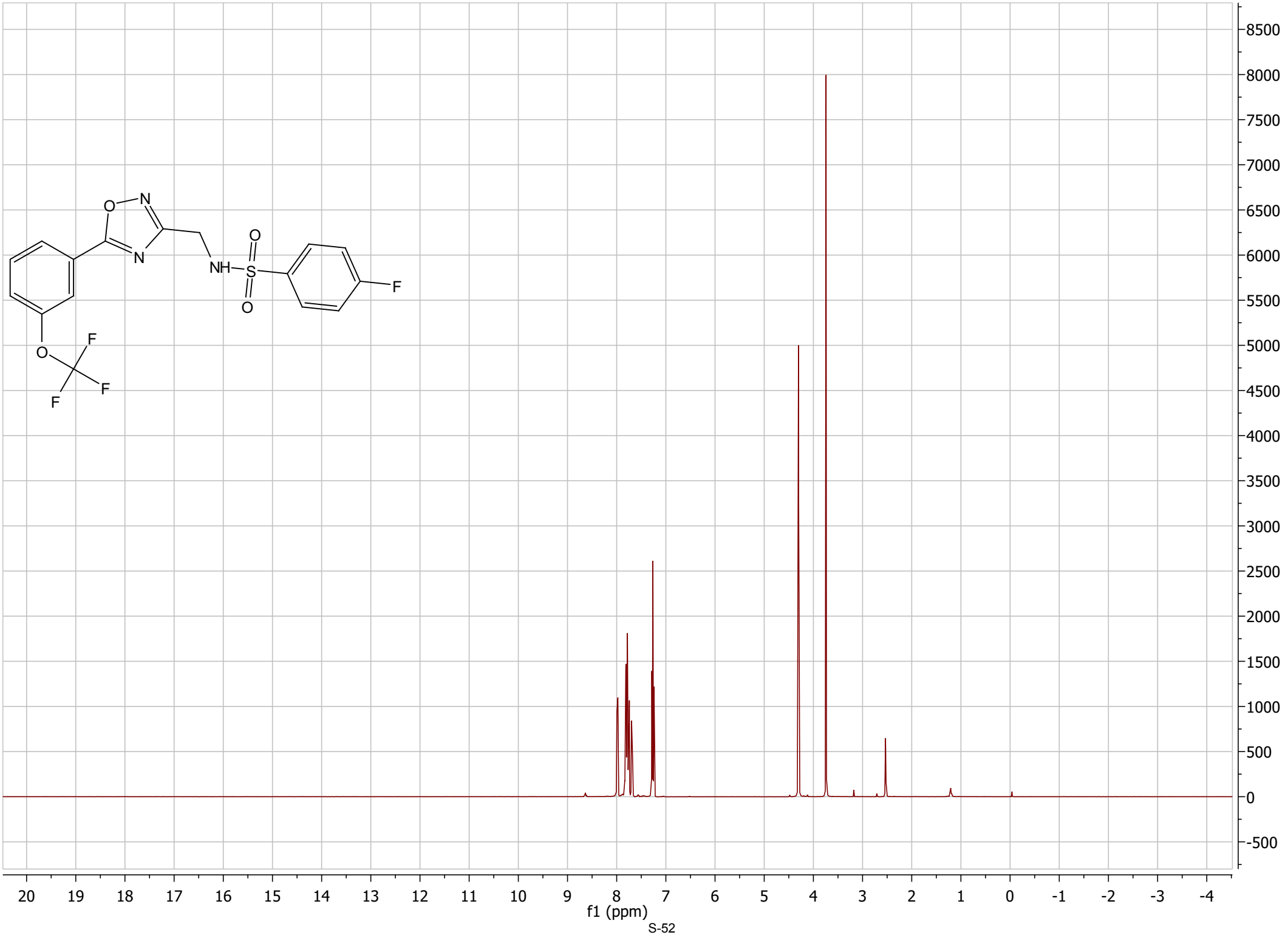
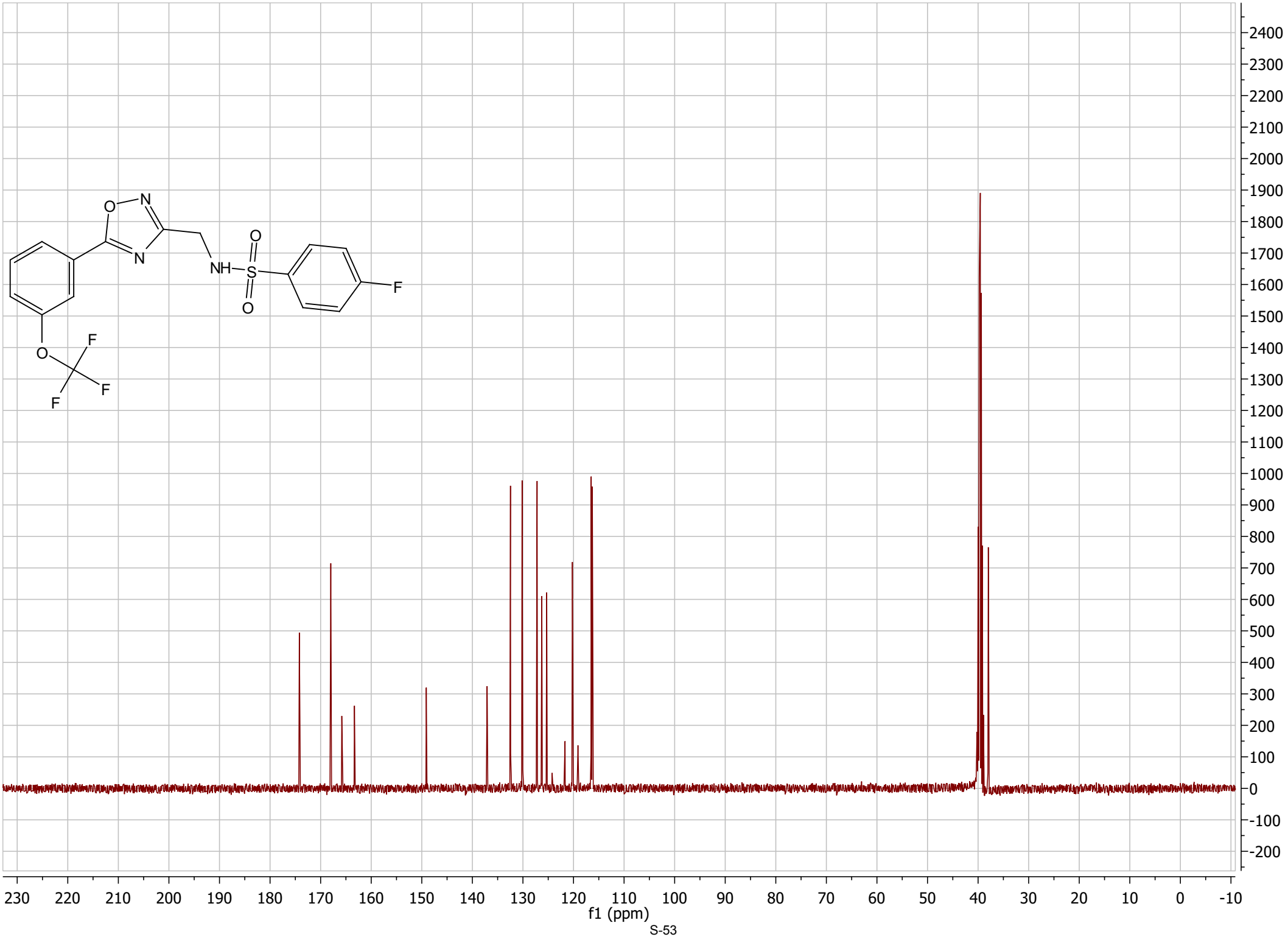
O
CH3
CH3
H3C
N
O
N
O
5500
5000
4500
4000
3500
3000
2500
2000
1500
1000
500
0
-500
20 19 18 17 16 15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1 -2 -3 -4
f1 (ppm)


NH
O
O
CH3
CH3
H3C
N
O
N
O
1500
1400
1300
1200
1100
1000
900
800
700
600
500
400
300
200
100
0
-100
230
220
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)


O
N
N
NH
S
O
O
F
O
F
F
F
8500
8000
7500
7000
6500
6000
5500
5000
4500
4000
3500
3000
2500
2000
1500
1000
500
0
-500
20 19 18 17 16 15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1 -2 -3 -4
f1 (ppm)


O
N
N
NH
S
O
O
F
O
F
F
F
2400
2300
2200
2100
2000
1900
1800
1700
1600
1500
1400
1300
1200
1100
1000
900
800
700
600
500
400
300
200
100
0
-100
-200
230
220
210
200
190
180
170
160
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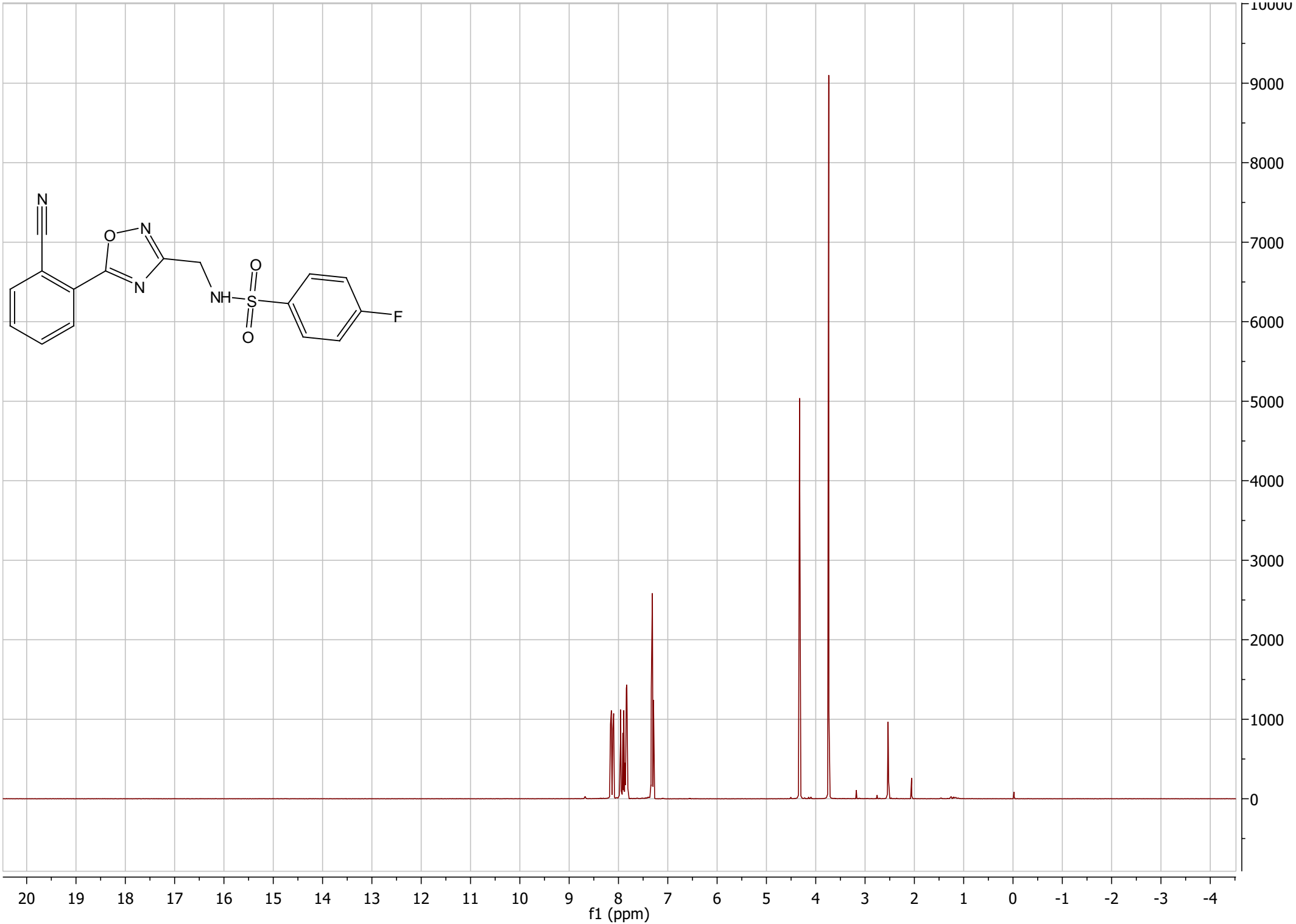
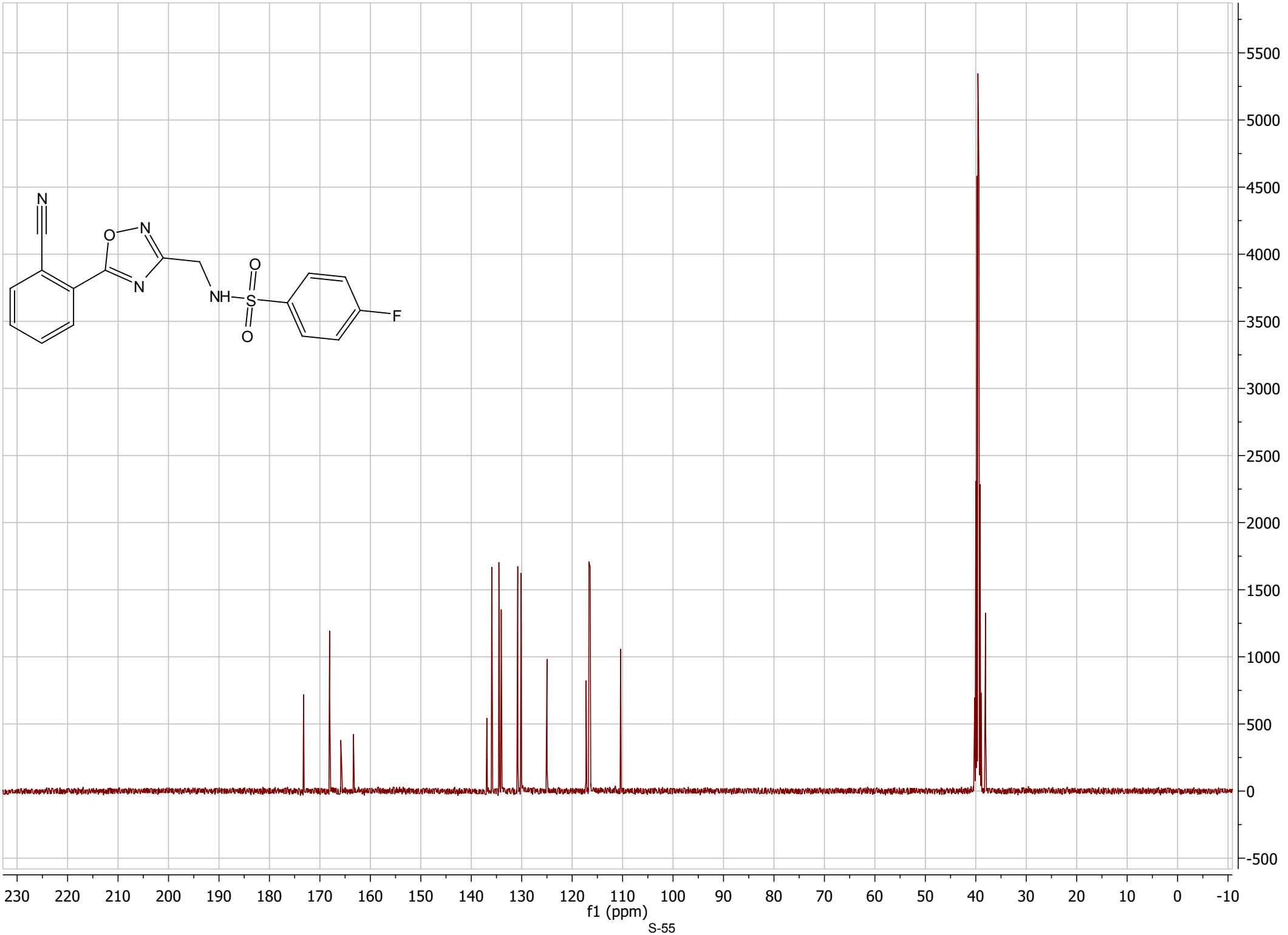
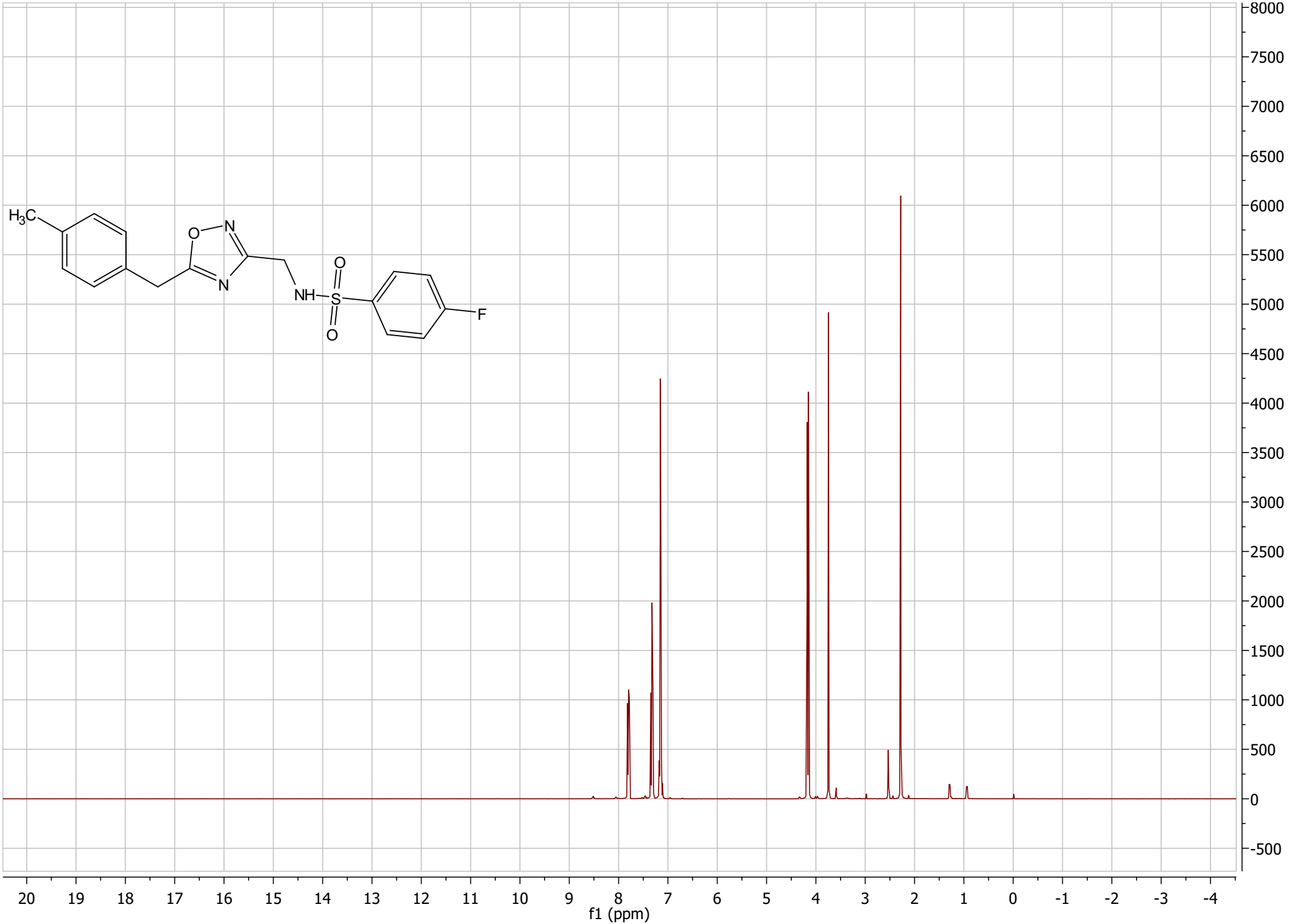
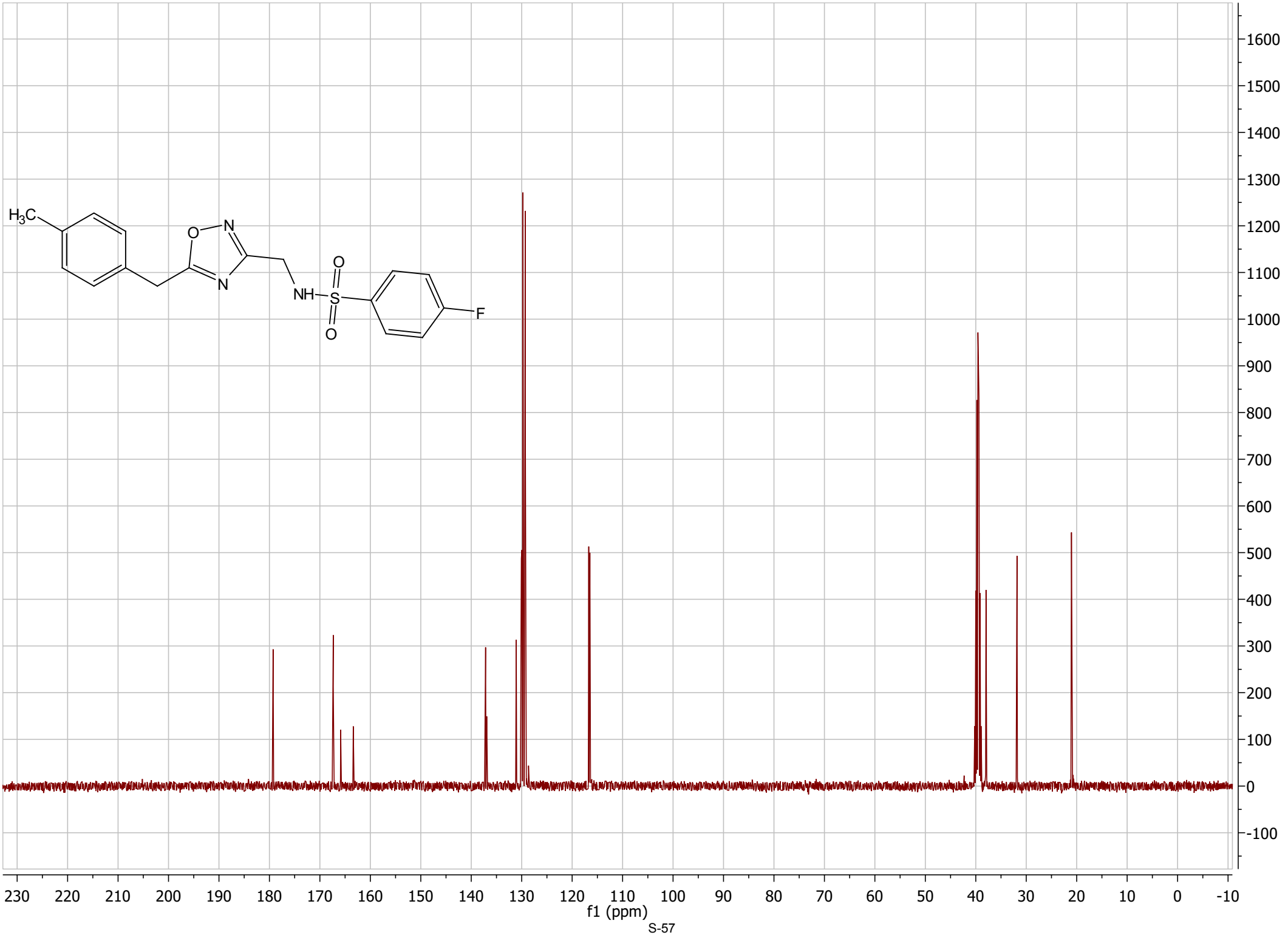
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)


N
O
N
N
NH
S
O
O
F
10000
9000
8000
7000
6000
5000
4000
3000
2000
1000
0
20 19 18 17 16 15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1 -2 -3 -4
f1 (ppm)


N
O
N
N
NH
S
O
O
F
5500
5000
4500
4000
3500
3000
2500
2000
1500
1000
500
0
-500
230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)


H3C
O
N
N
NH
S
O
O
F
8000
7500
7000
6500
6000
5500
5000
4500
4000
3500
3000
2500
2000
1500
1000
500
0
-500
20 19 18 17 16 15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1 -2 -3 -4
f1 (ppm)


H3C
O
N
N
NH
S
O
O
F
1600
1500
1400
1300
1200
1100
1000
900
800
700
600
500
400
300
200
100
0
-100
230
220
210
200
190
180
170
160
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140
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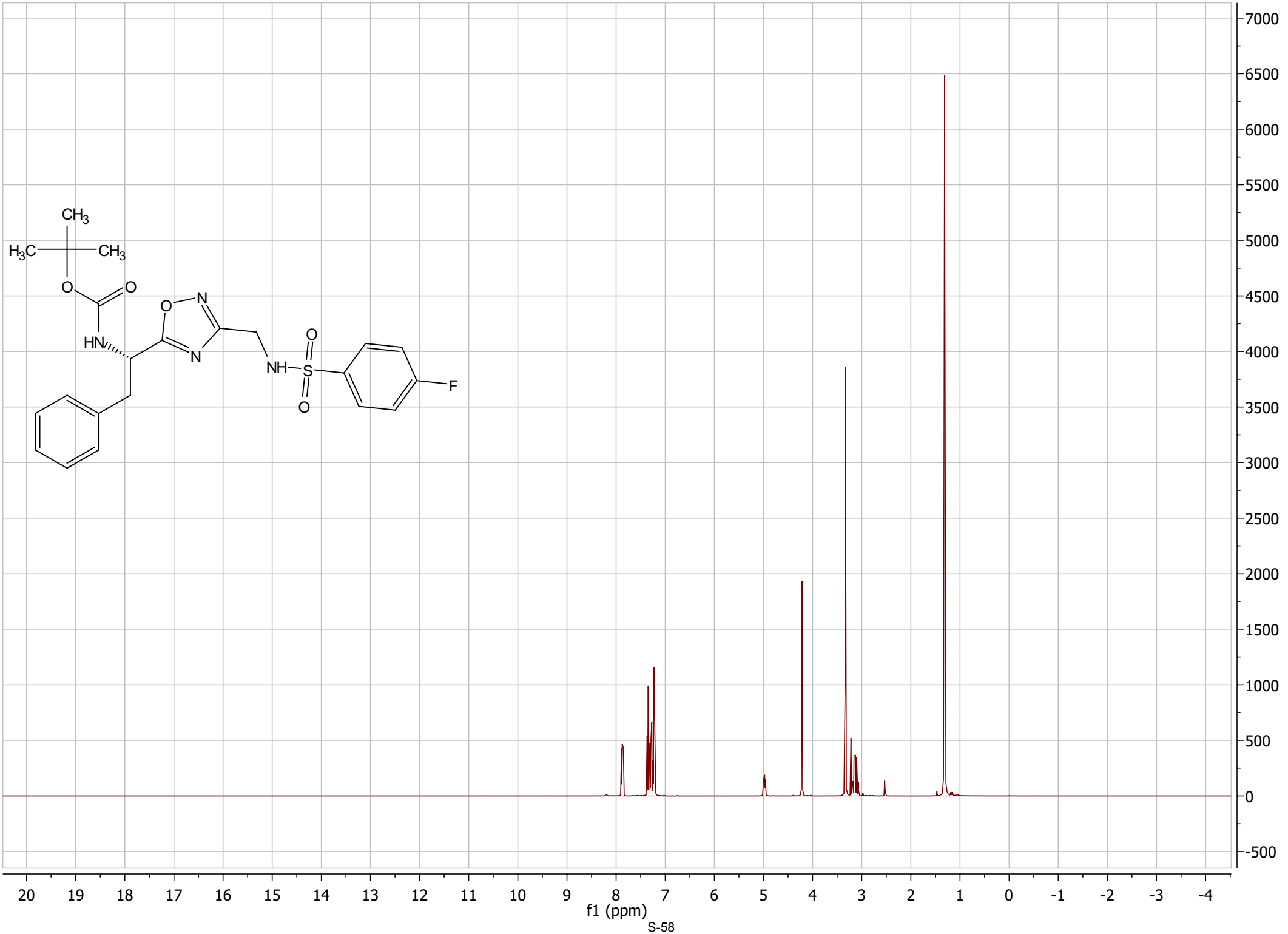
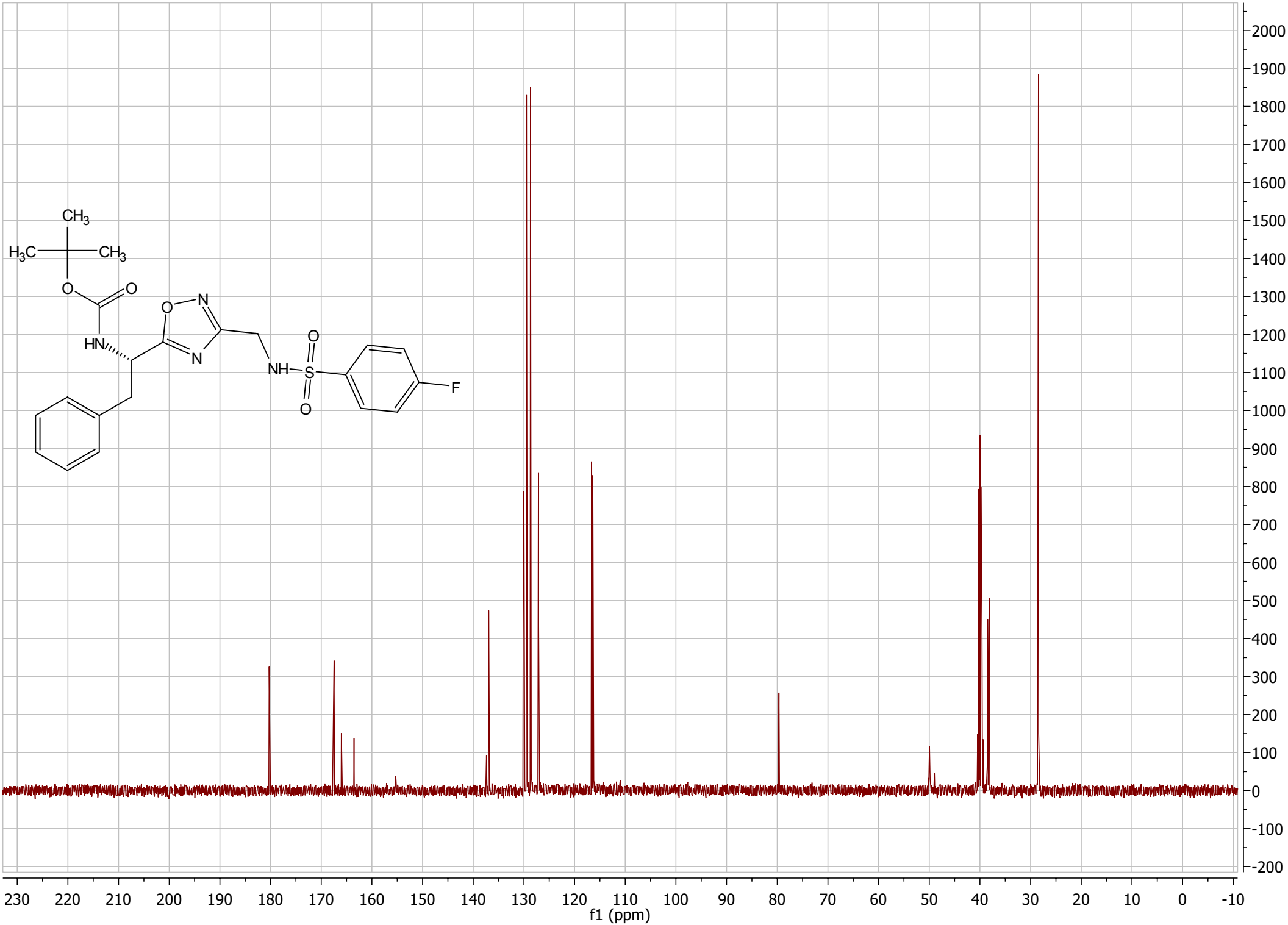
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)


CH3
H3C
CH3
O
O
HN
O
N
N
NH
S
O
O
F
7000
6500
6000
5500
5000
4500
4000
3500
3000
2500
2000
1500
1000
500
0
-500
20
19
18
17
16
15
14
13
12
11
10
9
8
7
6
5
4
3
2
1
0
-1
-2
-3
-4
f1 (ppm)


CH3
H3C
CH3
O
O
HN
O
N
N
NH
S
O
O
F
2000
1900
1800
1700
1600
1500
1400
1300
1200
1100
1000
900
800
700
600
500
400
300
200
100
0
-100
-200
230
220
210
200
190
180
170
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140
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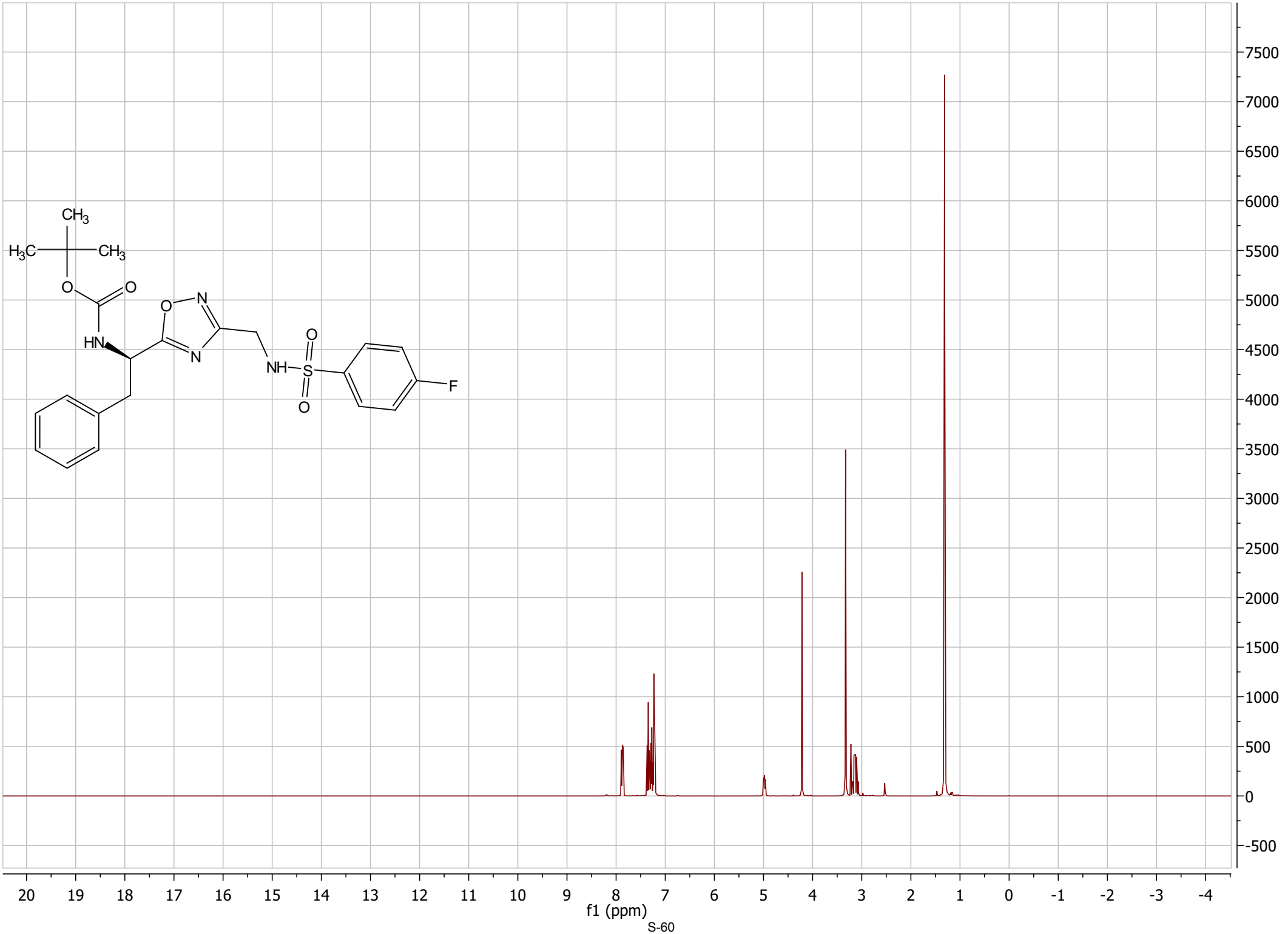
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)


CH3
H3C
CH3
O
O
HN
O
N
N
NH
S
O
O
F
7500
7000
6500
6000
5500
5000
4500
4000
3500
3000
2500
2000
1500
1000
500
0
-500
20
19
18
17
16
15
14
13
12
11
10
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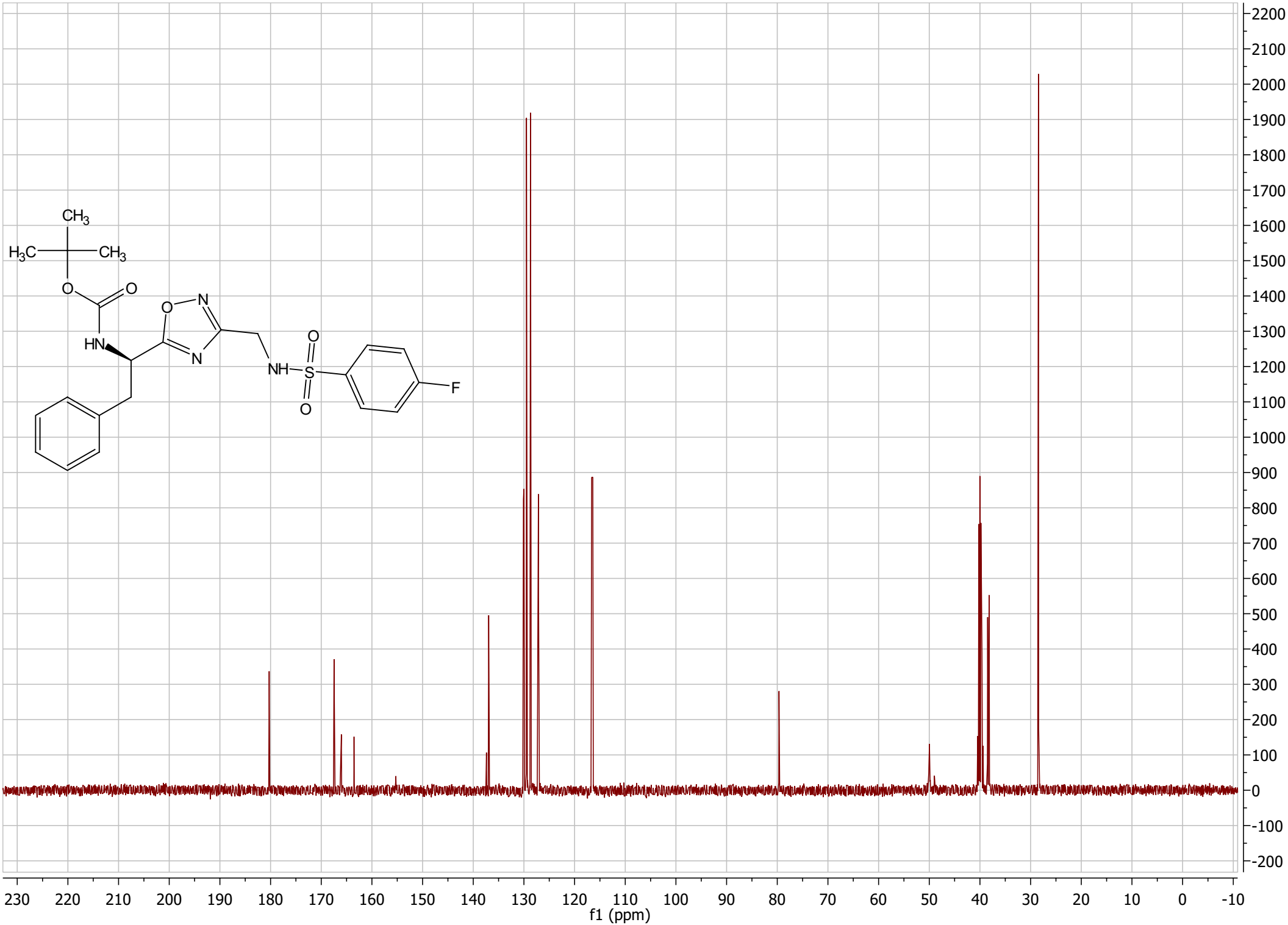
8
7
6
5
4
3
2
1
0
-1
-2
-3
-4
f1 (ppm)


CH3
H3C
CH3
O
O
HN
O
N
N
NH
S
O
O
F
2200
2100
2000
1900
1800
1700
1600
1500
1400
1300
1200
1100
1000
900
800
700
600
500
400
300
200
100
0
-100
-200
230
220
210
200
190
180
170
160
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140
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120
110
100
90
80
70
60
50
40
30
20
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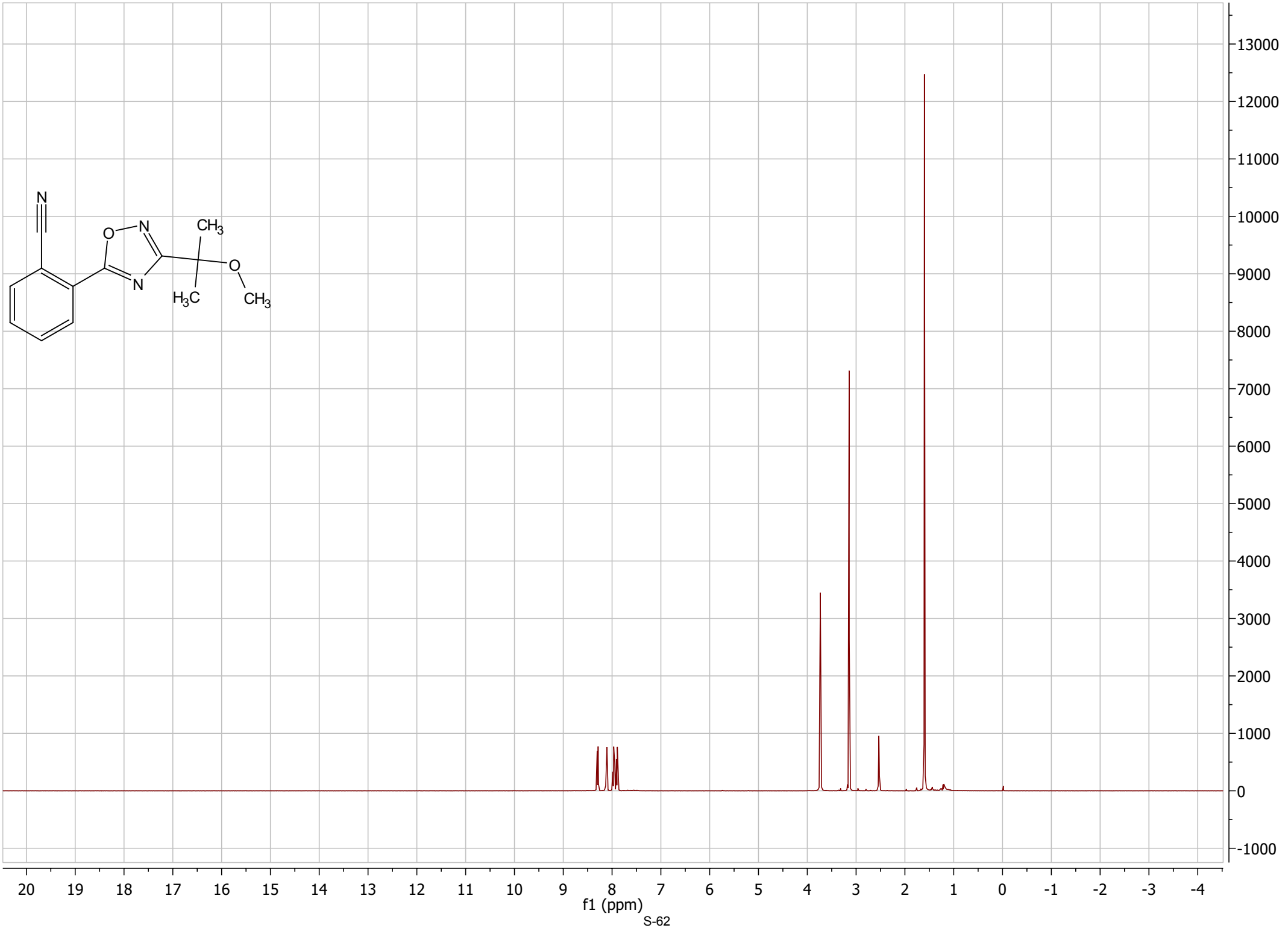
0
-10
f1 (ppm)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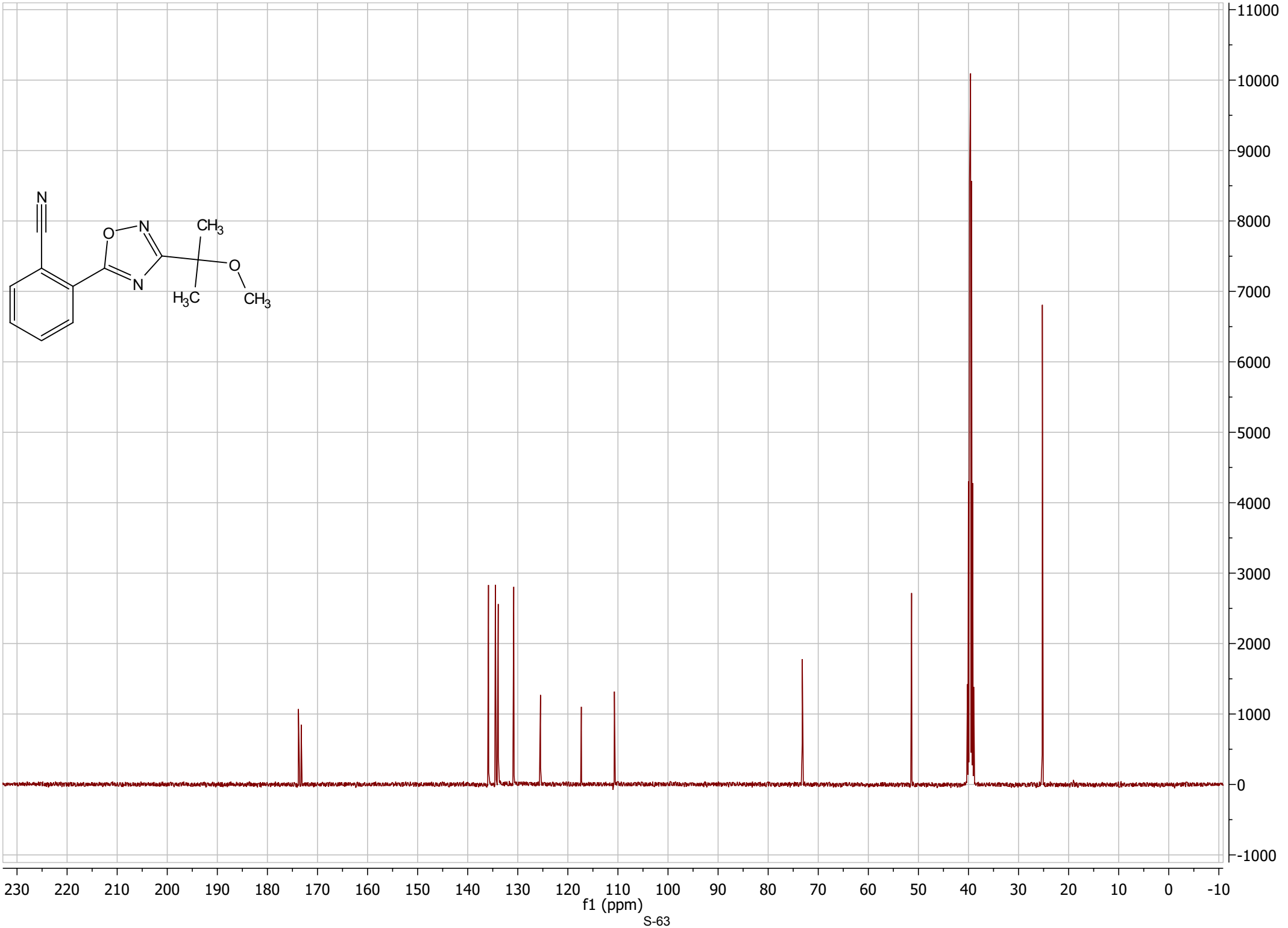
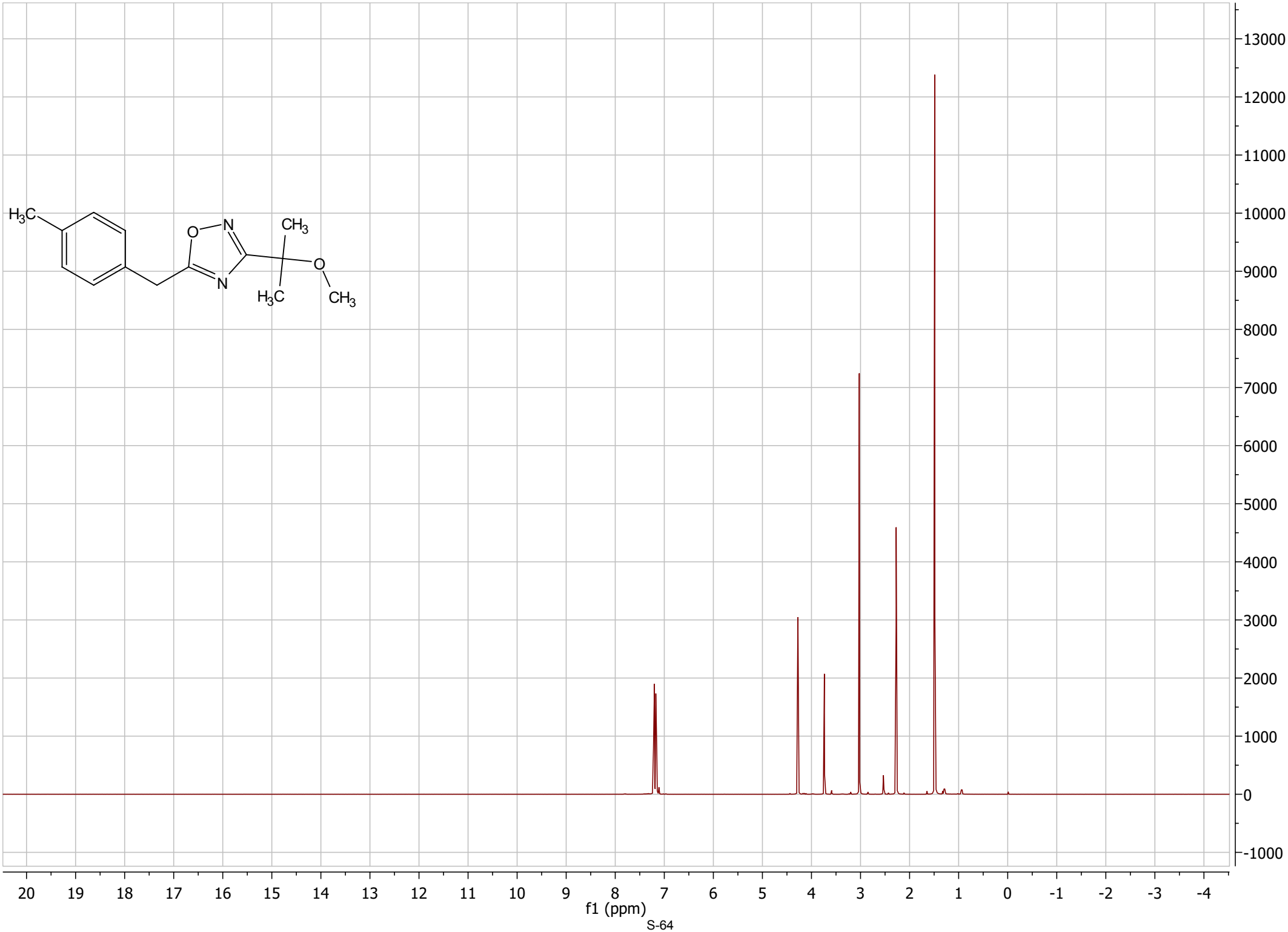
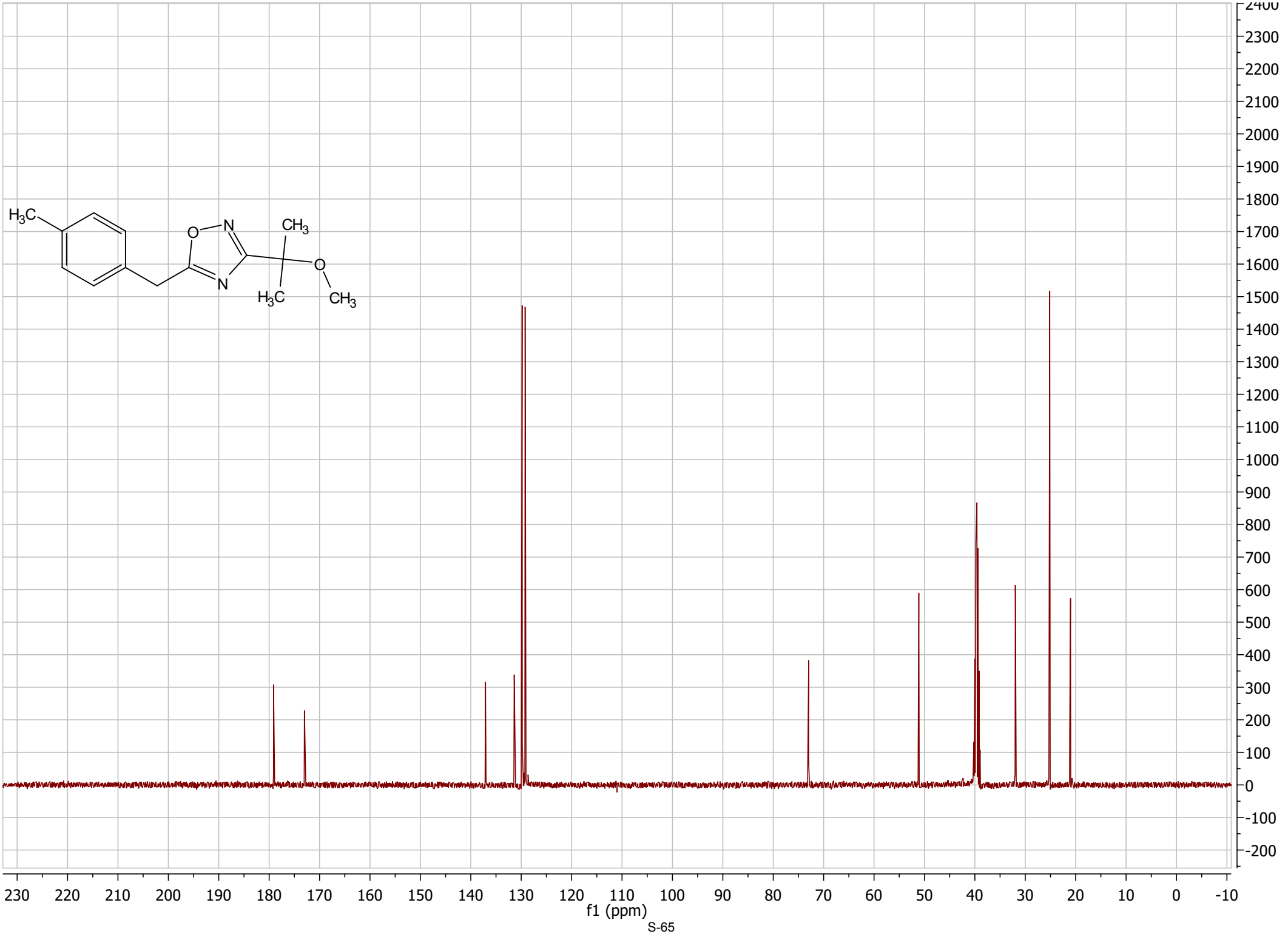
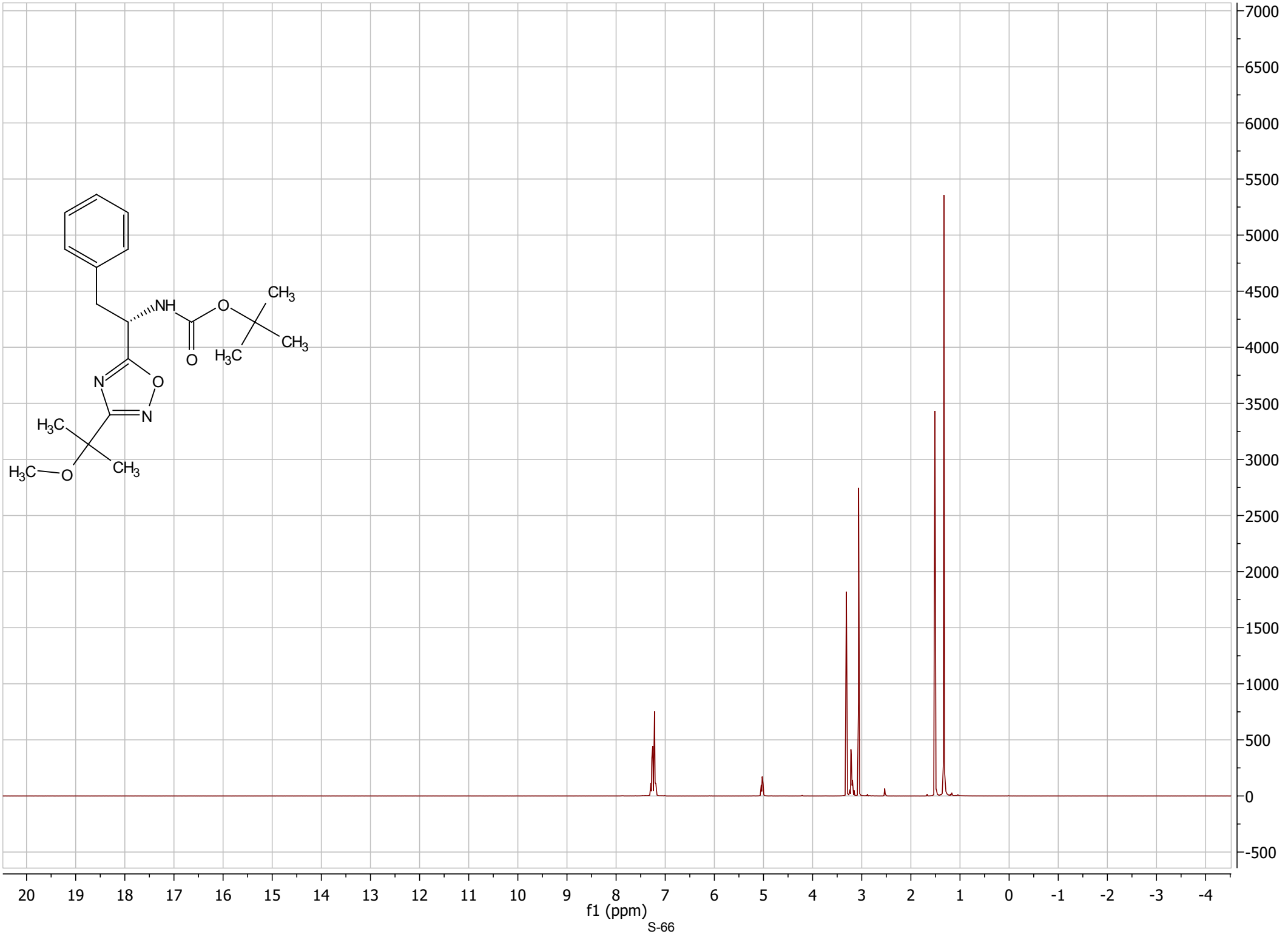
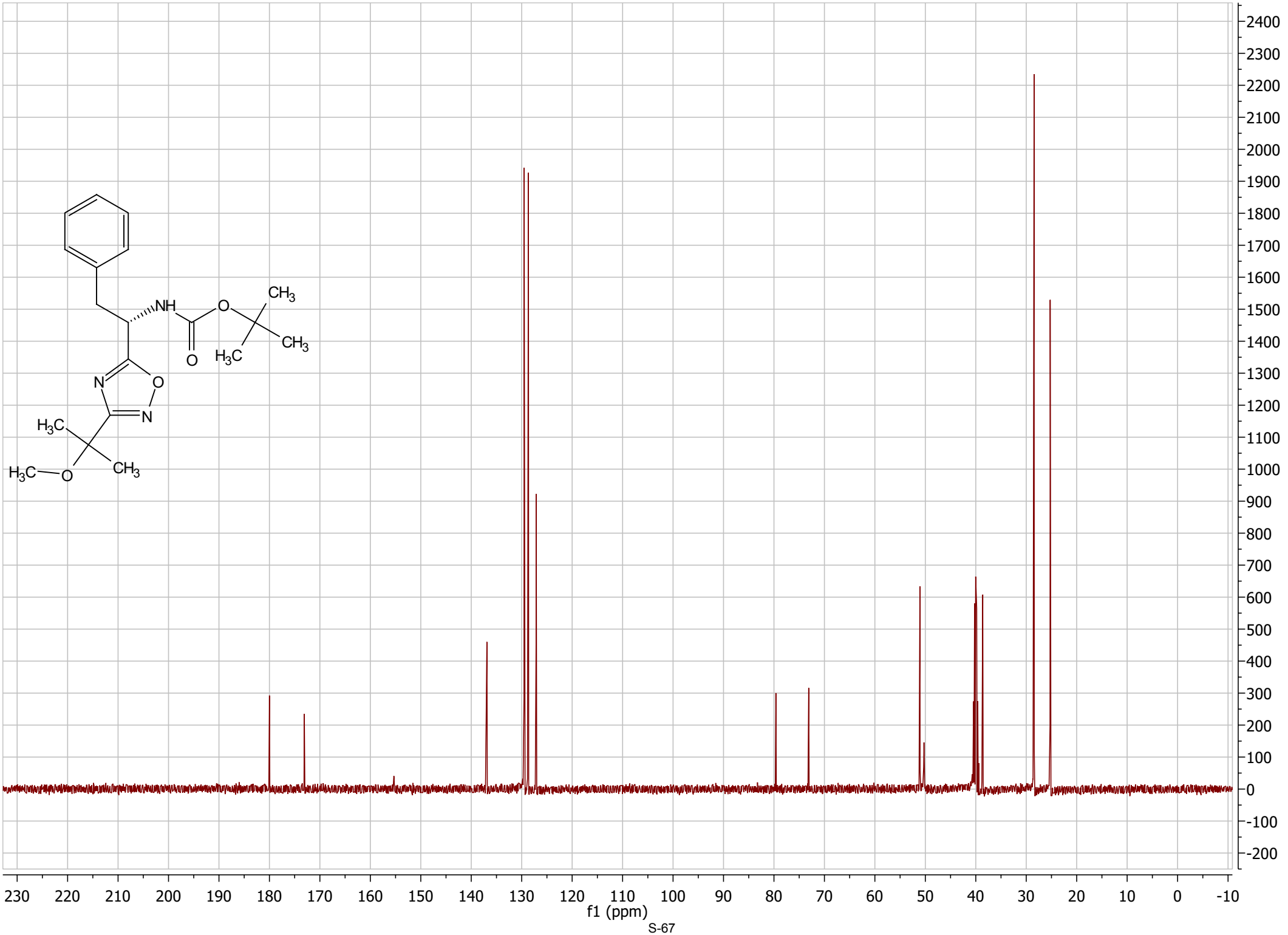
O
N
CH3
O
N
H3C
CH3
13000
12000
11000
10000
9000
8000
7000
6000
5000
4000
3000
2000
1000
0
-1000
20 19 18 17 16 15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1 -2 -3 -4
f1 (ppm)

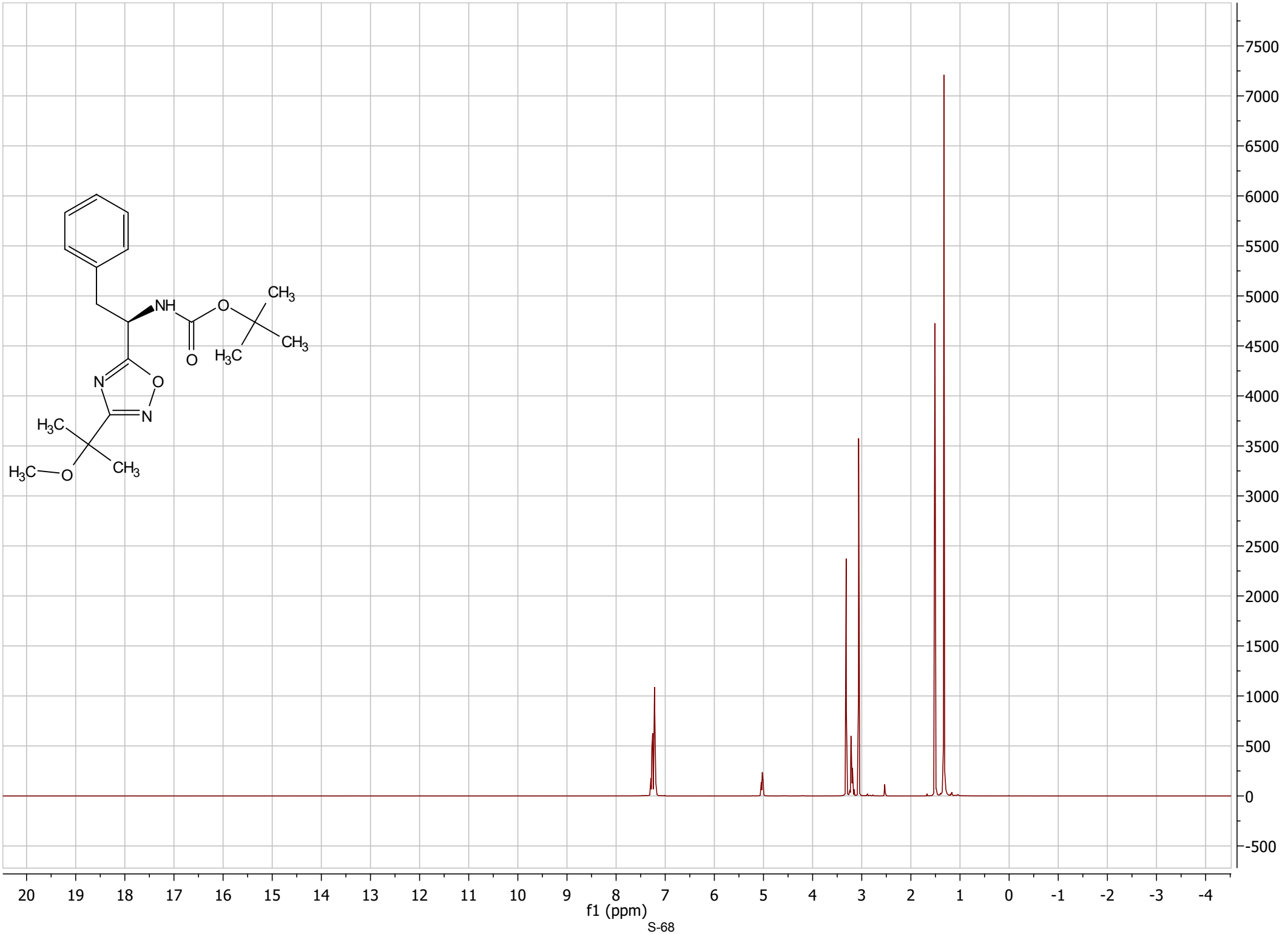

N
O
N
N
CH3
O
H3C
CH3
11000
10000
9000
8000
7000
6000
5000
4000
3000
2000
1000
0
-1000
230
220
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

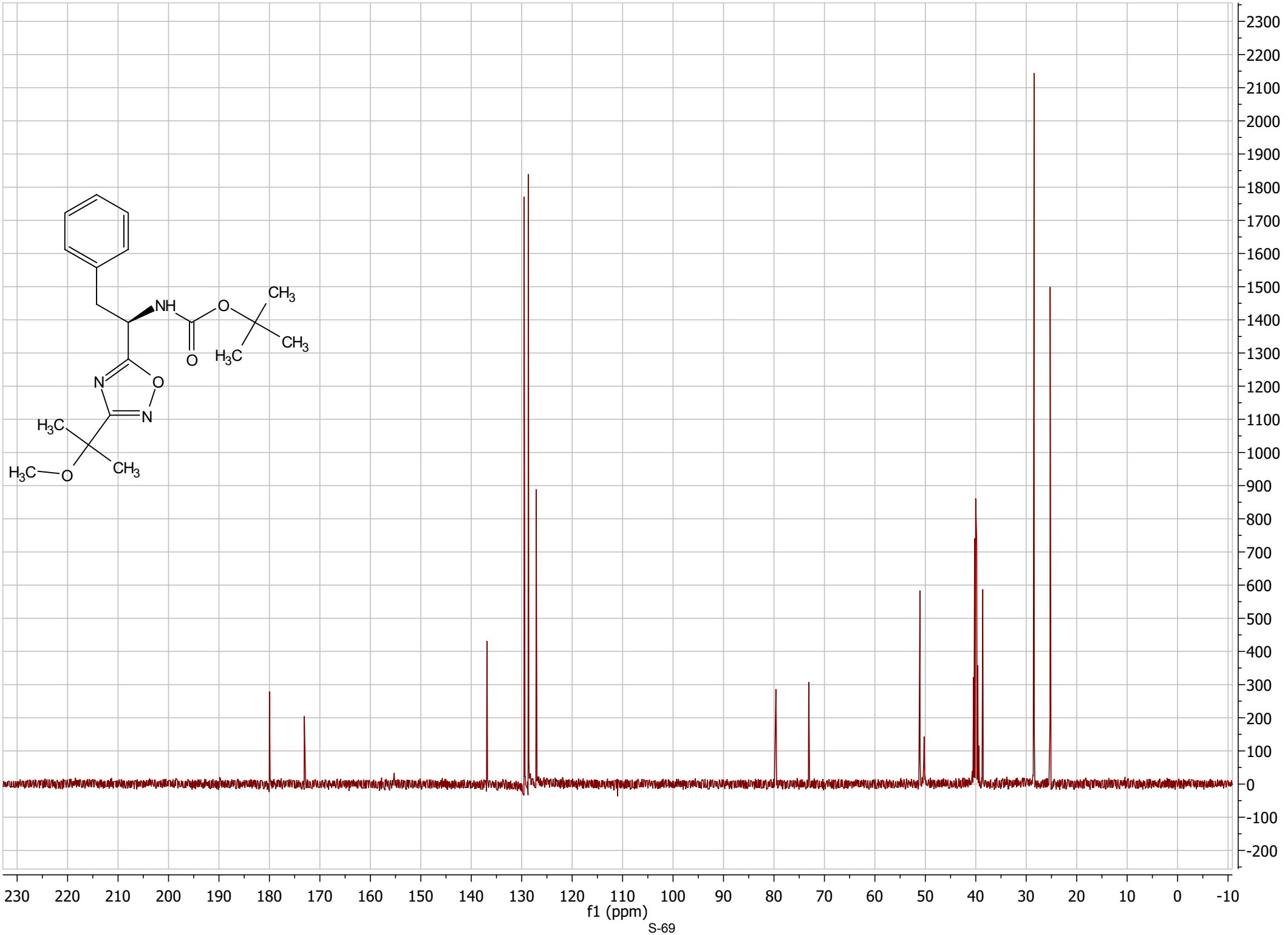

H3C
O
N
CH3
O
N
H3C
CH3
13000
12000
11000
10000
9000
8000
7000
6000
5000
4000
3000
2000
1000
0
-1000
20 19 18 17 16 15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1 -2 -3 -4
f1 (ppm)

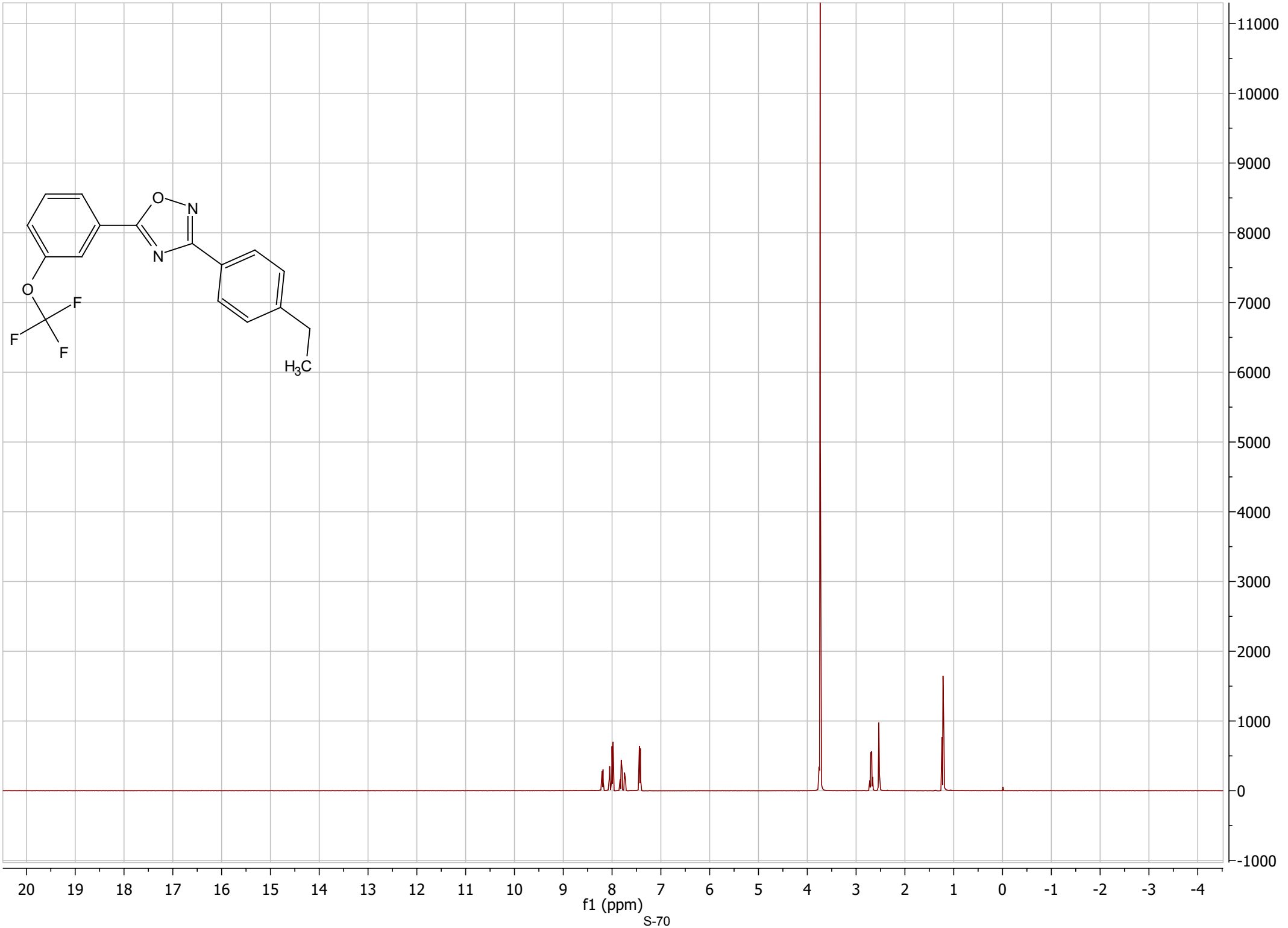

H3C
O
N
CH3
O
N
H3C
CH3
2400
2300
2200
2100
2000
1900
1800
1700
1600
1500
1400
1300
1200
1100
1000
900
800
700
600
500
400
300
200
100
0
-100
-200
230
220
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

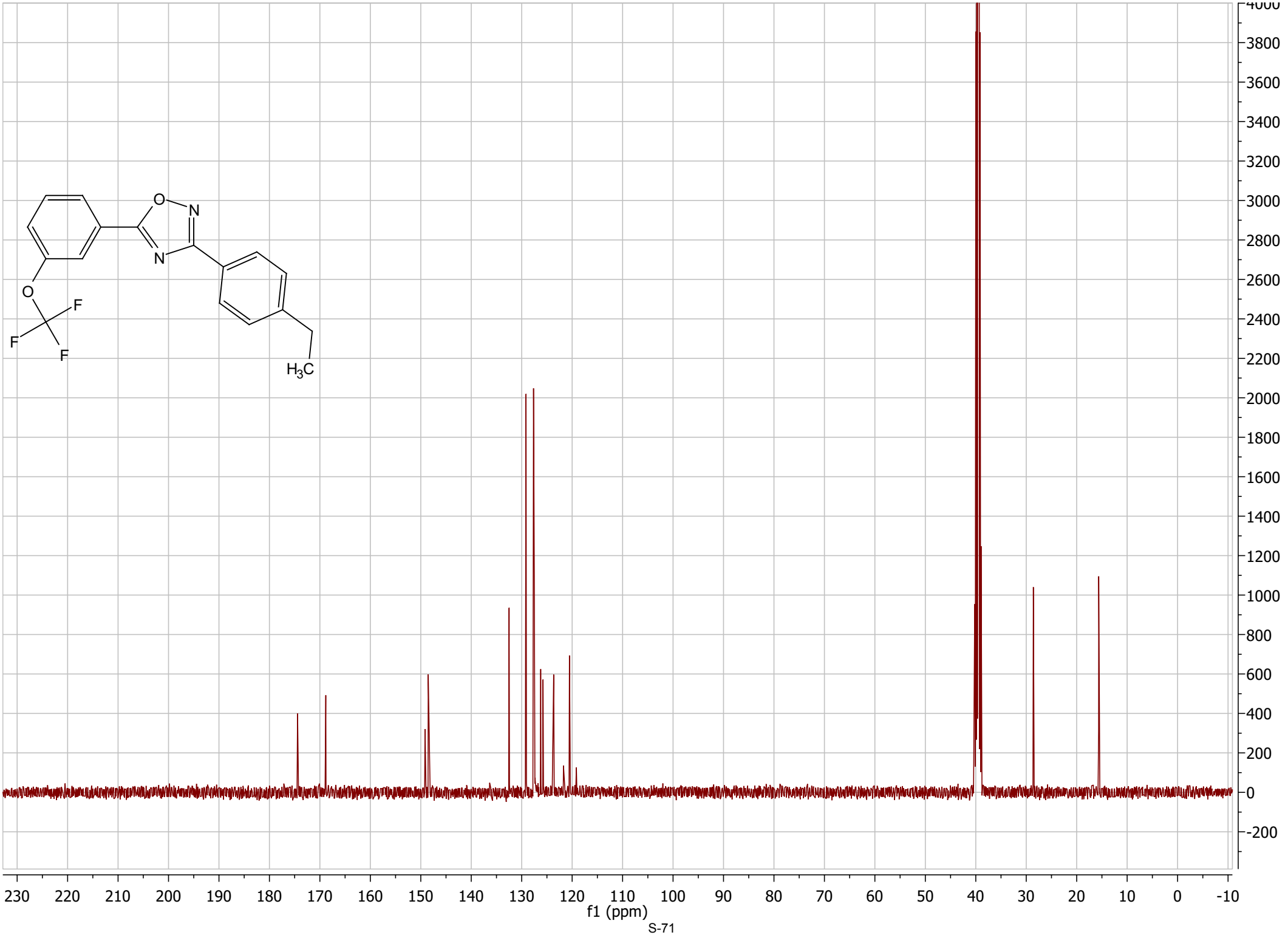

NH
O
O
CH3
CH3
H3C
N
O
N
H3C
H3C
O
CH3
7000
6500
6000
5500
5000
4500
4000
3500
3000
2500
2000
1500
1000
500
0
-500
20 19 18 17 16 15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1 -2 -3 -4
f1 (ppm)

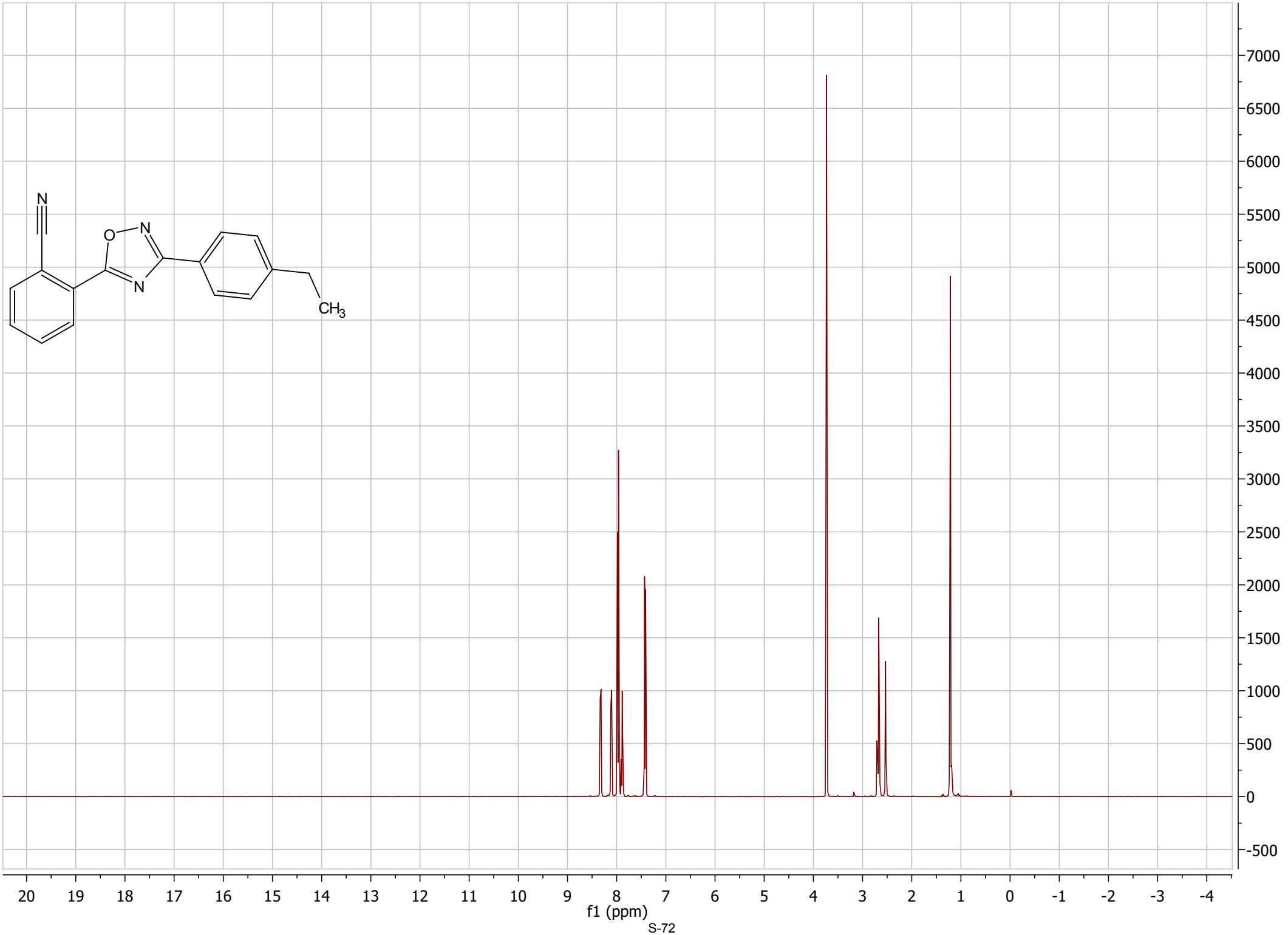

NH
O
O
CH3
CH3
H3C
N
O
N
H3C
H3C
O
CH3
2400
2300
2200
2100
2000
1900
1800
1700
1600
1500
1400
1300
1200
1100
1000
900
800
700
600
500
400
300
200
100
0
-100
-200
230
220
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

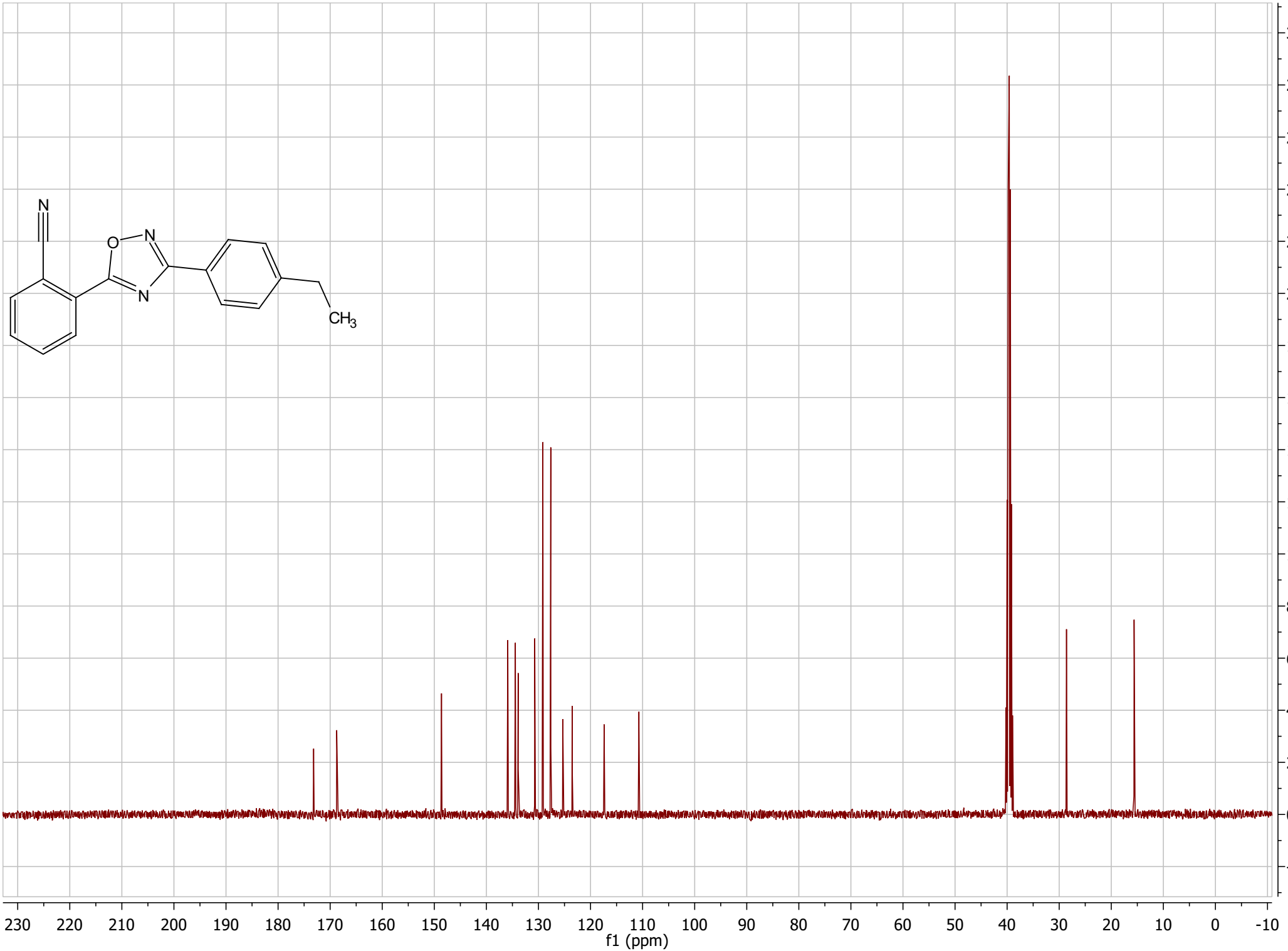

NH
O
O
CH3
CH3
H3C
N
O
N
H3C
H3C
O
CH3
7500
7000
6500
6000
5500
5000
4500
4000
3500
3000
2500
2000
1500
1000
500
0
-500
20 19 18 17 16 15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1 -2 -3 -4
f1 (ppm)

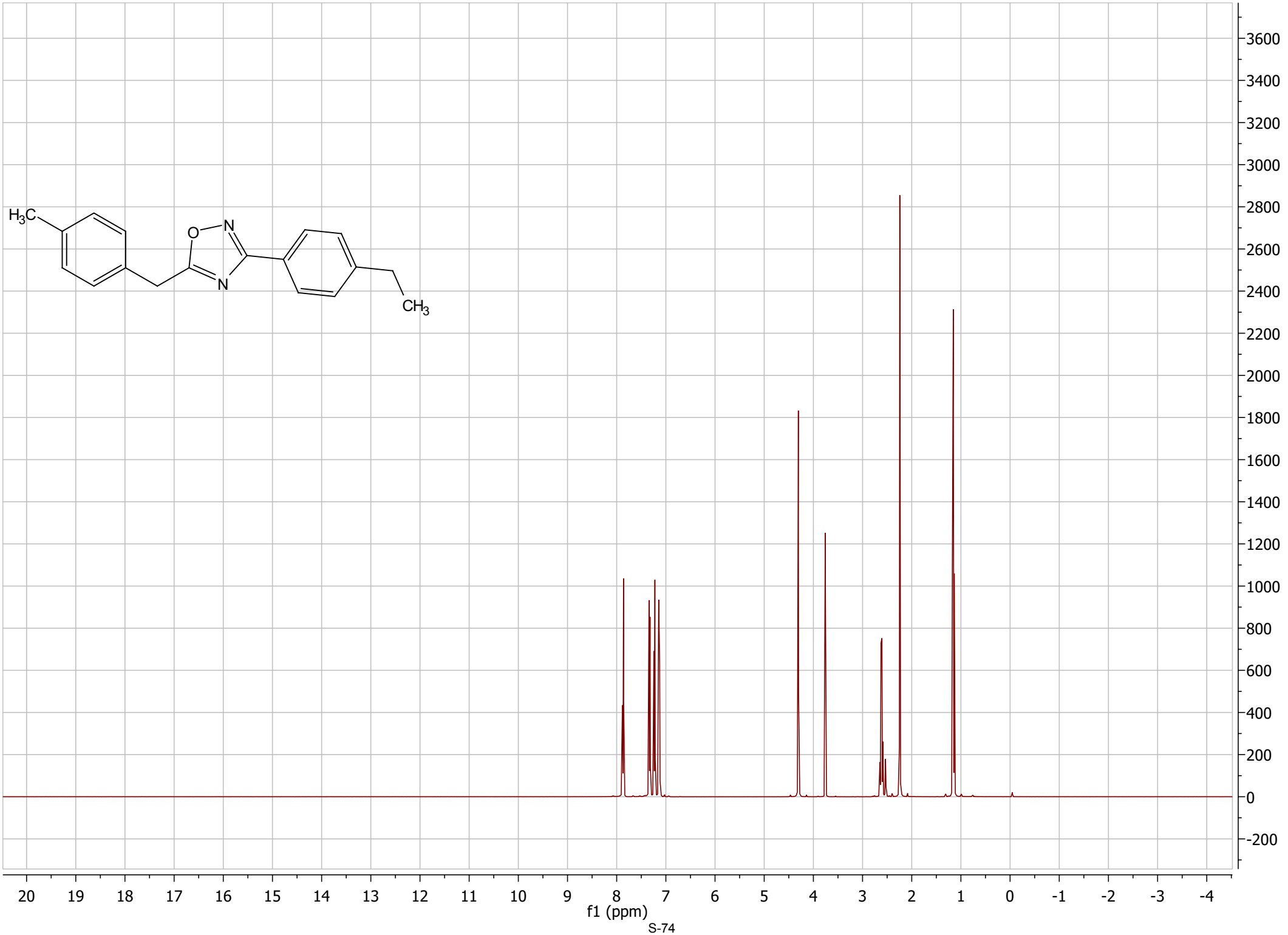

NH
O
O
CH3
CH3
H3C
N
O
N
H3C
H3C
O
CH3
2300
2200
2100
2000
1900
1800
1700
1600
1500
1400
1300
1200
1100
1000
900
800
700
600
500
400
300
200
100
0
-100
-200
230
220
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

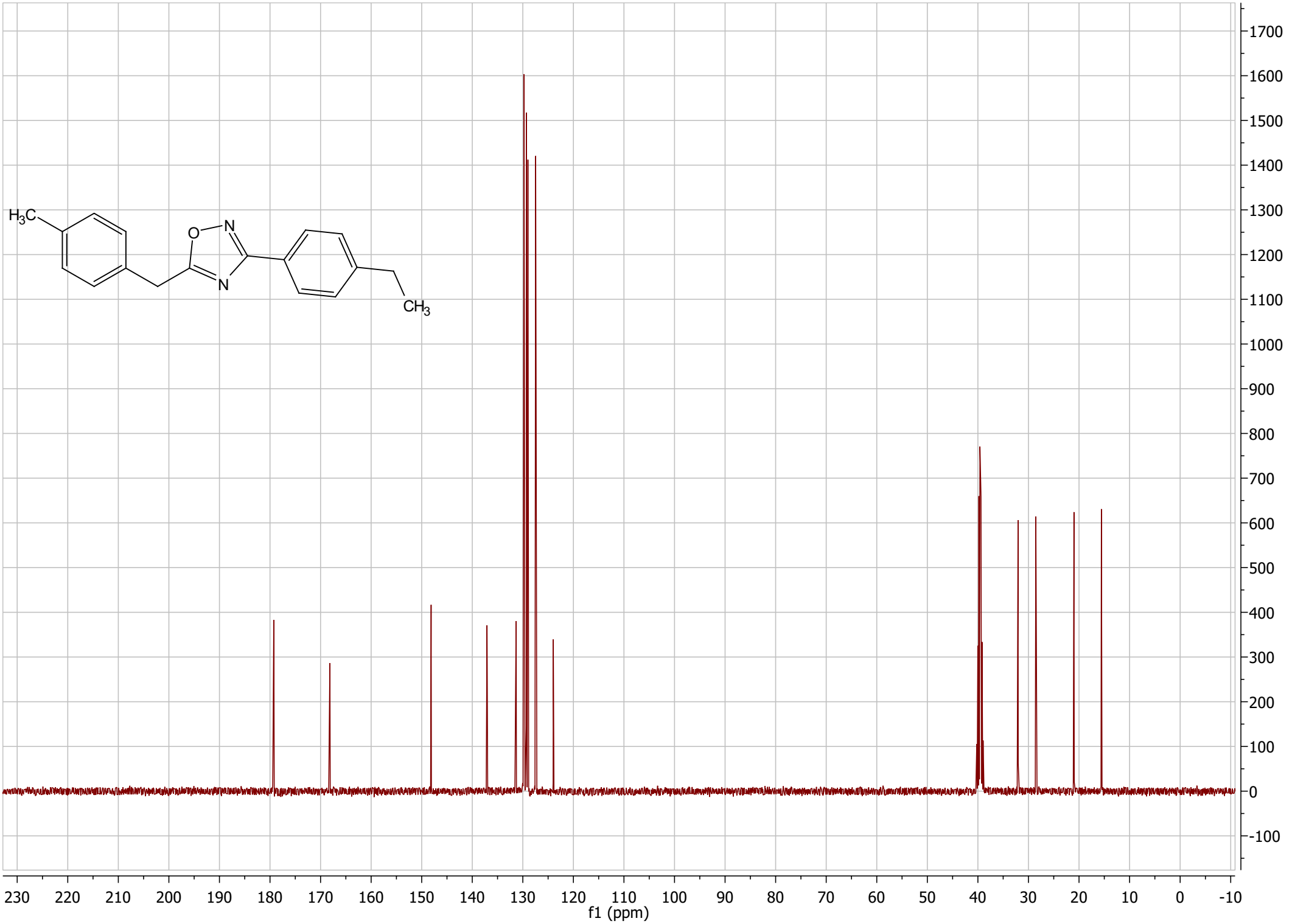

O
N
N
O
F
F
F
H3C
11000
10000
9000
8000
7000
6000
5000
4000
3000
2000
1000
0
-1000
20
19
18
17
16
15
14
13
12
11
10
9
8
7
6
5
4
3
2
1
0
-1
-2
-3
-4
f1 (ppm)


O
N
N
O
F
F
F
H3C
4000
3800
3600
3400
3200
3000
2800
2600
2400
2200
2000
1800
1600
1400
1200
1000
800
600
400
200
0
-200
230
220
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)


N
O
N
N
CH3
7000
6500
6000
5500
5000
4500
4000
3500
3000
2500
2000
1500
1000
500
0
-500
20
19
18
17
16
15
14
13
12
11
10
9
8
7
6
5
4
3
2
1
0
-1
-2
-3
-4
f1 (ppm)


N
O
N
N
CH3
3000
2800
2600
2400
2200
2000
1800
1600
1400
1200
1000
800
600
400
200
0
-200
230
220
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)


H3C
O
N
N
CH3
3600
3400
3200
3000
2800
2600
2400
2200
2000
1800
1600
1400
1200
1000
800
600
400
200
0
-200
20 19 18 17 16 15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1 -2 -3 -4
f1 (ppm)


H3C
O
N
N
CH3
1700
1600
1500
1400
1300
1200
1100
1000
900
800
700
600
500
400
300
200
100
0
-100
230
220
210
200
190
180
170
160
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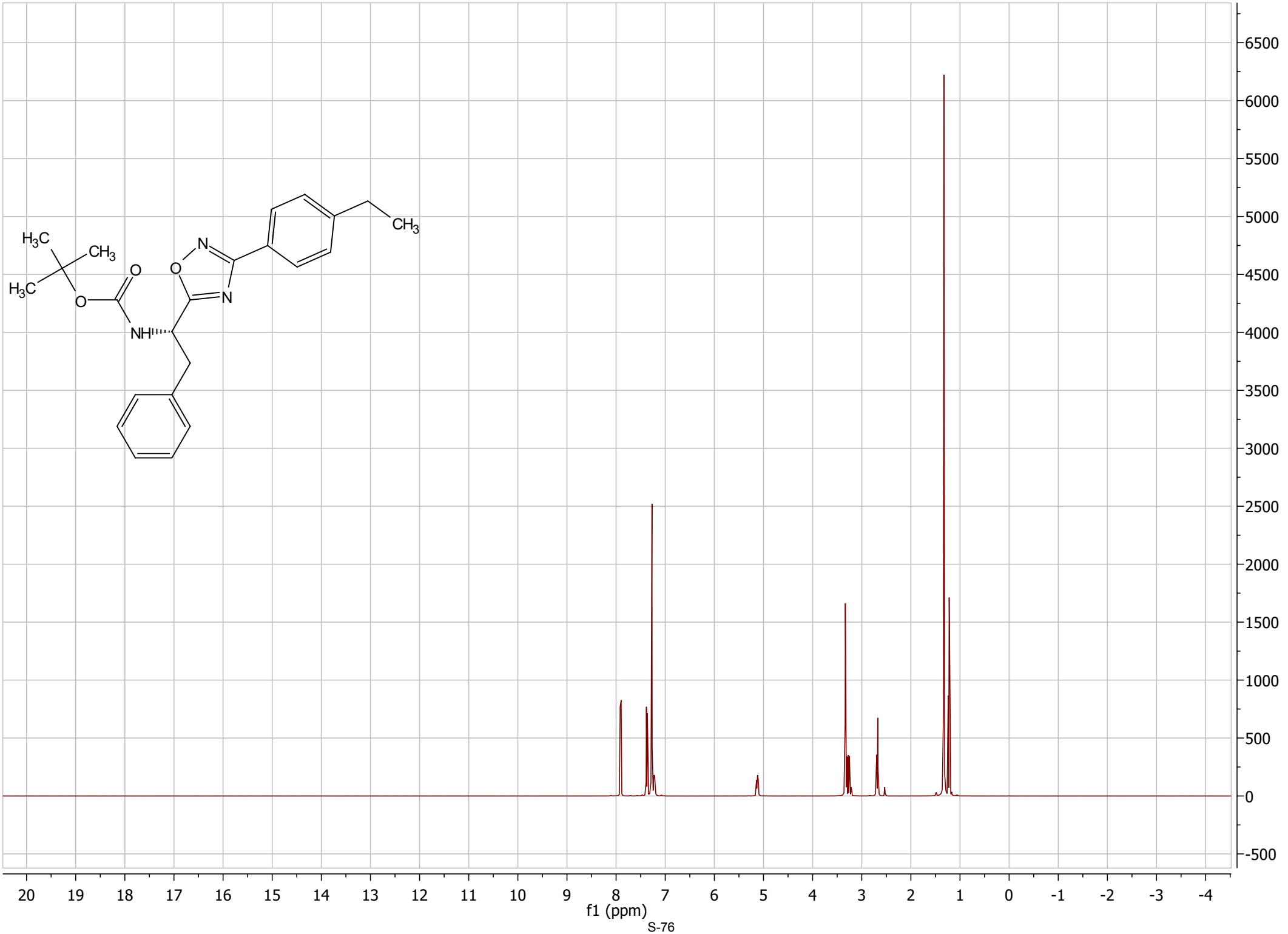
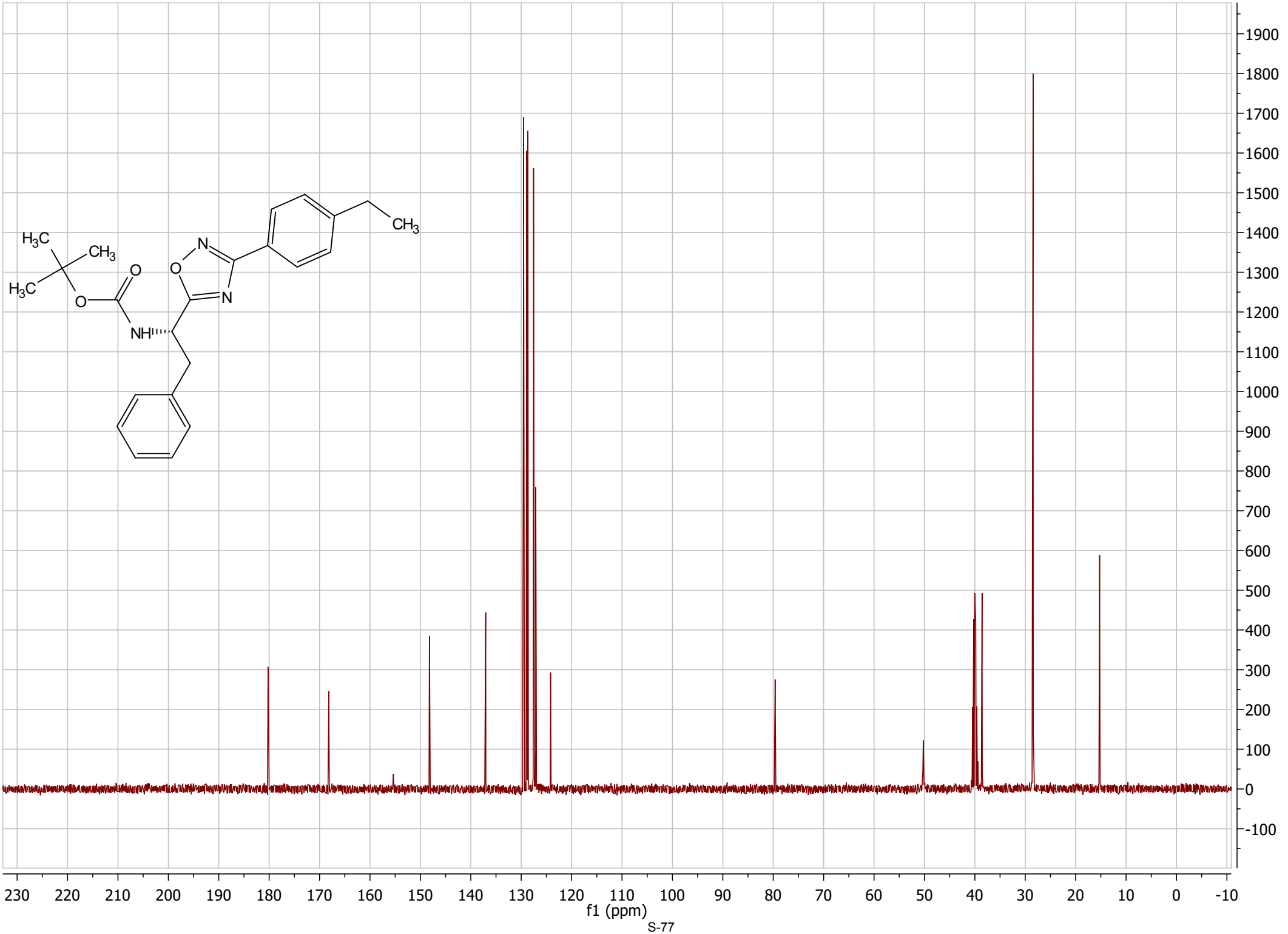
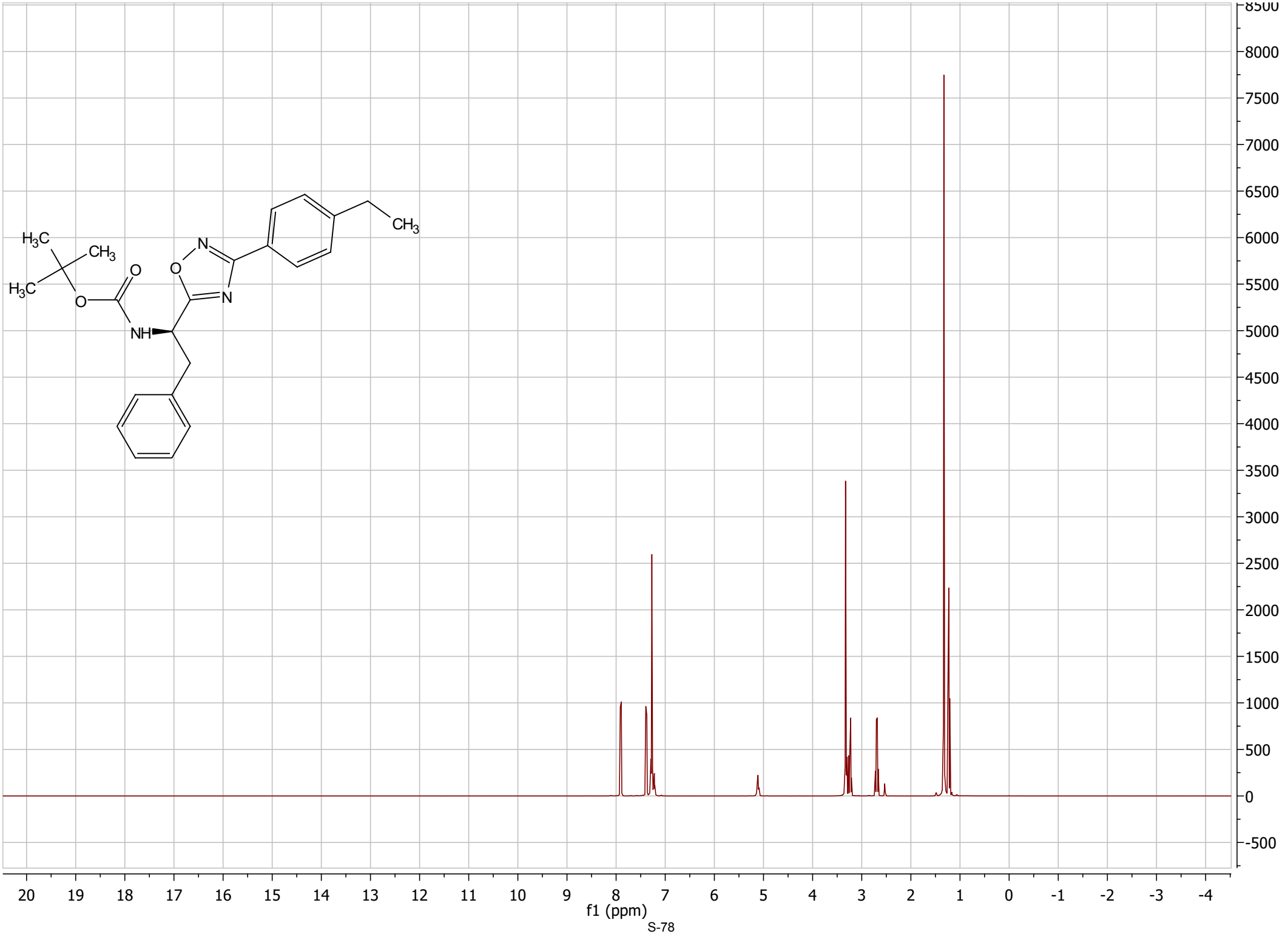
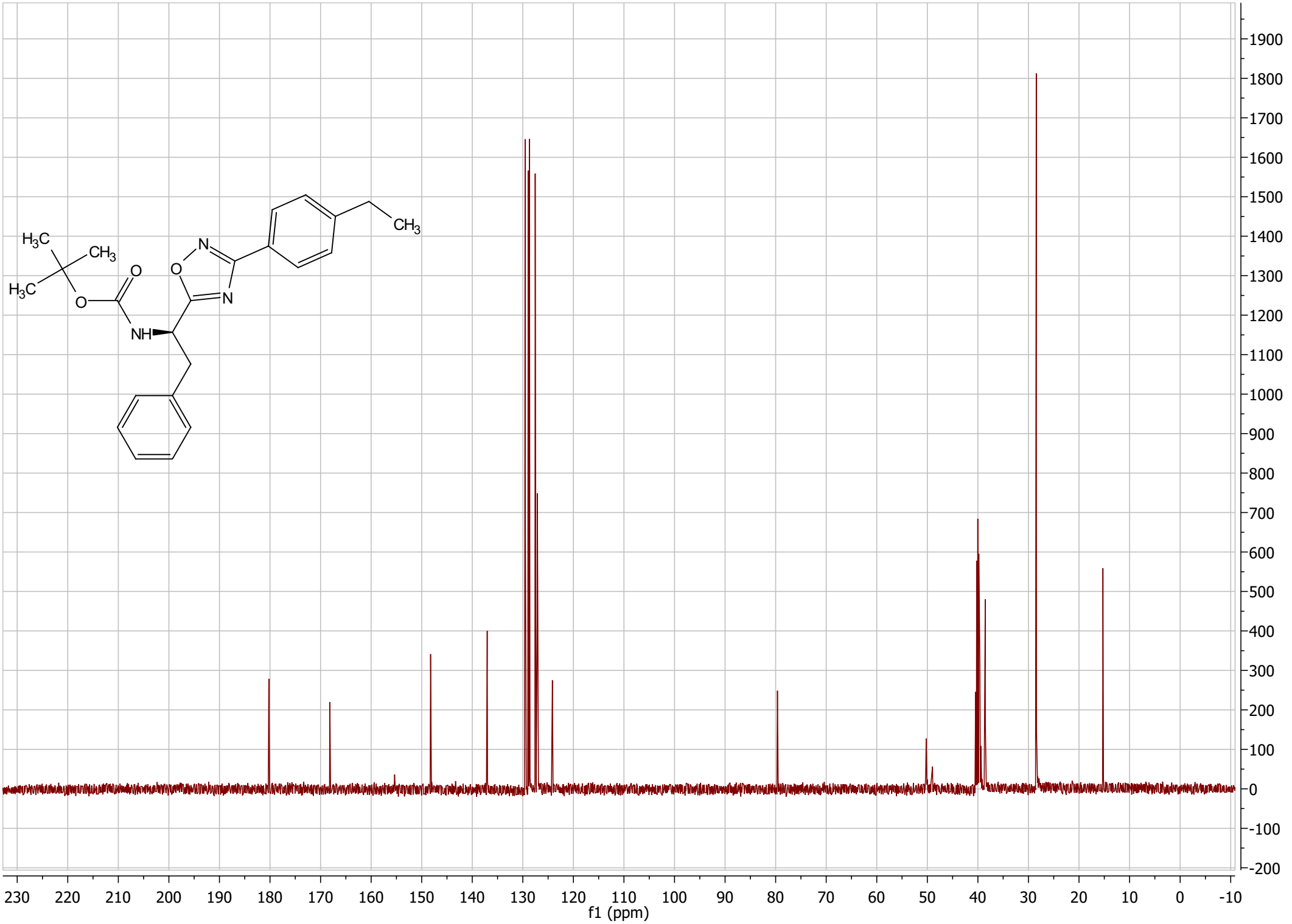
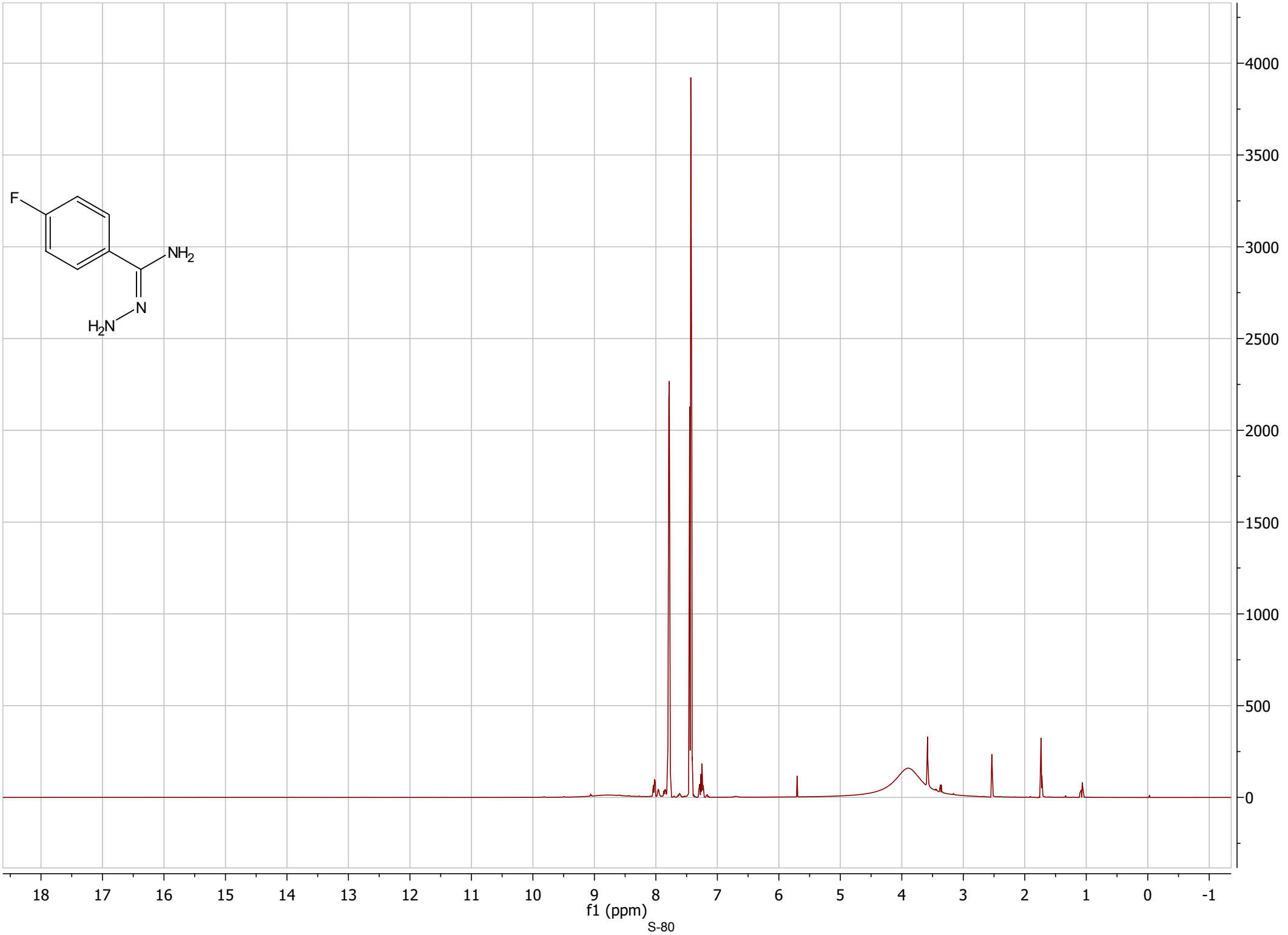
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

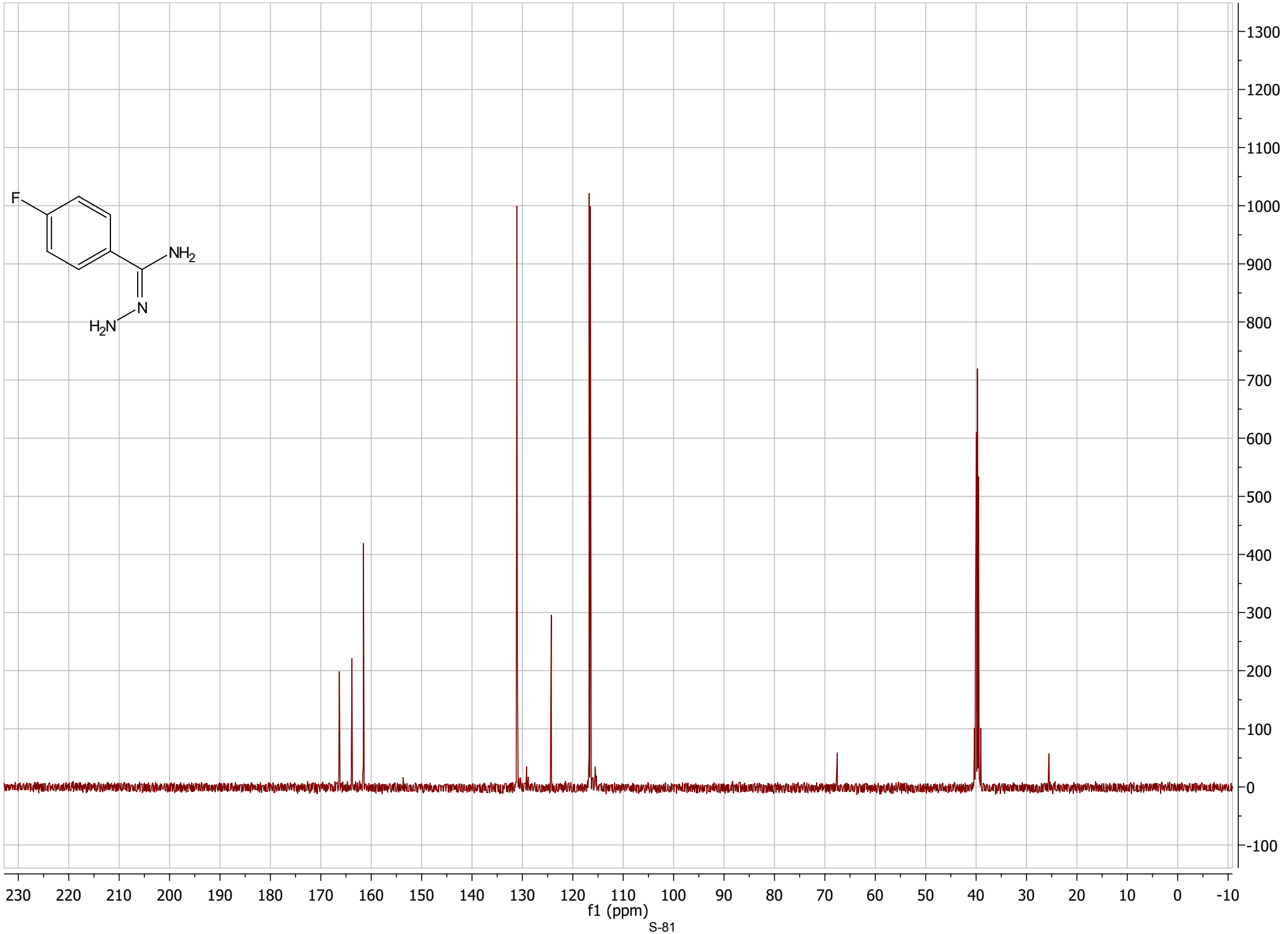

H3C
CH3
H3C
O
O
NH
O
N
N
CH3
6500
6000
5500
5000
4500
4000
3500
3000
2500
2000
1500
1000
500
0
-500
20 19 18 17 16 15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1 -2 -3 -4
f1 (ppm)

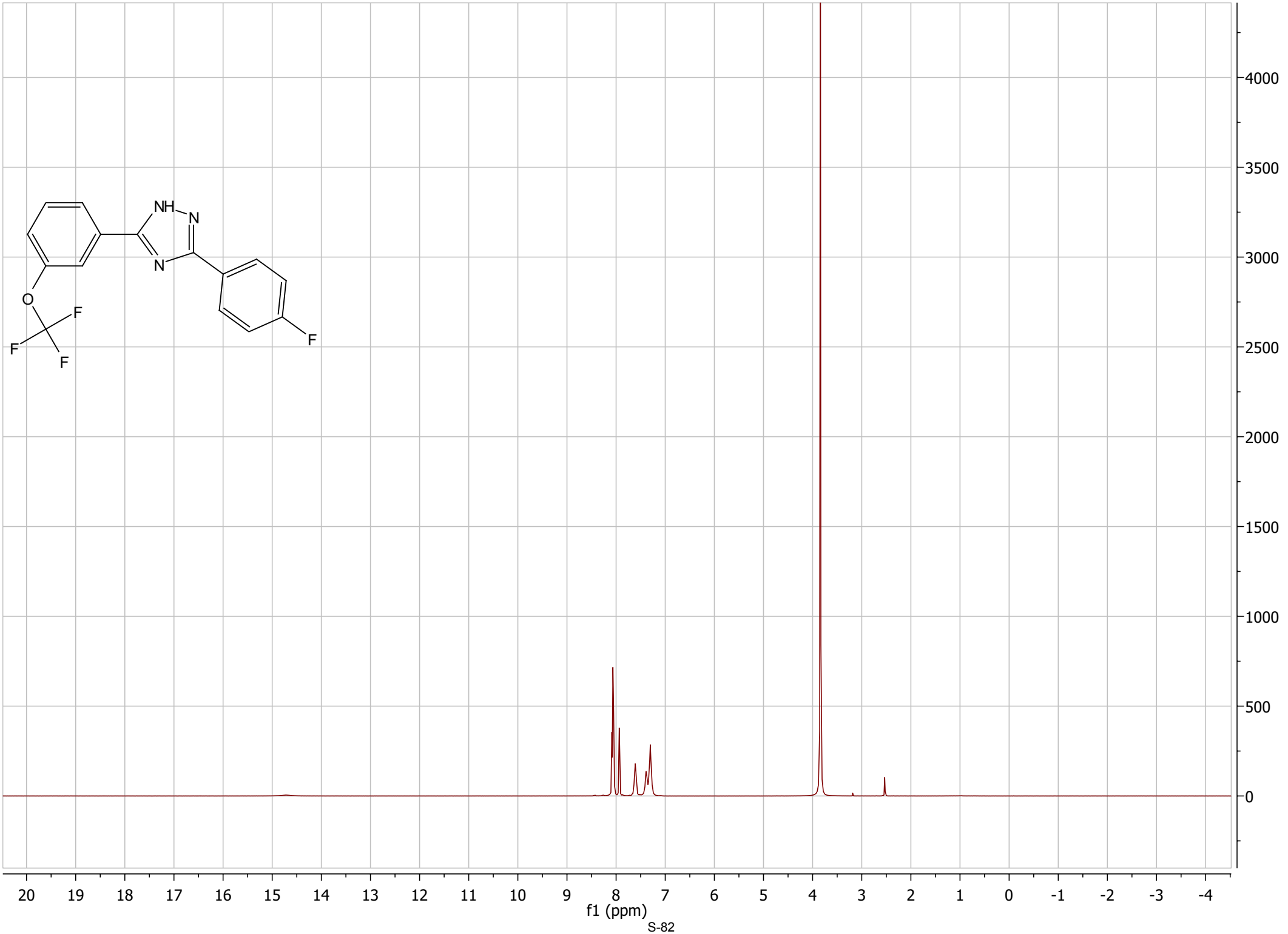

H3C
CH3
H3C
O
O
NH
O
N
N
CH3
1900
1800
1700
1600
1500
1400
1300
1200
1100
1000
900
800
700
600
500
400
300
200
100
0
-100
230
220
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

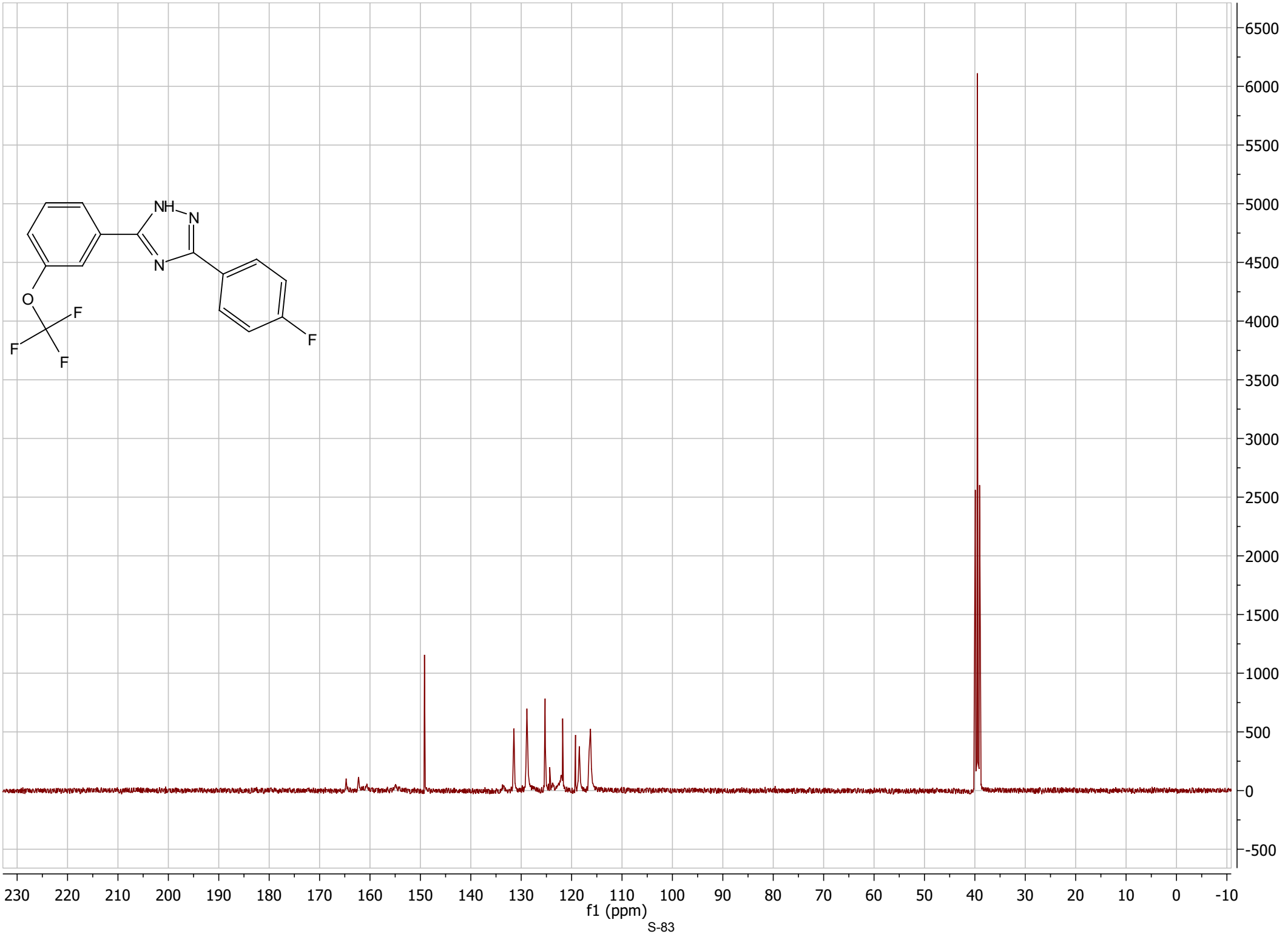

H3C
CH3
H3C
O
O
NH
O
N
N
CH3
8500
8000
7500
7000
6500
6000
5500
5000
4500
4000
3500
3000
2500
2000
1500
1000
500
0
-500
20 19 18 17 16 15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1 -2 -3 -4
f1 (ppm)

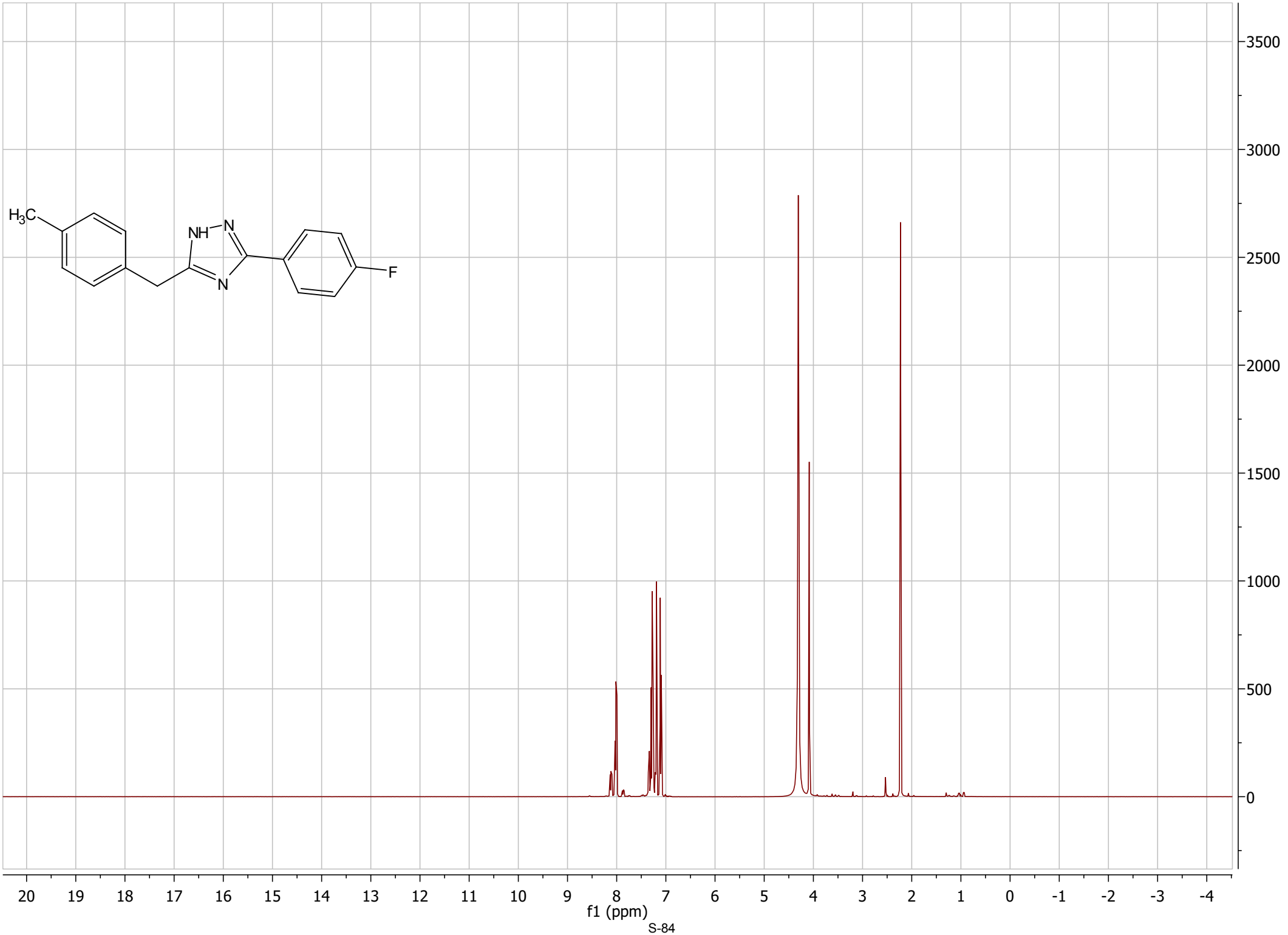

H3C
CH3
H3C
O
O
NH
O
N
N
CH3
1900
1800
1700
1600
1500
1400
1300
1200
1100
1000
900
800
700
600
500
400
300
200
100
0
-100
-200
230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

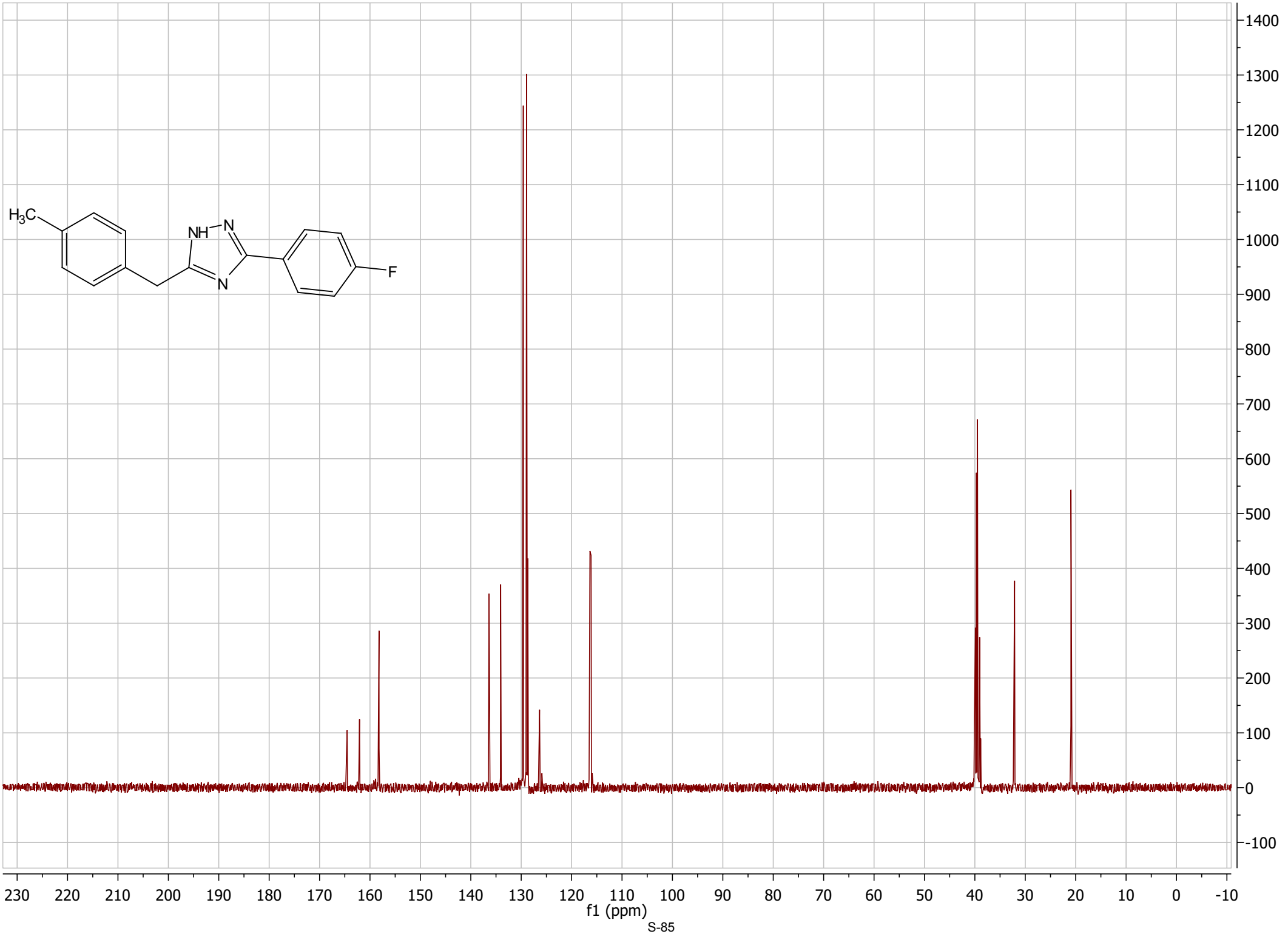

F
NH2
N
H2N
4000
3500
3000
2500
2000
1500
1000
500
0
18
17
16
15
14
13
12
11
10
9
8
7
6
5
4
3
2
1
0
-1
f1 (ppm)

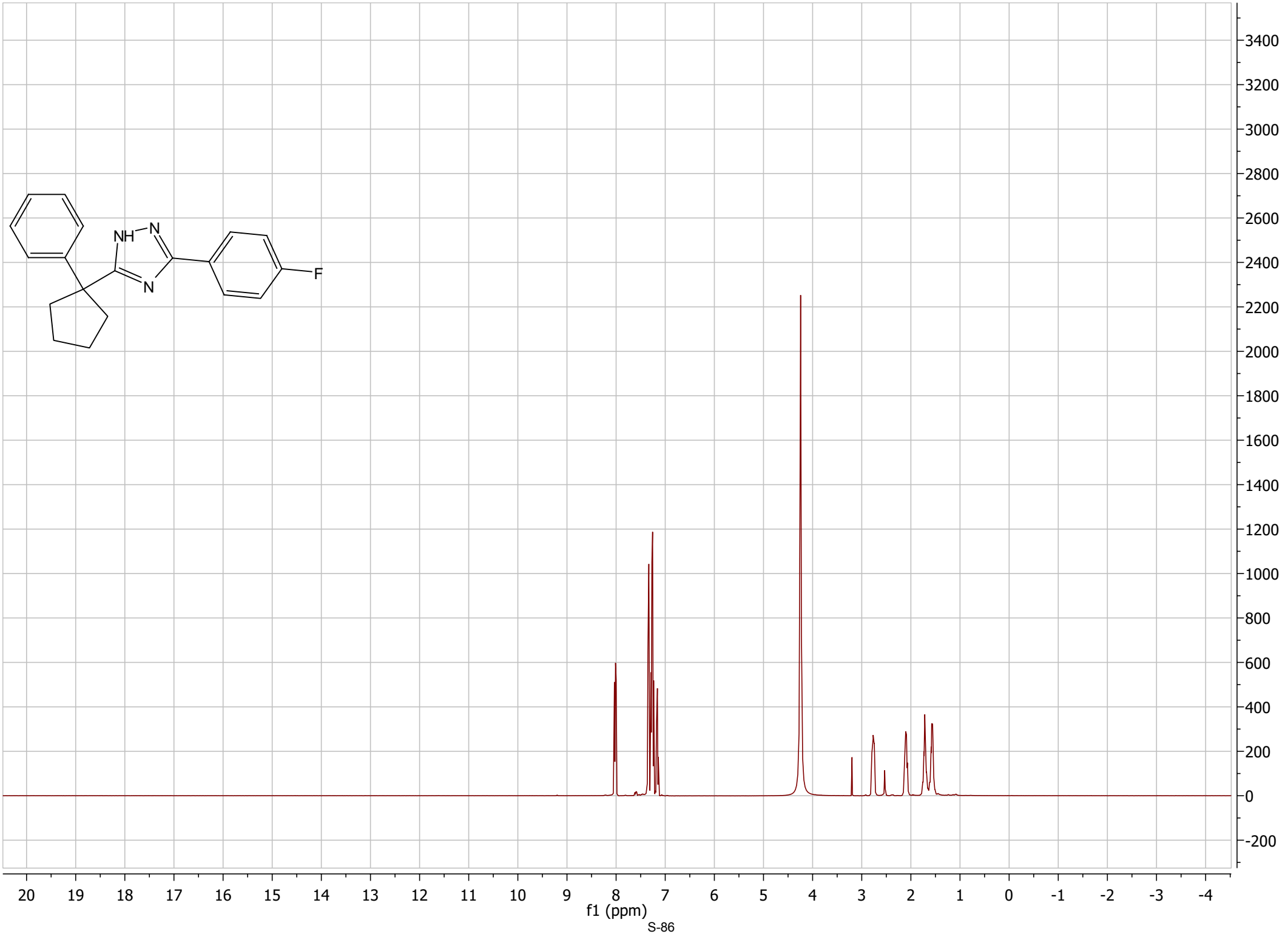

F
NH2
N
H2N
1300
1200
1100
1000
900
800
700
600
500
400
300
200
100
0
-100
230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

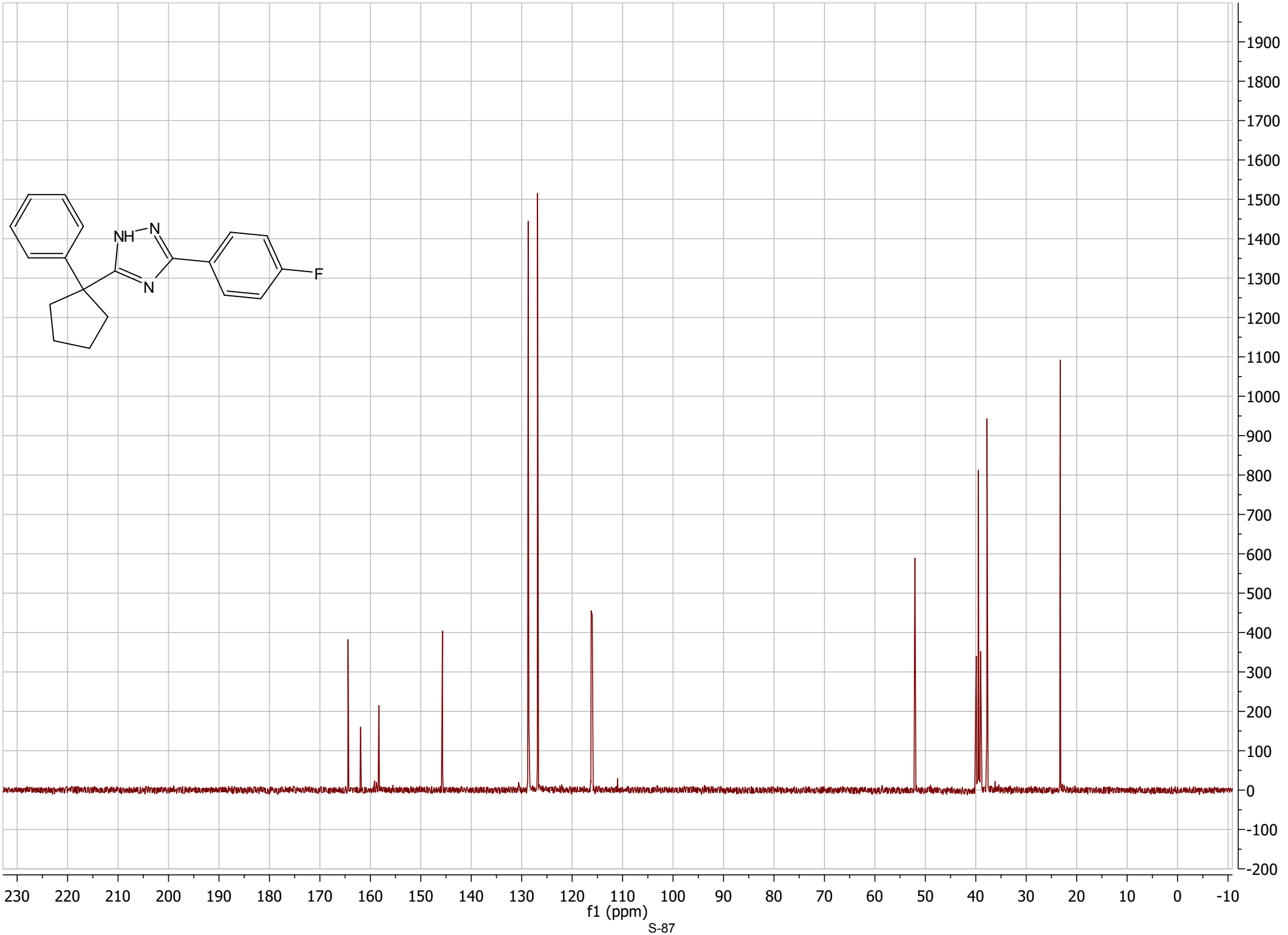

NH
N
N
O
F
F
F
F
4000
3500
3000
2500
2000
1500
1000
500
0
20
19
18
17
16
15
14
13
12
11
10
9
8
7
6
5
4
3
2
1
0
-1
-2
-3
-4
f1 (ppm)

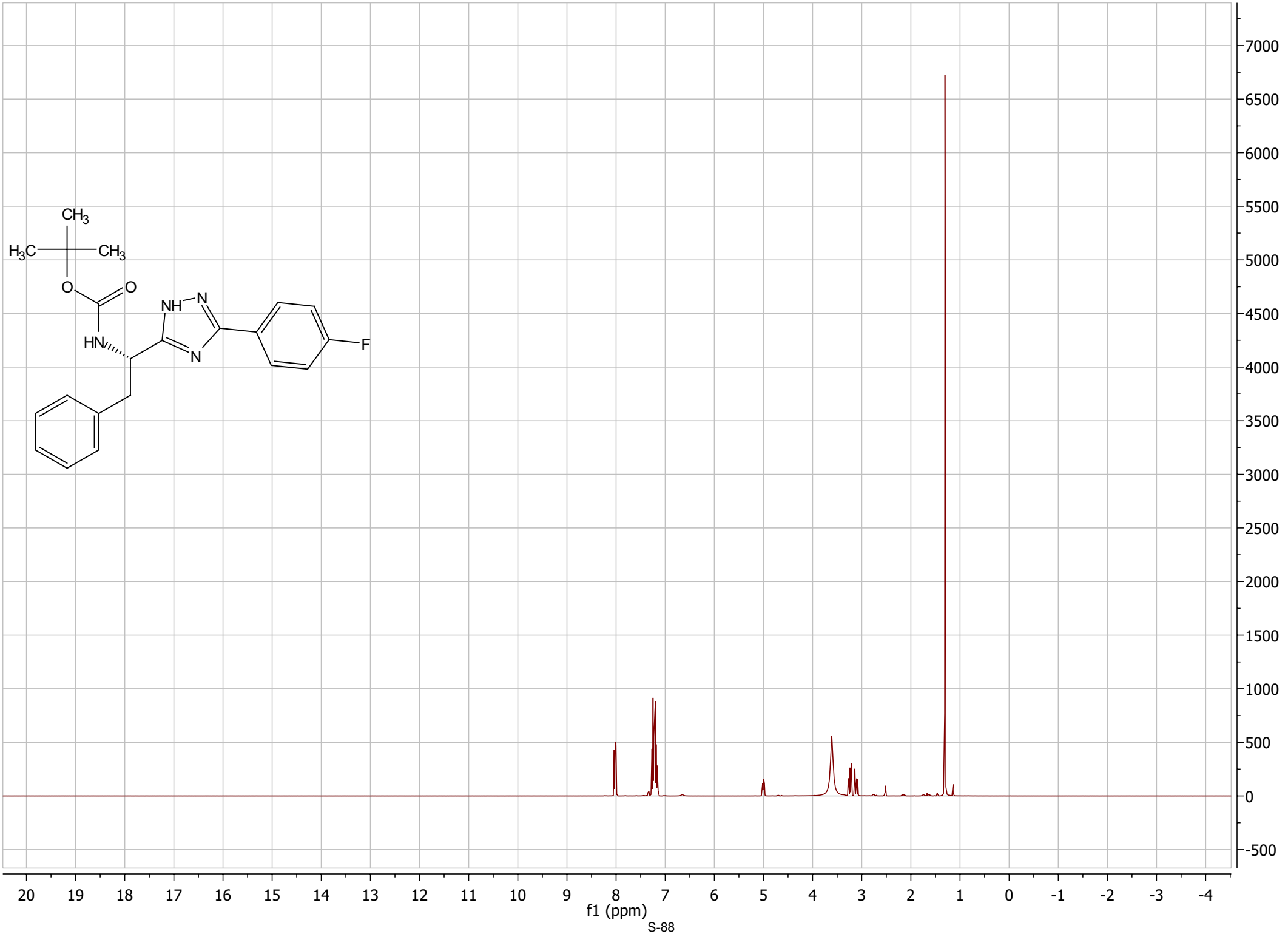

NH
N
N
O
F
F
F
F
6500
6000
5500
5000
4500
4000
3500
3000
2500
2000
1500
1000
500
0
-500
230
220
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

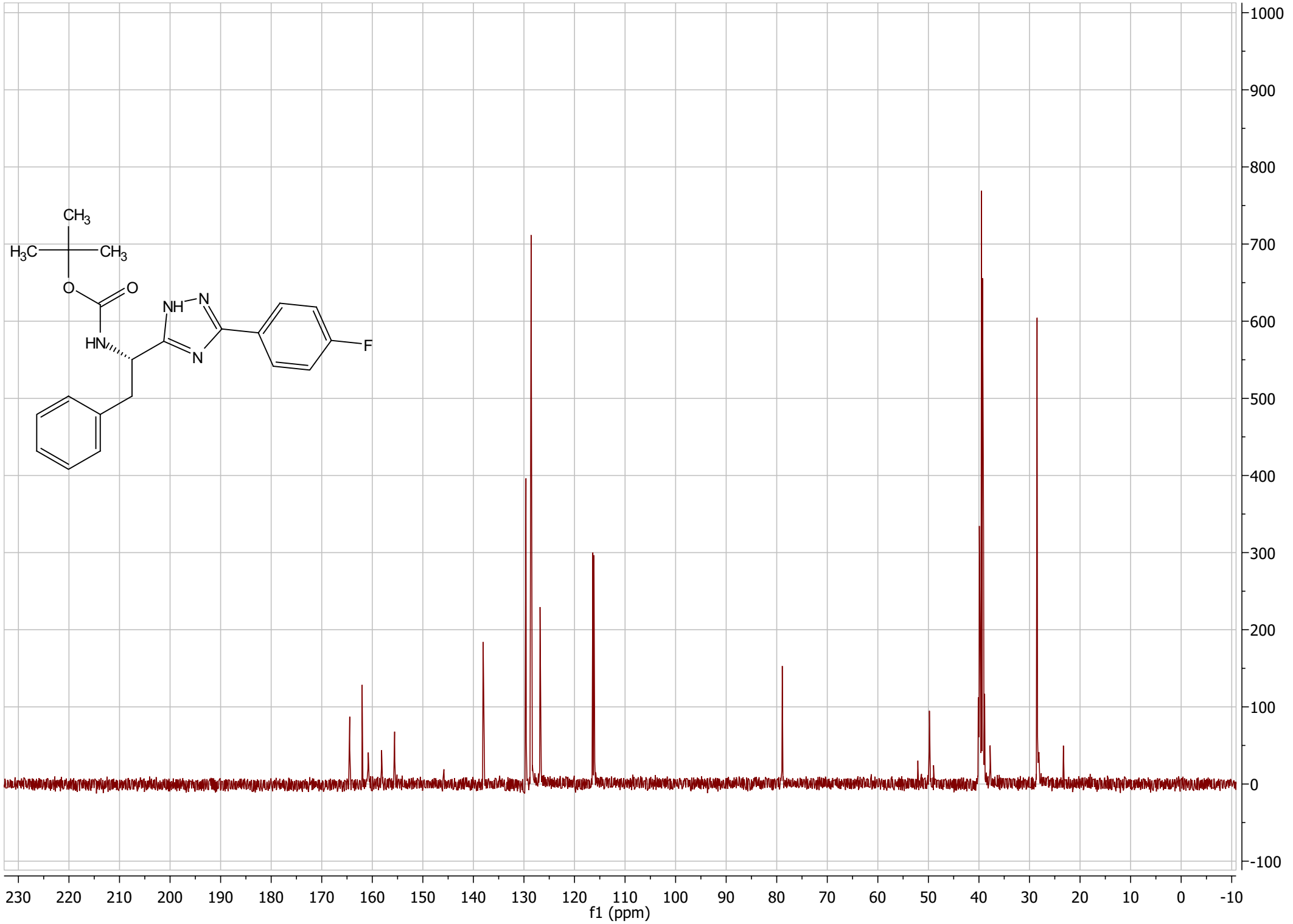

H3C
NH
N
N
F
3500
3000
2500
2000
1500
1000
500
0
20 19 18 17 16 15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1 -2 -3 -4
f1 (ppm)

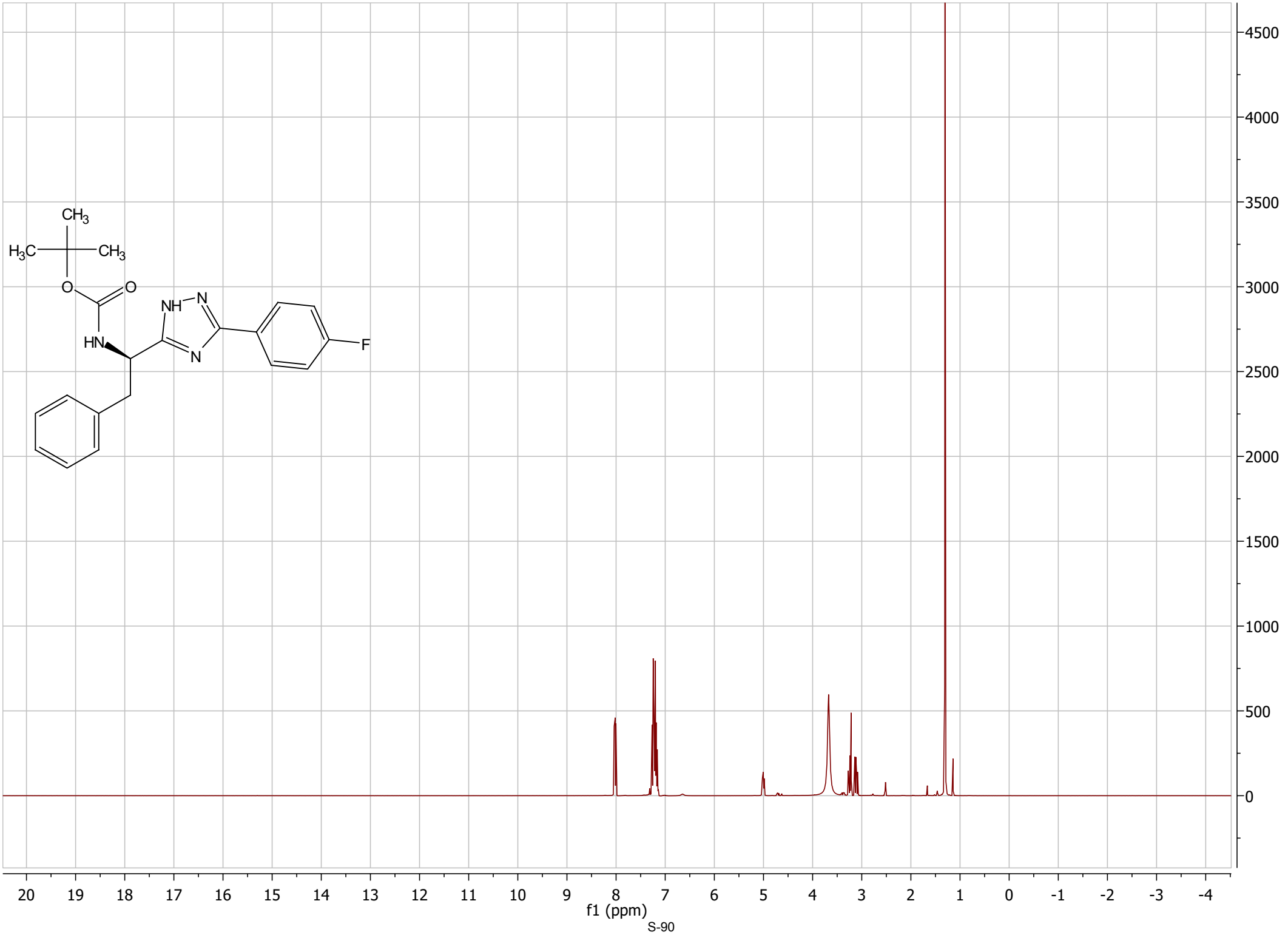

H3C
NH
N
N
F
1400
1300
1200
1100
1000
900
800
700
600
500
400
300
200
100
0
-100
230
220
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

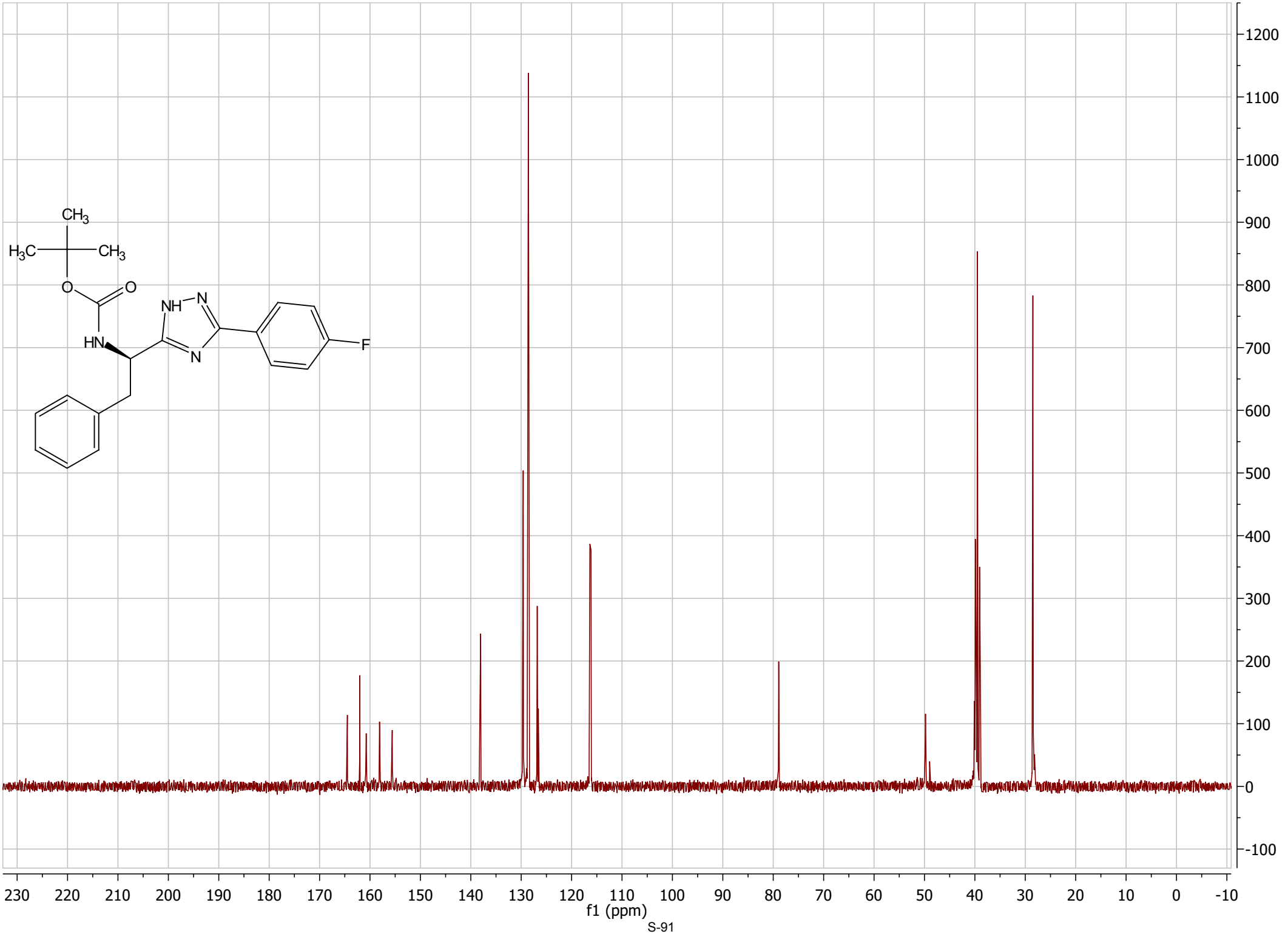

NH
N
N
F
3400
3200
3000
2800
2600
2400
2200
2000
1800
1600
1400
1200
1000
800
600
400
200
0
-200
20
19
18
17
16
15
14
13
12
11
10
9
8
7
6
5
4
3
2
1
0
-1
-2
-3
-4
f1 (ppm)


NH
N
N
F
1900
1800
1700
1600
1500
1400
1300
1200
1100
1000
900
800
700
600
500
400
300
200
100
0
-100
-200
230
220
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)


CH3
H3C
CH3
O
O
HN
NH
N
N
F
7000
6500
6000
5500
5000
4500
4000
3500
3000
2500
2000
1500
1000
500
0
-500
20 19 18 17 16 15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1 -2 -3 -4
f1 (ppm)


CH3
H3C
CH3
O
O
HN
NH
N
N
F
1000
900
800
700
600
500
400
300
200
100
0
-100
230
220
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)


CH3
H3C
CH3
O
O
HN
NH
N
N
F
4500
4000
3500
3000
2500
2000
1500
1000
500
0
20 19 18 17 16 15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1 -2 -3 -4
f1 (ppm)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H3C
CH3
O
O
HN
NH
N
N
F
1200
1100
1000
900
800
700
600
500
400
300
200
100
0
-100
230
220
210
200
190
180
170
160
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140
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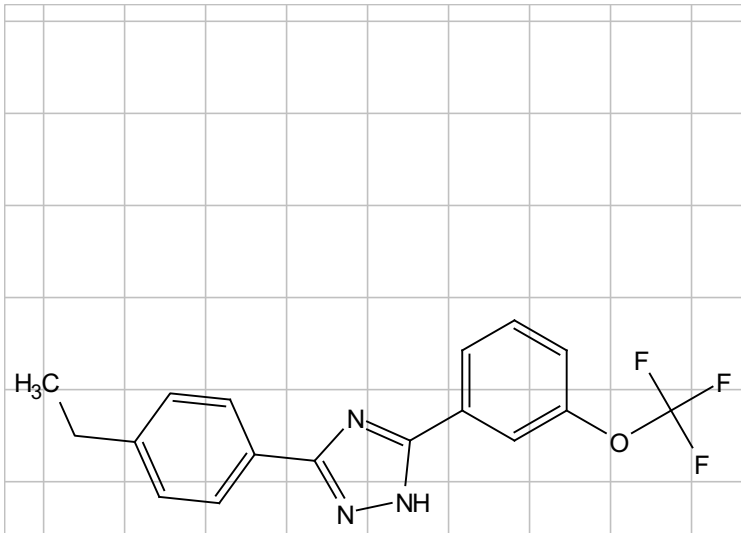
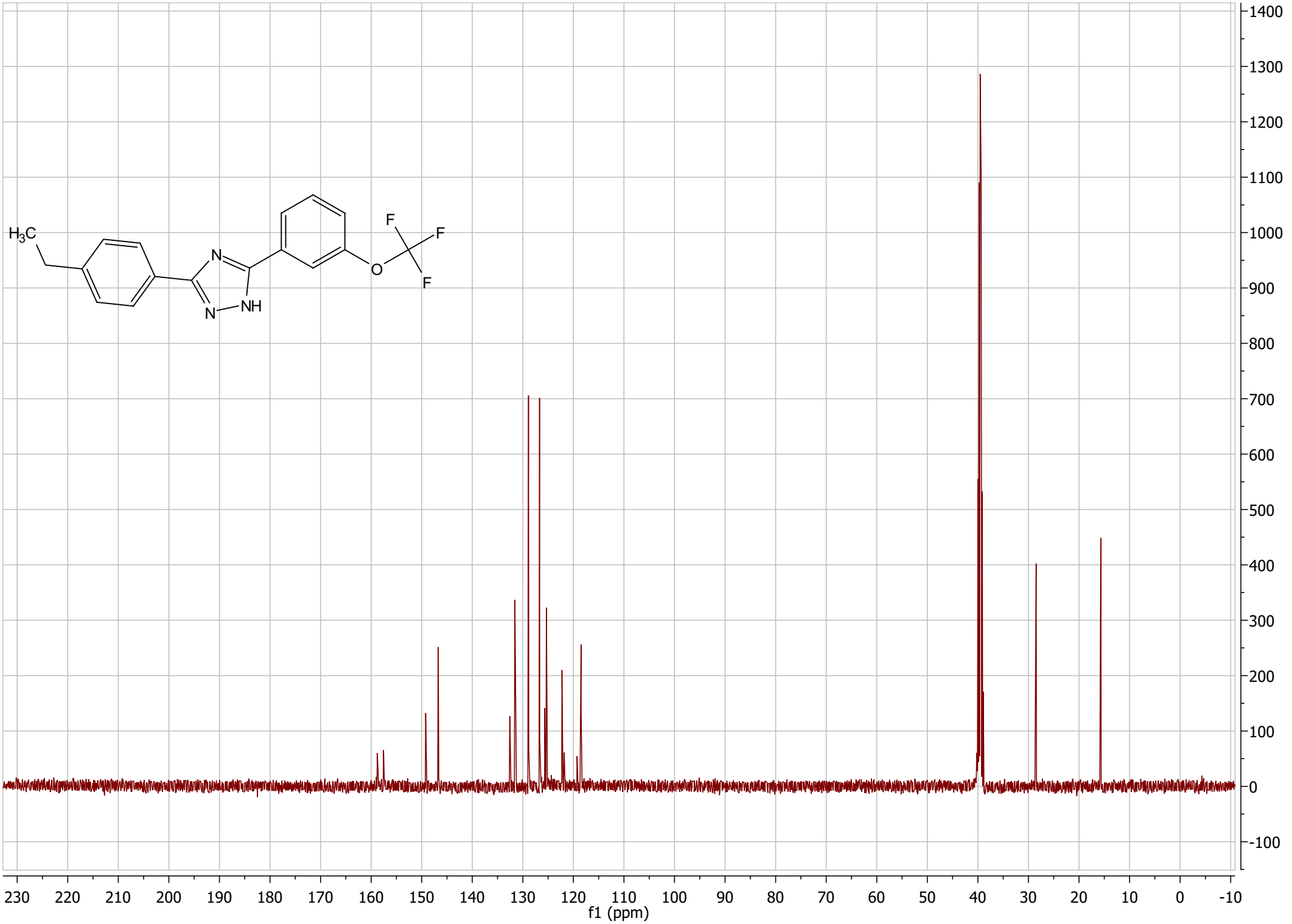
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)


H3C
N
NH
N
O
F
F
F

1400
1300
1200
1100
1000
900
800
700
600
500
400
300
200
100
0
-100
20
19
18
17
16
15
14
13
12
11
10
9
8
7
6
5
4
3
2
1
0
-1
-2
-3
-4
f1 (ppm)


H3C
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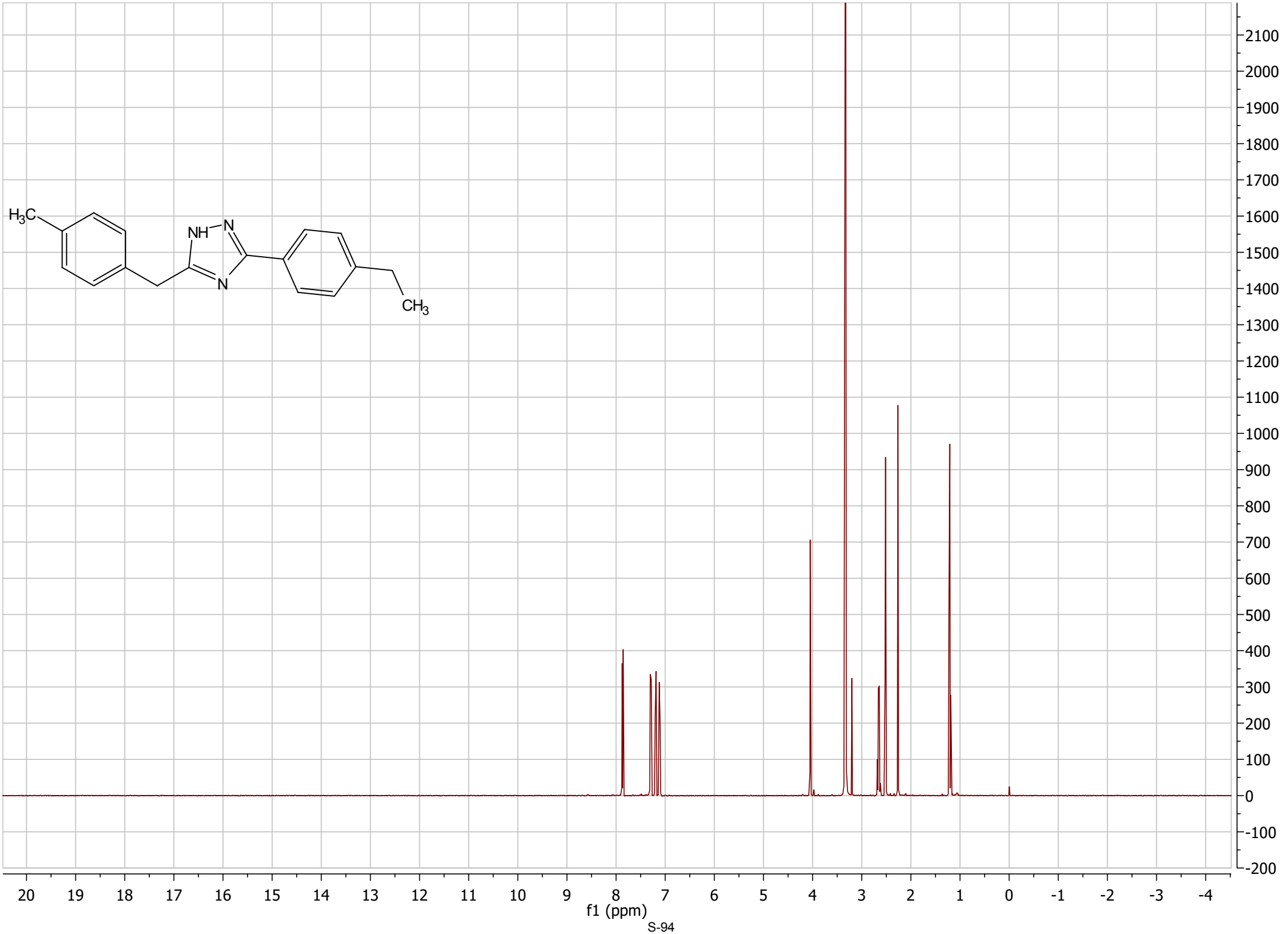
N
NH
O
F
F
F
1400
1300
1200
1100
1000
900
800
700
600
500
400
300
200
100
0
-100
230
220
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)


H3C
NH
N
N
CH3
2100
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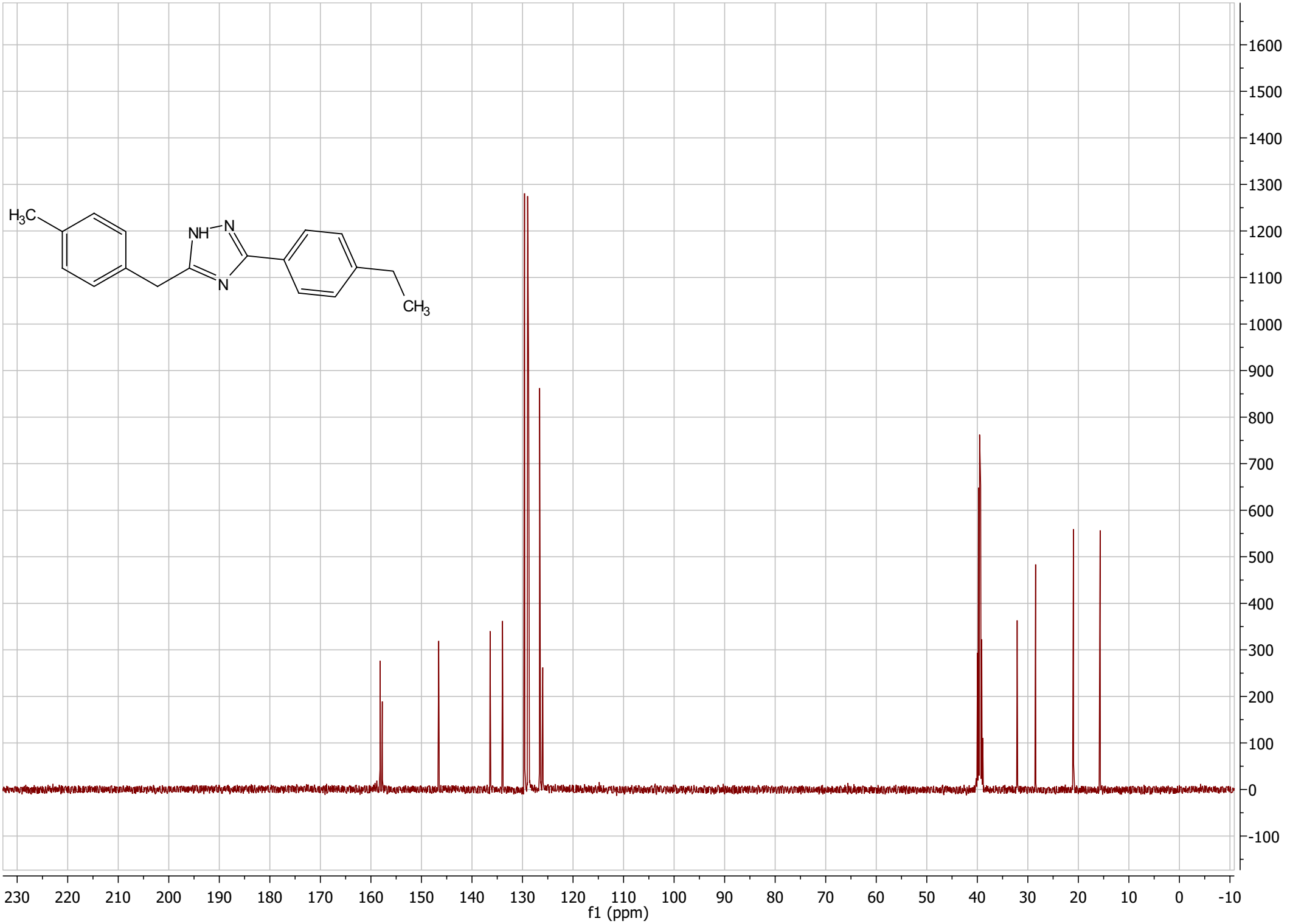
1900
1800
1700
1600
1500
1400
1300
1200
1100
1000
900
800
700
600
500
400
300
200
100
0
-100
-200
20 19 18 17 16 15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1 -2 -3 -4
f1 (ppm)


H3C
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N
N
CH3
1600
1500
1400
1300
1200
1100
1000
900
800
700
600
500
400
300
200
100
0
-100
230
220
210
200
190
180
170
160
150
140
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120
110
100
90
80
70
60
50
40
30
20
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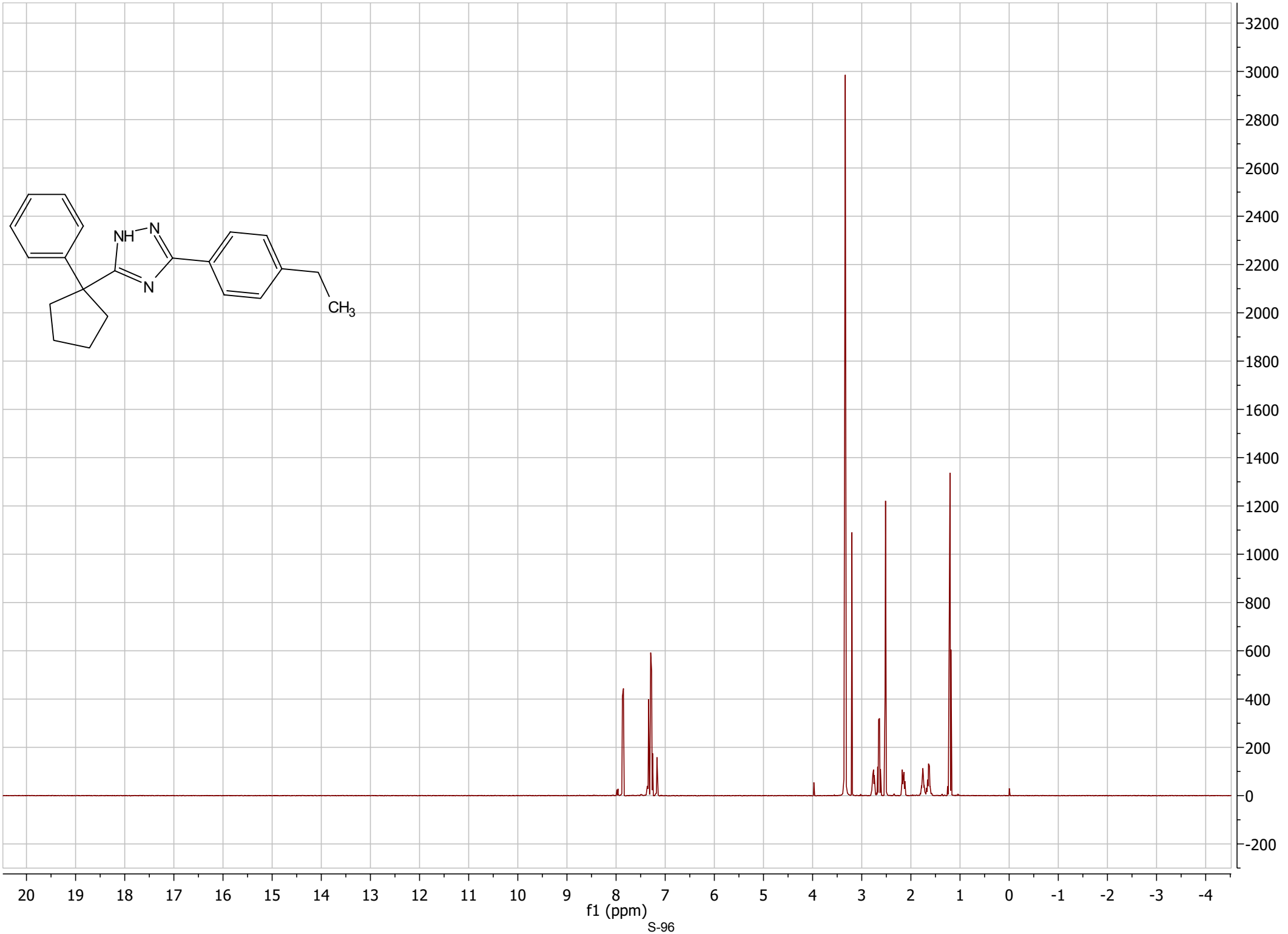
0
-10
f1 (ppm)


NH
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CH3
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2600
2400
2200
2000
1800
1600
1400
1200
1000
800
600
400
200
0
-200
20
19
18
17
16
15
14
13
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10
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7
6
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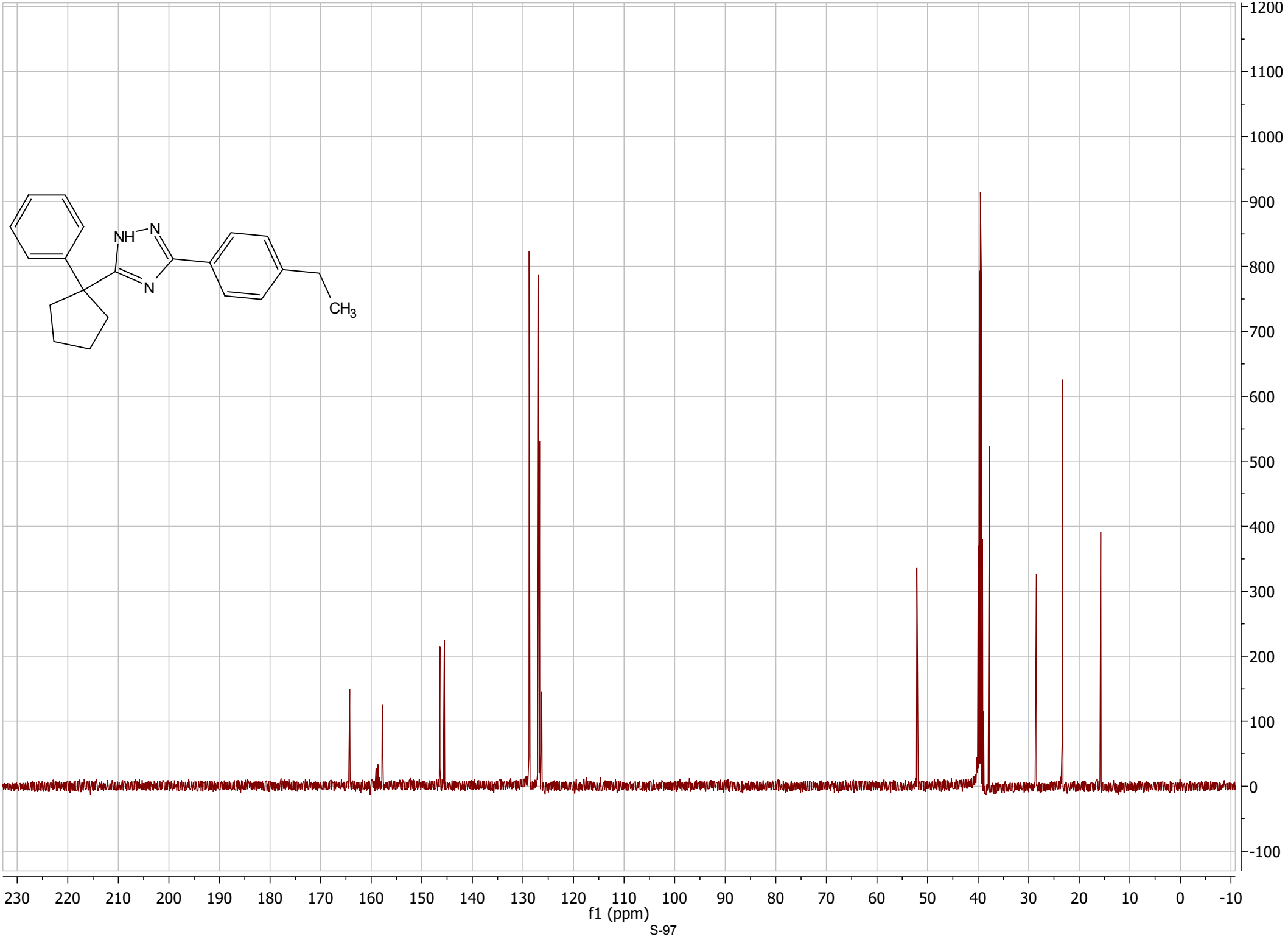
4
3
2
1
0
-1
-2
-3
-4
f1 (ppm)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CH3
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1100
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800
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500
400
300
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100
0
-100
230
220
210
200
190
180
170
160
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140
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120
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100
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80
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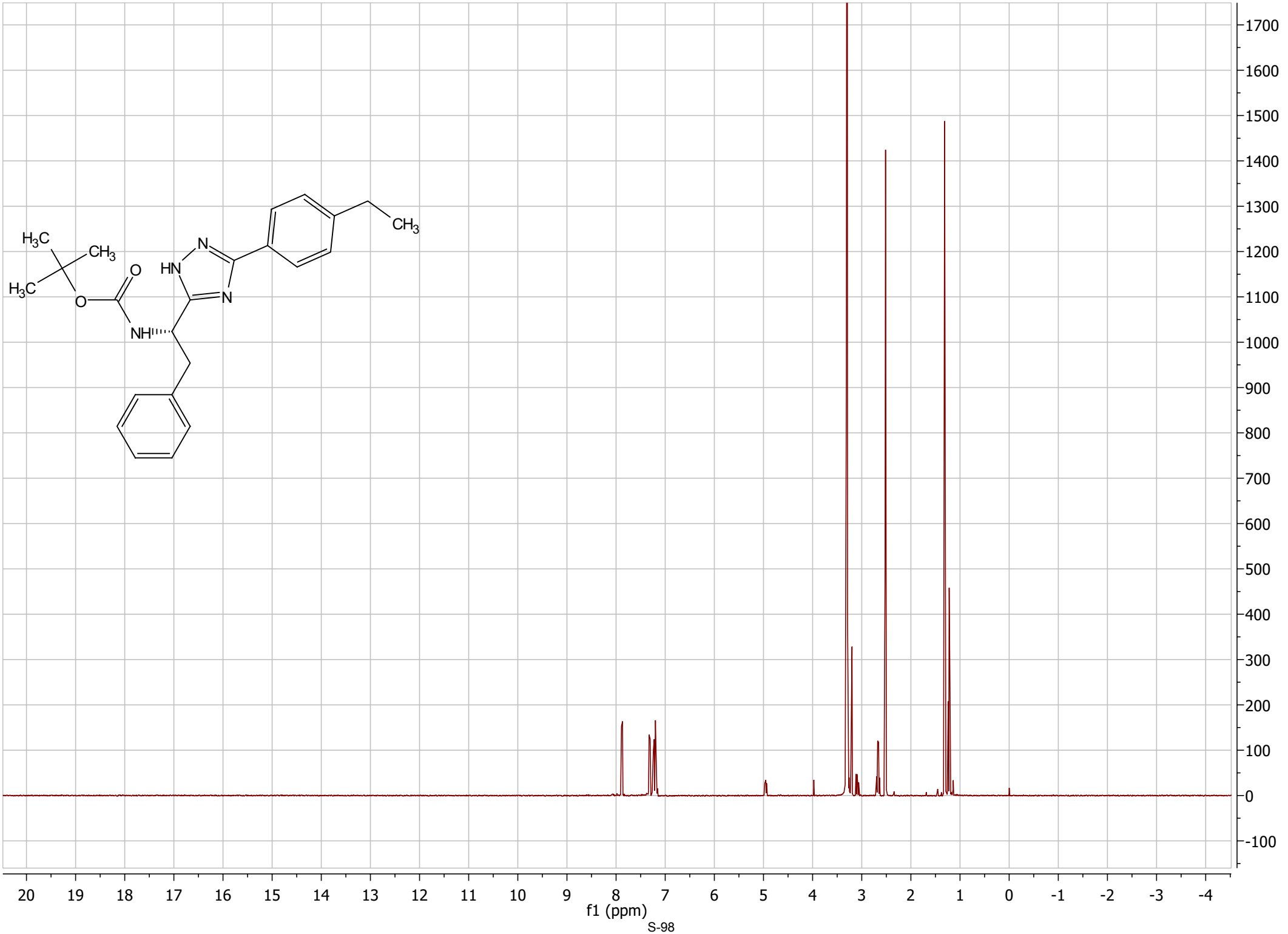
60
50
40
30
20
10
0
-10
f1 (ppm)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CH3
H3C
O
O
NH
HN
N
N
CH3
1700
1600
1500
1400
1300
1200
1100
1000
900
800
700
600
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400
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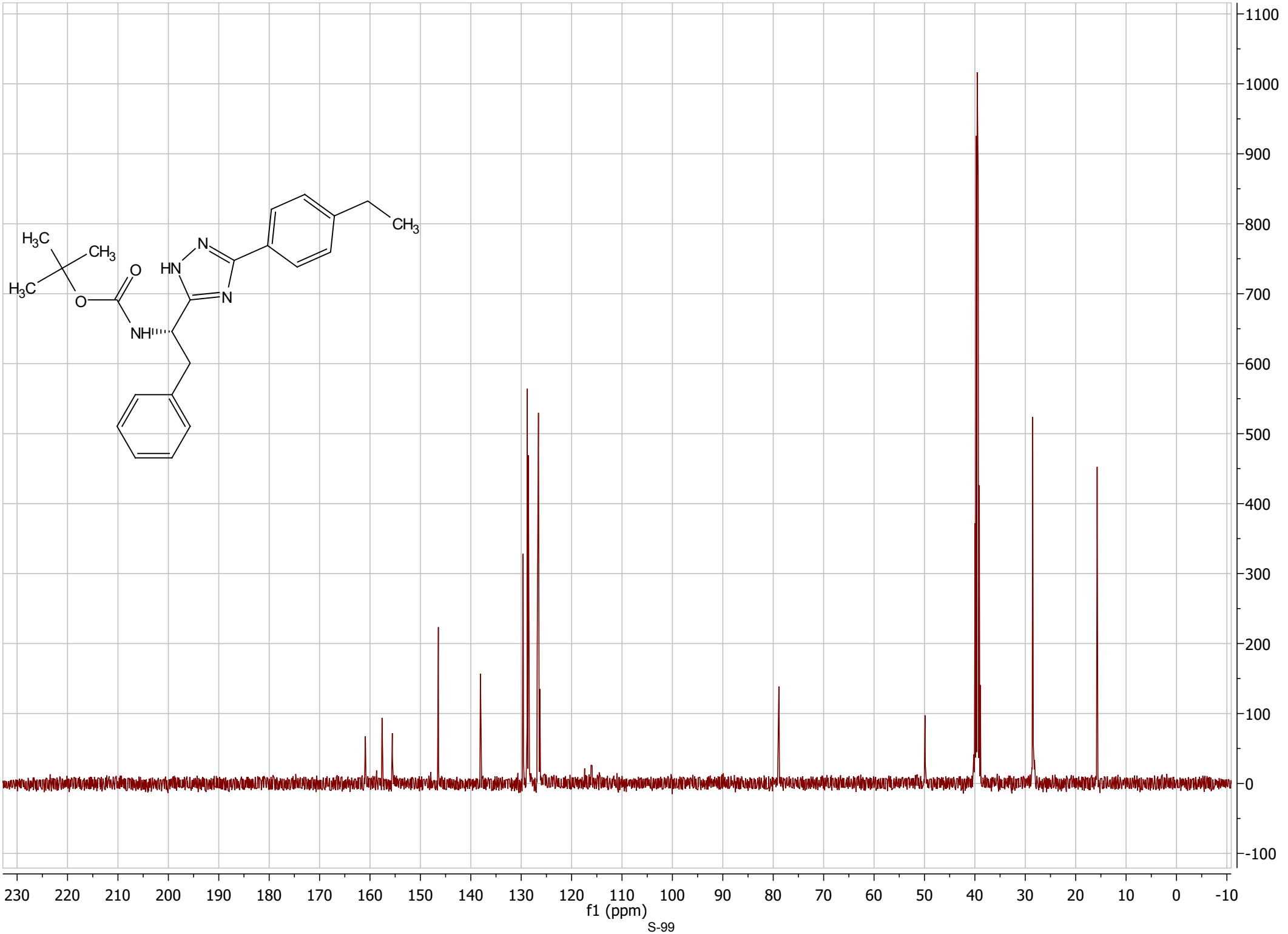
200
100
0
-100
20 19 18 17 16 15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1 -2 -3 -4
f1 (ppm)


H3C
CH3
H3C
O
O
NH
HN
N
N
CH3
1100
1000
900
800
700
600
500
400
300
200
100
0
-100
230
220
210
200
190
180
170
160
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140
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120
110
100
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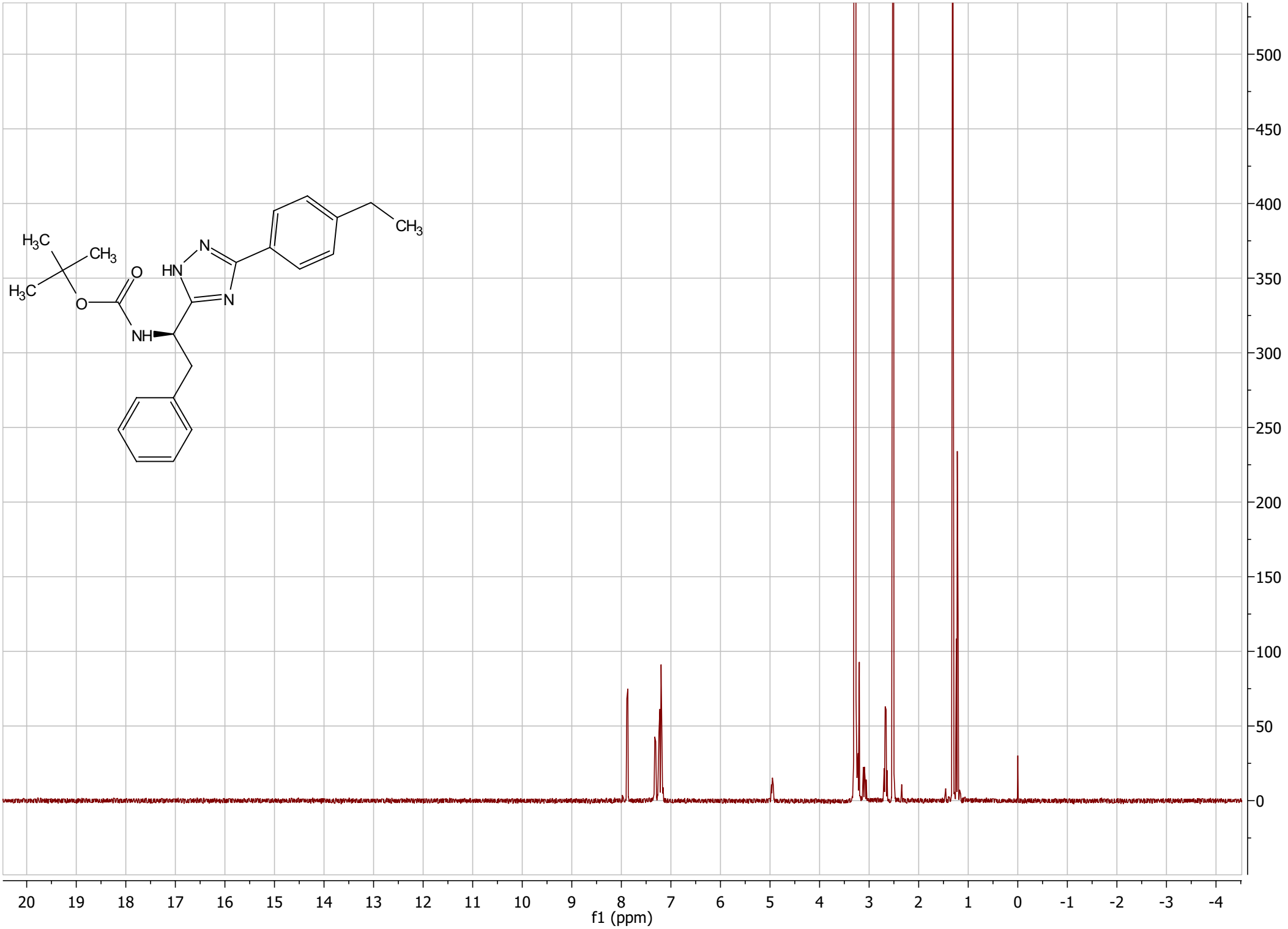
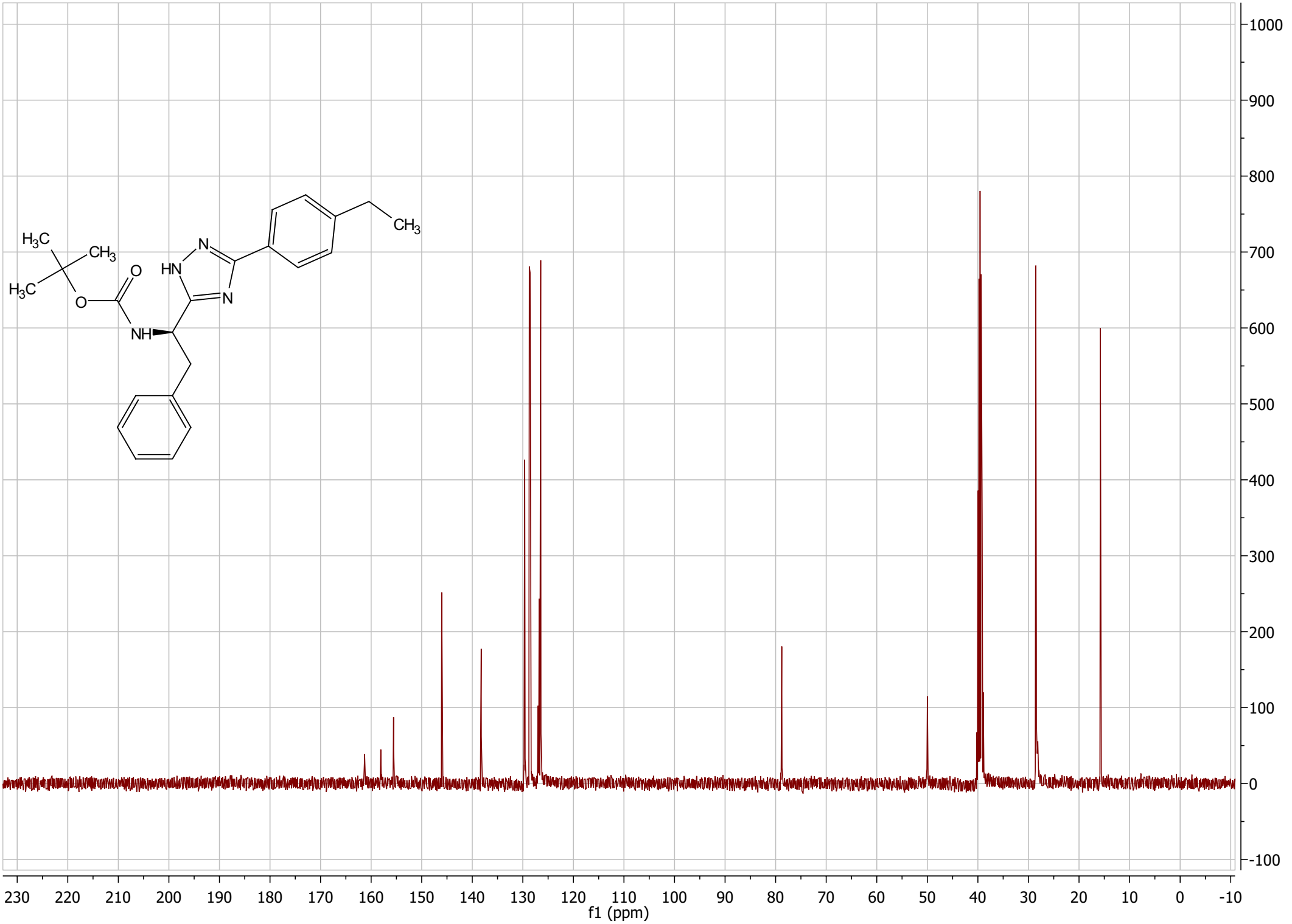
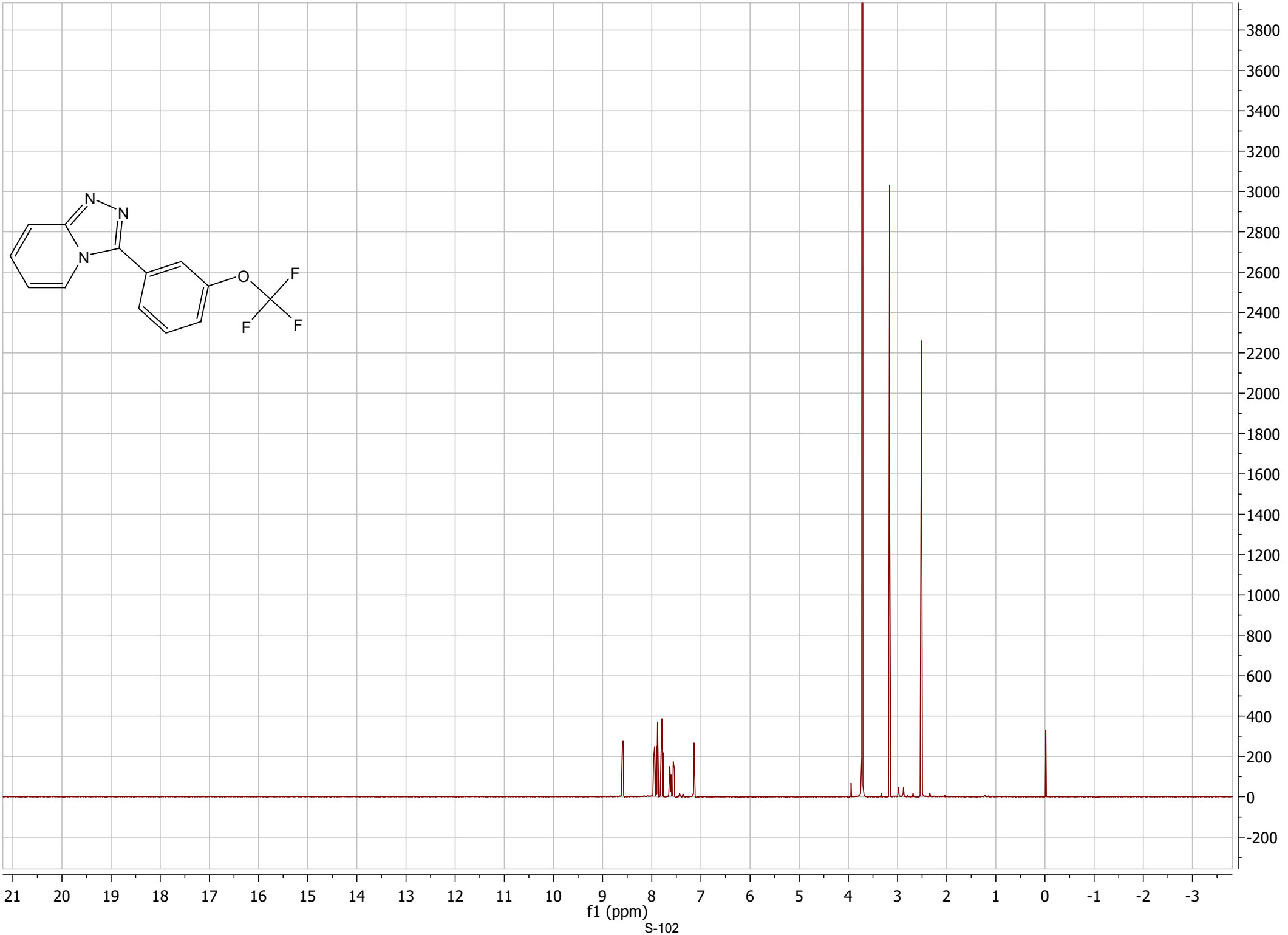
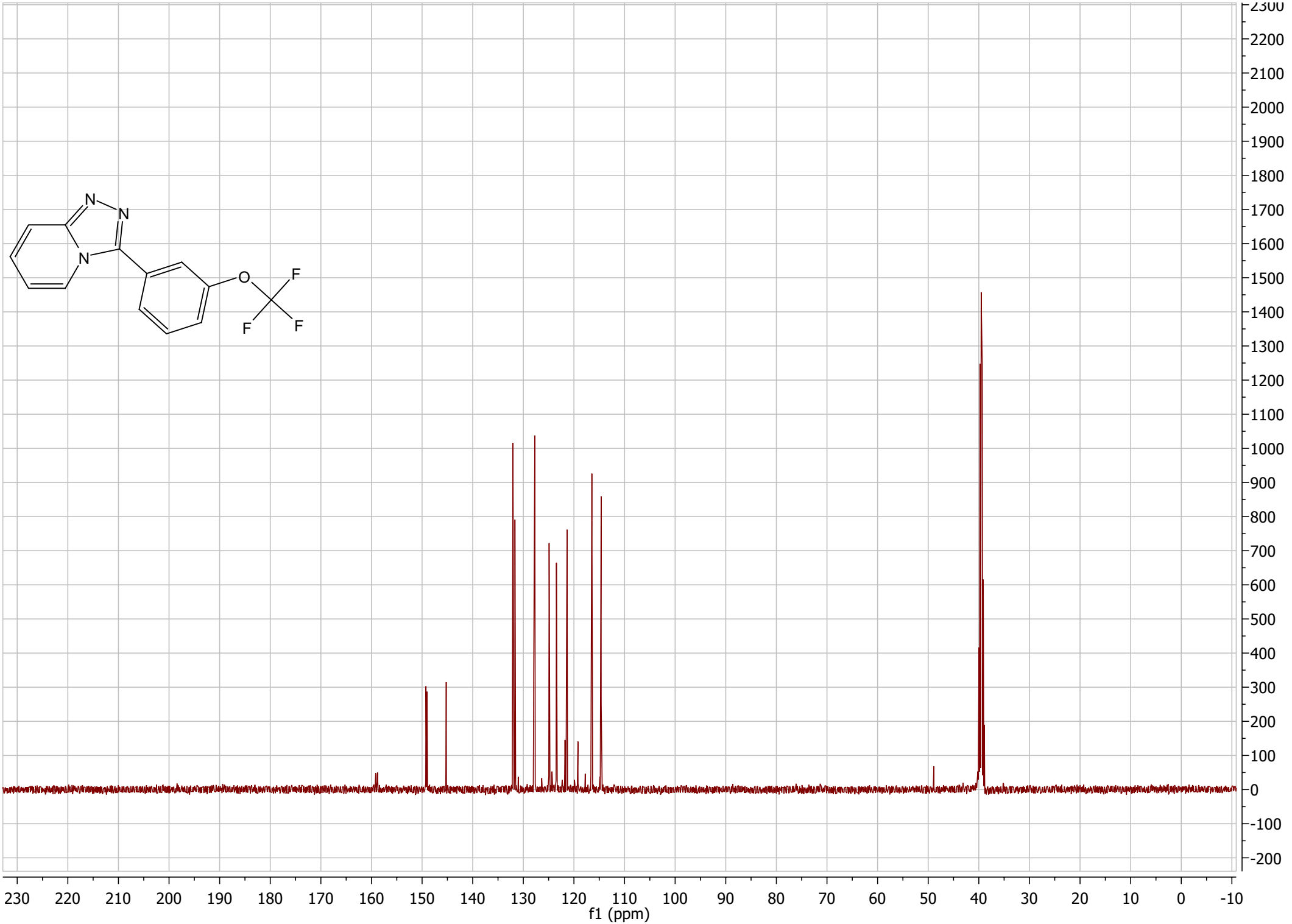
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)


H3C
CH3
H3C
O
O
NH
HN
N
N
CH3
500
450
400
350
300
250
200
150
100
50
0
20 19 18 17 16 15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1 -2 -3 -4
f1 (ppm)


H3C
CH3
H3C
O
O
NH
HN
N
N
CH3
1000
900
800
700
600
500
400
300
200
100
0
-100
230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)


N
N
N
O
F
F
F
3800
3600
3400
3200
3000
2800
2600
2400
2200
2000
1800
1600
1400
1200
1000
800
600
400
200
0
-200
21 20 19 18 17 16 15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1 -2 -3
f1 (ppm)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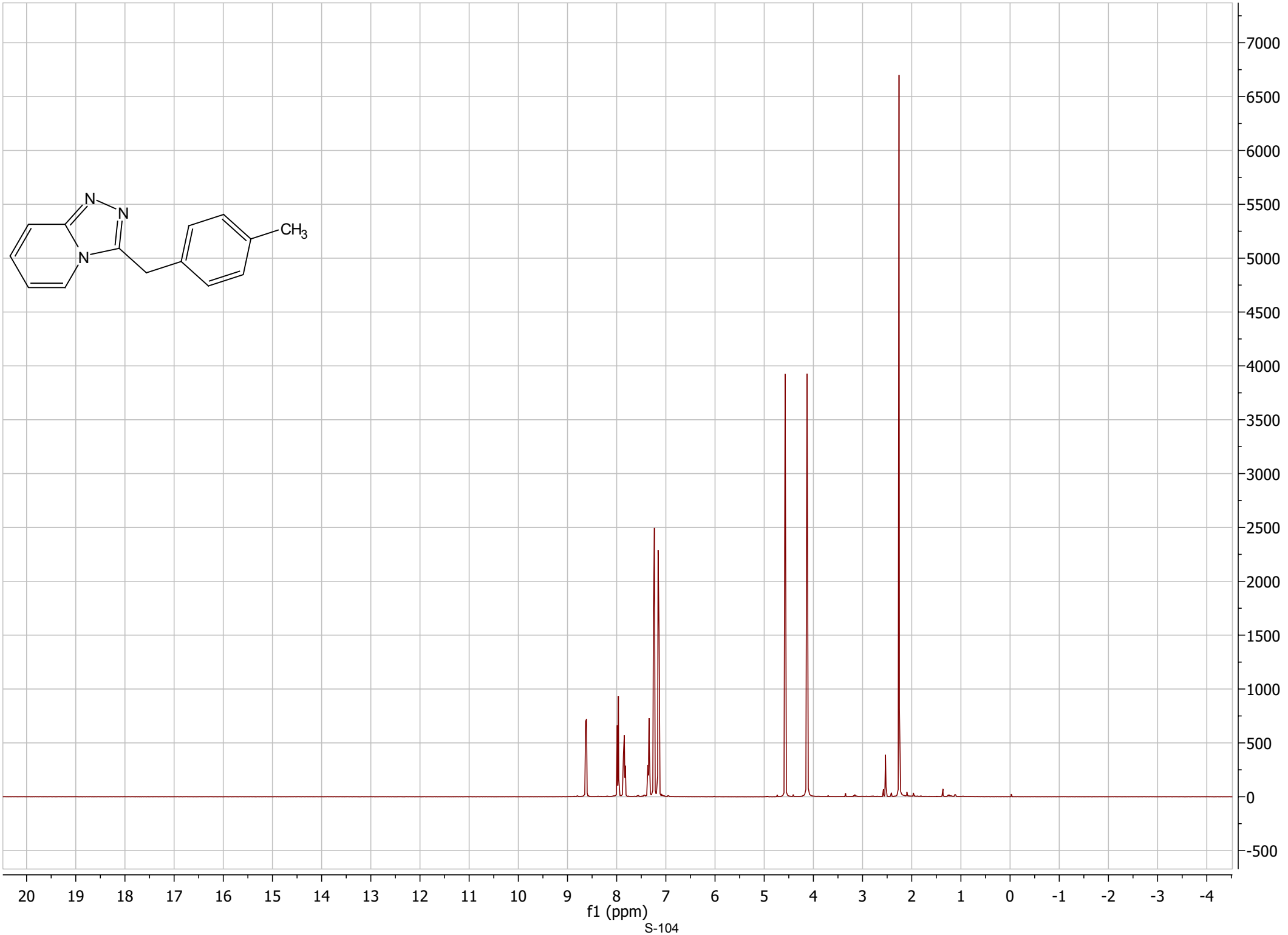
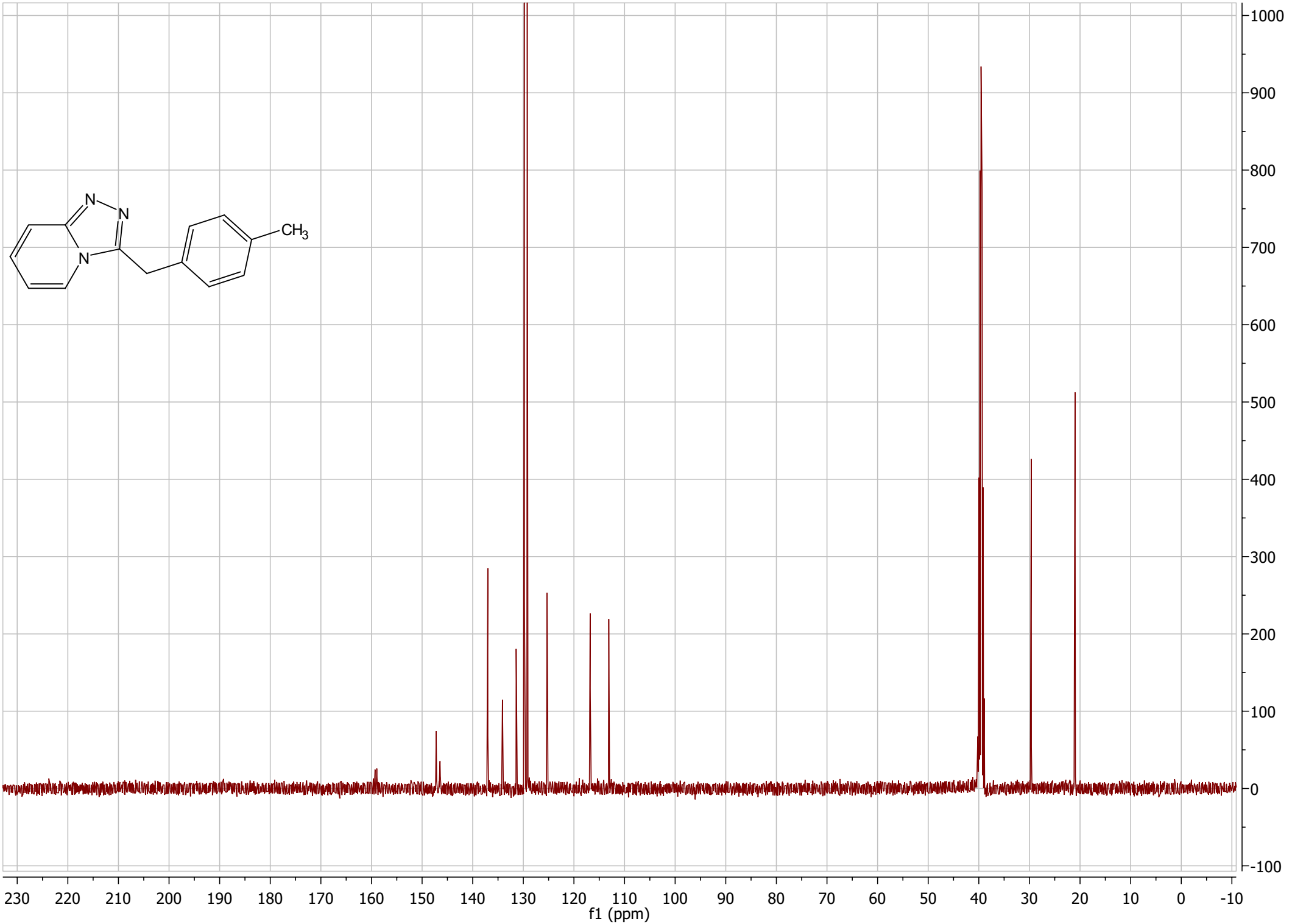
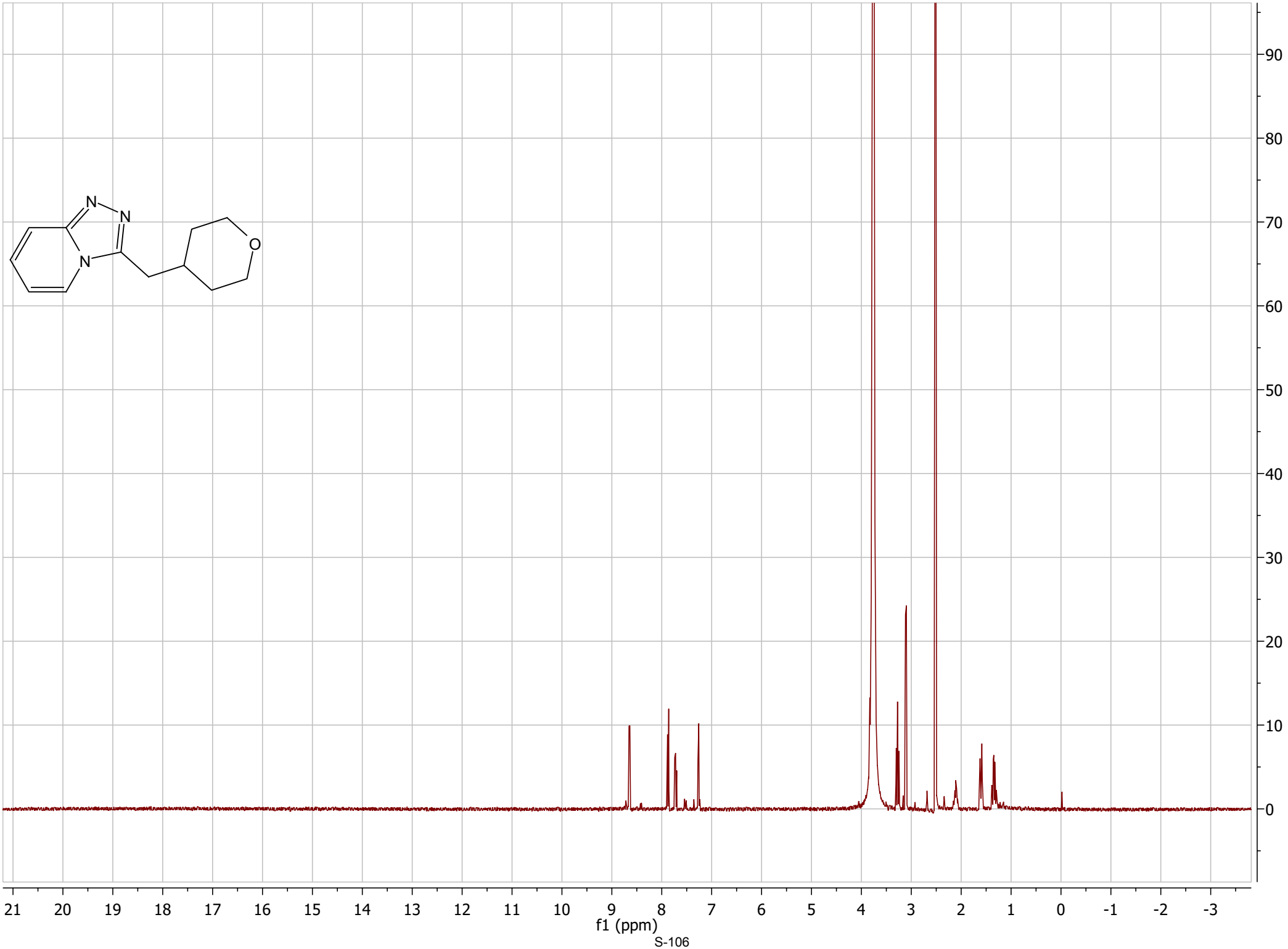
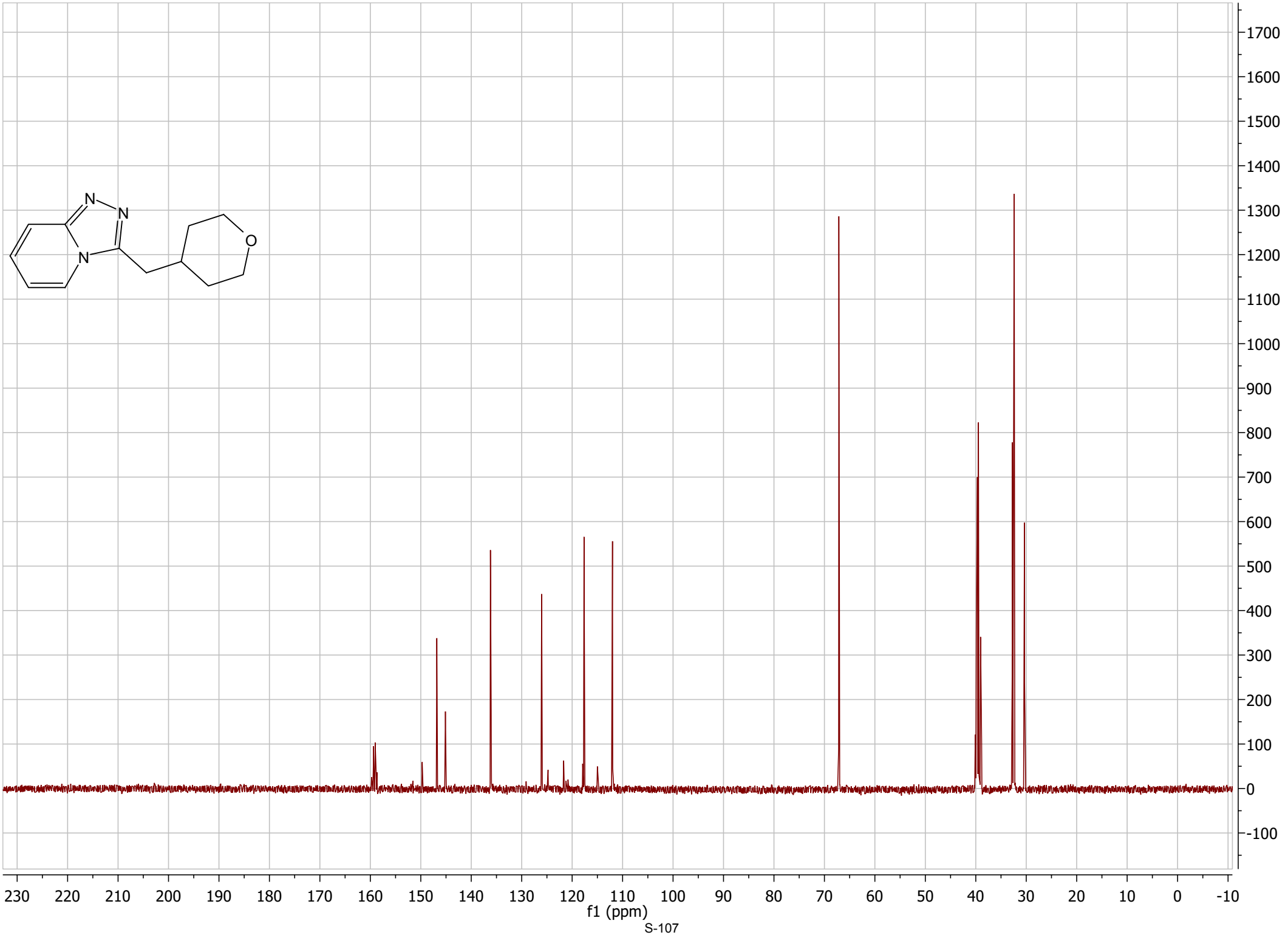
N
N
O
F
F
F
f1 (ppm)


N
N
N
CH3
7000
6500
6000
5500
5000
4500
4000
3500
3000
2500
2000
1500
1000
500
0
-500
20 19 18 17 16 15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1 -2 -3 -4
f1 (ppm)


N
N
N
CH3
1000
900
800
700
600
500
400
300
200
100
0
-100
230
220
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)


N
N
N
O
90
80
70
60
50
40
30
20
10
0
21
20
19
18
17
16
15
14
13
12
11
10
9
8
7
6
5
4
3
2
1
0
-1
-2
-3
f1 (ppm)


N
N
N
O
1700
1600
1500
1400
1300
1200
1100
1000
900
800
700
600
500
400
300
200
100
0
-100
230
220
210
200
190
180
170
160
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140
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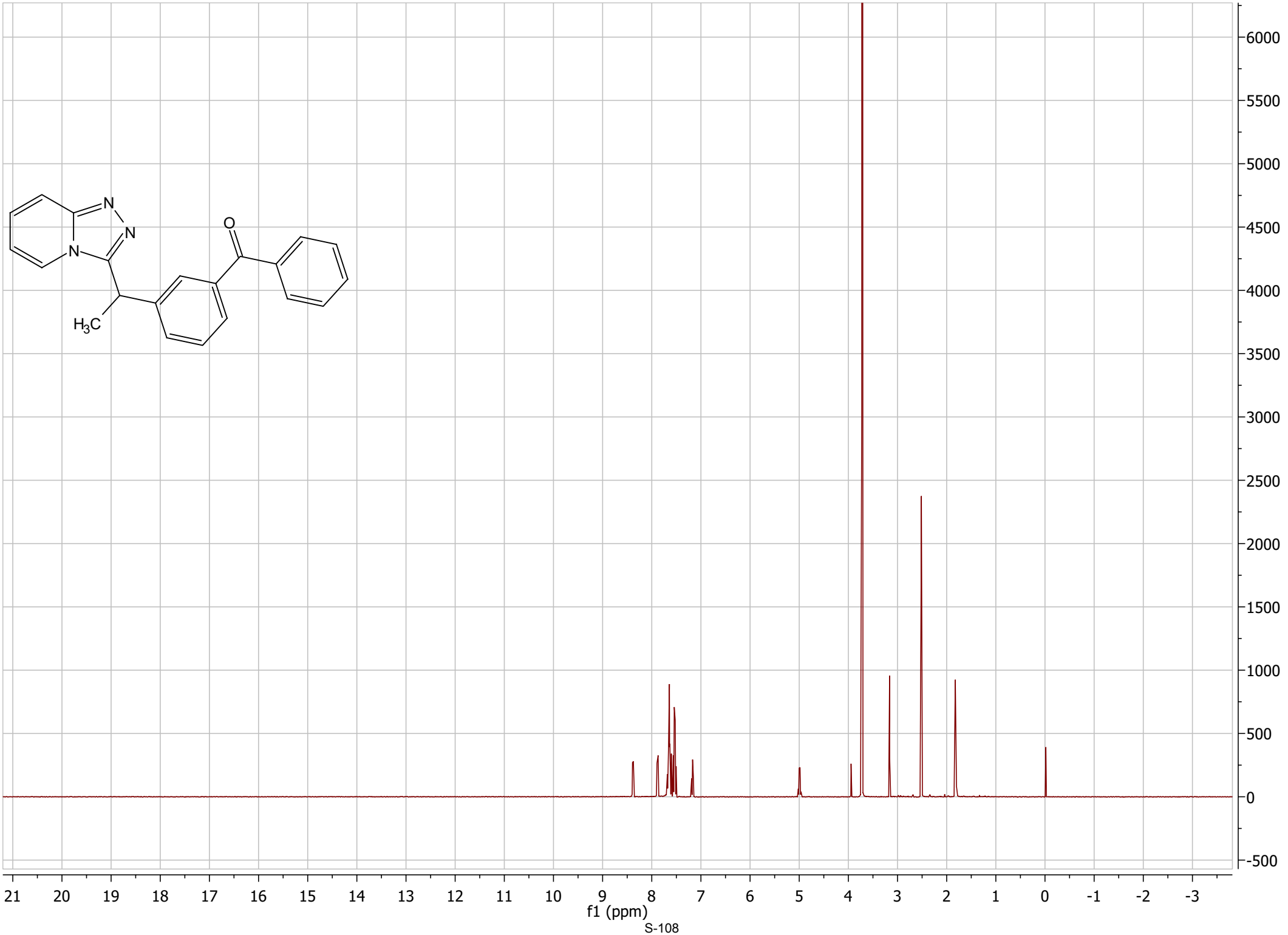
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)


N
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N
O
H3C
6000
5500
5000
4500
4000
3500
3000
2500
2000
1500
1000
500
0
-500
21
20
19
18
17
16
15
14
13
12
11
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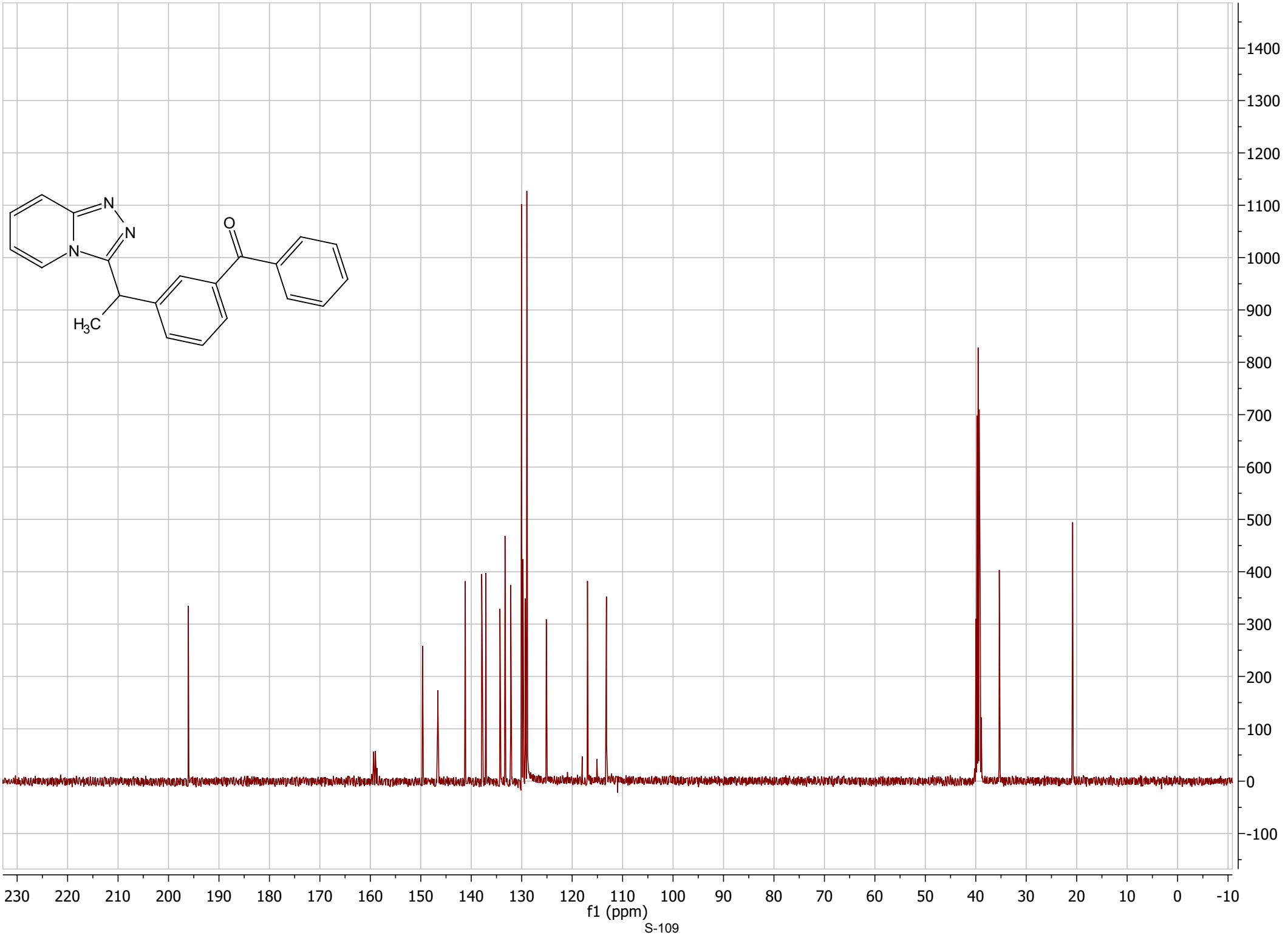
9
8
7
6
5
4
3
2
1
0
-1
-2
-3
f1 (ppm)


N
N
N
O
H3C
1400
1300
1200
1100
1000
900
800
700
600
500
400
300
200
100
0
-100
230
220
210
200
190
180
170
160
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140
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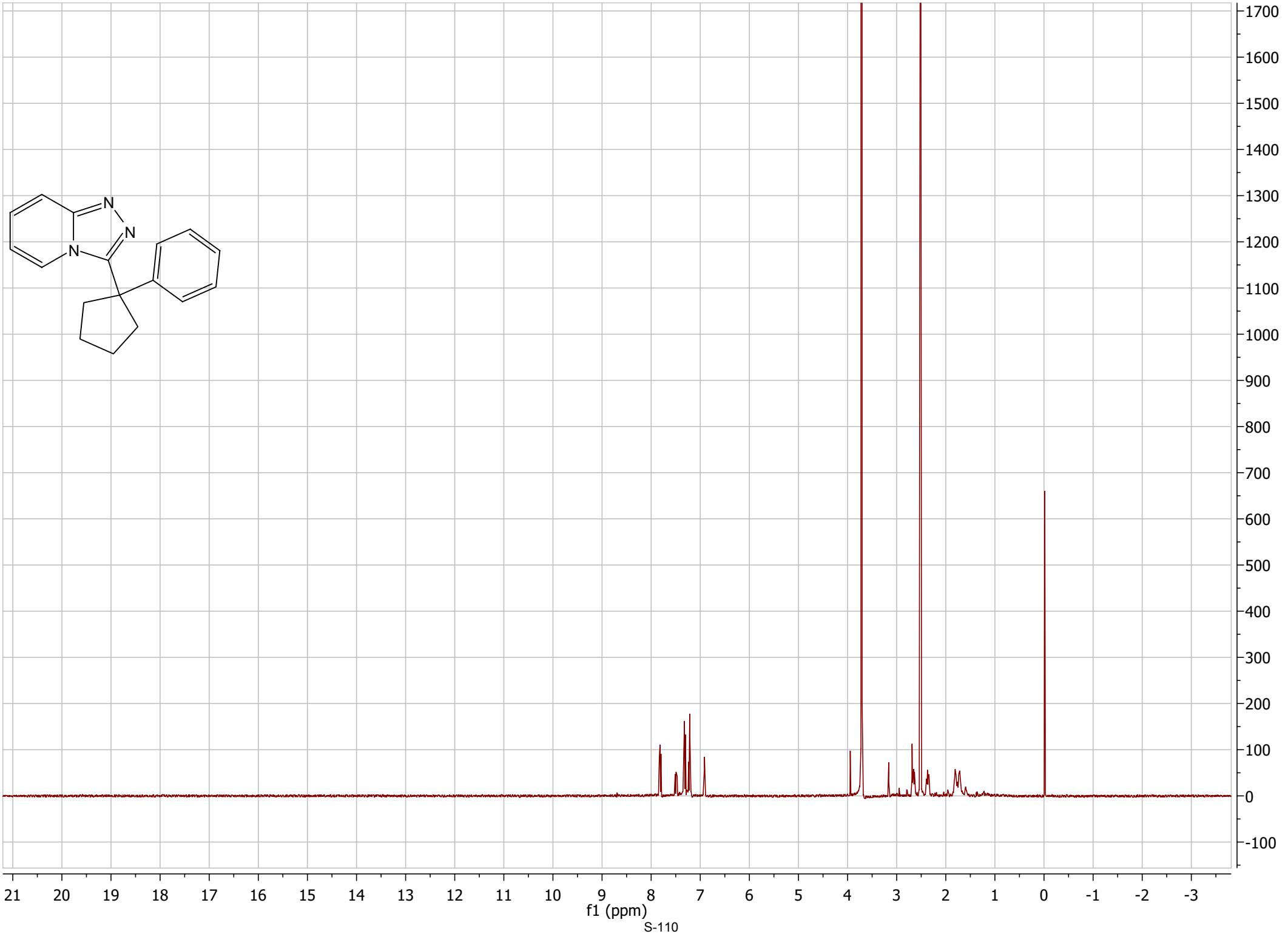
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)


N
N
N
1700
1600
1500
1400
1300
1200
1100
1000
900
800
700
600
500
400
300
200
100
0
-100
21
20
19
18
17
16
15
14
13
12
11
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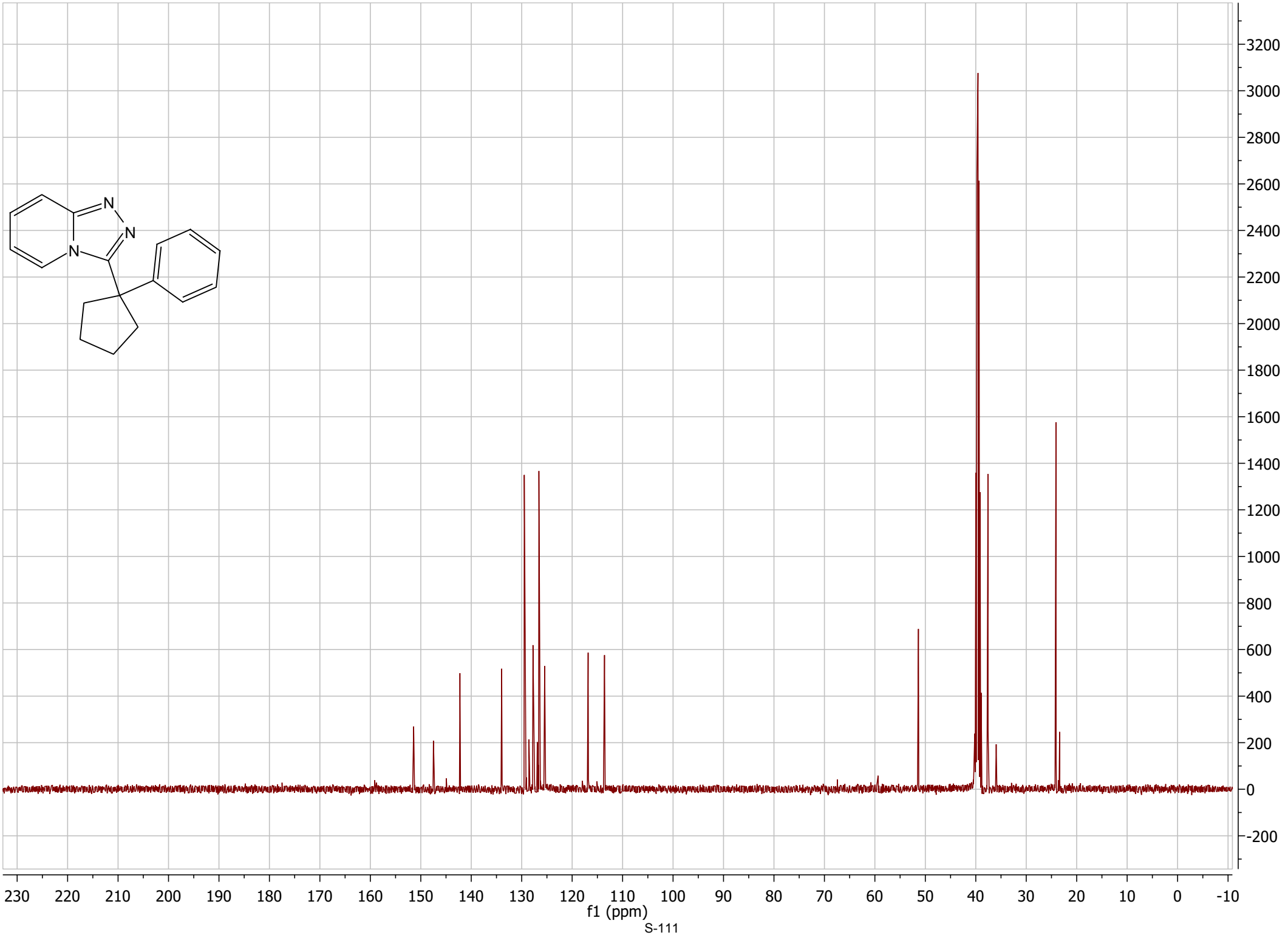
9
8
7
6
5
4
3
2
1
0
-1
-2
-3
f1 (ppm)


N
N
N
3200
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2800
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2400
2200
2000
1800
1600
1400
1200
1000
800
600
400
200
0
-200
230
220
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)